



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:52 PM GMT

PDB ID : 4JI6
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 : 3.55 Å(reported)

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

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

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

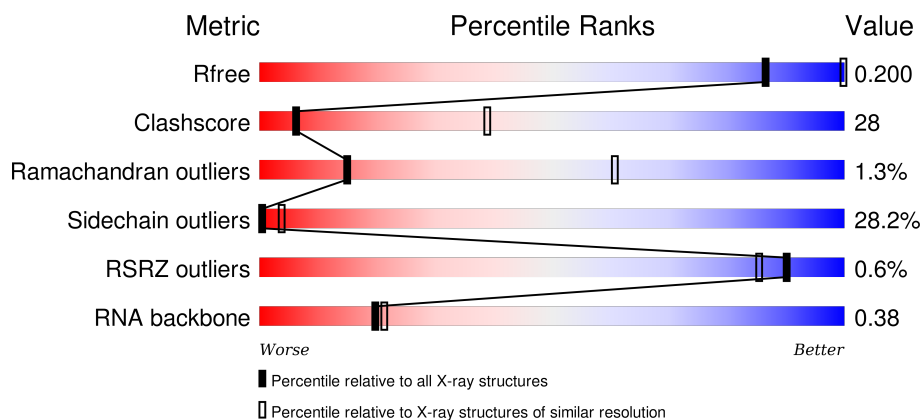
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)
RNA backbone	2183	1057 (4.30-2.80)

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

Mol	Chain	Length	Quality of chain
1	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
22	MG	A	1614	-	-	-	X
22	MG	A	1628	-	-	-	X
22	MG	A	1657	-	-	-	X
22	MG	A	1665	-	-	-	X
22	MG	A	1666	-	-	-	X
22	MG	A	1676	-	-	-	X
22	MG	A	1686	-	-	-	X
22	MG	A	1687	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1691	-	-	-	X
22	MG	A	1692	-	-	-	X
22	MG	A	1704	-	-	-	X
22	MG	A	1711	-	-	-	X
22	MG	A	1715	-	-	-	X
22	MG	A	1721	-	-	-	X
22	MG	A	1722	-	-	-	X
22	MG	A	1724	-	-	-	X
22	MG	A	1746	-	-	-	X
22	MG	A	1767	-	-	-	X
22	MG	A	1806	-	-	-	X
22	MG	A	1815	-	-	-	X
22	MG	A	1865	-	-	-	X
22	MG	A	1892	-	-	-	X
22	MG	A	1893	-	-	-	X
22	MG	A	1921	-	-	-	X
22	MG	A	1926	-	-	-	X
22	MG	A	1931	-	-	-	X
22	MG	A	1971	-	-	-	X
22	MG	A	1975	-	-	-	X
22	MG	N	102	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 53444 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	6	0
			32687	14559	6046	10562	1520			

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	S	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
			973	613	195	163	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	LEU	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	1	Total	Mg	0	0
			1	1		
22	G	1	Total	Mg	0	0
			1	1		
22	Q	2	Total	Mg	0	0
			2	2		
22	D	4	Total	Mg	0	0
			4	4		
22	K	1	Total	Mg	0	0
			1	1		
22	E	1	Total	Mg	0	0
			1	1		
22	H	1	Total	Mg	0	0
			1	1		
22	B	2	Total	Mg	0	0
			2	2		
22	I	2	Total	Mg	0	0
			2	2		
22	C	3	Total	Mg	0	0
			3	3		
22	A	377	Total	Mg	0	0
			377	377		
22	N	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	O	1	Total 1	Mg 1	0	0
22	L	1	Total 1	Mg 1	0	0
22	S	1	Total 1	Mg 1	0	0
22	F	1	Total 1	Mg 1	0	0

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1199	Total 1199	O 1199	0	0
24	C	6	Total 6	O 6	0	0
24	D	11	Total 11	O 11	0	0
24	E	7	Total 7	O 7	0	0
24	F	6	Total 6	O 6	0	0
24	G	6	Total 6	O 6	0	0
24	H	7	Total 7	O 7	0	0
24	I	1	Total 1	O 1	0	0
24	L	9	Total 9	O 9	0	0
24	M	2	Total 2	O 2	0	0
24	N	1	Total 1	O 1	0	0

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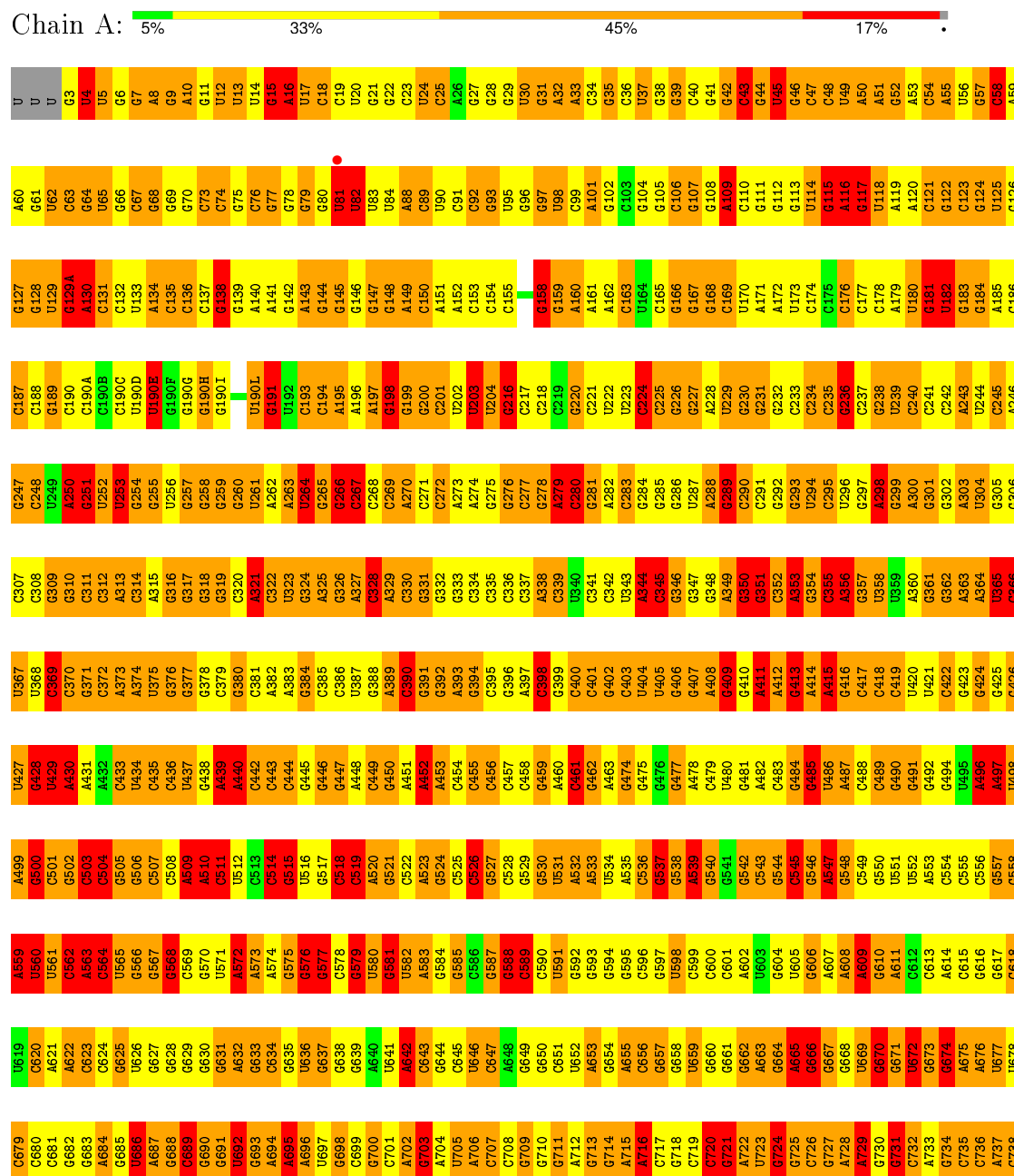
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	O	1	Total	O	0	0
			1	1		
24	P	3	Total	O	0	0
			3	3		
24	Q	6	Total	O	0	0
			6	6		

3 Residue-property plots

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

• Molecule 1: 16S rRNA

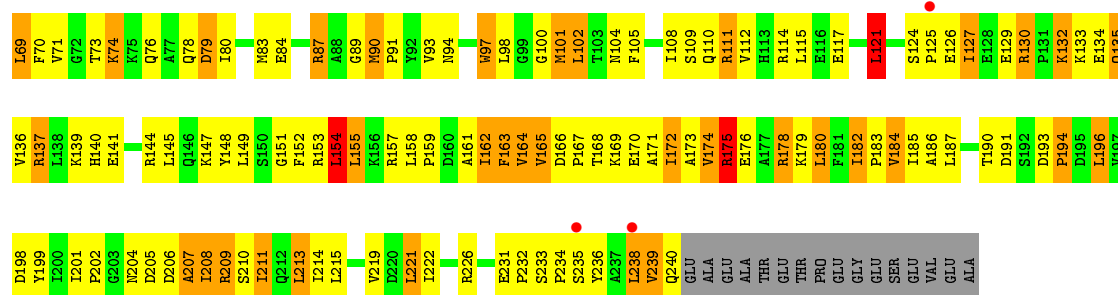


U1532	C1533	U1471	U406	G1347	A1287	A1235	G1164	C1103	U1040	C985	G925	A865	G799	G739
C1533	C1533	G1474	C1407	U1348	A1286	C1226	C1165	G1104	A1041	A986	G926	C866	G800	U740
A	A	G1475	A1408	A1349	A1289	A1227	G1166	A1105	G1042	A987	G927	C867	U801	G741
C	C	G1476	G1410	G1350	G1290	G1228	A1167	G1106	C1043	G988	G928	C868	A802	G742
U	U	G1477	G1411	C1352	U1292	A1229	A1168	C1107	A1044	C989	G929	C869	G803	U743
C	C	G1478	C1412	G1353	G1293	G1231	G1171	G1109	A1045	U991	G931	U870	U804	C744
U1480	U1414	C1354	A1413	C1354	G1294	U1232	C1172	A1110	A1046	U992	C932	C805	C745	G745
G1481	G1415	G1355	G1480	G1355	G1295	G1233	G1173	A1111	U1049	G993	A872	C806	A746	A747
U1541	G1416	G1356	G1481	G1356	C1296	C1234	G1174	A994	G1050	A994	G934	C808	C748	C748
U1542	G1417	A1357	G1482	G1357	G1297	U1235	G1175	C1113	C1051	C995	A935	C809	C749	C749
C1543	G1418	U1358	G1483	U1358	C1298	A1236	A1176	C1114	U1052	A996	G936	C810	G750	G750
U1544	C1484	C1359	C1484	C1359	A1299	G1237	G1177	C1115	G1053	U997	A937	C811	U751	U751
U1485	G1419	A1360	G1419	A1360	G1300	A1238	G1178	C1116	C1054	G998	A938	C812	G752	G752
H16	G1420	G1361	G1420	G1361	U1301	A1239	A1179	C1117	A1055	C999	G939	U813	A753	A753
F17	G1421	C1361A	G1421	C1361A	G1302	U1240	A1180	C1118	U1056	U1000	G940	A814	C754	C754
G18	G1422	C1362	G1422	C1362	G1303	G1241	G1181	C1119	G1057	A881	G941	A815	G755	G755
H19	G1423	A1363	G1423	A1363	G1304	C1242	G1182	G1120	G1058	G882	G942	A816	C756	C756
E20	C1424	U1364	C1424	U1364	G1305	C1243	A1183	U1121	C1059	C883	G943	C817	U757	U757
G1491	U1425	G1365	U1425	G1365	U1307	C1244	G1184	U1122	C1060	U884	G944	G818	G758	G758
A1492	C1426	C1366	C1426	C1366	U1308	A1245	G1185	A1123	G1061	A759	G945	A819	G759	G759
A1493	U1427	C1367	U1427	C1367	G1309	C1246	G1186	G1124	U1004	U886	A946	U820	G760	G760
G1494	A1428	G1368	G1494	G1368	G1309	U1247	G1187	U1125	C1063	G887	G947	G821	G761	G761
U1495	C1429	C1369	C1429	C1369	G1310	A1248	A1188	U1126	G1064	A888	C948	G822	C762	C762
C1496	G1430	G1370	G1430	G1370	G1311	C1249	C1189	G1127	U1065	C1008	A949	G823	G763	G763
G1497	G1431	G1371	G1431	G1371	G1312	A1250	G1190	C1128	C1066	G1009	U950	C824	C764	C764
U1498	G1432	U1372	G1432	U1372	U1313	A1251	A1191	C1129	A1067	G1010	G951	G825	G765	G765
A1499	A1433	G1373	A1433	G1373	C1314	A1252	C1192	A892	G1068	G1011	U952	C826	A766	A766
A1500	A1434	A1374	A1434	A1374	G1315	G1253	G1193	G1131	C1069	U1012	G953	U827	A767	A767
C1501	G1435	A1375	G1435	A1375	G1316	C1254	U1194	G1013	U1070	A768	G954	A828	A768	A768
A1502	U1436	U1376	U1436	U1376	C1317	G1255	C1195	A1014	C1071	A895	U955	G829	G769	G769
A1503	C1437	A1377	C1437	A1377	A1318	A1256	U1196	A1015	G1072	C896	U956	G830	C770	C770
G1504	G1438	C1378	G1504	C1378	A1319	U1257	G1197	U1016	U1073	C897	U957	U831	G771	G771
U1505	C1439	G1379	U1505	G1379	C1320	G1258	G1198	G1017	G1074	A898	A958	C832	U772	U772
U1506	C1440	U1380	U1506	C1380	C1321	C1259	G1199	C1018	C1075	C899	U959	U833	G773	G773
A1507	G1441	U1381	A1507	C1381	C1322	C1260	C1199	C1019	C1076	A900	U960	C834	G774	G774
G1508	G1442	C1382	G1508	C1382	G1323	A1261	A1201	C1140	G1077	U1020	U961	U835	G775	G775
C1509	G1443	C1383	C1509	C1383	A1324	C1262	G1202	C1141	U1078	G902	C962	G836	G776	G776
U1510	A1446	C1384	U1510	C1384	C1325	G1265	C1142	G1079	G1078	G1021	C963	G837	A777	A777
U1512	G1447	G1385	U1512	G1385	G1326	A1204	G1143	A1080	A1080	G1022	G903	G838	G778	G778
A1513	C1448	G1386	A1513	G1386	C1327	G1266	G1144	G1081	G1081	G1023	A964	C904	C779	C779
G1514	G1449	G1387	G1514	G1387	C1328	G1266	C1145	U1025	G1084	U1025	G966	G906	C840	A780
C1514	U1450	C1388	C1514	C1388	A1329	A1269	G1207	A1146	U1085	G1026	C967	A907	U841	A781
A1515	A1451	C1389	A1515	C1389	U1330	C1270	C1208	C1147	U1086	C1027	A968	C848	A782	A782
G1516	C1452	U1390	G1516	C1452	G1331	G1271	U1148	U1087	G1087	C1028	A969	C849	C783	C783
U1517	G1453	U1391	U1517	G1453	A1332	G1272	C1210	C1149	G1088	G1029	C970	U850	G784	G784
A1518	C1454	G1392	A1518	G1392	A1333	G1273	U1211	U1150	G1089	C1030	G971	G851	G785	G785
A1519	G1455	U1393	A1519	U1393	G1334	G1274	U1212	C912	U1090	G1030A	C972	G852	G786	G786
G1520	C1456	A1394	G1520	A1394	C1335	A1275	A1213	A1151	U1091	G1030B	G973	G853	A787	A787
R53	C1457	C1395	R53	C1395	G1336	G1276	C1214	C1153	A1092	G1030C	A974	G854	U788	U788
T54	G1460	A1396	T54	A1396	G1337	C1277	G1215	G1154	A1093	A1030D	A975	G855	U789	U789
U1522	G1461	C1397	U1522	C1397	G1338	U1278	G1216	G1155	G1094	G1031	G976	G856	A790	A790
C1523	C1462	A1398	C1523	A1398	A1339	A1279	C1217	U1156	U1095	G1032	A977	C857	A791	A791
G1524	C1463	C1399	G1524	C1399	A1340	A1280	C1218	A1157	C1096	G1033	A978	G858	A792	A792
U1525	G1464	C1399	U1525	G1464	U1341	U1281	G1219	C1158	C1097	G1034	C979	A859	U793	U793
G1526	C1465	G1400	G1526	G1400	C1342	C1282	U1159	U1159	C1098	A1035	C980	A860	A794	A794
C1527	G1466	C1401	C1527	G1466	G1343	G1283	G1221	G1160	G1099	G1036	U981	G861	C795	C795
U1528	G1467	C1402	U1528	C1402	C1344	A1284	G1222	C1161	C1100	C1037	U982	C862	C796	C796
G1529	A1468	C1403	G1529	C1403	C1345	A1285	C1223	C1162	A1101	C1038	A983	U863	C797	C797
G1530	G1469	C1404	G1530	C1404	A1346	A1286	G1224	C1163	A1102	C1039	C984	A864	G798	G798

● Molecule 2: RIBOSOMAL PROTEIN S2

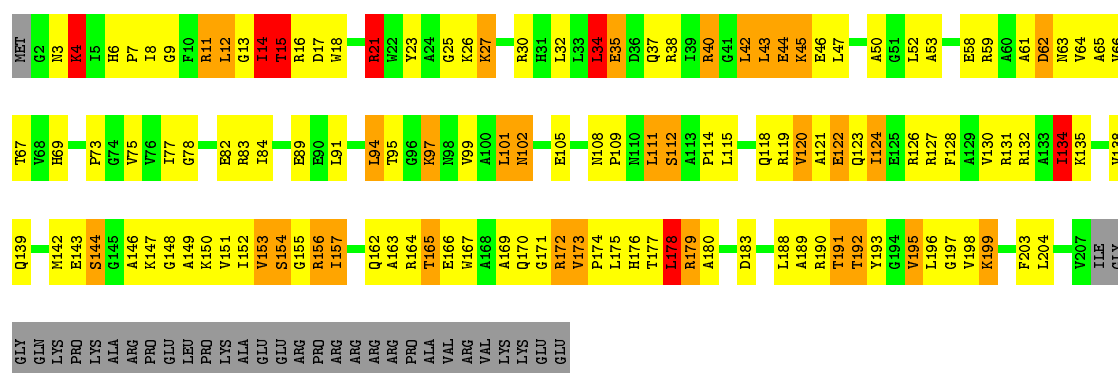


ME1	P40	V4L	G1U	I1E	T4R	V7	K3	E9	L10	L11	E12	V15	H16	F17	G18	H19	E20	R21	K22	R23	W24	N25	P26	R30	Y31	I32	Y33	A34	E35	R36	N37	G38	I39	H40	I41	I42	D43	L44	Q45	K46	T47	M48	E49	E50	L51	E52	R53	T54	I58	E59	D60	L61	R64	I68
-----	-----	-----	-----	-----	-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



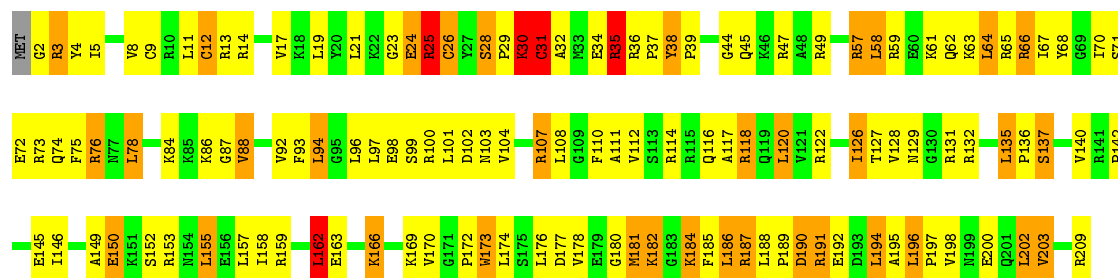
• Molecule 3: RIBOSOMAL PROTEIN S3

Chain C: 31% 38% 13% 14%



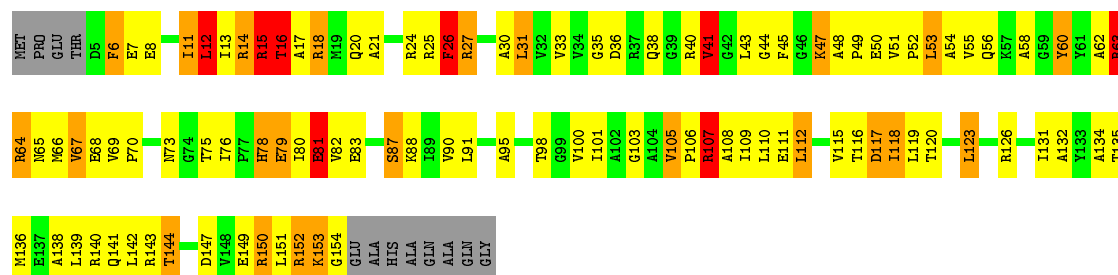
• Molecule 4: RIBOSOMAL PROTEIN S4

Chain D: 37% 44% 17%

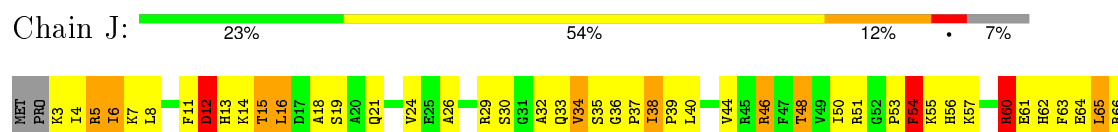


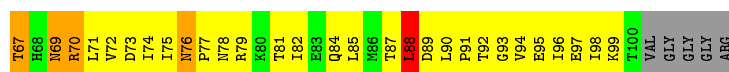
• Molecule 5: RIBOSOMAL PROTEIN S5

Chain E: 30% 44% 14% 5% 7%

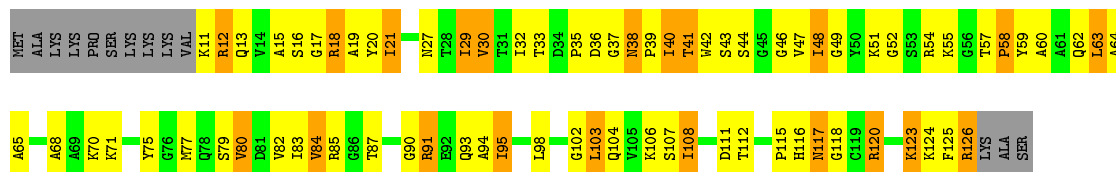


• Molecule 6: RIBOSOMAL PROTEIN S6

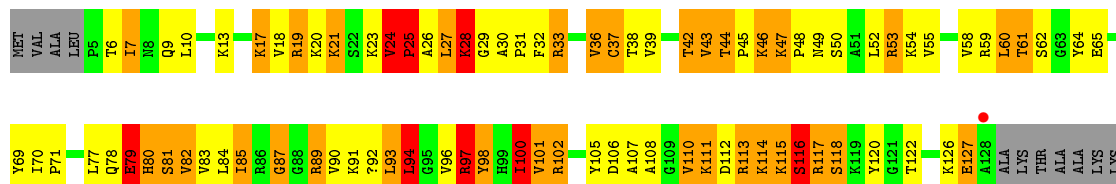
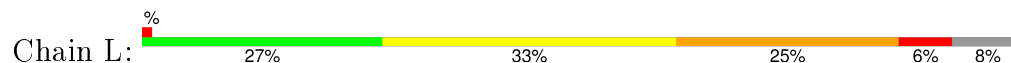




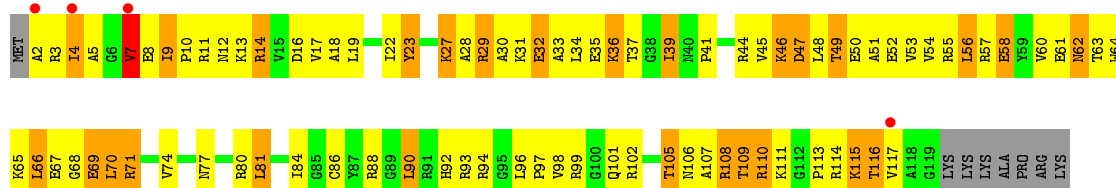
• Molecule 11: RIBOSOMAL PROTEIN S11



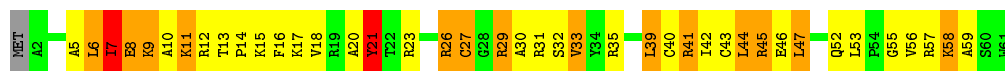
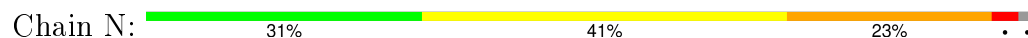
• Molecule 12: RIBOSOMAL PROTEIN S12



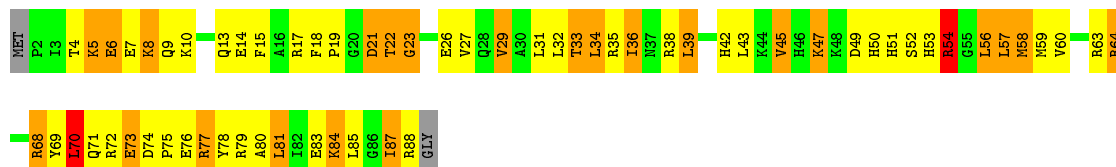
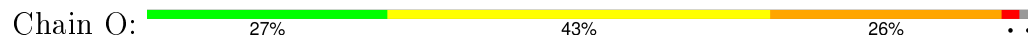
• Molecule 13: RIBOSOMAL PROTEIN S13



• Molecule 14: RIBOSOMAL PROTEIN S14



• Molecule 15: RIBOSOMAL PROTEIN S15



• Molecule 16: RIBOSOMAL PROTEIN S16





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.94Å 401.94Å 217.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.55 50.08 – 3.55	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-3.55) 98.3 (50.08-3.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1119)	Depositor
R, R_{free}	0.151 , 0.201 0.155 , 0.200	Depositor DCC
R_{free} test set	10475 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	127.6	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 153.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 209634 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53444	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, M2G, 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	1.77	785/36187 (2.2%)	2.98	5484/56471 (9.7%)
2	B	1.18	8/1935 (0.4%)	1.33	19/2609 (0.7%)
3	C	1.17	2/1636 (0.1%)	1.29	11/2205 (0.5%)
4	D	1.32	6/1733 (0.3%)	1.44	19/2318 (0.8%)
5	E	1.38	3/1162 (0.3%)	1.59	15/1564 (1.0%)
6	F	1.19	2/856 (0.2%)	1.40	12/1154 (1.0%)
7	G	0.98	1/1276 (0.1%)	1.13	4/1709 (0.2%)
8	H	1.23	2/1136 (0.2%)	1.38	8/1527 (0.5%)
9	I	0.94	0/1029	1.12	3/1379 (0.2%)
10	J	1.07	0/805	1.35	5/1082 (0.5%)
11	K	1.02	0/879	1.24	6/1187 (0.5%)
12	L	1.48	7/977 (0.7%)	1.59	17/1305 (1.3%)
13	M	0.88	1/947 (0.1%)	1.10	0/1270
14	N	1.02	1/501 (0.2%)	1.41	8/664 (1.2%)
15	O	1.07	0/740	1.30	7/987 (0.7%)
16	P	1.17	1/716 (0.1%)	1.30	3/963 (0.3%)
17	Q	1.35	2/836 (0.2%)	1.45	7/1117 (0.6%)
18	R	1.09	0/579	1.29	2/768 (0.3%)
19	S	0.89	0/661	1.28	7/890 (0.8%)
20	T	1.13	0/765	1.40	9/1007 (0.9%)
21	U	0.98	2/212 (0.9%)	0.97	0/277
All	All	1.58	823/55568 (1.5%)	2.58	5646/82453 (6.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	5
6	F	0	1
7	G	0	2
8	H	0	2
9	I	0	1
10	J	0	2
11	K	0	1
12	L	0	5
13	M	0	1
14	N	0	2
16	P	0	1
17	Q	0	1
18	R	0	1
19	S	0	2
20	T	0	2
All	All	0	36

All (823) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	975	A	N9-C4	-14.45	1.29	1.37
1	A	1493	A	N9-C4	13.90	1.46	1.37
4	D	12	CYS	CB-SG	13.89	2.05	1.82
1	A	768	A	N3-C4	-12.61	1.27	1.34
1	A	108	G	N1-C2	11.64	1.47	1.37
1	A	122	G	C5-C4	-11.60	1.30	1.38
1	A	22	G	N3-C4	-11.03	1.27	1.35
1	A	448	A	N9-C4	-10.96	1.31	1.37
1	A	1392	G	C6-N1	-10.92	1.31	1.39
1	A	262	A	N9-C4	-10.82	1.31	1.37
1	A	117	G	C6-O6	10.75	1.33	1.24
1	A	510	A	N3-C4	-10.72	1.28	1.34
1	A	733	A	N3-C4	-10.69	1.28	1.34
1	A	402	G	C6-N1	-10.63	1.32	1.39
1	A	510	A	N9-C4	-10.59	1.31	1.37
1	A	108	G	N9-C4	-10.45	1.29	1.38
1	A	439	A	N3-C4	-10.38	1.28	1.34
1	A	266	G	N9-C4	-10.30	1.29	1.38
1	A	134	A	N3-C4	-10.13	1.28	1.34
1	A	303	A	C5-C4	-10.10	1.31	1.38
1	A	1416	G	N9-C4	10.09	1.46	1.38
1	A	399	G	N1-C2	-9.99	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	G	N9-C8	-9.77	1.31	1.37
1	A	6	G	N9-C8	-9.75	1.31	1.37
1	A	1415	G	N3-C4	9.72	1.42	1.35
1	A	28	G	N7-C5	-9.69	1.33	1.39
1	A	1054	C	N3-C4	9.65	1.40	1.33
1	A	279	A	C5-C6	-9.64	1.32	1.41
1	A	1529	G	N9-C8	-9.64	1.31	1.37
1	A	325	A	N3-C4	-9.63	1.29	1.34
1	A	914	A	N3-C4	-9.61	1.29	1.34
1	A	768	A	N7-C5	-9.56	1.33	1.39
1	A	1415	G	C6-N1	9.54	1.46	1.39
12	L	26	ALA	CA-CB	9.53	1.72	1.52
1	A	563	A	N9-C4	-9.51	1.32	1.37
1	A	310	G	N7-C5	-9.50	1.33	1.39
1	A	566	G	C5-C6	-9.39	1.32	1.42
1	A	18	C	N1-C6	-9.35	1.31	1.37
1	A	117	G	C6-N1	9.26	1.46	1.39
1	A	722	A	N7-C5	-9.24	1.33	1.39
1	A	32	A	N3-C4	-9.17	1.29	1.34
1	A	185	A	N9-C4	-9.15	1.32	1.37
1	A	914	A	C6-N1	-9.14	1.29	1.35
1	A	322	C	N1-C6	-9.13	1.31	1.37
1	A	869	G	N7-C5	-9.11	1.33	1.39
1	A	563	A	N3-C4	-9.06	1.29	1.34
1	A	1357	A	N9-C4	-8.98	1.32	1.37
1	A	964	A	N3-C4	-8.95	1.29	1.34
1	A	964	A	N9-C4	-8.94	1.32	1.37
1	A	289	G	N7-C5	-8.93	1.33	1.39
1	A	1416	G	C5-C4	8.93	1.44	1.38
1	A	1340	A	N9-C4	-8.91	1.32	1.37
1	A	722	A	C5-C6	-8.89	1.33	1.41
1	A	266	G	N9-C8	8.89	1.44	1.37
1	A	778	G	C6-N1	-8.89	1.33	1.39
1	A	300	A	N3-C4	-8.86	1.29	1.34
1	A	929	G	C5-C4	-8.80	1.32	1.38
1	A	975	A	N3-C4	-8.79	1.29	1.34
1	A	120	A	N7-C5	-8.78	1.33	1.39
1	A	663	A	N3-C4	-8.78	1.29	1.34
1	A	279	A	N7-C5	-8.76	1.33	1.39
1	A	1529	G	N7-C5	-8.75	1.34	1.39
1	A	930	C	N1-C6	-8.74	1.31	1.37
1	A	29	G	N9-C4	-8.74	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	715	A	N9-C4	-8.73	1.32	1.37
1	A	746	A	N3-C4	-8.71	1.29	1.34
1	A	900	A	N9-C4	-8.63	1.32	1.37
1	A	828	A	N9-C4	-8.57	1.32	1.37
1	A	47	C	N1-C6	-8.55	1.32	1.37
1	A	714	G	N9-C8	-8.54	1.31	1.37
1	A	711	G	C5-C6	-8.53	1.33	1.42
1	A	285	G	N9-C4	-8.53	1.31	1.38
4	D	173	TRP	CB-CG	-8.51	1.34	1.50
1	A	711	G	N7-C5	-8.50	1.34	1.39
1	A	528	C	N1-C6	-8.48	1.32	1.37
1	A	859	A	N3-C4	-8.45	1.29	1.34
1	A	729	A	C6-N1	-8.43	1.29	1.35
1	A	329	A	N3-C4	-8.38	1.29	1.34
1	A	852	G	N9-C4	-8.33	1.31	1.38
1	A	228	A	N9-C4	-8.32	1.32	1.37
1	A	790	A	N3-C4	-8.31	1.29	1.34
1	A	819	A	C5-C6	-8.29	1.33	1.41
1	A	152	A	N9-C4	-8.28	1.32	1.37
1	A	122	G	C8-N7	-8.28	1.25	1.30
1	A	134	A	N9-C4	-8.27	1.32	1.37
1	A	724	G	C2-N3	8.22	1.39	1.32
1	A	44	G	C6-N1	-8.22	1.33	1.39
1	A	741	G	N9-C8	-8.20	1.32	1.37
1	A	279	A	N9-C4	-8.17	1.32	1.37
1	A	54	C	N1-C6	-8.15	1.32	1.37
1	A	438	G	C6-O6	8.13	1.31	1.24
1	A	923	A	N7-C5	-8.09	1.34	1.39
1	A	939	G	N7-C5	-8.08	1.34	1.39
1	A	544	G	C5-C6	-8.07	1.34	1.42
1	A	889	A	C6-N1	-8.07	1.29	1.35
1	A	117	G	N1-C2	8.06	1.44	1.37
1	A	872	A	N9-C8	-8.06	1.31	1.37
1	A	44	G	N7-C5	-8.06	1.34	1.39
1	A	1530	G	N7-C5	8.05	1.44	1.39
1	A	1530	G	C6-N1	8.05	1.45	1.39
1	A	22	G	C6-N1	-8.04	1.33	1.39
1	A	44	G	N9-C8	-8.04	1.32	1.37
1	A	109	A	N9-C4	-8.03	1.33	1.37
1	A	778	G	N3-C4	-8.01	1.29	1.35
1	A	1394	A	N3-C4	-8.01	1.30	1.34
1	A	900	A	N3-C4	-7.96	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	902	G	C6-N1	-7.93	1.33	1.39
1	A	1394	A	C6-N1	-7.93	1.30	1.35
1	A	566	G	C5-C4	-7.89	1.32	1.38
1	A	642	A	N3-C4	-7.87	1.30	1.34
1	A	1527	C	N1-C6	-7.87	1.32	1.37
1	A	111	G	N3-C4	-7.83	1.29	1.35
1	A	484	G	C6-N1	-7.81	1.34	1.39
4	D	150	GLU	CG-CD	7.80	1.63	1.51
1	A	722	A	C6-N1	-7.80	1.30	1.35
1	A	1250	A	N9-C4	-7.79	1.33	1.37
1	A	775	G	N1-C2	-7.76	1.31	1.37
1	A	730	G	N3-C4	-7.72	1.30	1.35
1	A	504	C	C4-C5	-7.71	1.36	1.43
1	A	403	C	N1-C6	-7.65	1.32	1.37
1	A	313	A	N9-C4	-7.65	1.33	1.37
1	A	810	C	N3-C4	-7.64	1.28	1.33
1	A	728	A	C6-N1	-7.63	1.30	1.35
1	A	865	A	N7-C5	-7.63	1.34	1.39
1	A	535	A	C6-N1	-7.61	1.30	1.35
1	A	1092	A	C6-N1	-7.60	1.30	1.35
1	A	889	A	N3-C4	-7.58	1.30	1.34
1	A	918	A	N7-C5	-7.58	1.34	1.39
1	A	741	G	C6-N1	-7.58	1.34	1.39
1	A	329	A	N7-C5	-7.54	1.34	1.39
5	E	16	THR	CA-CB	7.53	1.73	1.53
1	A	1502	A	C5-C6	-7.53	1.34	1.41
1	A	768	A	C6-N1	-7.53	1.30	1.35
1	A	291	C	C4-C5	-7.52	1.36	1.43
1	A	779	C	N3-C4	-7.52	1.28	1.33
1	A	801	U	C2-N3	-7.51	1.32	1.37
1	A	303	A	N9-C8	-7.50	1.31	1.37
1	A	45	U	C2-N3	-7.50	1.32	1.37
1	A	726	C	N1-C6	-7.49	1.32	1.37
1	A	971	G	N9-C8	-7.49	1.32	1.37
1	A	234	C	N3-C4	-7.48	1.28	1.33
1	A	484	G	C8-N7	-7.45	1.26	1.30
1	A	1527	C	N3-C4	-7.45	1.28	1.33
1	A	729	A	N3-C4	-7.44	1.30	1.34
1	A	748	C	N1-C2	7.44	1.47	1.40
1	A	399	G	C5-C4	-7.44	1.33	1.38
1	A	401	C	N3-C4	7.43	1.39	1.33
1	A	1125	U	P-O5'	7.42	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	G	N9-C8	-7.39	1.32	1.37
1	A	415	A	N9-C4	7.39	1.42	1.37
1	A	6	G	C8-N7	-7.38	1.26	1.30
1	A	566	G	N7-C5	-7.37	1.34	1.39
1	A	755	G	N7-C5	-7.35	1.34	1.39
1	A	1225	A	N3-C4	-7.35	1.30	1.34
1	A	694	A	N9-C4	-7.33	1.33	1.37
1	A	1353	G	C6-N1	-7.33	1.34	1.39
1	A	332	G	C2-N3	-7.33	1.26	1.32
1	A	713	G	N9-C8	-7.30	1.32	1.37
1	A	975	A	C5-C4	7.30	1.43	1.38
1	A	746	A	C6-N1	-7.30	1.30	1.35
1	A	550	G	C6-N1	-7.29	1.34	1.39
1	A	1513	A	C6-N6	-7.28	1.28	1.33
1	A	588	G	N9-C4	7.25	1.43	1.38
1	A	608	A	C5-C4	-7.25	1.33	1.38
1	A	59	A	N3-C4	-7.25	1.30	1.34
1	A	394	G	C5-C4	-7.22	1.33	1.38
1	A	983	A	N7-C5	-7.22	1.34	1.39
1	A	1392	G	N1-C2	-7.19	1.31	1.37
1	A	297	G	N3-C4	-7.18	1.30	1.35
1	A	644	G	N3-C4	-7.18	1.30	1.35
2	B	141	GLU	CG-CD	7.16	1.62	1.51
1	A	531	U	C4-O4	7.15	1.29	1.23
1	A	692	U	C2-N3	-7.15	1.32	1.37
1	A	673	G	N7-C5	7.14	1.43	1.39
1	A	120	A	C5-C6	-7.13	1.34	1.41
1	A	787	A	N7-C5	-7.12	1.34	1.39
1	A	632	A	C5-C6	-7.10	1.34	1.41
1	A	791	G	N9-C8	-7.10	1.32	1.37
1	A	1077	G	C2-N2	-7.09	1.27	1.34
1	A	385	C	N3-C4	-7.06	1.29	1.33
1	A	1401	G	C6-N1	-7.06	1.34	1.39
1	A	329	A	N9-C4	-7.05	1.33	1.37
1	A	833	U	C2-N3	-7.05	1.32	1.37
1	A	382	A	C6-N1	-7.05	1.30	1.35
1	A	298	A	N3-C4	-7.04	1.30	1.34
1	A	116	A	N9-C4	-7.04	1.33	1.37
1	A	310	G	N9-C8	-7.03	1.32	1.37
1	A	1075	C	N3-C4	-7.01	1.29	1.33
1	A	1280	A	N3-C4	-7.00	1.30	1.34
1	A	553	A	N3-C4	-6.99	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	156	TRP	CB-CG	6.99	1.62	1.50
1	A	408	A	N9-C4	6.99	1.42	1.37
1	A	878	G	C6-N1	-6.98	1.34	1.39
1	A	250	A	C5-C4	6.98	1.43	1.38
1	A	482	A	N7-C5	-6.97	1.35	1.39
1	A	802	A	N3-C4	-6.97	1.30	1.34
1	A	1176	A	N9-C4	6.97	1.42	1.37
1	A	741	G	N3-C4	-6.96	1.30	1.35
1	A	1481	U	C4-O4	6.95	1.29	1.23
1	A	1443	G	N9-C4	-6.95	1.32	1.38
1	A	588	G	N3-C4	6.92	1.40	1.35
1	A	352	C	N1-C6	-6.92	1.32	1.37
1	A	484	G	N1-C2	-6.91	1.32	1.37
1	A	299	G	N3-C4	-6.91	1.30	1.35
1	A	1202	G	N3-C4	-6.90	1.30	1.35
1	A	6	G	C6-O6	6.89	1.30	1.24
1	A	312	C	C2-O2	6.89	1.30	1.24
1	A	642	A	N7-C5	-6.88	1.35	1.39
1	A	1513	A	N9-C4	-6.88	1.33	1.37
1	A	117	G	C8-N7	-6.86	1.26	1.30
14	N	27	CYS	CB-SG	-6.86	1.70	1.82
1	A	1077	G	C2-N3	-6.86	1.27	1.32
1	A	482	A	N3-C4	-6.85	1.30	1.34
1	A	181	G	N7-C5	-6.85	1.35	1.39
1	A	267	C	C4-N4	-6.85	1.27	1.33
1	A	1468	A	N9-C4	-6.85	1.33	1.37
1	A	569	C	N1-C6	-6.85	1.33	1.37
1	A	981	U	C2-N3	6.80	1.42	1.37
1	A	1202	G	N9-C4	-6.78	1.32	1.38
1	A	28	G	N3-C4	-6.78	1.30	1.35
1	A	858	G	N7-C5	-6.78	1.35	1.39
1	A	663	A	N9-C4	-6.78	1.33	1.37
1	A	800	G	N3-C4	-6.77	1.30	1.35
1	A	1093	A	C6-N6	-6.77	1.28	1.33
1	A	109	A	N3-C4	-6.75	1.30	1.34
1	A	718	G	C2-N3	6.75	1.38	1.32
1	A	389	A	N7-C5	-6.72	1.35	1.39
1	A	865	A	N3-C4	-6.72	1.30	1.34
1	A	59	A	N9-C4	-6.71	1.33	1.37
1	A	789	U	C4-O4	6.71	1.29	1.23
1	A	406	G	N9-C4	6.70	1.43	1.38
1	A	297	G	C6-N1	-6.69	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	A	C5-C6	-6.68	1.35	1.41
1	A	1281	U	N1-C6	6.68	1.44	1.38
1	A	872	A	N7-C5	-6.68	1.35	1.39
1	A	1468	A	N3-C4	-6.68	1.30	1.34
1	A	31	G	N9-C8	-6.65	1.33	1.37
1	A	393	A	N9-C4	-6.65	1.33	1.37
1	A	500	G	N9-C4	-6.64	1.32	1.38
1	A	573	A	N7-C5	-6.63	1.35	1.39
1	A	1079	G	N9-C4	6.62	1.43	1.38
1	A	1101	A	C6-N6	6.62	1.39	1.33
1	A	1529	G	N3-C4	-6.62	1.30	1.35
1	A	1410	G	C8-N7	-6.62	1.26	1.30
1	A	355	C	N1-C6	-6.62	1.33	1.37
1	A	880	C	N3-C4	-6.61	1.29	1.33
1	A	331	G	N7-C5	-6.60	1.35	1.39
1	A	10	A	C6-N1	-6.58	1.30	1.35
1	A	15	G	N9-C4	6.58	1.43	1.38
3	C	105	GLU	CB-CG	6.57	1.64	1.52
1	A	204	U	C2-N3	6.57	1.42	1.37
1	A	694	A	N3-C4	-6.56	1.30	1.34
1	A	1497	G	N3-C4	-6.56	1.30	1.35
1	A	918	A	C5-C4	-6.56	1.34	1.38
1	A	912	C	N1-C6	-6.56	1.33	1.37
1	A	247	G	N3-C4	-6.55	1.30	1.35
1	A	394	G	N1-C2	-6.55	1.32	1.37
1	A	841	U	N1-C2	6.55	1.44	1.38
1	A	644	G	C5-C4	-6.55	1.33	1.38
1	A	907	A	C6-N1	-6.54	1.30	1.35
1	A	510	A	C5-C4	-6.54	1.34	1.38
1	A	108	G	C5-C6	-6.54	1.35	1.42
1	A	1390	U	C4-O4	6.54	1.28	1.23
1	A	712	A	C6-N1	-6.53	1.30	1.35
1	A	781	A	N9-C4	-6.53	1.33	1.37
1	A	385	C	N1-C6	-6.51	1.33	1.37
1	A	377	G	N1-C2	-6.51	1.32	1.37
1	A	1411	C	N1-C2	-6.51	1.33	1.40
1	A	385	C	C4-C5	-6.50	1.37	1.43
1	A	578	C	N3-C4	-6.49	1.29	1.33
1	A	367	U	C2-N3	-6.48	1.33	1.37
1	A	108	G	C2-N2	6.47	1.41	1.34
1	A	395	C	C4-C5	-6.47	1.37	1.43
1	A	553	A	N9-C4	-6.47	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	775	G	C5-C4	-6.47	1.33	1.38
1	A	310	G	C5-C4	-6.47	1.33	1.38
1	A	58	C	N3-C4	-6.46	1.29	1.33
1	A	802	A	N9-C4	-6.45	1.33	1.37
1	A	1468	A	C5-C4	-6.45	1.34	1.38
1	A	1139	G	C5-C6	6.45	1.48	1.42
1	A	9	G	N9-C8	-6.44	1.33	1.37
1	A	1497	G	N1-C2	-6.43	1.32	1.37
1	A	1497	G	C6-N1	-6.42	1.35	1.39
1	A	402	G	N3-C4	-6.42	1.30	1.35
1	A	1398	A	N9-C8	-6.42	1.32	1.37
1	A	248	C	N3-C4	-6.41	1.29	1.33
1	A	791	G	N3-C4	-6.41	1.30	1.35
1	A	408	A	N7-C5	-6.41	1.35	1.39
1	A	823	G	N9-C4	-6.41	1.32	1.38
1	A	725	G	C5-C6	-6.40	1.35	1.42
1	A	944	G	N9-C4	6.40	1.43	1.38
1	A	813	U	C4-O4	-6.40	1.18	1.23
1	A	1103	C	N1-C6	-6.40	1.33	1.37
1	A	1512	U	N3-C4	-6.39	1.32	1.38
1	A	1507	A	C6-N6	-6.38	1.28	1.33
1	A	737	A	N3-C4	-6.38	1.31	1.34
1	A	499	A	N9-C4	-6.37	1.34	1.37
1	A	357	G	N1-C2	-6.35	1.32	1.37
1	A	574	A	C5-C6	-6.34	1.35	1.41
1	A	566	G	C6-N1	-6.34	1.35	1.39
1	A	27	G	C5-C6	-6.34	1.36	1.42
1	A	566	G	N3-C4	-6.34	1.31	1.35
1	A	298	A	N7-C5	-6.33	1.35	1.39
1	A	1416	G	N3-C4	6.33	1.39	1.35
1	A	39	G	C5-C4	-6.32	1.33	1.38
1	A	267	C	N3-C4	-6.32	1.29	1.33
1	A	864	A	N3-C4	-6.32	1.31	1.34
1	A	730	G	C2-N3	-6.32	1.27	1.32
1	A	764	C	C5-C6	-6.31	1.29	1.34
1	A	860	A	C5-C4	-6.31	1.34	1.38
1	A	1107	C	N3-C4	-6.31	1.29	1.33
1	A	547	A	N3-C4	-6.30	1.31	1.34
1	A	260	G	N3-C4	-6.29	1.31	1.35
1	A	1111	A	N3-C4	-6.29	1.31	1.34
1	A	722	A	N3-C4	-6.29	1.31	1.34
1	A	666	G	C6-O6	6.28	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	G	C5-C6	-6.28	1.36	1.42
1	A	500	G	N7-C5	-6.27	1.35	1.39
1	A	1236	A	N9-C4	-6.27	1.34	1.37
1	A	740	U	C2-N3	-6.26	1.33	1.37
1	A	1341	U	N3-C4	-6.26	1.32	1.38
1	A	1350	A	C5-C4	-6.26	1.34	1.38
1	A	484	G	N9-C8	-6.25	1.33	1.37
1	A	120	A	N3-C4	-6.25	1.31	1.34
1	A	542	G	C6-N1	-6.24	1.35	1.39
1	A	58	C	C4-C5	-6.24	1.38	1.43
1	A	581	G	N7-C5	-6.24	1.35	1.39
1	A	643	C	C2-O2	6.24	1.30	1.24
1	A	798	G	N1-C2	-6.23	1.32	1.37
1	A	971	G	N3-C4	-6.22	1.31	1.35
1	A	605	U	C4-O4	-6.22	1.18	1.23
1	A	260	G	C6-O6	6.21	1.29	1.24
1	A	329	A	C6-N1	-6.21	1.31	1.35
1	A	1529	G	C5-C4	-6.20	1.34	1.38
1	A	578	C	C2-N3	-6.20	1.30	1.35
1	A	305	G	N7-C5	-6.19	1.35	1.39
1	A	48	C	N1-C6	-6.19	1.33	1.37
1	A	1093	A	C6-N1	-6.19	1.31	1.35
1	A	144	G	C6-N1	6.18	1.43	1.39
1	A	833	U	C2-O2	-6.18	1.16	1.22
1	A	1189	C	N1-C2	6.18	1.46	1.40
1	A	728	A	N3-C4	-6.18	1.31	1.34
2	B	141	GLU	CB-CG	6.17	1.63	1.52
1	A	28	G	N9-C8	-6.16	1.33	1.37
1	A	906	G	N7-C5	-6.16	1.35	1.39
1	A	543	C	N1-C6	-6.15	1.33	1.37
1	A	1168	A	N9-C4	6.15	1.41	1.37
1	A	1491	G	N9-C4	6.14	1.42	1.38
1	A	500	G	N1-C2	6.14	1.42	1.37
1	A	907	A	N3-C4	-6.14	1.31	1.34
1	A	617	G	N3-C4	-6.14	1.31	1.35
1	A	740	U	N1-C6	-6.14	1.32	1.38
1	A	775	G	C8-N7	-6.12	1.27	1.30
1	A	360	A	N9-C4	-6.12	1.34	1.37
1	A	1103	C	N3-C4	-6.12	1.29	1.33
1	A	172	A	N9-C4	-6.12	1.34	1.37
1	A	402	G	N1-C2	-6.12	1.32	1.37
1	A	44	G	N3-C4	-6.11	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	C	N1-C6	-6.11	1.33	1.37
1	A	277	C	N1-C6	-6.11	1.33	1.37
1	A	184	G	C8-N7	-6.10	1.27	1.30
1	A	895	G	C6-N1	-6.09	1.35	1.39
1	A	282	A	N9-C4	-6.09	1.34	1.37
1	A	485	G	N1-C2	-6.09	1.32	1.37
1	A	923	A	C5-C6	-6.09	1.35	1.41
1	A	1166	G	C5-C6	6.08	1.48	1.42
1	A	779	C	N1-C6	-6.07	1.33	1.37
1	A	733	A	C5-C6	-6.06	1.35	1.41
1	A	395	C	N1-C2	-6.05	1.34	1.40
1	A	505	G	C6-O6	-6.05	1.18	1.24
1	A	786	G	C5-C4	-6.05	1.34	1.38
1	A	61	G	C6-N1	6.05	1.43	1.39
1	A	1166	G	N9-C4	6.05	1.42	1.38
1	A	453	A	N9-C4	-6.05	1.34	1.37
1	A	1451	A	N9-C4	-6.04	1.34	1.37
1	A	509	A	N3-C4	-6.03	1.31	1.34
1	A	235	C	N1-C6	-6.03	1.33	1.37
1	A	1101	A	C5-C4	6.03	1.43	1.38
1	A	569	C	N3-C4	-6.02	1.29	1.33
1	A	803	G	C6-N1	-6.02	1.35	1.39
1	A	819	A	N7-C5	-6.02	1.35	1.39
1	A	1516[A]	G	N7-C5	6.02	1.42	1.39
1	A	1516[B]	G	N7-C5	6.02	1.42	1.39
1	A	714	G	C8-N7	-6.02	1.27	1.30
1	A	44	G	C8-N7	-6.01	1.27	1.30
1	A	299	G	N7-C5	-6.01	1.35	1.39
1	A	1200	C	N1-C6	-6.01	1.33	1.37
1	A	109	A	C6-N1	-6.00	1.31	1.35
3	C	105	GLU	CG-CD	6.00	1.60	1.51
1	A	1374	A	C6-N1	-6.00	1.31	1.35
1	A	740	U	N1-C2	-6.00	1.33	1.38
1	A	642	A	N9-C4	-5.99	1.34	1.37
1	A	196	A	N7-C5	5.99	1.42	1.39
1	A	168	G	N7-C5	-5.99	1.35	1.39
1	A	430	A	N7-C5	-5.99	1.35	1.39
1	A	658	G	C6-O6	5.98	1.29	1.24
1	A	41	G	C2-N3	-5.97	1.27	1.32
1	A	297	G	N9-C4	-5.97	1.33	1.38
1	A	768	A	C5-C6	-5.97	1.35	1.41
1	A	915	A	N9-C4	-5.97	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	919	A	N7-C5	-5.97	1.35	1.39
1	A	663	A	C6-N1	-5.96	1.31	1.35
1	A	6	G	C2-N2	-5.96	1.28	1.34
1	A	1302	U	N1-C2	5.96	1.44	1.38
1	A	245	C	N1-C6	-5.95	1.33	1.37
1	A	53	A	C6-N1	-5.95	1.31	1.35
1	A	781	A	C5-C4	-5.95	1.34	1.38
1	A	1198	G	N9-C4	-5.95	1.33	1.38
1	A	438	G	C5-C6	5.95	1.48	1.42
1	A	787	A	C5-C6	-5.95	1.35	1.41
1	A	1281	U	C2-N3	5.94	1.42	1.37
1	A	793	U	C4-C5	5.94	1.48	1.43
1	A	394	G	C6-N1	-5.94	1.35	1.39
1	A	873	A	C5-C4	-5.93	1.34	1.38
1	A	1157	A	N9-C4	5.93	1.41	1.37
1	A	291	C	N1-C6	-5.92	1.33	1.37
1	A	524	G	N9-C8	-5.92	1.33	1.37
1	A	897	C	N1-C6	-5.91	1.33	1.37
17	Q	24	GLU	CG-CD	5.89	1.60	1.51
1	A	1068	G	C6-O6	-5.89	1.18	1.24
1	A	1391	U	C2-O2	5.88	1.27	1.22
1	A	929	G	C2-N3	-5.88	1.28	1.32
1	A	193	C	N1-C6	-5.88	1.33	1.37
1	A	532	A	N7-C5	5.88	1.42	1.39
1	A	1528	U	C4-O4	-5.88	1.19	1.23
1	A	824	C	C4-C5	-5.87	1.38	1.43
13	M	7	VAL	CA-CB	5.87	1.67	1.54
1	A	768	A	N9-C4	-5.87	1.34	1.37
1	A	755	G	C5-C6	-5.86	1.36	1.42
1	A	255	G	C5-C4	-5.86	1.34	1.38
1	A	193	C	N3-C4	-5.86	1.29	1.33
1	A	1068	G	C5-C6	-5.85	1.36	1.42
1	A	1512	U	C2-N3	-5.85	1.33	1.37
1	A	355	C	N3-C4	-5.85	1.29	1.33
1	A	338	A	N3-C4	-5.85	1.31	1.34
1	A	1204	A	N9-C4	-5.85	1.34	1.37
12	L	7	ILE	CA-CB	-5.85	1.41	1.54
1	A	15	G	N9-C8	5.85	1.42	1.37
1	A	58	C	N1-C6	-5.84	1.33	1.37
1	A	1055	A	N7-C5	-5.84	1.35	1.39
1	A	826	C	N3-C4	-5.83	1.29	1.33
1	A	240	C	N1-C6	-5.83	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1188	A	N3-C4	-5.83	1.31	1.34
1	A	609	A	C5-C6	-5.83	1.35	1.41
1	A	402	G	N9-C8	-5.82	1.33	1.37
1	A	919	A	C5-C4	-5.82	1.34	1.38
1	A	669	U	C2-O2	5.82	1.27	1.22
1	A	703	G	C5-C6	5.82	1.48	1.42
1	A	1341	U	C2-N3	-5.82	1.33	1.37
1	A	276	G	C6-N1	-5.81	1.35	1.39
1	A	1401	G	N1-C2	-5.81	1.33	1.37
1	A	664	G	N9-C8	-5.80	1.33	1.37
1	A	327	A	C5-C6	-5.80	1.35	1.41
1	A	361	G	C5-C4	-5.80	1.34	1.38
1	A	511	C	N1-C6	-5.80	1.33	1.37
1	A	220	G	N9-C4	-5.80	1.33	1.38
1	A	584	G	N9-C4	-5.79	1.33	1.38
1	A	285	G	N3-C4	-5.79	1.31	1.35
1	A	218	C	N3-C4	-5.79	1.29	1.33
1	A	1392	G	C5-C4	-5.79	1.34	1.38
1	A	53	A	N3-C4	-5.78	1.31	1.34
1	A	1340	A	N3-C4	-5.78	1.31	1.34
1	A	1509	C	N3-C4	-5.78	1.29	1.33
1	A	440	A	N7-C5	-5.77	1.35	1.39
1	A	929	G	N3-C4	-5.77	1.31	1.35
4	D	150	GLU	CB-CG	5.77	1.63	1.52
1	A	118	U	C2-N3	-5.77	1.33	1.37
1	A	1509	C	N1-C6	-5.77	1.33	1.37
1	A	859	A	N9-C4	-5.77	1.34	1.37
1	A	1342	C	C2-O2	5.77	1.29	1.24
1	A	510	A	C6-N1	-5.76	1.31	1.35
1	A	1393	U	N1-C6	-5.76	1.32	1.38
1	A	297	G	C5-C4	-5.75	1.34	1.38
1	A	144	G	C5-C4	5.75	1.42	1.38
1	A	658	G	C8-N7	-5.75	1.27	1.30
1	A	622	A	C5-C6	-5.74	1.35	1.41
1	A	1251	A	N9-C4	-5.74	1.34	1.37
1	A	1308	U	C4-O4	5.74	1.28	1.23
1	A	634	C	N1-C6	-5.74	1.33	1.37
1	A	1542	U	N1-C6	-5.74	1.32	1.38
1	A	1415	G	C2-N3	5.74	1.37	1.32
1	A	748	C	N3-C4	5.73	1.38	1.33
1	A	327	A	N7-C5	-5.73	1.35	1.39
1	A	903	G	N1-C2	-5.73	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	C	N1-C6	-5.73	1.33	1.37
1	A	789	U	C4-C5	5.72	1.48	1.43
1	A	700	G	C6-O6	5.72	1.29	1.24
1	A	239	U	N1-C2	-5.72	1.33	1.38
1	A	1049	U	N1-C2	-5.72	1.33	1.38
1	A	1055	A	C5-C6	-5.72	1.35	1.41
1	A	1521	G	N7-C5	-5.71	1.35	1.39
1	A	356	A	N3-C4	-5.71	1.31	1.34
1	A	1227	A	N3-C4	-5.71	1.31	1.34
1	A	823	G	C8-N7	-5.71	1.27	1.30
1	A	22	G	C2-N3	-5.70	1.28	1.32
1	A	880	C	N1-C6	-5.70	1.33	1.37
1	A	1399	C	C4-N4	5.70	1.39	1.33
1	A	575	G	N1-C2	-5.70	1.33	1.37
1	A	267	C	C4-C5	-5.69	1.38	1.43
4	D	203	VAL	CA-CB	-5.69	1.42	1.54
1	A	1346	A	C3'-O3'	5.68	1.50	1.42
1	A	775	G	N9-C8	-5.67	1.33	1.37
1	A	344	A	C5-C4	5.67	1.42	1.38
1	A	377	G	C6-N1	-5.67	1.35	1.39
1	A	1084	G	N7-C5	-5.66	1.35	1.39
1	A	892	A	C5-C4	-5.66	1.34	1.38
1	A	122	G	N1-C2	-5.65	1.33	1.37
1	A	484	G	N7-C5	-5.65	1.35	1.39
1	A	888	G	N3-C4	-5.65	1.31	1.35
1	A	1433	A	N3-C4	-5.65	1.31	1.34
1	A	11	G	N1-C2	-5.64	1.33	1.37
1	A	1415	G	C6-O6	5.64	1.29	1.24
12	L	98	TYR	CZ-OH	5.64	1.47	1.37
4	D	31	CYS	CB-SG	-5.64	1.72	1.81
1	A	983	A	C5-C6	-5.63	1.35	1.41
1	A	508	C	N3-C4	-5.63	1.30	1.33
1	A	223	U	C2-N3	-5.63	1.33	1.37
1	A	377	G	C5-C4	-5.63	1.34	1.38
1	A	228	A	N3-C4	-5.62	1.31	1.34
1	A	1517[A]	G	N9-C8	-5.62	1.33	1.37
1	A	1517[B]	G	N9-C8	-5.62	1.33	1.37
1	A	239	U	N1-C6	-5.62	1.32	1.38
1	A	714	G	C5-C4	-5.62	1.34	1.38
1	A	1110	A	N7-C5	5.62	1.42	1.39
1	A	47	C	N3-C4	-5.62	1.30	1.33
1	A	499	A	N7-C5	-5.62	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	C	N1-C6	-5.62	1.33	1.37
1	A	832	C	N1-C6	-5.62	1.33	1.37
1	A	168	G	N3-C4	-5.61	1.31	1.35
1	A	244	U	N1-C6	-5.61	1.32	1.38
1	A	759	A	N3-C4	-5.61	1.31	1.34
1	A	133	U	C4-O4	5.61	1.28	1.23
1	A	733	A	C5-C4	-5.61	1.34	1.38
1	A	929	G	N1-C2	-5.60	1.33	1.37
1	A	714	G	N3-C4	-5.60	1.31	1.35
1	A	1079	G	C6-N1	-5.60	1.35	1.39
1	A	47	C	C2-N3	-5.60	1.31	1.35
1	A	51	A	C6-N6	-5.60	1.29	1.33
1	A	256	U	C2-N3	5.60	1.41	1.37
1	A	528	C	N3-C4	-5.59	1.30	1.33
1	A	504	C	C5-C6	-5.59	1.29	1.34
1	A	255	G	C5-C6	-5.59	1.36	1.42
1	A	806	C	N3-C4	-5.58	1.30	1.33
1	A	297	G	N7-C5	-5.58	1.35	1.39
1	A	728	A	C6-N6	-5.58	1.29	1.33
1	A	1087	G	C6-O6	5.58	1.29	1.24
1	A	88	A	N3-C4	-5.58	1.31	1.34
1	A	807	A	C5-C6	-5.58	1.36	1.41
1	A	1415	G	C5-C4	5.57	1.42	1.38
1	A	380	G	N9-C8	-5.57	1.33	1.37
1	A	411	A	N9-C4	-5.57	1.34	1.37
1	A	669	U	N1-C6	-5.57	1.32	1.38
1	A	814	A	N9-C4	-5.57	1.34	1.37
1	A	853	G	C2-N2	5.57	1.40	1.34
1	A	1530	G	N9-C8	5.56	1.41	1.37
21	U	6	ARG	CB-CG	5.56	1.67	1.52
1	A	543	C	N3-C4	-5.56	1.30	1.33
1	A	1525	G	N9-C4	5.55	1.42	1.38
1	A	176	C	N1-C6	-5.55	1.33	1.37
1	A	1279	A	N7-C5	-5.55	1.35	1.39
1	A	289	G	N9-C8	-5.55	1.33	1.37
1	A	303	A	N7-C5	-5.54	1.35	1.39
1	A	411	A	N3-C4	-5.54	1.31	1.34
1	A	1106	G	N1-C2	-5.54	1.33	1.37
1	A	584	G	C6-N1	-5.54	1.35	1.39
1	A	1437	C	C2-O2	5.54	1.29	1.24
1	A	1022	G	N9-C4	5.54	1.42	1.38
1	A	524	G	C5-C4	-5.53	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	35	GLU	CG-CD	5.53	1.60	1.51
1	A	39	G	N1-C2	-5.53	1.33	1.37
1	A	542	G	N1-C2	-5.53	1.33	1.37
1	A	184	G	N1-C2	-5.53	1.33	1.37
1	A	406	G	C6-N1	5.53	1.43	1.39
1	A	897	C	C5-C6	-5.52	1.29	1.34
1	A	908	A	N7-C5	-5.52	1.35	1.39
5	E	140	ARG	CB-CG	5.52	1.67	1.52
1	A	741	G	N1-C2	-5.51	1.33	1.37
1	A	116	A	N3-C4	-5.51	1.31	1.34
1	A	659	U	N3-C4	-5.50	1.33	1.38
1	A	1087	G	C6-N1	5.50	1.43	1.39
1	A	582	U	N1-C2	-5.50	1.33	1.38
1	A	1218	C	N3-C4	-5.50	1.30	1.33
1	A	1227	A	N9-C4	-5.49	1.34	1.37
1	A	730	G	C5-C4	-5.49	1.34	1.38
16	P	34	GLU	CG-CD	5.49	1.60	1.51
1	A	839	U	N1-C2	5.49	1.43	1.38
1	A	902	G	N1-C2	-5.49	1.33	1.37
1	A	828	A	N9-C8	-5.48	1.33	1.37
1	A	18	C	N3-C4	-5.48	1.30	1.33
1	A	1403	C	N1-C6	-5.48	1.33	1.37
1	A	328	C	C2-N3	-5.48	1.31	1.35
1	A	35	G	C8-N7	-5.48	1.27	1.30
1	A	963	G	N7-C5	-5.48	1.35	1.39
1	A	299	G	N9-C8	-5.47	1.34	1.37
1	A	227	G	C6-N1	-5.47	1.35	1.39
1	A	580	U	C4-O4	5.47	1.28	1.23
1	A	1338	G	C6-N1	-5.47	1.35	1.39
1	A	1093	A	C5-C6	-5.47	1.36	1.41
1	A	1077	G	N1-C2	-5.46	1.33	1.37
1	A	1525	G	C6-N1	-5.45	1.35	1.39
1	A	1408	A	C5-C4	5.45	1.42	1.38
1	A	30	U	C2-O2	5.45	1.27	1.22
1	A	577	G	C2-N3	-5.44	1.28	1.32
1	A	366	C	C2-O2	-5.44	1.19	1.24
1	A	1058	G	C6-N1	-5.44	1.35	1.39
1	A	1403	C	N1-C2	-5.43	1.34	1.40
1	A	704	A	N3-C4	-5.43	1.31	1.34
1	A	398	C	N3-C4	-5.42	1.30	1.33
12	L	37	CYS	CB-SG	-5.42	1.73	1.81
1	A	602	A	N7-C5	-5.42	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	784	C	C4-C5	-5.42	1.38	1.43
1	A	300	A	C6-N1	-5.42	1.31	1.35
1	A	533	A	C6-N1	-5.42	1.31	1.35
1	A	325	A	N1-C2	-5.41	1.29	1.34
1	A	1067	A	N3-C4	-5.41	1.31	1.34
1	A	130	A	C5-C6	-5.40	1.36	1.41
1	A	1387	G	N3-C4	-5.40	1.31	1.35
1	A	1127	G	N7-C5	-5.39	1.36	1.39
1	A	567	G	N3-C4	-5.39	1.31	1.35
1	A	874	G	N3-C4	-5.39	1.31	1.35
1	A	875	C	C4-C5	-5.39	1.38	1.43
1	A	515	G	N3-C4	-5.38	1.31	1.35
1	A	1069	C	C4-C5	-5.38	1.38	1.43
1	A	1516[A]	G	C2-N3	-5.38	1.28	1.32
1	A	1516[B]	G	C2-N3	-5.38	1.28	1.32
1	A	963	G	N3-C4	-5.38	1.31	1.35
1	A	1417	G	C5-C4	5.38	1.42	1.38
1	A	312	C	C4-C5	-5.38	1.38	1.43
1	A	453	A	N3-C4	-5.38	1.31	1.34
1	A	60	A	N3-C4	-5.37	1.31	1.34
1	A	379	C	N1-C6	-5.37	1.33	1.37
1	A	144	G	N1-C2	5.37	1.42	1.37
1	A	871	U	N1-C6	-5.37	1.33	1.38
1	A	363	A	C5-C6	-5.37	1.36	1.41
1	A	926	G	N1-C2	-5.36	1.33	1.37
1	A	1068	G	C6-N1	-5.36	1.35	1.39
1	A	1353	G	N1-C2	-5.36	1.33	1.37
1	A	878	G	N1-C2	-5.36	1.33	1.37
1	A	1500	A	N3-C4	-5.36	1.31	1.34
1	A	1502	A	N7-C5	-5.36	1.36	1.39
1	A	356	A	N9-C4	-5.35	1.34	1.37
1	A	108	G	N3-C4	-5.35	1.31	1.35
1	A	170	U	C4-O4	5.35	1.27	1.23
5	E	8	GLU	CG-CD	5.35	1.59	1.51
1	A	115	G	N9-C8	-5.35	1.34	1.37
1	A	44	G	C5-C4	-5.35	1.34	1.38
1	A	853	G	N7-C5	-5.34	1.36	1.39
1	A	703	G	N7-C5	5.34	1.42	1.39
1	A	1375	A	N9-C4	5.34	1.41	1.37
1	A	1516[A]	G	N9-C4	-5.34	1.33	1.38
1	A	1516[B]	G	N9-C4	-5.34	1.33	1.38
12	L	108	ALA	CA-CB	-5.34	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	G	N7-C5	-5.33	1.36	1.39
1	A	1125	U	O3'-P	5.33	1.67	1.61
1	A	388	G	N3-C4	-5.32	1.31	1.35
1	A	729	A	N1-C2	-5.32	1.29	1.34
1	A	1103	C	C2-O2	-5.32	1.19	1.24
1	A	954	G	C5-C4	-5.32	1.34	1.38
1	A	494	G	N7-C5	-5.31	1.36	1.39
1	A	28	G	C5-C4	-5.31	1.34	1.38
1	A	774	G	N1-C2	-5.31	1.33	1.37
1	A	1508	G	C2-N3	-5.31	1.28	1.32
1	A	117	G	C5-C4	5.30	1.42	1.38
1	A	1180	A	C5-C6	-5.30	1.36	1.41
1	A	1493	A	C5-C4	5.30	1.42	1.38
1	A	263	A	C5-C6	-5.30	1.36	1.41
2	B	164	VAL	CB-CG2	-5.30	1.41	1.52
1	A	1205	U	N1-C6	-5.29	1.33	1.38
1	A	66	G	N9-C4	-5.29	1.33	1.38
1	A	497	A	N9-C4	-5.29	1.34	1.37
1	A	829	G	N9-C4	-5.29	1.33	1.38
1	A	1521	G	C5-C4	-5.29	1.34	1.38
1	A	487	A	C5-C4	-5.29	1.35	1.38
1	A	1125	U	C2-N3	5.29	1.41	1.37
1	A	361	G	N9-C8	-5.29	1.34	1.37
1	A	341	C	N1-C6	5.28	1.40	1.37
1	A	533	A	N3-C4	-5.28	1.31	1.34
1	A	887	G	N9-C8	-5.28	1.34	1.37
2	B	94	ASN	CB-CG	-5.28	1.39	1.51
1	A	1308	U	C2-N3	5.28	1.41	1.37
1	A	578	C	N1-C6	-5.27	1.33	1.37
1	A	635	G	N9-C4	-5.27	1.33	1.38
21	U	6	ARG	CG-CD	5.27	1.65	1.51
1	A	550	G	N3-C4	-5.26	1.31	1.35
1	A	607	A	N3-C4	-5.26	1.31	1.34
1	A	798	G	C5-C4	-5.26	1.34	1.38
1	A	81	U	C2-N3	5.26	1.41	1.37
1	A	196	A	N9-C4	-5.26	1.34	1.37
1	A	231	G	N9-C4	-5.26	1.33	1.38
1	A	578	C	C5-C6	-5.26	1.30	1.34
1	A	352	C	P-O5'	-5.26	1.54	1.59
1	A	1104	G	C6-N1	-5.25	1.35	1.39
1	A	377	G	N3-C4	-5.25	1.31	1.35
1	A	585	G	C6-N1	-5.25	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	G	C5-C4	-5.24	1.34	1.38
1	A	172	A	N7-C5	-5.24	1.36	1.39
1	A	336	C	C2-O2	5.24	1.29	1.24
1	A	1529	G	C8-N7	-5.24	1.27	1.30
2	B	97	TRP	CG-CD2	-5.24	1.34	1.43
1	A	380	G	C5-C6	5.23	1.47	1.42
1	A	900	A	N7-C5	-5.23	1.36	1.39
1	A	1231	G	C5-C6	-5.23	1.37	1.42
1	A	1304	G	C5-C4	5.23	1.42	1.38
1	A	235	C	N3-C4	-5.23	1.30	1.33
1	A	636	U	C4-O4	5.23	1.27	1.23
1	A	298	A	N9-C4	-5.22	1.34	1.37
1	A	109	A	C6-N6	-5.22	1.29	1.33
1	A	185	A	N3-C4	-5.21	1.31	1.34
1	A	718	G	N9-C4	-5.21	1.33	1.38
1	A	769	G	N3-C4	-5.21	1.31	1.35
1	A	816	A	N7-C5	-5.21	1.36	1.39
1	A	430	A	C5-C6	-5.21	1.36	1.41
1	A	1276	G	C6-N1	5.21	1.43	1.39
1	A	1284	C	C2-O2	5.21	1.29	1.24
1	A	1350	A	C6-N1	-5.21	1.31	1.35
1	A	234	C	C2-N3	-5.21	1.31	1.35
1	A	139	G	C5-C4	-5.20	1.34	1.38
1	A	44	G	N1-C2	-5.20	1.33	1.37
1	A	29	G	N3-C4	-5.20	1.31	1.35
1	A	954	G	N9-C4	-5.20	1.33	1.38
1	A	1370	G	C6-O6	-5.20	1.19	1.24
1	A	281	G	N3-C4	-5.19	1.31	1.35
1	A	1392	G	N3-C4	-5.19	1.31	1.35
1	A	171	A	N9-C4	-5.19	1.34	1.37
2	B	165	VAL	CB-CG1	5.19	1.63	1.52
1	A	587	G	C5-C4	-5.19	1.34	1.38
1	A	504	C	N3-C4	-5.18	1.30	1.33
1	A	637	G	C6-O6	5.18	1.28	1.24
1	A	787	A	N3-C4	-5.18	1.31	1.34
1	A	462	G	N9-C4	5.18	1.42	1.38
1	A	875	C	N1-C6	-5.18	1.34	1.37
1	A	1490	C	N1-C6	5.18	1.40	1.37
1	A	383	A	N3-C4	-5.17	1.31	1.34
1	A	519	C	N3-C4	-5.17	1.30	1.33
1	A	703	G	N1-C2	-5.17	1.33	1.37
12	L	98	TYR	CE1-CZ	5.17	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	G	N3-C4	-5.17	1.31	1.35
1	A	61	G	N9-C4	-5.17	1.33	1.38
1	A	983	A	N3-C4	-5.17	1.31	1.34
1	A	1388	C	N1-C6	5.17	1.40	1.37
1	A	1501	C	C4-C5	-5.17	1.38	1.43
1	A	676	A	C5-C4	-5.17	1.35	1.38
1	A	560	U	C4-O4	5.17	1.27	1.23
1	A	635	G	N1-C2	5.16	1.41	1.37
2	B	97	TRP	CG-CD1	5.15	1.44	1.36
1	A	242	C	C2-N3	-5.15	1.31	1.35
1	A	902	G	C6-O6	-5.15	1.19	1.24
1	A	313	A	N3-C4	-5.15	1.31	1.34
1	A	111	G	C6-O6	5.14	1.28	1.24
1	A	410	G	N3-C4	-5.14	1.31	1.35
1	A	829	G	N3-C4	-5.14	1.31	1.35
1	A	281	G	C5-C6	-5.14	1.37	1.42
1	A	1093	A	N7-C5	-5.14	1.36	1.39
1	A	1158	C	N1-C6	-5.14	1.34	1.37
1	A	1279	A	C5-C6	-5.14	1.36	1.41
1	A	1502	A	C5'-C4'	-5.14	1.45	1.51
1	A	10	A	C6-N6	-5.13	1.29	1.33
1	A	21	G	C8-N7	-5.13	1.27	1.30
1	A	228	A	N7-C5	-5.13	1.36	1.39
1	A	1530	G	N9-C4	-5.13	1.33	1.38
1	A	922	G	C5-C6	-5.13	1.37	1.42
1	A	440	A	N3-C4	-5.13	1.31	1.34
1	A	826	C	C4-N4	-5.13	1.29	1.33
1	A	918	A	C5-C6	-5.13	1.36	1.41
1	A	730	G	N9-C8	-5.12	1.34	1.37
1	A	873	A	C5-C6	-5.12	1.36	1.41
1	A	1050	G	N7-C5	-5.11	1.36	1.39
1	A	535	A	C6-N6	-5.11	1.29	1.33
1	A	363	A	N9-C4	-5.11	1.34	1.37
1	A	1098	C	N1-C6	-5.11	1.34	1.37
1	A	718	G	N1-C2	5.11	1.41	1.37
1	A	1504	G	N3-C4	-5.10	1.31	1.35
1	A	602	A	C5-C6	-5.10	1.36	1.41
1	A	965	A	N7-C5	5.10	1.42	1.39
1	A	851	G	C6-O6	5.09	1.28	1.24
1	A	1338	G	N3-C4	-5.09	1.31	1.35
6	F	5	GLU	CD-OE2	5.09	1.31	1.25
1	A	293	G	C6-N1	-5.09	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	890	G	C5-C6	5.09	1.47	1.42
8	H	135	CYS	CB-SG	-5.09	1.73	1.81
1	A	854	G	C4'-O4'	-5.08	1.39	1.45
17	Q	9	VAL	CB-CG2	-5.08	1.42	1.52
1	A	28	G	C6-N1	-5.08	1.35	1.39
1	A	310	G	C5-C6	-5.08	1.37	1.42
1	A	344	A	N9-C4	5.08	1.40	1.37
1	A	769	G	C6-O6	5.08	1.28	1.24
1	A	1088	G	N1-C2	-5.07	1.33	1.37
1	A	1119	C	O3'-P	-5.07	1.55	1.61
1	A	1287	A	N7-C5	-5.07	1.36	1.39
1	A	260	G	C2-N3	-5.07	1.28	1.32
1	A	309	G	N7-C5	-5.07	1.36	1.39
6	F	23	LYS	CD-CE	5.06	1.64	1.51
1	A	362	G	N7-C5	-5.06	1.36	1.39
1	A	914	A	N7-C5	-5.06	1.36	1.39
1	A	1205	U	C2-N3	-5.06	1.34	1.37
1	A	198	G	C6-N1	-5.06	1.36	1.39
1	A	735	C	N1-C6	-5.06	1.34	1.37
1	A	950	U	C4-O4	5.05	1.27	1.23
1	A	288	A	N9-C4	-5.05	1.34	1.37
1	A	507	C	C2-O2	5.04	1.28	1.24
1	A	566	G	N1-C2	-5.04	1.33	1.37
1	A	50	A	N9-C4	-5.04	1.34	1.37
1	A	779	C	C2-N3	-5.04	1.31	1.35
1	A	784	C	N3-C4	-5.04	1.30	1.33
1	A	800	G	C6-N1	-5.04	1.36	1.39
1	A	1321	C	N3-C4	-5.04	1.30	1.33
8	H	134	ILE	CA-CB	-5.04	1.43	1.54
1	A	754	C	C2-N3	5.04	1.39	1.35
1	A	946	A	N3-C4	-5.04	1.31	1.34
1	A	913	A	C6-N1	-5.04	1.32	1.35
1	A	1136	U	C2-N3	5.04	1.41	1.37
1	A	651	C	C2-N3	5.03	1.39	1.35
1	A	827	U	C2-N3	5.03	1.41	1.37
1	A	306	G	C6-N1	5.03	1.43	1.39
1	A	245	C	N1-C2	-5.02	1.35	1.40
1	A	1288	A	N9-C4	-5.02	1.34	1.37
1	A	1247	U	C4-O4	5.02	1.27	1.23
1	A	1206	G	N3-C4	-5.02	1.31	1.35
1	A	548	G	C5-C6	-5.01	1.37	1.42
12	L	28	LYS	CB-CG	5.01	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	624	C	N1-C6	-5.01	1.34	1.37
1	A	764	C	N1-C6	-5.01	1.34	1.37
1	A	396	G	N3-C4	-5.00	1.31	1.35

All (5646) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1528	U	O5'-P-OP2	-27.91	77.21	110.70
1	A	279	A	N1-C6-N6	24.78	133.47	118.60
1	A	975	A	C2-N3-C4	-23.57	98.82	110.60
1	A	117	G	C5-C6-N1	-23.41	99.80	111.50
1	A	279	A	C5-N7-C8	-21.45	93.17	103.90
1	A	266	G	N3-C4-C5	20.89	139.04	128.60
1	A	117	G	N1-C6-O6	20.78	132.37	119.90
1	A	122	G	C8-N9-C4	20.55	114.62	106.40
1	A	711	G	N1-C6-O6	20.14	131.98	119.90
1	A	108	G	N1-C6-O6	20.04	131.92	119.90
1	A	122	G	N7-C8-N9	-19.84	103.18	113.10
1	A	279	A	C6-C5-N7	-19.75	118.47	132.30
1	A	730	G	C4-C5-N7	-19.46	103.02	110.80
1	A	730	G	N9-C4-C5	19.35	113.14	105.40
1	A	1504	G	O5'-P-OP1	-19.22	87.63	110.70
1	A	404	U	O5'-P-OP2	-18.71	88.25	110.70
1	A	401	C	N1-C2-O2	-18.57	107.76	118.90
1	A	1108	G	O5'-P-OP1	-18.48	88.52	110.70
1	A	1397	C	O5'-P-OP1	-18.44	88.57	110.70
1	A	1189	C	N1-C2-O2	18.43	129.96	118.90
1	A	234	C	C5-C6-N1	-18.29	111.85	121.00
1	A	371	G	O5'-P-OP1	-18.26	88.78	110.70
1	A	552	U	C5-C6-N1	-18.20	113.60	122.70
1	A	279	A	C4-C5-N7	18.20	119.80	110.70
1	A	555	C	O5'-P-OP2	-18.09	88.99	110.70
1	A	484	G	N3-C2-N2	17.87	132.41	119.90
1	A	624	C	C6-N1-C2	17.70	127.38	120.30
1	A	242	C	C5-C6-N1	-17.41	112.30	121.00
1	A	254	G	O5'-P-OP1	-17.35	89.89	110.70
1	A	518	C	O5'-P-OP1	-17.32	89.92	110.70
1	A	1411	C	C6-N1-C2	17.18	127.17	120.30
1	A	914	A	O5'-P-OP1	-17.15	90.12	110.70
1	A	1374	A	N1-C6-N6	-17.12	108.33	118.60
1	A	61	G	N1-C6-O6	17.06	130.13	119.90
1	A	279	A	N7-C8-N9	17.05	122.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	C	C6-N1-C2	16.98	127.09	120.30
1	A	266	G	N3-C4-N9	-16.89	115.87	126.00
1	A	880	C	C5-C6-N1	-16.72	112.64	121.00
1	A	975	A	C5-C6-N1	-16.69	109.35	117.70
1	A	484	G	N1-C2-N2	-16.54	101.32	116.20
1	A	1525	G	C8-N9-C4	-16.49	99.80	106.40
1	A	260	G	C8-N9-C4	-16.48	99.81	106.40
1	A	578	C	C2-N3-C4	-16.36	111.72	119.90
1	A	980	C	O5'-P-OP1	-16.30	91.03	105.70
1	A	833	U	C5-C6-N1	-16.15	114.62	122.70
1	A	300	A	N1-C6-N6	-16.13	108.92	118.60
1	A	122	G	C5-N7-C8	16.13	112.36	104.30
1	A	549	C	C6-N1-C2	16.09	126.73	120.30
1	A	779	C	C5-C6-N1	-16.06	112.97	121.00
1	A	1302	U	N3-C2-O2	-16.06	110.96	122.20
1	A	699	C	C6-N1-C2	16.05	126.72	120.30
1	A	279	A	C5-C6-N6	-16.05	110.86	123.70
1	A	496	A	O5'-P-OP1	-16.05	91.26	105.70
1	A	962	C	C6-N1-C2	15.98	126.69	120.30
1	A	599	C	C6-N1-C2	15.94	126.68	120.30
1	A	577	G	N3-C2-N2	-15.93	108.75	119.90
1	A	117	G	O5'-P-OP2	-15.93	91.37	105.70
1	A	1529	G	O5'-P-OP1	-15.87	91.42	105.70
1	A	819	A	N1-C6-N6	15.78	128.07	118.60
1	A	108	G	N3-C4-C5	15.65	136.43	128.60
1	A	872	A	O5'-P-OP1	-15.65	91.61	105.70
1	A	1493	A	C8-N9-C4	-15.58	99.57	105.80
1	A	578	C	C5-C6-N1	-15.58	113.21	121.00
1	A	242	C	N3-C4-C5	15.51	128.10	121.90
1	A	228	A	N1-C6-N6	-15.49	109.31	118.60
1	A	1050	G	N1-C6-O6	15.43	129.16	119.90
1	A	234	C	C6-N1-C2	15.41	126.47	120.30
1	A	922	G	N1-C6-O6	15.39	129.14	119.90
1	A	1202	G	N3-C4-N9	-15.36	116.78	126.00
1	A	242	C	C2-N3-C4	-15.32	112.24	119.90
1	A	766	A	O5'-P-OP2	-15.31	91.92	105.70
1	A	1411	C	N3-C2-O2	15.31	132.61	121.90
1	A	589	C	C6-N1-C2	-15.20	114.22	120.30
1	A	1063	C	N1-C2-O2	-15.19	109.78	118.90
1	A	889	A	N1-C6-N6	-15.17	109.50	118.60
1	A	332	G	N1-C6-O6	15.15	128.99	119.90
1	A	120	A	C2-N3-C4	-15.12	103.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1530	G	N3-C4-C5	15.12	136.16	128.60
1	A	300	A	N9-C4-C5	15.07	111.83	105.80
1	A	904	C	N3-C4-C5	15.07	127.93	121.90
1	A	1532	U	C5-C6-N1	15.06	130.23	122.70
1	A	372	C	N1-C2-O2	15.06	127.94	118.90
1	A	7	G	C5-C6-O6	-15.04	119.58	128.60
1	A	1079	G	C8-N9-C4	-15.04	100.38	106.40
1	A	10	A	N1-C6-N6	-15.04	109.58	118.60
1	A	9	G	O5'-P-OP2	-15.02	92.18	105.70
1	A	147	G	N1-C6-O6	15.01	128.91	119.90
1	A	117	G	C6-C5-N7	-15.00	121.40	130.40
1	A	438	G	C4-C5-N7	-15.00	104.80	110.80
1	A	1530	G	C4-N9-C1'	-14.91	107.12	126.50
1	A	1202	G	N9-C4-C5	14.85	111.34	105.40
1	A	1374	A	N9-C4-C5	14.78	111.71	105.80
1	A	228	A	N9-C4-C5	14.74	111.70	105.80
1	A	975	A	C5-N7-C8	-14.68	96.56	103.90
1	A	234	C	N3-C4-N4	-14.61	107.77	118.00
1	A	531	U	O5'-P-OP1	-14.57	92.59	105.70
1	A	711	G	C5-C6-O6	-14.56	119.86	128.60
1	A	902	G	N1-C6-O6	-14.55	111.17	119.90
1	A	572	A	N1-C6-N6	-14.53	109.88	118.60
1	A	1075	C	O5'-P-OP2	-14.48	92.67	105.70
1	A	108	G	C2-N3-C4	-14.45	104.67	111.90
1	A	578	C	N3-C4-C5	14.42	127.67	121.90
1	A	363	A	C5-C6-N6	-14.42	112.16	123.70
1	A	1516[A]	G	N3-C4-N9	-14.39	117.36	126.00
1	A	1516[B]	G	N3-C4-N9	-14.39	117.36	126.00
1	A	1290	G	N1-C6-O6	14.34	128.51	119.90
1	A	144	G	N1-C6-O6	14.34	128.50	119.90
1	A	363	A	N1-C6-N6	14.34	127.20	118.60
1	A	285	G	C2-N3-C4	-14.26	104.77	111.90
1	A	500	G	O5'-P-OP1	-14.24	92.88	105.70
1	A	1505	G	N3-C4-C5	-14.23	121.48	128.60
1	A	736	C	C6-N1-C2	-14.17	114.63	120.30
1	A	728	A	C8-N9-C4	-14.16	100.13	105.80
1	A	117	G	C8-N9-C1'	-14.16	108.59	127.00
1	A	825	G	O5'-P-OP1	-14.13	92.99	105.70
1	A	108	G	C5-C6-N1	-14.09	104.45	111.50
1	A	135	C	O5'-P-OP2	-14.09	93.02	105.70
1	A	1101	A	C5-C6-N1	-14.07	110.66	117.70
1	A	620	C	N3-C4-C5	14.04	127.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1530	G	N3-C4-N9	-14.04	117.57	126.00
1	A	34	C	C6-N1-C2	14.04	125.92	120.30
1	A	121	C	C6-N1-C2	13.99	125.90	120.30
1	A	117	G	N9-C4-C5	-13.96	99.82	105.40
1	A	260	G	N9-C4-C5	13.90	110.96	105.40
1	A	380	G	C4-C5-N7	-13.84	105.26	110.80
1	A	387	U	O5'-P-OP2	-13.82	93.26	105.70
1	A	889	A	N9-C4-C5	13.81	111.32	105.80
1	A	266	G	C5-N7-C8	-13.80	97.40	104.30
1	A	504	C	C6-N1-C2	-13.79	114.78	120.30
1	A	834	C	C5-C6-N1	-13.78	114.11	121.00
1	A	1528	U	O5'-P-OP1	13.73	127.18	110.70
1	A	725	G	N1-C6-O6	13.73	128.14	119.90
1	A	284	G	N1-C6-O6	13.71	128.13	119.90
1	A	873	A	O5'-P-OP2	-13.70	93.37	105.70
1	A	7	G	N1-C6-O6	13.68	128.11	119.90
1	A	790	A	N1-C2-N3	13.68	136.14	129.30
1	A	686	U	N1-C2-N3	13.66	123.10	114.90
1	A	241	C	C6-N1-C2	13.64	125.75	120.30
1	A	768	A	N1-C2-N3	13.63	136.12	129.30
1	A	1222	G	N1-C6-O6	13.61	128.06	119.90
1	A	564	C	N1-C2-O2	13.61	127.06	118.90
1	A	1378	C	N3-C4-C5	-13.61	116.46	121.90
1	A	834	C	O5'-P-OP2	-13.60	93.47	105.70
1	A	775	G	N3-C2-N2	13.59	129.41	119.90
1	A	1374	A	C8-N9-C4	-13.59	100.36	105.80
1	A	306	G	O5'-P-OP1	-13.54	93.52	105.70
1	A	228	A	C5-C6-N6	13.49	134.49	123.70
1	A	703	G	N3-C2-N2	13.47	129.33	119.90
1	A	711	G	C4-C5-N7	13.41	116.16	110.80
1	A	498	U	O5'-P-OP2	-13.39	93.65	105.70
1	A	552	U	C2-N3-C4	-13.37	118.98	127.00
1	A	117	G	C4-C5-C6	13.27	126.76	118.80
1	A	1222	G	C5-C6-N1	-13.27	104.87	111.50
1	A	1102	A	C8-N9-C4	-13.26	100.50	105.80
1	A	484	G	N3-C4-N9	13.25	133.95	126.00
1	A	27	G	C4-C5-N7	13.24	116.10	110.80
1	A	525	C	N3-C4-C5	13.16	127.17	121.90
1	A	247	G	N1-C6-O6	13.14	127.78	119.90
1	A	790	A	C4-C5-C6	13.14	123.57	117.00
1	A	1530	G	C8-N9-C1'	13.14	144.08	127.00
1	A	730	G	C5-C6-O6	13.13	136.48	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	740	U	C5-C6-N1	-13.12	116.14	122.70
1	A	711	G	C6-C5-N7	-13.09	122.55	130.40
1	A	436	C	O5'-P-OP1	-13.08	93.93	105.70
1	A	1302	U	N1-C2-O2	13.07	131.95	122.80
1	A	768	A	C4-C5-C6	13.06	123.53	117.00
1	A	1087	G	N1-C6-O6	13.05	127.73	119.90
1	A	544	G	C4-C5-N7	13.04	116.02	110.80
1	A	1350	A	N1-C6-N6	-13.01	110.79	118.60
1	A	6	G	N1-C2-N3	12.98	131.69	123.90
1	A	1411	C	C2-N1-C1'	-12.96	104.54	118.80
1	A	367	U	C5-C6-N1	-12.94	116.23	122.70
1	A	408	A	C8-N9-C4	-12.94	100.62	105.80
1	A	22	G	C8-N9-C4	-12.92	101.23	106.40
1	A	728	A	N1-C6-N6	-12.91	110.85	118.60
1	A	291	C	C6-N1-C2	-12.90	115.14	120.30
1	A	544	G	C5-C6-O6	-12.89	120.87	128.60
1	A	770	C	N3-C4-C5	12.88	127.05	121.90
1	A	729	A	C8-N9-C4	-12.86	100.66	105.80
1	A	662	G	N1-C6-O6	12.85	127.61	119.90
1	A	363	A	C5-N7-C8	-12.85	97.48	103.90
1	A	620	C	C6-N1-C2	12.84	125.44	120.30
1	A	907	A	N1-C6-N6	-12.83	110.90	118.60
1	A	549	C	N3-C4-C5	12.82	127.03	121.90
1	A	755	G	C6-C5-N7	-12.81	122.71	130.40
1	A	693	G	O5'-P-OP1	-12.81	94.17	105.70
1	A	1219	U	O5'-P-OP2	-12.78	94.20	105.70
1	A	981	U	C6-N1-C2	-12.77	113.34	121.00
1	A	1193	G	N1-C2-N3	12.77	131.56	123.90
1	A	746	A	N1-C2-N3	12.75	135.68	129.30
1	A	401	C	N3-C2-O2	12.75	130.82	121.90
1	A	402	G	N1-C2-N3	12.75	131.55	123.90
1	A	234	C	C2-N3-C4	-12.72	113.54	119.90
1	A	851	G	C5-C6-N1	-12.71	105.15	111.50
1	A	363	A	C4-C5-N7	12.69	117.05	110.70
1	A	775	G	N1-C2-N2	-12.68	104.79	116.20
1	A	794	A	O5'-P-OP2	-12.67	94.30	105.70
1	A	703	G	C8-N9-C4	12.63	111.45	106.40
1	A	880	C	C2-N3-C4	-12.62	113.59	119.90
1	A	43	C	O5'-P-OP1	-12.61	94.35	105.70
1	A	637	G	N1-C6-O6	12.59	127.46	119.90
1	A	299	G	C5-C6-O6	12.59	136.16	128.60
1	A	27	G	C5-C6-O6	-12.58	121.06	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	C	C4-C5-C6	12.56	123.68	117.40
1	A	834	C	C6-N1-C2	12.54	125.31	120.30
1	A	518	C	O5'-P-OP2	12.48	125.67	110.70
1	A	658	G	C8-N9-C1'	-12.48	110.78	127.00
1	A	975	A	N3-C4-C5	12.46	135.52	126.80
1	A	1231	G	N1-C6-O6	12.41	127.34	119.90
1	A	779	C	C6-N1-C2	12.36	125.25	120.30
1	A	1342	C	C6-N1-C2	12.36	125.25	120.30
1	A	577	G	N1-C2-N2	12.35	127.32	116.20
1	A	1390	U	N3-C4-C5	-12.35	107.19	114.60
5	E	14	ARG	NE-CZ-NH2	-12.35	114.13	120.30
1	A	662	G	C6-C5-N7	-12.34	122.99	130.40
1	A	231	G	N1-C6-O6	12.31	127.29	119.90
1	A	736	C	N3-C2-O2	-12.31	113.28	121.90
1	A	792	A	N1-C6-N6	12.31	125.98	118.60
1	A	283	C	N3-C4-C5	-12.30	116.98	121.90
1	A	613	C	O5'-P-OP1	-12.29	94.64	105.70
1	A	722	A	C2-N3-C4	-12.27	104.46	110.60
1	A	787	A	N1-C6-N6	12.27	125.96	118.60
1	A	1075	C	C5-C6-N1	-12.27	114.87	121.00
1	A	819	A	C5-C6-N6	-12.26	113.89	123.70
1	A	1377	A	N1-C2-N3	12.26	135.43	129.30
1	A	1227	A	N1-C6-N6	12.24	125.94	118.60
1	A	328	C	C6-N1-C2	12.24	125.19	120.30
1	A	252	U	N1-C2-O2	-12.23	114.24	122.80
1	A	1530	G	C6-C5-N7	12.23	137.74	130.40
1	A	1116	C	C6-N1-C2	12.23	125.19	120.30
1	A	108	G	C6-C5-N7	-12.23	123.06	130.40
1	A	321	A	O5'-P-OP2	-12.21	94.71	105.70
1	A	326	G	C5-C6-N1	-12.20	105.40	111.50
1	A	1395	C	C6-N1-C2	12.20	125.18	120.30
1	A	1209	C	C6-N1-C2	12.19	125.18	120.30
4	D	12	CYS	CA-CB-SG	12.17	135.91	114.00
1	A	401	C	N3-C4-N4	12.15	126.50	118.00
1	A	559	A	O5'-P-OP1	-12.14	94.77	105.70
1	A	1443	G	N3-C4-C5	12.07	134.63	128.60
1	A	331	G	N1-C6-O6	12.03	127.12	119.90
1	A	260	G	C5-C6-N1	-12.02	105.49	111.50
1	A	1397	C	OP1-P-OP2	11.99	137.59	119.60
1	A	746	A	N1-C6-N6	-11.99	111.41	118.60
1	A	120	A	C4-C5-C6	11.98	122.99	117.00
1	A	805	C	N3-C4-C5	11.98	126.69	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	G	O5'-P-OP2	-11.98	94.92	105.70
1	A	283	C	C5-C6-N1	11.97	126.98	121.00
1	A	1281	U	C5-C6-N1	11.96	128.68	122.70
1	A	1500	A	O5'-P-OP1	-11.95	94.95	105.70
1	A	1433	A	N1-C6-N6	-11.95	111.43	118.60
1	A	536	C	C6-N1-C2	-11.93	115.53	120.30
1	A	355	C	N1-C2-O2	-11.92	111.75	118.90
1	A	1097	C	C6-N1-C2	11.92	125.07	120.30
1	A	267	C	C6-N1-C2	-11.91	115.53	120.30
1	A	864	A	N9-C4-C5	11.90	110.56	105.80
1	A	24	U	C2-N3-C4	-11.89	119.86	127.00
1	A	720	C	N1-C2-O2	11.89	126.04	118.90
1	A	729	A	N9-C4-C5	11.87	110.55	105.80
1	A	728	A	N9-C4-C5	11.87	110.55	105.80
1	A	1509	C	C6-N1-C2	-11.87	115.55	120.30
1	A	1502	A	N1-C6-N6	11.85	125.71	118.60
1	A	283	C	C6-N1-C2	-11.85	115.56	120.30
1	A	945	G	C8-N9-C4	-11.84	101.66	106.40
1	A	939	G	C8-N9-C4	-11.84	101.67	106.40
1	A	692	U	C5-C6-N1	-11.82	116.79	122.70
1	A	746	A	C6-N1-C2	-11.82	111.51	118.60
1	A	378	G	N1-C6-O6	11.81	126.99	119.90
1	A	122	G	O5'-P-OP1	-11.81	95.07	105.70
1	A	36	C	C6-N1-C2	11.81	125.02	120.30
1	A	266	G	C4-C5-N7	11.79	115.52	110.80
1	A	291	C	C5-C6-N1	11.78	126.89	121.00
1	A	222	U	O5'-P-OP2	-11.77	95.11	105.70
1	A	669	U	O5'-P-OP2	-11.77	95.11	105.70
1	A	18	C	N3-C2-O2	-11.77	113.66	121.90
1	A	635	G	N1-C6-O6	11.76	126.96	119.90
1	A	892	A	C2-N3-C4	11.75	116.47	110.60
1	A	811	C	N3-C4-N4	-11.72	109.80	118.00
1	A	144	G	C5-C6-N1	-11.71	105.64	111.50
1	A	904	C	C6-N1-C2	11.71	124.98	120.30
1	A	778	G	N1-C2-N3	11.70	130.92	123.90
1	A	782	A	O5'-P-OP1	-11.70	95.17	105.70
1	A	578	C	C6-N1-C2	11.70	124.98	120.30
1	A	122	G	N3-C4-N9	11.70	133.02	126.00
1	A	298	A	C8-N9-C4	-11.70	101.12	105.80
1	A	670	G	O5'-P-OP2	-11.69	95.18	105.70
1	A	691	G	C8-N9-C4	-11.66	101.74	106.40
1	A	531	U	N3-C4-C5	-11.65	107.61	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1079	G	N3-C4-C5	-11.65	122.78	128.60
1	A	172	A	C2-N3-C4	-11.64	104.78	110.60
1	A	1530	G	C4-C5-C6	-11.62	111.83	118.80
1	A	686	U	C4-C5-C6	11.62	126.67	119.70
1	A	761	G	C2-N3-C4	-11.60	106.10	111.90
1	A	41	G	N3-C2-N2	-11.60	111.78	119.90
1	A	834	C	C2-N3-C4	-11.59	114.11	119.90
1	A	21	G	N3-C4-N9	11.59	132.95	126.00
1	A	294	U	O5'-P-OP1	-11.58	95.28	105.70
1	A	1231	G	C5-C6-O6	-11.56	121.66	128.60
1	A	380	G	C5-C6-O6	11.55	135.53	128.60
1	A	12	U	N3-C2-O2	-11.55	114.11	122.20
19	S	81	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	331	G	C6-C5-N7	-11.53	123.48	130.40
1	A	577	G	N9-C4-C5	11.53	110.01	105.40
1	A	1516[A]	G	N3-C4-C5	11.53	134.37	128.60
1	A	1516[B]	G	N3-C4-C5	11.53	134.37	128.60
1	A	673	G	O5'-P-OP1	-11.53	95.33	105.70
1	A	117	G	C2-N3-C4	-11.52	106.14	111.90
1	A	323	U	O5'-P-OP2	-11.52	95.33	105.70
1	A	18	C	C5-C6-N1	-11.51	115.25	121.00
1	A	285	G	N1-C6-O6	11.50	126.80	119.90
1	A	262	A	C5-N7-C8	-11.50	98.15	103.90
1	A	22	G	N9-C4-C5	11.49	110.00	105.40
1	A	485	G	N1-C6-O6	-11.49	113.01	119.90
1	A	818	G	O5'-P-OP1	-11.47	95.37	105.70
1	A	1287	A	N1-C6-N6	11.47	125.48	118.60
1	A	518	C	N1-C2-O2	11.46	125.78	118.90
1	A	913	A	N1-C6-N6	-11.46	111.72	118.60
1	A	117	G	C8-N9-C4	11.46	110.98	106.40
1	A	1075	C	C4-C5-C6	11.45	123.13	117.40
1	A	1098	C	C6-N1-C2	11.44	124.88	120.30
1	A	610	G	C8-N9-C4	-11.44	101.82	106.40
1	A	975	A	N7-C8-N9	11.42	119.51	113.80
1	A	520	A	O5'-P-OP2	-11.42	95.43	105.70
1	A	1392	G	N1-C6-O6	-11.41	113.05	119.90
1	A	886	G	C2-N3-C4	-11.41	106.19	111.90
1	A	1297	C	C6-N1-C2	11.41	124.86	120.30
1	A	982	U	N3-C2-O2	-11.41	114.22	122.20
1	A	1224	G	O5'-P-OP1	11.41	124.39	110.70
1	A	515	G	N1-C6-O6	11.39	126.74	119.90
1	A	779	C	C2-N3-C4	-11.38	114.21	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1102	A	N7-C8-N9	11.38	119.49	113.80
1	A	125	U	N3-C4-C5	-11.37	107.78	114.60
1	A	373	A	O5'-P-OP2	-11.36	95.47	105.70
1	A	703	G	N1-C2-N2	-11.36	105.98	116.20
1	A	975	A	N3-C4-N9	-11.36	118.31	127.40
1	A	768	A	C6-N1-C2	-11.35	111.79	118.60
1	A	398	C	N3-C4-N4	-11.34	110.06	118.00
1	A	888	G	C4-N9-C1'	11.34	141.24	126.50
1	A	1050	G	C6-C5-N7	-11.33	123.60	130.40
1	A	665	A	O5'-P-OP2	-11.32	95.51	105.70
1	A	309	G	O5'-P-OP1	-11.32	95.51	105.70
1	A	509	A	C8-N9-C4	-11.31	101.28	105.80
1	A	438	G	C5-N7-C8	11.30	109.95	104.30
1	A	1054	C	N3-C4-N4	11.28	125.90	118.00
1	A	1399	C	N1-C2-O2	-11.28	112.13	118.90
1	A	685	G	N3-C4-C5	11.27	134.23	128.60
1	A	1524	C	N1-C2-O2	-11.27	112.14	118.90
1	A	1220	G	N1-C6-O6	-11.27	113.14	119.90
1	A	317	G	N1-C6-O6	11.26	126.65	119.90
1	A	244	U	C5-C6-N1	-11.25	117.07	122.70
1	A	566	G	C4-C5-N7	11.25	115.30	110.80
1	A	438	G	C5-C6-O6	11.24	135.35	128.60
1	A	435	C	C6-N1-C2	-11.24	115.80	120.30
1	A	484	G	C8-N9-C1'	-11.23	112.41	127.00
1	A	326	G	OP1-P-O3'	-11.22	80.51	105.20
1	A	1276	G	C5-C6-O6	-11.22	121.87	128.60
1	A	970	C	O5'-P-OP1	-11.22	95.60	105.70
1	A	691	G	N9-C4-C5	11.22	109.89	105.40
1	A	390	C	N1-C2-O2	-11.21	112.17	118.90
1	A	1514	C	C6-N1-C2	11.20	124.78	120.30
1	A	755	G	C4-C5-N7	11.19	115.28	110.80
1	A	1276	G	N1-C6-O6	11.19	126.61	119.90
1	A	662	G	O5'-P-OP2	-11.19	95.63	105.70
1	A	730	G	C8-N9-C4	-11.16	101.93	106.40
1	A	1426	C	C6-N1-C2	11.16	124.77	120.30
1	A	24	U	C5-C6-N1	-11.16	117.12	122.70
1	A	883	C	N1-C2-O2	-11.16	112.20	118.90
1	A	517	G	C8-N9-C4	-11.16	101.94	106.40
1	A	444	C	N1-C2-O2	11.15	125.59	118.90
1	A	1202	G	N3-C2-N2	-11.15	112.09	119.90
1	A	1502	A	C2-N3-C4	-11.14	105.03	110.60
1	A	235	C	C5-C6-N1	-11.13	115.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	C	N3-C4-C5	11.13	126.35	121.90
1	A	664	G	C4-C5-N7	-11.13	106.35	110.80
1	A	523	A	N1-C6-N6	11.13	125.28	118.60
1	A	1166	G	C4-C5-N7	-11.13	106.35	110.80
1	A	55	A	N1-C6-N6	-11.12	111.93	118.60
1	A	730	G	N3-C2-N2	-11.12	112.12	119.90
1	A	266	G	C2-N3-C4	-11.11	106.34	111.90
1	A	234	C	N3-C4-C5	11.11	126.34	121.90
1	A	144	G	N3-C2-N2	-11.11	112.13	119.90
1	A	575	G	C5-C6-N1	11.10	117.05	111.50
1	A	725	G	C4-C5-N7	11.10	115.24	110.80
1	A	1104	G	N1-C2-N3	11.10	130.56	123.90
1	A	544	G	C6-C5-N7	-11.09	123.75	130.40
1	A	1374	A	C5-C6-N6	11.09	132.57	123.70
1	A	1071	C	C6-N1-C2	-11.09	115.86	120.30
1	A	134	A	N1-C2-N3	11.09	134.84	129.30
1	A	314	C	C5-C4-N4	-11.07	112.45	120.20
1	A	17	U	C5-C4-O4	-11.07	119.26	125.90
1	A	355	C	C6-N1-C2	-11.06	115.88	120.30
1	A	122	G	C8-N9-C1'	-11.05	112.63	127.00
1	A	975	A	N1-C2-N3	11.04	134.82	129.30
1	A	587	G	C2-N3-C4	11.03	117.42	111.90
1	A	1202	G	C8-N9-C4	-11.03	101.99	106.40
1	A	494	G	C8-N9-C4	-11.02	101.99	106.40
1	A	181	G	C6-C5-N7	-11.00	123.80	130.40
1	A	101	A	C8-N9-C4	-11.00	101.40	105.80
1	A	728	A	C6-N1-C2	-11.00	112.00	118.60
1	A	1166	G	C8-N9-C4	-11.00	102.00	106.40
1	A	1206	G	N1-C6-O6	11.00	126.50	119.90
1	A	727	G	N1-C6-O6	-10.99	113.31	119.90
1	A	536	C	N1-C2-O2	-10.99	112.31	118.90
1	A	622	A	C2-N3-C4	-10.98	105.11	110.60
1	A	224	C	N3-C2-O2	-10.97	114.22	121.90
1	A	120	A	C5-C6-N1	-10.96	112.22	117.70
1	A	1502	A	C4-C5-N7	10.96	116.18	110.70
1	A	1510	U	O5'-P-OP1	-10.96	95.84	105.70
1	A	587	G	C5-C6-N1	10.95	116.97	111.50
1	A	122	G	N9-C4-C5	-10.94	101.02	105.40
1	A	260	G	N3-C4-N9	-10.94	119.44	126.00
1	A	58	C	C6-N1-C2	-10.93	115.93	120.30
1	A	757	U	N3-C4-C5	-10.93	108.04	114.60
1	A	1227	A	C5-N7-C8	-10.93	98.44	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	G	N3-C4-N9	-10.93	119.44	126.00
1	A	580	U	N3-C4-C5	-10.93	108.05	114.60
1	A	793	U	C5-C6-N1	-10.92	117.24	122.70
1	A	1053	G	C4-N9-C1'	-10.92	112.31	126.50
1	A	127	G	N1-C6-O6	10.89	126.44	119.90
1	A	890	G	C4-C5-N7	-10.88	106.45	110.80
1	A	1350	A	C5-N7-C8	10.88	109.34	103.90
1	A	257	G	C2-N3-C4	-10.87	106.47	111.90
1	A	741	G	C4-N9-C1'	10.86	140.62	126.50
1	A	479	C	C6-N1-C2	-10.86	115.96	120.30
8	H	91	ARG	NE-CZ-NH2	-10.85	114.87	120.30
1	A	1050	G	C5-C6-N1	-10.85	106.08	111.50
1	A	39	G	C5-C6-O6	-10.84	122.09	128.60
1	A	713	G	C4-C5-N7	-10.84	106.46	110.80
1	A	522	C	C6-N1-C2	10.83	124.63	120.30
1	A	561	U	C6-N1-C2	10.83	127.50	121.00
1	A	1299	A	C2-N3-C4	-10.82	105.19	110.60
1	A	260	G	N7-C8-N9	10.82	118.51	113.10
1	A	1290	G	C5-C6-N1	-10.81	106.09	111.50
1	A	1493	A	N3-C4-C5	-10.81	119.23	126.80
1	A	1231	G	C6-C5-N7	-10.80	123.92	130.40
1	A	1507	A	N1-C6-N6	-10.80	112.12	118.60
1	A	1108	G	N1-C2-N3	10.79	130.37	123.90
1	A	864	A	C8-N9-C4	-10.78	101.49	105.80
1	A	300	A	N1-C2-N3	10.78	134.69	129.30
1	A	1338	G	C8-N9-C4	-10.77	102.09	106.40
1	A	1338	G	N1-C6-O6	-10.76	113.44	119.90
1	A	566	G	C6-C5-N7	-10.75	123.95	130.40
1	A	632	A	N1-C6-N6	10.75	125.05	118.60
1	A	274	A	O5'-P-OP2	-10.74	96.03	105.70
1	A	1532	U	C4-C5-C6	-10.73	113.26	119.70
1	A	284	G	C5-C6-O6	-10.72	122.17	128.60
1	A	1525	G	N7-C8-N9	10.70	118.45	113.10
1	A	1055	A	C5-C6-N6	-10.70	115.14	123.70
1	A	544	G	N1-C6-O6	10.69	126.31	119.90
1	A	130	A	N1-C6-N6	10.68	125.01	118.60
1	A	699	C	C2-N1-C1'	-10.68	107.05	118.80
1	A	819	A	C6-C5-N7	-10.68	124.82	132.30
1	A	1167	A	C5-C6-N6	10.68	132.24	123.70
1	A	1433	A	C6-N1-C2	-10.67	112.20	118.60
1	A	800	G	C8-N9-C4	-10.66	102.14	106.40
1	A	127	G	C5-C6-N1	-10.65	106.17	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1513	A	C8-N9-C4	10.65	110.06	105.80
1	A	782	A	O5'-P-OP2	10.64	123.47	110.70
1	A	795	C	C6-N1-C2	10.64	124.56	120.30
1	A	819	A	C4-C5-N7	10.64	116.02	110.70
1	A	922	G	C5-C6-O6	-10.63	122.22	128.60
1	A	672	U	N1-C2-O2	10.62	130.23	122.80
1	A	786	G	O5'-P-OP1	-10.62	96.14	105.70
1	A	851	G	C4-C5-C6	10.62	125.17	118.80
1	A	718	G	N9-C4-C5	-10.61	101.15	105.40
1	A	1350	A	N7-C8-N9	-10.62	108.49	113.80
1	A	1189	C	N3-C2-O2	-10.61	114.48	121.90
1	A	120	A	N1-C6-N6	10.60	124.96	118.60
1	A	725	G	C5-C6-O6	-10.59	122.25	128.60
1	A	860	A	C6-N1-C2	-10.58	112.25	118.60
1	A	234	C	C2-N1-C1'	-10.58	107.17	118.80
1	A	667	G	C5-C6-N1	-10.57	106.21	111.50
1	A	544	G	O5'-P-OP1	-10.57	96.19	105.70
1	A	398	C	C6-N1-C2	10.57	124.53	120.30
1	A	222	U	C5-C6-N1	-10.56	117.42	122.70
1	A	531	U	C5-C4-O4	10.56	132.24	125.90
1	A	865	A	C4-C5-C6	10.56	122.28	117.00
1	A	590	C	C6-N1-C2	10.55	124.52	120.30
1	A	1079	G	C6-C5-N7	-10.55	124.07	130.40
1	A	147	G	C2-N3-C4	-10.55	106.63	111.90
1	A	278	G	N3-C2-N2	-10.55	112.52	119.90
1	A	193	C	C5-C6-N1	-10.54	115.73	121.00
1	A	922	G	C6-C5-N7	-10.53	124.08	130.40
1	A	46	G	C8-N9-C4	-10.53	102.19	106.40
1	A	1166	G	N3-C4-C5	-10.53	123.33	128.60
1	A	550	G	C2-N3-C4	-10.53	106.64	111.90
1	A	1229	A	C2-N3-C4	-10.51	105.35	110.60
1	A	711	G	C5-N7-C8	-10.50	99.05	104.30
1	A	663	A	C2-N3-C4	-10.50	105.35	110.60
1	A	376	G	O5'-P-OP2	-10.49	96.25	105.70
1	A	757	U	C5-C4-O4	10.49	132.19	125.90
1	A	617	G	N1-C2-N3	10.48	130.19	123.90
1	A	120	A	C6-C5-N7	-10.48	124.97	132.30
1	A	1108	G	C2-N3-C4	-10.48	106.66	111.90
1	A	220	G	N1-C6-O6	10.47	126.18	119.90
1	A	297	G	N1-C6-O6	-10.47	113.62	119.90
1	A	484	G	N3-C4-C5	-10.47	123.36	128.60
1	A	288	A	C2-N3-C4	-10.47	105.36	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	740	U	O5'-P-OP2	-10.46	96.28	105.70
1	A	890	G	C5-C6-N1	-10.45	106.28	111.50
1	A	912	C	C4-C5-C6	10.45	122.62	117.40
1	A	292	G	C5-C6-N1	-10.44	106.28	111.50
1	A	1513	A	C2-N3-C4	-10.44	105.38	110.60
1	A	1168	A	C6-N1-C2	-10.44	112.34	118.60
1	A	27	G	C5-N7-C8	-10.43	99.08	104.30
1	A	736	C	N1-C2-N3	10.42	126.49	119.20
1	A	503	C	C6-N1-C2	10.41	124.47	120.30
1	A	793	U	C5-C4-O4	10.41	132.15	125.90
1	A	1531	A	N1-C6-N6	10.40	124.84	118.60
1	A	32	A	C6-N1-C2	-10.39	112.36	118.60
1	A	300	A	C5-C6-N6	10.39	132.01	123.70
1	A	529	G	O5'-P-OP2	-10.39	96.35	105.70
1	A	597	G	C2-N3-C4	-10.38	106.71	111.90
1	A	1502	A	C6-C5-N7	-10.36	125.05	132.30
1	A	312	C	N3-C4-C5	10.33	126.03	121.90
1	A	290	C	OP1-P-OP2	-10.33	104.11	119.60
1	A	889	A	C8-N9-C4	-10.33	101.67	105.80
1	A	741	G	N3-C4-C5	-10.33	123.44	128.60
1	A	300	A	C4-C5-N7	-10.32	105.54	110.70
1	A	552	U	N1-C2-N3	10.32	121.09	114.90
1	A	1103	C	C6-N1-C2	-10.31	116.17	120.30
1	A	181	G	N1-C6-O6	10.31	126.09	119.90
1	A	1443	G	C8-N9-C4	10.29	110.52	106.40
1	A	395	C	C5-C6-N1	10.28	126.14	121.00
1	A	484	G	C4-N9-C1'	10.29	139.87	126.50
1	A	542	G	N1-C6-O6	-10.28	113.73	119.90
1	A	332	G	C5-C6-O6	-10.28	122.43	128.60
1	A	1505	G	O5'-P-OP2	-10.27	96.45	105.70
1	A	241	C	C5-C6-N1	-10.27	115.87	121.00
1	A	790	A	C5-C6-N1	-10.26	112.57	117.70
1	A	834	C	N3-C4-C5	10.25	126.00	121.90
1	A	1112	C	C2-N3-C4	-10.25	114.78	119.90
1	A	22	G	N3-C4-N9	-10.24	119.85	126.00
1	A	871	U	N3-C2-O2	-10.24	115.03	122.20
1	A	399	G	N3-C4-N9	10.23	132.14	126.00
1	A	1338	G	N9-C4-C5	10.23	109.49	105.40
1	A	1054	C	C5-C6-N1	10.22	126.11	121.00
1	A	273	A	N1-C2-N3	10.22	134.41	129.30
1	A	751	U	O5'-P-OP1	-10.22	96.51	105.70
1	A	1338	G	C5-C6-O6	10.20	134.72	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	G	C8-N9-C1'	10.20	140.26	127.00
1	A	560	U	C5-C4-O4	10.20	132.02	125.90
1	A	392	G	O5'-P-OP2	-10.19	96.53	105.70
1	A	36	C	C5-C6-N1	-10.19	115.91	121.00
1	A	438	G	C5-C6-N1	-10.19	106.41	111.50
1	A	32	A	N1-C2-N3	10.18	134.39	129.30
1	A	566	G	C2-N3-C4	-10.18	106.81	111.90
1	A	730	G	C5-N7-C8	10.17	109.39	104.30
1	A	1079	G	O5'-P-OP2	-10.17	96.55	105.70
1	A	48	C	N3-C4-C5	-10.15	117.84	121.90
1	A	324	G	N1-C6-O6	10.15	125.99	119.90
1	A	548	G	N1-C6-O6	10.15	125.99	119.90
1	A	1290	G	C6-C5-N7	-10.15	124.31	130.40
14	N	6	LEU	CA-CB-CG	-10.15	91.96	115.30
1	A	61	G	O5'-P-OP1	-10.14	96.57	105.70
1	A	1091	U	O5'-P-OP2	-10.13	96.58	105.70
1	A	813	U	N3-C2-O2	10.13	129.29	122.20
1	A	38	G	O5'-P-OP1	-10.13	96.58	105.70
1	A	117	G	C4-N9-C1'	10.13	139.67	126.50
1	A	132	C	C5-C6-N1	-10.12	115.94	121.00
1	A	717	C	N1-C2-O2	-10.12	112.83	118.90
1	A	862	C	N3-C4-C5	10.13	125.95	121.90
1	A	703	G	N3-C4-N9	10.12	132.07	126.00
1	A	454	C	C6-N1-C2	10.12	124.35	120.30
1	A	896	C	C6-N1-C2	10.12	124.35	120.30
1	A	1442	G	C2-N3-C4	10.12	116.96	111.90
1	A	610	G	N3-C2-N2	-10.12	112.82	119.90
1	A	184	G	N3-C4-C5	-10.11	123.55	128.60
1	A	1104	G	C2-N3-C4	-10.10	106.85	111.90
1	A	1493	A	O4'-C1'-N9	10.10	116.28	108.20
1	A	1069	C	N3-C2-O2	10.10	128.97	121.90
1	A	1483	A	C5-C6-N1	-10.10	112.65	117.70
1	A	402	G	N1-C2-N2	-10.09	107.12	116.20
1	A	1079	G	C6-N1-C2	-10.08	119.05	125.10
1	A	379	C	N3-C4-C5	-10.08	117.87	121.90
1	A	658	G	C4-N9-C1'	10.07	139.59	126.50
1	A	316	G	N1-C6-O6	10.07	125.94	119.90
1	A	1287	A	C6-C5-N7	-10.07	125.25	132.30
1	A	888	G	C6-C5-N7	-10.07	124.36	130.40
1	A	406	G	O5'-P-OP2	-10.06	96.64	105.70
1	A	718	G	C8-N9-C4	10.06	110.43	106.40
1	A	268	C	O5'-P-OP2	10.06	122.77	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	987	G	C8-N9-C4	10.06	110.42	106.40
1	A	735	C	C2-N3-C4	-10.05	114.88	119.90
1	A	860	A	C5-C6-N1	10.05	122.72	117.70
1	A	374	A	C2-N3-C4	-10.04	105.58	110.60
1	A	888	G	C4-C5-C6	10.04	124.83	118.80
1	A	851	G	N1-C6-O6	10.04	125.92	119.90
1	A	865	A	C8-N9-C4	-10.04	101.78	105.80
1	A	233	C	O5'-P-OP2	-10.03	96.67	105.70
1	A	292	G	C4-C5-C6	10.03	124.82	118.80
1	A	292	G	N3-C2-N2	-10.03	112.88	119.90
1	A	111	G	C8-N9-C4	-10.02	102.39	106.40
1	A	299	G	N9-C4-C5	10.02	109.41	105.40
1	A	299	G	C4-C5-N7	-10.02	106.79	110.80
1	A	8	A	C5-C6-N1	10.02	122.71	117.70
1	A	572	A	N9-C4-C5	10.02	109.81	105.80
1	A	561	U	N1-C2-N3	-10.01	108.89	114.90
1	A	577	G	C8-N9-C4	-10.01	102.40	106.40
1	A	247	G	C5-C6-N1	-10.01	106.50	111.50
1	A	554	C	C6-N1-C2	9.99	124.30	120.30
1	A	1287	A	N7-C8-N9	9.99	118.80	113.80
1	A	1528	U	OP1-P-OP2	9.98	134.58	119.60
1	A	654	G	C8-N9-C4	-9.98	102.41	106.40
1	A	524	G	C2-N3-C4	9.98	116.89	111.90
1	A	1530	G	N1-C2-N2	9.98	125.18	116.20
1	A	132	C	C4-C5-C6	9.98	122.39	117.40
1	A	519	C	C4-C5-C6	9.97	122.38	117.40
1	A	890	G	O4'-C1'-N9	9.97	116.17	108.20
1	A	1433	A	O5'-P-OP1	-9.97	96.73	105.70
1	A	1530	G	N1-C2-N3	-9.97	117.92	123.90
1	A	1387	G	O5'-P-OP1	-9.96	96.73	105.70
1	A	800	G	N9-C4-C5	9.95	109.38	105.40
1	A	561	U	N1-C2-O2	9.93	129.75	122.80
1	A	116	A	C2-N3-C4	-9.93	105.64	110.60
1	A	659	U	C2-N3-C4	-9.92	121.05	127.00
1	A	908	A	C6-N1-C2	-9.92	112.65	118.60
1	A	224	C	N1-C2-O2	9.91	124.85	118.90
2	B	11	LEU	CA-CB-CG	9.91	138.09	115.30
1	A	635	G	C2-N3-C4	-9.91	106.95	111.90
1	A	667	G	N1-C6-O6	9.91	125.84	119.90
1	A	380	G	C5-N7-C8	9.90	109.25	104.30
1	A	35	G	C6-C5-N7	-9.90	124.46	130.40
1	A	372	C	N3-C4-C5	9.89	125.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	617	G	C2-N3-C4	-9.89	106.95	111.90
1	A	235	C	C4-C5-C6	9.89	122.34	117.40
1	A	1323	G	C2-N3-C4	-9.89	106.96	111.90
1	A	273	A	C2-N3-C4	-9.88	105.66	110.60
1	A	526	C	O5'-P-OP1	9.88	122.56	110.70
1	A	699	C	O5'-P-OP2	-9.88	96.81	105.70
1	A	1388	C	N3-C4-C5	9.88	125.85	121.90
1	A	24	U	N3-C4-C5	9.88	120.53	114.60
1	A	645	C	C6-N1-C2	9.88	124.25	120.30
1	A	1346	A	P-O3'-C3'	9.88	131.56	119.70
1	A	744	C	O5'-P-OP1	9.88	122.56	110.70
1	A	1101	A	C4-C5-C6	9.88	121.94	117.00
1	A	1533	C	N1-C2-O2	9.88	124.83	118.90
1	A	168	G	C5-C6-N1	-9.87	106.56	111.50
1	A	551	U	C6-N1-C2	9.87	126.92	121.00
1	A	922	G	C2-N3-C4	-9.87	106.97	111.90
1	A	19	C	O5'-P-OP2	-9.86	96.82	105.70
1	A	1394	A	N1-C2-N3	9.86	134.23	129.30
1	A	1131	G	C6-C5-N7	-9.86	124.48	130.40
1	A	126	G	C4-C5-N7	-9.86	106.86	110.80
1	A	225	C	O5'-P-OP1	9.86	122.53	110.70
1	A	518	C	N3-C2-O2	-9.85	115.00	121.90
1	A	21	G	N9-C4-C5	-9.85	101.46	105.40
1	A	789	U	N1-C2-N3	9.85	120.81	114.90
1	A	718	G	N1-C6-O6	9.84	125.80	119.90
1	A	1091	U	N3-C4-C5	-9.83	108.70	114.60
1	A	934	C	O5'-P-OP2	-9.83	96.85	105.70
1	A	566	G	N9-C4-C5	-9.82	101.47	105.40
1	A	1431	C	C6-N1-C2	-9.82	116.37	120.30
1	A	888	G	N1-C2-N3	9.82	129.79	123.90
1	A	120	A	N1-C2-N3	9.81	134.21	129.30
1	A	307	C	N1-C2-O2	9.81	124.79	118.90
1	A	317	G	C6-C5-N7	-9.81	124.52	130.40
20	T	62	LEU	CA-CB-CG	-9.80	92.76	115.30
1	A	1338	G	N3-C4-C5	-9.80	123.70	128.60
1	A	35	G	N9-C4-C5	-9.79	101.48	105.40
1	A	390	C	N3-C2-O2	9.80	128.76	121.90
1	A	1503	A	O5'-P-OP2	-9.79	96.89	105.70
1	A	729	A	N1-C6-N6	-9.79	112.72	118.60
1	A	735	C	N3-C4-C5	9.79	125.82	121.90
1	A	1439	C	C6-N1-C2	9.79	124.22	120.30
1	A	113	G	N1-C2-N3	9.79	129.77	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	C	C5-C6-N1	-9.79	116.11	121.00
1	A	714	G	C8-N9-C4	9.79	110.31	106.40
1	A	193	C	C2-N3-C4	-9.78	115.01	119.90
1	A	121	C	O5'-P-OP2	-9.78	96.90	105.70
1	A	299	G	N1-C2-N3	9.78	129.77	123.90
1	A	685	G	C4-N9-C1'	-9.78	113.79	126.50
1	A	759	A	C6-N1-C2	-9.78	112.73	118.60
1	A	1341	U	N3-C4-O4	-9.77	112.56	119.40
1	A	1502	A	C5-N7-C8	-9.77	99.01	103.90
1	A	355	C	N1-C2-N3	9.77	126.04	119.20
1	A	754	C	C5-C6-N1	9.77	125.88	121.00
1	A	934	C	C6-N1-C2	-9.76	116.39	120.30
1	A	902	G	C5-C6-N1	9.76	116.38	111.50
1	A	35	G	N1-C6-O6	9.75	125.75	119.90
1	A	314	C	C6-N1-C2	9.75	124.20	120.30
1	A	300	A	C6-N1-C2	-9.75	112.75	118.60
1	A	662	G	C5-C6-N1	-9.75	106.63	111.50
1	A	762	C	C2-N3-C4	-9.75	115.03	119.90
1	A	479	C	C2-N1-C1'	9.74	129.51	118.80
1	A	147	G	C6-C5-N7	-9.74	124.56	130.40
1	A	562	C	N1-C2-O2	9.74	124.74	118.90
1	A	1239	A	C8-N9-C4	9.73	109.69	105.80
1	A	322	C	C4-C5-C6	9.73	122.26	117.40
1	A	741	G	C8-N9-C1'	-9.73	114.36	127.00
1	A	759	A	N9-C4-C5	9.73	109.69	105.80
1	A	108	G	C4-C5-N7	9.72	114.69	110.80
1	A	540	G	C8-N9-C4	-9.72	102.51	106.40
1	A	972	C	OP1-P-OP2	-9.72	105.02	119.60
1	A	925	G	C2-N3-C4	-9.72	107.04	111.90
1	A	642	A	C6-N1-C2	-9.72	112.77	118.60
1	A	756	C	O5'-P-OP2	-9.71	96.96	105.70
1	A	757	U	N3-C2-O2	-9.71	115.40	122.20
1	A	379	C	N1-C2-O2	-9.71	113.07	118.90
1	A	910	C	C4-C5-C6	9.71	122.25	117.40
1	A	1030(B)	C	C2-N1-C1'	9.71	129.48	118.80
1	A	504	C	C5-C6-N1	9.69	125.84	121.00
1	A	574	A	C5-N7-C8	-9.69	99.06	103.90
1	A	945	G	N7-C8-N9	9.68	117.94	113.10
1	A	29	G	O5'-P-OP2	-9.67	97.00	105.70
1	A	285	G	C8-N9-C4	9.67	110.27	106.40
1	A	263	A	C5-C6-N6	-9.67	115.96	123.70
1	A	686	U	N3-C4-C5	-9.67	108.80	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1188	A	N1-C2-N3	9.66	134.13	129.30
1	A	378	G	C5-C6-O6	-9.66	122.81	128.60
1	A	560	U	C4-C5-C6	9.66	125.49	119.70
1	A	228	A	N3-C4-N9	-9.65	119.68	127.40
1	A	1269	A	O5'-P-OP2	-9.65	97.01	105.70
1	A	555	C	O5'-P-OP1	9.65	122.28	110.70
1	A	1053	G	N3-C4-C5	9.65	133.42	128.60
1	A	281	G	N1-C6-O6	9.64	125.69	119.90
1	A	637	G	C5-C6-N1	-9.64	106.68	111.50
1	A	761	G	N3-C4-C5	9.64	133.42	128.60
1	A	850	U	O5'-P-OP1	-9.64	97.02	105.70
1	A	741	G	C5-C6-O6	9.64	134.38	128.60
1	A	1443	G	C4-N9-C1'	-9.62	113.99	126.50
1	A	285	G	N3-C4-C5	9.62	133.41	128.60
1	A	694	A	C2-N3-C4	-9.62	105.79	110.60
1	A	444	C	N3-C2-O2	-9.62	115.17	121.90
1	A	1408	A	C5-C6-N1	-9.62	112.89	117.70
1	A	728	A	C5-C6-N1	9.62	122.51	117.70
1	A	1524	C	N3-C2-O2	9.62	128.63	121.90
1	A	674	G	N1-C2-N3	9.61	129.67	123.90
1	A	691	G	C4-C5-N7	-9.61	106.96	110.80
1	A	610	G	N9-C4-C5	9.60	109.24	105.40
1	A	725	G	C6-C5-N7	-9.60	124.64	130.40
1	A	1206	G	C2-N3-C4	-9.60	107.10	111.90
1	A	829	G	C2-N3-C4	-9.59	107.11	111.90
1	A	1275	A	C8-N9-C4	9.59	109.63	105.80
1	A	1075	C	N1-C2-N3	9.58	125.91	119.20
1	A	1279	A	C2-N3-C4	-9.58	105.81	110.60
1	A	549	C	C5-C6-N1	-9.58	116.21	121.00
1	A	981	U	C5-C6-N1	9.58	127.49	122.70
1	A	1287	A	C5-C6-N6	-9.58	116.03	123.70
1	A	729	A	N3-C4-C5	-9.57	120.10	126.80
1	A	61	G	C5-C6-N1	-9.56	106.72	111.50
1	A	769	G	N1-C6-O6	9.56	125.64	119.90
1	A	489	C	O5'-P-OP1	-9.56	97.10	105.70
1	A	1121	U	O5'-P-OP2	-9.56	97.10	105.70
1	A	1451	A	O4'-C1'-N9	-9.56	100.56	108.20
1	A	281	G	C5-C6-O6	-9.55	122.87	128.60
1	A	741	G	C4-C5-C6	9.55	124.53	118.80
1	A	20	U	C5-C4-O4	-9.55	120.17	125.90
1	A	456	C	O5'-P-OP2	-9.55	97.11	105.70
1	A	1399	C	N3-C4-C5	-9.55	118.08	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	757	U	C6-N1-C2	-9.54	115.27	121.00
1	A	127	G	O5'-P-OP2	-9.54	97.11	105.70
1	A	560	U	N1-C2-N3	9.54	120.62	114.90
1	A	1377	A	C2-N3-C4	-9.54	105.83	110.60
1	A	785	G	C4-C5-N7	9.54	114.61	110.80
1	A	306	G	N1-C6-O6	9.54	125.62	119.90
1	A	721	G	C8-N9-C4	9.53	110.21	106.40
1	A	871	U	N1-C2-O2	9.53	129.47	122.80
1	A	912	C	N3-C4-C5	-9.53	118.09	121.90
1	A	720	C	N3-C2-O2	-9.53	115.23	121.90
1	A	1529	G	N3-C2-N2	-9.52	113.23	119.90
1	A	809	G	C5-C6-N1	9.52	116.26	111.50
1	A	515	G	C6-C5-N7	-9.52	124.69	130.40
1	A	113	G	N1-C6-O6	9.51	125.61	119.90
1	A	674	G	C6-C5-N7	-9.51	124.69	130.40
1	A	741	G	N1-C2-N3	9.50	129.60	123.90
1	A	880	C	C4-C5-C6	9.50	122.15	117.40
1	A	125	U	C4-C5-C6	9.50	125.40	119.70
1	A	872	A	C4-C5-C6	9.49	121.75	117.00
1	A	301	G	O5'-P-OP1	-9.48	97.17	105.70
1	A	1128	C	N3-C4-C5	-9.48	118.11	121.90
1	A	279	A	C8-N9-C4	-9.47	102.01	105.80
1	A	593	G	C5-C6-N1	-9.47	106.76	111.50
1	A	915	A	O5'-P-OP1	-9.47	97.17	105.70
1	A	1323	G	N1-C6-O6	9.47	125.58	119.90
1	A	352	C	C5-C6-N1	-9.45	116.27	121.00
1	A	117	G	C6-N1-C2	9.45	130.77	125.10
1	A	218	C	C2-N3-C4	-9.44	115.18	119.90
1	A	279	A	C4-C5-C6	9.44	121.72	117.00
1	A	431	A	C8-N9-C4	9.44	109.58	105.80
1	A	1202	G	N1-C2-N2	9.44	124.69	116.20
1	A	1340	A	N1-C2-N3	9.43	134.01	129.30
1	A	1516[A]	G	N3-C2-N2	-9.43	113.30	119.90
1	A	1516[B]	G	N3-C2-N2	-9.43	113.30	119.90
1	A	1512	U	C5-C4-O4	9.43	131.56	125.90
1	A	298	A	N7-C8-N9	9.42	118.51	113.80
1	A	1335	C	N3-C4-N4	-9.42	111.41	118.00
1	A	1463	C	C6-N1-C2	9.42	124.07	120.30
1	A	1542	U	O5'-P-OP1	-9.41	97.23	105.70
1	A	579	G	C8-N9-C4	9.41	110.17	106.40
1	A	1222	G	C2-N3-C4	-9.41	107.19	111.90
1	A	1087	G	C6-C5-N7	-9.41	124.76	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	G	O5'-P-OP1	-9.40	97.24	105.70
1	A	1055	A	N1-C6-N6	9.40	124.24	118.60
1	A	327	A	C2-N3-C4	-9.40	105.90	110.60
1	A	474	G	N1-C6-O6	9.39	125.53	119.90
1	A	500	G	N1-C6-O6	9.39	125.53	119.90
1	A	712	A	N1-C6-N6	-9.39	112.97	118.60
1	A	927	G	C5-C6-N1	-9.39	106.81	111.50
1	A	1079	G	N7-C8-N9	9.39	117.79	113.10
1	A	295	C	N3-C2-O2	-9.38	115.33	121.90
1	A	1090	U	C4-C5-C6	9.38	125.33	119.70
1	A	1156	G	N1-C6-O6	-9.38	114.27	119.90
1	A	1168	A	N3-C4-C5	-9.38	120.24	126.80
1	A	198	G	N3-C4-C5	-9.37	123.92	128.60
1	A	1103	C	N1-C2-N3	9.37	125.76	119.20
1	A	1417	G	N7-C8-N9	9.37	117.78	113.10
1	A	566	G	O5'-P-OP1	-9.36	97.27	105.70
1	A	144	G	C2-N3-C4	-9.36	107.22	111.90
1	A	1271	G	C8-N9-C4	9.35	110.14	106.40
1	A	239	U	N3-C4-C5	-9.35	108.99	114.60
1	A	336	C	C6-N1-C2	9.35	124.04	120.30
1	A	551	U	C5-C6-N1	-9.35	118.03	122.70
1	A	880	C	C6-N1-C2	9.35	124.04	120.30
1	A	590	C	C5-C6-N1	-9.34	116.33	121.00
1	A	300	A	C8-N9-C4	-9.34	102.06	105.80
6	F	45	LEU	CA-CB-CG	-9.34	93.82	115.30
1	A	170	U	N3-C4-C5	-9.33	109.00	114.60
1	A	314	C	N3-C2-O2	9.33	128.43	121.90
1	A	701	C	N3-C4-C5	-9.33	118.17	121.90
1	A	1227	A	C6-C5-N7	-9.33	125.77	132.30
1	A	567	G	C2-N3-C4	-9.32	107.24	111.90
1	A	588	G	C8-N9-C4	-9.32	102.67	106.40
1	A	778	G	O5'-P-OP1	-9.32	97.31	105.70
1	A	993	G	N3-C4-N9	9.32	131.59	126.00
1	A	691	G	C5-C6-O6	9.32	134.19	128.60
1	A	299	G	OP2-P-O3'	9.31	125.69	105.20
1	A	1336	C	N1-C2-O2	9.31	124.48	118.90
1	A	575	G	O5'-P-OP2	-9.30	97.33	105.70
1	A	950	U	N3-C4-C5	-9.29	109.03	114.60
1	A	255	G	C5-C6-O6	-9.28	123.03	128.60
1	A	1293	G	C8-N9-C4	9.28	110.11	106.40
1	A	1532	U	N3-C2-O2	9.28	128.70	122.20
1	A	753	A	N1-C6-N6	-9.27	113.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	725	G	C2-N3-C4	-9.27	107.27	111.90
1	A	266	G	C4-N9-C1'	-9.27	114.45	126.50
1	A	1349	A	OP2-P-O3'	9.27	125.59	105.20
1	A	735	C	C5-C4-N4	-9.26	113.72	120.20
1	A	439	A	N9-C4-C5	9.26	109.50	105.80
1	A	404	U	O5'-P-OP1	9.25	121.80	110.70
1	A	1112	C	C5-C6-N1	-9.25	116.38	121.00
1	A	1365	G	C5-C6-O6	-9.25	123.05	128.60
1	A	1166	G	N9-C4-C5	9.25	109.10	105.40
1	A	1467	G	C2-N3-C4	9.24	116.52	111.90
1	A	35	G	C8-N9-C4	9.23	110.09	106.40
1	A	910	C	N3-C4-C5	-9.23	118.21	121.90
1	A	972	C	C6-N1-C2	9.23	123.99	120.30
1	A	584	G	N1-C6-O6	-9.22	114.37	119.90
1	A	1125	U	N3-C2-O2	9.21	128.65	122.20
3	C	179	ARG	N-CA-C	-9.22	86.12	111.00
1	A	290	C	O5'-P-OP2	-9.21	97.41	105.70
1	A	730	G	C6-C5-N7	9.21	135.92	130.40
1	A	526	C	C5-C6-N1	-9.20	116.40	121.00
1	A	547	A	N9-C4-C5	9.20	109.48	105.80
1	A	728	A	N1-C2-N3	9.21	133.90	129.30
1	A	1166	G	C5-C6-O6	9.20	134.12	128.60
1	A	317	G	C5-C6-O6	-9.20	123.08	128.60
1	A	319	G	C5-C6-N1	-9.20	106.90	111.50
1	A	1090	U	N1-C2-N3	9.20	120.42	114.90
1	A	352	C	C4-C5-C6	9.20	122.00	117.40
1	A	508	C	N3-C4-N4	-9.20	111.56	118.00
1	A	1167	A	C5-C6-N1	-9.20	113.10	117.70
1	A	108	G	C5-N7-C8	-9.20	99.70	104.30
1	A	703	G	C8-N9-C1'	-9.19	115.05	127.00
1	A	60	A	C4-C5-C6	9.19	121.59	117.00
1	A	501	C	C5-C6-N1	-9.19	116.41	121.00
1	A	741	G	N1-C2-N2	-9.19	107.93	116.20
1	A	816	A	OP1-P-OP2	9.18	133.38	119.60
1	A	896	C	N3-C4-C5	9.18	125.57	121.90
1	A	289	G	OP2-P-O3'	9.17	125.38	105.20
1	A	635	G	C5-C6-N1	-9.17	106.91	111.50
1	A	247	G	C4-C5-C6	9.17	124.30	118.80
1	A	1157	A	N1-C6-N6	-9.16	113.10	118.60
1	A	1166	G	N1-C6-O6	-9.16	114.40	119.90
1	A	201	C	C6-N1-C2	9.16	123.96	120.30
1	A	500	G	C5-C6-O6	-9.16	123.10	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	780	A	C5-C6-N6	-9.16	116.37	123.70
1	A	111	G	N3-C4-N9	-9.15	120.51	126.00
1	A	764	C	O5'-P-OP1	-9.15	97.46	105.70
1	A	284	G	N9-C4-C5	-9.15	101.74	105.40
1	A	1193	G	C4-C5-C6	9.15	124.29	118.80
1	A	382	A	N1-C2-N3	9.14	133.87	129.30
1	A	963	G	N1-C2-N3	9.14	129.38	123.90
1	A	1338	G	C4-C5-N7	-9.14	107.14	110.80
1	A	585	G	N1-C6-O6	-9.13	114.42	119.90
1	A	399	G	N3-C2-N2	9.13	126.29	119.90
1	A	670	G	N3-C4-N9	9.12	131.47	126.00
1	A	785	G	C5-C6-O6	-9.12	123.13	128.60
1	A	1516[A]	G	C8-N9-C1'	9.12	138.86	127.00
1	A	1516[B]	G	C8-N9-C1'	9.12	138.86	127.00
1	A	228	A	C8-N9-C4	-9.12	102.15	105.80
1	A	283	C	C2-N3-C4	9.12	124.46	119.90
1	A	545	C	C6-N1-C2	-9.12	116.65	120.30
1	A	821	G	N1-C2-N3	9.11	129.37	123.90
1	A	792	A	C5-C6-N6	-9.11	116.41	123.70
1	A	168	G	C4-C5-C6	9.11	124.27	118.80
1	A	864	A	N1-C6-N6	-9.11	113.14	118.60
1	A	755	G	C5-N7-C8	-9.11	99.75	104.30
1	A	1415	G	O5'-P-OP1	-9.11	97.50	105.70
1	A	61	G	C5-C6-O6	-9.09	123.14	128.60
1	A	1417	G	C8-N9-C4	-9.09	102.76	106.40
1	A	715	A	C5-C6-N1	9.09	122.25	117.70
1	A	111	G	N9-C4-C5	9.09	109.03	105.40
1	A	283	C	N3-C4-N4	9.09	124.36	118.00
1	A	406	G	C8-N9-C4	-9.09	102.76	106.40
1	A	1396	A	C2-N3-C4	-9.09	106.06	110.60
1	A	703	G	N1-C6-O6	-9.08	114.45	119.90
1	A	284	G	C2-N3-C4	-9.08	107.36	111.90
1	A	309	G	C8-N9-C4	-9.08	102.77	106.40
1	A	111	G	C5-C6-O6	9.08	134.05	128.60
1	A	729	A	C2-N3-C4	9.07	115.14	110.60
1	A	738	C	N3-C4-N4	9.07	124.35	118.00
1	A	1129	C	C6-N1-C2	-9.07	116.67	120.30
1	A	325	A	N9-C4-C5	9.06	109.43	105.80
1	A	671	G	C5-C6-O6	-9.06	123.17	128.60
1	A	654	G	N9-C4-C5	9.04	109.02	105.40
1	A	401	C	C5-C4-N4	-9.04	113.87	120.20
1	A	557	G	C8-N9-C4	-9.04	102.78	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	787	A	C6-C5-N7	-9.03	125.98	132.30
1	A	523	A	C5-N7-C8	-9.03	99.38	103.90
1	A	1075	C	C2-N3-C4	-9.03	115.38	119.90
1	A	1104	G	N7-C8-N9	9.03	117.61	113.10
1	A	1505	G	N3-C4-N9	9.02	131.41	126.00
1	A	266	G	C4-C5-C6	-9.02	113.39	118.80
1	A	277	C	O5'-P-OP1	-9.02	97.59	105.70
1	A	1305	G	C8-N9-C4	-9.02	102.79	106.40
1	A	15	G	C8-N9-C4	-9.01	102.80	106.40
1	A	190(G)	G	O5'-P-OP1	-9.01	97.59	105.70
1	A	1279	A	C5-N7-C8	-9.01	99.40	103.90
1	A	970	C	C6-N1-C2	9.00	123.90	120.30
1	A	247	G	N3-C2-N2	-9.00	113.60	119.90
1	A	607	A	C2-N3-C4	-8.99	106.10	110.60
1	A	281	G	C6-C5-N7	-8.99	125.00	130.40
1	A	933	G	C6-C5-N7	-8.98	125.01	130.40
1	A	712	A	N1-C2-N3	8.98	133.79	129.30
1	A	819	A	N9-C4-C5	-8.98	102.21	105.80
1	A	542	G	N3-C4-C5	-8.97	124.11	128.60
1	A	809	G	C2-N3-C4	8.97	116.39	111.90
1	A	1390	U	C6-N1-C2	-8.97	115.62	121.00
1	A	658	G	N3-C4-N9	8.96	131.38	126.00
1	A	918	A	N1-C6-N6	8.96	123.98	118.60
1	A	1090	U	C6-N1-C2	-8.96	115.62	121.00
1	A	848	C	C6-N1-C2	-8.96	116.72	120.30
1	A	184	G	C4-N9-C1'	8.96	138.14	126.50
1	A	387	U	N3-C4-O4	8.96	125.67	119.40
1	A	406	G	N1-C6-O6	8.96	125.27	119.90
1	A	659	U	N1-C2-N3	8.96	120.27	114.90
1	A	1506	U	C6-N1-C2	8.95	126.37	121.00
1	A	238	G	OP2-P-O3'	8.95	124.89	105.20
1	A	279	A	C2-N3-C4	-8.95	106.12	110.60
1	A	425	G	C4-C5-N7	-8.95	107.22	110.80
1	A	310	G	O5'-P-OP1	-8.95	97.65	105.70
1	A	1179	A	N1-C6-N6	-8.95	113.23	118.60
1	A	1181	G	N3-C2-N2	-8.95	113.64	119.90
1	A	1348	U	N1-C2-N3	8.94	120.27	114.90
1	A	1227	A	C4-C5-N7	8.94	115.17	110.70
1	A	503	C	O5'-P-OP2	-8.94	97.66	105.70
1	A	1539	C	C6-N1-C2	-8.94	116.73	120.30
1	A	562	C	C5-C6-N1	-8.93	116.53	121.00
1	A	45	U	N3-C2-O2	-8.93	115.95	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1501	C	O5'-P-OP1	-8.93	97.67	105.70
1	A	1131	G	C5-C6-N1	-8.93	107.04	111.50
1	A	1079	G	N1-C2-N3	8.92	129.25	123.90
1	A	1493	A	C2-N3-C4	8.92	115.06	110.60
1	A	108	G	N3-C4-N9	-8.92	120.65	126.00
1	A	748	C	N3-C4-N4	8.92	124.24	118.00
1	A	823	G	C2-N3-C4	-8.92	107.44	111.90
1	A	255	G	N1-C6-O6	8.91	125.25	119.90
1	A	1091	U	C4-C5-C6	8.91	125.05	119.70
1	A	1139	G	C5-C6-O6	8.91	133.95	128.60
1	A	564	C	O5'-P-OP2	-8.91	97.68	105.70
1	A	1414	U	C6-N1-C2	-8.91	115.65	121.00
1	A	1516[A]	G	C4-N9-C1'	-8.91	114.92	126.50
1	A	1516[B]	G	C4-N9-C1'	-8.91	114.92	126.50
1	A	654	G	N3-C4-N9	-8.91	120.66	126.00
1	A	886	G	N1-C2-N3	8.90	129.24	123.90
1	A	70	G	C8-N9-C4	8.90	109.96	106.40
1	A	553	A	C2-N3-C4	-8.90	106.15	110.60
1	A	889	A	C5-C6-N6	8.90	130.82	123.70
1	A	54	C	C6-N1-C2	8.90	123.86	120.30
17	Q	98	LEU	CA-CB-CG	8.90	135.76	115.30
1	A	685	G	N3-C4-N9	-8.89	120.67	126.00
1	A	499	A	N1-C6-N6	-8.89	113.27	118.60
17	Q	84	LEU	CA-CB-CG	-8.88	94.87	115.30
1	A	1517[A]	G	C8-N9-C4	8.88	109.95	106.40
1	A	1517[B]	G	C8-N9-C4	8.88	109.95	106.40
1	A	328	C	C5-C6-N1	-8.87	116.56	121.00
1	A	886	G	C6-C5-N7	-8.87	125.08	130.40
1	A	1131	G	N1-C6-O6	8.87	125.22	119.90
1	A	1502	A	O4'-C1'-N9	8.87	115.30	108.20
1	A	646	U	C5-C4-O4	8.87	131.22	125.90
1	A	402	G	C5-C6-O6	8.87	133.92	128.60
1	A	284	G	C8-N9-C4	8.86	109.94	106.40
1	A	753	A	N9-C4-C5	8.86	109.34	105.80
1	A	61	G	N3-C4-C5	8.86	133.03	128.60
1	A	169	C	N3-C4-C5	-8.85	118.36	121.90
1	A	322	C	N3-C4-C5	-8.85	118.36	121.90
1	A	307	C	N1-C2-N3	-8.85	113.01	119.20
1	A	299	G	C5-C6-N1	-8.85	107.08	111.50
1	A	632	A	C6-C5-N7	-8.84	126.11	132.30
1	A	1279	A	N1-C6-N6	8.84	123.91	118.60
1	A	892	A	C6-N1-C2	-8.84	113.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	890	G	C5-C6-O6	8.84	133.90	128.60
1	A	247	G	C6-C5-N7	-8.83	125.10	130.40
1	A	851	G	C4-N9-C1'	8.83	137.98	126.50
1	A	888	G	C8-N9-C1'	-8.83	115.52	127.00
1	A	505	G	C5-C6-N1	8.82	115.91	111.50
1	A	951	G	N1-C6-O6	8.82	125.19	119.90
1	A	1506	U	C5-C6-N1	-8.82	118.29	122.70
1	A	1288	A	N1-C6-N6	-8.82	113.31	118.60
1	A	288	A	N1-C2-N3	8.82	133.71	129.30
1	A	761	G	N1-C6-O6	8.82	125.19	119.90
1	A	260	G	C5-C6-O6	8.81	133.89	128.60
1	A	314	C	N1-C2-O2	-8.81	113.61	118.90
1	A	433	C	C6-N1-C2	-8.81	116.78	120.30
1	A	692	U	O5'-P-OP2	-8.81	97.77	105.70
1	A	484	G	C5-C6-O6	8.81	133.89	128.60
1	A	561	U	C6-N1-C1'	-8.81	108.87	121.20
1	A	1523	G	OP1-P-OP2	-8.81	106.39	119.60
1	A	553	A	N1-C6-N6	8.80	123.88	118.60
1	A	664	G	N1-C6-O6	-8.80	114.62	119.90
1	A	1087	G	C4-C5-C6	8.80	124.08	118.80
1	A	291	C	C2-N1-C1'	8.79	128.47	118.80
1	A	632	A	C5-N7-C8	-8.79	99.50	103.90
1	A	744	C	N3-C4-N4	8.79	124.16	118.00
1	A	1350	A	C4-C5-N7	-8.79	106.30	110.70
1	A	402	G	N1-C6-O6	-8.79	114.63	119.90
1	A	258	G	N1-C6-O6	8.78	125.17	119.90
1	A	593	G	C2-N3-C4	-8.78	107.51	111.90
1	A	632	A	C4-C5-N7	8.78	115.09	110.70
1	A	865	A	N1-C2-N3	8.78	133.69	129.30
1	A	1329	A	C8-N9-C4	-8.78	102.29	105.80
1	A	897	C	C6-N1-C2	8.78	123.81	120.30
1	A	111	G	C5-C6-N1	-8.78	107.11	111.50
1	A	1098	C	C5-C6-N1	-8.78	116.61	121.00
1	A	1329	A	OP1-P-O3'	8.78	124.51	105.20
1	A	292	G	N1-C6-O6	8.78	125.17	119.90
1	A	833	U	C2-N3-C4	-8.78	121.73	127.00
1	A	823	G	C4-C5-N7	8.77	114.31	110.80
1	A	1420	C	C6-N1-C2	-8.77	116.79	120.30
1	A	1258	G	C8-N9-C4	-8.77	102.89	106.40
1	A	372	C	N3-C2-O2	-8.77	115.76	121.90
1	A	770	C	OP1-P-OP2	-8.77	106.45	119.60
1	A	1215	G	C4-C5-N7	8.77	114.31	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	G	C2-N3-C4	-8.76	107.52	111.90
1	A	325	A	C8-N9-C4	-8.76	102.30	105.80
1	A	810	C	C5-C6-N1	-8.76	116.62	121.00
1	A	828	A	C8-N9-C4	8.76	109.30	105.80
1	A	253	U	O5'-P-OP2	-8.75	97.82	105.70
1	A	580	U	N3-C4-O4	8.75	125.53	119.40
1	A	1204	A	C2-N3-C4	-8.75	106.22	110.60
1	A	243	A	C8-N9-C4	-8.75	102.30	105.80
1	A	855	G	C2-N3-C4	-8.75	107.53	111.90
1	A	566	G	N1-C6-O6	8.74	125.15	119.90
1	A	1502	A	N7-C8-N9	8.74	118.17	113.80
1	A	1208	C	C6-N1-C2	8.74	123.80	120.30
1	A	1094	G	N3-C4-C5	-8.74	124.23	128.60
1	A	126	G	C5-C6-N1	-8.74	107.13	111.50
1	A	200	G	C2-N3-C4	-8.73	107.53	111.90
1	A	306	G	N3-C4-C5	8.73	132.97	128.60
1	A	1185	G	C8-N9-C4	-8.73	102.91	106.40
1	A	231	G	C5-C6-N1	-8.73	107.14	111.50
1	A	890	G	C4-C5-C6	8.73	124.04	118.80
1	A	813	U	C5-C4-O4	-8.73	120.66	125.90
1	A	267	C	N3-C4-C5	8.72	125.39	121.90
1	A	759	A	C8-N9-C4	-8.72	102.31	105.80
1	A	364	A	C2-N3-C4	-8.72	106.24	110.60
1	A	448	A	C2-N3-C4	-8.72	106.24	110.60
1	A	710	G	C6-C5-N7	-8.72	125.17	130.40
1	A	116	A	N1-C2-N3	8.72	133.66	129.30
1	A	1053	G	C8-N9-C1'	8.72	138.34	127.00
1	A	1182	G	N3-C4-C5	-8.72	124.24	128.60
1	A	1206	G	N3-C2-N2	-8.72	113.80	119.90
1	A	23	C	C6-N1-C2	8.71	123.78	120.30
1	A	1409	C	C5-C6-N1	8.71	125.35	121.00
1	A	303	A	C5-C6-N1	8.70	122.05	117.70
1	A	1259	C	N3-C4-C5	8.70	125.38	121.90
1	A	35	G	C5-C6-O6	-8.70	123.38	128.60
1	A	184	G	C8-N9-C1'	-8.70	115.69	127.00
1	A	515	G	C4-C5-N7	8.70	114.28	110.80
1	A	1488	G	C2-N3-C4	8.70	116.25	111.90
1	A	6	G	C8-N9-C1'	-8.69	115.70	127.00
1	A	823	G	N3-C4-C5	8.69	132.95	128.60
1	A	451	A	N1-C2-N3	8.69	133.65	129.30
1	A	496	A	O5'-P-OP2	8.69	121.12	110.70
1	A	1227	A	C5-C6-N6	-8.69	116.75	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	A	O5'-P-OP1	-8.68	97.89	105.70
1	A	1398	A	O5'-P-OP1	-8.68	97.89	105.70
1	A	155	C	O5'-P-OP1	-8.68	97.89	105.70
1	A	184	G	N1-C2-N2	-8.68	108.39	116.20
1	A	444	C	C2-N1-C1'	8.68	128.35	118.80
1	A	953	G	N1-C6-O6	-8.68	114.69	119.90
1	A	35	G	C8-N9-C1'	-8.68	115.72	127.00
1	A	900	A	N1-C2-N3	8.67	133.63	129.30
1	A	1287	A	C8-N9-C4	-8.67	102.33	105.80
1	A	147	G	C5-C6-N1	-8.67	107.17	111.50
1	A	1279	A	C6-C5-N7	-8.67	126.23	132.30
1	A	277	C	C6-N1-C2	8.66	123.77	120.30
1	A	494	G	N7-C8-N9	8.66	117.43	113.10
1	A	593	G	N1-C6-O6	8.66	125.10	119.90
1	A	872	A	N1-C2-N3	8.66	133.63	129.30
1	A	906	G	C6-C5-N7	-8.66	125.20	130.40
1	A	803	G	N1-C6-O6	-8.65	114.71	119.90
1	A	976	G	O5'-P-OP1	-8.65	97.91	105.70
1	A	1374	A	N1-C2-N3	8.65	133.63	129.30
1	A	548	G	C5-C6-O6	-8.65	123.41	128.60
1	A	913	A	C4-C5-N7	-8.65	106.38	110.70
1	A	306	G	OP1-P-OP2	8.65	132.57	119.60
1	A	544	G	O5'-P-OP2	8.64	121.07	110.70
1	A	733	A	N1-C2-N3	8.64	133.62	129.30
1	A	721	G	N7-C8-N9	-8.64	108.78	113.10
1	A	1244	C	C6-N1-C2	8.64	123.76	120.30
1	A	579	G	O5'-P-OP2	-8.64	97.92	105.70
1	A	1131	G	C4-C5-C6	8.64	123.98	118.80
1	A	500	G	OP2-P-O3'	8.63	124.20	105.20
1	A	977	A	C8-N9-C4	-8.63	102.35	105.80
1	A	284	G	OP2-P-O3'	8.63	124.19	105.20
1	A	1215	G	N1-C6-O6	8.63	125.08	119.90
1	A	241	C	C2-N3-C4	-8.62	115.59	119.90
1	A	552	U	C4-C5-C6	8.62	124.88	119.70
1	A	1348	U	N3-C2-O2	-8.62	116.16	122.20
1	A	531	U	C6-N1-C1'	8.62	133.27	121.20
1	A	666	G	C5-C6-N1	-8.62	107.19	111.50
1	A	748	C	C5-C4-N4	-8.62	114.17	120.20
1	A	1339	A	N1-C6-N6	-8.61	113.43	118.60
1	A	729	A	OP1-P-O3'	8.61	124.15	105.20
1	A	1125	U	C2-N1-C1'	-8.61	107.37	117.70
1	A	1101	A	C2-N3-C4	-8.61	106.30	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1363	A	C8-N9-C4	-8.61	102.36	105.80
1	A	674	G	N1-C2-N2	-8.61	108.45	116.20
1	A	1182	G	N3-C4-N9	8.60	131.16	126.00
1	A	364	A	P-O3'-C3'	8.60	130.02	119.70
1	A	484	G	N1-C6-O6	-8.60	114.74	119.90
1	A	748	C	C2-N1-C1'	8.60	128.26	118.80
1	A	714	G	C8-N9-C1'	-8.60	115.82	127.00
1	A	758	G	N3-C2-N2	8.60	125.92	119.90
1	A	810	C	N3-C4-N4	-8.60	111.98	118.00
1	A	722	A	C6-C5-N7	-8.59	126.28	132.30
1	A	907	A	N9-C4-C5	8.59	109.24	105.80
1	A	374	A	C5-C6-N1	-8.59	113.40	117.70
1	A	1520[A]	G	C4-N9-C1'	8.59	137.67	126.50
1	A	1520[B]	G	C4-N9-C1'	8.59	137.67	126.50
1	A	800	G	C5-C6-O6	8.59	133.75	128.60
1	A	984	C	N1-C2-O2	8.59	124.05	118.90
1	A	18	C	C2-N3-C4	-8.58	115.61	119.90
1	A	55	A	N9-C4-C5	8.58	109.23	105.80
1	A	172	A	C5-C6-N1	-8.58	113.41	117.70
1	A	1231	G	C4-C5-N7	8.58	114.23	110.80
1	A	790	A	C2-N3-C4	-8.58	106.31	110.60
1	A	108	G	N9-C1'-C2'	-8.57	102.57	112.00
1	A	150	C	C6-N1-C2	8.57	123.73	120.30
1	A	1509	C	N1-C2-N3	8.57	125.20	119.20
1	A	242	C	N3-C4-N4	-8.57	112.00	118.00
1	A	1034	G	C8-N9-C4	-8.57	102.97	106.40
1	A	46	G	N7-C8-N9	8.57	117.38	113.10
1	A	53	A	N1-C2-N3	8.57	133.58	129.30
1	A	1299	A	C5-C6-N1	-8.57	113.42	117.70
1	A	936	C	N3-C4-N4	8.57	124.00	118.00
1	A	1091	U	N3-C4-O4	8.56	125.39	119.40
1	A	1101	A	N1-C2-N3	8.56	133.58	129.30
1	A	1074	G	C2-N3-C4	8.56	116.18	111.90
1	A	9	G	N1-C6-O6	8.55	125.03	119.90
1	A	778	G	C4-C5-N7	-8.55	107.38	110.80
1	A	474	G	C2-N3-C4	-8.54	107.63	111.90
1	A	1411	C	N1-C2-N3	-8.54	113.22	119.20
1	A	1192	C	N3-C4-C5	8.54	125.32	121.90
1	A	223	U	C5-C6-N1	-8.54	118.43	122.70
1	A	894	G	C2-N3-C4	-8.54	107.63	111.90
1	A	352	C	OP2-P-O3'	8.54	123.98	105.20
1	A	710	G	N1-C6-O6	8.54	125.02	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	G	N1-C2-N2	-8.54	108.52	116.20
1	A	680	C	N3-C4-N4	8.53	123.97	118.00
1	A	40	C	O5'-P-OP1	-8.53	98.02	105.70
1	A	674	G	N3-C4-N9	8.53	131.12	126.00
1	A	482	A	N1-C2-N3	8.53	133.56	129.30
1	A	569	C	O4'-C1'-N1	-8.52	101.38	108.20
1	A	717	C	N3-C4-C5	-8.52	118.49	121.90
1	A	831	U	N3-C2-O2	8.52	128.16	122.20
1	A	354	G	C8-N9-C4	-8.51	103.00	106.40
1	A	531	U	N1-C2-N3	8.51	120.01	114.90
1	A	855	G	C8-N9-C4	8.51	109.81	106.40
1	A	341	C	C6-N1-C2	-8.51	116.90	120.30
1	A	28	G	C4-C5-C6	8.51	123.91	118.80
1	A	44	G	C8-N9-C1'	-8.51	115.94	127.00
1	A	228	A	C4-C5-N7	-8.51	106.45	110.70
1	A	416	G	C8-N9-C4	-8.51	103.00	106.40
1	A	814	A	O4'-C1'-N9	8.51	115.00	108.20
20	T	94	ALA	N-CA-C	-8.50	88.04	111.00
1	A	778	G	C5-C6-O6	8.50	133.70	128.60
1	A	671	G	C6-N1-C2	-8.50	120.00	125.10
1	A	918	A	C5-C6-N6	-8.50	116.90	123.70
1	A	974	A	C6-N1-C2	-8.50	113.50	118.60
1	A	198	G	N1-C6-O6	-8.49	114.80	119.90
1	A	663	A	N1-C2-N3	8.49	133.55	129.30
1	A	113	G	N3-C2-N2	-8.49	113.96	119.90
1	A	22	G	C5-C6-O6	8.49	133.69	128.60
1	A	282	A	C2-N3-C4	-8.49	106.36	110.60
1	A	575	G	N1-C6-O6	-8.49	114.81	119.90
1	A	854	G	N1-C6-O6	8.49	124.99	119.90
1	A	168	G	N1-C6-O6	8.48	124.99	119.90
1	A	364	A	C5-C6-N1	-8.48	113.46	117.70
1	A	724	G	C6-C5-N7	-8.48	125.31	130.40
1	A	1421	G	C8-N9-C4	-8.48	103.01	106.40
1	A	579	G	N1-C6-O6	8.48	124.99	119.90
1	A	632	A	C8-N9-C4	-8.48	102.41	105.80
1	A	1336	C	C2-N1-C1'	8.48	128.13	118.80
1	A	1433	A	C5-C6-N1	8.47	121.94	117.70
1	A	320	C	N3-C4-N4	8.47	123.93	118.00
1	A	661	G	C4-C5-N7	-8.47	107.41	110.80
1	A	889	A	N1-C2-N3	8.47	133.53	129.30
1	A	236	G	N1-C6-O6	-8.46	114.82	119.90
1	A	730	G	N1-C6-O6	-8.46	114.82	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1087	G	OP1-P-OP2	-8.46	106.90	119.60
1	A	1401	G	N1-C2-N2	-8.46	108.58	116.20
1	A	730	G	N3-C4-N9	-8.46	120.92	126.00
1	A	658	G	N1-C2-N2	-8.46	108.58	116.20
1	A	1259	C	C6-N1-C2	8.46	123.68	120.30
1	A	1451	A	C8-N9-C4	8.46	109.19	105.80
1	A	1206	G	C5-C6-N1	-8.46	107.27	111.50
1	A	557	G	N7-C8-N9	8.46	117.33	113.10
1	A	981	U	N3-C4-C5	-8.46	109.53	114.60
1	A	1374	A	C4-C5-N7	-8.45	106.47	110.70
1	A	204	U	C5-C6-N1	8.45	126.92	122.70
1	A	390	C	N3-C4-N4	8.45	123.91	118.00
1	A	645	C	N3-C4-C5	8.45	125.28	121.90
1	A	1003(A)	G	C4-N9-C1'	8.45	137.48	126.50
1	A	525	C	C6-N1-C2	8.44	123.68	120.30
1	A	965	A	C8-N9-C4	8.44	109.18	105.80
1	A	823	G	N1-C6-O6	8.44	124.96	119.90
1	A	610	G	N1-C2-N2	8.44	123.79	116.20
1	A	333	G	C5-C6-O6	-8.44	123.54	128.60
1	A	523	A	C4-C5-N7	8.44	114.92	110.70
1	A	789	U	O5'-P-OP2	-8.44	98.11	105.70
1	A	399	G	N3-C4-C5	-8.43	124.38	128.60
1	A	884	U	C5-C6-N1	-8.43	118.48	122.70
1	A	1297	C	N3-C4-C5	8.43	125.27	121.90
1	A	1112	C	C2-N1-C1'	-8.43	109.53	118.80
1	A	1121	U	C5-C6-N1	-8.43	118.48	122.70
1	A	671	G	C5-C6-N1	8.43	115.71	111.50
1	A	222	U	C6-N1-C2	8.43	126.06	121.00
1	A	577	G	C8-N9-C1'	8.43	137.96	127.00
1	A	348	G	N1-C6-O6	8.42	124.95	119.90
1	A	44	G	C4-C5-C6	8.42	123.85	118.80
1	A	125	U	N1-C2-N3	8.42	119.95	114.90
1	A	198	G	O5'-P-OP1	-8.42	98.12	105.70
1	A	482	A	C4-C5-C6	8.42	121.21	117.00
1	A	610	G	N7-C8-N9	8.42	117.31	113.10
1	A	375	U	C5-C6-N1	-8.41	118.49	122.70
1	A	740	U	C2-N1-C1'	-8.41	107.61	117.70
1	A	1104	G	C8-N9-C4	-8.41	103.04	106.40
1	A	1354	C	N1-C2-O2	-8.41	113.85	118.90
1	A	483	C	O5'-P-OP1	-8.40	98.14	105.70
1	A	109	A	C2-N3-C4	-8.40	106.40	110.60
1	A	922	G	C4-C5-N7	8.40	114.16	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1213	A	N1-C6-N6	-8.40	113.56	118.60
1	A	937	A	C8-N9-C4	-8.39	102.44	105.80
1	A	289	G	O5'-P-OP2	-8.39	98.15	105.70
1	A	388	G	C5-C6-N1	-8.39	107.30	111.50
1	A	1104	G	C6-C5-N7	-8.39	125.37	130.40
1	A	529	G	N1-C6-O6	8.39	124.93	119.90
1	A	125	U	C6-N1-C2	-8.39	115.97	121.00
1	A	607	A	N1-C2-N3	8.38	133.49	129.30
1	A	857	C	C6-N1-C2	-8.38	116.95	120.30
1	A	1158	C	C4-C5-C6	8.38	121.59	117.40
1	A	1340	A	C2-N3-C4	-8.38	106.41	110.60
1	A	1415	G	N3-C2-N2	8.38	125.77	119.90
1	A	1452	C	N1-C2-O2	8.38	123.93	118.90
1	A	1027	C	C6-N1-C2	-8.38	116.95	120.30
1	A	1497	G	C8-N9-C4	-8.38	103.05	106.40
1	A	1531	A	N7-C8-N9	8.38	117.99	113.80
1	A	763	G	C5-C6-N1	8.38	115.69	111.50
1	A	791	G	C4-C5-N7	-8.38	107.45	110.80
1	A	832	C	N3-C4-N4	8.38	123.86	118.00
1	A	479	C	N3-C2-O2	-8.38	116.04	121.90
1	A	686	U	N1-C2-O2	-8.37	116.94	122.80
1	A	264	U	N3-C2-O2	-8.37	116.34	122.20
1	A	35	G	N3-C4-N9	8.37	131.02	126.00
1	A	553	A	N1-C2-N3	8.36	133.48	129.30
1	A	571	U	O5'-P-OP2	8.36	120.73	110.70
1	A	903	G	C8-N9-C4	8.36	109.74	106.40
1	A	774	G	N1-C2-N2	-8.36	108.68	116.20
1	A	1148	U	N3-C2-O2	-8.36	116.35	122.20
1	A	685	G	C8-N9-C4	8.36	109.74	106.40
1	A	1287	A	C5-N7-C8	-8.36	99.72	103.90
1	A	127	G	C6-C5-N7	-8.35	125.39	130.40
1	A	981	U	N1-C2-O2	-8.35	116.96	122.80
1	A	1064	G	C5-N7-C8	-8.35	100.13	104.30
1	A	1488	G	C5-C6-O6	-8.35	123.59	128.60
1	A	360	A	C5-C6-N1	8.35	121.87	117.70
1	A	703	G	N7-C8-N9	-8.35	108.93	113.10
1	A	1516[A]	G	C2-N3-C4	-8.34	107.73	111.90
1	A	1516[B]	G	C2-N3-C4	-8.34	107.73	111.90
1	A	1158	C	N3-C2-O2	-8.34	116.06	121.90
1	A	1481	U	N3-C4-C5	-8.34	109.59	114.60
1	A	854	G	C2-N3-C4	-8.34	107.73	111.90
1	A	433	C	N3-C4-C5	-8.34	118.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	658	G	N9-C4-C5	-8.33	102.07	105.40
1	A	789	U	C5-C4-O4	8.33	130.90	125.90
1	A	524	G	N1-C2-N3	-8.32	118.91	123.90
1	A	544	G	C5-N7-C8	-8.32	100.14	104.30
1	A	672	U	N1-C2-N3	-8.32	109.91	114.90
1	A	907	A	N1-C2-N3	8.31	133.46	129.30
1	A	888	G	N1-C2-N2	-8.31	108.72	116.20
1	A	974	A	N1-C6-N6	-8.31	113.61	118.60
1	A	829	G	N3-C2-N2	-8.31	114.08	119.90
1	A	1509	C	C4-C5-C6	8.31	121.55	117.40
1	A	108	G	C5-C6-O6	-8.30	123.62	128.60
1	A	245	C	C6-N1-C2	8.30	123.62	120.30
1	A	285	G	C5-C6-N1	-8.30	107.35	111.50
1	A	47	C	C2-N3-C4	-8.30	115.75	119.90
1	A	1415	G	N9-C4-C5	-8.30	102.08	105.40
1	A	372	C	O5'-P-OP1	-8.30	98.23	105.70
1	A	670	G	N3-C4-C5	-8.30	124.45	128.60
1	A	331	G	C4-C5-C6	8.29	123.78	118.80
1	A	914	A	OP1-P-O3'	-8.29	86.95	105.20
1	A	1139	G	C4-C5-N7	-8.29	107.48	110.80
1	A	29	G	N3-C4-N9	-8.28	121.03	126.00
1	A	10	A	N7-C8-N9	-8.28	109.66	113.80
1	A	526	C	C4-C5-C6	8.28	121.54	117.40
1	A	1433	A	N9-C4-C5	8.28	109.11	105.80
1	A	800	G	O5'-P-OP1	-8.28	98.25	105.70
1	A	1269	A	O5'-P-OP1	8.28	120.64	110.70
1	A	803	G	C5-C6-N1	8.28	115.64	111.50
1	A	1394	A	C6-N1-C2	-8.27	113.64	118.60
1	A	509	A	N7-C8-N9	8.27	117.94	113.80
1	A	1493	A	N7-C8-N9	8.27	117.94	113.80
1	A	1501	C	C6-N1-C2	-8.27	116.99	120.30
1	A	1506	U	O5'-P-OP1	-8.26	98.26	105.70
1	A	520	A	C8-N9-C4	-8.26	102.50	105.80
1	A	126	G	C4-C5-C6	8.25	123.75	118.80
1	A	822	C	OP1-P-O3'	-8.25	87.04	105.20
1	A	860	A	C2-N3-C4	8.25	114.73	110.60
1	A	1389	C	O5'-P-OP1	-8.25	98.27	105.70
1	A	1417	G	N1-C6-O6	8.25	124.85	119.90
1	A	27	G	N1-C6-O6	8.25	124.85	119.90
1	A	231	G	C2-N3-C4	-8.25	107.78	111.90
1	A	307	C	C6-N1-C2	8.25	123.60	120.30
1	A	571	U	C6-N1-C2	-8.25	116.05	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	G	O5'-P-OP2	-8.25	98.28	105.70
1	A	241	C	N3-C4-C5	8.25	125.20	121.90
1	A	834	C	O5'-P-OP1	8.25	120.60	110.70
1	A	504	C	O5'-P-OP2	8.24	120.59	110.70
1	A	28	G	C6-C5-N7	-8.24	125.45	130.40
1	A	724	G	N3-C4-N9	8.24	130.95	126.00
1	A	1197	G	C6-C5-N7	-8.24	125.45	130.40
1	A	190(E)	U	C2-N3-C4	-8.24	122.06	127.00
1	A	750	G	C8-N9-C4	8.24	109.70	106.40
1	A	1127	G	C6-C5-N7	-8.24	125.46	130.40
1	A	342	C	C6-N1-C2	-8.24	117.00	120.30
1	A	666	G	C6-N1-C2	8.23	130.04	125.10
1	A	854	G	C5-C6-N1	-8.23	107.38	111.50
1	A	408	A	N7-C8-N9	8.23	117.92	113.80
1	A	718	G	C5-C6-O6	-8.23	123.66	128.60
1	A	668	G	N1-C2-N3	8.23	128.84	123.90
1	A	1520[A]	G	C8-N9-C1'	-8.23	116.30	127.00
1	A	1520[B]	G	C8-N9-C1'	-8.23	116.30	127.00
1	A	757	U	C4-C5-C6	8.23	124.64	119.70
1	A	542	G	C8-N9-C4	-8.22	103.11	106.40
1	A	1486	G	N3-C4-N9	8.22	130.93	126.00
1	A	1522	U	O5'-P-OP1	8.22	120.57	110.70
1	A	481	G	OP1-P-OP2	8.22	131.93	119.60
1	A	494	G	O5'-P-OP1	-8.22	98.30	105.70
1	A	517	G	N3-C4-C5	-8.22	124.49	128.60
1	A	44	G	C4-N9-C1'	8.22	137.18	126.50
1	A	392	G	C5-C6-O6	-8.21	123.67	128.60
1	A	692	U	C6-N1-C2	8.22	125.93	121.00
1	A	533	A	N1-C2-N3	8.21	133.41	129.30
1	A	109	A	C8-N9-C4	-8.21	102.52	105.80
1	A	252	U	N3-C2-O2	8.21	127.95	122.20
1	A	597	G	N1-C2-N3	8.21	128.83	123.90
1	A	713	G	N3-C4-C5	-8.21	124.49	128.60
1	A	367	U	C6-N1-C2	8.21	125.92	121.00
1	A	560	U	N3-C4-C5	-8.21	109.67	114.60
1	A	987	G	C5-C6-O6	-8.21	123.67	128.60
1	A	11	G	N1-C2-N2	-8.21	108.81	116.20
1	A	39	G	C4-C5-N7	8.20	114.08	110.80
1	A	1197	G	C4-C5-N7	8.20	114.08	110.80
1	A	1415	G	N1-C2-N3	-8.20	118.98	123.90
1	A	1341	U	N3-C2-O2	-8.19	116.46	122.20
1	A	439	A	C6-N1-C2	-8.19	113.69	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	A	O5'-P-OP1	-8.19	98.33	105.70
1	A	883	C	C2-N3-C4	-8.19	115.81	119.90
1	A	1203	C	N1-C2-O2	-8.19	113.99	118.90
1	A	1321	C	N3-C2-O2	-8.19	116.17	121.90
1	A	126	G	C5-N7-C8	8.19	108.39	104.30
1	A	858	G	C8-N9-C4	-8.19	103.12	106.40
1	A	303	A	C5-C6-N6	-8.18	117.15	123.70
2	B	213	LEU	CA-CB-CG	-8.18	96.48	115.30
1	A	262	A	C2-N3-C4	-8.18	106.51	110.60
1	A	1417	G	C6-C5-N7	-8.18	125.49	130.40
1	A	332	G	N1-C2-N2	8.18	123.56	116.20
1	A	662	G	C2-N3-C4	-8.18	107.81	111.90
1	A	790	A	C8-N9-C4	-8.18	102.53	105.80
1	A	1069	C	N1-C2-O2	-8.18	113.99	118.90
1	A	1435	G	C8-N9-C4	-8.18	103.13	106.40
1	A	562	C	C6-N1-C2	8.17	123.57	120.30
1	A	658	G	C6-C5-N7	-8.17	125.50	130.40
1	A	299	G	C8-N9-C4	-8.17	103.13	106.40
1	A	559	A	N1-C2-N3	8.17	133.38	129.30
1	A	888	G	C8-N9-C4	-8.17	103.13	106.40
1	A	1338	G	N1-C2-N3	8.17	128.80	123.90
1	A	1539	C	C5-C6-N1	8.17	125.08	121.00
1	A	399	G	N1-C2-N2	-8.16	108.85	116.20
1	A	744	C	OP1-P-OP2	-8.16	107.36	119.60
1	A	120	A	OP1-P-OP2	8.16	131.84	119.60
1	A	61	G	C2-N3-C4	-8.16	107.82	111.90
1	A	128	G	N1-C2-N3	8.16	128.79	123.90
1	A	529	G	C5-C6-N1	-8.15	107.42	111.50
1	A	1393	U	C4-C5-C6	8.15	124.59	119.70
1	A	184	G	N3-C4-N9	8.15	130.89	126.00
1	A	1530	G	OP1-P-OP2	8.15	131.83	119.60
1	A	230	G	C2-N3-C4	-8.15	107.83	111.90
1	A	403	C	C4-C5-C6	8.15	121.47	117.40
1	A	1429	C	N3-C4-C5	-8.15	118.64	121.90
1	A	378	G	OP1-P-OP2	-8.14	107.39	119.60
1	A	860	A	C5-C6-N6	-8.14	117.19	123.70
1	A	1466	C	C6-N1-C2	-8.14	117.04	120.30
1	A	245	C	N3-C4-C5	-8.14	118.64	121.90
1	A	889	A	C6-N1-C2	-8.14	113.72	118.60
1	A	632	A	N7-C8-N9	8.14	117.87	113.80
1	A	914	A	OP2-P-O3'	8.14	123.11	105.20
1	A	1234	C	C5-C6-N1	-8.14	116.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1513	A	N3-C4-C5	8.14	132.50	126.80
1	A	323	U	N1-C2-N3	8.13	119.78	114.90
1	A	661	G	C5-C6-O6	8.13	133.48	128.60
1	A	701	C	C2-N3-C4	8.13	123.97	119.90
1	A	884	U	C4-C5-C6	8.13	124.58	119.70
1	A	1452	C	C2-N1-C1'	8.13	127.75	118.80
1	A	1003(A)	G	C8-N9-C4	-8.13	103.15	106.40
1	A	234	C	C5-C4-N4	8.12	125.89	120.20
1	A	279	A	O4'-C1'-N9	-8.12	101.70	108.20
1	A	262	A	C4-C5-N7	8.12	114.76	110.70
1	A	1220	G	C5-C6-N1	8.12	115.56	111.50
1	A	314	C	C2-N3-C4	-8.12	115.84	119.90
1	A	893	C	C6-N1-C2	8.12	123.55	120.30
1	A	1077	G	N1-C6-O6	8.12	124.77	119.90
1	A	48	C	C2-N3-C4	8.11	123.96	119.90
1	A	64	G	N3-C4-N9	8.11	130.87	126.00
1	A	713	G	C5-C6-O6	8.11	133.47	128.60
1	A	190(E)	U	O5'-P-OP2	-8.11	98.40	105.70
1	A	64	G	N3-C2-N2	8.11	125.58	119.90
1	A	263	A	C4-C5-N7	8.11	114.75	110.70
1	A	813	U	OP1-P-O3'	-8.11	87.37	105.20
1	A	1180	A	C5-N7-C8	-8.11	99.85	103.90
1	A	724	G	N3-C4-C5	-8.10	124.55	128.60
1	A	539	A	N1-C6-N6	-8.10	113.74	118.60
1	A	1050	G	O5'-P-OP1	-8.10	98.41	105.70
1	A	1399	C	N3-C4-N4	8.10	123.67	118.00
1	A	1227	A	N1-C2-N3	8.09	133.34	129.30
4	D	162	LEU	CA-CB-CG	-8.09	96.69	115.30
1	A	167	G	N1-C6-O6	8.09	124.75	119.90
1	A	768	A	C2-N3-C4	-8.09	106.56	110.60
1	A	552	U	OP2-P-O3'	8.09	122.99	105.20
1	A	499	A	C5-C6-N6	8.08	130.17	123.70
1	A	664	G	N3-C4-C5	-8.08	124.56	128.60
3	C	4	LYS	N-CA-C	8.08	132.82	111.00
1	A	230	G	C8-N9-C4	8.08	109.63	106.40
1	A	918	A	C4-C5-C6	8.08	121.04	117.00
1	A	526	C	C2-N3-C4	-8.08	115.86	119.90
1	A	574	A	C4-C5-N7	8.08	114.74	110.70
1	A	1488	G	C5-C6-N1	8.08	115.54	111.50
1	A	1529	G	C4-C5-C6	8.08	123.65	118.80
1	A	285	G	C6-C5-N7	-8.08	125.55	130.40
1	A	779	C	N3-C4-N4	-8.08	112.35	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	851	G	C8-N9-C1'	-8.08	116.50	127.00
1	A	1075	C	N1-C2-O2	-8.08	114.05	118.90
1	A	1167	A	N9-C4-C5	8.07	109.03	105.80
1	A	1504	G	OP2-P-O3'	8.07	122.96	105.20
1	A	45	U	C5-C6-N1	-8.07	118.67	122.70
1	A	703	G	C5-C6-O6	8.07	133.44	128.60
1	A	840	C	OP1-P-OP2	-8.07	107.50	119.60
1	A	395	C	N3-C2-O2	8.06	127.54	121.90
1	A	1376	U	N3-C2-O2	-8.06	116.56	122.20
1	A	317	G	N9-C4-C5	-8.06	102.18	105.40
1	A	335	C	C6-N1-C2	-8.06	117.08	120.30
1	A	1222	G	C6-C5-N7	-8.06	125.57	130.40
1	A	711	G	N3-C2-N2	-8.05	114.26	119.90
1	A	1310	G	N1-C6-O6	8.05	124.73	119.90
1	A	1526	G	N3-C2-N2	-8.05	114.26	119.90
1	A	829	G	N1-C6-O6	8.05	124.73	119.90
1	A	1513	A	N7-C8-N9	-8.05	109.78	113.80
1	A	768	A	C6-C5-N7	-8.04	126.67	132.30
1	A	807	A	C2-N3-C4	-8.04	106.58	110.60
1	A	248	C	C5-C6-N1	-8.04	116.98	121.00
1	A	559	A	P-O3'-C3'	8.04	129.35	119.70
1	A	779	C	C2-N1-C1'	-8.04	109.95	118.80
1	A	1505	G	C8-N9-C4	-8.04	103.18	106.40
1	A	856	C	N1-C2-O2	-8.04	114.08	118.90
1	A	820	U	C6-N1-C2	8.04	125.82	121.00
1	A	402	G	C2-N3-C4	-8.03	107.88	111.90
1	A	521	G	C5-C6-N1	8.03	115.52	111.50
1	A	796	C	C6-N1-C2	8.03	123.51	120.30
1	A	829	G	OP1-P-OP2	8.03	131.65	119.60
1	A	185	A	C8-N9-C4	8.03	109.01	105.80
1	A	257	G	C5-C6-N1	-8.03	107.49	111.50
1	A	632	A	C5-C6-N6	-8.03	117.28	123.70
1	A	789	U	N3-C4-C5	-8.02	109.79	114.60
1	A	908	A	C5-C6-N1	8.02	121.71	117.70
1	A	279	A	N9-C4-C5	-8.02	102.59	105.80
1	A	608	A	O5'-P-OP2	-8.02	98.48	105.70
1	A	1195	C	N3-C4-C5	8.01	125.11	121.90
1	A	1502	A	C5-C6-N1	-8.01	113.69	117.70
1	A	61	G	N3-C2-N2	-8.01	114.29	119.90
1	A	325	A	C6-N1-C2	-8.01	113.79	118.60
1	A	1030(B)	C	N1-C2-O2	8.01	123.70	118.90
1	A	1118	C	C6-N1-C2	-8.00	117.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1411	C	N1-C2-O2	-8.00	114.10	118.90
1	A	509	A	C6-N1-C2	-8.00	113.80	118.60
1	A	627	G	C8-N9-C4	-8.00	103.20	106.40
1	A	1090	U	N3-C4-C5	-8.00	109.80	114.60
1	A	320	C	N3-C2-O2	8.00	127.50	121.90
1	A	788	U	C5-C6-N1	-8.00	118.70	122.70
1	A	755	G	N1-C6-O6	7.99	124.69	119.90
1	A	913	A	C5-N7-C8	7.99	107.90	103.90
1	A	864	A	C5-C6-N6	7.99	130.09	123.70
1	A	1335	C	C5-C4-N4	7.99	125.79	120.20
1	A	831	U	C5-C4-O4	-7.99	121.11	125.90
1	A	1223	C	C6-N1-C2	-7.99	117.10	120.30
1	A	11	G	O5'-P-OP1	7.99	120.28	110.70
1	A	106	C	OP2-P-O3'	7.99	122.77	105.20
1	A	332	G	N3-C2-N2	-7.99	114.31	119.90
1	A	1493	A	N9-C4-C5	7.98	108.99	105.80
1	A	633	G	N1-C6-O6	7.98	124.69	119.90
1	A	892	A	N3-C4-C5	-7.98	121.21	126.80
1	A	900	A	C2-N3-C4	-7.98	106.61	110.60
1	A	1232	U	N1-C2-N3	7.98	119.69	114.90
1	A	263	A	C5-N7-C8	-7.98	99.91	103.90
1	A	576	G	N3-C4-C5	-7.98	124.61	128.60
1	A	113	G	C5-C6-O6	-7.97	123.81	128.60
1	A	181	G	C4-C5-C6	7.97	123.58	118.80
1	A	316	G	C6-C5-N7	-7.97	125.62	130.40
1	A	703	G	N9-C4-C5	-7.97	102.21	105.40
1	A	104	G	C6-C5-N7	-7.97	125.62	130.40
1	A	571	U	OP1-P-OP2	-7.97	107.64	119.60
1	A	775	G	C8-N9-C4	7.97	109.59	106.40
1	A	1507	A	C5-C6-N1	7.97	121.69	117.70
1	A	934	C	N3-C4-C5	-7.97	118.71	121.90
1	A	238	G	OP1-P-O3'	-7.96	87.68	105.20
1	A	355	C	OP1-P-OP2	7.96	131.55	119.60
1	A	918	A	C6-C5-N7	-7.96	126.72	132.30
1	A	220	G	C2-N3-C4	-7.96	107.92	111.90
1	A	900	A	OP1-P-OP2	-7.96	107.66	119.60
1	A	1198	G	N1-C2-N3	7.96	128.68	123.90
1	A	623	C	C6-N1-C2	7.96	123.48	120.30
1	A	727	G	N9-C4-C5	7.96	108.58	105.40
1	A	656	C	C5-C4-N4	-7.96	114.63	120.20
1	A	34	C	N3-C2-O2	7.96	127.47	121.90
1	A	389	A	C8-N9-C4	-7.96	102.62	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	A	C6-N1-C2	-7.96	113.83	118.60
1	A	1124	G	C8-N9-C4	-7.95	103.22	106.40
1	A	1504	G	N9-C4-C5	7.95	108.58	105.40
1	A	1121	U	C6-N1-C2	7.95	125.77	121.00
1	A	554	C	C5-C6-N1	-7.95	117.03	121.00
1	A	575	G	C2-N3-C4	7.95	115.87	111.90
1	A	762	C	N3-C4-N4	-7.95	112.44	118.00
1	A	1054	C	C2-N1-C1'	7.95	127.54	118.80
1	A	23	C	N1-C2-O2	-7.94	114.13	118.90
1	A	39	G	C5-C6-N1	7.94	115.47	111.50
1	A	294	U	C5-C6-N1	-7.94	118.73	122.70
1	A	547	A	C8-N9-C4	-7.94	102.62	105.80
1	A	604	G	O5'-P-OP1	-7.94	98.56	105.70
1	A	32	A	C5-C6-N6	-7.94	117.35	123.70
1	A	316	G	C5-C6-N1	-7.93	107.53	111.50
1	A	550	G	N1-C2-N3	7.93	128.66	123.90
1	A	1063	C	N3-C2-O2	7.93	127.45	121.90
1	A	1335	C	C2-N1-C1'	-7.93	110.07	118.80
1	A	168	G	C6-C5-N7	-7.93	125.64	130.40
1	A	549	C	C2-N3-C4	-7.93	115.93	119.90
1	A	181	G	C4-N9-C1'	7.93	136.81	126.50
1	A	789	U	C4-C5-C6	7.93	124.46	119.70
1	A	62	U	C4-C5-C6	7.92	124.45	119.70
1	A	776	G	OP1-P-O3'	7.92	122.63	105.20
1	A	1528	U	OP1-P-O3'	7.92	122.63	105.20
1	A	811	C	C2-N1-C1'	-7.92	110.09	118.80
1	A	4	U	C5-C6-N1	7.91	126.66	122.70
1	A	1106	G	N1-C2-N2	-7.91	109.08	116.20
1	A	170	U	C4-C5-C6	7.91	124.44	119.70
1	A	532	A	C8-N9-C4	7.91	108.96	105.80
1	A	101	A	N1-C2-N3	7.91	133.25	129.30
1	A	510	A	N9-C4-C5	7.91	108.96	105.80
1	A	1378	C	C4-C5-C6	7.90	121.35	117.40
1	A	658	G	C8-N9-C4	7.90	109.56	106.40
1	A	673	G	N3-C4-N9	-7.90	121.26	126.00
1	A	1079	G	C4-C5-C6	7.90	123.54	118.80
1	A	67	C	C5-C6-N1	-7.90	117.05	121.00
1	A	702	A	O5'-P-OP2	-7.90	98.59	105.70
1	A	818	G	OP2-P-O3'	7.90	122.57	105.20
1	A	1257	U	N1-C2-O2	7.89	128.33	122.80
1	A	675	A	N1-C2-N3	7.89	133.24	129.30
1	A	295	C	N1-C2-O2	7.89	123.63	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	G	N1-C6-O6	7.89	124.63	119.90
1	A	1533	C	C6-N1-C2	-7.88	117.15	120.30
5	E	63	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	283	C	C2-N1-C1'	7.88	127.47	118.80
1	A	438	G	N9-C4-C5	7.88	108.55	105.40
1	A	1410	G	C2-N3-C4	7.88	115.84	111.90
1	A	589	C	N3-C4-C5	-7.88	118.75	121.90
1	A	657	G	N1-C6-O6	7.88	124.63	119.90
1	A	1290	G	C2-N3-C4	-7.88	107.96	111.90
1	A	889	A	C4-C5-N7	-7.87	106.76	110.70
1	A	326	G	OP2-P-O3'	7.87	122.51	105.20
1	A	67	C	C6-N1-C2	7.87	123.45	120.30
1	A	1030	C	N1-C2-O2	7.86	123.62	118.90
1	A	1076	C	C6-N1-C2	-7.86	117.16	120.30
1	A	173	U	N1-C2-O2	7.86	128.30	122.80
1	A	374	A	N1-C6-N6	7.86	123.32	118.60
1	A	815	A	OP1-P-OP2	-7.86	107.81	119.60
1	A	380	G	O5'-P-OP2	-7.86	98.63	105.70
1	A	813	U	N3-C4-C5	7.86	119.32	114.60
1	A	1336	C	C2-N3-C4	7.86	123.83	119.90
1	A	1124	G	N3-C4-C5	-7.86	124.67	128.60
1	A	888	G	N3-C4-C5	-7.86	124.67	128.60
1	A	333	G	C4-C5-N7	7.86	113.94	110.80
1	A	492	G	C8-N9-C4	-7.85	103.26	106.40
1	A	713	G	N1-C6-O6	-7.85	115.19	119.90
1	A	562	C	C4-C5-C6	7.85	121.33	117.40
1	A	764	C	C2-N1-C1'	7.85	127.43	118.80
1	A	6	G	C4-C5-C6	7.85	123.51	118.80
1	A	291	C	N3-C4-N4	7.85	123.49	118.00
1	A	444	C	C6-N1-C2	-7.85	117.16	120.30
1	A	1303	C	N3-C2-O2	-7.85	116.41	121.90
1	A	22	G	N7-C8-N9	7.84	117.02	113.10
1	A	363	A	N9-C4-C5	-7.84	102.66	105.80
1	A	1053	G	N1-C2-N2	7.84	123.25	116.20
1	A	448	A	C5-N7-C8	-7.84	99.98	103.90
1	A	127	G	C2-N3-C4	-7.83	107.98	111.90
1	A	285	G	N9-C4-C5	-7.83	102.27	105.40
1	A	1333	A	N1-C2-N3	7.83	133.22	129.30
20	T	20	LEU	CA-CB-CG	-7.83	97.28	115.30
1	A	1104	G	N1-C2-N2	-7.83	109.15	116.20
1	A	190(E)	U	N3-C2-O2	-7.83	116.72	122.20
1	A	484	G	C6-C5-N7	-7.83	125.70	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1462	G	C8-N9-C4	7.83	109.53	106.40
1	A	60	A	C5-C6-N1	-7.83	113.79	117.70
1	A	336	C	C5-C4-N4	-7.83	114.72	120.20
1	A	1043	C	C6-N1-C2	-7.83	117.17	120.30
1	A	25	C	O5'-P-OP2	-7.82	98.66	105.70
1	A	420	U	O5'-P-OP1	-7.82	98.66	105.70
1	A	919	A	P-O3'-C3'	7.82	129.08	119.70
1	A	643	C	C6-N1-C2	7.81	123.43	120.30
1	A	109	A	N1-C2-N3	7.81	133.20	129.30
1	A	419	C	C6-N1-C2	-7.81	117.18	120.30
1	A	1185	G	N7-C8-N9	7.80	117.00	113.10
1	A	490	G	N3-C4-N9	7.80	130.68	126.00
1	A	423	G	C4-C5-N7	7.80	113.92	110.80
1	A	1258	G	N3-C4-C5	-7.80	124.70	128.60
1	A	1279	A	N7-C8-N9	7.80	117.70	113.80
1	A	741	G	C4-C5-N7	-7.80	107.68	110.80
1	A	907	A	O5'-P-OP2	-7.80	98.68	105.70
1	A	680	C	N3-C4-C5	-7.79	118.78	121.90
1	A	1139	G	N1-C6-O6	-7.79	115.22	119.90
1	A	1512	U	N1-C2-N3	7.79	119.58	114.90
1	A	408	A	C4-C5-C6	7.79	120.90	117.00
1	A	44	G	C6-C5-N7	-7.79	125.73	130.40
1	A	1352	C	N3-C4-C5	-7.79	118.78	121.90
1	A	1502	A	OP2-P-O3'	7.79	122.34	105.20
1	A	10	A	C5-N7-C8	7.79	107.79	103.90
1	A	147	G	C5-C6-O6	-7.79	123.93	128.60
1	A	448	A	N3-C4-C5	7.79	132.25	126.80
1	A	822	C	OP2-P-O3'	7.79	122.34	105.20
1	A	698	G	N3-C2-N2	-7.79	114.45	119.90
1	A	1452	C	C6-N1-C1'	-7.79	111.46	120.80
1	A	134	A	C2-N3-C4	-7.78	106.71	110.60
1	A	220	G	C6-C5-N7	-7.78	125.73	130.40
1	A	1156	G	C4-C5-N7	-7.78	107.69	110.80
1	A	1350	A	O5'-P-OP2	-7.78	98.70	105.70
1	A	147	G	N3-C2-N2	-7.78	114.45	119.90
1	A	897	C	C5-C4-N4	-7.78	114.75	120.20
1	A	1149	C	C6-N1-C2	-7.77	117.19	120.30
1	A	22	G	C5-C6-N1	-7.77	107.61	111.50
1	A	398	C	N3-C4-C5	7.77	125.01	121.90
1	A	1112	C	N1-C2-O2	-7.77	114.24	118.90
1	A	379	C	C4-C5-C6	7.77	121.28	117.40
1	A	865	A	C5-C6-N1	-7.77	113.82	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	807	A	N1-C6-N6	7.77	123.26	118.60
1	A	225	C	O5'-P-OP2	-7.76	98.71	105.70
1	A	532	A	N7-C8-N9	-7.76	109.92	113.80
1	A	22	G	N1-C2-N3	7.76	128.56	123.90
1	A	74	C	O5'-P-OP1	7.76	120.01	110.70
1	A	312	C	N1-C2-N3	-7.76	113.77	119.20
1	A	356	A	OP1-P-OP2	7.76	131.24	119.60
1	A	1417	G	C5-C6-N1	-7.76	107.62	111.50
1	A	789	U	O5'-P-OP1	7.76	120.01	110.70
1	A	236	G	C5-C6-O6	7.75	133.25	128.60
1	A	1310	G	C5-C6-N1	-7.74	107.63	111.50
1	A	1069	C	N3-C4-N4	7.74	123.42	118.00
1	A	231	G	N3-C4-C5	7.74	132.47	128.60
1	A	687	A	OP2-P-O3'	-7.74	88.18	105.20
1	A	791	G	C5-C6-N1	-7.74	107.63	111.50
1	A	1339	A	C5-C6-N1	7.74	121.57	117.70
1	A	1543	C	N1-C2-O2	-7.73	114.26	118.90
1	A	1392	G	N1-C2-N2	-7.73	109.24	116.20
1	A	1393	U	N3-C4-C5	-7.73	109.96	114.60
1	A	862	C	C6-N1-C2	7.73	123.39	120.30
1	A	12	U	N1-C2-N3	7.72	119.53	114.90
1	A	760	G	N3-C2-N2	-7.72	114.49	119.90
1	A	787	A	C4-C5-C6	7.72	120.86	117.00
1	A	811	C	N3-C4-C5	7.72	124.99	121.90
1	A	507	C	C6-N1-C2	7.72	123.39	120.30
1	A	273	A	N1-C6-N6	-7.72	113.97	118.60
1	A	133	U	C5-C6-N1	-7.72	118.84	122.70
1	A	911	U	N3-C2-O2	-7.71	116.80	122.20
1	A	853	G	N1-C2-N3	-7.71	119.27	123.90
1	A	1065	U	P-O3'-C3'	7.71	128.96	119.70
1	A	199	G	N1-C2-N3	7.71	128.53	123.90
1	A	918	A	C6-N1-C2	-7.71	113.97	118.60
1	A	738	C	C5-C4-N4	-7.71	114.80	120.20
1	A	1227	A	N7-C8-N9	7.71	117.66	113.80
1	A	567	G	C5-C6-N1	-7.71	107.65	111.50
1	A	761	G	C5-N7-C8	-7.71	100.45	104.30
1	A	1500	A	O5'-P-OP2	7.71	119.95	110.70
1	A	729	A	OP2-P-O3'	-7.70	88.25	105.20
1	A	913	A	C5-C6-N6	7.70	129.86	123.70
1	A	1151	A	O5'-P-OP2	-7.70	98.77	105.70
1	A	602	A	C8-N9-C4	-7.70	102.72	105.80
1	A	5	U	N3-C4-C5	-7.70	109.98	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	G	C2-N3-C4	-7.70	108.05	111.90
1	A	662	G	C4-C5-C6	7.70	123.42	118.80
1	A	1279	A	C4-C5-N7	7.70	114.55	110.70
1	A	42	G	N3-C2-N2	-7.69	114.52	119.90
1	A	829	G	O5'-P-OP2	-7.69	98.78	105.70
1	A	44	G	O5'-P-OP1	-7.69	98.78	105.70
1	A	1130	A	O5'-P-OP2	-7.69	98.78	105.70
1	A	442	C	C6-N1-C2	7.69	123.37	120.30
1	A	1341	U	C5-C4-O4	7.69	130.51	125.90
1	A	814	A	N1-C2-N3	7.68	133.14	129.30
1	A	289	G	C4-N9-C1'	7.68	136.48	126.50
1	A	980	C	O5'-P-OP2	7.68	119.92	110.70
1	A	319	G	N1-C6-O6	7.67	124.50	119.90
1	A	383	A	N9-C4-C5	7.67	108.87	105.80
1	A	833	U	N1-C2-N3	7.67	119.50	114.90
1	A	945	G	C5-N7-C8	-7.67	100.46	104.30
1	A	1533	C	N3-C2-O2	-7.67	116.53	121.90
1	A	1376	U	C6-N1-C2	-7.67	116.40	121.00
1	A	702	A	C8-N9-C4	7.67	108.87	105.80
1	A	1399	C	C4-C5-C6	7.67	121.23	117.40
1	A	307	C	C4-C5-C6	-7.66	113.57	117.40
1	A	811	C	C5-C6-N1	-7.66	117.17	121.00
1	A	1093	A	C8-N9-C4	-7.66	102.73	105.80
1	A	886	G	C5-C6-N1	-7.66	107.67	111.50
1	A	1525	G	N3-C4-C5	-7.66	124.77	128.60
1	A	1532	U	C5-C4-O4	-7.66	121.30	125.90
1	A	293	G	C2-N3-C4	-7.66	108.07	111.90
1	A	598	U	N3-C4-O4	7.66	124.76	119.40
1	A	387	U	N3-C4-C5	-7.66	110.01	114.60
1	A	329	A	C2-N3-C4	-7.65	106.78	110.60
1	A	1377	A	C5-C6-N6	7.65	129.82	123.70
1	A	1198	G	N1-C2-N2	-7.65	109.32	116.20
1	A	1342	C	N3-C2-O2	7.65	127.25	121.90
1	A	225	C	C4-C5-C6	7.65	121.22	117.40
1	A	889	A	O5'-P-OP2	-7.65	98.82	105.70
1	A	55	A	C4-C5-N7	-7.64	106.88	110.70
1	A	325	A	O5'-P-OP1	-7.64	98.82	105.70
1	A	344	A	N7-C8-N9	7.64	117.62	113.80
1	A	880	C	N3-C4-C5	7.64	124.96	121.90
19	S	81	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	37	U	N3-C2-O2	-7.64	116.85	122.20
1	A	108	G	N3-C2-N2	-7.64	114.55	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	G	N3-C4-C5	-7.64	124.78	128.60
1	A	778	G	C4-C5-C6	7.64	123.38	118.80
1	A	856	C	C5-C4-N4	-7.64	114.86	120.20
1	A	1405	G	N1-C2-N3	7.64	128.48	123.90
1	A	449	C	N1-C2-O2	-7.63	114.32	118.90
1	A	1234	C	C6-N1-C2	7.63	123.35	120.30
1	A	1486	G	C8-N9-C4	7.63	109.45	106.40
1	A	1491	G	N3-C4-N9	7.63	130.58	126.00
1	A	832	C	N3-C4-C5	-7.63	118.85	121.90
1	A	1502	A	N9-C4-C5	-7.63	102.75	105.80
1	A	832	C	OP2-P-O3'	7.63	121.98	105.20
1	A	115	G	P-O3'-C3'	7.63	128.85	119.70
1	A	965	A	O5'-P-OP2	-7.63	98.84	105.70
1	A	780	A	C2-N3-C4	7.62	114.41	110.60
1	A	352	C	N1-C2-O2	-7.62	114.33	118.90
1	A	474	G	C5-C6-N1	-7.62	107.69	111.50
1	A	982	U	C4-C5-C6	7.62	124.27	119.70
1	A	686	U	C5-C4-O4	7.62	130.47	125.90
1	A	885	G	OP1-P-O3'	-7.62	88.44	105.20
1	A	1249	C	C4-C5-C6	7.62	121.21	117.40
1	A	430	A	N1-C6-N6	7.62	123.17	118.60
1	A	607	A	C5-C6-N1	-7.62	113.89	117.70
1	A	1045	C	N3-C4-C5	7.61	124.94	121.90
1	A	601	C	C5-C6-N1	-7.61	117.19	121.00
1	A	610	G	C5-N7-C8	-7.61	100.50	104.30
1	A	677	U	N1-C2-N3	7.61	119.47	114.90
1	A	1515[A]	C	C6-N1-C2	7.61	123.34	120.30
1	A	1515[B]	C	C6-N1-C2	7.61	123.34	120.30
1	A	610	G	O5'-P-OP1	-7.61	98.86	105.70
1	A	44	G	N1-C2-N2	-7.60	109.36	116.20
1	A	735	C	C6-N1-C2	7.60	123.34	120.30
1	A	1180	A	C2-N3-C4	-7.60	106.80	110.60
1	A	1222	G	N3-C2-N2	-7.60	114.58	119.90
1	A	1513	A	C4-N9-C1'	-7.60	112.62	126.30
1	A	1531	A	C4-C5-N7	7.59	114.50	110.70
1	A	354	G	N1-C6-O6	7.59	124.45	119.90
1	A	1412	C	C6-N1-C2	7.59	123.34	120.30
1	A	1210	C	C6-N1-C2	7.59	123.34	120.30
1	A	880	C	N3-C2-O2	-7.59	116.59	121.90
1	A	1350	A	C2-N3-C4	7.59	114.39	110.60
1	A	235	C	N3-C2-O2	-7.58	116.59	121.90
1	A	262	A	N3-C4-C5	7.58	132.11	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1235	U	N1-C2-O2	-7.58	117.49	122.80
1	A	33	A	C8-N9-C4	7.58	108.83	105.80
1	A	451	A	C2-N3-C4	-7.58	106.81	110.60
1	A	934	C	O5'-P-OP1	7.58	119.79	110.70
1	A	946	A	C6-N1-C2	-7.58	114.05	118.60
1	A	884	U	C2-N3-C4	-7.58	122.45	127.00
1	A	1054	C	C5-C4-N4	-7.58	114.90	120.20
1	A	308	C	N3-C2-O2	7.57	127.20	121.90
1	A	1433	A	OP2-P-O3'	7.57	121.86	105.20
1	A	983	A	C8-N9-C4	-7.57	102.77	105.80
1	A	1306	A	O5'-P-OP2	-7.57	98.89	105.70
1	A	530	G	C6-C5-N7	-7.57	125.86	130.40
1	A	267	C	C2-N3-C4	-7.57	116.12	119.90
1	A	1531	A	C5-N7-C8	-7.56	100.12	103.90
1	A	1359	C	O5'-P-OP1	-7.56	98.89	105.70
1	A	810	C	C2-N3-C4	-7.56	116.12	119.90
1	A	981	U	N3-C4-O4	7.56	124.69	119.40
1	A	955	U	O5'-P-OP2	7.55	119.77	110.70
1	A	669	U	N1-C2-N3	-7.55	110.37	114.90
1	A	593	G	C6-C5-N7	-7.55	125.87	130.40
1	A	1336	C	C6-N1-C1'	-7.55	111.74	120.80
1	A	230	G	C5-C6-N1	-7.55	107.73	111.50
1	A	608	A	C5-C6-N1	7.54	121.47	117.70
1	A	851	G	N3-C2-N2	-7.54	114.62	119.90
1	A	1137	C	C6-N1-C2	-7.54	117.28	120.30
1	A	1442	G	N3-C4-C5	-7.54	124.83	128.60
1	A	746	A	N9-C4-C5	7.54	108.82	105.80
1	A	762	C	N1-C2-N3	7.54	124.48	119.20
1	A	532	A	N1-C6-N6	-7.54	114.08	118.60
1	A	753	A	C4-C5-N7	-7.54	106.93	110.70
1	A	1515[A]	C	O5'-P-OP1	7.54	119.75	110.70
1	A	1515[B]	C	O5'-P-OP1	7.54	119.75	110.70
5	E	53	LEU	CA-CB-CG	-7.54	97.97	115.30
1	A	635	G	C6-C5-N7	-7.54	125.88	130.40
1	A	851	G	N1-C2-N3	7.54	128.42	123.90
1	A	1328	C	C6-N1-C2	7.54	123.31	120.30
1	A	681	C	C6-N1-C2	7.53	123.31	120.30
1	A	546	G	C6-N1-C2	-7.53	120.58	125.10
1	A	29	G	OP1-P-OP2	7.53	130.89	119.60
1	A	124	G	C2-N3-C4	-7.53	108.14	111.90
1	A	303	A	C2-N3-C4	7.53	114.36	110.60
1	A	486	U	N1-C2-N3	7.53	119.42	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	888	G	N7-C8-N9	7.53	116.86	113.10
1	A	915	A	OP2-P-O3'	7.53	121.75	105.20
1	A	1087	G	C5-C6-N1	-7.53	107.74	111.50
1	A	129(A)	G	P-O3'-C3'	7.52	128.73	119.70
1	A	1390	U	C4-C5-C6	7.52	124.21	119.70
1	A	692	U	N3-C2-O2	-7.52	116.93	122.20
1	A	198	G	C6-N1-C2	-7.52	120.59	125.10
1	A	793	U	N3-C4-O4	-7.52	114.14	119.40
1	A	1003(A)	G	N7-C8-N9	7.52	116.86	113.10
1	A	1067	A	C5-C6-N1	-7.52	113.94	117.70
1	A	1218	C	C2-N3-C4	-7.52	116.14	119.90
1	A	361	G	C8-N9-C4	7.52	109.41	106.40
1	A	388	G	N1-C6-O6	7.52	124.41	119.90
1	A	927	G	C6-N1-C2	7.52	129.61	125.10
1	A	1345	U	N3-C4-C5	-7.52	110.09	114.60
1	A	964	A	C2-N3-C4	-7.52	106.84	110.60
1	A	1505	G	P-O3'-C3'	7.52	128.72	119.70
1	A	793	U	OP1-P-O3'	7.51	121.73	105.20
1	A	1482	G	C5-C6-O6	7.51	133.11	128.60
1	A	230	G	N9-C4-C5	-7.51	102.40	105.40
1	A	127	G	C4-C5-C6	7.51	123.31	118.80
1	A	567	G	N1-C6-O6	7.51	124.41	119.90
1	A	962	C	C5-C6-N1	-7.51	117.25	121.00
1	A	1508	G	C4-C5-N7	7.51	113.80	110.80
1	A	694	A	C5-C6-N1	-7.50	113.95	117.70
1	A	769	G	O5'-P-OP2	-7.50	98.95	105.70
1	A	1168	A	C5-C6-N1	7.50	121.45	117.70
1	A	827	U	C4-C5-C6	7.50	124.20	119.70
1	A	578	C	N3-C4-N4	-7.50	112.75	118.00
1	A	993	G	N3-C4-C5	-7.50	124.85	128.60
1	A	244	U	C4-C5-C6	7.50	124.20	119.70
1	A	750	G	N9-C4-C5	-7.50	102.40	105.40
1	A	913	A	N9-C4-C5	7.50	108.80	105.80
1	A	1235	U	C4-C5-C6	7.50	124.20	119.70
1	A	687	A	OP1-P-O3'	7.49	121.68	105.20
1	A	561	U	C5-C4-O4	-7.49	121.41	125.90
1	A	310	G	O5'-P-OP2	-7.49	98.96	105.70
1	A	356	A	O5'-P-OP1	-7.49	98.96	105.70
1	A	841	U	C5-C6-N1	7.49	126.44	122.70
1	A	1087	G	O5'-P-OP1	7.49	119.68	110.70
1	A	104	G	C4-C5-C6	7.48	123.29	118.80
1	A	233	C	C5-C6-N1	-7.48	117.26	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	G	O5'-P-OP2	-7.48	98.97	105.70
1	A	890	G	C5-N7-C8	7.48	108.04	104.30
1	A	797	C	C5-C6-N1	-7.48	117.26	121.00
1	A	927	G	O5'-P-OP1	-7.48	98.97	105.70
11	K	48	ILE	CB-CA-C	-7.48	96.65	111.60
17	Q	25	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	1389	C	C2-N3-C4	-7.47	116.16	119.90
1	A	396	G	C8-N9-C4	-7.47	103.41	106.40
1	A	975	A	C6-C5-N7	-7.47	127.07	132.30
1	A	125	U	N3-C4-O4	7.47	124.63	119.40
1	A	915	A	C2-N3-C4	-7.47	106.87	110.60
1	A	378	G	C4-C5-N7	7.47	113.79	110.80
1	A	417	C	N1-C2-O2	-7.46	114.42	118.90
1	A	818	G	OP1-P-OP2	7.46	130.79	119.60
1	A	111	G	N7-C8-N9	7.46	116.83	113.10
1	A	530	G	N1-C6-O6	7.46	124.38	119.90
1	A	335	C	N3-C2-O2	-7.46	116.68	121.90
1	A	106	C	O5'-P-OP2	-7.46	98.99	105.70
1	A	294	U	O5'-P-OP2	7.46	119.65	110.70
1	A	699	C	N3-C4-C5	7.46	124.88	121.90
1	A	922	G	OP1-P-O3'	7.46	121.61	105.20
1	A	1189	C	C2-N1-C1'	7.46	127.00	118.80
1	A	535	A	O5'-P-OP2	-7.46	98.99	105.70
1	A	881	G	C8-N9-C4	7.46	109.38	106.40
1	A	462	G	N3-C4-C5	-7.46	124.87	128.60
1	A	1504	G	C8-N9-C4	-7.46	103.42	106.40
1	A	101	A	N7-C8-N9	7.45	117.53	113.80
1	A	1388	C	N3-C4-N4	-7.45	112.78	118.00
1	A	21	G	N3-C2-N2	7.45	125.11	119.90
1	A	762	C	N3-C2-O2	-7.45	116.69	121.90
1	A	531	U	N1-C2-O2	-7.45	117.59	122.80
1	A	1368	G	C8-N9-C1'	-7.45	117.32	127.00
1	A	532	A	C6-C5-N7	7.44	137.51	132.30
1	A	647	C	C6-N1-C2	-7.44	117.33	120.30
1	A	285	G	N1-C2-N3	7.43	128.36	123.90
1	A	658	G	C5-C6-N1	-7.43	107.78	111.50
1	A	1357	A	C2-N3-C4	-7.43	106.88	110.60
1	A	336	C	N3-C2-O2	7.43	127.10	121.90
1	A	1257	U	C6-N1-C1'	-7.43	110.79	121.20
1	A	913	A	OP1-P-O3'	7.43	121.54	105.20
1	A	584	G	C5-C6-O6	7.43	133.06	128.60
1	A	713	G	C5-N7-C8	7.43	108.01	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	831	U	C6-N1-C2	7.42	125.45	121.00
1	A	1126	U	C6-N1-C1'	7.42	131.59	121.20
1	A	1225	A	OP1-P-OP2	7.42	130.74	119.60
1	A	790	A	C6-C5-N7	-7.42	127.10	132.30
1	A	1346	A	N1-C2-N3	7.42	133.01	129.30
1	A	248	C	C2-N1-C1'	-7.42	110.64	118.80
1	A	1162	C	C6-N1-C2	7.42	123.27	120.30
1	A	133	U	C5-C4-O4	7.42	130.35	125.90
1	A	930	C	C4-C5-C6	7.42	121.11	117.40
1	A	1390	U	N1-C2-O2	-7.42	117.61	122.80
1	A	1527	C	C4-C5-C6	7.41	121.11	117.40
1	A	44	G	OP1-P-OP2	7.41	130.72	119.60
1	A	130	A	C4-C5-N7	7.41	114.41	110.70
1	A	486	U	N1-C2-O2	-7.41	117.61	122.80
1	A	1062	U	OP2-P-O3'	7.41	121.50	105.20
1	A	1064	G	C8-N9-C4	-7.41	103.44	106.40
1	A	769	G	C6-C5-N7	-7.41	125.95	130.40
1	A	281	G	N1-C2-N3	7.41	128.34	123.90
1	A	566	G	C8-N9-C4	7.41	109.36	106.40
1	A	1333	A	C6-N1-C2	-7.40	114.16	118.60
1	A	1453	G	N3-C4-N9	7.40	130.44	126.00
1	A	390	C	C5-C4-N4	-7.40	115.02	120.20
1	A	1057	G	C6-N1-C2	-7.40	120.66	125.10
1	A	193	C	OP2-P-O3'	7.40	121.48	105.20
1	A	755	G	N7-C8-N9	7.40	116.80	113.10
1	A	763	G	C5-C6-O6	-7.40	124.16	128.60
1	A	1287	A	C4-N9-C1'	7.40	139.61	126.30
1	A	1405	G	C2-N3-C4	-7.40	108.20	111.90
1	A	1521	G	C5-C6-O6	-7.40	124.16	128.60
1	A	1159	U	C2-N1-C1'	-7.39	108.83	117.70
1	A	1299	A	C6-C5-N7	-7.39	127.12	132.30
1	A	42	G	C4-C5-N7	-7.39	107.84	110.80
1	A	882	C	O5'-P-OP2	-7.39	99.05	105.70
1	A	677	U	C5-C4-O4	7.39	130.33	125.90
1	A	360	A	C5-N7-C8	-7.39	100.21	103.90
1	A	794	A	C5-C6-N1	7.39	121.39	117.70
1	A	879	C	N1-C2-O2	-7.38	114.47	118.90
1	A	673	G	C6-C5-N7	7.38	134.83	130.40
1	A	64	G	C4-N9-C1'	7.38	136.09	126.50
1	A	439	A	N1-C2-N3	7.38	132.99	129.30
1	A	1171	G	C8-N9-C4	-7.38	103.45	106.40
1	A	374	A	N1-C2-N3	7.38	132.99	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	C	C2-N3-C4	7.38	123.59	119.90
1	A	1544	U	N3-C4-O4	-7.38	114.23	119.40
1	A	1050	G	C4-C5-C6	7.38	123.22	118.80
1	A	1056	U	O5'-P-OP2	-7.38	99.06	105.70
1	A	1409	C	C4-C5-C6	-7.37	113.71	117.40
1	A	194	C	C6-N1-C2	7.37	123.25	120.30
1	A	266	G	C6-N1-C2	7.37	129.52	125.10
1	A	1290	G	C4-C5-C6	7.37	123.22	118.80
1	A	1494	G	C4-C5-N7	-7.37	107.85	110.80
1	A	64	G	C8-N9-C1'	-7.37	117.42	127.00
1	A	567	G	C8-N9-C4	7.37	109.35	106.40
1	A	922	G	N1-C2-N3	7.37	128.32	123.90
1	A	572	A	C6-C5-N7	7.36	137.46	132.30
1	A	280	C	N3-C4-C5	-7.36	118.95	121.90
12	L	52	LEU	CA-CB-CG	-7.36	98.37	115.30
1	A	101	A	N9-C4-C5	7.36	108.74	105.80
1	A	112	G	OP1-P-OP2	7.36	130.64	119.60
1	A	408	A	N3-C4-C5	-7.36	121.65	126.80
1	A	942	G	OP2-P-O3'	7.36	121.39	105.20
1	A	1120	G	C8-N9-C4	-7.36	103.46	106.40
1	A	484	G	C4-C5-C6	7.35	123.21	118.80
1	A	693	G	N1-C2-N3	7.35	128.31	123.90
1	A	1074	G	N1-C2-N3	-7.35	119.49	123.90
4	D	76	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	336	C	N1-C2-N3	-7.35	114.06	119.20
1	A	1179	A	C5-C6-N6	7.35	129.58	123.70
1	A	651	C	N3-C2-O2	7.35	127.04	121.90
1	A	1075	C	C5-C4-N4	7.35	125.34	120.20
1	A	1229	A	O5'-P-OP1	7.34	119.51	110.70
1	A	1506	U	C6-N1-C1'	-7.34	110.92	121.20
1	A	277	C	C2-N1-C1'	-7.34	110.72	118.80
1	A	304	U	N3-C4-C5	7.34	119.01	114.60
1	A	400	C	C4-C5-C6	-7.34	113.73	117.40
1	A	239	U	N3-C4-O4	7.34	124.54	119.40
1	A	1156	G	C5-C6-O6	7.34	133.00	128.60
1	A	479	C	N1-C2-O2	7.34	123.30	118.90
1	A	667	G	C2-N3-C4	-7.34	108.23	111.90
1	A	703	G	C5-N7-C8	7.34	107.97	104.30
1	A	1167	A	N3-C4-N9	-7.34	121.53	127.40
1	A	1345	U	N3-C4-O4	7.34	124.54	119.40
1	A	1531	A	C6-C5-N7	-7.34	127.16	132.30
1	A	291	C	C5-C4-N4	-7.33	115.07	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	A	C6-C5-N7	-7.33	127.17	132.30
1	A	864	A	OP1-P-O3'	7.33	121.33	105.20
1	A	672	U	N3-C4-O4	-7.33	114.27	119.40
1	A	721	G	C5-N7-C8	7.33	107.97	104.30
1	A	364	A	N1-C6-N6	7.33	123.00	118.60
1	A	69	G	C8-N9-C4	7.33	109.33	106.40
15	O	34	LEU	CA-CB-CG	-7.32	98.45	115.30
1	A	676	A	O5'-P-OP2	-7.32	99.11	105.70
1	A	1211	U	C5-C6-N1	-7.32	119.04	122.70
1	A	297	G	C5-C6-O6	7.32	132.99	128.60
1	A	833	U	O5'-P-OP1	7.32	119.48	110.70
1	A	841	U	C6-N1-C2	-7.31	116.61	121.00
1	A	1215	G	C6-C5-N7	-7.31	126.01	130.40
1	A	45	U	C5-C4-O4	7.31	130.28	125.90
15	O	34	LEU	CB-CG-CD1	7.31	123.42	111.00
1	A	543	C	N3-C2-O2	-7.31	116.79	121.90
1	A	750	G	C5-C6-O6	-7.31	124.22	128.60
1	A	1401	G	N3-C2-N2	7.31	125.01	119.90
1	A	583	A	N1-C6-N6	7.30	122.98	118.60
1	A	1521	G	N3-C4-N9	7.30	130.38	126.00
1	A	133	U	C4-C5-C6	7.30	124.08	119.70
1	A	284	G	OP1-P-O3'	-7.30	89.14	105.20
1	A	446	G	C8-N9-C4	-7.30	103.48	106.40
1	A	572	A	C5-C6-N6	7.30	129.54	123.70
1	A	1011	G	C8-N9-C4	-7.30	103.48	106.40
1	A	1204	A	C8-N9-C4	7.30	108.72	105.80
1	A	64	G	C6-C5-N7	-7.30	126.02	130.40
1	A	198	G	C4-C5-N7	-7.29	107.88	110.80
4	D	76	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	744	C	N3-C2-O2	7.29	127.00	121.90
1	A	805	C	C4-C5-C6	-7.29	113.75	117.40
1	A	1030(C)	G	O5'-P-OP2	-7.29	99.14	105.70
3	C	178	LEU	CA-CB-CG	7.29	132.07	115.30
1	A	895	G	C5-C6-N1	7.29	115.14	111.50
1	A	1128	C	O5'-P-OP2	-7.29	99.14	105.70
1	A	732	C	N1-C2-O2	7.29	123.27	118.90
1	A	1199	U	C6-N1-C2	7.29	125.37	121.00
1	A	1438	G	C6-C5-N7	-7.29	126.03	130.40
1	A	1497	G	N1-C2-N3	7.29	128.27	123.90
1	A	1097	C	N3-C4-C5	7.29	124.81	121.90
1	A	486	U	O5'-P-OP2	-7.29	99.14	105.70
1	A	855	G	N3-C4-C5	7.29	132.24	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	726	C	OP1-P-O3'	7.28	121.22	105.20
1	A	1282	C	C6-N1-C2	7.28	123.21	120.30
1	A	1392	G	N1-C2-N3	7.28	128.27	123.90
1	A	544	G	C2-N3-C4	-7.28	108.26	111.90
1	A	711	G	N7-C8-N9	7.28	116.74	113.10
1	A	1310	G	C4-C5-C6	7.28	123.17	118.80
1	A	113	G	C6-C5-N7	-7.28	126.03	130.40
1	A	581	G	C4-C5-N7	7.28	113.71	110.80
1	A	1414	U	OP1-P-O3'	7.28	121.21	105.20
1	A	196	A	C4-C5-C6	-7.27	113.36	117.00
1	A	398	C	C2-N1-C1'	-7.27	110.80	118.80
1	A	938	A	N1-C6-N6	-7.27	114.24	118.60
1	A	403	C	C5-C6-N1	-7.27	117.37	121.00
1	A	560	U	C5-C6-N1	-7.27	119.07	122.70
1	A	657	G	C5-C6-O6	-7.27	124.24	128.60
1	A	685	G	C8-N9-C1'	7.27	136.45	127.00
1	A	775	G	N1-C6-O6	-7.27	115.54	119.90
1	A	859	A	N1-C2-N3	7.27	132.93	129.30
1	A	1079	G	N1-C2-N2	-7.27	109.66	116.20
1	A	1366	C	C4-C5-C6	7.26	121.03	117.40
1	A	796	C	N1-C2-N3	-7.26	114.12	119.20
1	A	1410	G	N1-C6-O6	-7.26	115.54	119.90
1	A	780	A	C6-N1-C2	-7.26	114.24	118.60
1	A	733	A	C6-N1-C2	-7.26	114.25	118.60
1	A	1342	C	C2-N1-C1'	-7.26	110.82	118.80
1	A	1116	C	C5-C6-N1	-7.26	117.37	121.00
1	A	415	A	OP1-P-O3'	7.25	121.16	105.20
12	L	81	SER	N-CA-C	-7.25	91.41	111.00
1	A	599	C	C5-C6-N1	-7.25	117.37	121.00
1	A	1175	G	C2-N3-C4	-7.25	108.27	111.90
6	F	86	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	A	1201	A	P-O3'-C3'	7.25	128.40	119.70
1	A	630	G	N1-C6-O6	-7.25	115.55	119.90
1	A	670	G	C4-N9-C1'	7.25	135.92	126.50
1	A	319	G	C8-N9-C4	-7.25	103.50	106.40
1	A	1095	U	C6-N1-C2	-7.25	116.65	121.00
1	A	1310	G	C6-C5-N7	-7.24	126.06	130.40
1	A	664	G	C5-C6-O6	7.24	132.94	128.60
1	A	1464	G	N1-C6-O6	7.24	124.24	119.90
1	A	715	A	C6-N1-C2	-7.24	114.26	118.60
1	A	1211	U	C5-C4-O4	7.24	130.24	125.90
1	A	1234	C	C2-N3-C4	-7.24	116.28	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	531	U	C4-C5-C6	7.23	124.04	119.70
1	A	982	U	N1-C2-N3	7.23	119.24	114.90
1	A	1128	C	C6-N1-C2	-7.23	117.41	120.30
1	A	266	G	N7-C8-N9	7.23	116.71	113.10
1	A	601	C	C6-N1-C2	7.23	123.19	120.30
1	A	733	A	N1-C6-N6	7.23	122.94	118.60
1	A	907	A	C5-C6-N6	7.23	129.48	123.70
1	A	792	A	C6-C5-N7	-7.23	127.24	132.30
1	A	1414	U	N3-C4-C5	-7.23	110.27	114.60
1	A	1093	A	OP1-P-OP2	7.22	130.44	119.60
1	A	6	G	C4-N9-C1'	7.22	135.89	126.50
1	A	216	G	C4-N9-C1'	-7.22	117.11	126.50
1	A	584	G	OP2-P-O3'	7.22	121.09	105.20
1	A	1244	C	N3-C4-C5	7.22	124.79	121.90
1	A	194	C	N3-C4-C5	7.22	124.79	121.90
1	A	1076	C	N3-C2-O2	-7.22	116.85	121.90
1	A	1079	G	C4-N9-C1'	7.22	135.88	126.50
1	A	23	C	N3-C2-O2	7.22	126.95	121.90
1	A	11	G	N1-C6-O6	-7.21	115.57	119.90
1	A	1513	A	C4-C5-C6	-7.21	113.39	117.00
1	A	1365	G	C5-C6-N1	7.21	115.11	111.50
1	A	180	U	O5'-P-OP2	7.21	119.35	110.70
1	A	382	A	N1-C6-N6	-7.21	114.27	118.60
1	A	800	G	N7-C8-N9	7.21	116.70	113.10
1	A	851	G	C6-C5-N7	-7.21	126.07	130.40
1	A	1086	U	O5'-P-OP2	-7.21	99.21	105.70
1	A	1416	G	N1-C6-O6	7.21	124.23	119.90
1	A	679	C	OP1-P-O3'	-7.21	89.34	105.20
1	A	819	A	C5-N7-C8	-7.21	100.30	103.90
1	A	881	G	N1-C2-N3	7.21	128.22	123.90
1	A	119	A	N1-C2-N3	7.21	132.90	129.30
1	A	1126	U	N1-C2-O2	-7.21	117.76	122.80
1	A	130	A	C6-C5-N7	-7.20	127.26	132.30
1	A	1005	A	N7-C8-N9	7.20	117.40	113.80
1	A	1094	G	N3-C4-N9	7.20	130.32	126.00
1	A	731	G	C5-C6-O6	-7.20	124.28	128.60
1	A	1237	C	C2-N3-C4	-7.20	116.30	119.90
1	A	7	G	C4-C5-N7	7.20	113.68	110.80
1	A	332	G	C4-C5-N7	7.20	113.68	110.80
1	A	1271	G	N9-C4-C5	-7.20	102.52	105.40
1	A	814	A	C2-N3-C4	-7.19	107.00	110.60
1	A	1410	G	C8-N9-C1'	-7.19	117.65	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	G	N3-C2-N2	-7.19	114.87	119.90
1	A	480	U	C4-C5-C6	7.19	124.01	119.70
1	A	769	G	N1-C2-N3	7.19	128.22	123.90
1	A	793	U	N1-C2-N3	7.19	119.21	114.90
1	A	1215	G	C5-C6-O6	-7.19	124.29	128.60
1	A	608	A	C2-N3-C4	7.19	114.19	110.60
1	A	1486	G	N3-C4-C5	-7.19	125.01	128.60
1	A	722	A	C4-C5-C6	7.19	120.59	117.00
1	A	43	C	N1-C2-O2	-7.19	114.59	118.90
1	A	126	G	N1-C2-N3	7.19	128.21	123.90
1	A	532	A	C4-C5-C6	-7.19	113.41	117.00
1	A	587	G	N1-C6-O6	-7.19	115.59	119.90
1	A	752	G	C5-C6-O6	7.19	132.91	128.60
1	A	984	C	N3-C2-O2	-7.18	116.87	121.90
1	A	501	C	C4-C5-C6	7.18	120.99	117.40
1	A	1401	G	N1-C6-O6	-7.18	115.59	119.90
1	A	727	G	C5-C6-O6	7.18	132.91	128.60
1	A	1088	G	N3-C4-N9	7.18	130.31	126.00
1	A	298	A	C5-N7-C8	-7.18	100.31	103.90
1	A	384	G	C5-C6-O6	-7.18	124.29	128.60
1	A	1433	A	OP1-P-O3'	-7.18	89.41	105.20
1	A	1501	C	C5-C6-N1	7.18	124.59	121.00
1	A	761	G	C4-C5-N7	7.18	113.67	110.80
1	A	1376	U	N1-C2-N3	7.18	119.21	114.90
1	A	1434	A	N7-C8-N9	-7.18	110.21	113.80
1	A	929	G	C5-C6-N1	7.18	115.09	111.50
1	A	1157	A	C4-C5-N7	-7.18	107.11	110.70
1	A	1491	G	C5-C6-O6	-7.18	124.29	128.60
1	A	795	C	C5-C6-N1	-7.17	117.41	121.00
1	A	598	U	C6-N1-C2	7.17	125.30	121.00
1	A	885	G	C2-N3-C4	-7.17	108.31	111.90
1	A	1030(B)	C	C5-C6-N1	7.17	124.59	121.00
1	A	617	G	N1-C2-N2	-7.17	109.75	116.20
1	A	111	G	OP1-P-OP2	7.17	130.35	119.60
1	A	1390	U	N3-C4-O4	7.17	124.42	119.40
1	A	53	A	O5'-P-OP2	7.16	119.30	110.70
1	A	908	A	C5-C6-N6	-7.16	117.97	123.70
1	A	1516[A]	G	N9-C4-C5	7.16	108.27	105.40
1	A	1516[B]	G	N9-C4-C5	7.16	108.27	105.40
1	A	61	G	O5'-P-OP2	7.16	119.29	110.70
1	A	649	G	OP2-P-O3'	7.16	120.95	105.20
1	A	1087	G	C4-N9-C1'	7.16	135.81	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	C	N3-C4-C5	7.16	124.76	121.90
1	A	564	C	N3-C4-C5	7.16	124.76	121.90
1	A	811	C	C5-C4-N4	7.16	125.21	120.20
1	A	1053	G	C5-C6-O6	-7.16	124.31	128.60
1	A	1162	C	C2-N1-C1'	-7.16	110.92	118.80
1	A	1167	A	C2-N3-C4	-7.16	107.02	110.60
1	A	1276	G	C6-C5-N7	-7.16	126.11	130.40
1	A	1415	G	N3-C4-N9	7.15	130.29	126.00
1	A	70	G	N9-C4-C5	-7.15	102.54	105.40
1	A	380	G	C4-C5-C6	7.15	123.09	118.80
1	A	558	G	OP1-P-OP2	-7.15	108.87	119.60
1	A	1093	A	C5-C6-N1	7.15	121.28	117.70
4	D	31	CYS	C-N-CA	7.15	139.58	121.70
1	A	437	U	C5-C6-N1	-7.15	119.12	122.70
1	A	834	C	N3-C4-N4	-7.15	113.00	118.00
1	A	945	G	N9-C4-C5	7.15	108.26	105.40
1	A	1248	A	N1-C6-N6	7.15	122.89	118.60
1	A	1143	G	C4-C5-N7	-7.15	107.94	110.80
12	L	102	ARG	NE-CZ-NH1	-7.15	116.73	120.30
1	A	671	G	N3-C4-N9	7.14	130.29	126.00
1	A	884	U	N1-C2-N3	7.14	119.19	114.90
1	A	1005	A	C8-N9-C4	-7.14	102.94	105.80
1	A	425	G	N1-C6-O6	-7.14	115.61	119.90
1	A	535	A	N1-C6-N6	-7.14	114.32	118.60
1	A	509	A	C2'-C3'-O3'	7.14	125.20	109.50
1	A	572	A	C4-C5-N7	-7.13	107.13	110.70
1	A	292	G	C4-C5-N7	-7.13	107.95	110.80
1	A	393	A	N1-C6-N6	7.13	122.88	118.60
1	A	515	G	C5-N7-C8	-7.13	100.73	104.30
1	A	865	A	C2-N3-C4	-7.13	107.03	110.60
1	A	1287	A	C4-C5-N7	7.13	114.27	110.70
1	A	306	G	C2-N3-C4	-7.13	108.33	111.90
1	A	551	U	OP2-P-O3'	7.13	120.89	105.20
1	A	1286	A	O5'-P-OP1	-7.13	99.28	105.70
1	A	664	G	C5-N7-C8	7.13	107.86	104.30
1	A	109	A	C5-N7-C8	-7.13	100.34	103.90
1	A	669	U	C6-N1-C2	7.13	125.28	121.00
1	A	40	C	N3-C2-O2	7.12	126.89	121.90
1	A	953	G	C5-C6-O6	7.12	132.88	128.60
1	A	263	A	N1-C6-N6	7.12	122.87	118.60
1	A	754	C	C6-N1-C2	-7.12	117.45	120.30
1	A	1067	A	C5-C6-N6	7.12	129.40	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	G	N9-C4-C5	7.12	108.25	105.40
1	A	1299	A	N1-C6-N6	7.12	122.87	118.60
1	A	740	U	C6-N1-C2	7.12	125.27	121.00
1	A	1505	G	C2-N3-C4	7.12	115.46	111.90
1	A	776	G	N1-C6-O6	-7.12	115.63	119.90
1	A	248	C	C6-N1-C2	7.12	123.15	120.30
1	A	813	U	OP2-P-O3'	7.12	120.86	105.20
1	A	1249	C	C5-C6-N1	-7.12	117.44	121.00
1	A	1359	C	N3-C4-N4	7.12	122.98	118.00
1	A	462	G	N1-C6-O6	-7.11	115.63	119.90
1	A	559	A	C6-N1-C2	-7.11	114.33	118.60
1	A	709	G	C6-C5-N7	-7.11	126.13	130.40
1	A	810	C	N3-C4-C5	7.11	124.75	121.90
1	A	1374	A	C6-N1-C2	-7.11	114.33	118.60
1	A	135	C	N3-C4-C5	-7.11	119.06	121.90
1	A	670	G	N1-C2-N2	-7.11	109.80	116.20
1	A	1530	G	C6-N1-C2	7.11	129.37	125.10
1	A	132	C	N1-C2-O2	-7.11	114.63	118.90
1	A	780	A	OP1-P-OP2	-7.11	108.93	119.60
1	A	1096	C	C5-C4-N4	-7.11	115.22	120.20
1	A	1341	U	C5-C6-N1	-7.11	119.14	122.70
1	A	62	U	N3-C4-C5	-7.11	110.33	114.60
1	A	1092	A	O5'-P-OP2	-7.11	99.30	105.70
2	B	23	ARG	N-CA-C	-7.11	91.81	111.00
1	A	1093	A	N1-C6-N6	-7.11	114.34	118.60
1	A	549	C	C2-N1-C1'	-7.10	110.99	118.80
1	A	402	G	OP2-P-O3'	7.10	120.82	105.20
1	A	1542	U	N1-C2-N3	-7.10	110.64	114.90
12	L	53	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	740	U	C2-N3-C4	-7.10	122.74	127.00
1	A	791	G	C4-C5-C6	7.10	123.06	118.80
1	A	1168	A	N1-C2-N3	7.10	132.85	129.30
1	A	1310	G	N1-C2-N3	7.10	128.16	123.90
1	A	1320	C	N3-C4-C5	-7.10	119.06	121.90
1	A	10	A	C5-C6-N6	7.10	129.38	123.70
1	A	597	G	C5-C6-N1	-7.10	107.95	111.50
1	A	1410	G	N3-C4-C5	-7.10	125.05	128.60
1	A	1034	G	N7-C8-N9	7.09	116.65	113.10
1	A	710	G	C4-C5-C6	7.09	123.05	118.80
1	A	802	A	N1-C2-N3	7.09	132.84	129.30
20	T	13	LEU	CB-CA-C	-7.09	96.73	110.20
1	A	310	G	OP1-P-OP2	7.09	130.23	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	31	LEU	CA-CB-CG	-7.09	99.00	115.30
1	A	540	G	C6-C5-N7	-7.08	126.15	130.40
1	A	557	G	N1-C2-N3	7.08	128.15	123.90
1	A	562	C	O5'-P-OP1	-7.08	99.32	105.70
1	A	865	A	N7-C8-N9	7.08	117.34	113.80
1	A	1092	A	C8-N9-C4	-7.08	102.97	105.80
1	A	1408	A	C4-C5-C6	7.08	120.54	117.00
1	A	299	G	C4-C5-C6	7.08	123.05	118.80
1	A	1211	U	N3-C4-O4	-7.08	114.45	119.40
1	A	1505	G	C4-C5-C6	7.08	123.05	118.80
1	A	55	A	O5'-P-OP1	-7.07	99.33	105.70
1	A	216	G	N1-C6-O6	7.07	124.14	119.90
1	A	750	G	N3-C4-N9	7.07	130.24	126.00
2	B	196	LEU	CB-CG-CD1	-7.07	98.97	111.00
1	A	794	A	C6-N1-C2	-7.07	114.36	118.60
1	A	1105	A	C6-N1-C2	-7.07	114.36	118.60
1	A	1354	C	C6-N1-C2	7.07	123.13	120.30
1	A	514	C	C6-N1-C2	-7.07	117.47	120.30
1	A	1389	C	N3-C4-C5	7.07	124.73	121.90
1	A	881	G	OP2-P-O3'	7.06	120.74	105.20
1	A	1368	G	N3-C4-N9	7.06	130.24	126.00
1	A	833	U	C4-C5-C6	7.06	123.94	119.70
1	A	511	C	N1-C2-O2	-7.06	114.66	118.90
1	A	610	G	N3-C4-N9	-7.06	121.76	126.00
1	A	41	G	O5'-P-OP1	-7.06	99.35	105.70
1	A	134	A	OP2-P-O3'	7.06	120.72	105.20
1	A	914	A	N1-C2-N3	7.06	132.83	129.30
1	A	286	G	C5-C6-O6	-7.05	124.37	128.60
1	A	1416	G	C8-N9-C4	-7.05	103.58	106.40
1	A	1073	U	O5'-P-OP1	-7.05	99.35	105.70
1	A	1499	A	C6-N1-C2	-7.05	114.37	118.60
1	A	904	C	N3-C4-N4	-7.05	113.07	118.00
1	A	1416	G	N3-C4-C5	-7.05	125.08	128.60
1	A	823	G	C5-N7-C8	-7.05	100.78	104.30
1	A	859	A	O5'-P-OP1	-7.05	99.36	105.70
1	A	1515[A]	C	N1-C2-N3	-7.05	114.27	119.20
1	A	1515[B]	C	N1-C2-N3	-7.05	114.27	119.20
1	A	762	C	C5-C6-N1	-7.04	117.48	121.00
1	A	319	G	C4-C5-C6	7.04	123.03	118.80
1	A	474	G	N1-C2-N3	7.04	128.13	123.90
1	A	1030(B)	C	C6-N1-C2	-7.04	117.48	120.30
1	A	61	G	C8-N9-C4	7.04	109.22	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	658	G	C4-C5-C6	7.04	123.02	118.80
1	A	1180	A	C4-C5-N7	7.04	114.22	110.70
1	A	435	C	C5-C6-N1	7.04	124.52	121.00
1	A	724	G	O5'-P-OP2	7.04	119.15	110.70
1	A	736	C	C4-C5-C6	7.04	120.92	117.40
1	A	1094	G	C2-N3-C4	7.04	115.42	111.90
1	A	744	C	C5-C4-N4	-7.04	115.27	120.20
1	A	312	C	C6-N1-C2	7.03	123.11	120.30
1	A	779	C	N3-C4-C5	7.03	124.71	121.90
1	A	1053	G	C8-N9-C4	7.03	109.21	106.40
1	A	803	G	C6-N1-C2	-7.03	120.88	125.10
1	A	417	C	N3-C2-O2	7.03	126.82	121.90
1	A	937	A	N9-C4-C5	7.03	108.61	105.80
1	A	292	G	C4-N9-C1'	7.03	135.63	126.50
1	A	953	G	C8-N9-C1'	-7.03	117.86	127.00
1	A	1377	A	N1-C6-N6	-7.03	114.38	118.60
1	A	6	G	C4-C5-N7	-7.03	107.99	110.80
1	A	1526	G	C6-N1-C2	-7.03	120.89	125.10
1	A	1353	G	C5-C6-N1	7.02	115.01	111.50
1	A	635	G	N3-C4-C5	7.02	132.11	128.60
1	A	28	G	C8-N9-C4	-7.02	103.59	106.40
1	A	793	U	C2-N1-C1'	-7.02	109.28	117.70
1	A	19	C	C4-C5-C6	7.02	120.91	117.40
1	A	448	A	O5'-P-OP2	-7.02	99.38	105.70
1	A	686	U	C6-N1-C2	-7.02	116.79	121.00
1	A	1045	C	C4-C5-C6	-7.02	113.89	117.40
1	A	502	G	OP1-P-OP2	-7.02	109.08	119.60
1	A	15	G	O5'-P-OP1	-7.01	99.39	105.70
1	A	21	G	C2-N3-C4	7.01	115.41	111.90
1	A	295	C	C4-C5-C6	7.01	120.91	117.40
1	A	833	U	N3-C2-O2	-7.01	117.29	122.20
1	A	919	A	N1-C2-N3	-7.01	125.79	129.30
1	A	1182	G	C4-N9-C1'	7.01	135.62	126.50
1	A	1338	G	C6-N1-C2	-7.01	120.89	125.10
1	A	353	A	N1-C6-N6	-7.01	114.39	118.60
1	A	692	U	N1-C2-O2	7.01	127.71	122.80
1	A	42	G	N9-C4-C5	7.01	108.20	105.40
1	A	184	G	C4-C5-C6	7.01	123.01	118.80
1	A	342	C	N3-C4-C5	-7.01	119.10	121.90
1	A	1368	G	N9-C4-C5	-7.01	102.60	105.40
1	A	822	C	O5'-P-OP1	7.01	119.11	110.70
1	A	88	A	C8-N9-C4	-7.01	103.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	A	N7-C8-N9	7.01	117.30	113.80
1	A	398	C	C5-C6-N1	-7.00	117.50	121.00
1	A	829	G	N3-C4-C5	7.00	132.10	128.60
1	A	1232	U	C6-N1-C2	-7.00	116.80	121.00
1	A	1416	G	N7-C8-N9	7.00	116.60	113.10
1	A	547	A	OP1-P-O3'	7.00	120.60	105.20
1	A	797	C	O5'-P-OP1	7.00	119.10	110.70
1	A	1410	G	N3-C4-N9	7.00	130.20	126.00
1	A	6	G	N1-C2-N2	-6.99	109.91	116.20
1	A	130	A	C5-C6-N6	-6.99	118.11	123.70
1	A	733	A	C5-C6-N6	-6.99	118.11	123.70
1	A	774	G	N1-C2-N3	6.99	128.10	123.90
1	A	1486	G	N7-C8-N9	-6.99	109.60	113.10
1	A	1205	U	N3-C2-O2	-6.99	117.31	122.20
1	A	428	G	C8-N9-C4	-6.99	103.61	106.40
1	A	1491	G	C6-C5-N7	-6.99	126.21	130.40
1	A	926	G	N1-C2-N3	6.99	128.09	123.90
1	A	658	G	O5'-P-OP2	-6.99	99.41	105.70
1	A	686	U	C6-N1-C1'	6.99	130.98	121.20
1	A	1168	A	N1-C6-N6	-6.99	114.41	118.60
1	A	176	C	C6-N1-C2	6.98	123.09	120.30
1	A	73	C	N1-C2-O2	-6.98	114.71	118.90
1	A	108	G	N1-C2-N2	6.98	122.48	116.20
1	A	199	G	C2-N3-C4	-6.98	108.41	111.90
1	A	964	A	O4'-C1'-N9	-6.98	102.62	108.20
1	A	1053	G	O5'-P-OP1	-6.98	99.42	105.70
1	A	1416	G	N3-C4-N9	6.98	130.19	126.00
1	A	1450	U	C4-C5-C6	6.98	123.89	119.70
1	A	18	C	N1-C2-N3	6.98	124.08	119.20
1	A	872	A	C6-N1-C2	-6.98	114.41	118.60
1	A	6	G	C2-N3-C4	-6.97	108.41	111.90
1	A	982	U	C6-N1-C2	-6.97	116.82	121.00
1	A	41	G	N1-C6-O6	6.97	124.08	119.90
5	E	107	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	A	1401	G	N3-C4-C5	-6.97	125.12	128.60
1	A	42	G	C4-C5-C6	6.97	122.98	118.80
1	A	450	G	N1-C6-O6	6.97	124.08	119.90
1	A	662	G	C4-C5-N7	6.97	113.59	110.80
1	A	1066	C	O5'-P-OP1	-6.97	99.43	105.70
1	A	1193	G	C2-N3-C4	-6.96	108.42	111.90
1	A	354	G	N3-C2-N2	-6.96	115.03	119.90
1	A	757	U	N1-C2-N3	6.96	119.08	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	805	C	C5-C4-N4	-6.96	115.33	120.20
1	A	146	G	C8-N9-C4	6.96	109.18	106.40
1	A	1176	A	C8-N9-C4	-6.96	103.02	105.80
1	A	231	G	C6-C5-N7	-6.96	126.22	130.40
1	A	519	C	N3-C4-C5	-6.96	119.12	121.90
1	A	1249	C	N3-C4-C5	-6.96	119.12	121.90
1	A	693	G	C2-N3-C4	-6.96	108.42	111.90
1	A	309	G	N7-C8-N9	6.96	116.58	113.10
1	A	656	C	N3-C4-C5	6.95	124.68	121.90
1	A	1093	A	P-O3'-C3'	6.95	128.04	119.70
1	A	1287	A	C4-C5-C6	6.95	120.48	117.00
1	A	21	G	C5-C6-O6	-6.95	124.43	128.60
1	A	167	G	O5'-P-OP1	-6.95	99.44	105.70
1	A	962	C	N1-C2-N3	-6.95	114.33	119.20
1	A	1350	A	C6-C5-N7	6.95	137.16	132.30
1	A	691	G	N3-C4-C5	-6.95	125.13	128.60
1	A	987	G	N1-C6-O6	6.95	124.07	119.90
1	A	1079	G	N3-C4-N9	6.95	130.17	126.00
1	A	1112	C	N3-C4-C5	6.95	124.68	121.90
1	A	1254	C	N1-C2-O2	-6.95	114.73	118.90
1	A	862	C	OP1-P-OP2	6.95	130.02	119.60
1	A	963	G	C2-N3-C4	-6.95	108.43	111.90
1	A	1051	C	C6-N1-C2	6.95	123.08	120.30
1	A	1192	C	C4-C5-C6	-6.95	113.93	117.40
1	A	306	G	C8-N9-C4	6.94	109.18	106.40
1	A	344	A	C8-N9-C4	-6.94	103.02	105.80
1	A	569	C	C5-C6-N1	-6.94	117.53	121.00
1	A	587	G	C6-C5-N7	6.94	134.56	130.40
1	A	712	A	O5'-P-OP1	-6.94	99.45	105.70
1	A	1336	C	N3-C4-N4	6.94	122.86	118.00
1	A	1401	G	N3-C4-N9	6.94	130.16	126.00
1	A	778	G	N9-C4-C5	6.94	108.17	105.40
1	A	797	C	C2-N3-C4	-6.94	116.43	119.90
1	A	976	G	C8-N9-C4	6.94	109.17	106.40
1	A	1053	G	N1-C6-O6	6.94	124.06	119.90
1	A	413	G	O4'-C1'-N9	6.93	113.75	108.20
1	A	41	G	C8-N9-C4	-6.93	103.63	106.40
1	A	1058	G	N3-C2-N2	6.93	124.75	119.90
1	A	1125	U	C6-N1-C2	6.93	125.16	121.00
1	A	365	U	N3-C2-O2	-6.93	117.35	122.20
1	A	1139	G	N3-C4-C5	-6.93	125.14	128.60
1	A	1434	A	O5'-P-OP1	6.93	119.01	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	C	C5-C4-N4	-6.92	115.36	120.20
1	A	860	A	N3-C4-C5	-6.92	121.95	126.80
1	A	1385	G	C2-N3-C4	-6.92	108.44	111.90
1	A	443	C	C5-C6-N1	-6.92	117.54	121.00
1	A	880	C	N3-C4-N4	-6.92	113.16	118.00
1	A	1233	G	O5'-P-OP1	6.92	119.00	110.70
1	A	263	A	C5-C6-N1	6.92	121.16	117.70
1	A	929	G	C5-C6-O6	-6.92	124.45	128.60
12	L	36	VAL	CB-CA-C	-6.92	98.26	111.40
1	A	507	C	N1-C2-N3	-6.91	114.36	119.20
1	A	636	U	O5'-P-OP1	-6.91	99.48	105.70
1	A	983	A	N7-C8-N9	6.91	117.26	113.80
1	A	987	G	N9-C4-C5	-6.91	102.64	105.40
1	A	1315	U	O5'-P-OP2	-6.91	99.48	105.70
1	A	36	C	C2-N3-C4	-6.91	116.44	119.90
1	A	717	C	N3-C2-O2	6.91	126.74	121.90
1	A	780	A	C5-C6-N1	6.91	121.16	117.70
1	A	1410	G	C4-N9-C1'	6.91	135.49	126.50
1	A	823	G	C6-C5-N7	-6.91	126.26	130.40
1	A	1020	U	C6-N1-C2	-6.91	116.86	121.00
1	A	391	G	OP2-P-O3'	6.91	120.39	105.20
1	A	695	A	N1-C6-N6	6.91	122.74	118.60
1	A	380	G	N9-C4-C5	6.90	108.16	105.40
1	A	697	U	C2-N1-C1'	-6.90	109.42	117.70
1	A	1202	G	C4-C5-N7	-6.90	108.04	110.80
1	A	1415	G	C2-N3-C4	6.90	115.35	111.90
1	A	1206	G	N1-C2-N3	6.90	128.04	123.90
1	A	1397	C	O5'-P-OP2	6.90	118.98	110.70
16	P	55	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	A	538	G	OP2-P-O3'	6.90	120.37	105.20
1	A	600	C	OP2-P-O3'	6.90	120.37	105.20
1	A	673	G	N3-C4-C5	6.90	132.05	128.60
1	A	540	G	N7-C8-N9	6.89	116.55	113.10
1	A	659	U	N3-C4-C5	6.89	118.74	114.60
1	A	1425	U	C5-C4-O4	6.89	130.03	125.90
1	A	1524	C	O5'-P-OP2	6.89	118.97	110.70
1	A	1281	U	C2-N3-C4	6.89	131.13	127.00
1	A	1354	C	N3-C2-O2	6.89	126.72	121.90
1	A	277	C	C5-C6-N1	-6.88	117.56	121.00
1	A	724	G	N3-C2-N2	6.88	124.72	119.90
1	A	776	G	O5'-P-OP1	-6.88	99.50	105.70
1	A	61	G	C6-C5-N7	-6.88	126.27	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1237	C	O5'-P-OP2	-6.88	99.50	105.70
1	A	711	G	N3-C4-C5	6.88	132.04	128.60
1	A	927	G	N1-C6-O6	6.88	124.03	119.90
1	A	1322	C	OP1-P-OP2	-6.88	109.28	119.60
1	A	606	G	N3-C4-N9	6.88	130.13	126.00
1	A	1065	U	OP2-P-O3'	6.88	120.33	105.20
1	A	1286	A	C5-N7-C8	-6.88	100.46	103.90
1	A	1435	G	N7-C8-N9	6.88	116.54	113.10
1	A	1443	G	N3-C4-N9	-6.88	121.87	126.00
1	A	788	U	C4-C5-C6	6.88	123.83	119.70
1	A	1542	U	N1-C2-O2	6.88	127.61	122.80
1	A	901	A	C2-N3-C4	-6.87	107.16	110.60
1	A	922	G	N3-C2-N2	-6.87	115.09	119.90
1	A	1058	G	N9-C4-C5	-6.87	102.65	105.40
1	A	1131	G	C4-N9-C1'	6.87	135.44	126.50
1	A	1281	U	N3-C2-O2	6.87	127.01	122.20
1	A	58	C	C5-C6-N1	6.87	124.44	121.00
1	A	613	C	O5'-P-OP2	6.87	118.95	110.70
1	A	724	G	N7-C8-N9	6.87	116.54	113.10
1	A	821	G	C2-N3-C4	-6.87	108.46	111.90
1	A	1234	C	N3-C4-C5	6.87	124.65	121.90
1	A	243	A	N1-C2-N3	6.87	132.74	129.30
1	A	689	C	C6-N1-C2	6.87	123.05	120.30
1	A	108	G	C6-N1-C2	6.87	129.22	125.10
1	A	331	G	N3-C4-N9	6.87	130.12	126.00
1	A	793	U	O5'-P-OP2	-6.87	99.52	105.70
1	A	763	G	C6-N1-C2	-6.86	120.98	125.10
1	A	1145	C	N3-C4-N4	-6.86	113.20	118.00
1	A	1032	G	O4'-C1'-N9	-6.86	102.71	108.20
1	A	1053	G	N3-C2-N2	-6.86	115.10	119.90
1	A	552	U	N1-C2-O2	-6.86	118.00	122.80
1	A	570	G	OP1-P-OP2	-6.86	109.31	119.60
1	A	756	C	N3-C4-N4	6.86	122.80	118.00
1	A	977	A	N7-C8-N9	6.86	117.23	113.80
1	A	430	A	C5-C6-N6	-6.86	118.22	123.70
1	A	1520[A]	G	C6-C5-N7	-6.86	126.29	130.40
1	A	1520[B]	G	C6-C5-N7	-6.86	126.29	130.40
1	A	892	A	C5-C6-N1	6.85	121.13	117.70
1	A	44	G	N1-C2-N3	6.85	128.01	123.90
1	A	577	G	C6-C5-N7	6.85	134.51	130.40
1	A	1392	G	C5-C6-O6	6.85	132.71	128.60
1	A	658	G	N1-C2-N3	6.85	128.01	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	785	G	N9-C4-C5	-6.85	102.66	105.40
1	A	176	C	OP2-P-O3'	6.85	120.27	105.20
1	A	410	G	N9-C4-C5	6.85	108.14	105.40
1	A	684	A	C8-N9-C4	-6.85	103.06	105.80
1	A	232	G	C4-C5-N7	6.85	113.54	110.80
1	A	521	G	C2-N3-C4	6.85	115.32	111.90
1	A	1227	A	C2-N3-C4	-6.85	107.18	110.60
1	A	60	A	O5'-P-OP1	-6.84	99.54	105.70
1	A	144	G	N3-C4-C5	6.84	132.02	128.60
1	A	1362	C	C5-C4-N4	6.84	124.99	120.20
1	A	89	C	O5'-P-OP2	-6.84	99.54	105.70
1	A	320	C	C2-N3-C4	6.84	123.32	119.90
1	A	1477	C	N3-C4-C5	-6.84	119.16	121.90
1	A	7	G	N9-C4-C5	-6.84	102.67	105.40
1	A	617	G	C6-C5-N7	-6.84	126.30	130.40
1	A	872	A	O5'-P-OP2	6.84	118.90	110.70
1	A	445	G	C4-C5-N7	6.83	113.53	110.80
1	A	317	G	O5'-P-OP2	-6.83	99.55	105.70
1	A	328	C	O4'-C1'-N1	6.83	113.67	108.20
1	A	624	C	N1-C2-N3	-6.83	114.42	119.20
1	A	711	G	N1-C2-N2	6.83	122.35	116.20
1	A	140	A	O5'-P-OP2	6.83	118.89	110.70
1	A	172	A	N1-C2-N3	6.83	132.71	129.30
1	A	1383	C	OP2-P-O3'	6.83	120.22	105.20
1	A	1414	U	C5-C6-N1	6.83	126.11	122.70
1	A	671	G	N3-C4-C5	-6.82	125.19	128.60
1	A	1425	U	C5-C6-N1	-6.82	119.29	122.70
1	A	716	A	N1-C6-N6	6.82	122.69	118.60
1	A	806	C	C4-C5-C6	6.82	120.81	117.40
1	A	937	A	N1-C6-N6	-6.82	114.51	118.60
1	A	975	A	N1-C6-N6	6.82	122.69	118.60
1	A	1493	A	C6-N1-C2	-6.82	114.51	118.60
1	A	700	G	C5-C6-N1	-6.82	108.09	111.50
1	A	1053	G	N3-C4-N9	-6.82	121.91	126.00
1	A	1525	G	C4-N9-C1'	6.82	135.36	126.50
1	A	332	G	OP1-P-OP2	6.81	129.82	119.60
1	A	1499	A	N1-C2-N3	6.81	132.71	129.30
1	A	29	G	C5-N7-C8	-6.81	100.89	104.30
1	A	643	C	N1-C2-N3	-6.81	114.43	119.20
1	A	15	G	C2-N3-C4	6.81	115.30	111.90
1	A	624	C	C5-C6-N1	-6.81	117.60	121.00
1	A	875	C	C5-C4-N4	-6.81	115.44	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	G	N3-C2-N2	6.81	124.66	119.90
1	A	298	A	C2-N3-C4	-6.81	107.20	110.60
1	A	272	C	N1-C2-O2	6.80	122.98	118.90
1	A	1512	U	N3-C4-O4	-6.80	114.64	119.40
4	D	64	LEU	CB-CG-CD1	-6.80	99.44	111.00
1	A	53	A	O5'-P-OP1	-6.80	99.58	105.70
1	A	230	G	N1-C6-O6	6.80	123.98	119.90
1	A	362	G	N1-C6-O6	6.80	123.98	119.90
1	A	1276	G	N9-C4-C5	-6.80	102.68	105.40
1	A	1054	C	O4'-C1'-N1	6.80	113.64	108.20
1	A	1206	G	C6-C5-N7	-6.80	126.32	130.40
1	A	558	G	O5'-P-OP1	6.80	118.86	110.70
1	A	288	A	C5-C6-N6	6.80	129.14	123.70
1	A	334	C	N1-C2-O2	-6.80	114.82	118.90
1	A	727	G	C8-N9-C4	-6.80	103.68	106.40
1	A	946	A	C5-C6-N6	-6.80	118.26	123.70
1	A	929	G	C6-N1-C2	-6.79	121.02	125.10
1	A	1090	U	N3-C2-O2	-6.79	117.44	122.20
1	A	1516[A]	G	C6-C5-N7	6.79	134.48	130.40
1	A	1516[B]	G	C6-C5-N7	6.79	134.48	130.40
1	A	137	C	N3-C4-C5	-6.79	119.18	121.90
1	A	406	G	O5'-P-OP1	6.79	118.85	110.70
1	A	130	A	N9-C4-C5	-6.79	103.08	105.80
1	A	1284	C	N1-C2-O2	6.79	122.97	118.90
1	A	333	G	N9-C4-C5	-6.79	102.69	105.40
1	A	1145	C	C5-C6-N1	-6.79	117.61	121.00
1	A	230	G	N1-C2-N3	6.78	127.97	123.90
1	A	436	C	OP1-P-OP2	6.78	129.77	119.60
1	A	718	G	C6-C5-N7	-6.78	126.33	130.40
1	A	722	A	N1-C2-N3	6.78	132.69	129.30
1	A	150	C	N3-C2-O2	6.78	126.65	121.90
1	A	258	G	C6-C5-N7	-6.78	126.33	130.40
1	A	331	G	C5-C6-O6	-6.78	124.53	128.60
1	A	484	G	N9-C4-C5	-6.78	102.69	105.40
1	A	522	C	C2-N1-C1'	-6.78	111.34	118.80
1	A	304	U	O5'-P-OP2	-6.78	99.60	105.70
1	A	830	G	N1-C6-O6	6.78	123.97	119.90
1	A	1087	G	C5-C6-O6	-6.78	124.53	128.60
1	A	1222	G	C4-C5-C6	6.78	122.87	118.80
1	A	650	G	C4-C5-N7	-6.78	108.09	110.80
1	A	770	C	O5'-P-OP2	6.78	118.83	110.70
1	A	247	G	N1-C2-N3	6.77	127.97	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	531	U	C2-N1-C1'	-6.77	109.57	117.70
1	A	106	C	OP1-P-O3'	-6.77	90.30	105.20
1	A	402	G	C6-N1-C2	-6.77	121.04	125.10
1	A	294	U	C6-N1-C2	6.77	125.06	121.00
1	A	1494	G	N1-C6-O6	-6.77	115.84	119.90
1	A	220	G	C5-C6-O6	-6.76	124.54	128.60
1	A	452	A	O4'-C1'-N9	6.76	113.61	108.20
1	A	589	C	C5-C6-N1	6.76	124.38	121.00
1	A	886	G	O4'-C1'-N9	6.76	113.61	108.20
1	A	938	A	C8-N9-C4	-6.76	103.09	105.80
1	A	923	A	C4-C5-N7	6.76	114.08	110.70
1	A	1481	U	C4-C5-C6	6.76	123.76	119.70
1	A	447	G	N9-C4-C5	-6.76	102.70	105.40
1	A	732	C	N3-C2-O2	-6.76	117.17	121.90
1	A	203	U	O4'-C1'-N1	-6.76	102.79	108.20
1	A	398	C	C5-C4-N4	6.76	124.93	120.20
1	A	1461	G	C8-N9-C4	6.76	109.10	106.40
1	A	589	C	N1-C2-N3	6.76	123.93	119.20
1	A	903	G	C6-N1-C2	-6.76	121.05	125.10
1	A	1362	C	N3-C4-N4	-6.76	113.27	118.00
1	A	423	G	N9-C4-C5	-6.75	102.70	105.40
1	A	184	G	N3-C2-N2	6.75	124.63	119.90
1	A	196	A	C8-N9-C4	6.75	108.50	105.80
1	A	795	C	OP1-P-O3'	-6.75	90.34	105.20
9	I	56	LEU	CA-CB-CG	6.75	130.83	115.30
1	A	259	G	N1-C2-N3	6.75	127.95	123.90
1	A	1240	U	N1-C2-N3	6.75	118.95	114.90
1	A	1379	G	C6-C5-N7	-6.75	126.35	130.40
1	A	1114	C	N3-C4-C5	6.75	124.60	121.90
1	A	380	G	N3-C4-C5	-6.75	125.23	128.60
1	A	1280	A	OP1-P-OP2	6.75	129.72	119.60
1	A	133	U	N3-C4-C5	-6.75	110.55	114.60
1	A	10	A	O5'-P-OP2	-6.74	99.63	105.70
1	A	1281	U	C6-N1-C2	-6.74	116.95	121.00
1	A	672	U	N3-C4-C5	6.74	118.64	114.60
1	A	349	A	C2-N3-C4	-6.74	107.23	110.60
1	A	730	G	N1-C2-N2	6.74	122.27	116.20
1	A	755	G	C2-N3-C4	-6.74	108.53	111.90
4	D	94	LEU	CA-CB-CG	-6.74	99.80	115.30
1	A	272	C	O5'-P-OP1	-6.74	99.64	105.70
1	A	525	C	C4-C5-C6	-6.74	114.03	117.40
1	A	858	G	OP1-P-O3'	-6.74	90.37	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	865	A	C6-C5-N7	-6.74	127.58	132.30
1	A	1218	C	N3-C4-C5	6.74	124.60	121.90
1	A	1366	C	N3-C2-O2	-6.74	117.18	121.90
1	A	1066	C	N1-C2-O2	-6.74	114.86	118.90
1	A	10	A	C6-N1-C2	-6.74	114.56	118.60
1	A	181	G	C8-N9-C4	-6.74	103.71	106.40
1	A	517	G	N7-C8-N9	6.74	116.47	113.10
1	A	584	G	N3-C2-N2	6.73	124.61	119.90
1	A	362	G	C6-C5-N7	-6.73	126.36	130.40
1	A	1054	C	N3-C4-C5	-6.73	119.21	121.90
1	A	1525	G	N9-C4-C5	6.73	108.09	105.40
1	A	715	A	C5-N7-C8	-6.73	100.53	103.90
1	A	914	A	N9-C4-C5	6.73	108.49	105.80
1	A	1108	G	N1-C2-N2	-6.73	110.14	116.20
1	A	1476	G	N1-C6-O6	6.73	123.94	119.90
1	A	768	A	N9-C4-C5	6.73	108.49	105.80
1	A	168	G	O5'-P-OP1	-6.73	99.64	105.70
1	A	911	U	C5-C4-O4	6.73	129.94	125.90
1	A	1304	G	C5-C6-N1	-6.73	108.14	111.50
1	A	972	C	O5'-P-OP2	6.73	118.77	110.70
1	A	1116	C	C2-N1-C1'	-6.73	111.40	118.80
1	A	1120	G	N7-C8-N9	6.73	116.46	113.10
1	A	284	G	C6-C5-N7	-6.72	126.36	130.40
1	A	580	U	C4-C5-C6	6.72	123.73	119.70
6	F	23	LYS	CD-CE-NZ	6.72	127.17	111.70
1	A	389	A	N3-C4-C5	-6.72	122.09	126.80
1	A	674	G	C6-N1-C2	-6.72	121.07	125.10
1	A	711	G	C2-N3-C4	-6.72	108.54	111.90
1	A	148	G	C4-C5-C6	6.72	122.83	118.80
1	A	747	C	C5-C6-N1	-6.72	117.64	121.00
1	A	52	G	OP2-P-O3'	6.72	119.98	105.20
1	A	673	G	C4-C5-C6	-6.72	114.77	118.80
1	A	265	G	N1-C2-N2	-6.71	110.16	116.20
1	A	1078	U	N3-C2-O2	-6.71	117.50	122.20
1	A	1498	UR3	P-O3'-C3'	6.71	127.75	119.70
1	A	109	A	OP1-P-OP2	6.71	129.66	119.60
1	A	29	G	N3-C4-C5	6.71	131.95	128.60
1	A	1308	U	N3-C4-C5	-6.71	110.58	114.60
1	A	722	A	N1-C6-N6	6.71	122.62	118.60
1	A	902	G	OP1-P-OP2	6.71	129.66	119.60
1	A	975	A	C4-C5-N7	6.71	114.05	110.70
1	A	993	G	O5'-P-OP1	-6.71	99.67	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	G	C6-C5-N7	-6.70	126.38	130.40
1	A	882	C	C5-C6-N1	-6.70	117.65	121.00
1	A	132	C	OP2-P-O3'	6.70	119.94	105.20
1	A	305	G	N1-C2-N2	-6.70	110.17	116.20
1	A	786	G	C2-N3-C4	6.70	115.25	111.90
1	A	951	G	C5-C6-O6	-6.70	124.58	128.60
1	A	1093	A	O5'-P-OP1	-6.70	99.67	105.70
1	A	1442	G	C5-C6-N1	6.70	114.85	111.50
1	A	367	U	C2-N3-C4	-6.69	122.98	127.00
1	A	1095	U	C5-C6-N1	6.69	126.05	122.70
1	A	294	U	C5-C4-O4	-6.69	121.89	125.90
1	A	711	G	C5-C6-N1	-6.69	108.15	111.50
1	A	731	G	C4-C5-N7	6.69	113.48	110.80
1	A	944	G	N3-C4-C5	-6.69	125.25	128.60
1	A	1181	G	N9-C4-C5	6.69	108.08	105.40
1	A	1342	C	N1-C2-N3	-6.69	114.52	119.20
1	A	712	A	C6-N1-C2	-6.69	114.59	118.60
1	A	939	G	N9-C4-C5	6.69	108.08	105.40
1	A	1416	G	C6-C5-N7	-6.69	126.39	130.40
1	A	10	A	C5-C6-N1	6.69	121.04	117.70
1	A	148	G	N1-C2-N3	6.69	127.91	123.90
1	A	1508	G	C8-N9-C4	-6.69	103.72	106.40
1	A	88	A	C4-C5-C6	6.68	120.34	117.00
1	A	718	G	C4-C5-N7	6.68	113.47	110.80
1	A	1002	G	C4-N9-C1'	-6.68	117.81	126.50
1	A	873	A	C2-N3-C4	6.68	113.94	110.60
1	A	856	C	N3-C2-O2	6.68	126.58	121.90
1	A	900	A	C6-N1-C2	-6.68	114.59	118.60
1	A	1482	G	C5-C6-N1	-6.68	108.16	111.50
1	A	362	G	C4-N9-C1'	6.68	135.18	126.50
1	A	549	C	O5'-P-OP2	-6.68	99.69	105.70
1	A	829	G	C5-C6-N1	-6.68	108.16	111.50
1	A	1015	A	N1-C6-N6	-6.68	114.59	118.60
1	A	357	G	N1-C6-O6	-6.67	115.90	119.90
1	A	900	A	O5'-P-OP1	6.67	118.71	110.70
1	A	372	C	O5'-P-OP2	6.67	118.71	110.70
1	A	785	G	C5-C6-N1	6.67	114.84	111.50
1	A	1273	G	N3-C4-C5	-6.67	125.27	128.60
1	A	1529	G	N1-C6-O6	6.67	123.90	119.90
1	A	105	G	N1-C6-O6	6.67	123.90	119.90
1	A	177	C	C6-N1-C2	6.67	122.97	120.30
1	A	914	A	C8-N9-C4	-6.67	103.13	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	C	C4-C5-C6	6.67	120.73	117.40
1	A	32	A	N1-C6-N6	6.67	122.60	118.60
1	A	1482	G	C4-C5-N7	-6.66	108.14	110.80
1	A	1240	U	C5-C6-N1	-6.66	119.37	122.70
1	A	55	A	C6-N1-C2	-6.66	114.60	118.60
1	A	616	G	N1-C6-O6	6.66	123.90	119.90
1	A	654	G	N1-C6-O6	-6.66	115.90	119.90
12	L	24	VAL	N-CA-CB	-6.66	96.85	111.50
1	A	372	C	C2-N1-C1'	6.66	126.12	118.80
1	A	660	G	C5-C6-N1	-6.66	108.17	111.50
1	A	1417	G	C4-C5-C6	6.66	122.79	118.80
1	A	1198	G	C2-N3-C4	-6.66	108.57	111.90
1	A	793	U	C4-C5-C6	6.65	123.69	119.70
1	A	193	C	C6-N1-C2	6.65	122.96	120.30
1	A	1155	G	N1-C6-O6	6.65	123.89	119.90
1	A	1157	A	C2-N3-C4	6.65	113.93	110.60
1	A	987	G	N7-C8-N9	-6.65	109.78	113.10
1	A	1273	G	N3-C4-N9	6.65	129.99	126.00
1	A	1475	G	C5-C6-N1	-6.65	108.17	111.50
1	A	273	A	OP2-P-O3'	6.65	119.83	105.20
1	A	380	G	N1-C6-O6	-6.65	115.91	119.90
1	A	975	A	C6-N1-C2	6.65	122.59	118.60
1	A	1093	A	N9-C4-C5	6.65	108.46	105.80
1	A	1378	C	C2-N3-C4	6.64	123.22	119.90
1	A	17	U	C2-N3-C4	-6.64	123.02	127.00
1	A	113	G	C2-N3-C4	-6.64	108.58	111.90
1	A	1125	U	O5'-P-OP2	6.64	118.67	110.70
1	A	1106	G	N3-C2-N2	6.64	124.55	119.90
1	A	429	U	N1-C2-O2	6.64	127.45	122.80
1	A	819	A	C2-N3-C4	-6.64	107.28	110.60
1	A	944	G	C8-N9-C4	-6.64	103.75	106.40
1	A	1525	G	C6-C5-N7	-6.64	126.42	130.40
1	A	24	U	O5'-P-OP1	6.63	118.66	110.70
1	A	397	A	C6-N1-C2	-6.63	114.62	118.60
1	A	561	U	N3-C4-C5	6.63	118.58	114.60
1	A	936	C	C5-C4-N4	-6.63	115.56	120.20
1	A	1126	U	C2-N1-C1'	-6.63	109.74	117.70
1	A	1104	G	C5-N7-C8	-6.63	100.98	104.30
1	A	20	U	C5-C6-N1	-6.63	119.39	122.70
1	A	372	C	P-O5'-C5'	-6.63	110.30	120.90
1	A	543	C	C4-C5-C6	6.63	120.71	117.40
1	A	609	A	OP2-P-O3'	6.63	119.78	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1508	G	OP2-P-O3'	6.63	119.78	105.20
1	A	294	U	C2-N3-C4	-6.63	123.02	127.00
1	A	935	A	C8-N9-C4	-6.62	103.15	105.80
1	A	1188	A	C2-N3-C4	-6.62	107.29	110.60
1	A	1329	A	N9-C4-C5	6.62	108.45	105.80
1	A	1442	G	N3-C4-N9	6.62	129.97	126.00
1	A	1180	A	N7-C8-N9	6.62	117.11	113.80
1	A	1434	A	C8-N9-C4	6.62	108.45	105.80
1	A	388	G	C6-C5-N7	-6.62	126.43	130.40
1	A	485	G	C5-C6-N1	6.62	114.81	111.50
1	A	505	G	N1-C6-O6	-6.62	115.93	119.90
1	A	1257	U	C2-N1-C1'	6.62	125.64	117.70
1	A	1183	A	C2-N3-C4	-6.62	107.29	110.60
1	A	325	A	C5-C6-N1	6.61	121.01	117.70
1	A	675	A	N1-C6-N6	6.61	122.57	118.60
1	A	700	G	C8-N9-C4	6.61	109.05	106.40
1	A	1209	C	N1-C2-N3	-6.61	114.57	119.20
1	A	1379	G	OP2-P-O3'	6.61	119.75	105.20
1	A	408	A	O5'-P-OP1	-6.61	99.75	105.70
1	A	1230	C	N3-C4-N4	6.61	122.63	118.00
1	A	1295	G	N1-C6-O6	6.61	123.87	119.90
10	J	88	LEU	N-CA-C	6.61	128.85	111.00
1	A	194	C	C2-N3-C4	-6.61	116.59	119.90
1	A	701	C	OP1-P-O3'	6.61	119.74	105.20
1	A	1520[A]	G	N3-C4-C5	-6.61	125.30	128.60
1	A	1520[B]	G	N3-C4-C5	-6.61	125.30	128.60
1	A	11	G	N1-C2-N3	6.61	127.86	123.90
1	A	104	G	N1-C2-N3	6.61	127.86	123.90
1	A	643	C	C5-C4-N4	-6.60	115.58	120.20
1	A	669	U	OP2-P-O3'	6.60	119.73	105.20
1	A	42	G	C5-C6-N1	-6.60	108.20	111.50
1	A	418	C	N3-C4-C5	6.60	124.54	121.90
1	A	1486	G	C5-N7-C8	6.60	107.60	104.30
1	A	1080	A	C5-C6-N1	6.60	121.00	117.70
1	A	1181	G	N3-C4-N9	-6.60	122.04	126.00
1	A	123	C	C5-C6-N1	6.60	124.30	121.00
1	A	1175	G	N1-C2-N3	6.60	127.86	123.90
1	A	1529	G	C4-N9-C1'	6.60	135.08	126.50
1	A	856	C	C6-N1-C2	6.60	122.94	120.30
1	A	942	G	C5-C6-N1	-6.60	108.20	111.50
1	A	1514	C	N3-C4-C5	6.60	124.54	121.90
1	A	553	A	C4-C5-C6	6.59	120.30	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1139	G	N9-C4-C5	6.59	108.04	105.40
1	A	104	G	C2-N3-C4	-6.59	108.61	111.90
1	A	218	C	C5-C6-N1	-6.59	117.70	121.00
1	A	304	U	C2-N3-C4	-6.59	123.05	127.00
1	A	1230	C	N3-C4-C5	-6.59	119.26	121.90
1	A	1159	U	C6-N1-C2	6.59	124.95	121.00
1	A	806	C	N3-C2-O2	-6.59	117.29	121.90
1	A	831	U	N1-C2-N3	-6.59	110.95	114.90
1	A	840	C	N1-C2-O2	6.59	122.85	118.90
1	A	886	G	N1-C6-O6	6.59	123.85	119.90
1	A	1235	U	N1-C2-N3	6.59	118.85	114.90
1	A	1316	G	N1-C6-O6	6.59	123.85	119.90
1	A	1331	G	C8-N9-C4	-6.59	103.77	106.40
1	A	1381	U	C6-N1-C2	-6.59	117.05	121.00
1	A	233	C	C2-N3-C4	-6.58	116.61	119.90
1	A	238	G	C2-N3-C4	-6.58	108.61	111.90
1	A	286	G	N1-C6-O6	6.58	123.85	119.90
1	A	524	G	C8-N9-C1'	-6.58	118.44	127.00
1	A	169	C	N1-C2-O2	6.58	122.85	118.90
1	A	194	C	C5-C6-N1	-6.58	117.71	121.00
1	A	779	C	C4-C5-C6	6.58	120.69	117.40
1	A	1108	G	O4'-C1'-N9	-6.58	102.94	108.20
1	A	1386	G	O5'-P-OP1	6.58	118.60	110.70
1	A	588	G	N1-C6-O6	6.58	123.85	119.90
1	A	243	A	C6-N1-C2	-6.58	114.65	118.60
1	A	434	U	C6-N1-C2	-6.58	117.05	121.00
1	A	971	G	C8-N9-C4	6.58	109.03	106.40
1	A	1167	A	N1-C6-N6	-6.58	114.66	118.60
1	A	1198	G	N1-C6-O6	-6.57	115.96	119.90
12	L	97	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	A	1049	U	N3-C2-O2	6.57	126.80	122.20
1	A	1089	G	C8-N9-C4	-6.57	103.77	106.40
1	A	9	G	C5-C6-O6	-6.57	124.66	128.60
1	A	658	G	N1-C6-O6	6.57	123.84	119.90
1	A	909	A	C5-N7-C8	-6.57	100.61	103.90
1	A	404	U	OP2-P-O3'	6.57	119.65	105.20
1	A	488	C	C5-C6-N1	6.57	124.28	121.00
1	A	748	C	C6-N1-C2	-6.57	117.67	120.30
1	A	879	C	C2-N3-C4	-6.57	116.62	119.90
1	A	1030	C	C6-N1-C2	-6.57	117.67	120.30
1	A	1495	U	C6-N1-C2	6.57	124.94	121.00
1	A	688	G	O5'-P-OP1	-6.57	99.79	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1359	C	C5-C4-N4	-6.56	115.61	120.20
1	A	650	G	N3-C2-N2	-6.56	115.31	119.90
1	A	1003(A)	G	N3-C4-C5	-6.56	125.32	128.60
1	A	667	G	N3-C4-C5	6.56	131.88	128.60
1	A	974	A	N3-C4-C5	-6.56	122.21	126.80
1	A	228	A	C2-N3-C4	-6.56	107.32	110.60
1	A	364	A	C6-C5-N7	-6.56	127.71	132.30
1	A	267	C	C2-N1-C1'	6.56	126.01	118.80
1	A	608	A	N1-C6-N6	-6.56	114.67	118.60
1	A	98	U	OP1-P-OP2	-6.55	109.77	119.60
1	A	385	C	O5'-P-OP1	-6.55	99.80	105.70
1	A	396	G	N7-C8-N9	6.55	116.38	113.10
1	A	871	U	P-O3'-C3'	6.55	127.57	119.70
1	A	950	U	C2-N3-C4	6.55	130.93	127.00
1	A	1178	G	C8-N9-C4	-6.55	103.78	106.40
1	A	52	G	N3-C2-N2	-6.55	115.31	119.90
1	A	768	A	C8-N9-C4	-6.55	103.18	105.80
1	A	1433	A	N1-C2-N3	6.55	132.58	129.30
1	A	278	G	N9-C4-C5	6.55	108.02	105.40
1	A	395	C	O5'-P-OP1	-6.55	99.81	105.70
1	A	116	A	C8-N9-C4	6.55	108.42	105.80
1	A	646	U	O4'-C1'-N1	6.55	113.44	108.20
1	A	1340	A	N1-C6-N6	-6.55	114.67	118.60
1	A	203	U	O5'-P-OP1	-6.55	99.81	105.70
1	A	287	U	N3-C4-O4	6.55	123.98	119.40
1	A	971	G	N1-C6-O6	6.55	123.83	119.90
1	A	1184	G	C4-C5-N7	-6.55	108.18	110.80
1	A	1227	A	O4'-C1'-N9	-6.55	102.96	108.20
1	A	685	G	C5-C6-N1	-6.54	108.23	111.50
1	A	1506	U	OP1-P-OP2	6.54	129.42	119.60
1	A	53	A	N1-C6-N6	-6.54	114.68	118.60
1	A	312	C	C4-C5-C6	-6.54	114.13	117.40
1	A	566	G	N1-C2-N2	-6.54	110.31	116.20
1	A	670	G	C8-N9-C1'	-6.54	118.50	127.00
1	A	728	A	N7-C8-N9	6.54	117.07	113.80
1	A	778	G	C2-N3-C4	-6.54	108.63	111.90
1	A	1415	G	C6-N1-C2	6.54	129.02	125.10
1	A	1488	G	N3-C4-N9	6.54	129.92	126.00
1	A	1544	U	C6-N1-C2	-6.54	117.08	121.00
1	A	190(I)	G	O5'-P-OP1	6.54	118.54	110.70
1	A	508	C	C5-C4-N4	6.54	124.77	120.20
1	A	559	A	C4-C5-C6	6.54	120.27	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	G	C5-C6-N1	6.54	114.77	111.50
1	A	734	G	C8-N9-C4	-6.54	103.79	106.40
1	A	1202	G	N3-C4-C5	6.54	131.87	128.60
1	A	787	A	C5-C6-N1	-6.53	114.43	117.70
1	A	1491	G	C4-C5-N7	6.53	113.41	110.80
1	A	236	G	N3-C2-N2	6.53	124.47	119.90
1	A	1030(B)	C	C6-N1-C1'	-6.53	112.97	120.80
1	A	352	C	C6-N1-C2	6.53	122.91	120.30
1	A	557	G	C5-N7-C8	-6.53	101.04	104.30
1	A	1505	G	C4-N9-C1'	6.53	134.99	126.50
1	A	316	G	C4-C5-C6	6.53	122.72	118.80
1	A	12	U	C5-C4-O4	6.52	129.81	125.90
1	A	297	G	C6-N1-C2	-6.52	121.19	125.10
1	A	759	A	N1-C6-N6	-6.52	114.69	118.60
1	A	402	G	C4-C5-N7	-6.52	108.19	110.80
1	A	811	C	OP1-P-O3'	-6.52	90.85	105.20
1	A	574	A	C8-N9-C4	-6.52	103.19	105.80
1	A	802	A	C2-N3-C4	-6.52	107.34	110.60
1	A	907	A	C6-N1-C2	-6.52	114.69	118.60
1	A	232	G	N3-C2-N2	6.52	124.46	119.90
1	A	1128	C	C4-C5-C6	6.52	120.66	117.40
1	A	782	A	C2-N3-C4	-6.52	107.34	110.60
1	A	825	G	C8-N9-C4	6.52	109.01	106.40
1	A	413	G	N1-C2-N3	-6.51	119.99	123.90
1	A	1276	G	N3-C4-N9	6.51	129.91	126.00
1	A	48	C	O5'-P-OP1	-6.51	99.84	105.70
1	A	1167	A	C8-N9-C4	-6.51	103.20	105.80
1	A	1257	U	N1-C2-N3	-6.51	111.00	114.90
1	A	642	A	C5-C6-N6	-6.50	118.50	123.70
1	A	1521	G	C8-N9-C1'	-6.50	118.54	127.00
1	A	40	C	O5'-P-OP2	6.50	118.50	110.70
1	A	717	C	N3-C4-N4	6.50	122.55	118.00
1	A	1189	C	O5'-P-OP2	6.50	118.50	110.70
1	A	1323	G	N3-C4-C5	6.50	131.85	128.60
12	L	117	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	725	G	C5-N7-C8	-6.50	101.05	104.30
1	A	1021	G	C2-N3-C4	6.50	115.15	111.90
1	A	1157	A	C5-N7-C8	6.50	107.15	103.90
1	A	102	G	C6-C5-N7	-6.50	126.50	130.40
1	A	397	A	N7-C8-N9	6.50	117.05	113.80
1	A	1211	U	N3-C2-O2	-6.50	117.65	122.20
1	A	395	C	N1-C2-O2	-6.49	115.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	974	A	C4-C5-N7	-6.49	107.45	110.70
1	A	1075	C	O5'-P-OP1	6.49	118.49	110.70
1	A	1143	G	C5-C6-O6	6.49	132.50	128.60
1	A	1276	G	C4-C5-N7	6.49	113.40	110.80
1	A	10	A	C4-C5-N7	-6.49	107.46	110.70
1	A	60	A	N1-C2-N3	6.49	132.54	129.30
1	A	64	G	N3-C4-C5	-6.49	125.36	128.60
1	A	311	C	C5-C4-N4	6.49	124.74	120.20
1	A	540	G	N3-C4-C5	-6.49	125.36	128.60
1	A	1515[A]	C	O5'-P-OP2	-6.49	99.86	105.70
1	A	1515[B]	C	O5'-P-OP2	-6.49	99.86	105.70
1	A	34	C	C5-C6-N1	-6.49	117.76	121.00
1	A	352	C	C2-N3-C4	-6.49	116.66	119.90
1	A	474	G	C6-C5-N7	-6.49	126.51	130.40
1	A	520	A	N1-C2-N3	6.49	132.54	129.30
1	A	791	G	C8-N9-C1'	-6.49	118.57	127.00
1	A	575	G	N7-C8-N9	-6.48	109.86	113.10
1	A	636	U	N3-C4-O4	6.48	123.94	119.40
1	A	974	A	C5-C6-N1	6.48	120.94	117.70
1	A	1215	G	C5-N7-C8	-6.48	101.06	104.30
1	A	983	A	C6-C5-N7	-6.48	127.77	132.30
1	A	636	U	N3-C4-C5	-6.48	110.72	114.60
1	A	22	G	OP2-P-O3'	6.47	119.45	105.20
1	A	1108	G	OP1-P-OP2	6.47	129.31	119.60
1	A	1145	C	C5-C4-N4	6.47	124.73	120.20
1	A	813	U	C4-C5-C6	-6.47	115.82	119.70
1	A	1525	G	C4-C5-C6	6.47	122.68	118.80
1	A	278	G	N3-C4-N9	-6.47	122.12	126.00
1	A	927	G	N7-C8-N9	6.47	116.33	113.10
1	A	1338	G	C4-N9-C1'	6.47	134.91	126.50
1	A	517	G	N9-C4-C5	6.47	107.99	105.40
1	A	896	C	N3-C2-O2	6.47	126.43	121.90
1	A	1211	U	O5'-P-OP1	-6.47	99.88	105.70
1	A	364	A	C8-N9-C4	-6.47	103.21	105.80
1	A	652	U	C5-C4-O4	-6.47	122.02	125.90
1	A	686	U	O5'-P-OP2	-6.47	99.88	105.70
1	A	1379	G	C4-C5-C6	6.47	122.68	118.80
1	A	1380	U	P-O3'-C3'	6.47	127.46	119.70
1	A	1398	A	OP1-P-OP2	6.47	129.30	119.60
1	A	1515[A]	C	N3-C2-O2	6.47	126.43	121.90
1	A	1515[B]	C	N3-C2-O2	6.47	126.43	121.90
1	A	637	G	C6-C5-N7	-6.46	126.52	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	906	G	C4-C5-C6	6.46	122.68	118.80
1	A	1113	C	N3-C4-N4	-6.46	113.48	118.00
12	L	94	LEU	CA-CB-CG	-6.46	100.44	115.30
1	A	6	G	C5-C6-N1	-6.46	108.27	111.50
1	A	1336	C	N1-C2-N3	-6.46	114.68	119.20
1	A	715	A	C2-N3-C4	-6.46	107.37	110.60
1	A	237	C	OP2-P-O3'	6.46	119.41	105.20
1	A	252	U	C6-N1-C1'	6.46	130.24	121.20
1	A	298	A	C5-C6-N1	-6.46	114.47	117.70
7	G	9	VAL	CB-CA-C	-6.46	99.13	111.40
1	A	1000	U	C5-C6-N1	6.46	125.93	122.70
1	A	1291	G	N1-C6-O6	6.46	123.77	119.90
1	A	1530	G	O5'-P-OP2	-6.45	99.89	105.70
1	A	153	C	N3-C4-C5	-6.45	119.32	121.90
1	A	154	C	C6-N1-C2	-6.45	117.72	120.30
1	A	969	A	O5'-P-OP1	6.45	118.44	110.70
1	A	1199	U	C5-C6-N1	-6.45	119.47	122.70
1	A	1193	G	N1-C2-N2	-6.45	110.40	116.20
1	A	1111	A	N1-C2-N3	6.45	132.52	129.30
1	A	690	G	C5-C6-N1	-6.45	108.28	111.50
1	A	321	A	C2-N3-C4	-6.44	107.38	110.60
1	A	365	U	OP1-P-O3'	6.44	119.37	105.20
1	A	744	C	C5-C6-N1	6.44	124.22	121.00
1	A	1190	G	N3-C4-C5	-6.44	125.38	128.60
1	A	674	G	C2-N3-C4	-6.44	108.68	111.90
1	A	790	A	C4-N9-C1'	6.44	137.89	126.30
1	A	1200	C	C6-N1-C2	-6.44	117.72	120.30
1	A	585	G	C5-C6-O6	6.44	132.46	128.60
1	A	854	G	C6-C5-N7	-6.44	126.54	130.40
1	A	1397	C	N3-C4-C5	6.44	124.48	121.90
1	A	1080	A	N1-C6-N6	-6.44	114.74	118.60
1	A	1337	G	N1-C6-O6	6.44	123.76	119.90
1	A	791	G	C5-C6-O6	6.44	132.46	128.60
1	A	780	A	N1-C6-N6	6.43	122.46	118.60
1	A	942	G	C4-C5-N7	-6.43	108.23	110.80
1	A	27	G	N7-C8-N9	6.43	116.31	113.10
1	A	218	C	N3-C2-O2	-6.43	117.40	121.90
1	A	479	C	N3-C4-N4	6.43	122.50	118.00
1	A	627	G	N9-C4-C5	6.43	107.97	105.40
1	A	897	C	OP2-P-O3'	6.43	119.34	105.20
1	A	709	G	O5'-P-OP1	6.43	118.41	110.70
1	A	775	G	C5-C6-O6	6.43	132.46	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	14	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	A	198	G	O4'-C1'-N9	-6.43	103.06	108.20
1	A	946	A	C2-N3-C4	6.43	113.81	110.60
1	A	204	U	C2-N1-C1'	6.42	125.41	117.70
1	A	1220	G	C6-C5-N7	6.42	134.25	130.40
1	A	1368	G	C6-C5-N7	-6.42	126.55	130.40
1	A	1393	U	N3-C4-O4	6.42	123.90	119.40
1	A	1398	A	O5'-P-OP2	-6.42	99.92	105.70
1	A	325	A	N1-C6-N6	-6.42	114.75	118.60
1	A	338	A	N1-C2-N3	6.42	132.51	129.30
1	A	1286	A	N7-C8-N9	6.42	117.01	113.80
1	A	890	G	N3-C4-C5	-6.42	125.39	128.60
1	A	1092	A	C5-C6-N6	6.42	128.83	123.70
1	A	1389	C	O5'-P-OP2	6.42	118.40	110.70
1	A	1410	G	N3-C2-N2	6.42	124.39	119.90
1	A	746	A	C4-C5-N7	-6.41	107.49	110.70
1	A	1129	C	C5-C6-N1	6.41	124.21	121.00
1	A	1200	C	N3-C4-C5	-6.41	119.33	121.90
1	A	47	C	C5-C6-N1	-6.41	117.79	121.00
1	A	443	C	C2-N3-C4	-6.41	116.69	119.90
1	A	150	C	O5'-P-OP1	6.41	118.39	110.70
1	A	1064	G	N7-C8-N9	6.41	116.31	113.10
1	A	81	U	OP1-P-OP2	6.41	129.21	119.60
1	A	282	A	C5-C6-N1	-6.41	114.50	117.70
1	A	582	U	N1-C2-O2	-6.41	118.31	122.80
1	A	814	A	OP2-P-O3'	6.41	119.30	105.20
1	A	825	G	N3-C4-C5	6.41	131.80	128.60
1	A	983	A	C2-N3-C4	-6.41	107.39	110.60
1	A	626	U	C5-C4-O4	-6.41	122.06	125.90
1	A	1202	G	C8-N9-C1'	6.41	135.33	127.00
1	A	1509	C	OP2-P-O3'	6.41	119.29	105.20
1	A	515	G	C5-C6-N1	-6.40	108.30	111.50
1	A	646	U	N3-C2-O2	-6.40	117.72	122.20
1	A	1049	U	C5-C4-O4	-6.40	122.06	125.90
1	A	168	G	C2-N3-C4	-6.40	108.70	111.90
1	A	902	G	C5-C6-O6	6.40	132.44	128.60
1	A	19	C	O5'-P-OP1	6.40	118.38	110.70
1	A	239	U	N1-C2-O2	-6.40	118.32	122.80
1	A	309	G	C2-N3-C4	6.40	115.10	111.90
1	A	1078	U	N3-C4-O4	6.40	123.88	119.40
1	A	1387	G	N1-C2-N3	6.40	127.74	123.90
1	A	562	C	N3-C2-O2	-6.40	117.42	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	711	G	C8-N9-C4	-6.40	103.84	106.40
1	A	1483	A	N1-C6-N6	6.40	122.44	118.60
1	A	54	C	C5-C6-N1	-6.40	117.80	121.00
1	A	76	C	N1-C2-O2	-6.40	115.06	118.90
1	A	302	G	O5'-P-OP1	-6.40	99.94	105.70
1	A	531	U	C6-N1-C2	-6.40	117.16	121.00
1	A	829	G	C8-N9-C4	6.40	108.96	106.40
1	A	1130	A	N7-C8-N9	6.40	117.00	113.80
1	A	422	C	C5-C6-N1	-6.39	117.80	121.00
1	A	429	U	O4'-C1'-N1	6.39	113.32	108.20
1	A	545	C	C4-C5-C6	6.39	120.60	117.40
1	A	1020	U	N3-C4-C5	-6.39	110.76	114.60
14	N	21	TYR	CB-CA-C	6.39	123.19	110.40
1	A	198	G	C5-N7-C8	6.39	107.50	104.30
1	A	281	G	N3-C4-N9	6.39	129.84	126.00
1	A	575	G	C6-N1-C2	-6.39	121.27	125.10
1	A	804	U	O4'-C1'-N1	6.39	113.31	108.20
1	A	908	A	N1-C2-N3	6.39	132.50	129.30
1	A	935	A	N7-C8-N9	6.39	117.00	113.80
1	A	1064	G	C8-N9-C1'	6.39	135.31	127.00
1	A	661	G	C5-C6-N1	-6.39	108.30	111.50
1	A	1022	G	C4-C5-N7	-6.39	108.24	110.80
1	A	1050	G	C5-C6-O6	-6.39	124.77	128.60
1	A	1105	A	O5'-P-OP2	-6.39	99.95	105.70
7	G	59	LEU	CA-CB-CG	-6.39	100.60	115.30
1	A	320	C	N1-C2-N3	-6.39	114.73	119.20
1	A	396	G	N3-C4-N9	-6.39	122.17	126.00
1	A	699	C	O5'-P-OP1	6.39	118.36	110.70
1	A	1205	U	C2-N3-C4	-6.39	123.17	127.00
1	A	1219	U	C5-C6-N1	-6.39	119.51	122.70
1	A	108	G	N9-C4-C5	-6.38	102.85	105.40
1	A	903	G	C8-N9-C1'	-6.38	118.70	127.00
1	A	970	C	O5'-P-OP2	6.38	118.36	110.70
1	A	190(A)	C	N3-C4-C5	-6.38	119.35	121.90
1	A	852	G	O5'-P-OP2	-6.38	99.95	105.70
1	A	886	G	C4-C5-C6	6.38	122.63	118.80
1	A	1378	C	C5-C4-N4	6.38	124.67	120.20
1	A	63	C	C6-N1-C2	6.38	122.85	120.30
1	A	606	G	N9-C4-C5	-6.38	102.85	105.40
1	A	1057	G	N1-C2-N3	6.38	127.73	123.90
1	A	1497	G	N7-C8-N9	6.38	116.29	113.10
1	A	243	A	N9-C4-C5	6.38	108.35	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1368	G	N1-C2-N2	-6.38	110.46	116.20
1	A	633	G	OP2-P-O3'	6.37	119.22	105.20
1	A	821	G	N3-C2-N2	-6.37	115.44	119.90
1	A	1121	U	N3-C2-O2	6.37	126.66	122.20
1	A	204	U	C6-N1-C2	-6.37	117.18	121.00
1	A	292	G	O4'-C1'-N9	-6.37	103.10	108.20
1	A	309	G	N3-C4-C5	-6.37	125.42	128.60
1	A	716	A	C5-C6-N6	-6.37	118.60	123.70
1	A	849	C	C6-N1-C2	-6.37	117.75	120.30
1	A	963	G	C6-C5-N7	-6.37	126.58	130.40
1	A	358	U	N3-C2-O2	-6.37	117.74	122.20
1	A	1197	G	N1-C2-N3	6.37	127.72	123.90
1	A	446	G	N9-C4-C5	6.37	107.95	105.40
1	A	564	C	N3-C2-O2	-6.37	117.44	121.90
1	A	724	G	C8-N9-C4	-6.37	103.85	106.40
1	A	422	C	O5'-P-OP2	-6.37	99.97	105.70
1	A	1159	U	N3-C4-O4	-6.37	114.94	119.40
1	A	754	C	N3-C2-O2	6.37	126.36	121.90
1	A	1144	G	C5-C6-N1	-6.37	108.32	111.50
1	A	1396	A	OP1-P-OP2	6.37	129.15	119.60
1	A	1526	G	C8-N9-C4	-6.37	103.85	106.40
1	A	462	G	N1-C2-N2	-6.36	110.47	116.20
1	A	1429	C	C6-N1-C2	-6.36	117.75	120.30
5	E	81	GLU	CB-CA-C	-6.36	97.67	110.40
1	A	383	A	C4-C5-N7	-6.36	107.52	110.70
1	A	657	G	O5'-P-OP1	6.36	118.33	110.70
1	A	1067	A	C2-N3-C4	-6.36	107.42	110.60
1	A	307	C	C2-N3-C4	6.36	123.08	119.90
1	A	639	G	C5-C6-O6	-6.36	124.78	128.60
1	A	855	G	C5-C6-O6	6.36	132.42	128.60
1	A	949	A	O4'-C1'-N9	-6.36	103.11	108.20
1	A	48	C	N3-C4-N4	6.36	122.45	118.00
1	A	181	G	C5-C6-N1	-6.36	108.32	111.50
1	A	909	A	C5-C6-N6	-6.36	118.61	123.70
1	A	919	A	C2-N3-C4	6.36	113.78	110.60
1	A	959	A	C8-N9-C4	6.36	108.34	105.80
1	A	1022	G	N3-C4-C5	-6.36	125.42	128.60
1	A	186	C	N3-C2-O2	-6.35	117.45	121.90
1	A	878	G	O5'-P-OP2	-6.35	99.98	105.70
1	A	954	G	N3-C4-C5	6.35	131.78	128.60
1	A	963	G	N1-C2-N2	-6.35	110.48	116.20
1	A	75	G	N1-C6-O6	6.35	123.71	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	G	C8-N9-C1'	-6.35	118.75	127.00
1	A	1055	A	C6-C5-N7	-6.35	127.86	132.30
1	A	774	G	N3-C4-N9	6.35	129.81	126.00
1	A	1205	U	N1-C2-N3	6.35	118.71	114.90
1	A	1350	A	C8-N9-C4	6.35	108.34	105.80
1	A	19	C	N1-C2-N3	6.34	123.64	119.20
1	A	218	C	N3-C4-N4	-6.34	113.56	118.00
1	A	510	A	N3-C4-N9	-6.34	122.32	127.40
1	A	622	A	N3-C4-C5	6.34	131.24	126.80
1	A	685	G	C2-N3-C4	-6.34	108.73	111.90
1	A	978	A	N1-C2-N3	6.34	132.47	129.30
1	A	576	G	C4-N9-C1'	6.34	134.75	126.50
1	A	317	G	N3-C4-N9	6.34	129.81	126.00
1	A	611	A	N1-C6-N6	-6.34	114.80	118.60
1	A	930	C	O5'-P-OP2	-6.34	99.99	105.70
1	A	1111	A	C6-N1-C2	-6.34	114.80	118.60
1	A	27	G	C6-C5-N7	-6.34	126.60	130.40
1	A	106	C	N3-C4-C5	-6.34	119.36	121.90
1	A	200	G	C8-N9-C4	6.34	108.94	106.40
1	A	409	G	C6-C5-N7	-6.34	126.60	130.40
1	A	969	A	C8-N9-C4	6.34	108.34	105.80
1	A	1139	G	C8-N9-C4	-6.34	103.86	106.40
1	A	19	C	C2-N3-C4	-6.34	116.73	119.90
1	A	780	A	P-O3'-C3'	6.34	127.30	119.70
1	A	1235	U	C5-C6-N1	-6.34	119.53	122.70
1	A	354	G	N7-C8-N9	6.33	116.27	113.10
1	A	1401	G	C5-C6-N1	6.33	114.67	111.50
1	A	944	G	C5-C6-O6	6.33	132.40	128.60
1	A	1529	G	N1-C2-N2	6.33	121.90	116.20
1	A	585	G	N1-C2-N3	6.33	127.70	123.90
1	A	1310	G	C4-N9-C1'	6.33	134.73	126.50
1	A	1497	G	C4-N9-C1'	6.33	134.73	126.50
1	A	252	U	C2-N1-C1'	-6.33	110.10	117.70
1	A	706	A	N1-C2-N3	6.33	132.47	129.30
1	A	1102	A	C5-C6-N1	6.33	120.86	117.70
1	A	502	G	C5-C6-N1	6.33	114.66	111.50
1	A	692	U	N3-C4-O4	-6.33	114.97	119.40
1	A	920	U	N1-C2-N3	-6.33	111.11	114.90
1	A	1118	C	C5-C6-N1	6.33	124.16	121.00
1	A	1539	C	N3-C4-N4	6.33	122.43	118.00
1	A	670	G	N3-C2-N2	6.32	124.33	119.90
1	A	925	G	N1-C6-O6	6.32	123.69	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1104	G	OP1-P-OP2	6.32	129.08	119.60
1	A	232	G	C6-C5-N7	-6.32	126.61	130.40
1	A	246	A	C8-N9-C4	6.32	108.33	105.80
1	A	904	C	C2-N3-C4	-6.32	116.74	119.90
1	A	974	A	C5-N7-C8	6.32	107.06	103.90
1	A	331	G	C5-C6-N1	-6.32	108.34	111.50
1	A	360	A	C5-C6-N6	-6.32	118.65	123.70
1	A	608	A	O5'-P-OP1	6.32	118.28	110.70
1	A	622	A	N1-C6-N6	6.32	122.39	118.60
1	A	1544	U	N1-C2-N3	6.32	118.69	114.90
1	A	568	G	O5'-P-OP2	6.31	118.28	110.70
1	A	404	U	N1-C2-N3	6.31	118.69	114.90
1	A	159	G	C8-N9-C4	-6.31	103.88	106.40
1	A	354	G	O5'-P-OP1	-6.31	100.02	105.70
1	A	710	G	N3-C4-N9	6.31	129.79	126.00
1	A	1379	G	N1-C6-O6	6.31	123.69	119.90
1	A	360	A	C6-N1-C2	-6.31	114.81	118.60
1	A	1247	U	N3-C4-C5	-6.31	110.82	114.60
1	A	20	U	C6-N1-C2	6.30	124.78	121.00
1	A	837	G	C5-C6-O6	-6.30	124.82	128.60
1	A	891	U	OP1-P-OP2	6.30	129.06	119.60
1	A	1327	C	C5-C6-N1	-6.30	117.85	121.00
1	A	1450	U	N3-C4-C5	-6.30	110.82	114.60
1	A	852	G	N3-C4-C5	6.30	131.75	128.60
1	A	1503	A	OP1-P-O3'	6.30	119.07	105.20
1	A	302	G	N1-C2-N3	6.30	127.68	123.90
1	A	379	C	N3-C4-N4	6.30	122.41	118.00
1	A	403	C	O5'-P-OP2	-6.30	100.03	105.70
1	A	55	A	N1-C2-N3	6.30	132.45	129.30
1	A	118	U	N3-C4-O4	-6.30	114.99	119.40
1	A	841	U	N1-C2-O2	6.30	127.21	122.80
1	A	499	A	N3-C4-N9	-6.29	122.36	127.40
1	A	31	G	C8-N9-C4	6.29	108.92	106.40
1	A	668	G	C2-N3-C4	-6.29	108.75	111.90
2	B	11	LEU	CB-CG-CD1	6.29	121.70	111.00
1	A	673	G	C8-N9-C1'	6.29	135.18	127.00
1	A	1491	G	N1-C6-O6	6.29	123.67	119.90
14	N	39	LEU	CA-CB-CG	-6.29	100.83	115.30
1	A	6	G	C6-N1-C2	-6.29	121.33	125.10
1	A	1426	C	N1-C2-N3	-6.29	114.80	119.20
1	A	686	U	C5-C6-N1	-6.29	119.56	122.70
1	A	759	A	N3-C4-C5	-6.29	122.40	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1104	G	C4-C5-C6	6.29	122.57	118.80
1	A	1450	U	O5'-P-OP2	-6.29	100.04	105.70
1	A	1408	A	N1-C2-N3	6.29	132.44	129.30
1	A	19	C	C2-N1-C1'	6.29	125.71	118.80
1	A	523	A	C5-C6-N6	-6.29	118.67	123.70
1	A	674	G	N9-C4-C5	-6.29	102.89	105.40
1	A	772	U	C6-N1-C2	-6.29	117.23	121.00
1	A	1126	U	N3-C2-O2	6.28	126.60	122.20
1	A	1493	A	N1-C6-N6	-6.28	114.83	118.60
1	A	1310	G	C8-N9-C1'	-6.28	118.83	127.00
1	A	1524	C	P-O5'-C5'	-6.28	110.85	120.90
1	A	15	G	P-O3'-C3'	6.28	127.24	119.70
1	A	815	A	O4'-C1'-N9	6.28	113.22	108.20
5	E	152	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	A	548	G	C6-C5-N7	-6.28	126.63	130.40
1	A	618	C	OP1-P-OP2	6.28	129.01	119.60
1	A	1162	C	N3-C4-N4	-6.28	113.61	118.00
1	A	122	G	OP1-P-O3'	6.28	119.01	105.20
1	A	983	A	C5-N7-C8	-6.28	100.76	103.90
4	D	96	LEU	CA-CB-CG	-6.28	100.86	115.30
1	A	63	C	O5'-P-OP2	-6.27	100.05	105.70
8	H	13	ILE	CB-CA-C	-6.27	99.06	111.60
1	A	1061	G	N3-C2-N2	-6.27	115.51	119.90
1	A	308	C	N1-C2-O2	-6.27	115.14	118.90
1	A	1294	G	C8-N9-C4	6.27	108.91	106.40
1	A	1521	G	N9-C4-C5	-6.27	102.89	105.40
1	A	265	G	N3-C2-N2	6.27	124.29	119.90
1	A	575	G	N3-C4-C5	-6.27	125.47	128.60
1	A	646	U	C6-N1-C2	-6.26	117.24	121.00
1	A	1054	C	C6-N1-C1'	-6.26	113.28	120.80
1	A	1060	C	C4-C5-C6	6.26	120.53	117.40
1	A	36	C	O5'-P-OP2	-6.26	100.06	105.70
1	A	52	G	N1-C2-N2	6.26	121.83	116.20
1	A	1277	C	C2-N1-C1'	6.26	125.69	118.80
1	A	226	G	C5-C6-N1	-6.26	108.37	111.50
1	A	1468	A	C6-N1-C2	-6.26	114.84	118.60
1	A	228	A	N1-C2-N3	6.26	132.43	129.30
1	A	298	A	N9-C4-C5	6.26	108.30	105.80
1	A	364	A	O5'-P-OP2	6.26	118.21	110.70
3	C	21	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	5	U	O5'-P-OP1	-6.25	100.07	105.70
1	A	270	A	C5-C6-N1	6.25	120.83	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	641	U	C5-C4-O4	-6.25	122.15	125.90
1	A	41	G	N1-C2-N2	6.25	121.83	116.20
1	A	61	G	N9-C4-C5	-6.25	102.90	105.40
1	A	216	G	C5-C6-O6	-6.25	124.85	128.60
1	A	411	A	N1-C6-N6	6.25	122.35	118.60
4	D	30	LYS	N-CA-C	6.25	127.88	111.00
1	A	272	C	C2-N1-C1'	6.25	125.67	118.80
1	A	281	G	C6-N1-C2	-6.25	121.35	125.10
1	A	550	G	N1-C2-N2	-6.25	110.58	116.20
1	A	736	C	C2-N3-C4	-6.25	116.78	119.90
1	A	982	U	C2-N1-C1'	6.25	125.19	117.70
1	A	1252	A	C8-N9-C4	6.25	108.30	105.80
1	A	41	G	C5-C6-O6	-6.24	124.85	128.60
1	A	1088	G	N3-C4-C5	-6.24	125.48	128.60
1	A	1350	A	C5-C6-N1	6.24	120.82	117.70
1	A	1491	G	O4'-C1'-N9	6.24	113.19	108.20
1	A	261	U	N3-C4-C5	-6.24	110.86	114.60
1	A	557	G	C6-C5-N7	-6.24	126.66	130.40
1	A	588	G	OP1-P-O3'	6.24	118.92	105.20
1	A	663	A	C5-C6-N1	-6.24	114.58	117.70
1	A	1064	G	C4-C5-N7	6.24	113.30	110.80
1	A	504	C	C5-C4-N4	-6.24	115.83	120.20
1	A	442	C	C5-C6-N1	-6.24	117.88	121.00
1	A	869	G	C8-N9-C4	-6.24	103.91	106.40
1	A	971	G	C4-C5-C6	6.24	122.54	118.80
1	A	1193	G	C5-C6-N1	-6.24	108.38	111.50
1	A	221	C	C2-N1-C1'	6.23	125.66	118.80
1	A	319	G	N3-C2-N2	-6.23	115.54	119.90
1	A	1085	U	P-O3'-C3'	6.23	127.18	119.70
1	A	388	G	C4-C5-C6	6.23	122.54	118.80
1	A	867	G	C5-C6-O6	-6.23	124.86	128.60
1	A	270	A	C8-N9-C4	-6.23	103.31	105.80
1	A	446	G	N3-C2-N2	-6.23	115.54	119.90
1	A	1127	G	N1-C6-O6	6.23	123.64	119.90
1	A	396	G	N9-C4-C5	6.23	107.89	105.40
1	A	254	G	OP1-P-OP2	6.23	128.94	119.60
1	A	282	A	OP2-P-O3'	6.23	118.90	105.20
1	A	329	A	C6-C5-N7	-6.23	127.94	132.30
1	A	1168	A	N9-C4-C5	6.23	108.29	105.80
1	A	35	G	N1-C2-N3	6.23	127.64	123.90
1	A	37	U	N1-C2-N3	6.22	118.63	114.90
1	A	948	C	O5'-P-OP2	-6.22	100.10	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1261	A	N1-C6-N6	6.22	122.33	118.60
1	A	299	G	C2-N3-C4	-6.22	108.79	111.90
1	A	672	U	C4-C5-C6	-6.22	115.97	119.70
1	A	251	G	N9-C4-C5	-6.22	102.91	105.40
1	A	301	G	N1-C2-N2	6.22	121.80	116.20
1	A	301	G	N9-C4-C5	6.22	107.89	105.40
1	A	716	A	C4-C5-N7	6.22	113.81	110.70
1	A	750	G	C5-C6-N1	6.22	114.61	111.50
1	A	1092	A	N9-C4-C5	6.22	108.29	105.80
1	A	1381	U	N3-C4-C5	-6.22	110.87	114.60
1	A	221	C	N3-C4-C5	-6.21	119.41	121.90
1	A	535	A	N9-C4-C5	6.21	108.29	105.80
1	A	783	C	C6-N1-C2	6.21	122.79	120.30
1	A	1453	G	C8-N9-C1'	-6.21	118.92	127.00
1	A	360	A	O5'-P-OP1	-6.21	100.11	105.70
1	A	1057	G	N1-C6-O6	-6.21	116.17	119.90
1	A	1345	U	C4-C5-C6	6.21	123.43	119.70
1	A	176	C	C5-C4-N4	-6.21	115.86	120.20
1	A	800	G	OP1-P-OP2	6.21	128.91	119.60
1	A	1039	C	N1-C2-O2	6.21	122.62	118.90
1	A	1109	C	N3-C4-C5	6.21	124.38	121.90
1	A	1287	A	N3-C4-N9	6.21	132.37	127.40
1	A	1503	A	N1-C2-N3	6.21	132.40	129.30
1	A	1539	C	C2-N3-C4	6.21	123.00	119.90
1	A	110	C	O5'-P-OP1	-6.21	100.11	105.70
1	A	1455	G	N1-C2-N3	6.21	127.62	123.90
1	A	548	G	C2-N3-C4	-6.20	108.80	111.90
1	A	1271	G	N3-C4-C5	6.20	131.70	128.60
1	A	129(A)	G	N1-C6-O6	6.20	123.62	119.90
1	A	187	C	N3-C4-C5	-6.20	119.42	121.90
1	A	559	A	O4'-C1'-N9	-6.20	103.24	108.20
1	A	1334	G	C8-N9-C4	-6.20	103.92	106.40
1	A	65	U	OP1-P-O3'	6.20	118.84	105.20
1	A	198	G	N3-C4-N9	6.20	129.72	126.00
1	A	1236	A	C2-N3-C4	-6.20	107.50	110.60
1	A	1443	G	C8-N9-C1'	6.20	135.06	127.00
1	A	454	C	N1-C2-N3	-6.20	114.86	119.20
1	A	766	A	C2-N3-C4	-6.20	107.50	110.60
1	A	861	G	O5'-P-OP1	-6.20	100.12	105.70
1	A	1076	C	N3-C4-C5	6.20	124.38	121.90
1	A	1193	G	C6-N1-C2	-6.20	121.38	125.10
1	A	1539	C	N3-C4-C5	-6.20	119.42	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	100	ILE	CB-CA-C	-6.20	99.20	111.60
1	A	397	A	C8-N9-C4	-6.20	103.32	105.80
1	A	736	C	O4'-C1'-N1	6.20	113.16	108.20
1	A	369	C	O5'-P-OP2	-6.20	100.12	105.70
1	A	431	A	OP2-P-O3'	6.20	118.83	105.20
1	A	833	U	C6-N1-C2	6.19	124.72	121.00
1	A	451	A	C4-C5-C6	6.19	120.10	117.00
1	A	598	U	C5-C4-O4	-6.19	122.19	125.90
1	A	316	G	C8-N9-C1'	-6.19	118.95	127.00
1	A	442	C	C2-N3-C4	-6.19	116.81	119.90
1	A	818	G	C4-C5-N7	-6.19	108.33	110.80
1	A	1202	G	C5-C6-N1	-6.19	108.41	111.50
1	A	1354	C	C2-N1-C1'	-6.19	111.99	118.80
1	A	1118	C	N1-C2-O2	-6.19	115.19	118.90
1	A	812	C	OP2-P-O3'	6.18	118.81	105.20
1	A	928	G	OP2-P-O3'	6.18	118.81	105.20
1	A	931	C	C2-N3-C4	6.18	122.99	119.90
1	A	1144	G	C8-N9-C4	6.18	108.87	106.40
1	A	543	C	C6-N1-C2	-6.18	117.83	120.30
1	A	897	C	C2-N3-C4	-6.18	116.81	119.90
1	A	1337	G	C6-C5-N7	-6.18	126.69	130.40
1	A	395	C	C4-C5-C6	-6.18	114.31	117.40
1	A	1493	A	C4-N9-C1'	6.18	137.43	126.30
2	B	180	LEU	CB-CG-CD1	6.18	121.51	111.00
1	A	726	C	C6-N1-C2	-6.18	117.83	120.30
1	A	939	G	N7-C8-N9	6.18	116.19	113.10
1	A	1371	G	C4-C5-N7	6.18	113.27	110.80
1	A	1463	C	O5'-P-OP2	-6.18	100.14	105.70
1	A	1508	G	C5-N7-C8	-6.18	101.21	104.30
1	A	169	C	C2-N3-C4	6.18	122.99	119.90
1	A	710	G	C5-C6-O6	-6.18	124.89	128.60
1	A	937	A	C5-C6-N6	6.18	128.64	123.70
1	A	780	A	N3-C4-C5	-6.18	122.48	126.80
1	A	1084	G	C8-N9-C4	-6.17	103.93	106.40
1	A	1396	A	C5-C6-N1	-6.17	114.61	117.70
1	A	1193	G	C4-N9-C1'	6.17	134.53	126.50
1	A	965	A	N7-C8-N9	-6.17	110.71	113.80
1	A	688	G	OP1-P-OP2	6.17	128.85	119.60
1	A	1162	C	N3-C4-C5	6.17	124.37	121.90
1	A	288	A	OP2-P-O3'	6.17	118.77	105.20
1	A	576	G	C4-C5-C6	6.17	122.50	118.80
1	A	129	U	N1-C2-N3	-6.16	111.20	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	G	N3-C2-N2	-6.16	115.59	119.90
1	A	1186	G	C8-N9-C4	-6.16	103.94	106.40
1	A	423	G	N3-C4-N9	6.16	129.70	126.00
1	A	503	C	O5'-P-OP1	6.16	118.09	110.70
1	A	511	C	N1-C2-N3	6.16	123.51	119.20
1	A	593	G	C4-C5-C6	6.16	122.49	118.80
1	A	1515[A]	C	C4-C5-C6	-6.16	114.32	117.40
1	A	1515[B]	C	C4-C5-C6	-6.16	114.32	117.40
1	A	416	G	N7-C8-N9	6.16	116.18	113.10
1	A	499	A	N9-C4-C5	6.16	108.26	105.80
1	A	699	C	N3-C4-N4	-6.16	113.69	118.00
1	A	1014	A	C2-N3-C4	6.15	113.68	110.60
1	A	830	G	C5-C6-O6	-6.15	124.91	128.60
1	A	1197	G	C5-N7-C8	-6.15	101.22	104.30
1	A	1531	A	C8-N9-C4	-6.15	103.34	105.80
1	A	1182	G	C8-N9-C1'	-6.15	119.00	127.00
1	A	1364	U	N3-C4-C5	6.15	118.29	114.60
1	A	109	A	N7-C8-N9	6.15	116.88	113.80
1	A	770	C	C2-N3-C4	-6.15	116.83	119.90
1	A	919	A	C8-N9-C4	-6.15	103.34	105.80
1	A	172	A	OP1-P-OP2	-6.15	110.38	119.60
1	A	429	U	O5'-P-OP2	6.15	118.08	110.70
1	A	1194	U	C5-C4-O4	-6.15	122.21	125.90
1	A	32	A	C6-C5-N7	-6.15	128.00	132.30
1	A	425	G	C5-N7-C8	6.15	107.37	104.30
1	A	582	U	C6-N1-C2	-6.15	117.31	121.00
1	A	759	A	N1-C2-N3	6.15	132.37	129.30
1	A	1057	G	C5-C6-N1	6.15	114.57	111.50
1	A	1391	U	OP1-P-OP2	-6.14	110.39	119.60
1	A	461	C	OP2-P-O3'	6.14	118.71	105.20
1	A	715	A	OP1-P-O3'	6.14	118.71	105.20
1	A	953	G	C4-N9-C1'	6.14	134.49	126.50
1	A	21	G	C5-C6-N1	6.14	114.57	111.50
1	A	1279	A	C5-C6-N1	-6.14	114.63	117.70
1	A	1486	G	C8-N9-C1'	-6.14	119.02	127.00
1	A	357	G	O5'-P-OP2	-6.14	100.18	105.70
1	A	1370	G	N3-C2-N2	-6.14	115.61	119.90
1	A	127	G	OP1-P-OP2	6.13	128.80	119.60
1	A	232	G	C5-N7-C8	-6.13	101.23	104.30
1	A	646	U	N1-C2-N3	6.13	118.58	114.90
1	A	364	A	C4-C5-C6	6.13	120.07	117.00
1	A	123	C	N3-C4-N4	6.13	122.29	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	583	A	C4-C5-C6	6.13	120.06	117.00
1	A	896	C	C2-N1-C1'	-6.13	112.06	118.80
1	A	35	G	C4-C5-C6	6.13	122.48	118.80
1	A	631	G	O5'-P-OP2	-6.13	100.19	105.70
1	A	1168	A	C2-N3-C4	6.13	113.67	110.60
1	A	1389	C	C5-C4-N4	-6.13	115.91	120.20
1	A	1438	G	N1-C6-O6	6.13	123.58	119.90
1	A	196	A	O5'-P-OP1	-6.13	100.19	105.70
1	A	544	G	N9-C4-C5	-6.13	102.95	105.40
1	A	684	A	N7-C8-N9	6.13	116.86	113.80
1	A	801	U	N3-C4-O4	-6.13	115.11	119.40
1	A	1149	C	C5-C6-N1	6.13	124.06	121.00
1	A	1189	C	C6-N1-C1'	-6.13	113.45	120.80
1	A	112	G	O5'-P-OP2	-6.12	100.19	105.70
1	A	675	A	C2-N3-C4	-6.12	107.54	110.60
1	A	45	U	N3-C4-O4	-6.12	115.11	119.40
1	A	286	G	N3-C2-N2	-6.12	115.61	119.90
1	A	439	A	OP1-P-OP2	-6.12	110.42	119.60
1	A	1003(A)	G	C8-N9-C1'	-6.12	119.04	127.00
1	A	318	G	C6-C5-N7	-6.12	126.73	130.40
1	A	687	A	O4'-C1'-N9	6.12	113.10	108.20
1	A	830	G	C8-N9-C4	6.12	108.85	106.40
1	A	556	C	C5-C4-N4	-6.12	115.92	120.20
1	A	1058	G	C6-C5-N7	-6.12	126.73	130.40
1	A	497	A	O5'-P-OP1	-6.12	100.19	105.70
1	A	1340	A	OP1-P-OP2	6.12	128.78	119.60
1	A	662	G	C4-N9-C1'	6.12	134.45	126.50
1	A	691	G	C4-C5-C6	6.12	122.47	118.80
1	A	1346	A	N1-C6-N6	-6.12	114.93	118.60
1	A	229	U	N3-C4-O4	6.11	123.68	119.40
1	A	289	G	C8-N9-C1'	-6.11	119.05	127.00
1	A	681	C	N3-C4-N4	6.11	122.28	118.00
1	A	816	A	O5'-P-OP1	-6.11	100.20	105.70
1	A	867	G	N3-C2-N2	-6.11	115.62	119.90
1	A	1225	A	C4-C5-C6	6.11	120.06	117.00
1	A	620	C	C4-C5-C6	-6.11	114.34	117.40
1	A	1505	G	O5'-P-OP1	6.11	118.03	110.70
1	A	490	G	N3-C4-C5	-6.11	125.55	128.60
1	A	1530	G	O4'-C1'-N9	6.11	113.09	108.20
1	A	363	A	C6-C5-N7	-6.11	128.02	132.30
1	A	1183	A	O4'-C1'-N9	6.11	113.08	108.20
1	A	298	A	N1-C2-N3	6.11	132.35	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	C	OP1-P-O3'	6.11	118.63	105.20
1	A	1373	G	N3-C4-C5	-6.11	125.55	128.60
1	A	1387	G	OP1-P-O3'	6.11	118.63	105.20
1	A	517	G	OP1-P-O3'	6.10	118.63	105.20
1	A	438	G	C6-N1-C2	6.10	128.76	125.10
1	A	1338	G	N1-C2-N2	-6.10	110.71	116.20
1	A	289	G	C6-C5-N7	-6.10	126.74	130.40
1	A	1055	A	C4-C5-N7	6.10	113.75	110.70
1	A	276	G	C6-N1-C2	-6.10	121.44	125.10
1	A	574	A	N7-C8-N9	6.10	116.85	113.80
1	A	641	U	C2-N3-C4	-6.10	123.34	127.00
1	A	10	A	OP1-P-OP2	6.10	128.75	119.60
1	A	1312	G	C2-N3-C4	-6.10	108.85	111.90
1	A	1390	U	N1-C2-N3	6.09	118.56	114.90
1	A	293	G	O5'-P-OP1	6.09	118.01	110.70
1	A	1075	C	N3-C4-N4	-6.09	113.74	118.00
1	A	1239	A	N9-C4-C5	-6.09	103.36	105.80
1	A	664	G	N9-C4-C5	6.09	107.84	105.40
1	A	900	A	C5-N7-C8	-6.09	100.86	103.90
1	A	938	A	N9-C4-C5	6.09	108.24	105.80
1	A	1092	A	N1-C6-N6	-6.09	114.95	118.60
1	A	1544	U	C5-C4-O4	6.09	129.55	125.90
1	A	688	G	C8-N9-C1'	-6.09	119.08	127.00
1	A	851	G	C2-N3-C4	-6.09	108.86	111.90
1	A	406	G	C2-N3-C4	6.09	114.94	111.90
1	A	1051	C	N3-C4-N4	-6.09	113.74	118.00
1	A	1308	U	N3-C4-O4	6.09	123.66	119.40
1	A	654	G	OP1-P-OP2	6.08	128.73	119.60
1	A	1124	G	N7-C8-N9	6.08	116.14	113.10
1	A	42	G	C8-N9-C4	-6.08	103.97	106.40
1	A	341	C	C5-C6-N1	6.08	124.04	121.00
1	A	406	G	OP2-P-O3'	6.08	118.58	105.20
1	A	654	G	N3-C2-N2	-6.08	115.64	119.90
1	A	699	C	C4-C5-C6	-6.08	114.36	117.40
1	A	710	G	C4-N9-C1'	6.08	134.41	126.50
1	A	1480	G	C5-C6-N1	-6.08	108.46	111.50
1	A	197	A	N1-C6-N6	-6.08	114.95	118.60
1	A	450	G	N3-C2-N2	-6.08	115.64	119.90
1	A	501	C	C2-N3-C4	-6.08	116.86	119.90
1	A	511	C	O5'-P-OP2	-6.08	100.23	105.70
1	A	558	G	C8-N9-C4	6.08	108.83	106.40
1	A	789	U	N1-C2-O2	-6.08	118.54	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1525	G	N1-C2-N3	6.08	127.55	123.90
1	A	158	G	C8-N9-C4	-6.08	103.97	106.40
1	A	230	G	N1-C2-N2	-6.08	110.73	116.20
1	A	7	G	C8-N9-C4	6.08	108.83	106.40
1	A	976	G	N7-C8-N9	-6.08	110.06	113.10
1	A	1220	G	C2-N3-C4	6.08	114.94	111.90
1	A	1452	C	N3-C2-O2	-6.08	117.65	121.90
1	A	702	A	O5'-P-OP1	6.08	117.99	110.70
1	A	539	A	C5-C6-N1	6.08	120.74	117.70
1	A	702	A	N7-C8-N9	-6.08	110.76	113.80
1	A	1526	G	N9-C4-C5	6.08	107.83	105.40
1	A	108	G	C8-N9-C1'	-6.07	119.11	127.00
1	A	662	G	N7-C8-N9	6.07	116.14	113.10
1	A	892	A	C5-C6-N6	-6.07	118.84	123.70
1	A	128	G	C8-N9-C1'	-6.07	119.11	127.00
1	A	383	A	N1-C6-N6	-6.07	114.96	118.60
1	A	1112	C	N3-C4-N4	-6.07	113.75	118.00
1	A	1423	G	N3-C2-N2	-6.07	115.65	119.90
1	A	564	C	C6-N1-C2	6.07	122.73	120.30
1	A	248	C	N3-C4-N4	-6.07	113.75	118.00
1	A	894	G	N9-C4-C5	-6.07	102.97	105.40
1	A	423	G	C6-C5-N7	-6.07	126.76	130.40
1	A	500	G	N3-C2-N2	-6.07	115.66	119.90
1	A	566	G	C5-C6-O6	-6.07	124.96	128.60
1	A	715	A	C5-C6-N6	-6.07	118.85	123.70
1	A	1205	U	C5-C6-N1	-6.07	119.67	122.70
1	A	1543	C	OP2-P-O3'	6.07	118.54	105.20
1	A	515	G	C5-C6-O6	-6.06	124.96	128.60
1	A	933	G	N1-C2-N3	6.06	127.54	123.90
1	A	36	C	O5'-P-OP1	6.06	117.97	110.70
1	A	317	G	O5'-P-OP1	6.06	117.97	110.70
1	A	423	G	C5-C6-O6	-6.06	124.96	128.60
1	A	697	U	OP2-P-O3'	6.06	118.54	105.20
1	A	740	U	N1-C2-N3	6.06	118.54	114.90
1	A	1185	G	C5-C6-N1	-6.06	108.47	111.50
1	A	281	G	N9-C4-C5	-6.06	102.98	105.40
1	A	147	G	C4-C5-C6	6.06	122.44	118.80
1	A	1410	G	C5-C6-O6	6.06	132.24	128.60
1	A	689	C	O5'-P-OP2	-6.06	100.25	105.70
1	A	1090	U	N3-C4-O4	6.06	123.64	119.40
1	A	1335	C	C5-C6-N1	-6.06	117.97	121.00
1	A	183	G	N3-C4-C5	-6.06	125.57	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1350	A	O5'-P-OP1	6.06	117.97	110.70
1	A	746	A	C5-C6-N1	6.05	120.73	117.70
1	A	857	C	N3-C4-N4	6.05	122.24	118.00
1	A	1467	G	C5-C6-N1	6.05	114.53	111.50
1	A	625	G	N3-C2-N2	-6.05	115.66	119.90
1	A	1208	C	N3-C4-C5	6.05	124.32	121.90
1	A	523	A	N9-C4-C5	-6.05	103.38	105.80
1	A	646	U	OP2-P-O3'	6.05	118.52	105.20
1	A	797	C	O5'-P-OP2	-6.05	100.25	105.70
1	A	1126	U	N3-C4-O4	-6.05	115.16	119.40
15	O	79	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	50	A	OP1-P-OP2	6.05	128.67	119.60
1	A	246	A	N7-C8-N9	-6.05	110.78	113.80
1	A	55	A	C5-C6-N6	6.05	128.54	123.70
1	A	258	G	C5-C6-O6	-6.05	124.97	128.60
1	A	419	C	N3-C2-O2	-6.05	117.67	121.90
1	A	814	A	OP1-P-OP2	-6.05	110.53	119.60
1	A	953	G	N3-C2-N2	6.05	124.13	119.90
1	A	1211	U	O4'-C1'-N1	6.05	113.04	108.20
1	A	1249	C	C6-N1-C2	6.05	122.72	120.30
1	A	268	C	O5'-P-OP1	-6.04	100.26	105.70
1	A	650	G	N9-C4-C5	6.04	107.82	105.40
1	A	487	A	C6-N1-C2	-6.04	114.98	118.60
1	A	21	G	C8-N9-C4	6.04	108.82	106.40
1	A	635	G	O5'-P-OP1	-6.04	100.26	105.70
1	A	892	A	N3-C4-N9	6.04	132.23	127.40
1	A	184	G	C5-N7-C8	6.04	107.32	104.30
1	A	303	A	C6-N1-C2	-6.04	114.98	118.60
1	A	447	G	C6-C5-N7	-6.04	126.78	130.40
1	A	753	A	C5-C6-N6	6.04	128.53	123.70
1	A	548	G	C4-C5-N7	6.04	113.22	110.80
1	A	620	C	C2-N3-C4	-6.04	116.88	119.90
1	A	1203	C	C5-C6-N1	-6.04	117.98	121.00
1	A	106	C	C6-N1-C2	-6.04	117.89	120.30
1	A	428	G	C5-C6-O6	6.04	132.22	128.60
1	A	696	A	C2-N3-C4	-6.04	107.58	110.60
1	A	322	C	N1-C2-O2	-6.03	115.28	118.90
1	A	447	G	N3-C4-N9	6.03	129.62	126.00
1	A	505	G	C6-N1-C2	-6.03	121.48	125.10
1	A	721	G	N3-C4-N9	6.03	129.62	126.00
1	A	956	U	C5-C6-N1	-6.03	119.68	122.70
1	A	1255	G	C5-C6-O6	-6.03	124.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	G	N3-C4-C5	-6.03	125.58	128.60
1	A	761	G	C5-C6-N1	-6.03	108.48	111.50
1	A	1505	G	C4-C5-N7	-6.03	108.39	110.80
1	A	183	G	C6-N1-C2	-6.03	121.48	125.10
1	A	570	G	OP1-P-O3'	6.03	118.46	105.20
1	A	317	G	C4-C5-N7	6.03	113.21	110.80
1	A	254	G	OP2-P-O3'	6.02	118.45	105.20
1	A	320	C	C5-C4-N4	-6.02	115.98	120.20
1	A	1095	U	N3-C4-C5	-6.02	110.99	114.60
1	A	28	G	OP1-P-OP2	6.02	128.63	119.60
1	A	620	C	N3-C4-N4	-6.02	113.79	118.00
1	A	230	G	C6-C5-N7	-6.02	126.79	130.40
1	A	519	C	C5-C6-N1	-6.02	117.99	121.00
1	A	579	G	N9-C4-C5	-6.02	102.99	105.40
1	A	597	G	C4-C5-C6	6.02	122.41	118.80
1	A	1377	A	N9-C4-C5	6.02	108.21	105.80
1	A	257	G	C6-C5-N7	-6.02	126.79	130.40
1	A	113	G	C6-N1-C2	-6.01	121.49	125.10
1	A	236	G	N1-C2-N2	-6.01	110.79	116.20
1	A	408	A	C6-C5-N7	-6.01	128.09	132.30
1	A	902	G	C6-C5-N7	6.01	134.01	130.40
1	A	627	G	N3-C4-N9	-6.01	122.39	126.00
1	A	856	C	C2-N3-C4	-6.01	116.89	119.90
1	A	872	A	OP2-P-O3'	6.01	118.42	105.20
1	A	941	G	N1-C6-O6	6.01	123.51	119.90
1	A	316	G	C2-N3-C4	-6.01	108.90	111.90
1	A	1266	G	N3-C4-C5	6.01	131.60	128.60
1	A	641	U	C6-N1-C1'	-6.01	112.79	121.20
1	A	973	G	N9-C4-C5	6.01	107.80	105.40
17	Q	70	ARG	NE-CZ-NH1	-6.01	117.30	120.30
1	A	319	G	C6-C5-N7	-6.00	126.80	130.40
1	A	528	C	OP2-P-O3'	6.00	118.41	105.20
1	A	439	A	C4-C5-N7	-6.00	107.70	110.70
1	A	654	G	N7-C8-N9	6.00	116.10	113.10
1	A	814	A	C6-N1-C2	-6.00	115.00	118.60
1	A	1398	A	C2-N3-C4	6.00	113.60	110.60
1	A	233	C	C6-N1-C2	6.00	122.70	120.30
1	A	447	G	C8-N9-C1'	-6.00	119.20	127.00
1	A	1463	C	C5-C6-N1	-6.00	118.00	121.00
1	A	888	G	C6-N1-C2	-6.00	121.50	125.10
1	A	1189	C	C2-N3-C4	6.00	122.90	119.90
1	A	875	C	N3-C4-C5	6.00	124.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1342	C	O5'-P-OP2	-6.00	100.30	105.70
1	A	1191	A	O5'-P-OP1	-6.00	100.30	105.70
1	A	783	C	N3-C2-O2	5.99	126.10	121.90
1	A	1112	C	C6-N1-C1'	5.99	127.99	120.80
1	A	139	G	C5-C6-N1	5.99	114.50	111.50
1	A	949	A	C2-N3-C4	-5.99	107.60	110.60
1	A	309	G	C5-C6-O6	-5.99	125.01	128.60
1	A	622	A	C4-C5-N7	5.99	113.69	110.70
1	A	782	A	N1-C2-N3	5.99	132.29	129.30
1	A	990	C	C5-C6-N1	5.99	123.99	121.00
5	E	123	LEU	CA-CB-CG	-5.99	101.53	115.30
1	A	971	G	N1-C2-N3	5.99	127.49	123.90
1	A	443	C	C6-N1-C2	5.98	122.69	120.30
1	A	92	C	N3-C4-C5	-5.98	119.51	121.90
1	A	115	G	C6-N1-C2	-5.98	121.51	125.10
1	A	724	G	N1-C2-N2	-5.98	110.81	116.20
1	A	753	A	C2-N3-C4	5.98	113.59	110.60
1	A	1054	C	C2-N3-C4	5.98	122.89	119.90
19	S	31	ILE	N-CA-C	-5.98	94.85	111.00
1	A	229	U	C4-C5-C6	5.98	123.29	119.70
1	A	498	U	O5'-P-OP1	5.98	117.88	110.70
1	A	646	U	O5'-P-OP2	-5.98	100.32	105.70
1	A	727	G	C8-N9-C1'	5.98	134.78	127.00
1	A	755	G	C5-C6-O6	-5.98	125.01	128.60
1	A	502	G	N7-C8-N9	-5.98	110.11	113.10
1	A	579	G	C5-C6-O6	-5.98	125.01	128.60
1	A	1368	G	C4-N9-C1'	5.98	134.27	126.50
1	A	706	A	C2-N3-C4	-5.98	107.61	110.60
1	A	1161	C	C4-C5-C6	5.98	120.39	117.40
1	A	257	G	N1-C2-N3	5.98	127.49	123.90
1	A	368	U	C6-N1-C2	-5.98	117.41	121.00
1	A	481	G	C5-C6-N1	5.98	114.49	111.50
1	A	915	A	OP1-P-OP2	5.98	128.56	119.60
1	A	1483	A	C2-N3-C4	-5.98	107.61	110.60
1	A	820	U	OP2-P-O3'	5.97	118.34	105.20
1	A	863	U	C5-C6-N1	-5.97	119.71	122.70
1	A	329	A	C8-N9-C4	-5.97	103.41	105.80
1	A	377	G	N1-C6-O6	-5.97	116.32	119.90
1	A	557	G	C6-N1-C2	-5.97	121.52	125.10
1	A	1107	C	N3-C4-C5	5.97	124.29	121.90
1	A	1376	U	N3-C4-C5	-5.97	111.02	114.60
1	A	485	G	C5-C6-O6	5.97	132.18	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	858	G	P-O3'-C3'	5.97	126.86	119.70
1	A	858	G	N7-C8-N9	5.97	116.09	113.10
1	A	864	A	C4-C5-N7	-5.97	107.71	110.70
1	A	1355	G	N3-C4-C5	-5.97	125.61	128.60
1	A	298	A	OP2-P-O3'	5.97	118.33	105.20
1	A	282	A	N3-C4-C5	5.97	130.98	126.80
1	A	1049	U	N1-C2-O2	-5.97	118.62	122.80
1	A	1204	A	O5'-P-OP2	5.97	117.86	110.70
1	A	198	G	C5-C6-N1	5.97	114.48	111.50
1	A	371	G	N1-C6-O6	-5.97	116.32	119.90
1	A	1002	G	C6-C5-N7	5.97	133.98	130.40
1	A	222	U	O5'-P-OP1	5.96	117.86	110.70
1	A	383	A	C4-C5-C6	5.96	119.98	117.00
1	A	403	C	OP1-P-O3'	5.96	118.32	105.20
1	A	1340	A	C6-N1-C2	-5.96	115.02	118.60
1	A	1413	A	O5'-P-OP1	-5.96	100.33	105.70
1	A	594	G	C5-C6-N1	5.96	114.48	111.50
1	A	1367	C	N1-C2-O2	-5.96	115.32	118.90
11	K	125	PHE	N-CA-C	5.96	127.10	111.00
1	A	276	G	N1-C2-N3	5.96	127.48	123.90
1	A	1084	G	C5-C6-O6	5.96	132.18	128.60
1	A	264	U	C2-N1-C1'	5.96	124.85	117.70
1	A	515	G	C2-N3-C4	-5.96	108.92	111.90
1	A	1216	G	C5-C6-N1	-5.96	108.52	111.50
1	A	1288	A	C5-C6-N6	5.96	128.47	123.70
1	A	724	G	C4-C5-C6	5.96	122.37	118.80
1	A	1416	G	C4-C5-C6	5.96	122.37	118.80
1	A	1520[A]	G	N3-C4-N9	5.96	129.57	126.00
1	A	1520[B]	G	N3-C4-N9	5.96	129.57	126.00
1	A	329	A	O5'-P-OP2	5.95	117.84	110.70
1	A	691	G	N1-C6-O6	-5.95	116.33	119.90
16	P	26	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	221	C	C4-C5-C6	5.95	120.38	117.40
1	A	353	A	OP2-P-O3'	5.95	118.29	105.20
1	A	93	G	N1-C6-O6	5.95	123.47	119.90
1	A	434	U	C5-C6-N1	5.95	125.67	122.70
4	D	88	VAL	CB-CA-C	-5.95	100.10	111.40
1	A	184	G	C5-C6-O6	5.95	132.17	128.60
1	A	227	G	C2-N3-C4	-5.95	108.93	111.90
1	A	385	C	C6-N1-C2	-5.95	117.92	120.30
1	A	1101	A	N1-C6-N6	5.95	122.17	118.60
1	A	389	A	C4-C5-C6	5.95	119.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	A	C6-C5-N7	-5.95	128.14	132.30
1	A	884	U	N3-C2-O2	-5.95	118.04	122.20
1	A	1520[A]	G	C4-C5-C6	5.95	122.37	118.80
1	A	1520[B]	G	C4-C5-C6	5.95	122.37	118.80
1	A	38	G	N1-C6-O6	5.94	123.47	119.90
1	A	318	G	C5-C6-N1	-5.94	108.53	111.50
1	A	22	G	O5'-P-OP2	5.94	117.83	110.70
1	A	1195	C	C5-C4-N4	-5.94	116.04	120.20
1	A	1335	C	C6-N1-C1'	5.94	127.93	120.80
1	A	1521	G	C6-C5-N7	-5.94	126.83	130.40
1	A	1523	G	OP2-P-O3'	5.94	118.27	105.20
6	F	72	VAL	CB-CA-C	-5.94	100.11	111.40
6	F	87	ARG	NE-CZ-NH1	5.94	123.27	120.30
12	L	85	ILE	CG1-CB-CG2	-5.94	98.32	111.40
1	A	190(H)	G	C5-C6-O6	-5.94	125.04	128.60
1	A	1493	A	C5-C6-N1	5.94	120.67	117.70
1	A	23	C	C5-C6-N1	-5.94	118.03	121.00
1	A	309	G	OP1-P-O3'	5.94	118.27	105.20
1	A	687	A	C2-N3-C4	5.94	113.57	110.60
1	A	914	A	C4-C5-C6	5.94	119.97	117.00
1	A	35	G	N1-C2-N2	-5.94	110.86	116.20
1	A	68	G	C8-N9-C4	5.94	108.78	106.40
1	A	575	G	C6-C5-N7	5.94	133.96	130.40
1	A	663	A	N3-C4-N9	-5.94	122.65	127.40
1	A	753	A	N3-C4-C5	-5.94	122.64	126.80
1	A	863	U	OP1-P-OP2	5.94	128.50	119.60
1	A	706	A	N1-C6-N6	5.93	122.16	118.60
1	A	1077	G	C5-C6-O6	-5.93	125.04	128.60
1	A	1379	G	C2-N3-C4	-5.93	108.93	111.90
1	A	1440	C	N3-C2-O2	5.93	126.05	121.90
1	A	1050	G	C4-C5-N7	5.93	113.17	110.80
1	A	1255	G	C4-C5-N7	5.93	113.17	110.80
1	A	1323	G	N3-C2-N2	-5.93	115.75	119.90
1	A	55	A	OP2-P-O3'	5.93	118.24	105.20
1	A	285	G	C4-C5-N7	5.93	113.17	110.80
1	A	506	G	N1-C2-N3	5.93	127.46	123.90
1	A	651	C	O5'-P-OP2	-5.93	100.36	105.70
1	A	718	G	C2-N3-C4	-5.93	108.94	111.90
1	A	406	G	N7-C8-N9	5.93	116.06	113.10
1	A	800	G	OP2-P-O3'	5.93	118.24	105.20
1	A	1364	U	C6-N1-C2	5.93	124.56	121.00
1	A	275	G	N1-C6-O6	5.93	123.46	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	737	A	C5-C6-N1	-5.93	114.74	117.70
1	A	1452	C	OP1-P-O3'	5.93	118.24	105.20
19	S	79	THR	N-CA-C	5.93	127.00	111.00
1	A	24	U	O5'-P-OP2	-5.92	100.37	105.70
1	A	305	G	C5-C6-N1	-5.92	108.54	111.50
1	A	440	A	C8-N9-C4	-5.92	103.43	105.80
1	A	1060	C	N1-C2-O2	-5.92	115.35	118.90
1	A	1087	G	N7-C8-N9	5.92	116.06	113.10
1	A	1395	C	OP1-P-OP2	5.92	128.49	119.60
1	A	23	C	OP2-P-O3'	5.92	118.23	105.20
1	A	791	G	C4-N9-C1'	5.92	134.20	126.50
1	A	925	G	N1-C2-N3	5.92	127.45	123.90
1	A	1274	G	C8-N9-C4	5.92	108.77	106.40
1	A	1462	G	N7-C8-N9	-5.92	110.14	113.10
1	A	1175	G	N1-C6-O6	5.92	123.45	119.90
1	A	1205	U	OP1-P-OP2	5.92	128.48	119.60
1	A	129(A)	G	C5-C6-O6	-5.92	125.05	128.60
1	A	715	A	C4-C5-N7	5.92	113.66	110.70
1	A	182	U	N3-C4-O4	5.92	123.54	119.40
1	A	646	U	C4-C5-C6	5.92	123.25	119.70
1	A	903	G	N3-C4-N9	5.92	129.55	126.00
1	A	1011	G	N7-C8-N9	5.92	116.06	113.10
1	A	1223	C	C5-C6-N1	5.92	123.96	121.00
1	A	292	G	C8-N9-C1'	-5.92	119.31	127.00
1	A	673	G	C4-N9-C1'	-5.92	118.81	126.50
1	A	854	G	C6-N1-C2	5.92	128.65	125.10
1	A	522	C	N3-C2-O2	5.91	126.04	121.90
1	A	707	C	C2-N1-C1'	5.91	125.31	118.80
1	A	273	A	C5-C6-N6	5.91	128.43	123.70
1	A	290	C	C5-C6-N1	5.91	123.95	121.00
1	A	1157	A	N3-C4-C5	-5.91	122.66	126.80
1	A	25	C	C6-N1-C2	5.91	122.66	120.30
1	A	316	G	N9-C4-C5	-5.91	103.04	105.40
1	A	903	G	N1-C2-N2	-5.91	110.88	116.20
1	A	1252	A	OP2-P-O3'	5.91	118.20	105.20
1	A	284	G	C4-C5-N7	5.91	113.16	110.80
1	A	730	G	OP2-P-O3'	5.91	118.20	105.20
1	A	1440	C	C5-C4-N4	-5.91	116.06	120.20
1	A	379	C	C6-N1-C2	-5.91	117.94	120.30
1	A	380	G	C5-C6-N1	-5.91	108.55	111.50
1	A	496	A	C6-N1-C2	5.91	122.14	118.60
1	A	776	G	C8-N9-C4	5.91	108.76	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	791	G	C5-N7-C8	5.91	107.25	104.30
1	A	811	C	OP2-P-O3'	5.91	118.19	105.20
1	A	1357	A	N1-C2-N3	5.91	132.25	129.30
1	A	857	C	N3-C4-C5	-5.90	119.54	121.90
1	A	898	G	C5-C6-N1	-5.90	108.55	111.50
1	A	332	G	N3-C4-C5	5.90	131.55	128.60
1	A	1409	C	N1-C2-O2	5.90	122.44	118.90
1	A	30	U	O5'-P-OP1	-5.90	100.39	105.70
1	A	1417	G	OP1-P-OP2	-5.90	110.75	119.60
1	A	971	G	C5-C6-N1	-5.90	108.55	111.50
1	A	1429	C	N1-C2-O2	-5.90	115.36	118.90
1	A	1476	G	C5-C6-N1	-5.90	108.55	111.50
1	A	655	A	C5-C6-N1	-5.90	114.75	117.70
1	A	969	A	C5-C6-N6	-5.90	118.98	123.70
1	A	1236	A	N1-C2-N3	5.90	132.25	129.30
1	A	181	G	C8-N9-C1'	-5.89	119.34	127.00
1	A	775	G	N3-C4-N9	5.89	129.54	126.00
1	A	346	G	N3-C4-C5	5.89	131.54	128.60
1	A	482	A	C6-C5-N7	-5.89	128.18	132.30
1	A	220	G	C4-C5-N7	5.89	113.16	110.80
1	A	545	C	N3-C2-O2	-5.89	117.78	121.90
1	A	1524	C	OP1-P-OP2	-5.89	110.77	119.60
1	A	588	G	N3-C2-N2	-5.89	115.78	119.90
1	A	1091	U	OP1-P-OP2	5.89	128.43	119.60
1	A	1411	C	C6-N1-C1'	5.89	127.86	120.80
1	A	148	G	C6-C5-N7	-5.89	126.87	130.40
1	A	255	G	C6-C5-N7	-5.89	126.87	130.40
1	A	375	U	C6-N1-C2	5.89	124.53	121.00
1	A	588	G	N7-C8-N9	5.89	116.04	113.10
1	A	906	G	C4-N9-C1'	5.89	134.15	126.50
1	A	198	G	C8-N9-C1'	-5.88	119.35	127.00
1	A	1336	C	C5-C6-N1	5.88	123.94	121.00
1	A	1379	G	C5-C6-N1	-5.88	108.56	111.50
1	A	372	C	C4-C5-C6	-5.88	114.46	117.40
1	A	1435	G	C6-C5-N7	-5.88	126.87	130.40
7	G	101	LEU	CB-CG-CD1	5.88	121.00	111.00
1	A	69	G	C2-N3-C4	-5.88	108.96	111.90
1	A	614	A	N1-C6-N6	5.88	122.13	118.60
20	T	96	GLY	N-CA-C	5.88	127.80	113.10
1	A	395	C	C6-N1-C2	-5.88	117.95	120.30
1	A	1056	U	C5-C6-N1	5.88	125.64	122.70
1	A	1443	G	C4-C5-C6	-5.88	115.27	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	G	C5-N7-C8	-5.88	101.36	104.30
1	A	801	U	C6-N1-C2	5.88	124.53	121.00
1	A	1032	G	C4-N9-C1'	-5.88	118.86	126.50
1	A	1190	G	N3-C4-N9	5.88	129.53	126.00
1	A	301	G	OP1-P-O3'	5.87	118.12	105.20
1	A	332	G	C5-C6-N1	-5.87	108.56	111.50
1	A	424	G	C6-C5-N7	5.87	133.92	130.40
1	A	780	A	C8-N9-C4	-5.87	103.45	105.80
1	A	1092	A	C2-N3-C4	-5.87	107.66	110.60
1	A	1203	C	C2-N3-C4	-5.87	116.96	119.90
1	A	437	U	C4-C5-C6	5.87	123.22	119.70
1	A	363	A	C5-C6-N1	5.87	120.63	117.70
1	A	653	A	C2-N3-C4	5.87	113.53	110.60
1	A	837	G	OP2-P-O3'	5.87	118.11	105.20
1	A	916	G	C6-N1-C2	-5.87	121.58	125.10
1	A	1465	C	N1-C2-O2	5.87	122.42	118.90
1	A	807	A	C4-C5-N7	5.87	113.63	110.70
1	A	146	G	N7-C8-N9	-5.87	110.17	113.10
1	A	199	G	C6-N1-C2	-5.87	121.58	125.10
1	A	245	C	OP2-P-O3'	5.87	118.10	105.20
1	A	478	A	N1-C6-N6	5.87	122.12	118.60
1	A	860	A	N3-C4-N9	5.87	132.09	127.40
1	A	1354	C	C5-C6-N1	-5.87	118.07	121.00
1	A	714	G	N9-C4-C5	-5.86	103.05	105.40
1	A	609	A	C6-C5-N7	-5.86	128.20	132.30
1	A	867	G	N3-C4-C5	-5.86	125.67	128.60
1	A	1512	U	N3-C2-O2	-5.86	118.10	122.20
1	A	885	G	OP2-P-O3'	5.86	118.09	105.20
1	A	1094	G	C5-C6-N1	5.86	114.43	111.50
1	A	428	G	N3-C4-N9	-5.86	122.49	126.00
1	A	1340	A	N9-C4-C5	5.86	108.14	105.80
1	A	152	A	N3-C4-C5	5.86	130.90	126.80
1	A	1427	U	C5-C6-N1	-5.86	119.77	122.70
1	A	1027	C	O4'-C1'-N1	5.85	112.88	108.20
1	A	506	G	N1-C6-O6	5.85	123.41	119.90
1	A	872	A	C4-C5-N7	-5.85	107.77	110.70
1	A	882	C	N1-C2-O2	-5.85	115.39	118.90
1	A	1350	A	C5-C6-N6	5.85	128.38	123.70
1	A	53	A	C2-N3-C4	-5.85	107.67	110.60
1	A	198	G	C4-N9-C1'	5.85	134.11	126.50
1	A	852	G	N3-C4-N9	-5.85	122.49	126.00
1	A	552	U	C6-N1-C2	5.85	124.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	910	C	N3-C4-N4	5.85	122.09	118.00
1	A	1222	G	N7-C8-N9	5.85	116.03	113.10
1	A	111	G	C5-N7-C8	-5.85	101.38	104.30
1	A	649	G	C5-C6-O6	-5.85	125.09	128.60
1	A	647	C	O5'-P-OP2	-5.84	100.44	105.70
1	A	865	A	N9-C4-C5	5.84	108.14	105.80
1	A	1391	U	C5-C4-O4	5.84	129.41	125.90
1	A	14	U	N3-C2-O2	-5.84	118.11	122.20
1	A	118	U	N3-C4-C5	5.84	118.10	114.60
1	A	189	G	C8-N9-C4	5.84	108.74	106.40
1	A	487	A	C5-C6-N1	5.84	120.62	117.70
1	A	787	A	OP1-P-OP2	5.84	128.36	119.60
1	A	916	G	C5-C6-N1	5.84	114.42	111.50
1	A	998	G	N3-C2-N2	-5.84	115.81	119.90
1	A	231	G	C4-C5-N7	5.84	113.14	110.80
1	A	376	G	O5'-P-OP1	5.84	117.70	110.70
1	A	553	A	O5'-P-OP1	5.84	117.70	110.70
1	A	498	U	N1-C2-O2	-5.83	118.72	122.80
1	A	643	C	N3-C4-N4	5.83	122.08	118.00
1	A	1067	A	N1-C2-N3	5.83	132.22	129.30
1	A	709	G	N1-C6-O6	5.83	123.40	119.90
1	A	1346	A	N9-C4-C5	5.83	108.13	105.80
1	A	186	C	N1-C2-O2	5.83	122.40	118.90
1	A	661	G	N1-C2-N3	5.83	127.40	123.90
1	A	1055	A	C5-C6-N1	5.83	120.61	117.70
12	L	43	VAL	CB-CA-C	-5.83	100.32	111.40
1	A	674	G	C5-C6-O6	-5.83	125.10	128.60
1	A	183	G	C4-N9-C1'	5.83	134.08	126.50
1	A	775	G	O5'-P-OP1	-5.83	100.45	105.70
1	A	44	G	N3-C4-N9	5.83	129.50	126.00
1	A	153	C	N3-C4-N4	5.83	122.08	118.00
1	A	326	G	C4-C5-C6	5.83	122.30	118.80
10	J	54	PHE	N-CA-C	5.83	126.73	111.00
1	A	37	U	OP1-P-OP2	5.83	128.34	119.60
1	A	1349	A	C2-N3-C4	-5.83	107.69	110.60
1	A	1058	G	O5'-P-OP2	-5.82	100.46	105.70
6	F	65	VAL	CB-CA-C	-5.82	100.34	111.40
1	A	718	G	OP1-P-OP2	-5.82	110.87	119.60
1	A	388	G	C2-N3-C4	-5.82	108.99	111.90
1	A	439	A	N1-C6-N6	-5.82	115.11	118.60
1	A	894	G	C8-N9-C4	5.82	108.73	106.40
1	A	110	C	N3-C4-N4	5.82	122.07	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	698	G	N3-C4-N9	-5.82	122.51	126.00
1	A	1171	G	C4-C5-C6	5.82	122.29	118.80
1	A	1281	U	C4-C5-C6	-5.82	116.21	119.70
1	A	722	A	C5-C6-N1	-5.81	114.79	117.70
1	A	792	A	C5-N7-C8	-5.81	100.99	103.90
1	A	185	A	C2-N3-C4	-5.81	107.69	110.60
1	A	329	A	C5-N7-C8	-5.81	100.99	103.90
1	A	565	U	N3-C4-O4	5.81	123.47	119.40
1	A	405	U	OP1-P-O3'	5.81	117.98	105.20
1	A	606	G	C8-N9-C4	5.81	108.72	106.40
1	A	747	C	C2-N3-C4	-5.81	116.99	119.90
1	A	1117	G	N3-C4-N9	5.81	129.49	126.00
1	A	872	A	C5-N7-C8	5.81	106.81	103.90
1	A	923	A	N1-C6-N6	5.81	122.08	118.60
1	A	21	G	C8-N9-C1'	-5.81	119.45	127.00
1	A	232	G	N7-C8-N9	5.81	116.00	113.10
1	A	1244	C	N3-C4-N4	-5.81	113.94	118.00
1	A	1435	G	N1-C6-O6	5.81	123.38	119.90
1	A	509	A	C5-N7-C8	-5.81	101.00	103.90
1	A	894	G	C5-C6-N1	-5.81	108.60	111.50
1	A	1401	G	C6-N1-C2	-5.81	121.62	125.10
1	A	333	G	C4-C5-C6	-5.80	115.32	118.80
1	A	510	A	N1-C6-N6	-5.80	115.12	118.60
1	A	322	C	N3-C4-N4	5.80	122.06	118.00
1	A	480	U	N3-C4-C5	-5.80	111.12	114.60
14	N	7	ILE	CB-CA-C	5.80	123.20	111.60
1	A	542	G	C2-N3-C4	5.80	114.80	111.90
1	A	606	G	N3-C2-N2	5.80	123.96	119.90
1	A	642	A	N1-C2-N3	5.80	132.20	129.30
1	A	243	A	N7-C8-N9	5.80	116.70	113.80
1	A	1149	C	N1-C2-O2	-5.80	115.42	118.90
1	A	714	G	N7-C8-N9	-5.80	110.20	113.10
1	A	792	A	C4-C5-N7	5.80	113.60	110.70
1	A	827	U	N3-C4-C5	-5.80	111.12	114.60
1	A	980	C	C6-N1-C2	-5.80	117.98	120.30
1	A	1408	A	C2-N3-C4	-5.80	107.70	110.60
1	A	1131	G	N7-C8-N9	5.79	116.00	113.10
1	A	668	G	C5-C6-O6	5.79	132.08	128.60
1	A	685	G	C6-N1-C2	5.79	128.58	125.10
1	A	828	A	N7-C8-N9	-5.79	110.90	113.80
1	A	1287	A	N3-C4-C5	-5.79	122.74	126.80
1	A	1015	A	N9-C4-C5	5.79	108.12	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	G	C5-C6-N1	-5.79	108.61	111.50
1	A	1392	G	C6-N1-C2	-5.79	121.63	125.10
1	A	607	A	N1-C6-N6	5.79	122.07	118.60
5	E	12	LEU	CB-CG-CD2	5.79	120.84	111.00
1	A	296	U	N1-C2-N3	5.79	118.37	114.90
1	A	308	C	O5'-P-OP2	5.79	117.64	110.70
1	A	406	G	C5-C6-O6	-5.79	125.13	128.60
1	A	436	C	C2-N1-C1'	5.79	125.17	118.80
17	Q	90	ILE	CB-CA-C	-5.79	100.03	111.60
1	A	721	G	OP1-P-OP2	5.78	128.28	119.60
1	A	920	U	C4-C5-C6	-5.78	116.23	119.70
1	A	931	C	C5-C6-N1	5.78	123.89	121.00
1	A	104	G	N1-C6-O6	5.78	123.37	119.90
1	A	331	G	C4-N9-C1'	5.78	134.01	126.50
1	A	622	A	C5-N7-C8	-5.78	101.01	103.90
1	A	1113	C	C2-N1-C1'	-5.78	112.44	118.80
1	A	317	G	C4-C5-C6	5.78	122.27	118.80
1	A	675	A	C4-C5-C6	5.78	119.89	117.00
1	A	1050	G	O5'-P-OP2	5.78	117.64	110.70
20	T	62	LEU	CB-CG-CD1	-5.78	101.18	111.00
1	A	459	G	O5'-P-OP1	-5.78	100.50	105.70
1	A	780	A	N7-C8-N9	5.78	116.69	113.80
1	A	839	U	C2-N1-C1'	5.78	124.63	117.70
1	A	59	A	C5-N7-C8	-5.78	101.01	103.90
1	A	145	G	C5-C6-O6	-5.78	125.14	128.60
1	A	721	G	C2-N3-C4	5.78	114.79	111.90
1	A	807	A	C6-C5-N7	-5.78	128.26	132.30
1	A	123	C	N1-C1'-C2'	-5.77	105.65	112.00
1	A	297	G	N9-C4-C5	5.77	107.71	105.40
1	A	958	A	C2-N3-C4	-5.77	107.71	110.60
1	A	1485	U	O4'-C1'-N1	5.77	112.82	108.20
1	A	381	C	OP1-P-OP2	-5.77	110.94	119.60
1	A	1255	G	O5'-P-OP1	-5.77	100.50	105.70
1	A	193	C	N3-C4-N4	-5.77	113.96	118.00
1	A	280	C	C5-C6-N1	-5.77	118.11	121.00
1	A	598	U	O5'-P-OP2	-5.77	100.51	105.70
1	A	674	G	C4-C5-C6	5.77	122.26	118.80
1	A	252	U	O5'-P-OP2	-5.77	100.51	105.70
1	A	372	C	C6-N1-C1'	-5.77	113.88	120.80
1	A	703	G	N3-C4-C5	-5.77	125.72	128.60
1	A	731	G	C5-N7-C8	-5.77	101.42	104.30
1	A	946	A	N3-C4-C5	-5.77	122.76	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	16	HIS	N-CA-C	5.77	126.58	111.00
1	A	778	G	C4-N9-C1'	5.77	134.00	126.50
1	A	692	U	C2-N3-C4	-5.77	123.54	127.00
1	A	181	G	N7-C8-N9	5.76	115.98	113.10
1	A	182	U	C5-C4-O4	-5.76	122.44	125.90
1	A	764	C	O5'-P-OP2	5.76	117.62	110.70
1	A	823	G	C5-C6-N1	-5.76	108.62	111.50
8	H	129	VAL	CB-CA-C	-5.76	100.45	111.40
1	A	809	G	C6-C5-N7	5.76	133.86	130.40
1	A	53	A	C6-N1-C2	-5.76	115.14	118.60
1	A	517	G	C5-C6-O6	5.76	132.06	128.60
1	A	1147	C	C6-N1-C2	-5.76	118.00	120.30
1	A	1199	U	N3-C2-O2	5.76	126.23	122.20
1	A	1348	U	OP1-P-O3'	5.76	117.87	105.20
3	C	25	GLY	N-CA-C	-5.76	98.70	113.10
1	A	134	A	N9-C4-C5	5.76	108.10	105.80
1	A	339	C	N3-C4-N4	5.76	122.03	118.00
1	A	576	G	C8-N9-C4	-5.76	104.10	106.40
1	A	758	G	C4-C5-N7	5.76	113.10	110.80
1	A	225	C	C2-N3-C4	-5.76	117.02	119.90
1	A	324	G	C4-C5-N7	5.76	113.10	110.80
1	A	1416	G	C4-N9-C1'	5.76	133.99	126.50
1	A	720	C	N3-C4-C5	5.76	124.20	121.90
1	A	1460	A	C5-C6-N1	5.75	120.58	117.70
1	A	572	A	C5-C6-N1	5.75	120.58	117.70
1	A	66	G	C8-N9-C4	5.75	108.70	106.40
1	A	895	G	N1-C6-O6	-5.75	116.45	119.90
1	A	947	G	N1-C2-N3	5.75	127.35	123.90
1	A	1305	G	N7-C8-N9	5.75	115.97	113.10
1	A	176	C	N3-C4-N4	5.75	122.03	118.00
1	A	1237	C	C5-C6-N1	-5.75	118.13	121.00
1	A	109	A	N9-C4-C5	5.75	108.10	105.80
1	A	1181	G	C4-C5-N7	-5.75	108.50	110.80
1	A	1306	A	C8-N9-C4	5.75	108.10	105.80
1	A	903	G	C5-C6-N1	5.75	114.37	111.50
1	A	1338	G	O5'-P-OP1	-5.75	100.53	105.70
1	A	1463	C	N1-C1'-C2'	-5.75	105.68	112.00
1	A	14	U	C5-C6-N1	-5.74	119.83	122.70
1	A	32	A	C5-N7-C8	-5.74	101.03	103.90
1	A	517	G	N1-C6-O6	-5.74	116.45	119.90
1	A	1494	G	C5-C6-O6	5.74	132.05	128.60
12	L	24	VAL	C-N-CD	-5.74	107.97	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	27	CYS	CA-CB-SG	-5.74	103.66	114.00
1	A	84	U	O5'-P-OP2	5.74	117.59	110.70
1	A	4	U	C2-N1-C1'	5.74	124.59	117.70
1	A	577	G	C6-N1-C2	-5.74	121.66	125.10
1	A	108	G	C4-C5-C6	5.74	122.24	118.80
1	A	271	C	C5-C4-N4	-5.74	116.18	120.20
1	A	410	G	C5-C6-O6	5.74	132.04	128.60
1	A	486	U	C2-N3-C4	-5.74	123.56	127.00
1	A	1331	G	N3-C4-C5	-5.74	125.73	128.60
2	B	17	PHE	CB-CA-C	5.74	121.88	110.40
1	A	599	C	N1-C2-N3	-5.74	115.18	119.20
5	E	144	THR	CB-CA-C	-5.74	96.11	111.60
1	A	871	U	C2-N1-C1'	5.74	124.58	117.70
1	A	881	G	C2-N3-C4	-5.74	109.03	111.90
1	A	867	G	C6-N1-C2	-5.73	121.66	125.10
1	A	1423	G	N3-C4-N9	-5.73	122.56	126.00
1	A	251	G	C5-C6-N1	-5.73	108.63	111.50
1	A	933	G	C4-C5-C6	5.73	122.24	118.80
1	A	976	G	C2-N3-C4	-5.73	109.03	111.90
1	A	580	U	C6-N1-C2	-5.73	117.56	121.00
1	A	1004	A	O4'-C1'-N9	5.73	112.78	108.20
1	A	1255	G	N1-C6-O6	5.73	123.34	119.90
1	A	878	G	N1-C2-N2	-5.73	111.05	116.20
1	A	1405	G	C6-C5-N7	-5.73	126.96	130.40
1	A	496	A	N1-C6-N6	5.72	122.03	118.60
1	A	567	G	N3-C2-N2	-5.72	115.89	119.90
1	A	882	C	C6-N1-C2	5.72	122.59	120.30
1	A	1211	U	N1-C2-N3	5.72	118.33	114.90
1	A	1287	A	C6-N1-C2	-5.72	115.17	118.60
1	A	1423	G	N1-C6-O6	5.72	123.33	119.90
1	A	1491	G	N7-C8-N9	5.72	115.96	113.10
1	A	118	U	C4-C5-C6	-5.72	116.27	119.70
1	A	444	C	C5-C6-N1	5.72	123.86	121.00
1	A	592	G	N1-C2-N3	5.72	127.33	123.90
1	A	41	G	O5'-P-OP2	5.72	117.56	110.70
1	A	238	G	O5'-P-OP2	-5.72	100.55	105.70
1	A	308	C	OP1-P-OP2	-5.72	111.02	119.60
1	A	922	G	C5-C6-N1	-5.72	108.64	111.50
1	A	328	C	C2-N1-C1'	-5.72	112.51	118.80
1	A	1416	G	OP1-P-O3'	5.72	117.78	105.20
6	F	80	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	401	C	N3-C4-C5	-5.71	119.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	A	C6-C5-N7	-5.71	128.30	132.30
1	A	559	A	N3-C4-C5	-5.71	122.80	126.80
1	A	780	A	N3-C4-N9	5.71	131.97	127.40
1	A	1197	G	C5-C6-O6	-5.71	125.17	128.60
14	N	31	ARG	C-N-CA	-5.71	107.42	121.70
1	A	327	A	C5-N7-C8	-5.71	101.04	103.90
1	A	506	G	C8-N9-C1'	-5.71	119.57	127.00
1	A	499	A	C2-N3-C4	-5.71	107.74	110.60
1	A	825	G	N3-C2-N2	-5.71	115.90	119.90
1	A	1103	C	C2-N3-C4	-5.71	117.04	119.90
1	A	625	G	O5'-P-OP1	-5.71	100.56	105.70
1	A	1323	G	C6-C5-N7	-5.71	126.97	130.40
1	A	64	G	C4-C5-C6	5.71	122.22	118.80
1	A	190(H)	G	OP2-P-O3'	5.71	117.76	105.20
1	A	614	A	C5-C6-N6	-5.71	119.13	123.70
1	A	1506	U	C5-C4-O4	-5.71	122.47	125.90
1	A	1529	G	O5'-P-OP2	5.71	117.55	110.70
1	A	182	U	O5'-P-OP2	-5.71	100.56	105.70
1	A	804	U	C2-N1-C1'	-5.71	110.85	117.70
1	A	1023	G	N1-C6-O6	-5.71	116.48	119.90
1	A	17	U	N3-C4-O4	5.70	123.39	119.40
1	A	193	C	N3-C4-C5	5.70	124.18	121.90
1	A	242	C	OP2-P-O3'	5.70	117.75	105.20
1	A	686	U	O4'-C1'-N1	5.70	112.76	108.20
1	A	1051	C	C2-N1-C1'	-5.70	112.53	118.80
1	A	1520[A]	G	N1-C2-N3	5.70	127.32	123.90
1	A	1520[B]	G	N1-C2-N3	5.70	127.32	123.90
1	A	1197	G	N1-C6-O6	5.70	123.32	119.90
1	A	714	G	C4-C5-C6	5.70	122.22	118.80
1	A	1181	G	N1-C2-N2	5.70	121.33	116.20
1	A	239	U	OP1-P-OP2	5.70	128.15	119.60
1	A	520	A	N7-C8-N9	5.70	116.65	113.80
1	A	1208	C	N1-C2-O2	5.70	122.32	118.90
1	A	1230	C	C2-N3-C4	5.70	122.75	119.90
10	J	44	VAL	CB-CA-C	-5.70	100.57	111.40
1	A	144	G	N3-C4-N9	-5.70	122.58	126.00
1	A	1366	C	N1-C2-N3	5.70	123.19	119.20
1	A	119	A	C2-N3-C4	-5.69	107.75	110.60
1	A	247	G	C4-N9-C1'	5.69	133.90	126.50
1	A	735	C	C5-C6-N1	-5.69	118.15	121.00
1	A	829	G	O4'-C1'-N9	-5.69	103.65	108.20
1	A	267	C	N1-C2-N3	5.69	123.18	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	659	U	N3-C4-O4	-5.69	115.42	119.40
1	A	138	G	O4'-C1'-N9	5.69	112.75	108.20
1	A	183	G	OP1-P-OP2	-5.69	111.07	119.60
1	A	993	G	C8-N9-C1'	-5.69	119.61	127.00
1	A	317	G	C8-N9-C1'	-5.69	119.61	127.00
1	A	477	G	C6-C5-N7	-5.69	126.99	130.40
1	A	918	A	N3-C4-C5	-5.69	122.82	126.80
1	A	1478	C	C6-N1-C2	-5.69	118.03	120.30
1	A	1491	G	N3-C4-C5	-5.69	125.76	128.60
1	A	663	A	C5-C6-N6	5.69	128.25	123.70
1	A	1182	G	C6-C5-N7	-5.69	126.99	130.40
1	A	318	G	N1-C2-N3	5.68	127.31	123.90
1	A	1374	A	N7-C8-N9	5.68	116.64	113.80
1	A	1486	G	C2-N3-C4	5.68	114.74	111.90
1	A	1539	C	C2-N1-C1'	5.68	125.05	118.80
1	A	1328	C	N3-C4-C5	5.68	124.17	121.90
1	A	996	A	N9-C4-C5	5.68	108.07	105.80
1	A	147	G	N1-C2-N3	5.68	127.31	123.90
1	A	583	A	C6-C5-N7	-5.68	128.32	132.30
1	A	928	G	OP1-P-OP2	-5.68	111.08	119.60
1	A	223	U	N3-C2-O2	-5.68	118.23	122.20
1	A	678	U	OP2-P-O3'	5.68	117.69	105.20
1	A	801	U	C5-C6-N1	-5.68	119.86	122.70
1	A	857	C	N1-C2-O2	-5.68	115.50	118.90
1	A	1106	G	C6-C5-N7	-5.68	126.99	130.40
1	A	389	A	C2-N3-C4	5.67	113.44	110.60
1	A	1124	G	N3-C4-N9	5.67	129.40	126.00
1	A	1403	C	O5'-P-OP1	-5.67	100.59	105.70
1	A	289	G	C4-C5-C6	5.67	122.20	118.80
1	A	524	G	C4-N9-C1'	5.67	133.87	126.50
1	A	1129	C	OP2-P-O3'	5.67	117.68	105.20
1	A	1475	G	C8-N9-C4	-5.67	104.13	106.40
1	A	761	G	N3-C4-N9	-5.67	122.60	126.00
1	A	336	C	N3-C4-C5	5.67	124.17	121.90
1	A	591	U	N3-C2-O2	-5.67	118.23	122.20
1	A	1033	G	C2-N3-C4	5.67	114.73	111.90
1	A	183	G	N3-C4-N9	5.67	129.40	126.00
1	A	796	C	N1-C2-O2	5.67	122.30	118.90
1	A	1103	C	N1-C2-O2	-5.67	115.50	118.90
1	A	1176	A	N7-C8-N9	5.67	116.63	113.80
1	A	1349	A	OP1-P-O3'	-5.67	92.73	105.20
1	A	1497	G	N3-C4-C5	-5.67	125.77	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	G	C4-C5-N7	5.66	113.06	110.80
1	A	536	C	N1-C2-N3	5.66	123.17	119.20
1	A	1530	G	C8-N9-C4	5.66	108.67	106.40
1	A	1376	U	C4-C5-C6	5.66	123.10	119.70
1	A	934	C	N1-C2-O2	-5.66	115.50	118.90
1	A	973	G	C6-N1-C2	-5.66	121.70	125.10
1	A	606	G	C8-N9-C1'	-5.66	119.64	127.00
1	A	761	G	N1-C2-N3	5.66	127.30	123.90
1	A	932	C	OP1-P-O3'	5.66	117.65	105.20
1	A	979	C	N3-C4-N4	5.66	121.96	118.00
1	A	235	C	C2-N3-C4	-5.66	117.07	119.90
1	A	260	G	C4-C5-N7	-5.66	108.54	110.80
1	A	748	C	C6-N1-C1'	-5.66	114.01	120.80
1	A	417	C	N3-C4-N4	5.65	121.96	118.00
1	A	200	G	N1-C2-N3	5.65	127.29	123.90
1	A	450	G	N1-C2-N2	5.65	121.29	116.20
1	A	685	G	N7-C8-N9	-5.65	110.27	113.10
1	A	73	C	OP2-P-O3'	5.65	117.63	105.20
1	A	134	A	P-O3'-C3'	5.65	126.48	119.70
1	A	136	C	C5-C4-N4	-5.65	116.24	120.20
1	A	333	G	N1-C6-O6	5.65	123.29	119.90
1	A	730	G	C5-C6-N1	-5.65	108.67	111.50
1	A	758	G	N1-C2-N2	-5.65	111.11	116.20
1	A	815	A	O5'-P-OP2	5.65	117.48	110.70
1	A	990	C	C5-C4-N4	-5.65	116.24	120.20
1	A	1212	U	O4'-C1'-N1	5.65	112.72	108.20
4	D	159	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	230	G	C8-N9-C1'	-5.65	119.66	127.00
1	A	670	G	C6-C5-N7	-5.65	127.01	130.40
1	A	1462	G	C6-C5-N7	5.65	133.79	130.40
1	A	59	A	N1-C6-N6	-5.65	115.21	118.60
1	A	409	G	C8-N9-C4	-5.65	104.14	106.40
1	A	482	A	C6-N1-C2	-5.65	115.21	118.60
1	A	1374	A	N3-C4-C5	-5.65	122.85	126.80
1	A	126	G	C8-N9-C4	5.64	108.66	106.40
1	A	272	C	C6-N1-C1'	-5.64	114.03	120.80
1	A	1014	A	N1-C6-N6	-5.64	115.21	118.60
1	A	1058	G	C8-N9-C4	5.64	108.66	106.40
1	A	1466	C	C5-C6-N1	5.64	123.82	121.00
1	A	1107	C	C6-N1-C2	5.64	122.56	120.30
1	A	569	C	P-O3'-C3'	-5.64	112.93	119.70
1	A	638	G	N1-C6-O6	-5.64	116.52	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	A	N7-C8-N9	-5.64	110.98	113.80
1	A	807	A	C5-N7-C8	-5.64	101.08	103.90
1	A	1090	U	C2-N1-C1'	5.64	124.47	117.70
1	A	89	C	O5'-P-OP1	5.64	117.46	110.70
1	A	1331	G	O4'-C1'-N9	5.64	112.71	108.20
1	A	1003	G	N1-C6-O6	-5.63	116.52	119.90
1	A	1078	U	C2-N1-C1'	5.63	124.46	117.70
1	A	1253	G	C2-N3-C4	5.63	114.72	111.90
15	O	23	GLY	N-CA-C	5.63	127.19	113.10
17	Q	67	LYS	CD-CE-NZ	5.63	124.66	111.70
1	A	811	C	C6-N1-C1'	5.63	127.56	120.80
1	A	1416	G	C5-C6-N1	-5.63	108.68	111.50
1	A	933	G	N3-C4-N9	5.63	129.38	126.00
1	A	1418	A	N1-C6-N6	5.63	121.98	118.60
1	A	1503	A	O5'-P-OP1	5.63	117.46	110.70
1	A	542	G	C5-C6-O6	5.63	131.98	128.60
1	A	1193	G	C6-C5-N7	-5.63	127.02	130.40
1	A	251	G	O4'-C1'-N9	-5.63	103.70	108.20
1	A	455	C	C6-N1-C2	5.63	122.55	120.30
1	A	508	C	OP2-P-O3'	5.63	117.58	105.20
1	A	787	A	C2-N3-C4	-5.63	107.79	110.60
1	A	1071	C	C5-C6-N1	5.63	123.81	121.00
1	A	180	U	C6-N1-C2	5.63	124.38	121.00
1	A	794	A	OP1-P-OP2	-5.63	111.16	119.60
1	A	1022	G	N1-C6-O6	-5.63	116.52	119.90
1	A	1494	G	C5-N7-C8	5.62	107.11	104.30
1	A	153	C	C6-N1-C2	-5.62	118.05	120.30
1	A	564	C	C6-N1-C1'	-5.62	114.05	120.80
1	A	1411	C	N1-C1'-C2'	-5.62	105.81	112.00
12	L	115	LYS	C-N-CA	-5.62	107.65	121.70
1	A	290	C	C6-N1-C2	-5.62	118.05	120.30
1	A	9	G	O5'-P-OP1	5.62	117.44	110.70
1	A	79	G	N1-C6-O6	5.62	123.27	119.90
1	A	170	U	N1-C2-O2	-5.62	118.87	122.80
1	A	650	G	N3-C4-N9	-5.62	122.63	126.00
1	A	1435	G	OP2-P-O3'	5.62	117.56	105.20
6	F	43	LEU	CB-CG-CD2	5.62	120.55	111.00
1	A	883	C	N3-C4-C5	5.62	124.15	121.90
1	A	1517[A]	G	O4'-C1'-N9	-5.62	103.71	108.20
1	A	1517[B]	G	O4'-C1'-N9	-5.62	103.71	108.20
1	A	224	C	C6-N1-C1'	-5.62	114.06	120.80
1	A	715	A	C4-C5-C6	-5.62	114.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	882	C	OP2-P-O3'	5.62	117.55	105.20
1	A	1198	G	C5-C6-O6	5.62	131.97	128.60
1	A	1437	C	N3-C2-O2	5.62	125.83	121.90
1	A	165	C	C6-N1-C2	-5.61	118.06	120.30
1	A	386	C	C5-C4-N4	-5.61	116.27	120.20
1	A	474	G	C4-C5-C6	5.61	122.17	118.80
1	A	946	A	O5'-P-OP2	-5.61	100.65	105.70
1	A	1192	C	N3-C2-O2	5.61	125.83	121.90
1	A	1254	C	C4-C5-C6	5.61	120.21	117.40
1	A	1275	A	N7-C8-N9	-5.61	110.99	113.80
1	A	1325	C	N3-C4-C5	-5.61	119.65	121.90
1	A	200	G	C5-C6-N1	-5.61	108.69	111.50
1	A	538	G	O5'-P-OP1	5.61	117.44	110.70
1	A	758	G	O4'-C1'-N9	-5.61	103.71	108.20
1	A	853	G	C6-C5-N7	-5.61	127.03	130.40
1	A	65	U	O4'-C1'-N1	-5.61	103.71	108.20
1	A	355	C	C2-N3-C4	-5.61	117.09	119.90
1	A	367	U	C2-N1-C1'	-5.61	110.97	117.70
1	A	1482	G	N3-C4-N9	-5.61	122.63	126.00
1	A	674	G	C4-C5-N7	5.61	113.04	110.80
1	A	1195	C	C6-N1-C2	5.61	122.54	120.30
20	T	13	LEU	CB-CG-CD1	5.61	120.53	111.00
1	A	407	G	N7-C8-N9	5.61	115.90	113.10
1	A	1187	G	N1-C2-N3	5.61	127.26	123.90
1	A	1423	G	N3-C4-C5	5.61	131.40	128.60
1	A	1517[A]	G	O5'-P-OP1	-5.61	100.66	105.70
1	A	1517[B]	G	O5'-P-OP1	-5.61	100.66	105.70
2	B	175	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	28	G	N3-C4-C5	-5.60	125.80	128.60
1	A	257	G	N3-C4-C5	5.60	131.40	128.60
1	A	1189	C	C5-C6-N1	5.60	123.80	121.00
1	A	1339	A	C6-N1-C2	-5.60	115.24	118.60
1	A	1364	U	C2-N3-C4	-5.60	123.64	127.00
1	A	1395	C	C5-C6-N1	-5.60	118.20	121.00
1	A	681	C	C5-C4-N4	-5.60	116.28	120.20
1	A	1058	G	C4-C5-N7	5.60	113.04	110.80
1	A	256	U	C5-C6-N1	-5.60	119.90	122.70
1	A	567	G	N1-C2-N3	5.60	127.26	123.90
1	A	588	G	C4-C5-C6	5.60	122.16	118.80
1	A	714	G	N3-C4-N9	5.60	129.36	126.00
1	A	145	G	N1-C6-O6	5.60	123.26	119.90
1	A	564	C	OP1-P-O3'	5.60	117.52	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	984	C	C6-N1-C1'	-5.60	114.08	120.80
1	A	4	U	N1-C2-O2	5.59	126.72	122.80
1	A	324	G	C5-C6-N1	-5.59	108.70	111.50
1	A	25	C	C4-C5-C6	5.59	120.20	117.40
1	A	262	A	N1-C6-N6	5.59	121.95	118.60
1	A	579	G	N7-C8-N9	-5.59	110.30	113.10
1	A	74	C	OP1-P-OP2	-5.59	111.22	119.60
1	A	250	A	N1-C2-N3	5.59	132.09	129.30
1	A	408	A	OP2-P-O3'	5.59	117.50	105.20
1	A	435	C	N3-C4-C5	-5.59	119.66	121.90
1	A	1098	C	C2-N1-C1'	-5.59	112.65	118.80
1	A	1309	G	C5-C6-N1	5.59	114.30	111.50
1	A	677	U	N3-C4-C5	-5.59	111.25	114.60
1	A	462	G	N3-C4-N9	5.59	129.35	126.00
1	A	566	G	N7-C8-N9	-5.59	110.31	113.10
1	A	1287	A	C8-N9-C1'	-5.59	117.64	127.70
1	A	1216	G	N1-C6-O6	5.58	123.25	119.90
1	A	1507	A	C2-N3-C4	5.58	113.39	110.60
1	A	18	C	N1-C2-O2	5.58	122.25	118.90
1	A	609	A	N1-C6-N6	5.58	121.95	118.60
1	A	954	G	N3-C4-N9	-5.58	122.65	126.00
1	A	1022	G	C2-N3-C4	5.58	114.69	111.90
1	A	1405	G	N1-C6-O6	5.58	123.25	119.90
1	A	1508	G	O5'-P-OP1	-5.58	100.68	105.70
1	A	167	G	C4-C5-C6	5.58	122.15	118.80
1	A	477	G	C8-N9-C4	-5.58	104.17	106.40
1	A	803	G	O5'-P-OP1	-5.58	100.68	105.70
4	D	120	LEU	CA-CB-CG	-5.58	102.46	115.30
1	A	764	C	C6-N1-C1'	-5.58	114.10	120.80
1	A	697	U	C6-N1-C1'	5.58	129.01	121.20
1	A	839	U	C5-C6-N1	5.58	125.49	122.70
1	A	1051	C	N3-C4-C5	5.58	124.13	121.90
1	A	1221	G	C8-N9-C4	5.58	108.63	106.40
1	A	232	G	C4-N9-C1'	5.58	133.75	126.50
1	A	351	G	C5-C6-N1	5.57	114.29	111.50
1	A	356	A	OP1-P-O3'	5.57	117.46	105.20
1	A	532	A	C4-N9-C1'	-5.57	116.27	126.30
1	A	1206	G	C4-C5-C6	5.57	122.14	118.80
1	A	839	U	N1-C2-O2	5.57	126.70	122.80
1	A	542	G	C5-C6-N1	5.57	114.28	111.50
1	A	953	G	N3-C4-C5	-5.57	125.81	128.60
1	A	1087	G	N3-C2-N2	-5.57	116.00	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	U	OP2-P-O3'	5.57	117.45	105.20
1	A	189	G	N7-C8-N9	-5.57	110.32	113.10
1	A	224	C	C2-N1-C1'	5.57	124.92	118.80
1	A	434	U	N3-C4-O4	5.57	123.30	119.40
1	A	535	A	N3-C4-C5	-5.57	122.90	126.80
1	A	678	U	N3-C4-O4	-5.57	115.50	119.40
1	A	1468	A	C5-C6-N1	5.57	120.48	117.70
1	A	23	C	C2-N1-C1'	-5.57	112.68	118.80
1	A	253	U	N1-C2-N3	5.57	118.24	114.90
1	A	316	G	C4-N9-C1'	5.57	133.74	126.50
4	D	155	LEU	CA-CB-CG	-5.57	102.50	115.30
1	A	66	G	C2-N3-C4	-5.56	109.12	111.90
1	A	946	A	N1-C6-N6	5.56	121.94	118.60
1	A	1168	A	C8-N9-C4	-5.56	103.58	105.80
1	A	1188	A	C5-C6-N1	-5.56	114.92	117.70
1	A	914	A	O5'-P-OP2	5.56	117.37	110.70
1	A	15	G	N3-C4-C5	-5.56	125.82	128.60
1	A	113	G	OP2-P-O3'	5.56	117.43	105.20
1	A	113	G	C4-C5-C6	5.56	122.14	118.80
1	A	1507	A	O5'-P-OP1	-5.56	100.70	105.70
1	A	784	C	C6-N1-C2	-5.56	118.08	120.30
1	A	109	A	OP2-P-O3'	5.56	117.42	105.20
1	A	28	G	O5'-P-OP1	-5.55	100.70	105.70
1	A	135	C	C6-N1-C2	-5.55	118.08	120.30
1	A	139	G	N1-C6-O6	-5.55	116.57	119.90
1	A	1084	G	N1-C2-N3	-5.55	120.57	123.90
1	A	1127	G	C4-C5-C6	5.55	122.13	118.80
1	A	1467	G	N1-C2-N3	-5.55	120.57	123.90
1	A	959	A	N7-C8-N9	-5.55	111.02	113.80
1	A	1245	A	C8-N9-C4	5.55	108.02	105.80
1	A	4	U	C6-N1-C2	-5.55	117.67	121.00
1	A	76	C	OP1-P-O3'	5.55	117.41	105.20
1	A	184	G	C4-C5-N7	-5.55	108.58	110.80
1	A	222	U	C2-N3-C4	-5.55	123.67	127.00
1	A	576	G	N1-C2-N3	5.55	127.23	123.90
1	A	659	U	C5-C6-N1	-5.55	119.92	122.70
1	A	944	G	N1-C6-O6	-5.55	116.57	119.90
1	A	1053	G	N7-C8-N9	-5.55	110.32	113.10
1	A	1161	C	N3-C4-C5	-5.55	119.68	121.90
1	A	1303	C	C6-N1-C2	-5.55	118.08	120.30
1	A	904	C	C4-C5-C6	-5.55	114.62	117.40
1	A	909	A	C4-C5-N7	5.55	113.47	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1318	A	N1-C2-N3	5.55	132.07	129.30
1	A	674	G	C4-N9-C1'	5.55	133.71	126.50
1	A	410	G	C4-C5-N7	-5.55	108.58	110.80
1	A	766	A	OP1-P-OP2	5.55	127.92	119.60
1	A	1224	G	P-O3'-C3'	5.55	126.36	119.70
1	A	198	G	OP1-P-O3'	-5.54	93.00	105.20
1	A	188	C	N3-C4-C5	-5.54	119.68	121.90
1	A	1094	G	C6-N1-C2	-5.54	121.78	125.10
1	A	1406	U	N3-C4-O4	5.54	123.28	119.40
16	P	73	LEU	CA-CB-CG	-5.54	102.55	115.30
1	A	169	C	OP1-P-O3'	5.54	117.39	105.20
1	A	520	A	N9-C4-C5	5.54	108.02	105.80
1	A	574	A	C5-C6-N1	5.54	120.47	117.70
1	A	734	G	N9-C4-C5	5.54	107.62	105.40
19	S	5	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	1386	G	O5'-P-OP2	-5.54	100.72	105.70
3	C	14	ILE	CG1-CB-CG2	5.54	123.58	111.40
1	A	1002	G	C8-N9-C1'	5.53	134.19	127.00
1	A	989	C	N3-C4-C5	-5.53	119.69	121.90
1	A	20	U	C2-N3-C4	-5.53	123.68	127.00
1	A	326	G	C2-N3-C4	-5.53	109.13	111.90
1	A	485	G	C2-N3-C4	5.53	114.67	111.90
1	A	912	C	N3-C4-N4	5.53	121.87	118.00
1	A	1030	C	C5-C6-N1	5.53	123.77	121.00
1	A	1045	C	N1-C2-O2	5.53	122.22	118.90
4	D	25	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	57	G	N1-C2-N3	5.53	127.22	123.90
1	A	258	G	C4-C5-N7	5.53	113.01	110.80
1	A	397	A	N1-C2-N3	5.53	132.06	129.30
1	A	528	C	OP1-P-OP2	5.53	127.89	119.60
1	A	715	A	N1-C2-N3	5.53	132.06	129.30
1	A	724	G	C4-N9-C1'	5.53	133.69	126.50
1	A	981	U	N1-C2-N3	5.53	118.22	114.90
7	G	99	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	309	G	O5'-P-OP2	5.53	117.33	110.70
1	A	404	U	C6-N1-C2	-5.53	117.68	121.00
1	A	425	G	C5-C6-O6	5.53	131.92	128.60
1	A	1100	C	N1-C2-O2	5.53	122.22	118.90
1	A	1124	G	C6-C5-N7	-5.53	127.08	130.40
6	F	87	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	479	C	C5-C6-N1	5.52	123.76	121.00
1	A	1015	A	C5-C6-N6	5.52	128.12	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	A	N1-C2-N3	5.52	132.06	129.30
1	A	903	G	N1-C2-N3	5.52	127.21	123.90
1	A	10	A	N1-C2-N3	5.52	132.06	129.30
1	A	409	G	C4-C5-C6	5.52	122.11	118.80
1	A	605	U	N3-C4-C5	5.52	117.91	114.60
1	A	637	G	C8-N9-C1'	-5.52	119.82	127.00
1	A	1499	A	C5-C6-N6	-5.52	119.28	123.70
1	A	578	C	N3-C2-O2	-5.52	118.04	121.90
1	A	690	G	C4-C5-C6	5.52	122.11	118.80
1	A	750	G	N7-C8-N9	-5.52	110.34	113.10
1	A	1184	G	C5-N7-C8	5.52	107.06	104.30
1	A	1521	G	C4-N9-C1'	5.52	133.68	126.50
1	A	497	A	C8-N9-C4	-5.52	103.59	105.80
1	A	1526	G	OP2-P-O3'	5.52	117.34	105.20
1	A	358	U	N1-C2-N3	5.52	118.21	114.90
1	A	1159	U	C5-C6-N1	-5.52	119.94	122.70
1	A	147	G	C4-C5-N7	5.51	113.00	110.80
1	A	982	U	OP1-P-OP2	-5.51	111.33	119.60
1	A	35	G	C4-C5-N7	5.51	113.00	110.80
1	A	135	C	O5'-P-OP1	5.51	117.31	110.70
1	A	725	G	N9-C4-C5	-5.51	103.19	105.40
1	A	905	U	OP2-P-O3'	5.51	117.33	105.20
1	A	190(H)	G	C4-C5-N7	5.51	113.00	110.80
1	A	855	G	N1-C6-O6	-5.51	116.59	119.90
1	A	1438	G	N3-C4-N9	5.51	129.31	126.00
1	A	1507	A	N9-C4-C5	5.51	108.00	105.80
2	B	180	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	A	587	G	C6-N1-C2	-5.51	121.79	125.10
1	A	699	C	N1-C2-N3	-5.51	115.34	119.20
1	A	1197	G	C2-N3-C4	-5.51	109.14	111.90
1	A	1527	C	N3-C4-C5	-5.51	119.70	121.90
1	A	818	G	O5'-P-OP2	5.51	117.31	110.70
1	A	230	G	O5'-P-OP2	5.51	117.31	110.70
1	A	583	A	N7-C8-N9	5.51	116.55	113.80
1	A	670	G	O5'-P-OP1	5.51	117.31	110.70
1	A	1069	C	C5-C4-N4	-5.51	116.35	120.20
1	A	500	G	C2-N3-C4	-5.50	109.15	111.90
1	A	1435	G	C5-N7-C8	-5.50	101.55	104.30
1	A	1489	G	N3-C4-C5	-5.50	125.85	128.60
1	A	1512	U	C5-C6-N1	-5.50	119.95	122.70
1	A	832	C	O5'-P-OP1	5.50	117.30	110.70
1	A	918	A	N3-C4-N9	5.50	131.80	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1277	C	C6-N1-C1'	-5.50	114.20	120.80
1	A	323	U	C6-N1-C2	-5.50	117.70	121.00
1	A	354	G	C6-C5-N7	-5.50	127.10	130.40
1	A	358	U	C4-C5-C6	5.50	123.00	119.70
1	A	1316	G	C5-C6-O6	-5.50	125.30	128.60
1	A	1363	A	N7-C8-N9	5.50	116.55	113.80
1	A	1492	A	C8-N9-C4	-5.50	103.60	105.80
1	A	248	C	O5'-P-OP2	-5.50	100.75	105.70
1	A	793	U	N3-C2-O2	-5.50	118.35	122.20
1	A	1521	G	N1-C6-O6	5.50	123.20	119.90
1	A	69	G	N9-C4-C5	-5.50	103.20	105.40
1	A	407	G	C2-N3-C4	-5.50	109.15	111.90
1	A	1512	U	C6-N1-C1'	5.50	128.90	121.20
1	A	250	A	OP1-P-OP2	-5.50	111.35	119.60
1	A	385	C	C4-C5-C6	5.50	120.15	117.40
1	A	759	A	C5-C6-N1	5.50	120.45	117.70
1	A	1167	A	C6-N1-C2	5.50	121.90	118.60
1	A	1349	A	O5'-P-OP1	-5.50	100.75	105.70
1	A	1543	C	OP1-P-OP2	5.50	127.84	119.60
1	A	351	G	C8-N9-C4	-5.50	104.20	106.40
1	A	996	A	C4-C5-N7	-5.50	107.95	110.70
1	A	1422	G	N3-C2-N2	-5.50	116.05	119.90
1	A	1533	C	C2-N1-C1'	5.50	124.84	118.80
1	A	324	G	C5-C6-O6	-5.49	125.30	128.60
1	A	514	C	O5'-P-OP2	-5.49	100.76	105.70
1	A	642	A	N1-C6-N6	5.49	121.90	118.60
1	A	795	C	OP2-P-O3'	5.49	117.29	105.20
1	A	190(H)	G	N7-C8-N9	5.49	115.85	113.10
1	A	546	G	P-O3'-C3'	5.49	126.29	119.70
1	A	641	U	C2-N1-C1'	5.49	124.29	117.70
1	A	407	G	C5-N7-C8	-5.49	101.56	104.30
1	A	806	C	C5-C4-N4	5.49	124.04	120.20
1	A	1328	C	C5-C6-N1	-5.49	118.25	121.00
1	A	1435	G	C5-C6-O6	-5.49	125.31	128.60
1	A	378	G	C6-C5-N7	-5.49	127.11	130.40
1	A	584	G	N1-C2-N2	-5.49	111.26	116.20
1	A	637	G	C4-C5-C6	5.49	122.09	118.80
1	A	811	C	C2-N3-C4	-5.49	117.16	119.90
1	A	117	G	O4'-C1'-N9	-5.49	103.81	108.20
1	A	269	C	N3-C4-N4	-5.49	114.16	118.00
1	A	346	G	N3-C4-N9	-5.49	122.71	126.00
1	A	1089	G	C2-N3-C4	5.49	114.64	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	727	G	C6-C5-N7	5.48	133.69	130.40
1	A	1032	G	C8-N9-C1'	5.48	134.13	127.00
1	A	8	A	C8-N9-C4	-5.48	103.61	105.80
1	A	269	C	N3-C4-C5	5.48	124.09	121.90
1	A	799	G	C2-N3-C4	-5.48	109.16	111.90
1	A	1345	U	O4'-C1'-N1	5.48	112.59	108.20
1	A	666	G	N3-C2-N2	5.48	123.74	119.90
1	A	774	G	C6-C5-N7	-5.48	127.11	130.40
1	A	176	C	N1-C2-N3	-5.48	115.36	119.20
1	A	318	G	N1-C6-O6	5.48	123.19	119.90
1	A	733	A	C4-C5-N7	5.48	113.44	110.70
1	A	890	G	OP1-P-OP2	5.48	127.82	119.60
1	A	292	G	N1-C2-N3	5.48	127.19	123.90
1	A	1064	G	N3-C4-N9	-5.48	122.71	126.00
1	A	16	A	C2-N3-C4	-5.47	107.86	110.60
1	A	35	G	C4-N9-C1'	5.47	133.62	126.50
1	A	851	G	OP1-P-OP2	5.47	127.81	119.60
1	A	933	G	N1-C6-O6	5.47	123.19	119.90
1	A	957	U	C5-C6-N1	-5.47	119.96	122.70
1	A	314	C	O4'-C1'-N1	-5.47	103.82	108.20
1	A	1376	U	C2-N1-C1'	5.47	124.27	117.70
1	A	1063	C	O5'-P-OP2	-5.47	100.78	105.70
1	A	1392	G	C5-C6-N1	5.47	114.24	111.50
1	A	380	G	N1-C2-N3	5.47	127.18	123.90
1	A	422	C	C6-N1-C2	5.47	122.49	120.30
1	A	190(G)	G	N1-C6-O6	5.47	123.18	119.90
1	A	448	A	N3-C4-N9	-5.47	123.03	127.40
1	A	830	G	C4-N9-C1'	-5.47	119.39	126.50
1	A	1371	G	C6-C5-N7	-5.47	127.12	130.40
1	A	318	G	C4-C5-C6	5.46	122.08	118.80
1	A	533	A	C4-C5-C6	5.46	119.73	117.00
1	A	781	A	C5-C6-N1	5.46	120.43	117.70
1	A	1469	G	N9-C4-C5	5.46	107.58	105.40
2	B	165	VAL	CG1-CB-CG2	5.46	119.64	110.90
1	A	691	G	O4'-C1'-N9	5.46	112.57	108.20
1	A	357	G	C5-C6-N1	5.46	114.23	111.50
1	A	482	A	C2-N3-C4	-5.46	107.87	110.60
1	A	557	G	C2-N3-C4	-5.46	109.17	111.90
1	A	609	A	C8-N9-C4	-5.46	103.61	105.80
1	A	886	G	C8-N9-C4	-5.46	104.22	106.40
1	A	1514	C	C5-C6-N1	-5.46	118.27	121.00
1	A	434	U	N3-C4-C5	-5.46	111.32	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	G	N3-C4-C5	5.46	131.33	128.60
1	A	1319	A	C8-N9-C4	-5.46	103.62	105.80
1	A	1528	U	N3-C4-C5	5.46	117.88	114.60
1	A	1106	G	C4-C5-N7	5.46	112.98	110.80
1	A	35	G	OP1-P-O3'	-5.46	93.20	105.20
1	A	266	G	OP1-P-O3'	5.46	117.21	105.20
2	B	191	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	582	U	N1-C2-N3	5.46	118.17	114.90
1	A	1030	C	N3-C2-O2	-5.46	118.08	121.90
1	A	121	C	C5-C6-N1	-5.45	118.27	121.00
1	A	259	G	C6-N1-C2	-5.45	121.83	125.10
1	A	281	G	C4-C5-C6	5.45	122.07	118.80
1	A	790	A	N7-C8-N9	5.45	116.53	113.80
1	A	876	G	C5-C6-N1	-5.45	108.77	111.50
1	A	1100	C	C2-N1-C1'	5.45	124.80	118.80
1	A	1122	U	N1-C2-N3	5.45	118.17	114.90
1	A	40	C	N1-C2-O2	-5.45	115.63	118.90
1	A	1015	A	C8-N9-C4	-5.45	103.62	105.80
1	A	425	G	N9-C4-C5	5.45	107.58	105.40
1	A	818	G	C5-N7-C8	5.45	107.02	104.30
1	A	362	G	C5-C6-N1	-5.45	108.78	111.50
1	A	435	C	OP1-P-O3'	5.45	117.18	105.20
1	A	620	C	C5-C6-N1	-5.45	118.28	121.00
1	A	1453	G	N3-C4-C5	-5.45	125.88	128.60
1	A	1529	G	C4-C5-N7	-5.45	108.62	110.80
1	A	96	G	C8-N9-C4	5.45	108.58	106.40
1	A	216	G	N3-C4-C5	5.45	131.32	128.60
1	A	888	G	N3-C4-N9	5.45	129.27	126.00
3	C	34	LEU	CA-CB-CG	5.45	127.82	115.30
8	H	36	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	301	G	C8-N9-C4	-5.44	104.22	106.40
1	A	1495	U	C5-C6-N1	-5.44	119.98	122.70
18	R	53	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	A	511	C	N3-C4-C5	-5.44	119.72	121.90
1	A	948	C	C5-C6-N1	-5.44	118.28	121.00
1	A	992	U	P-O3'-C3'	5.44	126.23	119.70
1	A	1236	A	C8-N9-C4	5.44	107.98	105.80
1	A	1413	A	C8-N9-C4	5.44	107.98	105.80
1	A	1497	G	N1-C2-N2	-5.44	111.30	116.20
1	A	254	G	N9-C4-C5	-5.44	103.22	105.40
1	A	1477	C	N3-C4-N4	5.44	121.81	118.00
1	A	772	U	OP1-P-OP2	5.44	127.76	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	A	N3-C4-N9	-5.44	123.05	127.40
1	A	121	C	N1-C2-N3	-5.44	115.39	119.20
1	A	778	G	C6-N1-C2	-5.44	121.84	125.10
1	A	813	U	N1-C2-O2	-5.44	118.99	122.80
1	A	382	A	OP2-P-O3'	5.44	117.16	105.20
1	A	502	G	C8-N9-C4	5.44	108.58	106.40
1	A	1289	A	N1-C2-N3	-5.44	126.58	129.30
1	A	1323	G	C5-C6-N1	-5.44	108.78	111.50
2	B	23	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	607	A	C4-C5-C6	5.43	119.72	117.00
1	A	623	C	C2-N3-C4	-5.43	117.18	119.90
1	A	768	A	OP1-P-OP2	-5.43	111.45	119.60
1	A	800	G	N3-C4-N9	-5.43	122.74	126.00
1	A	825	G	C4-N9-C1'	-5.43	119.43	126.50
1	A	1087	G	C8-N9-C1'	-5.43	119.93	127.00
1	A	1102	A	C5-N7-C8	-5.43	101.18	103.90
1	A	821	G	N9-C4-C5	5.43	107.57	105.40
1	A	854	G	N3-C4-C5	5.43	131.32	128.60
1	A	866	C	C6-N1-C2	-5.43	118.13	120.30
1	A	975	A	N9-C1'-C2'	-5.43	106.02	112.00
1	A	41	G	N7-C8-N9	5.43	115.81	113.10
1	A	1394	A	C4-C5-C6	5.43	119.72	117.00
1	A	642	A	C8-N9-C4	-5.43	103.63	105.80
1	A	1463	C	N3-C4-C5	5.43	124.07	121.90
1	A	524	G	N1-C2-N2	5.43	121.09	116.20
1	A	922	G	C5-N7-C8	-5.43	101.59	104.30
1	A	9	G	C8-N9-C4	5.43	108.57	106.40
1	A	485	G	N3-C4-C5	-5.43	125.89	128.60
1	A	740	U	C4-C5-C6	5.43	122.96	119.70
1	A	1299	A	C4-C5-C6	5.43	119.71	117.00
1	A	101	A	C4-C5-C6	5.42	119.71	117.00
1	A	129	U	C6-N1-C2	5.42	124.25	121.00
1	A	326	G	N1-C6-O6	5.42	123.15	119.90
1	A	546	G	N1-C2-N3	5.42	127.16	123.90
1	A	837	G	C4-C5-N7	5.42	112.97	110.80
4	D	196	LEU	CB-CG-CD2	5.42	120.22	111.00
1	A	633	G	N1-C2-N2	5.42	121.08	116.20
1	A	674	G	C8-N9-C1'	-5.42	119.95	127.00
1	A	195	A	N7-C8-N9	-5.42	111.09	113.80
1	A	296	U	OP1-P-O3'	5.42	117.13	105.20
1	A	685	G	C6-C5-N7	5.42	133.65	130.40
1	A	680	C	N1-C2-O2	-5.42	115.65	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	G	C4-C5-C6	-5.42	115.55	118.80
1	A	1030(C)	G	N3-C4-C5	5.42	131.31	128.60
1	A	189	G	O5'-P-OP1	5.42	117.20	110.70
1	A	288	A	C5-C6-N1	-5.42	114.99	117.70
1	A	395	C	C6-N1-C1'	5.42	127.30	120.80
1	A	614	A	C5-N7-C8	-5.42	101.19	103.90
1	A	883	C	OP2-P-O3'	5.42	117.11	105.20
1	A	951	G	C4-C5-N7	5.42	112.97	110.80
1	A	54	C	C4-C5-C6	5.41	120.11	117.40
1	A	874	G	O5'-P-OP2	-5.41	100.83	105.70
1	A	984	C	C6-N1-C2	5.41	122.47	120.30
1	A	1030	C	C2-N1-C1'	5.41	124.75	118.80
1	A	1087	G	N3-C4-C5	-5.41	125.89	128.60
4	D	26	CYS	N-CA-C	-5.41	96.38	111.00
1	A	117	G	OP1-P-OP2	5.41	127.72	119.60
1	A	479	C	N3-C4-C5	-5.41	119.73	121.90
1	A	713	G	OP1-P-O3'	5.41	117.11	105.20
1	A	998	G	N3-C4-N9	-5.41	122.75	126.00
12	L	27	LEU	CB-CG-CD2	5.41	120.20	111.00
1	A	11	G	OP2-P-O3'	5.41	117.10	105.20
1	A	251	G	OP1-P-O3'	5.41	117.10	105.20
1	A	531	U	O5'-P-OP2	5.41	117.19	110.70
1	A	974	A	N1-C2-N3	5.41	132.00	129.30
1	A	1078	U	OP2-P-O3'	5.41	117.10	105.20
1	A	1479	C	N3-C4-C5	-5.41	119.74	121.90
1	A	1522	U	C5-C6-N1	-5.41	119.99	122.70
1	A	44	G	N3-C4-C5	-5.41	125.90	128.60
1	A	299	G	N1-C2-N2	-5.41	111.33	116.20
1	A	393	A	OP1-P-OP2	-5.41	111.49	119.60
1	A	1187	G	O5'-P-OP2	-5.41	100.83	105.70
1	A	1464	G	C2-N3-C4	-5.41	109.20	111.90
1	A	78	G	C8-N9-C4	-5.41	104.24	106.40
1	A	228	A	C8-N9-C1'	5.41	137.43	127.70
1	A	485	G	N3-C2-N2	5.41	123.68	119.90
1	A	1098	C	N3-C4-N4	-5.41	114.22	118.00
1	A	216	G	C8-N9-C1'	5.40	134.03	127.00
1	A	368	U	C2-N1-C1'	5.40	124.18	117.70
1	A	599	C	C5-C4-N4	-5.40	116.42	120.20
1	A	622	A	N9-C4-C5	-5.40	103.64	105.80
1	A	299	G	N1-C6-O6	-5.40	116.66	119.90
1	A	333	G	C8-N9-C4	5.40	108.56	106.40
1	A	498	U	C6-N1-C2	-5.40	117.76	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1338	G	C4-C5-C6	5.40	122.04	118.80
1	A	1493	A	N3-C4-N9	5.40	131.72	127.40
1	A	424	G	N1-C6-O6	-5.40	116.66	119.90
1	A	741	G	N9-C4-C5	5.40	107.56	105.40
1	A	1486	G	O5'-P-OP2	-5.40	100.84	105.70
1	A	58	C	O5'-P-OP1	-5.40	100.84	105.70
1	A	841	U	O4'-C1'-N1	5.40	112.52	108.20
1	A	76	C	N3-C2-O2	5.40	125.68	121.90
1	A	775	G	N9-C4-C5	-5.40	103.24	105.40
1	A	786	G	OP1-P-OP2	5.40	127.70	119.60
1	A	830	G	C2-N3-C4	-5.40	109.20	111.90
1	A	1087	G	C8-N9-C4	-5.40	104.24	106.40
1	A	1277	C	N1-C2-O2	5.40	122.14	118.90
1	A	256	U	N1-C2-O2	-5.40	119.02	122.80
1	A	483	C	OP1-P-OP2	5.40	127.69	119.60
1	A	921	U	N1-C2-N3	-5.40	111.66	114.90
1	A	1471	G	C4-C5-N7	-5.40	108.64	110.80
1	A	588	G	P-O3'-C3'	5.39	126.17	119.70
1	A	1481	U	C5-C4-O4	5.39	129.14	125.90
1	A	126	G	C8-N9-C1'	-5.39	119.99	127.00
1	A	447	G	C8-N9-C4	5.39	108.56	106.40
1	A	744	C	C2-N3-C4	5.39	122.60	119.90
1	A	1229	A	N1-C6-N6	5.39	121.83	118.60
1	A	856	C	O5'-P-OP1	5.39	117.17	110.70
1	A	1266	G	C2-N3-C4	-5.39	109.20	111.90
1	A	59	A	C5-C6-N1	5.39	120.39	117.70
1	A	530	G	C4-C5-C6	5.39	122.03	118.80
1	A	532	A	C5-C6-N1	5.39	120.39	117.70
1	A	542	G	N9-C4-C5	5.39	107.56	105.40
1	A	1281	U	C6-N1-C1'	5.39	128.75	121.20
1	A	974	A	O4'-C1'-N9	-5.39	103.89	108.20
1	A	1021	G	C5-C6-N1	5.39	114.19	111.50
1	A	9	G	OP1-P-OP2	5.38	127.68	119.60
1	A	193	C	O5'-P-OP1	5.38	117.16	110.70
1	A	428	G	N1-C6-O6	-5.38	116.67	119.90
1	A	438	G	C6-C5-N7	5.38	133.63	130.40
1	A	518	C	C2-N1-C1'	5.38	124.72	118.80
1	A	796	C	O5'-P-OP2	-5.38	100.85	105.70
1	A	1531	A	C5-C6-N6	-5.38	119.39	123.70
1	A	112	G	N1-C6-O6	5.38	123.13	119.90
1	A	144	G	N1-C2-N2	5.38	121.04	116.20
1	A	770	C	N3-C4-N4	-5.38	114.23	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1051	C	C5-C6-N1	-5.38	118.31	121.00
1	A	449	C	N3-C4-C5	-5.38	119.75	121.90
1	A	829	G	N1-C2-N3	5.38	127.13	123.90
1	A	1008	C	C5-C6-N1	5.38	123.69	121.00
1	A	1499	A	C5-C6-N1	5.38	120.39	117.70
1	A	264	U	N1-C2-O2	5.38	126.56	122.80
1	A	284	G	N7-C8-N9	-5.38	110.41	113.10
1	A	336	C	C4-C5-C6	-5.38	114.71	117.40
1	A	530	G	C4-N9-C1'	5.38	133.49	126.50
1	A	703	G	OP1-P-OP2	5.38	127.67	119.60
1	A	754	C	N1-C2-O2	-5.38	115.67	118.90
1	A	1084	G	C2-N3-C4	5.38	114.59	111.90
1	A	1329	A	OP2-P-O3'	-5.38	93.37	105.20
1	A	170	U	C5-C4-O4	5.38	129.12	125.90
1	A	703	G	C4-N9-C1'	5.38	133.49	126.50
1	A	1242	C	C6-N1-C2	-5.38	118.15	120.30
1	A	614	A	C4-C5-N7	5.37	113.39	110.70
1	A	858	G	OP2-P-O3'	5.37	117.02	105.20
1	A	190(E)	U	N1-C2-N3	5.37	118.12	114.90
5	E	69	VAL	C-N-CD	5.37	139.68	128.40
1	A	623	C	C5-C6-N1	-5.37	118.31	121.00
1	A	972	C	C5-C6-N1	-5.37	118.31	121.00
1	A	1529	G	O4'-C1'-N9	5.37	112.50	108.20
1	A	637	G	N3-C2-N2	-5.37	116.14	119.90
1	A	690	G	C6-C5-N7	-5.37	127.18	130.40
1	A	729	A	C6-N1-C2	-5.37	115.38	118.60
1	A	741	G	N1-C6-O6	-5.37	116.68	119.90
1	A	577	G	C4-N9-C1'	-5.37	119.52	126.50
1	A	1121	U	C2-N1-C1'	-5.37	111.26	117.70
1	A	1348	U	C2-N3-C4	-5.37	123.78	127.00
1	A	1467	G	OP1-P-OP2	5.37	127.65	119.60
11	K	63	LEU	CA-CB-CG	-5.37	102.96	115.30
1	A	107	G	O5'-P-OP1	5.37	117.14	110.70
1	A	290	C	C5-C4-N4	-5.37	116.44	120.20
1	A	1195	C	OP2-P-O3'	5.37	117.00	105.20
1	A	379	C	N1-C2-N3	5.36	122.95	119.20
1	A	873	A	OP1-P-OP2	5.36	127.64	119.60
1	A	1131	G	C8-N9-C1'	-5.36	120.03	127.00
1	A	1506	U	O5'-P-OP2	-5.36	100.88	105.70
1	A	280	C	O5'-P-OP2	-5.36	100.88	105.70
1	A	414	A	N1-C6-N6	-5.36	115.39	118.60
1	A	490	G	OP1-P-OP2	5.36	127.64	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	695	A	O5'-P-OP1	5.36	117.13	110.70
1	A	123	C	C6-N1-C2	-5.36	118.16	120.30
1	A	186	C	C5-C6-N1	-5.36	118.32	121.00
1	A	661	G	N3-C2-N2	-5.36	116.15	119.90
1	A	1113	C	C5-C4-N4	5.36	123.95	120.20
1	A	1239	A	N7-C8-N9	-5.36	111.12	113.80
1	A	1295	G	C5-C6-O6	-5.36	125.39	128.60
1	A	1303	C	N1-C2-O2	5.36	122.11	118.90
1	A	755	G	C4-C5-C6	5.35	122.01	118.80
1	A	1193	G	N3-C4-C5	-5.35	125.92	128.60
1	A	36	C	OP1-P-O3'	-5.35	93.43	105.20
1	A	272	C	C5-C4-N4	-5.35	116.45	120.20
1	A	1163	C	C6-N1-C2	-5.35	118.16	120.30
1	A	1363	A	OP1-P-OP2	5.35	127.63	119.60
1	A	1387	G	N3-C2-N2	-5.35	116.15	119.90
1	A	1075	C	C6-N1-C1'	5.35	127.22	120.80
1	A	166	G	N1-C2-N3	5.35	127.11	123.90
1	A	568	G	O4'-C1'-N9	-5.35	103.92	108.20
1	A	767	A	P-O3'-C3'	5.35	126.12	119.70
1	A	982	U	N1-C2-O2	5.35	126.55	122.80
1	A	1415	G	C8-N9-C4	5.35	108.54	106.40
1	A	1420	C	N1-C2-N3	5.35	122.94	119.20
14	N	31	ARG	N-CA-C	5.35	125.44	111.00
1	A	104	G	C8-N9-C4	-5.35	104.26	106.40
1	A	405	U	OP1-P-OP2	-5.35	111.58	119.60
1	A	871	U	C4-C5-C6	5.35	122.91	119.70
1	A	1503	A	C2-N3-C4	-5.35	107.93	110.60
9	I	44	VAL	CB-CA-C	-5.35	101.24	111.40
1	A	66	G	N3-C4-C5	5.35	131.27	128.60
1	A	756	C	OP1-P-OP2	5.35	127.62	119.60
1	A	36	C	N3-C4-C5	5.34	124.04	121.90
1	A	190(L)	U	O5'-P-OP1	-5.34	100.89	105.70
1	A	485	G	C6-N1-C2	-5.34	121.89	125.10
1	A	512	U	N1-C2-N3	5.34	118.11	114.90
1	A	548	G	N3-C4-C5	5.34	131.27	128.60
1	A	904	C	C5-C6-N1	-5.34	118.33	121.00
1	A	1030(B)	C	C2-N3-C4	5.34	122.57	119.90
9	I	109	VAL	CB-CA-C	-5.34	101.25	111.40
1	A	351	G	C5-N7-C8	-5.34	101.63	104.30
1	A	1094	G	C4-N9-C1'	5.34	133.44	126.50
1	A	290	C	N3-C4-N4	5.34	121.74	118.00
1	A	382	A	C6-N1-C2	-5.34	115.40	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	710	G	C8-N9-C1'	-5.34	120.06	127.00
1	A	1483	A	C6-N1-C2	5.34	121.80	118.60
15	O	54	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	332	G	N9-C4-C5	-5.34	103.27	105.40
1	A	1062	U	C5-C6-N1	-5.34	120.03	122.70
1	A	46	G	N1-C2-N3	5.34	127.10	123.90
1	A	1204	A	N1-C2-N3	5.33	131.97	129.30
1	A	1381	U	C5-C4-O4	5.33	129.10	125.90
1	A	657	G	C6-C5-N7	-5.33	127.20	130.40
1	A	694	A	N3-C4-C5	5.33	130.53	126.80
1	A	1193	G	C4-C5-N7	-5.33	108.67	110.80
1	A	1491	G	C8-N9-C4	-5.33	104.27	106.40
1	A	21	G	C4-C5-N7	5.33	112.93	110.80
1	A	424	G	C4-C5-C6	-5.33	115.60	118.80
1	A	789	U	C5-C6-N1	-5.33	120.03	122.70
1	A	856	C	N3-C4-C5	5.33	124.03	121.90
1	A	1290	G	C5-C6-O6	-5.33	125.40	128.60
14	N	44	LEU	CB-CG-CD1	5.33	120.06	111.00
1	A	131	C	N3-C4-C5	-5.33	119.77	121.90
1	A	730	G	N3-C4-C5	-5.33	125.94	128.60
1	A	883	C	C2-N1-C1'	-5.33	112.94	118.80
1	A	955	U	C4-C5-C6	5.33	122.90	119.70
1	A	837	G	N3-C4-N9	5.33	129.20	126.00
1	A	1062	U	C5-C4-O4	5.33	129.10	125.90
1	A	53	A	N9-C4-C5	5.33	107.93	105.80
1	A	318	G	C2-N3-C4	-5.33	109.24	111.90
1	A	1063	C	C6-N1-C2	-5.33	118.17	120.30
1	A	1332	A	O5'-P-OP2	-5.33	100.91	105.70
8	H	63	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	A	546	G	OP1-P-OP2	-5.33	111.61	119.60
1	A	836	G	C8-N9-C4	-5.33	104.27	106.40
1	A	1323	G	O5'-P-OP1	-5.33	100.91	105.70
1	A	1500	A	C2-N3-C4	5.33	113.26	110.60
1	A	1533	C	C5-C6-N1	5.33	123.66	121.00
1	A	204	U	C2-N3-C4	5.32	130.19	127.00
1	A	552	U	C2-N1-C1'	-5.32	111.31	117.70
1	A	557	G	OP1-P-O3'	5.32	116.91	105.20
1	A	1514	C	N1-C2-N3	-5.32	115.47	119.20
1	A	310	G	C6-C5-N7	-5.32	127.21	130.40
1	A	956	U	N3-C2-O2	-5.32	118.47	122.20
1	A	1511	G	OP1-P-OP2	5.32	127.58	119.60
1	A	50	A	C2-N3-C4	-5.32	107.94	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	G	C5-C6-O6	-5.32	125.41	128.60
1	A	195	A	C6-N1-C2	-5.32	115.41	118.60
1	A	228	A	O4'-C1'-N9	5.32	112.46	108.20
1	A	350	G	OP1-P-O3'	5.32	116.91	105.20
1	A	577	G	C5-C6-O6	-5.32	125.41	128.60
1	A	1409	C	C6-N1-C2	-5.32	118.17	120.30
1	A	564	C	N1-C2-N3	-5.32	115.48	119.20
1	A	969	A	N9-C4-C5	-5.32	103.67	105.80
1	A	1192	C	C6-N1-C2	5.32	122.43	120.30
1	A	289	G	N3-C4-C5	-5.32	125.94	128.60
1	A	537	G	C5-C6-O6	-5.32	125.41	128.60
1	A	813	U	N1-C2-N3	-5.32	111.71	114.90
1	A	823	G	N9-C4-C5	-5.32	103.27	105.40
1	A	999	C	C6-N1-C2	5.32	122.43	120.30
1	A	1433	A	C4-C5-N7	-5.32	108.04	110.70
8	H	112	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	A	330	C	C6-N1-C2	-5.32	118.17	120.30
1	A	504	C	N3-C4-N4	5.32	121.72	118.00
1	A	679	C	O5'-P-OP1	-5.32	100.92	105.70
1	A	975	A	C5-C6-N6	5.32	127.95	123.70
1	A	1186	G	N3-C2-N2	-5.32	116.18	119.90
1	A	1232	U	C2-N1-C1'	5.32	124.08	117.70
1	A	1294	G	C4-C5-C6	-5.32	115.61	118.80
1	A	1328	C	C2-N3-C4	-5.31	117.24	119.90
1	A	560	U	N3-C2-O2	-5.31	118.48	122.20
1	A	98	U	N3-C4-O4	-5.31	115.68	119.40
1	A	399	G	C2-N3-C4	5.31	114.56	111.90
1	A	1339	A	C6-C5-N7	5.31	136.02	132.30
1	A	1505	G	C2'-C3'-O3'	5.31	122.20	113.70
1	A	200	G	N3-C4-C5	5.31	131.25	128.60
1	A	252	U	N3-C4-C5	-5.31	111.41	114.60
1	A	362	G	C4-C5-C6	5.31	121.98	118.80
1	A	698	G	O5'-P-OP2	-5.31	100.92	105.70
1	A	755	G	C4-N9-C1'	5.31	133.40	126.50
1	A	1216	G	C2-N3-C4	-5.31	109.25	111.90
1	A	1469	G	N1-C6-O6	-5.31	116.71	119.90
1	A	82	U	OP1-P-O3'	5.31	116.88	105.20
1	A	281	G	C4-C5-N7	5.31	112.92	110.80
1	A	293	G	N1-C2-N3	5.31	127.08	123.90
1	A	423	G	N1-C6-O6	5.31	123.08	119.90
1	A	662	G	OP1-P-OP2	5.31	127.56	119.60
1	A	720	C	OP1-P-OP2	5.31	127.56	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	854	G	O5'-P-OP1	-5.31	100.92	105.70
1	A	1156	G	N9-C4-C5	5.31	107.52	105.40
1	A	1193	G	C8-N9-C1'	-5.31	120.10	127.00
1	A	1432	G	OP1-P-OP2	5.31	127.56	119.60
10	J	60	ARG	N-CA-C	5.31	125.33	111.00
1	A	261	U	OP1-P-OP2	-5.31	111.64	119.60
1	A	805	C	C6-N1-C2	5.31	122.42	120.30
1	A	1417	G	O5'-P-OP2	5.31	117.07	110.70
12	L	110	VAL	CB-CA-C	-5.31	101.32	111.40
1	A	19	C	N3-C4-N4	5.30	121.71	118.00
1	A	53	A	OP1-P-OP2	-5.30	111.64	119.60
1	A	145	G	C4-C5-N7	5.30	112.92	110.80
1	A	377	G	OP1-P-O3'	5.30	116.87	105.20
1	A	630	G	OP2-P-O3'	5.30	116.87	105.20
1	A	1108	G	C4-C5-C6	5.30	121.98	118.80
1	A	1143	G	C4-C5-C6	5.30	121.98	118.80
1	A	1349	A	N1-C6-N6	5.30	121.78	118.60
1	A	61	G	N1-C2-N2	5.30	120.97	116.20
1	A	535	A	C5-C6-N1	5.30	120.35	117.70
1	A	902	G	C6-N1-C2	-5.30	121.92	125.10
1	A	633	G	C5-C6-O6	-5.30	125.42	128.60
1	A	1477	C	C6-N1-C2	-5.30	118.18	120.30
1	A	195	A	C5-N7-C8	5.30	106.55	103.90
1	A	733	A	C5-N7-C8	-5.30	101.25	103.90
1	A	791	G	N1-C2-N3	5.29	127.08	123.90
1	A	239	U	C4-C5-C6	5.29	122.88	119.70
1	A	1075	C	C2-N1-C1'	-5.29	112.98	118.80
1	A	1157	A	N9-C4-C5	5.29	107.92	105.80
8	H	100	ILE	CB-CA-C	-5.29	101.01	111.60
1	A	122	G	N3-C4-C5	-5.29	125.95	128.60
1	A	216	G	C8-N9-C4	5.29	108.52	106.40
1	A	975	A	C8-N9-C4	-5.29	103.68	105.80
1	A	1385	G	C5-C6-N1	-5.29	108.85	111.50
1	A	1529	G	N9-C4-C5	5.29	107.52	105.40
11	K	103	LEU	CA-CB-CG	-5.29	103.13	115.30
1	A	446	G	N7-C8-N9	5.29	115.74	113.10
1	A	572	A	O5'-P-OP2	-5.29	100.94	105.70
1	A	817	C	O4'-C1'-N1	-5.29	103.97	108.20
1	A	1166	G	C5-N7-C8	5.29	106.94	104.30
1	A	126	G	N7-C8-N9	-5.29	110.46	113.10
1	A	396	G	C5-N7-C8	-5.29	101.66	104.30
1	A	443	C	N3-C4-C5	5.29	124.01	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	731	G	N1-C6-O6	5.29	123.07	119.90
1	A	778	G	N3-C4-C5	-5.29	125.96	128.60
1	A	1213	A	C5-C6-N1	5.29	120.34	117.70
1	A	284	G	N3-C4-C5	5.28	131.24	128.60
1	A	649	G	OP1-P-O3'	-5.28	93.58	105.20
1	A	1067	A	N9-C4-C5	5.28	107.91	105.80
3	C	178	LEU	N-CA-C	-5.28	96.74	111.00
19	S	9	VAL	CB-CA-C	-5.28	101.36	111.40
1	A	1460	A	C6-N1-C2	-5.28	115.43	118.60
1	A	39	G	N9-C1'-C2'	-5.28	106.19	112.00
1	A	760	G	N3-C4-N9	-5.28	122.83	126.00
1	A	954	G	C4-N9-C1'	-5.28	119.64	126.50
1	A	1066	C	N3-C4-C5	-5.28	119.79	121.90
1	A	1327	C	C6-N1-C2	5.28	122.41	120.30
1	A	801	U	N3-C4-C5	5.28	117.77	114.60
1	A	29	G	C2-N3-C4	-5.28	109.26	111.90
1	A	51	A	C2-N3-C4	-5.28	107.96	110.60
1	A	818	G	N9-C4-C5	5.28	107.51	105.40
1	A	883	C	C5-C6-N1	-5.28	118.36	121.00
1	A	1063	C	OP1-P-O3'	5.28	116.81	105.20
1	A	204	U	N3-C4-O4	5.28	123.09	119.40
1	A	479	C	C6-N1-C1'	-5.28	114.47	120.80
1	A	536	C	C5-C6-N1	5.28	123.64	121.00
1	A	567	G	N3-C4-C5	5.28	131.24	128.60
1	A	594	G	C6-N1-C2	-5.28	121.93	125.10
1	A	1506	U	OP2-P-O3'	5.28	116.81	105.20
1	A	1529	G	C8-N9-C1'	-5.28	120.14	127.00
2	B	19	HIS	CB-CA-C	5.28	120.95	110.40
1	A	198	G	N1-C2-N3	5.27	127.06	123.90
1	A	361	G	C5-C6-N1	5.27	114.14	111.50
1	A	362	G	C8-N9-C1'	-5.27	120.14	127.00
1	A	168	G	O5'-P-OP2	5.27	117.03	110.70
1	A	292	G	C6-C5-N7	-5.27	127.24	130.40
1	A	311	C	C6-N1-C1'	5.27	127.13	120.80
1	A	444	C	C6-N1-C1'	-5.27	114.47	120.80
1	A	963	G	C4-C5-C6	5.27	121.96	118.80
1	A	1011	G	N3-C4-C5	-5.27	125.96	128.60
1	A	1160	G	C5-C6-N1	-5.27	108.86	111.50
1	A	306	G	C5-C6-N1	-5.27	108.86	111.50
1	A	786	G	N1-C2-N3	-5.27	120.74	123.90
1	A	1231	G	C5-N7-C8	-5.27	101.66	104.30
1	A	353	A	N9-C4-C5	5.27	107.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1542	U	O5'-P-OP2	5.27	117.02	110.70
1	A	53	A	C4-C5-N7	-5.27	108.07	110.70
1	A	752	G	N3-C2-N2	5.27	123.59	119.90
1	A	1366	C	C6-N1-C2	-5.27	118.19	120.30
1	A	494	G	OP1-P-O3'	5.26	116.78	105.20
1	A	578	C	OP2-P-O3'	5.26	116.78	105.20
1	A	655	A	C4-C5-C6	5.26	119.63	117.00
1	A	1225	A	C5-N7-C8	5.26	106.53	103.90
1	A	255	G	N7-C8-N9	-5.26	110.47	113.10
1	A	1391	U	C2-N1-C1'	-5.26	111.39	117.70
1	A	370	C	OP1-P-O3'	5.26	116.78	105.20
1	A	327	A	OP1-P-OP2	5.26	127.49	119.60
1	A	601	C	C2-N3-C4	-5.26	117.27	119.90
1	A	861	G	OP1-P-OP2	5.26	127.49	119.60
1	A	1066	C	N3-C2-O2	5.26	125.58	121.90
1	A	1265	G	N3-C4-C5	-5.26	125.97	128.60
1	A	707	C	C6-N1-C1'	-5.26	114.49	120.80
1	A	883	C	N1-C2-N3	5.26	122.88	119.20
1	A	1386	G	N1-C6-O6	5.26	123.06	119.90
1	A	1409	C	C5-C4-N4	-5.26	116.52	120.20
1	A	1513	A	C5-C6-N1	5.26	120.33	117.70
20	T	38	LYS	CD-CE-NZ	5.26	123.79	111.70
1	A	1053	G	C6-C5-N7	5.25	133.55	130.40
1	A	506	G	N9-C4-C5	-5.25	103.30	105.40
1	A	510	A	C5-C6-N6	5.25	127.90	123.70
1	A	576	G	C4-C5-N7	-5.25	108.70	110.80
1	A	852	G	C4-N9-C1'	-5.25	119.67	126.50
1	A	1333	A	C4-C5-C6	5.25	119.63	117.00
1	A	78	G	N1-C6-O6	5.25	123.05	119.90
1	A	345	C	N1-C2-O2	5.25	122.05	118.90
1	A	520	A	C5-N7-C8	-5.25	101.28	103.90
1	A	667	G	N3-C2-N2	-5.25	116.22	119.90
1	A	714	G	C6-C5-N7	-5.25	127.25	130.40
1	A	1068	G	C5-C6-O6	-5.25	125.45	128.60
1	A	61	G	C5-N7-C8	-5.25	101.67	104.30
1	A	276	G	OP1-P-OP2	5.25	127.47	119.60
1	A	608	A	C6-N1-C2	-5.25	115.45	118.60
1	A	1401	G	C4-N9-C1'	5.25	133.32	126.50
1	A	172	A	C5-C6-N6	5.25	127.90	123.70
1	A	562	C	OP1-P-O3'	5.25	116.75	105.20
1	A	896	C	OP2-P-O3'	5.25	116.75	105.20
1	A	1010	G	N3-C2-N2	-5.25	116.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1142	G	C5-C6-N1	5.25	114.12	111.50
1	A	1308	U	N1-C2-O2	-5.25	119.13	122.80
1	A	1377	A	C4-C5-N7	-5.25	108.08	110.70
1	A	134	A	C4-C5-C6	5.25	119.62	117.00
1	A	374	A	C6-C5-N7	-5.25	128.63	132.30
1	A	431	A	C2-N3-C4	-5.25	107.98	110.60
1	A	607	A	O4'-C1'-N9	-5.25	104.00	108.20
1	A	716	A	N9-C4-C5	-5.25	103.70	105.80
1	A	797	C	C6-N1-C2	5.25	122.40	120.30
1	A	1053	G	C4-C5-C6	-5.25	115.65	118.80
1	A	990	C	N1-C2-N3	-5.25	115.53	119.20
1	A	73	C	N3-C2-O2	5.24	125.57	121.90
1	A	429	U	N3-C4-O4	5.24	123.07	119.40
1	A	651	C	OP1-P-OP2	5.24	127.47	119.60
1	A	985	C	O5'-P-OP1	-5.24	100.98	105.70
1	A	37	U	C4-C5-C6	5.24	122.84	119.70
1	A	221	C	C6-N1-C1'	-5.24	114.51	120.80
1	A	451	A	C5-C6-N1	-5.24	115.08	117.70
1	A	625	G	N1-C2-N2	5.24	120.92	116.20
1	A	769	G	C5-C6-O6	-5.24	125.45	128.60
1	A	1185	G	N1-C6-O6	5.24	123.05	119.90
1	A	1502	A	C6-N1-C2	5.24	121.74	118.60
1	A	462	G	N1-C2-N3	5.24	127.04	123.90
1	A	888	G	C5-C6-N1	-5.24	108.88	111.50
1	A	259	G	N3-C2-N2	-5.24	116.23	119.90
1	A	1012	U	C5-C4-O4	5.24	129.04	125.90
1	A	130	A	C5-N7-C8	-5.23	101.28	103.90
1	A	383	A	C6-N1-C2	-5.23	115.46	118.60
1	A	758	G	O5'-P-OP2	5.23	116.98	110.70
1	A	863	U	C2-N3-C4	-5.23	123.86	127.00
1	A	1469	G	C8-N9-C1'	5.23	133.80	127.00
1	A	311	C	C4-C5-C6	5.23	120.02	117.40
1	A	377	G	O5'-P-OP1	5.23	116.98	110.70
1	A	654	G	C5-N7-C8	-5.23	101.69	104.30
1	A	718	G	N3-C4-C5	5.23	131.22	128.60
1	A	442	C	N3-C4-C5	5.23	123.99	121.90
1	A	316	G	N1-C2-N3	5.23	127.04	123.90
1	A	790	A	N9-C4-C5	5.23	107.89	105.80
1	A	867	G	OP2-P-O3'	5.23	116.70	105.20
1	A	1125	U	N1-C2-N3	-5.23	111.76	114.90
1	A	1375	A	C5-C6-N6	-5.23	119.52	123.70
5	E	142	LEU	CB-CG-CD1	-5.23	102.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	A	N9-C4-C5	5.23	107.89	105.80
1	A	226	G	N1-C2-N3	5.23	127.04	123.90
1	A	970	C	N3-C4-N4	-5.23	114.34	118.00
1	A	1102	A	N3-C4-C5	-5.23	123.14	126.80
1	A	32	A	OP2-P-O3'	5.22	116.69	105.20
1	A	477	G	N7-C8-N9	5.22	115.71	113.10
1	A	488	C	C5-C4-N4	-5.22	116.54	120.20
1	A	1063	C	O5'-P-OP1	5.22	116.97	110.70
1	A	1071	C	C6-N1-C1'	5.22	127.07	120.80
1	A	1174	G	O5'-P-OP1	5.22	116.97	110.70
1	A	1280	A	N1-C2-N3	5.22	131.91	129.30
1	A	1516[A]	G	C5-C6-N1	-5.22	108.89	111.50
1	A	1516[B]	G	C5-C6-N1	-5.22	108.89	111.50
1	A	55	A	C8-N9-C4	-5.22	103.71	105.80
1	A	120	A	O5'-P-OP2	-5.22	101.00	105.70
1	A	627	G	N7-C8-N9	5.22	115.71	113.10
1	A	1197	G	C4-N9-C1'	5.22	133.29	126.50
11	K	91	ARG	N-CA-C	-5.22	96.90	111.00
1	A	482	A	C8-N9-C4	-5.22	103.71	105.80
1	A	1281	U	OP2-P-O3'	5.22	116.69	105.20
8	H	36	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	A	43	C	OP1-P-OP2	5.22	127.43	119.60
1	A	427	U	C6-N1-C2	-5.22	117.87	121.00
1	A	962	C	C2-N1-C1'	-5.22	113.06	118.80
18	R	72	ARG	NE-CZ-NH2	-5.22	117.69	120.30
20	T	102	GLY	N-CA-C	-5.22	100.05	113.10
1	A	425	G	C6-C5-N7	5.22	133.53	130.40
1	A	598	U	OP1-P-OP2	5.22	127.42	119.60
1	A	793	U	C6-N1-C1'	5.22	128.50	121.20
1	A	920	U	C6-N1-C2	5.22	124.13	121.00
1	A	1180	A	C8-N9-C4	-5.22	103.71	105.80
1	A	1294	G	C5-C6-N1	5.22	114.11	111.50
10	J	40	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	261	U	C6-N1-C2	-5.21	117.87	121.00
1	A	424	G	C5-C6-N1	5.21	114.11	111.50
1	A	642	A	C6-C5-N7	-5.21	128.65	132.30
1	A	809	G	C4-C5-C6	-5.21	115.67	118.80
1	A	930	C	C2-N3-C4	-5.21	117.29	119.90
1	A	288	A	N3-C4-N9	-5.21	123.23	127.40
1	A	323	U	C4-C5-C6	5.21	122.83	119.70
1	A	363	A	N7-C8-N9	5.21	116.41	113.80
1	A	664	G	C2-N3-C4	5.21	114.51	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	957	U	N1-C2-O2	-5.21	119.15	122.80
1	A	1225	A	C8-N9-C1'	-5.21	118.32	127.70
1	A	1283	G	N3-C2-N2	-5.21	116.25	119.90
2	B	33	TYR	CA-CB-CG	5.21	123.30	113.40
1	A	709	G	C4-C5-C6	5.21	121.93	118.80
1	A	663	A	N9-C4-C5	5.21	107.88	105.80
1	A	1509	C	N3-C4-C5	-5.21	119.82	121.90
1	A	117	G	N3-C4-N9	5.21	129.12	126.00
1	A	196	A	C4-N9-C1'	-5.21	116.93	126.30
1	A	674	G	N3-C4-C5	-5.21	126.00	128.60
1	A	930	C	N1-C2-N3	5.21	122.84	119.20
1	A	1224	G	C8-N9-C4	-5.21	104.32	106.40
1	A	1346	A	C5-C6-N6	5.21	127.86	123.70
1	A	521	G	C8-N9-C4	5.21	108.48	106.40
1	A	22	G	O5'-P-OP1	-5.20	101.02	105.70
1	A	57	G	OP2-P-O3'	5.20	116.65	105.20
1	A	110	C	C5-C6-N1	5.20	123.60	121.00
1	A	185	A	N3-C4-C5	5.20	130.44	126.80
1	A	491	G	C5-C6-N1	-5.20	108.90	111.50
1	A	819	A	OP2-P-O3'	5.20	116.65	105.20
1	A	872	A	N3-C4-C5	-5.20	123.16	126.80
1	A	1106	G	N3-C4-N9	5.20	129.12	126.00
1	A	45	U	N1-C2-N3	5.20	118.02	114.90
1	A	269	C	C5-C6-N1	-5.20	118.40	121.00
1	A	270	A	C5-N7-C8	-5.20	101.30	103.90
1	A	746	A	C5-C6-N6	5.20	127.86	123.70
1	A	933	G	C4-N9-C1'	5.20	133.26	126.50
1	A	1059	C	N1-C2-O2	-5.20	115.78	118.90
1	A	1077	G	C4-C5-N7	5.20	112.88	110.80
1	A	1105	A	N3-C4-C5	-5.20	123.16	126.80
1	A	717	C	C4-C5-C6	5.20	120.00	117.40
1	A	1189	C	N1-C2-N3	-5.20	115.56	119.20
3	C	134	ILE	CB-CA-C	-5.20	101.20	111.60
1	A	508	C	N1-C2-O2	5.20	122.02	118.90
1	A	697	U	N1-C2-O2	-5.20	119.16	122.80
1	A	886	G	N7-C8-N9	5.20	115.70	113.10
1	A	960	U	C2-N1-C1'	5.20	123.94	117.70
1	A	1352	C	C4-C5-C6	5.20	120.00	117.40
5	E	26	PHE	CB-CA-C	-5.20	100.01	110.40
1	A	24	U	N3-C2-O2	-5.20	118.56	122.20
1	A	196	A	N3-C4-C5	5.20	130.44	126.80
1	A	238	G	N1-C2-N3	5.20	127.02	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	C	N3-C2-O2	5.20	125.54	121.90
1	A	753	A	C8-N9-C4	-5.20	103.72	105.80
1	A	1107	C	C5-C6-N1	-5.20	118.40	121.00
2	B	207	ALA	N-CA-C	5.20	125.03	111.00
1	A	338	A	C6-N1-C2	-5.19	115.48	118.60
1	A	105	G	C5-C6-O6	-5.19	125.48	128.60
1	A	143	A	N1-C6-N6	5.19	121.72	118.60
1	A	180	U	N3-C4-O4	5.19	123.03	119.40
1	A	1341	U	C2-N3-C4	-5.19	123.88	127.00
1	A	1438	G	N9-C4-C5	-5.19	103.32	105.40
6	F	61	LEU	CA-CB-CG	5.19	127.24	115.30
15	O	81	LEU	CA-CB-CG	-5.19	103.36	115.30
1	A	282	A	N1-C6-N6	5.19	121.71	118.60
1	A	646	U	C6-N1-C1'	5.19	128.47	121.20
1	A	913	A	C6-C5-N7	5.19	135.93	132.30
19	S	81	ARG	CD-NE-CZ	5.19	130.87	123.60
1	A	46	G	C5-N7-C8	-5.19	101.70	104.30
1	A	327	A	C6-C5-N7	-5.19	128.67	132.30
1	A	447	G	OP2-P-O3'	5.19	116.61	105.20
1	A	1120	G	C6-C5-N7	-5.19	127.29	130.40
1	A	1497	G	C6-C5-N7	-5.19	127.29	130.40
1	A	27	G	C5-C6-N1	5.19	114.09	111.50
1	A	167	G	O5'-P-OP2	5.19	116.92	110.70
1	A	327	A	C4-C5-N7	5.19	113.29	110.70
1	A	431	A	N7-C8-N9	-5.19	111.21	113.80
1	A	769	G	C5-C6-N1	-5.19	108.91	111.50
1	A	1283	G	C5-N7-C8	5.19	106.89	104.30
1	A	1435	G	N3-C2-N2	-5.19	116.27	119.90
6	F	47	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	134	A	C5-C6-N1	-5.18	115.11	117.70
1	A	361	G	N7-C8-N9	-5.18	110.51	113.10
1	A	764	C	N3-C2-O2	-5.18	118.27	121.90
1	A	1527	C	O5'-P-OP2	-5.18	101.03	105.70
1	A	446	G	OP2-P-O3'	5.18	116.60	105.20
1	A	903	G	N7-C8-N9	-5.18	110.51	113.10
1	A	968	A	N1-C6-N6	5.18	121.71	118.60
1	A	1021	G	O4'-C1'-N9	5.18	112.35	108.20
1	A	1149	C	C6-N1-C1'	5.18	127.02	120.80
1	A	801	U	C2-N3-C4	-5.18	123.89	127.00
1	A	97	G	N1-C2-N3	5.18	127.01	123.90
1	A	132	C	C2-N3-C4	-5.18	117.31	119.90
1	A	946	A	N3-C4-N9	5.18	131.54	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1039	C	N3-C4-C5	-5.18	119.83	121.90
1	A	129	U	C2-N1-C1'	-5.18	111.49	117.70
1	A	190(G)	G	C5-C6-N1	-5.18	108.91	111.50
1	A	485	G	N1-C2-N2	-5.18	111.54	116.20
1	A	759	A	C4-C5-N7	-5.18	108.11	110.70
1	A	8	A	C4-C5-C6	-5.18	114.41	117.00
1	A	128	G	C4-N9-C1'	5.18	133.23	126.50
1	A	576	G	N9-C4-C5	5.18	107.47	105.40
1	A	1507	A	OP2-P-O3'	5.18	116.59	105.20
1	A	582	U	C6-N1-C1'	5.17	128.44	121.20
1	A	1281	U	O5'-P-OP1	-5.17	101.04	105.70
1	A	570	G	O5'-P-OP2	5.17	116.91	110.70
1	A	737	A	C2-N3-C4	-5.17	108.01	110.60
1	A	810	C	N3-C2-O2	-5.17	118.28	121.90
1	A	875	C	O5'-P-OP2	-5.17	101.04	105.70
1	A	755	G	C8-N9-C4	-5.17	104.33	106.40
1	A	1173	G	C2-N3-C4	-5.17	109.31	111.90
1	A	190(D)	U	N1-C2-O2	5.17	126.42	122.80
1	A	1104	G	OP2-P-O3'	5.17	116.57	105.20
1	A	1496	C	N1-C2-O2	-5.17	115.80	118.90
1	A	97	G	C8-N9-C4	-5.17	104.33	106.40
1	A	407	G	C8-N9-C4	-5.17	104.33	106.40
1	A	521	G	N1-C6-O6	-5.17	116.80	119.90
1	A	594	G	C8-N9-C4	5.17	108.47	106.40
1	A	824	C	OP1-P-O3'	5.17	116.57	105.20
1	A	994	A	OP1-P-O3'	5.17	116.57	105.20
1	A	1052	U	C5-C6-N1	-5.17	120.12	122.70
1	A	840	C	O4'-C1'-N1	5.17	112.33	108.20
1	A	857	C	N1-C2-N3	5.17	122.82	119.20
1	A	676	A	C5-N7-C8	5.17	106.48	103.90
1	A	368	U	N1-C2-N3	5.16	118.00	114.90
1	A	438	G	OP2-P-O3'	5.16	116.56	105.20
1	A	849	C	C5-C6-N1	5.16	123.58	121.00
1	A	509	A	N1-C2-N3	5.16	131.88	129.30
1	A	818	G	C2-N3-C4	5.16	114.48	111.90
1	A	12	U	C4-C5-C6	5.16	122.80	119.70
1	A	1098	C	OP1-P-OP2	5.16	127.34	119.60
1	A	1109	C	C2-N3-C4	-5.16	117.32	119.90
1	A	25	C	N3-C2-O2	5.16	125.51	121.90
1	A	241	C	C2-N1-C1'	-5.16	113.13	118.80
1	A	970	C	N3-C4-C5	5.16	123.96	121.90
1	A	1454	G	O5'-P-OP2	-5.16	101.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1002	G	N3-C4-N9	-5.16	122.91	126.00
1	A	190(H)	G	N1-C6-O6	5.16	122.99	119.90
1	A	1421	G	N7-C8-N9	5.16	115.68	113.10
1	A	183	G	C6-C5-N7	-5.15	127.31	130.40
1	A	191	G	N1-C2-N3	5.15	126.99	123.90
1	A	389	A	N9-C4-C5	5.15	107.86	105.80
1	A	712	A	OP2-P-O3'	5.15	116.54	105.20
1	A	1353	G	C6-N1-C2	-5.15	122.01	125.10
1	A	68	G	N7-C8-N9	-5.15	110.52	113.10
1	A	497	A	N7-C8-N9	5.15	116.38	113.80
1	A	563	A	N1-C2-N3	5.15	131.88	129.30
1	A	389	A	P-O3'-C3'	5.15	125.88	119.70
1	A	497	A	OP1-P-OP2	5.15	127.33	119.60
1	A	575	G	C5-N7-C8	5.15	106.88	104.30
1	A	729	A	C4-N9-C1'	5.15	135.57	126.30
1	A	149	A	N1-C2-N3	5.15	131.87	129.30
1	A	677	U	C4-C5-C6	5.15	122.79	119.70
1	A	1505	G	N7-C8-N9	5.15	115.67	113.10
1	A	276	G	N7-C8-N9	-5.15	110.53	113.10
1	A	519	C	N1-C2-N3	5.15	122.80	119.20
1	A	785	G	C5-N7-C8	-5.15	101.73	104.30
1	A	1382	C	N3-C4-N4	-5.15	114.40	118.00
1	A	1254	C	N1-C2-N3	5.15	122.80	119.20
3	C	124	ILE	CB-CA-C	-5.15	101.31	111.60
1	A	129(A)	G	N7-C8-N9	5.14	115.67	113.10
1	A	255	G	N3-C2-N2	-5.14	116.30	119.90
1	A	1144	G	N1-C6-O6	5.14	122.99	119.90
1	A	1532	U	N1-C2-N3	-5.14	111.81	114.90
1	A	184	G	N1-C2-N3	5.14	126.99	123.90
1	A	306	G	C5-C6-O6	-5.14	125.51	128.60
1	A	927	G	C5-N7-C8	-5.14	101.73	104.30
1	A	1111	A	C8-N9-C4	5.14	107.86	105.80
1	A	1334	G	C6-N1-C2	-5.14	122.01	125.10
1	A	1409	C	N3-C2-O2	-5.14	118.30	121.90
1	A	1525	G	OP1-P-OP2	-5.14	111.89	119.60
1	A	650	G	C5-N7-C8	5.14	106.87	104.30
4	D	12	CYS	N-CA-C	-5.14	97.12	111.00
1	A	866	C	O5'-P-OP1	-5.14	101.08	105.70
1	A	909	A	N1-C6-N6	5.14	121.68	118.60
1	A	1367	C	C6-N1-C2	-5.14	118.24	120.30
1	A	511	C	C4-C5-C6	5.14	119.97	117.40
1	A	553	A	C5-N7-C8	-5.14	101.33	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	993	G	C5-C6-N1	5.14	114.07	111.50
1	A	1451	A	N9-C4-C5	-5.14	103.75	105.80
1	A	1509	C	C2-N3-C4	-5.14	117.33	119.90
1	A	1539	C	N1-C2-O2	5.14	121.98	118.90
2	B	20	GLU	N-CA-C	5.14	124.87	111.00
1	A	354	G	O5'-P-OP2	5.13	116.86	110.70
1	A	360	A	C4-C5-N7	5.13	113.27	110.70
1	A	449	C	C6-N1-C2	-5.13	118.25	120.30
1	A	1528	U	C5-C6-N1	-5.13	120.13	122.70
1	A	257	G	N9-C4-C5	-5.13	103.35	105.40
1	A	451	A	N1-C6-N6	5.13	121.68	118.60
1	A	651	C	N1-C2-O2	-5.13	115.82	118.90
1	A	1156	G	C5-N7-C8	5.13	106.87	104.30
1	A	1503	A	C5-C6-N1	-5.13	115.14	117.70
1	A	131	C	C4-C5-C6	5.13	119.97	117.40
1	A	357	G	C8-N9-C4	5.13	108.45	106.40
1	A	1414	U	C5'-C4'-C3'	-5.13	107.79	116.00
1	A	364	A	OP1-P-OP2	-5.13	111.91	119.60
1	A	462	G	C4-N9-C1'	5.13	133.17	126.50
1	A	892	A	O5'-P-OP1	-5.13	101.08	105.70
1	A	1036	G	N3-C4-N9	5.13	129.08	126.00
1	A	1143	G	N1-C2-N3	5.13	126.98	123.90
1	A	1381	U	OP2-P-O3'	5.13	116.48	105.20
1	A	367	U	OP2-P-O3'	5.12	116.47	105.20
1	A	662	G	C5-N7-C8	-5.12	101.74	104.30
1	A	741	G	C5-C6-N1	-5.12	108.94	111.50
1	A	691	G	N7-C8-N9	5.12	115.66	113.10
1	A	1121	U	N1-C2-O2	-5.12	119.21	122.80
1	A	1363	A	C6-N1-C2	-5.12	115.53	118.60
2	B	121	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	581	G	N9-C4-C5	-5.12	103.35	105.40
1	A	1168	A	C4-C5-N7	-5.12	108.14	110.70
1	A	1392	G	C2-N3-C4	-5.12	109.34	111.90
1	A	447	G	N1-C6-O6	5.12	122.97	119.90
1	A	1468	A	C8-N9-C4	5.12	107.85	105.80
1	A	1512	U	C2-N1-C1'	-5.12	111.56	117.70
12	L	58	VAL	CB-CA-C	-5.12	101.67	111.40
1	A	12	U	C6-N1-C2	-5.12	117.93	121.00
1	A	109	A	N9-C1'-C2'	5.12	120.65	114.00
1	A	787	A	C5-C6-N6	-5.12	119.61	123.70
1	A	1164	G	O5'-P-OP2	-5.12	101.09	105.70
1	A	378	G	N9-C4-C5	-5.12	103.35	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	C	P-O5'-C5'	-5.12	112.72	120.90
1	A	517	G	C4-C5-C6	5.12	121.87	118.80
1	A	1055	A	C6-N1-C2	-5.12	115.53	118.60
1	A	1077	G	N9-C4-C5	-5.12	103.35	105.40
1	A	10	A	C6-C5-N7	5.11	135.88	132.30
1	A	47	C	N3-C2-O2	-5.11	118.32	121.90
1	A	635	G	C4-C5-C6	5.11	121.87	118.80
1	A	610	G	C8-N9-C1'	5.11	133.65	127.00
1	A	1421	G	N9-C4-C5	5.11	107.44	105.40
1	A	278	G	N1-C2-N2	5.11	120.80	116.20
1	A	344	A	O4'-C1'-N9	-5.11	104.11	108.20
1	A	539	A	C6-N1-C2	-5.11	115.53	118.60
1	A	568	G	OP2-P-O3'	5.11	116.44	105.20
1	A	646	U	N3-C4-C5	-5.11	111.53	114.60
1	A	667	G	C6-C5-N7	-5.11	127.33	130.40
1	A	923	A	C5-C6-N6	-5.11	119.61	123.70
1	A	1197	G	N1-C2-N2	-5.11	111.60	116.20
1	A	109	A	C6-N1-C2	-5.11	115.54	118.60
1	A	279	A	C4-N9-C1'	5.11	135.49	126.30
1	A	403	C	N3-C4-C5	-5.11	119.86	121.90
1	A	570	G	C4-N9-C1'	5.11	133.14	126.50
1	A	977	A	N9-C4-C5	5.11	107.84	105.80
1	A	1131	G	O5'-P-OP2	-5.11	101.10	105.70
1	A	1204	A	C5-C6-N1	-5.11	115.15	117.70
1	A	1399	C	C5-C6-N1	-5.11	118.45	121.00
1	A	29	G	OP2-P-O3'	5.11	116.43	105.20
1	A	78	G	C4-C5-C6	5.11	121.86	118.80
1	A	264	U	O5'-P-OP1	5.11	116.83	110.70
1	A	696	A	O4'-C1'-N9	-5.11	104.12	108.20
1	A	768	A	O5'-P-OP2	5.11	116.83	110.70
1	A	781	A	P-O3'-C3'	5.11	125.83	119.70
1	A	851	G	C4-C5-N7	-5.11	108.76	110.80
1	A	1093	A	C6-N1-C2	-5.11	115.54	118.60
1	A	1116	C	OP1-P-O3'	5.11	116.43	105.20
1	A	768	A	C4-N9-C1'	5.10	135.49	126.30
1	A	1505	G	N1-C2-N3	5.10	126.96	123.90
15	O	70	LEU	CA-CB-CG	-5.10	103.56	115.30
1	A	114	U	N3-C2-O2	-5.10	118.63	122.20
1	A	127	G	C8-N9-C1'	-5.10	120.37	127.00
1	A	297	G	C4-C5-N7	-5.10	108.76	110.80
1	A	710	G	N3-C4-C5	-5.10	126.05	128.60
1	A	763	G	C4-C5-N7	5.10	112.84	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1182	G	C4-C5-C6	5.10	121.86	118.80
1	A	1299	A	C5-N7-C8	-5.10	101.35	103.90
1	A	1450	U	OP1-P-O3'	5.10	116.43	105.20
1	A	1493	A	C4-C5-C6	5.10	119.55	117.00
5	E	15	ARG	NE-CZ-NH1	5.10	122.85	120.30
5	E	41	VAL	CB-CA-C	-5.10	101.70	111.40
1	A	553	A	OP2-P-O3'	5.10	116.42	105.20
1	A	910	C	N1-C2-O2	-5.10	115.84	118.90
1	A	113	G	C4-N9-C1'	5.10	133.13	126.50
1	A	505	G	N9-C4-C5	5.10	107.44	105.40
1	A	731	G	OP1-P-OP2	-5.10	111.95	119.60
1	A	961	U	C5-C4-O4	-5.10	122.84	125.90
1	A	969	A	O4'-C1'-N9	-5.10	104.12	108.20
1	A	1173	G	N3-C4-C5	5.10	131.15	128.60
1	A	282	A	O5'-P-OP2	5.10	116.82	110.70
1	A	867	G	N1-C6-O6	5.10	122.96	119.90
1	A	234	C	C4-C5-C6	5.09	119.95	117.40
1	A	506	G	O4'-C1'-N9	-5.09	104.12	108.20
1	A	604	G	N1-C6-O6	5.09	122.96	119.90
1	A	637	G	C2-N3-C4	-5.09	109.35	111.90
1	A	907	A	C4-C5-N7	-5.09	108.15	110.70
1	A	1027	C	C5-C6-N1	5.09	123.55	121.00
1	A	1053	G	O5'-P-OP2	5.09	116.81	110.70
1	A	1158	C	N1-C2-N3	5.09	122.77	119.20
1	A	331	G	C8-N9-C1'	-5.09	120.38	127.00
1	A	330	C	C4-C5-C6	5.09	119.94	117.40
1	A	685	G	C5-C6-O6	5.09	131.66	128.60
1	A	841	U	N3-C2-O2	-5.09	118.64	122.20
1	A	1077	G	N3-C2-N2	-5.09	116.33	119.90
1	A	1505	G	C6-N1-C2	-5.09	122.05	125.10
1	A	222	U	N3-C4-O4	-5.09	115.84	119.40
1	A	338	A	N9-C4-C5	5.09	107.84	105.80
1	A	409	G	C4-N9-C1'	5.09	133.12	126.50
1	A	874	G	C8-N9-C4	5.09	108.44	106.40
1	A	1168	A	N3-C4-N9	5.09	131.47	127.40
1	A	1412	C	N3-C4-C5	5.09	123.94	121.90
1	A	1432	G	C5-C6-N1	-5.09	108.96	111.50
1	A	1526	G	N7-C8-N9	5.09	115.64	113.10
1	A	190(A)	C	N3-C4-N4	5.09	121.56	118.00
1	A	1452	C	N3-C4-N4	5.09	121.56	118.00
1	A	46	G	O5'-P-OP1	-5.09	101.12	105.70
1	A	737	A	C4-C5-C6	5.09	119.54	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	G	C4-C5-N7	5.08	112.83	110.80
1	A	1112	C	C6-N1-C2	5.08	122.33	120.30
1	A	1363	A	N9-C4-C5	5.08	107.83	105.80
1	A	149	A	C4-C5-C6	5.08	119.54	117.00
1	A	371	G	C5-C6-O6	5.08	131.65	128.60
1	A	518	C	P-O3'-C3'	5.08	125.80	119.70
1	A	765	G	O5'-P-OP1	-5.08	101.12	105.70
1	A	1063	C	N1-C2-N3	5.08	122.76	119.20
1	A	1259	C	N1-C2-O2	5.08	121.95	118.90
1	A	252	U	C5-C4-O4	5.08	128.95	125.90
1	A	498	U	N3-C4-C5	-5.08	111.55	114.60
1	A	1057	G	C4-C5-N7	-5.08	108.77	110.80
1	A	1504	G	C4-C5-N7	-5.08	108.77	110.80
2	B	154	LEU	CA-CB-CG	-5.08	103.61	115.30
1	A	964	A	C5-C6-N1	-5.08	115.16	117.70
1	A	392	G	C8-N9-C4	5.08	108.43	106.40
1	A	419	C	O5'-P-OP1	5.08	116.79	110.70
1	A	1217	C	O5'-P-OP1	-5.08	101.13	105.70
1	A	1504	G	C5-C6-O6	5.08	131.65	128.60
1	A	1511	G	C8-N9-C4	-5.08	104.37	106.40
1	A	220	G	N3-C4-C5	5.08	131.14	128.60
1	A	820	U	C5-C6-N1	-5.08	120.16	122.70
1	A	1103	C	OP1-P-OP2	5.08	127.22	119.60
1	A	287	U	C5-C4-O4	-5.08	122.86	125.90
1	A	301	G	N3-C2-N2	-5.08	116.35	119.90
1	A	935	A	C5-N7-C8	-5.08	101.36	103.90
1	A	1231	G	C4-C5-C6	5.08	121.84	118.80
1	A	290	C	C2-N1-C1'	5.07	124.38	118.80
1	A	598	U	N1-C2-N3	-5.07	111.86	114.90
1	A	738	C	C5-C6-N1	5.07	123.54	121.00
1	A	1137	C	N1-C2-O2	5.07	121.94	118.90
1	A	528	C	O5'-P-OP1	-5.07	101.14	105.70
1	A	996	A	C8-N9-C4	-5.07	103.77	105.80
1	A	1406	U	C5-C4-O4	-5.07	122.86	125.90
1	A	28	G	N1-C6-O6	5.07	122.94	119.90
1	A	478	A	C5-C6-N6	-5.07	119.64	123.70
1	A	952	U	C5-C4-O4	-5.07	122.86	125.90
1	A	35	G	C2-N3-C4	-5.07	109.37	111.90
1	A	190(G)	G	OP2-P-O3'	5.07	116.35	105.20
1	A	572	A	C8-N9-C1'	5.07	136.82	127.70
1	A	598	U	N3-C2-O2	5.07	125.75	122.20
1	A	737	A	C8-N9-C4	-5.07	103.77	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	748	C	N1-C2-O2	5.07	121.94	118.90
1	A	900	A	N1-C6-N6	5.07	121.64	118.60
1	A	911	U	C4-C5-C6	5.07	122.74	119.70
1	A	996	A	C4-C5-C6	5.07	119.53	117.00
1	A	1137	C	N3-C2-O2	-5.07	118.35	121.90
4	D	34	GLU	CA-C-N	-5.07	106.05	117.20
1	A	70	G	N1-C6-O6	5.07	122.94	119.90
1	A	284	G	N1-C2-N3	5.07	126.94	123.90
1	A	609	A	C4-C5-N7	5.07	113.23	110.70
1	A	868	C	OP2-P-O3'	5.07	116.34	105.20
1	A	920	U	N3-C4-C5	5.07	117.64	114.60
1	A	926	G	C6-N1-C2	-5.07	122.06	125.10
1	A	964	A	N3-C4-C5	5.07	130.35	126.80
1	A	60	A	N9-C4-C5	5.06	107.83	105.80
1	A	371	G	O5'-P-OP2	5.06	116.78	110.70
1	A	1248	A	C8-N9-C4	5.06	107.83	105.80
1	A	1252	A	OP1-P-OP2	-5.06	112.00	119.60
1	A	60	A	C8-N9-C4	-5.06	103.78	105.80
1	A	938	A	N7-C8-N9	5.06	116.33	113.80
1	A	974	A	C2-N3-C4	5.06	113.13	110.60
1	A	1117	G	N3-C2-N2	5.06	123.44	119.90
1	A	1131	G	O5'-P-OP1	5.06	116.78	110.70
1	A	190(E)	U	N3-C4-C5	5.06	117.64	114.60
1	A	350	G	C5-N7-C8	-5.06	101.77	104.30
1	A	430	A	OP1-P-OP2	5.06	127.19	119.60
1	A	853	G	C8-N9-C4	-5.06	104.38	106.40
1	A	909	A	N7-C8-N9	5.06	116.33	113.80
1	A	1119	C	N1-C2-N3	-5.06	115.66	119.20
1	A	978	A	C4-C5-C6	5.06	119.53	117.00
1	A	1232	U	C4-C5-C6	5.06	122.73	119.70
1	A	1321	C	C5-C4-N4	5.06	123.74	120.20
4	D	120	LEU	CB-CG-CD1	5.06	119.60	111.00
1	A	240	C	C2-N3-C4	-5.06	117.37	119.90
1	A	251	G	C8-N9-C1'	-5.05	120.43	127.00
1	A	305	G	C6-C5-N7	-5.05	127.37	130.40
1	A	800	G	N1-C2-N3	5.05	126.93	123.90
1	A	918	A	O5'-P-OP1	-5.05	101.15	105.70
1	A	12	U	N1-C2-O2	5.05	126.34	122.80
1	A	144	G	C6-C5-N7	-5.05	127.37	130.40
1	A	379	C	O4'-C1'-N1	5.05	112.24	108.20
1	A	758	G	OP2-P-O3'	5.05	116.32	105.20
1	A	1055	A	OP2-P-O3'	5.05	116.32	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1289	A	C2-N3-C4	5.05	113.13	110.60
1	A	1403	C	O4'-C1'-N1	-5.05	104.16	108.20
1	A	233	C	OP1-P-OP2	5.05	127.18	119.60
1	A	551	U	P-O3'-C3'	5.05	125.76	119.70
1	A	724	G	OP1-P-O3'	5.05	116.31	105.20
1	A	1054	C	N1-C2-O2	5.05	121.93	118.90
1	A	31	G	N7-C8-N9	-5.05	110.58	113.10
1	A	270	A	N7-C8-N9	5.05	116.32	113.80
1	A	319	G	OP2-P-O3'	5.05	116.31	105.20
1	A	1023	G	C2-N3-C4	5.05	114.42	111.90
1	A	1122	U	N3-C2-O2	-5.05	118.67	122.20
1	A	1302	U	C2-N1-C1'	5.05	123.76	117.70
1	A	1385	G	N1-C2-N3	5.05	126.93	123.90
1	A	1475	G	N7-C8-N9	5.05	115.62	113.10
1	A	124	G	N3-C4-C5	5.05	131.12	128.60
1	A	327	A	C5-C6-N1	-5.05	115.18	117.70
1	A	98	U	N3-C4-C5	5.05	117.63	114.60
1	A	240	C	OP1-P-OP2	5.05	127.17	119.60
1	A	1256	A	N1-C6-N6	5.05	121.63	118.60
1	A	1492	A	O4'-C1'-N9	5.05	112.24	108.20
1	A	271	C	N3-C4-N4	5.04	121.53	118.00
1	A	793	U	C2-N3-C4	-5.04	123.97	127.00
1	A	303	A	OP1-P-OP2	5.04	127.17	119.60
1	A	762	C	N3-C4-C5	5.04	123.92	121.90
1	A	805	C	N1-C2-N3	-5.04	115.67	119.20
1	A	841	U	C2-N3-C4	5.04	130.03	127.00
1	A	890	G	C1'-O4'-C4'	-5.04	105.86	109.90
1	A	33	A	N9-C4-C5	-5.04	103.78	105.80
1	A	480	U	N3-C4-O4	5.04	122.93	119.40
1	A	878	G	C4-C5-N7	5.04	112.82	110.80
1	A	1508	G	N7-C8-N9	5.04	115.62	113.10
1	A	504	C	OP1-P-OP2	-5.04	112.04	119.60
1	A	666	G	OP1-P-OP2	5.04	127.16	119.60
1	A	907	A	C2-N3-C4	-5.04	108.08	110.60
1	A	1365	G	C4-C5-N7	5.04	112.82	110.80
1	A	382	A	C4-C5-N7	-5.04	108.18	110.70
1	A	583	A	C5-C6-N1	-5.04	115.18	117.70
1	A	1331	G	N9-C4-C5	5.04	107.42	105.40
1	A	231	G	C5-C6-O6	-5.04	125.58	128.60
1	A	562	C	C6-N1-C1'	-5.04	114.76	120.80
1	A	567	G	P-O3'-C3'	-5.04	113.66	119.70
1	A	1093	A	C8-N9-C1'	5.04	136.77	127.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1489	G	C2-N3-C4	5.04	114.42	111.90
3	C	27	LYS	CD-CE-NZ	5.04	123.28	111.70
1	A	13	U	N1-C2-O2	-5.04	119.28	122.80
1	A	544	G	N1-C2-N3	5.04	126.92	123.90
1	A	675	A	O5'-P-OP1	-5.04	101.17	105.70
1	A	1037	C	C2-N3-C4	5.04	122.42	119.90
1	A	675	A	C6-C5-N7	-5.03	128.78	132.30
1	A	743	U	N3-C2-O2	5.03	125.72	122.20
1	A	859	A	C8-N9-C4	5.03	107.81	105.80
1	A	1341	U	N1-C2-N3	5.03	117.92	114.90
1	A	567	G	N7-C8-N9	-5.03	110.58	113.10
1	A	1033	G	C5-C6-N1	5.03	114.02	111.50
1	A	29	G	N7-C8-N9	5.03	115.62	113.10
1	A	661	G	N9-C4-C5	5.03	107.41	105.40
1	A	933	G	N1-C2-N2	-5.03	111.67	116.20
1	A	1088	G	O5'-P-OP1	5.03	116.74	110.70
1	A	714	G	C4-N9-C1'	5.03	133.04	126.50
1	A	712	A	N9-C4-C5	5.03	107.81	105.80
1	A	1077	G	C5'-C4'-O4'	5.03	115.13	109.10
1	A	190(C)	C	OP1-P-OP2	5.03	127.14	119.60
1	A	429	U	C5-C4-O4	-5.03	122.89	125.90
1	A	1178	G	N3-C4-C5	-5.03	126.09	128.60
1	A	1244	C	N1-C2-O2	5.03	121.92	118.90
1	A	1319	A	C2-N3-C4	-5.03	108.09	110.60
1	A	1349	A	N1-C2-N3	5.03	131.81	129.30
1	A	1418	A	N9-C4-C5	-5.03	103.79	105.80
1	A	1200	C	C4-C5-C6	5.02	119.91	117.40
1	A	124	G	C5-N7-C8	-5.02	101.79	104.30
1	A	380	G	OP2-P-O3'	5.02	116.25	105.20
1	A	660	G	C6-N1-C2	5.02	128.11	125.10
1	A	664	G	N7-C8-N9	-5.02	110.59	113.10
1	A	729	A	O5'-P-OP1	5.02	116.73	110.70
1	A	733	A	C2-N3-C4	-5.02	108.09	110.60
1	A	869	G	N1-C2-N2	-5.02	111.68	116.20
1	A	399	G	C6-C5-N7	-5.02	127.39	130.40
1	A	688	G	C4-N9-C1'	5.02	133.03	126.50
1	A	890	G	C5'-C4'-O4'	5.02	115.12	109.10
1	A	139	G	C6-N1-C2	-5.02	122.09	125.10
1	A	181	G	C5-C6-O6	-5.02	125.59	128.60
1	A	276	G	C8-N9-C4	5.02	108.41	106.40
1	A	309	G	C5-C6-N1	5.02	114.01	111.50
1	A	571	U	N1-C2-N3	5.02	117.91	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	830	G	N3-C4-C5	5.02	131.11	128.60
1	A	1240	U	C5-C4-O4	5.02	128.91	125.90
1	A	13	U	C4-C5-C6	5.02	122.71	119.70
1	A	549	C	N3-C4-N4	-5.02	114.49	118.00
1	A	581	G	N3-C2-N2	5.02	123.41	119.90
1	A	752	G	N1-C6-O6	-5.02	116.89	119.90
1	A	1022	G	C5-N7-C8	5.02	106.81	104.30
1	A	1076	C	N1-C2-O2	5.02	121.91	118.90
1	A	1134	G	N3-C2-N2	-5.02	116.39	119.90
1	A	626	U	N3-C4-C5	5.02	117.61	114.60
1	A	810	C	O5'-P-OP1	-5.02	101.19	105.70
1	A	1479	C	C5-C6-N1	5.02	123.51	121.00
1	A	218	C	N1-C2-N3	5.01	122.71	119.20
1	A	500	G	N1-C2-N2	5.01	120.71	116.20
1	A	729	A	C4-C5-C6	5.01	119.51	117.00
1	A	871	U	C6-N1-C1'	-5.01	114.18	121.20
1	A	1488	G	N1-C2-N3	-5.01	120.89	123.90
1	A	311	C	C2-N1-C1'	-5.01	113.29	118.80
1	A	587	G	N3-C4-C5	-5.01	126.09	128.60
1	A	693	G	C6-N1-C2	-5.01	122.09	125.10
1	A	799	G	N1-C6-O6	5.01	122.91	119.90
1	A	953	G	O5'-P-OP2	-5.01	101.19	105.70
1	A	1350	A	C6-N1-C2	-5.01	115.59	118.60
1	A	269	C	O4'-C1'-N1	5.01	112.21	108.20
1	A	1084	G	C4-C5-N7	-5.01	108.80	110.80
1	A	617	G	C5-C6-N1	-5.01	109.00	111.50
1	A	933	G	N7-C8-N9	5.01	115.61	113.10
1	A	944	G	OP2-P-O3'	5.01	116.22	105.20
1	A	984	C	C5-C6-N1	-5.01	118.50	121.00
1	A	990	C	C2-N3-C4	5.01	122.40	119.90
1	A	547	A	C5-C6-N6	5.01	127.71	123.70
1	A	776	G	C4-N9-C1'	-5.01	119.99	126.50
1	A	892	A	C4-N9-C1'	5.01	135.31	126.30
1	A	1028	C	C6-N1-C1'	5.01	126.81	120.80
1	A	1090	U	OP2-P-O3'	5.01	116.22	105.20
1	A	1348	U	C6-N1-C2	-5.01	118.00	121.00
1	A	257	G	C8-N9-C4	5.01	108.40	106.40
1	A	304	U	C6-N1-C2	5.01	124.00	121.00
1	A	373	A	O5'-C5'-C4'	5.01	121.21	111.70
1	A	551	U	N3-C4-C5	5.01	117.60	114.60
1	A	662	G	C8-N9-C1'	-5.01	120.49	127.00
1	A	756	C	C5-C4-N4	-5.01	116.69	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1028	C	C2-N1-C1'	-5.01	113.29	118.80
1	A	1154	G	C5-C6-N1	5.01	114.00	111.50
1	A	1321	C	C6-N1-C2	-5.01	118.30	120.30
1	A	1414	U	C2-N3-C4	5.01	130.00	127.00
1	A	230	G	C4-C5-C6	5.00	121.80	118.80
1	A	941	G	C5-C6-O6	-5.00	125.60	128.60
1	A	1257	U	O5'-P-OP2	-5.00	101.20	105.70
1	A	13	U	N3-C2-O2	5.00	125.70	122.20
1	A	160	A	C2-N3-C4	-5.00	108.10	110.60
1	A	251	G	N3-C4-N9	5.00	129.00	126.00
1	A	573	A	N7-C8-N9	5.00	116.30	113.80
1	A	887	G	N3-C2-N2	-5.00	116.40	119.90
1	A	1143	G	C5-C6-N1	-5.00	109.00	111.50
1	A	1288	A	N3-C4-N9	-5.00	123.40	127.40
1	A	1455	G	OP2-P-O3'	5.00	116.21	105.20
6	F	21	LEU	CA-CB-CG	-5.00	103.79	115.30
11	K	21	ILE	CB-CA-C	-5.00	101.59	111.60
1	A	57	G	N3-C4-C5	-5.00	126.10	128.60
1	A	67	C	N3-C4-C5	5.00	123.90	121.90
1	A	196	A	C6-C5-N7	5.00	135.80	132.30
1	A	426	G	C5-C6-N1	5.00	114.00	111.50
1	A	535	A	C8-N9-C4	-5.00	103.80	105.80
1	A	574	A	C4-C5-C6	-5.00	114.50	117.00
1	A	661	G	O5'-P-OP2	5.00	116.70	110.70
1	A	956	U	C2-N3-C4	-5.00	124.00	127.00

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	8	LYS	Peptide
2	B	89	GLY	Peptide
3	C	154	SER	Peptide
3	C	166	GLU	Peptide
3	C	178	LEU	Mainchain
3	C	179	ARG	Peptide
3	C	3	ASN	Peptide
4	D	195	ALA	Peptide
4	D	29	PRO	Peptide
4	D	3	ARG	Peptide
4	D	30	LYS	Peptide
4	D	35	ARG	Peptide

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Mol	Chain	Res	Type	Group
6	F	99	ALA	Peptide
7	G	13	GLN	Peptide
7	G	154	TYR	Peptide
8	H	62	TYR	Peptide
8	H	90	GLY	Peptide
9	I	126	SER	Peptide
10	J	12	ASP	Peptide
10	J	88	LEU	Peptide
11	K	102	GLY	Peptide
12	L	116	SER	Peptide
12	L	24	VAL	Peptide
12	L	25	PRO	Peptide
12	L	46	LYS	Peptide
12	L	87	GLY	Peptide
13	M	105	THR	Peptide
14	N	30	ALA	Peptide
14	N	7	ILE	Peptide
16	P	81	ARG	Peptide
17	Q	13	ASP	Peptide
18	R	21	LYS	Peptide
19	S	4	SER	Peptide
19	S	7	LYS	Peptide
20	T	12	ALA	Peptide
20	T	93	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32687	0	16508	1072	0
2	B	1900	0	1951	144	0
3	C	1612	0	1677	118	0
4	D	1703	0	1763	124	0
5	E	1146	0	1207	94	0
6	F	843	0	857	77	0
7	G	1257	0	1296	101	0
8	H	1116	0	1177	90	0
9	I	1010	0	1037	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	792	0	835	75	0
11	K	864	0	881	66	0
12	L	973	0	1062	83	0
13	M	937	0	995	88	0
14	N	492	0	529	48	0
15	O	729	0	768	66	0
16	P	700	0	720	54	0
17	Q	823	0	891	68	0
18	R	574	0	644	58	1
19	S	647	0	673	83	0
20	T	763	0	861	54	0
21	U	208	0	221	12	0
22	A	377	0	0	0	0
22	B	2	0	0	0	0
22	C	3	0	0	0	0
22	D	4	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	G	1	0	0	0	0
22	H	1	0	0	0	0
22	I	2	0	0	0	0
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	N	2	0	0	0	0
22	O	1	0	0	0	0
22	P	1	0	0	0	0
22	Q	2	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	1199	0	0	56	0
24	C	6	0	0	0	0
24	D	11	0	0	0	0
24	E	7	0	0	0	0
24	F	6	0	0	1	0
24	G	6	0	0	0	0
24	H	7	0	0	1	0
24	I	1	0	0	0	0
24	L	9	0	0	1	0
24	M	2	0	0	1	0
24	N	1	0	0	0	0
24	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	P	3	0	0	0	0
24	Q	6	0	0	2	0
All	All	53444	0	36553	2457	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 28.

All (2457) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:CYS:SG	4:D:12:CYS:CB	2.05	1.44
11:K:120:ARG:HB3	11:K:120:ARG:HH11	1.22	1.02
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.37	1.01
15:O:70:LEU:HB3	15:O:78:TYR:HB2	1.44	0.99
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.31	0.96
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.48	0.95
1:A:1162:C:N4	1:A:1174:G:O6	1.99	0.94
4:D:188:LEU:HD23	4:D:189:PRO:HD2	1.49	0.94
19:S:7:LYS:HD3	19:S:7:LYS:H	1.31	0.93
1:A:547:A:OP2	4:D:2:GLY:N	2.00	0.93
19:S:80:TYR:HE1	19:S:81:ARG:HD3	1.29	0.93
7:G:117:ALA:HA	7:G:120:ILE:HG12	1.51	0.92
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.50	0.91
10:J:4:ILE:HB	10:J:74:ILE:HB	1.50	0.91
19:S:80:TYR:CE1	19:S:81:ARG:HD3	2.05	0.91
1:A:664:G:H22	1:A:741:G:H1	1.09	0.91
20:T:93:GLU:N	20:T:93:GLU:OE1	2.05	0.90
1:A:998:G:N2	1:A:1043:C:O2	2.05	0.90
2:B:204:ASN:HD21	2:B:207:ALA:HB3	1.35	0.89
1:A:1523:G:OP1	11:K:123:LYS:NZ	2.05	0.89
3:C:35:GLU:HG3	3:C:95:THR:HG21	1.53	0.88
1:A:1515[A]:C:N3	1:A:1520[A]:G:N2	2.22	0.88
9:I:55:ALA:HA	9:I:58:HIS:HB2	1.53	0.88
1:A:1005:A:H1'	1:A:1026:G:H1	1.37	0.88
12:L:83:VAL:HG21	12:L:100:ILE:HD13	1.57	0.86
4:D:36:ARG:HB2	4:D:38:TYR:CE2	2.08	0.86
1:A:1007:C:N4	1:A:1023:G:O6	2.08	0.86
13:M:12:ASN:H	13:M:45:VAL:HB	1.41	0.86
1:A:579:G:H5'	1:A:728:A:H1'	1.58	0.86
1:A:1127:G:N2	1:A:1145:C:N3	2.24	0.85
13:M:5:ALA:N	13:M:8:GLU:OE1	2.08	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1490:C:H2'	1:A:1491:G:H5'	1.59	0.85
21:U:13:ILE:HA	21:U:22:ARG:HH21	1.41	0.85
3:C:21:ARG:HH11	3:C:21:ARG:HB3	1.41	0.84
1:A:1425:U:H2'	1:A:1426:C:C6	2.13	0.83
1:A:1402:4OC:HM43	1:A:1403:C:C4	2.12	0.83
1:A:263:A:OP2	20:T:79:ARG:NH1	2.10	0.83
2:B:9:GLU:OE2	2:B:10:LEU:N	2.11	0.83
14:N:9:LYS:HD2	14:N:23:ARG:HD2	1.60	0.83
1:A:141:A:H1'	1:A:182:U:O2	1.78	0.83
1:A:575:G:H4'	1:A:576:G:H5''	1.60	0.83
1:A:81:U:H2'	1:A:82:U:H5''	1.59	0.83
12:L:27:LEU:O	12:L:29:GLY:N	2.11	0.83
4:D:104:VAL:HG21	4:D:140:VAL:HG21	1.59	0.82
6:F:7:ASN:HD21	18:R:34:TYR:HE1	1.26	0.82
10:J:19:SER:HB3	10:J:91:PRO:HG2	1.61	0.82
20:T:56:MET:HE1	20:T:85:MET:HG2	1.62	0.82
1:A:895:G:N2	24:A:2471:HOH:O	2.13	0.82
14:N:32:SER:O	14:N:40:CYS:HA	1.81	0.81
12:L:27:LEU:HG	12:L:28:LYS:H	1.46	0.81
1:A:545:C:OP2	4:D:62:GLN:NE2	2.12	0.81
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.59	0.81
5:E:11:ILE:HG22	5:E:31:LEU:HB3	1.63	0.81
1:A:1226:C:H5''	19:S:80:TYR:CD2	2.16	0.80
8:H:11:THR:O	8:H:15:ASN:ND2	2.14	0.80
1:A:1100:C:N4	24:A:2914:HOH:O	2.07	0.80
4:D:197:PRO:HD2	4:D:198:VAL:HG23	1.62	0.80
1:A:427:U:OP2	4:D:36:ARG:NH2	2.14	0.80
1:A:279:A:H8	1:A:279:A:H5'	1.47	0.80
2:B:97:TRP:HH2	2:B:176:GLU:OE1	1.65	0.79
11:K:79:SER:OG	11:K:104:GLN:O	2.00	0.79
18:R:74:ARG:HB3	18:R:81:PHE:CE2	2.17	0.79
1:A:443:C:H42	1:A:491:G:H1	1.29	0.79
10:J:38:ILE:HG13	10:J:71:LEU:HB3	1.64	0.79
13:M:47:ASP:N	13:M:47:ASP:OD1	2.08	0.79
1:A:1162:C:N3	1:A:1175:G:N2	2.31	0.79
20:T:33:ILE:HD13	20:T:63:ILE:HG12	1.65	0.79
1:A:936:C:O2	1:A:1379:G:N2	2.16	0.78
1:A:677:U:H3	1:A:713:G:H22	1.31	0.78
6:F:5:GLU:HB3	6:F:62:TRP:HE1	1.47	0.78
1:A:444:C:O2	1:A:490:G:N2	2.11	0.78
1:A:227:G:O2'	24:A:2623:HOH:O	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:34:VAL:HG13	10:J:74:ILE:HA	1.64	0.78
1:A:664:G:OP1	18:R:64:ARG:HD2	1.84	0.78
6:F:15:ASP:OD2	6:F:17:SER:N	2.16	0.78
1:A:1182:G:H4'	1:A:1183:A:H5''	1.64	0.78
1:A:664:G:N2	1:A:741:G:H1	1.80	0.78
1:A:1403:C:H2'	1:A:1403:C:O2	1.83	0.78
18:R:38:GLU:O	18:R:42:ARG:NH1	2.17	0.78
15:O:4:THR:OG1	15:O:7:GLU:HG3	1.84	0.78
1:A:856:C:H2'	1:A:857:C:H5''	1.66	0.77
13:M:5:ALA:HA	13:M:61:GLU:HG3	1.64	0.77
1:A:1002:G:N7	1:A:1003:G:N2	2.33	0.77
3:C:14:ILE:O	3:C:16:ARG:N	2.16	0.77
1:A:1005:A:H61	1:A:1023:G:H22	1.32	0.77
1:A:434:U:H2'	1:A:435:C:H6	1.48	0.77
4:D:30:LYS:O	4:D:32:ALA:N	2.18	0.77
1:A:1152:A:H5''	10:J:13:HIS:CE1	2.20	0.77
1:A:1033:G:H3'	1:A:1034:G:H8	1.49	0.77
9:I:6:GLY:HA3	9:I:83:ARG:HB2	1.66	0.77
19:S:49:ILE:HG21	19:S:71:LEU:HD11	1.67	0.77
2:B:111:ARG:HH11	2:B:111:ARG:HG3	1.50	0.76
4:D:118:ARG:HG3	4:D:118:ARG:HH21	1.48	0.76
1:A:740:U:O2'	1:A:741:G:H5'	1.85	0.76
11:K:12:ARG:HE	11:K:40:ILE:HD11	1.51	0.76
11:K:40:ILE:HG13	11:K:75:TYR:HD2	1.51	0.76
1:A:869:G:C8	24:A:3090:HOH:O	2.39	0.76
10:J:5:ARG:HD2	10:J:99:LYS:HB2	1.64	0.76
15:O:36:ILE:HG13	15:O:59:MET:HE3	1.68	0.76
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.66	0.76
1:A:1313:U:O4	19:S:4:SER:OG	2.04	0.75
1:A:1262:C:H42	1:A:1273:G:H1	1.33	0.75
13:M:80:ARG:HH21	13:M:81:LEU:HD23	1.51	0.75
12:L:25:PRO:HB2	12:L:64:TYR:HE2	1.50	0.75
17:Q:61:GLU:HA	17:Q:71:PHE:CE2	2.21	0.75
15:O:77:ARG:HG2	15:O:77:ARG:HH11	1.52	0.75
6:F:30:LEU:HD23	6:F:35:ALA:HB3	1.68	0.75
13:M:11:ARG:HA	13:M:45:VAL:HG21	1.67	0.75
1:A:414:A:H2'	1:A:415:A:C8	2.22	0.75
1:A:1451:A:H5'	1:A:1452:C:H5	1.52	0.75
1:A:1435:G:H2'	1:A:1436:U:C6	2.22	0.75
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.02	0.75
1:A:673:G:H2'	1:A:674:G:C8	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.27	0.74
9:I:89:ASN:HB3	9:I:92:TYR:CD1	2.21	0.74
1:A:1103:C:H5''	2:B:98:LEU:HD22	1.68	0.74
5:E:64:ARG:HH21	5:E:65:ASN:HB2	1.52	0.74
12:L:24:VAL:HG22	12:L:98:TYR:CE2	2.22	0.74
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.69	0.74
13:M:23:TYR:HB3	13:M:67:GLU:H	1.52	0.74
1:A:411:A:OP1	4:D:30:LYS:NZ	2.20	0.74
4:D:28:SER:OG	4:D:30:LYS:N	2.19	0.74
1:A:1195:C:H5''	1:A:1196:U:OP2	1.87	0.74
14:N:35:ARG:HH11	14:N:35:ARG:HG2	1.53	0.74
15:O:26:GLU:O	15:O:29:VAL:HG12	1.87	0.74
2:B:47:THR:OG1	2:B:202:PRO:O	2.06	0.74
7:G:111:ARG:HH21	7:G:123:GLU:HA	1.49	0.74
12:L:25:PRO:C	12:L:27:LEU:H	1.91	0.73
1:A:720:C:H5''	1:A:721:G:H5''	1.70	0.73
1:A:127:G:H1	1:A:234:C:H42	1.33	0.73
5:E:131:ILE:O	5:E:134:ALA:HB3	1.88	0.73
1:A:403:C:OP1	4:D:137:SER:OG	2.05	0.73
1:A:1127:G:H1	1:A:1145:C:H42	1.36	0.73
1:A:933:G:OP2	7:G:3:ARG:HB2	1.89	0.73
4:D:31:CYS:SG	4:D:31:CYS:O	2.47	0.73
1:A:322:C:H4'	20:T:23:ARG:HD2	1.69	0.73
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.24	0.73
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.71	0.73
13:M:71:ARG:HB3	13:M:71:ARG:HH11	1.53	0.73
1:A:977:A:H2'	1:A:978:A:H5''	1.71	0.73
4:D:63:LYS:O	4:D:67:ILE:HG13	1.89	0.73
1:A:1441:G:H4'	1:A:1442:G:C5	2.23	0.73
1:A:363:A:OP1	12:L:61:THR:OG1	2.03	0.72
1:A:363:A:O2'	1:A:364:A:H5'	1.89	0.72
9:I:34:ASN:N	9:I:34:ASN:OD1	2.18	0.72
1:A:1505:G:H4'	1:A:1506:U:H5''	1.71	0.72
4:D:36:ARG:HB2	4:D:38:TYR:HE2	1.55	0.72
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.71	0.72
2:B:132:LYS:HA	2:B:135:GLN:HB2	1.72	0.72
1:A:1489:G:H8	1:A:1489:G:OP2	1.71	0.72
1:A:1032:G:H3'	1:A:1033:G:H5''	1.70	0.72
10:J:11:PHE:HE2	10:J:67:THR:HG23	1.54	0.72
1:A:981:U:H2'	1:A:982:U:H5	1.55	0.72
1:A:869:G:N7	24:A:3090:HOH:O	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:41:VAL:HG12	19:S:42:PRO:HD2	1.72	0.72
18:R:88:LYS:NZ	18:R:88:LYS:OXT	2.15	0.72
8:H:15:ASN:HD22	8:H:15:ASN:H	1.37	0.71
1:A:875:C:H1'	8:H:15:ASN:OD1	1.88	0.71
1:A:1196:U:O2'	24:A:2127:HOH:O	2.07	0.71
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.22	0.71
1:A:1124:G:OP1	10:J:33:GLN:NE2	2.23	0.71
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.71	0.71
18:R:42:ARG:HH11	18:R:42:ARG:HG3	1.55	0.71
1:A:184:G:H1	1:A:193:C:H42	1.38	0.71
16:P:48:TRP:CD1	16:P:48:TRP:N	2.56	0.71
1:A:414:A:H2'	1:A:415:A:H8	1.56	0.71
1:A:235:C:N4	24:A:2070:HOH:O	2.24	0.71
1:A:1527:C:H2'	1:A:1528:U:C6	2.26	0.71
12:L:55:VAL:HG12	12:L:69:TYR:HA	1.73	0.71
7:G:73:MET:HG2	7:G:90:GLU:HA	1.73	0.71
7:G:15:ASP:HB3	7:G:24:THR:HG22	1.72	0.71
10:J:34:VAL:HG22	10:J:75:ILE:H	1.53	0.70
1:A:695:A:H2'	1:A:696:A:C8	2.24	0.70
21:U:13:ILE:HD12	21:U:22:ARG:HE	1.56	0.70
9:I:9:ARG:HB2	9:I:14:VAL:HA	1.72	0.70
6:F:87:ARG:HH11	6:F:87:ARG:HG3	1.56	0.70
7:G:87:VAL:HG21	7:G:154:TYR:HB2	1.72	0.70
12:L:47:LYS:CG	12:L:48:PRO:HD3	2.21	0.70
1:A:1005:A:N6	1:A:1024:G:O2'	2.25	0.70
15:O:81:LEU:O	15:O:81:LEU:HD23	1.92	0.70
1:A:447:G:H2'	1:A:485:G:N2	2.07	0.70
1:A:662:G:H2'	1:A:663:A:C8	2.25	0.70
1:A:263:A:O2'	1:A:264:U:H5'	1.92	0.70
9:I:48:GLU:OE1	9:I:51:ARG:HD2	1.92	0.70
14:N:14:PRO:O	14:N:15:LYS:HB3	1.92	0.70
1:A:779:C:O2'	1:A:780:A:H5'	1.91	0.69
9:I:77:ILE:O	9:I:81:ILE:HG12	1.91	0.69
1:A:1525:G:H5''	1:A:1525:G:H8	1.56	0.69
5:E:73:ASN:O	5:E:73:ASN:ND2	2.25	0.69
1:A:1057:G:H4'	3:C:197:GLY:H	1.58	0.69
20:T:87:LYS:O	20:T:91:LEU:HB2	1.91	0.69
1:A:758:G:N7	24:A:3191:HOH:O	2.25	0.69
3:C:35:GLU:OE2	3:C:97:LYS:NZ	2.25	0.69
1:A:1126:U:O4	1:A:1127:G:N2	2.25	0.69
1:A:1322:C:H4'	1:A:1323:G:OP1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1413:A:H61	1:A:1487:G:H1	1.40	0.69
1:A:1033:G:H3'	1:A:1034:G:C8	2.27	0.69
18:R:27:GLY:O	18:R:29:PHE:HB3	1.93	0.69
1:A:1169:A:N6	1:A:1171:G:N3	2.40	0.69
16:P:47:ASP:N	16:P:47:ASP:OD1	2.17	0.69
9:I:16:ARG:HB2	9:I:64:THR:HG23	1.75	0.69
1:A:500:G:C5	1:A:546:G:N2	2.60	0.69
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.73	0.69
1:A:849:C:N4	24:A:2521:HOH:O	2.25	0.69
15:O:50:HIS:O	15:O:53:HIS:N	2.25	0.69
9:I:50:LEU:HD22	9:I:55:ALA:HB3	1.75	0.69
6:F:12:PRO:HG3	6:F:58:GLY:HA2	1.75	0.69
1:A:56:U:H2'	1:A:57:G:C8	2.27	0.69
18:R:74:ARG:HB3	18:R:81:PHE:HE2	1.55	0.69
1:A:927:G:O2'	1:A:1503:A:N7	2.26	0.69
3:C:58:GLU:H	3:C:65:ALA:HB3	1.58	0.69
1:A:344:A:H5''	1:A:345:C:H5	1.57	0.69
18:R:44:LEU:HD11	18:R:79:LEU:HD22	1.74	0.69
10:J:57:LYS:O	10:J:60:ARG:NH1	2.25	0.69
6:F:3:ARG:NH1	6:F:64:GLN:OE1	2.25	0.69
1:A:1231:G:H2'	1:A:1232:U:H6	1.57	0.68
21:U:13:ILE:HD12	21:U:22:ARG:NE	2.07	0.68
14:N:9:LYS:HE2	14:N:12:ARG:HH12	1.59	0.68
1:A:1332:A:H2'	1:A:1333:A:H8	1.57	0.68
19:S:18:LYS:HE3	19:S:31:ILE:HG12	1.75	0.68
4:D:38:TYR:HD2	4:D:38:TYR:H	1.41	0.68
10:J:92:THR:OG1	10:J:93:GLY:N	2.26	0.68
15:O:4:THR:HG1	15:O:7:GLU:HG3	1.56	0.68
1:A:1196:U:H1'	24:A:2842:HOH:O	1.94	0.68
1:A:435:C:O2'	24:A:2527:HOH:O	2.10	0.68
19:S:22:LEU:HD11	19:S:27:GLU:HA	1.75	0.68
1:A:669:U:H2'	1:A:670:G:C8	2.28	0.68
1:A:1124:G:H1	1:A:1149:C:H42	1.41	0.68
18:R:26:LEU:HD11	18:R:42:ARG:HE	1.58	0.68
2:B:69:LEU:HB3	2:B:162:ILE:HD11	1.76	0.68
1:A:690:G:N7	11:K:55:LYS:NZ	2.36	0.68
21:U:6:ARG:HB3	21:U:15:ARG:HH12	1.59	0.68
8:H:104:ARG:HG3	8:H:104:ARG:HH11	1.59	0.68
8:H:105:ARG:NH2	24:H:304:HOH:O	2.26	0.67
5:E:110:LEU:HD22	5:E:115:VAL:HG21	1.76	0.67
5:E:116:THR:OG1	5:E:117:ASP:N	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:G:O3'	9:I:69:GLY:HA3	1.94	0.67
3:C:134:ILE:HD11	3:C:153:VAL:HG22	1.76	0.67
19:S:53:ASN:HD22	19:S:56:GLN:HG3	1.58	0.67
1:A:1413:A:H3'	1:A:1414:U:H5''	1.77	0.67
1:A:689:C:P	11:K:46:GLY:HA3	2.33	0.67
3:C:188:LEU:HD22	3:C:189:ALA:N	2.10	0.67
16:P:26:ARG:HH11	16:P:26:ARG:HG2	1.59	0.67
4:D:107:ARG:NH1	4:D:114:ARG:HH22	1.92	0.67
1:A:1379:G:O2'	1:A:1380:U:H5'	1.95	0.67
1:A:457:C:H2'	1:A:458:C:H6	1.59	0.67
1:A:1405:G:O6	1:A:1493:A:N6	2.27	0.67
1:A:1439:C:OP1	20:T:38:LYS:HE2	1.94	0.67
7:G:41:ARG:HB2	7:G:41:ARG:NH1	2.10	0.67
17:Q:37:LYS:O	17:Q:38:ARG:HD3	1.95	0.66
3:C:61:ALA:O	3:C:63:ASN:ND2	2.28	0.66
1:A:1030(C):G:N2	1:A:1030(D):A:H61	1.93	0.66
13:M:90:LEU:HA	13:M:93:ARG:HG2	1.76	0.66
1:A:1191:A:H5''	3:C:4:LYS:HE3	1.76	0.66
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.60	0.66
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.60	0.66
1:A:1519[B]:MA6:H5'	1:A:1520[B]:G:OP2	1.96	0.66
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.75	0.66
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.11	0.66
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.29	0.66
6:F:23:LYS:HD2	6:F:42:GLU:OE1	1.96	0.66
1:A:418:C:H2'	1:A:419:C:H6	1.60	0.66
1:A:518:C:H2'	1:A:530:G:C8	2.31	0.66
1:A:1347:G:H5''	9:I:107:ARG:HG3	1.76	0.66
8:H:15:ASN:ND2	8:H:15:ASN:H	1.93	0.66
1:A:405:U:O4	4:D:2:GLY:HA3	1.96	0.66
12:L:113:ARG:HH11	12:L:116:SER:H	1.41	0.66
1:A:982:U:OP2	14:N:23:ARG:NH2	2.29	0.66
1:A:1221:G:H4'	19:S:77:THR:HG21	1.78	0.66
1:A:1128:C:O2'	1:A:1130:A:OP1	2.13	0.66
19:S:36:ARG:NH2	19:S:75:ALA:O	2.29	0.66
1:A:875:C:O2'	8:H:14:ARG:NH1	2.28	0.66
1:A:127:G:H1	1:A:234:C:N4	1.93	0.66
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.30	0.66
9:I:118:LYS:O	9:I:120:ARG:N	2.28	0.66
1:A:365:U:H5''	1:A:366:C:OP1	1.95	0.66
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:G:H5'	1:A:1358:U:O2'	1.96	0.66
1:A:1423:G:H1	1:A:1477:C:H42	1.44	0.66
15:O:26:GLU:N	15:O:26:GLU:OE2	2.29	0.66
1:A:1054:C:H3'	24:A:2923:HOH:O	1.96	0.66
1:A:670:G:H1	1:A:736:C:H42	1.44	0.66
1:A:1309:G:OP2	13:M:99:ARG:NH2	2.29	0.66
1:A:1448:C:H42	1:A:1455:G:H1	1.41	0.66
1:A:44:G:H1	1:A:398:C:H42	1.44	0.66
1:A:1039:C:H2'	1:A:1040:U:C6	2.31	0.66
11:K:40:ILE:HG13	11:K:75:TYR:CD2	2.30	0.65
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.30	0.65
17:Q:97:SER:O	17:Q:98:LEU:HD12	1.95	0.65
3:C:6:HIS:HD2	3:C:9:GLY:H	1.44	0.65
21:U:6:ARG:HB3	21:U:15:ARG:NH1	2.11	0.65
13:M:56:LEU:O	13:M:60:VAL:HG23	1.97	0.65
1:A:858:G:H5'	1:A:858:G:H8	1.61	0.65
3:C:155:GLY:HA2	3:C:157:ILE:HG12	1.79	0.65
1:A:1518[A]:MA6:N6	1:A:1519[A]:MA6:H103	2.12	0.65
1:A:1442:G:C5	1:A:1446:A:C6	2.84	0.65
12:L:47:LYS:HG3	12:L:48:PRO:HD3	1.79	0.65
9:I:108:VAL:HG12	9:I:109:VAL:H	1.60	0.65
2:B:112:VAL:HG23	2:B:149:LEU:HD13	1.79	0.65
15:O:5:LYS:HE2	15:O:5:LYS:H	1.62	0.65
6:F:40:VAL:HG22	6:F:63:TYR:CD1	2.31	0.65
2:B:73:THR:HG22	2:B:169:LYS:HE3	1.78	0.65
19:S:22:LEU:HD12	19:S:47:HIS:HE1	1.62	0.65
5:E:105:VAL:HG23	5:E:106:PRO:HD3	1.78	0.65
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.78	0.65
20:T:50:GLU:HB2	20:T:99:LEU:HD13	1.78	0.65
1:A:1148:U:H2'	1:A:1149:C:O4'	1.97	0.65
2:B:58:ILE:HG22	2:B:221:LEU:HD12	1.79	0.65
8:H:120:THR:OG1	8:H:123:GLU:HG3	1.96	0.64
2:B:147:LYS:HE2	2:B:148:TYR:CZ	2.33	0.64
1:A:503:C:OP2	12:L:116:SER:OG	2.09	0.64
1:A:1425:U:H2'	1:A:1426:C:H6	1.63	0.64
1:A:1196:U:O2'	1:A:1197:G:OP1	2.15	0.64
1:A:976:G:OP2	1:A:1358:U:O2'	2.15	0.64
1:A:1476:G:H2'	1:A:1477:C:H6	1.63	0.64
4:D:162:LEU:HD22	4:D:181:MET:HG3	1.80	0.64
7:G:85:TYR:HD1	7:G:154:TYR:CE1	2.16	0.64
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.07	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.79	0.64
15:O:5:LYS:O	15:O:8:LYS:HB3	1.98	0.64
9:I:28:VAL:HG22	9:I:63:ILE:HD11	1.80	0.64
1:A:1415:G:H2'	1:A:1416:G:H8	1.63	0.64
1:A:922:G:H2'	1:A:923:A:C8	2.33	0.64
13:M:11:ARG:HH11	13:M:45:VAL:HG12	1.62	0.64
10:J:57:LYS:HG2	10:J:60:ARG:HH12	1.63	0.64
1:A:337:C:N4	24:A:2569:HOH:O	2.31	0.64
19:S:39:THR:HA	19:S:70:LYS:HA	1.79	0.64
1:A:1277:C:H2'	1:A:1279:A:C8	2.33	0.64
13:M:49:THR:N	13:M:52:GLU:OE1	2.28	0.64
19:S:43:GLU:H	19:S:43:GLU:CD	2.01	0.64
1:A:1425:U:H3	1:A:1475:G:H1	1.45	0.64
17:Q:7:THR:O	17:Q:23:VAL:HG13	1.98	0.64
1:A:779:C:C2'	1:A:780:A:H5'	2.28	0.64
5:E:7:GLU:HB3	5:E:112:LEU:HD21	1.80	0.64
2:B:54:THR:HG21	2:B:201:ILE:HD11	1.78	0.64
13:M:62:ASN:OD1	13:M:62:ASN:N	2.30	0.64
1:A:1408:A:H2'	1:A:1409:C:C2	2.31	0.64
14:N:23:ARG:HA	14:N:29:ARG:O	1.98	0.64
1:A:1413:A:C3'	1:A:1414:U:H5''	2.27	0.64
1:A:965:A:C2	1:A:969:A:C2	2.85	0.64
2:B:132:LYS:HG2	2:B:135:GLN:OE1	1.98	0.64
1:A:98:U:O2'	1:A:99:C:H5'	1.98	0.64
1:A:1244:C:H42	1:A:1293:G:H1	1.46	0.64
1:A:518:C:O2'	12:L:50:SER:HB3	1.98	0.63
1:A:1119:C:H2'	1:A:1120:G:H8	1.64	0.63
1:A:1532:U:H3'	1:A:1532:U:H6	1.63	0.63
5:E:64:ARG:HE	5:E:65:ASN:HB2	1.64	0.63
10:J:57:LYS:HG2	10:J:60:ARG:NH1	2.13	0.63
1:A:1147:C:O2	9:I:16:ARG:NH1	2.32	0.63
1:A:1062:U:H2'	1:A:1063:C:C6	2.32	0.63
1:A:1316:G:N1	1:A:1319:A:OP2	2.30	0.63
1:A:1256:A:OP2	3:C:26:LYS:NZ	2.31	0.63
1:A:544:G:P	4:D:59:ARG:HH22	2.21	0.63
1:A:1375:A:OP1	7:G:28:ASN:ND2	2.29	0.63
1:A:1320:C:N3	19:S:36:ARG:HG3	2.13	0.63
1:A:1318:A:H4'	19:S:10:PHE:CE2	2.33	0.63
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.31	0.63
7:G:78:ARG:HH12	7:G:156:TRP:HB2	1.63	0.63
19:S:53:ASN:HB2	19:S:56:GLN:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:C:H2'	1:A:1098:C:H6	1.64	0.63
7:G:121:ALA:O	7:G:125:MET:HB2	1.98	0.63
8:H:40:ALA:HB2	8:H:45:ILE:HD11	1.79	0.63
7:G:114:ARG:HB2	7:G:115:ARG:HD3	1.79	0.63
12:L:6:THR:HG23	12:L:9:GLN:HG3	1.80	0.63
1:A:106:C:C2'	1:A:107:G:H5'	2.29	0.63
1:A:849:C:H2'	1:A:850:U:H6	1.63	0.63
1:A:1217:C:H2'	1:A:1218:C:H6	1.64	0.63
16:P:34:GLU:OE2	16:P:55:ARG:HD2	1.99	0.63
1:A:4:U:H6	1:A:4:U:H5''	1.62	0.63
1:A:168:G:C2	1:A:169:C:C5	2.86	0.63
11:K:54:ARG:O	11:K:57:THR:HG22	1.99	0.63
8:H:20:TYR:HD1	8:H:65:TYR:CE1	2.17	0.63
7:G:84:ASN:OD1	7:G:84:ASN:N	2.31	0.63
6:F:15:ASP:N	6:F:18:GLN:OE1	2.22	0.62
1:A:705:U:H5''	1:A:706:A:OP2	1.99	0.62
1:A:773:G:H1	1:A:806:C:H42	1.46	0.62
20:T:16:HIS:O	20:T:20:LEU:HD12	1.99	0.62
12:L:25:PRO:C	12:L:27:LEU:N	2.53	0.62
9:I:35:GLU:HA	9:I:38:GLN:HB2	1.81	0.62
5:E:36:ASP:O	5:E:38:GLN:HG2	1.98	0.62
1:A:1338:G:H2'	1:A:1339:A:C8	2.34	0.62
1:A:1279:A:O2'	1:A:1281:U:OP2	2.17	0.62
6:F:41:GLU:HB3	6:F:43:LEU:HD11	1.81	0.62
4:D:196:LEU:N	4:D:196:LEU:HD23	2.15	0.62
11:K:120:ARG:HH11	11:K:120:ARG:CB	2.07	0.62
3:C:188:LEU:HD21	3:C:195:VAL:HG23	1.82	0.62
1:A:631:G:OP1	8:H:98:LYS:NZ	2.33	0.62
10:J:61:GLU:OE2	14:N:45:ARG:HD2	2.00	0.62
1:A:1023:G:N3	1:A:1023:G:H2'	2.15	0.62
1:A:80:G:H2'	1:A:81:U:H5'	1.82	0.62
1:A:443:C:N4	1:A:491:G:H1	1.97	0.62
1:A:322:C:H2'	1:A:323:U:C6	2.34	0.62
1:A:1392:G:H21	1:A:1502:A:H8	1.47	0.62
1:A:343:U:O2'	1:A:346:G:O6	2.16	0.62
4:D:88:VAL:O	4:D:92:VAL:HG23	2.00	0.62
15:O:64:ARG:HD2	15:O:88:ARG:HH12	1.65	0.62
1:A:317:G:O2'	1:A:318:G:H5'	2.00	0.62
3:C:59:ARG:HD3	3:C:64:VAL:HG22	1.81	0.61
1:A:1221:G:H1'	19:S:54:GLY:HA3	1.83	0.61
1:A:669:U:H2'	1:A:670:G:H8	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:LYS:NZ	4:D:72:GLU:OE2	2.31	0.61
1:A:7:G:H5''	24:A:2358:HOH:O	1.99	0.61
18:R:79:LEU:HD23	18:R:80:PRO:HD2	1.82	0.61
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.32	0.61
1:A:1348:U:H4'	9:I:120:ARG:HG3	1.82	0.61
16:P:3:LYS:HD3	16:P:65:GLN:HB3	1.82	0.61
13:M:105:THR:OG1	13:M:106:ASN:HB2	2.00	0.61
20:T:42:GLN:HG3	20:T:46:GLU:OE1	2.00	0.61
1:A:1443:G:H5''	1:A:1446:A:H5'	1.81	0.61
1:A:736:C:H5''	18:R:72:ARG:HH21	1.65	0.61
1:A:1409:C:H6	1:A:1409:C:H3'	1.65	0.61
7:G:149:ARG:HD3	11:K:59:TYR:CE1	2.36	0.61
1:A:248:C:H42	1:A:276:G:H1	1.48	0.61
1:A:966:M2G:HM13	1:A:967:5MC:C1'	2.22	0.61
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.15	0.61
1:A:1326:C:OP1	21:U:12:LYS:HE3	2.00	0.61
3:C:153:VAL:HG12	3:C:198:VAL:HG22	1.81	0.61
3:C:17:ASP:OD1	3:C:18:TRP:N	2.32	0.61
5:E:43:LEU:O	5:E:62:ALA:HA	2.00	0.61
2:B:214:ILE:N	2:B:214:ILE:HD13	2.15	0.61
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.36	0.61
1:A:967:5MC:O2'	9:I:128:ARG:NH1	2.33	0.61
1:A:44:G:H1	1:A:398:C:N4	1.98	0.61
1:A:1080:A:OP2	5:E:47:LYS:NZ	2.28	0.61
1:A:1314:C:OP2	19:S:6:LYS:HD3	2.01	0.61
1:A:1126:U:O4	1:A:1127:G:C2	2.53	0.61
10:J:6:ILE:HG13	10:J:72:VAL:HB	1.82	0.61
8:H:53:VAL:HB	8:H:58:TYR:HD1	1.64	0.61
1:A:257:G:H1	1:A:269:C:H42	1.47	0.61
10:J:19:SER:HB2	10:J:89:ASP:OD2	1.99	0.61
5:E:149:GLU:O	5:E:153:LYS:HB3	2.00	0.61
13:M:12:ASN:H	13:M:45:VAL:CB	2.13	0.61
3:C:150:LYS:HA	3:C:169:ALA:HB2	1.83	0.61
6:F:25:ILE:HA	6:F:28:ARG:HD2	1.83	0.61
11:K:106:LYS:O	11:K:107:SER:HB3	2.00	0.61
1:A:1410:G:O6	1:A:1490:C:N4	2.30	0.60
10:J:5:ARG:HG3	10:J:99:LYS:H	1.65	0.60
10:J:11:PHE:CE2	10:J:67:THR:HG23	2.37	0.60
10:J:12:ASP:OD2	10:J:15:THR:HG23	2.01	0.60
19:S:5:LEU:HD13	19:S:10:PHE:HB2	1.83	0.60
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.34	0.60
20:T:10:LEU:HD23	20:T:12:ALA:N	2.16	0.60
5:E:15:ARG:HH11	5:E:15:ARG:CG	2.13	0.60
11:K:57:THR:HG23	11:K:60:ALA:H	1.65	0.60
1:A:1491:G:N7	1:A:1492:A:N6	2.50	0.60
1:A:323:U:O3'	20:T:22:ARG:HD2	2.02	0.60
2:B:132:LYS:HE3	2:B:135:GLN:HB3	1.84	0.60
3:C:130:VAL:HG11	3:C:153:VAL:HG21	1.83	0.60
7:G:70:LYS:HE2	7:G:96:GLN:HE21	1.66	0.60
8:H:11:THR:CG2	8:H:15:ASN:HD21	2.14	0.60
9:I:27:THR:O	9:I:63:ILE:HG12	2.02	0.60
9:I:4:TYR:CE1	9:I:88:TYR:HD1	2.19	0.60
6:F:14:LEU:HD13	6:F:19:LEU:HA	1.82	0.60
18:R:53:ARG:HH12	18:R:59:SER:HA	1.65	0.60
7:G:57:GLU:HB2	7:G:60:LYS:HG3	1.84	0.60
1:A:363:A:C2'	1:A:364:A:H5'	2.32	0.60
8:H:4:ASP:OD1	8:H:6:ILE:N	2.34	0.60
15:O:54:ARG:NH1	15:O:58:MET:SD	2.75	0.60
8:H:11:THR:HG22	8:H:15:ASN:HD21	1.66	0.60
1:A:1378:C:OP2	7:G:7:ALA:HB3	2.02	0.60
4:D:172:PRO:HD2	4:D:173:TRP:CE3	2.37	0.60
1:A:778:G:H8	1:A:778:G:O5'	1.85	0.60
1:A:1001:A:H2'	1:A:1002:G:O4'	2.02	0.60
13:M:67:GLU:O	13:M:71:ARG:HG3	2.02	0.60
7:G:95:ARG:NE	7:G:99:LEU:HD21	2.17	0.60
2:B:87:ARG:HD3	2:B:234:PRO:HG2	1.84	0.60
3:C:40:ARG:O	3:C:44:GLU:HB2	2.02	0.60
1:A:3:G:H1	4:D:87:GLY:H	1.49	0.60
2:B:100:GLY:O	2:B:102:LEU:N	2.35	0.59
8:H:81:HIS:HB2	8:H:138:TRP:O	2.01	0.59
8:H:37:ARG:HH11	8:H:37:ARG:HB3	1.67	0.59
13:M:23:TYR:CD2	13:M:70:LEU:HD12	2.37	0.59
1:A:1256:A:N6	1:A:1278:U:OP2	2.35	0.59
1:A:1119:C:H2'	1:A:1120:G:C8	2.37	0.59
1:A:725:G:H2'	1:A:726:C:H6	1.66	0.59
16:P:10:GLY:H	16:P:16:HIS:H	1.50	0.59
20:T:43:LEU:HD13	20:T:51:GLU:HB3	1.84	0.59
1:A:1010:G:N2	1:A:1020:U:H1'	2.17	0.59
1:A:1426:C:H2'	1:A:1427:U:C6	2.37	0.59
18:R:26:LEU:HD11	18:R:42:ARG:NE	2.16	0.59
15:O:22:THR:OG1	15:O:23:GLY:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:101:ILE:O	5:E:120:THR:HB	2.00	0.59
17:Q:29:HIS:O	17:Q:31:LEU:N	2.35	0.59
2:B:80:ILE:HG21	2:B:211:ILE:HG22	1.84	0.59
1:A:1286:A:H2'	1:A:1287:A:H4'	1.83	0.59
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.84	0.59
2:B:180:LEU:HB2	2:B:182:ILE:HG13	1.85	0.59
6:F:74:ASP:HA	6:F:77:ARG:HB3	1.84	0.59
1:A:499:A:H4'	1:A:500:G:H5'	1.83	0.59
1:A:937:A:H1'	1:A:1379:G:N2	2.18	0.59
6:F:39:LYS:HG2	6:F:40:VAL:H	1.67	0.59
7:G:75:VAL:HA	7:G:87:VAL:O	2.03	0.59
1:A:362:G:H5''	12:L:61:THR:HG21	1.83	0.59
1:A:376:G:H5''	16:P:5:ARG:HD2	1.84	0.59
1:A:15:G:H5'	1:A:15:G:H8	1.66	0.59
9:I:50:LEU:O	9:I:54:ASP:N	2.29	0.59
1:A:1191:A:H2'	1:A:1192:C:C6	2.38	0.59
6:F:37:VAL:HG22	6:F:65:VAL:HG12	1.84	0.59
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.85	0.59
18:R:82:THR:OG1	18:R:83:GLU:N	2.33	0.59
12:L:19:ARG:H	12:L:19:ARG:HD2	1.67	0.59
1:A:198:G:H5''	1:A:198:G:H8	1.68	0.59
7:G:78:ARG:NH1	7:G:154:TYR:O	2.35	0.59
1:A:737:A:OP1	6:F:92:LYS:HB2	2.02	0.59
10:J:8:LEU:HD22	10:J:96:ILE:HG22	1.83	0.59
10:J:78:ASN:OD1	10:J:79:ARG:N	2.27	0.59
1:A:369:C:O2'	1:A:370:C:H5'	2.03	0.59
11:K:95:ILE:O	11:K:98:LEU:N	2.34	0.59
19:S:10:PHE:HE2	19:S:37:ARG:HD3	1.68	0.59
9:I:50:LEU:HD13	9:I:55:ALA:HB3	1.85	0.59
1:A:81:U:C2'	1:A:82:U:H5''	2.33	0.59
1:A:1333:A:H2'	1:A:1334:G:O4'	2.03	0.59
4:D:57:ARG:HB3	4:D:202:LEU:HD12	1.85	0.59
1:A:1406:U:H2'	1:A:1407:5MC:C6	2.37	0.58
14:N:32:SER:HB2	14:N:41:ARG:HB3	1.84	0.58
1:A:254:G:OP1	17:Q:67:LYS:O	2.21	0.58
13:M:65:LYS:HD3	13:M:69:GLU:HG2	1.85	0.58
1:A:1329:A:P	13:M:28:ALA:HB3	2.43	0.58
20:T:46:GLU:HB3	20:T:48:LYS:HE3	1.84	0.58
8:H:73:ASP:N	8:H:74:PRO:HD3	2.17	0.58
2:B:17:PHE:CE1	2:B:18:GLY:O	2.56	0.58
1:A:646:U:H2'	1:A:647:C:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:112:LEU:HD12	8:H:112:LEU:N	2.18	0.58
15:O:39:LEU:O	15:O:42:HIS:HB3	2.03	0.58
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.67	0.58
1:A:250:A:H5'	1:A:250:A:C8	2.38	0.58
7:G:41:ARG:HH11	7:G:41:ARG:HB2	1.68	0.58
9:I:108:VAL:HG12	9:I:109:VAL:HG23	1.86	0.58
5:E:15:ARG:HH11	5:E:15:ARG:HG2	1.68	0.58
9:I:91:ASP:N	9:I:91:ASP:OD1	2.36	0.58
1:A:664:G:N2	1:A:741:G:H22	2.01	0.58
13:M:50:GLU:OE2	13:M:54:VAL:N	2.36	0.58
1:A:858:G:H5'	1:A:858:G:C8	2.38	0.58
1:A:514:C:C2'	1:A:515:G:H5'	2.33	0.58
12:L:81:SER:HA	24:L:304:HOH:O	2.03	0.58
1:A:946:A:H2'	1:A:947:G:C8	2.37	0.58
1:A:1097:C:H2'	1:A:1098:C:C6	2.38	0.58
15:O:39:LEU:O	15:O:42:HIS:N	2.36	0.58
10:J:21:GLN:HA	10:J:24:VAL:HG12	1.85	0.58
15:O:70:LEU:O	15:O:72:ARG:N	2.37	0.58
1:A:1226:C:H4'	19:S:80:TYR:CE2	2.37	0.58
9:I:50:LEU:HA	9:I:53:VAL:HG22	1.85	0.58
9:I:112:LYS:NZ	9:I:113:LYS:O	2.36	0.58
1:A:1055:A:H1'	3:C:156:ARG:NH2	2.18	0.58
17:Q:10:VAL:HG23	17:Q:55:ASP:O	2.03	0.58
1:A:350:G:O2'	1:A:351:G:H5'	2.04	0.58
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.69	0.58
1:A:981:U:H2'	1:A:982:U:C5	2.38	0.58
1:A:265:G:C4	1:A:267:C:H5	2.21	0.58
12:L:27:LEU:C	12:L:29:GLY:H	2.04	0.58
5:E:6:PHE:CE2	5:E:36:ASP:HB3	2.38	0.58
11:K:47:VAL:HG12	11:K:48:ILE:N	2.18	0.58
4:D:145:GLU:OE1	4:D:182:LYS:NZ	2.32	0.58
18:R:70:ILE:O	18:R:74:ARG:HG3	2.03	0.58
8:H:89:PRO:HA	8:H:92:ARG:HH11	1.68	0.58
11:K:58:PRO:HB3	11:K:93:GLN:HG3	1.85	0.58
1:A:1499:A:H1'	1:A:1520[A]:G:OP1	2.03	0.58
1:A:1392:G:N2	1:A:1502:A:H8	2.02	0.58
11:K:21:ILE:HD13	11:K:94:ALA:HB3	1.86	0.58
1:A:1427:U:H2'	1:A:1428:A:C8	2.39	0.58
1:A:409:G:N2	1:A:433:C:O2	2.35	0.58
1:A:858:G:C8	24:A:3092:HOH:O	2.57	0.58
1:A:1504:G:C3'	1:A:1505:G:H5'	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1533:C:H2'	1:A:1533:C:O2	2.03	0.58
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.69	0.58
19:S:35:SER:O	19:S:35:SER:OG	2.21	0.58
12:L:94:LEU:O	12:L:94:LEU:HG	2.03	0.58
6:F:5:GLU:HB3	6:F:62:TRP:NE1	2.16	0.57
2:B:111:ARG:NH1	2:B:111:ARG:HG3	2.14	0.57
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.38	0.57
1:A:1143:G:H2'	1:A:1144:G:H8	1.68	0.57
19:S:22:LEU:HD22	19:S:25:LYS:HB2	1.86	0.57
13:M:12:ASN:N	13:M:45:VAL:HB	2.16	0.57
14:N:9:LYS:HG2	14:N:12:ARG:HH12	1.68	0.57
1:A:1375:A:P	7:G:28:ASN:HD22	2.27	0.57
6:F:21:LEU:HG	6:F:21:LEU:O	2.00	0.57
1:A:1319:A:OP1	19:S:5:LEU:HD12	2.04	0.57
1:A:737:A:H2'	1:A:738:C:C6	2.38	0.57
8:H:106:GLY:HA2	8:H:122:ARG:NH2	2.18	0.57
2:B:178:ARG:HH11	2:B:178:ARG:HA	1.69	0.57
5:E:26:PHE:N	5:E:26:PHE:CD1	2.72	0.57
1:A:949:A:C2	1:A:1233:G:N3	2.73	0.57
15:O:80:ALA:HA	15:O:83:GLU:HB2	1.87	0.57
1:A:682:G:H1	1:A:708:C:H42	1.51	0.57
19:S:5:LEU:HA	19:S:6:LYS:HE3	1.87	0.57
2:B:98:LEU:O	2:B:101:MET:HG2	2.04	0.57
9:I:48:GLU:N	9:I:49:PRO:HD2	2.19	0.57
1:A:737:A:H1'	6:F:73:ASN:OD1	2.05	0.57
10:J:61:GLU:OE1	14:N:58:LYS:HE3	2.04	0.57
17:Q:56:VAL:HB	17:Q:78:GLU:CB	2.35	0.57
8:H:21:LYS:O	8:H:63:LEU:HD23	2.05	0.57
12:L:111:LYS:O	12:L:112:ASP:HB2	2.05	0.57
1:A:837:G:H2'	1:A:838:G:H5'	1.86	0.57
9:I:69:GLY:O	9:I:73:GLN:HG3	2.05	0.57
16:P:59:TRP:HB3	16:P:64:ALA:HB2	1.87	0.57
8:H:20:TYR:HA	8:H:65:TYR:CE1	2.40	0.57
1:A:1233:G:OP2	9:I:124:GLN:HB3	2.03	0.57
19:S:3:ARG:HG2	19:S:4:SER:N	2.19	0.57
19:S:51:VAL:O	19:S:57:HIS:HA	2.05	0.57
2:B:17:PHE:CD1	2:B:18:GLY:O	2.57	0.57
2:B:124:SER:HB2	2:B:126:GLU:HG2	1.86	0.57
1:A:1070:U:H2'	1:A:1071:C:C6	2.39	0.57
1:A:10:A:H61	1:A:24:U:H3	1.53	0.57
1:A:1314:C:H41	19:S:4:SER:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:85:ARG:NE	8:H:87:SER:O	2.38	0.57
5:E:79:GLU:O	5:E:80:ILE:HB	2.05	0.57
15:O:4:THR:HG23	15:O:7:GLU:OE2	2.03	0.57
1:A:409:G:OP1	4:D:24:GLU:O	2.23	0.57
1:A:1332:A:H2'	1:A:1333:A:C8	2.38	0.57
3:C:155:GLY:O	3:C:156:ARG:HB2	2.04	0.57
1:A:1008:C:H42	1:A:1022:G:N2	2.03	0.57
1:A:1041:A:H2'	1:A:1042:G:C8	2.40	0.57
16:P:4:ILE:HD11	16:P:60:LEU:HD21	1.87	0.57
1:A:203:U:H5'	1:A:203:U:H6	1.69	0.57
3:C:14:ILE:HB	3:C:15:THR:HG23	1.85	0.56
1:A:413:G:H8	1:A:428:G:H21	1.51	0.56
8:H:121:ASP:OD2	8:H:121:ASP:N	2.38	0.56
17:Q:86:GLU:O	17:Q:90:ILE:HG13	2.03	0.56
13:M:4:ILE:H	13:M:8:GLU:CD	2.09	0.56
5:E:151:LEU:O	5:E:154:GLY:N	2.34	0.56
3:C:191:THR:HG22	3:C:192:THR:HG23	1.87	0.56
4:D:36:ARG:N	4:D:37:PRO:HD3	2.20	0.56
1:A:260:G:H2'	1:A:261:U:H6	1.70	0.56
3:C:8:ILE:HG22	3:C:9:GLY:N	2.20	0.56
1:A:411:A:O2'	1:A:412:A:H4'	2.06	0.56
11:K:12:ARG:NE	11:K:40:ILE:HD11	2.21	0.56
9:I:111:ARG:NH1	9:I:112:LYS:O	2.37	0.56
7:G:154:TYR:N	7:G:154:TYR:HD2	2.03	0.56
2:B:69:LEU:HB3	2:B:162:ILE:CD1	2.35	0.56
5:E:116:THR:OG1	5:E:117:ASP:OD2	2.19	0.56
1:A:377:G:OP1	16:P:3:LYS:NZ	2.37	0.56
1:A:684:A:H1'	11:K:38:ASN:HB3	1.87	0.56
19:S:15:LEU:HD23	19:S:15:LEU:H	1.71	0.56
1:A:1125:U:H5''	24:A:2983:HOH:O	2.05	0.56
14:N:26:ARG:HD2	14:N:43:CYS:SG	2.44	0.56
14:N:26:ARG:HH12	14:N:47:LEU:HD22	1.70	0.56
20:T:74:LYS:HB2	20:T:76:ALA:H	1.70	0.56
1:A:130:A:H1'	1:A:263:A:O2'	2.04	0.56
6:F:7:ASN:OD1	6:F:7:ASN:N	2.34	0.56
2:B:33:TYR:HE2	2:B:44:LEU:HD12	1.69	0.56
1:A:1489:G:OP2	1:A:1489:G:C8	2.57	0.56
2:B:126:GLU:HB3	2:B:129:GLU:OE1	2.05	0.56
5:E:30:ALA:O	5:E:45:PHE:HA	2.05	0.56
20:T:14:LYS:O	20:T:17:ARG:HB3	2.06	0.56
6:F:100:ASN:HA	18:R:23:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:A:H2'	1:A:1016:A:C8	2.39	0.56
4:D:98:GLU:OE1	4:D:107:ARG:NH1	2.36	0.56
13:M:48:LEU:HD22	13:M:53:VAL:HG22	1.87	0.56
8:H:104:ARG:NH1	8:H:104:ARG:HG3	2.18	0.56
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.87	0.56
1:A:1089:G:C5	1:A:1090:U:C5	2.94	0.56
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.36	0.56
6:F:10:LEU:H	6:F:10:LEU:HD12	1.69	0.56
1:A:527:7MG:H81	1:A:527:7MG:H5''	1.87	0.56
1:A:986:A:H5''	1:A:987:G:OP2	2.05	0.56
5:E:64:ARG:NH2	5:E:65:ASN:HB2	2.20	0.56
18:R:85:LEU:HD23	18:R:88:LYS:HG2	1.87	0.56
3:C:120:VAL:HG12	3:C:198:VAL:HG11	1.88	0.56
3:C:151:VAL:HG12	3:C:152:ILE:H	1.71	0.56
15:O:49:ASP:OD1	15:O:52:SER:OG	2.21	0.56
1:A:984:C:H2'	1:A:985:C:H6	1.71	0.56
5:E:52:PRO:HG2	5:E:53:LEU:H	1.70	0.56
13:M:65:LYS:HG3	13:M:70:LEU:HD23	1.87	0.56
1:A:672:U:H2'	1:A:672:U:O2	2.06	0.56
1:A:106:C:H2'	1:A:107:G:H5'	1.87	0.56
8:H:20:TYR:CZ	8:H:76:PRO:HD2	2.40	0.56
2:B:126:GLU:O	2:B:130:ARG:NH2	2.38	0.56
17:Q:90:ILE:HG22	17:Q:94:ASN:HD21	1.70	0.56
7:G:16:LEU:HD22	9:I:44:VAL:HB	1.86	0.56
2:B:15:VAL:HG13	2:B:209:ARG:HB3	1.88	0.56
14:N:21:TYR:HE2	14:N:23:ARG:HE	1.52	0.56
6:F:83:ASP:HA	24:F:302:HOH:O	2.06	0.56
5:E:27:ARG:HB3	5:E:27:ARG:CZ	2.36	0.56
13:M:53:VAL:O	13:M:57:ARG:HB2	2.06	0.56
1:A:489:C:H2'	1:A:490:G:H8	1.71	0.56
1:A:1350:A:OP2	9:I:118:LYS:NZ	2.23	0.56
6:F:43:LEU:O	6:F:46:ARG:NH2	2.39	0.56
17:Q:29:HIS:CD2	17:Q:30:PRO:HD2	2.40	0.56
1:A:1075:C:O2'	1:A:1076:C:H5'	2.06	0.56
21:U:12:LYS:HB3	21:U:22:ARG:HG3	1.88	0.56
1:A:17:U:H2'	1:A:18:C:C6	2.41	0.56
1:A:1513:A:H2'	1:A:1514:C:C6	2.41	0.56
1:A:309:G:H1'	1:A:608:A:C2	2.41	0.56
1:A:892:A:H2'	1:A:893:C:O4'	2.06	0.56
12:L:27:LEU:CG	12:L:28:LYS:H	2.17	0.55
1:A:1443:G:H5''	1:A:1446:A:C5'	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:G:N2	1:A:760:G:N7	2.54	0.55
6:F:91:VAL:HG12	6:F:92:LYS:O	2.06	0.55
1:A:1357:A:H5''	1:A:1358:U:OP2	2.07	0.55
12:L:82:VAL:H	12:L:106:ASP:HB2	1.71	0.55
1:A:414:A:C2	1:A:415:A:C4	2.95	0.55
1:A:415:A:H5''	1:A:416:G:OP2	2.07	0.55
4:D:24:GLU:O	4:D:25:ARG:HB3	2.06	0.55
1:A:57:G:H2'	1:A:58:C:C6	2.41	0.55
4:D:173:TRP:O	4:D:186:LEU:HG	2.06	0.55
2:B:100:GLY:O	2:B:104:ASN:N	2.37	0.55
1:A:325:A:H2'	1:A:326:G:O4'	2.06	0.55
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.89	0.55
1:A:500:G:C6	1:A:546:G:C2	2.94	0.55
20:T:81:LYS:O	20:T:85:MET:HG3	2.07	0.55
5:E:65:ASN:ND2	5:E:65:ASN:O	2.39	0.55
1:A:925:G:O2'	1:A:927:G:OP1	2.23	0.55
1:A:1277:C:H2'	1:A:1279:A:H8	1.69	0.55
1:A:859:A:H2'	1:A:860:A:H5'	1.88	0.55
1:A:867:G:H5''	1:A:867:G:H8	1.71	0.55
4:D:118:ARG:NH2	4:D:118:ARG:HG3	2.21	0.55
1:A:977:A:C2'	1:A:978:A:H5''	2.35	0.55
18:R:32:ARG:O	18:R:69:THR:HG21	2.06	0.55
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.88	0.55
11:K:43:SER:HA	11:K:47:VAL:HG21	1.88	0.55
1:A:608:A:H2'	1:A:609:A:O4'	2.07	0.55
1:A:148:G:H2'	1:A:149:A:H8	1.71	0.55
19:S:40:ILE:HB	19:S:67:VAL:O	2.07	0.55
12:L:28:LYS:HB3	12:L:30:ALA:HB2	1.88	0.55
18:R:26:LEU:HD21	18:R:42:ARG:HD3	1.88	0.55
4:D:24:GLU:HG2	4:D:25:ARG:N	2.21	0.55
16:P:36:ILE:HD12	16:P:56:ALA:HB2	1.87	0.55
3:C:119:ARG:HH11	3:C:119:ARG:HG3	1.71	0.55
2:B:236:TYR:O	2:B:239:VAL:HG23	2.07	0.55
1:A:437:U:H5''	4:D:155:LEU:HD11	1.88	0.55
1:A:664:G:H22	1:A:741:G:H22	1.55	0.55
1:A:1403:C:O2	1:A:1403:C:C2'	2.53	0.55
6:F:15:ASP:OD2	6:F:16:GLN:N	2.40	0.55
6:F:26:ILE:CG2	6:F:63:TYR:HE2	2.20	0.55
18:R:87:ARG:O	18:R:88:LYS:HB2	2.07	0.55
6:F:12:PRO:HG2	6:F:57:GLN:HG3	1.88	0.55
11:K:107:SER:C	11:K:108:ILE:HG12	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:GLU:HG3	2:B:23:ARG:HD2	1.88	0.55
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.41	0.55
7:G:62:PHE:HD1	7:G:124:LEU:HD22	1.71	0.55
1:A:579:G:H2'	1:A:580:U:C6	2.41	0.55
5:E:64:ARG:HE	5:E:65:ASN:CB	2.20	0.55
1:A:1423:G:H1	1:A:1477:C:N4	2.03	0.55
18:R:52:PRO:O	18:R:56:THR:HG23	2.06	0.55
1:A:496:A:H4'	1:A:497:A:H5''	1.88	0.55
1:A:1448:C:N4	1:A:1455:G:H1	2.05	0.55
17:Q:90:ILE:O	17:Q:94:ASN:ND2	2.39	0.55
12:L:82:VAL:HG22	12:L:105:TYR:HB3	1.88	0.55
4:D:99:SER:O	4:D:140:VAL:HG23	2.06	0.55
5:E:75:THR:C	5:E:76:ILE:HD13	2.28	0.55
11:K:59:TYR:O	11:K:63:LEU:HG	2.06	0.55
1:A:8:A:N6	4:D:209:ARG:HB2	2.22	0.55
1:A:312:C:H2'	1:A:313:A:C8	2.41	0.55
10:J:38:ILE:HG22	10:J:39:PRO:HD2	1.88	0.55
3:C:151:VAL:HG12	3:C:152:ILE:N	2.22	0.55
1:A:1060:C:H5'	14:N:45:ARG:NH2	2.22	0.55
17:Q:90:ILE:HG22	17:Q:94:ASN:ND2	2.22	0.55
3:C:119:ARG:HG3	3:C:119:ARG:NH1	2.20	0.55
1:A:560:U:H4'	1:A:561:U:H5''	1.88	0.55
2:B:171:ALA:O	2:B:174:VAL:HG12	2.06	0.54
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.89	0.54
1:A:417:C:H2'	1:A:418:C:C6	2.42	0.54
1:A:1116:C:H42	1:A:1184:G:H1	1.53	0.54
4:D:149:ALA:HB3	4:D:152:SER:HB3	1.89	0.54
4:D:107:ARG:NH1	4:D:114:ARG:NH2	2.55	0.54
1:A:1518[A]:MA6:C6	1:A:1519[A]:MA6:H103	2.38	0.54
1:A:1003:G:H4'	1:A:1003(A):G:N7	2.23	0.54
2:B:97:TRP:CH2	2:B:176:GLU:OE1	2.54	0.54
1:A:935:A:N6	7:G:3:ARG:HG2	2.22	0.54
9:I:17:VAL:HG11	9:I:81:ILE:HD13	1.89	0.54
20:T:10:LEU:HD23	20:T:12:ALA:H	1.72	0.54
4:D:150:GLU:N	4:D:150:GLU:OE1	2.40	0.54
1:A:766:A:H8	1:A:766:A:H5'	1.73	0.54
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.89	0.54
10:J:4:ILE:HD12	10:J:74:ILE:HG21	1.89	0.54
1:A:737:A:H2'	1:A:738:C:H6	1.73	0.54
1:A:1532:U:H3'	1:A:1532:U:C6	2.41	0.54
8:H:20:TYR:HD1	8:H:65:TYR:CD1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:G:H5''	1:A:350:G:H8	1.72	0.54
2:B:130:ARG:H	2:B:130:ARG:HD2	1.72	0.54
2:B:70:PHE:HE2	2:B:163:PHE:CD1	2.25	0.54
1:A:364:A:H61	12:L:28:LYS:HE3	1.71	0.54
13:M:23:TYR:CE2	13:M:70:LEU:HD12	2.42	0.54
1:A:542:G:C4	1:A:543:C:C5	2.95	0.54
1:A:609:A:N6	24:A:2173:HOH:O	2.09	0.54
4:D:65:ARG:HG3	4:D:75:PHE:CG	2.43	0.54
1:A:62:U:H2'	1:A:63:C:C6	2.43	0.54
1:A:537:G:OP1	12:L:113:ARG:NH2	2.41	0.54
1:A:4:U:H4'	1:A:5:U:OP2	2.06	0.54
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.40	0.54
17:Q:56:VAL:HB	17:Q:78:GLU:HB2	1.90	0.54
19:S:64:GLU:O	19:S:67:VAL:HG23	2.07	0.54
1:A:1118:C:H5''	9:I:104:ARG:HG3	1.89	0.54
7:G:89:MET:HA	7:G:155:ARG:NH2	2.22	0.54
13:M:13:LYS:HD2	13:M:17:VAL:HG11	1.90	0.54
1:A:375:U:H5	24:A:3172:HOH:O	1.89	0.54
20:T:100:ILE:HG22	20:T:102:GLY:N	2.23	0.54
1:A:116:A:H5''	24:A:2008:HOH:O	2.08	0.54
12:L:53:ARG:HH12	12:L:92:OTD:CG	2.20	0.54
1:A:362:G:N7	24:A:2487:HOH:O	2.33	0.54
6:F:7:ASN:ND2	18:R:34:TYR:HE1	2.02	0.54
1:A:1366:C:H2'	1:A:1367:C:C6	2.43	0.54
1:A:560:U:H5'	1:A:566:G:N2	2.22	0.54
3:C:77:ILE:HG22	3:C:78:GLY:O	2.08	0.54
15:O:45:VAL:HA	15:O:47:LYS:NZ	2.22	0.54
2:B:10:LEU:O	2:B:10:LEU:HD22	2.08	0.54
17:Q:57:VAL:HG12	17:Q:75:ARG:O	2.08	0.54
6:F:99:ALA:HB3	18:R:31:LEU:HG	1.90	0.54
2:B:53:ARG:HG3	2:B:54:THR:N	2.21	0.54
1:A:370:C:C2'	1:A:371:G:H5'	2.38	0.54
11:K:80:VAL:HG23	11:K:103:LEU:HB3	1.90	0.54
7:G:31:MET:HB3	7:G:39:ALA:HB2	1.90	0.54
7:G:45:ASP:HA	7:G:48:LYS:HD3	1.90	0.54
1:A:474:G:OP2	16:P:75:ARG:HD3	2.07	0.54
13:M:108:ARG:O	13:M:111:LYS:N	2.41	0.54
1:A:3:G:C8	4:D:86:LYS:HE2	2.43	0.54
1:A:45:U:H2'	1:A:46:G:C8	2.42	0.54
8:H:35:ILE:HG22	8:H:36:LEU:N	2.23	0.54
15:O:39:LEU:HD13	15:O:56:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:G:H4'	15:O:69:TYR:OH	2.08	0.53
1:A:950:U:H2'	1:A:951:G:C8	2.43	0.53
9:I:80:GLY:HA2	9:I:83:ARG:HG3	1.91	0.53
6:F:26:ILE:HG21	6:F:63:TYR:CE2	2.43	0.53
1:A:1527:C:H2'	1:A:1528:U:H6	1.72	0.53
1:A:1021:G:H2'	1:A:1021:G:N3	2.22	0.53
16:P:40:ASP:OD1	16:P:44:THR:HG23	2.09	0.53
8:H:97:VAL:HA	8:H:100:ILE:HD11	1.91	0.53
8:H:25:ASP:OD1	8:H:25:ASP:N	2.41	0.53
11:K:124:LYS:O	11:K:124:LYS:HG2	2.06	0.53
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.41	0.53
1:A:581:G:O2'	1:A:582:U:H5'	2.07	0.53
1:A:518:C:H2'	1:A:530:G:N7	2.23	0.53
10:J:79:ARG:O	10:J:82:ILE:N	2.40	0.53
15:O:56:LEU:O	15:O:60:VAL:HG23	2.08	0.53
1:A:142:G:H2'	1:A:143:A:C8	2.43	0.53
3:C:139:GLN:O	3:C:143:GLU:HG3	2.08	0.53
6:F:47:ARG:O	6:F:48:LEU:HD23	2.08	0.53
17:Q:83:ASP:N	17:Q:83:ASP:OD2	2.37	0.53
13:M:2:ALA:O	13:M:10:PRO:HD2	2.09	0.53
10:J:6:ILE:HG22	10:J:97:GLU:O	2.08	0.53
10:J:5:ARG:CG	10:J:99:LYS:H	2.21	0.53
6:F:2:ARG:NH1	6:F:69:GLU:HG2	2.24	0.53
1:A:1226:C:H5''	19:S:80:TYR:CE2	2.42	0.53
1:A:1127:G:H8	1:A:1127:G:H3'	1.73	0.53
2:B:31:TYR:CD2	2:B:202:PRO:HG3	2.42	0.53
1:A:447:G:H2'	1:A:485:G:H22	1.73	0.53
1:A:1167:A:H2'	1:A:1168:A:C8	2.44	0.53
17:Q:22:LEU:HD12	17:Q:23:VAL:N	2.23	0.53
20:T:14:LYS:HB2	20:T:17:ARG:NH2	2.23	0.53
1:A:1280:A:OP1	10:J:7:LYS:NZ	2.41	0.53
1:A:620:C:H2'	1:A:621:A:O4'	2.07	0.53
1:A:363:A:H62	12:L:28:LYS:HD3	1.72	0.53
1:A:826:C:H2'	1:A:827:U:H6	1.73	0.53
1:A:250:A:H4'	1:A:251:G:O5'	2.09	0.53
1:A:1503:A:H4'	1:A:1504:G:OP2	2.09	0.53
5:E:75:THR:O	5:E:76:ILE:HD13	2.09	0.53
1:A:166:G:H2'	1:A:167:G:H8	1.74	0.53
7:G:143:ARG:HB2	7:G:143:ARG:NH1	2.24	0.53
17:Q:13:ASP:H	17:Q:14:LYS:HD2	1.74	0.53
12:L:36:VAL:HG12	12:L:37:CYS:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:U:H2'	1:A:637:G:C8	2.44	0.53
1:A:748:C:O5'	1:A:748:C:H6	1.92	0.53
1:A:839:U:O2	1:A:839:U:H3'	2.08	0.53
1:A:500:G:N7	1:A:546:G:N2	2.56	0.53
1:A:265:G:N2	1:A:267:C:H5'	2.23	0.53
1:A:1169:A:C6	1:A:1171:G:H1'	2.43	0.53
18:R:56:THR:OG1	18:R:58:LEU:HD12	2.09	0.53
13:M:39:ILE:O	13:M:41:PRO:HD3	2.09	0.53
11:K:20:TYR:CZ	11:K:83:ILE:HD12	2.44	0.53
1:A:728:A:H2'	1:A:729:A:C8	2.44	0.53
13:M:19:LEU:HD23	13:M:22:ILE:HD13	1.90	0.53
17:Q:62:SER:HB3	17:Q:72:ARG:HE	1.74	0.53
19:S:28:LYS:HD3	19:S:31:ILE:HG13	1.91	0.53
1:A:1020:U:H2'	1:A:1021:G:O4'	2.09	0.53
1:A:794:A:H2'	1:A:795:C:C6	2.44	0.53
1:A:1067:A:H3'	1:A:1094:G:OP1	2.08	0.53
1:A:1360:A:H2'	1:A:1361:G:H5'	1.90	0.53
6:F:76:ALA:O	6:F:80:ARG:HG3	2.08	0.53
1:A:1490:C:C2'	1:A:1491:G:H5'	2.36	0.53
1:A:1099:G:H2'	1:A:1100:C:C6	2.43	0.53
4:D:9:CYS:SG	4:D:31:CYS:O	2.67	0.53
12:L:44:THR:HG22	12:L:45:PRO:HD2	1.91	0.53
7:G:95:ARG:O	7:G:99:LEU:HG	2.08	0.53
1:A:1125:U:H5''	24:A:2985:HOH:O	2.08	0.53
20:T:28:ALA:HA	20:T:31:SER:OG	2.08	0.53
1:A:1011:G:N2	1:A:1019:C:H1'	2.24	0.53
1:A:114:U:O2'	1:A:115:G:H5'	2.09	0.53
2:B:172:ILE:H	2:B:172:ILE:HD12	1.74	0.53
7:G:56:GLN:N	7:G:56:GLN:OE1	2.41	0.53
1:A:1004:A:N7	1:A:1037:C:N3	2.57	0.53
2:B:108:ILE:O	2:B:111:ARG:HB2	2.09	0.53
1:A:1392:G:N2	1:A:1502:A:C8	2.77	0.53
5:E:35:GLY:CA	5:E:112:LEU:HD22	2.39	0.53
2:B:16:HIS:CB	2:B:210:SER:HB2	2.39	0.53
11:K:58:PRO:HG3	11:K:90:GLY:N	2.23	0.53
1:A:1014:A:H4'	19:S:14:HIS:CE1	2.44	0.53
1:A:76:C:C2'	1:A:77:G:H5'	2.38	0.53
1:A:585:G:H8	1:A:585:G:O5'	1.92	0.53
12:L:89:ARG:HH21	12:L:97:ARG:HG3	1.74	0.52
1:A:1502:A:H3'	1:A:1503:A:H5''	1.89	0.52
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:114:ARG:O	7:G:119:ARG:NH1	2.42	0.52
7:G:115:ARG:H	7:G:115:ARG:NE	2.06	0.52
1:A:250:A:H5'	1:A:250:A:H8	1.74	0.52
5:E:64:ARG:O	5:E:65:ASN:HB3	2.10	0.52
19:S:18:LYS:HE3	19:S:31:ILE:HG23	1.90	0.52
11:K:44:SER:HG	11:K:46:GLY:H	1.55	0.52
3:C:155:GLY:HA2	3:C:157:ILE:CG1	2.38	0.52
2:B:147:LYS:HG2	2:B:148:TYR:CD1	2.44	0.52
1:A:543:C:O2'	1:A:544:G:H5'	2.08	0.52
1:A:828:A:OP1	1:A:828:A:H4'	2.08	0.52
4:D:102:ASP:OD1	4:D:103:ASN:N	2.41	0.52
19:S:44:MET:O	19:S:47:HIS:HB2	2.08	0.52
10:J:5:ARG:O	10:J:98:ILE:HG23	2.08	0.52
3:C:58:GLU:HB2	3:C:65:ALA:HB2	1.91	0.52
16:P:52:ASP:OD2	16:P:55:ARG:HB2	2.09	0.52
1:A:276:G:O2'	1:A:277:C:H5'	2.10	0.52
1:A:683:G:H3'	1:A:684:A:H8	1.75	0.52
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.91	0.52
1:A:1492:A:C8	1:A:1492:A:H3'	2.44	0.52
9:I:19:LEU:HB3	9:I:59:PHE:CE2	2.45	0.52
17:Q:70:ARG:O	17:Q:71:PHE:HD2	1.91	0.52
9:I:124:GLN:HG3	9:I:125:TYR:N	2.24	0.52
17:Q:13:ASP:HA	24:Q:306:HOH:O	2.08	0.52
1:A:226:G:N2	24:A:2625:HOH:O	2.17	0.52
1:A:821:G:C2'	1:A:822:C:H5'	2.39	0.52
12:L:83:VAL:CG2	12:L:100:ILE:HG23	2.38	0.52
2:B:161:ALA:HA	2:B:182:ILE:HG22	1.90	0.52
1:A:514:C:H2'	1:A:515:G:H5'	1.92	0.52
11:K:17:GLY:HA2	11:K:35:PRO:HG3	1.91	0.52
2:B:125:PRO:O	2:B:127:ILE:HG13	2.09	0.52
11:K:85:ARG:HA	11:K:112:THR:OG1	2.10	0.52
1:A:299:G:C6	1:A:300:A:C6	2.98	0.52
4:D:146:ILE:HD12	4:D:146:ILE:H	1.73	0.52
1:A:265:G:C5	1:A:267:C:C5	2.98	0.52
1:A:1378:C:C5	1:A:1379:G:C4	2.97	0.52
1:A:1151:A:H1'	1:A:1152:A:C8	2.45	0.52
1:A:1391:U:H2'	1:A:1392:G:C8	2.45	0.52
7:G:78:ARG:NH1	7:G:156:TRP:HB2	2.24	0.52
6:F:97:PHE:HB2	18:R:32:ARG:NH1	2.25	0.52
8:H:13:ILE:O	8:H:17:THR:HG23	2.10	0.52
1:A:706:A:O4'	11:K:29:ILE:HD11	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:VAL:HA	2:B:139:LYS:HB3	1.90	0.52
1:A:688:G:C5	1:A:700:G:C2	2.98	0.52
1:A:1251:A:H2'	1:A:1252:A:O4'	2.10	0.52
1:A:576:G:H3'	1:A:577:G:H5''	1.92	0.52
1:A:322:C:H2'	1:A:323:U:H6	1.75	0.52
3:C:18:TRP:HZ2	14:N:56:VAL:O	1.93	0.52
2:B:16:HIS:ND1	2:B:17:PHE:O	2.42	0.52
4:D:191:ARG:HD3	4:D:192:GLU:OE1	2.09	0.52
1:A:510:A:P	24:A:2093:HOH:O	2.67	0.52
7:G:13:GLN:HB3	7:G:14:PRO:O	2.10	0.52
11:K:115:PRO:C	11:K:117:ASN:H	2.12	0.52
8:H:61:VAL:HG12	8:H:61:VAL:O	2.09	0.52
19:S:5:LEU:CD1	19:S:10:PHE:HB2	2.40	0.52
4:D:13:ARG:HG2	4:D:38:TYR:O	2.09	0.52
1:A:981:U:H5'	14:N:21:TYR:CE1	2.45	0.52
14:N:41:ARG:HG2	14:N:42:ILE:N	2.24	0.52
1:A:978:A:H1'	1:A:1322:C:O2	2.10	0.52
1:A:1502:A:H2	1:A:1505:G:H1	1.57	0.52
1:A:56:U:H2'	1:A:57:G:H8	1.71	0.52
5:E:138:ALA:O	5:E:141:GLN:HB2	2.08	0.52
20:T:40:ALA:HB2	20:T:55:ILE:HG22	1.90	0.52
1:A:257:G:C2	1:A:270:A:C2	2.98	0.52
1:A:1030(C):G:H21	1:A:1030(D):A:H61	1.57	0.52
1:A:1121:U:O2'	1:A:1122:U:H5'	2.09	0.52
1:A:767:A:H2'	1:A:768:A:O4'	2.10	0.52
7:G:154:TYR:N	7:G:154:TYR:CD2	2.77	0.52
5:E:40:ARG:HB3	5:E:66:MET:HE1	1.93	0.52
1:A:122:G:C2'	1:A:123:C:H5'	2.39	0.52
1:A:939:G:H2'	1:A:940:C:C6	2.44	0.52
1:A:793:U:O2	1:A:1516[A]:G:H4'	2.10	0.51
15:O:4:THR:HA	15:O:5:LYS:HZ1	1.75	0.51
1:A:1330:U:H2'	1:A:1331:G:H5'	1.92	0.51
1:A:144:G:H1	1:A:178:C:H42	1.58	0.51
1:A:1254:C:O4'	1:A:1356:G:H5''	2.10	0.51
4:D:200:GLU:O	4:D:203:VAL:N	2.37	0.51
3:C:102:ASN:OD1	3:C:102:ASN:N	2.42	0.51
15:O:68:ARG:O	15:O:71:GLN:N	2.43	0.51
10:J:4:ILE:HB	10:J:74:ILE:CB	2.34	0.51
18:R:87:ARG:CG	18:R:88:LYS:H	2.23	0.51
1:A:1381:U:C6	7:G:156:TRP:HZ2	2.28	0.51
6:F:12:PRO:CG	6:F:57:GLN:HG3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:A:H2'	1:A:1192:C:H6	1.75	0.51
1:A:1278:U:C5'	1:A:1279:A:H5'	2.40	0.51
7:G:115:ARG:H	7:G:115:ARG:CD	2.23	0.51
11:K:57:THR:O	11:K:60:ALA:HB3	2.09	0.51
1:A:706:A:C1'	11:K:29:ILE:HD11	2.39	0.51
11:K:33:THR:HG21	11:K:37:GLY:HA2	1.91	0.51
18:R:45:SER:HB2	18:R:46:GLU:OE2	2.10	0.51
1:A:564:C:H5''	1:A:565:U:OP2	2.10	0.51
1:A:615:C:O5'	1:A:615:C:H6	1.94	0.51
1:A:931:C:H2'	1:A:931:C:O2	2.09	0.51
2:B:162:ILE:O	2:B:185:ILE:HB	2.10	0.51
5:E:103:GLY:O	5:E:106:PRO:HD2	2.10	0.51
1:A:1278:U:H5''	1:A:1279:A:H5'	1.91	0.51
1:A:1510:U:H2'	1:A:1511:G:C8	2.45	0.51
1:A:463:A:H4'	16:P:82:GLN:HB2	1.92	0.51
15:O:22:THR:O	15:O:27:VAL:HG11	2.09	0.51
3:C:150:LYS:CG	3:C:169:ALA:HB2	2.40	0.51
13:M:74:VAL:O	13:M:77:ASN:HB2	2.10	0.51
8:H:122:ARG:NH1	8:H:125:ARG:HH22	2.07	0.51
1:A:1340:A:O2'	9:I:127:LYS:NZ	2.43	0.51
1:A:1071:C:H2'	1:A:1072:G:H8	1.76	0.51
12:L:84:LEU:HD13	12:L:105:TYR:HE1	1.75	0.51
1:A:1465:C:H2'	1:A:1466:C:O4'	2.11	0.51
6:F:78:GLU:HA	6:F:81:ILE:HG13	1.91	0.51
9:I:126:SER:O	9:I:128:ARG:N	2.43	0.51
1:A:1315:U:H2'	1:A:1316:G:O4'	2.11	0.51
1:A:259:G:H2'	1:A:260:G:O4'	2.10	0.51
1:A:1503:A:H61	1:A:1533:C:N4	2.08	0.51
1:A:735:C:H2'	1:A:736:C:H6	1.76	0.51
11:K:44:SER:OG	11:K:46:GLY:N	2.34	0.51
3:C:4:LYS:NZ	3:C:4:LYS:HB2	2.26	0.51
13:M:51:ALA:O	13:M:55:ARG:HD3	2.10	0.51
2:B:16:HIS:HB3	2:B:210:SER:HB2	1.91	0.51
1:A:149:A:H2'	1:A:150:C:C6	2.46	0.51
19:S:40:ILE:HD13	19:S:62:ILE:HD11	1.91	0.51
1:A:877:C:H5''	8:H:88:LYS:HD3	1.92	0.51
19:S:32:LYS:H	19:S:32:LYS:NZ	2.09	0.51
1:A:1226:C:H4'	19:S:80:TYR:CZ	2.46	0.51
12:L:25:PRO:HA	12:L:27:LEU:H	1.76	0.51
1:A:321:A:O2'	1:A:322:C:H5'	2.10	0.51
1:A:1205:U:O2'	3:C:195:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1497:G:O2'	1:A:1498:UR3:H5'	2.10	0.51
1:A:804:U:H5''	1:A:805:C:OP2	2.10	0.51
11:K:120:ARG:NH2	11:K:126:ARG:NH1	2.59	0.51
1:A:135:C:C5	1:A:136:C:C5	2.98	0.51
18:R:56:THR:OG1	18:R:57:GLY:N	2.43	0.51
1:A:963:G:H5'	24:A:2606:HOH:O	2.11	0.51
1:A:216:G:O2'	1:A:217:C:O4'	2.29	0.51
1:A:1366:C:O3'	10:J:60:ARG:NH2	2.44	0.51
1:A:1305:G:N2	1:A:1331:G:H1'	2.26	0.51
7:G:47:CYS:HB3	7:G:58:PRO:CB	2.41	0.51
1:A:1085:U:N3	24:A:2258:HOH:O	2.34	0.51
6:F:45:LEU:HD21	6:F:59:TYR:HD1	1.76	0.51
1:A:13:U:O2	1:A:914:A:H3'	2.11	0.51
1:A:189:G:H2'	1:A:190:C:C6	2.46	0.51
16:P:12:LYS:O	16:P:13:HIS:HB2	2.11	0.51
10:J:75:ILE:HA	10:J:77:PRO:HG3	1.92	0.51
6:F:26:ILE:O	6:F:30:LEU:HB2	2.11	0.51
2:B:17:PHE:CD1	2:B:18:GLY:N	2.79	0.51
1:A:566:G:N2	24:A:3183:HOH:O	2.40	0.51
2:B:136:VAL:HG13	2:B:139:LYS:HD3	1.93	0.51
1:A:1157:A:C6	1:A:1180:A:C6	2.99	0.51
2:B:71:VAL:HG13	2:B:93:VAL:HB	1.93	0.51
1:A:82:U:O2'	1:A:83:U:H5'	2.10	0.51
7:G:70:LYS:HG2	7:G:96:GLN:HG2	1.93	0.51
17:Q:17:LYS:HG2	17:Q:47:PRO:O	2.11	0.51
16:P:28:ARG:HG2	16:P:29:ASP:OD2	2.10	0.51
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.92	0.51
1:A:1314:C:H2'	1:A:1315:U:C6	2.47	0.50
13:M:4:ILE:HG22	13:M:57:ARG:HA	1.93	0.50
6:F:16:GLN:HA	6:F:16:GLN:OE1	2.11	0.50
13:M:80:ARG:NH2	13:M:81:LEU:HD23	2.23	0.50
1:A:253:U:H2'	1:A:254:G:H8	1.76	0.50
17:Q:87:LYS:HE2	17:Q:91:ARG:HG3	1.94	0.50
10:J:26:ALA:HA	10:J:29:ARG:HH21	1.76	0.50
16:P:53:VAL:HG23	16:P:54:GLU:N	2.25	0.50
3:C:142:MET:SD	3:C:148:GLY:HA2	2.50	0.50
10:J:76:ASN:N	10:J:77:PRO:HD3	2.26	0.50
1:A:434:U:H2'	1:A:435:C:C6	2.38	0.50
10:J:50:ILE:HD13	10:J:60:ARG:HD3	1.93	0.50
5:E:78:HIS:HE1	5:E:143:ARG:HB2	1.77	0.50
7:G:46:ALA:O	7:G:49:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:C:O2'	1:A:807:A:H5'	2.11	0.50
14:N:26:ARG:HH12	14:N:47:LEU:CD2	2.23	0.50
1:A:147:G:C2	1:A:148:G:C8	2.99	0.50
16:P:75:ARG:HG3	16:P:80:PHE:HB2	1.92	0.50
20:T:67:ALA:O	20:T:73:HIS:ND1	2.39	0.50
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.92	0.50
19:S:29:ARG:NH1	19:S:48:THR:OG1	2.42	0.50
2:B:79:ASP:OD2	2:B:79:ASP:N	2.21	0.50
1:A:1162:C:N4	1:A:1174:G:C6	2.77	0.50
13:M:4:ILE:CD1	13:M:22:ILE:HD11	2.42	0.50
12:L:25:PRO:HB2	12:L:64:TYR:CE2	2.39	0.50
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.15	0.50
2:B:101:MET:HB2	2:B:152:PHE:CZ	2.45	0.50
1:A:129:U:O3'	1:A:129(A):G:H3'	2.10	0.50
3:C:195:VAL:C	3:C:196:LEU:HD12	2.32	0.50
1:A:390:C:H2'	1:A:391:G:C8	2.46	0.50
1:A:452:A:H1'	1:A:453:A:C8	2.45	0.50
1:A:579:G:H2'	1:A:580:U:H6	1.75	0.50
1:A:279:A:C8	1:A:279:A:H5'	2.38	0.50
15:O:4:THR:HG1	15:O:6:GLU:HG2	1.76	0.50
15:O:4:THR:HG1	15:O:7:GLU:H	1.59	0.50
1:A:1128:C:H4'	9:I:16:ARG:HH22	1.76	0.50
18:R:58:LEU:HD23	18:R:62:GLU:OE1	2.12	0.50
10:J:26:ALA:HB1	10:J:84:GLN:HB3	1.93	0.50
1:A:1521:G:H2'	1:A:1522:U:O4'	2.11	0.50
1:A:1144:G:H2'	1:A:1145:C:C5	2.47	0.50
1:A:576:G:H3'	1:A:577:G:C5'	2.42	0.50
20:T:56:MET:CE	20:T:85:MET:HG2	2.38	0.50
1:A:1150:U:C2'	1:A:1151:A:H5'	2.41	0.50
12:L:42:THR:HA	12:L:53:ARG:O	2.10	0.50
5:E:51:VAL:O	5:E:54:ALA:HB3	2.12	0.50
15:O:69:TYR:CE2	15:O:73:GLU:HG2	2.46	0.50
1:A:390:C:O3'	16:P:28:ARG:NH2	2.44	0.50
1:A:642:A:H2'	1:A:643:C:H6	1.77	0.50
7:G:102:ARG:O	7:G:106:GLN:HG2	2.12	0.50
1:A:663:A:H61	1:A:742:G:H1	1.60	0.50
1:A:362:G:N2	1:A:364:A:H3'	2.27	0.50
1:A:324:G:OP1	20:T:22:ARG:HD3	2.11	0.50
7:G:27:ILE:HD13	7:G:40:ALA:HA	1.93	0.50
2:B:167:PRO:HG3	2:B:186:ALA:CB	2.42	0.50
1:A:692:U:H5''	1:A:797:C:H5'	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:10:ARG:HD3	9:I:75:ASP:HB2	1.94	0.50
1:A:37:U:O2'	1:A:500:G:H4'	2.12	0.50
8:H:86:ILE:HG22	8:H:93:VAL:HG21	1.93	0.50
1:A:1171:G:O2'	1:A:1172:C:H5'	2.11	0.50
16:P:26:ARG:HG2	16:P:26:ARG:NH1	2.25	0.50
2:B:17:PHE:HD1	2:B:18:GLY:N	2.10	0.50
2:B:121:LEU:O	2:B:124:SER:OG	2.28	0.50
1:A:1017:G:H2'	1:A:1018:C:O4'	2.12	0.50
1:A:691:G:H2'	1:A:692:U:H6	1.77	0.50
2:B:24:TRP:CG	2:B:25:ASN:N	2.80	0.50
1:A:1162:C:N3	1:A:1175:G:C2	2.79	0.50
1:A:499:A:H4'	1:A:500:G:OP1	2.11	0.50
14:N:35:ARG:NH1	14:N:35:ARG:HG2	2.20	0.50
1:A:1414:U:C4	1:A:1415:G:N7	2.79	0.50
8:H:17:THR:HA	8:H:65:TYR:OH	2.11	0.50
8:H:9:MET:O	8:H:13:ILE:HG12	2.12	0.50
1:A:955:U:H1'	1:A:1227:A:H61	1.77	0.50
1:A:620:C:C2	4:D:135:LEU:HD22	2.47	0.50
1:A:1516[B]:G:C2	1:A:1518[B]:MA6:OP1	2.64	0.50
1:A:429:U:H4'	1:A:430:A:O5'	2.12	0.50
2:B:105:PHE:O	2:B:108:ILE:N	2.45	0.50
1:A:859:A:C2'	1:A:860:A:H5'	2.42	0.50
1:A:505:G:H5'	1:A:534:U:H2'	1.92	0.50
13:M:4:ILE:HD11	13:M:10:PRO:HG3	1.93	0.49
1:A:1059:C:N4	24:A:2658:HOH:O	2.44	0.49
1:A:1031:G:H2'	1:A:1032:G:C5	2.47	0.49
3:C:21:ARG:NH1	3:C:21:ARG:HB3	2.19	0.49
6:F:87:ARG:NH1	6:F:87:ARG:HG3	2.25	0.49
1:A:1190:G:H5'	3:C:176:HIS:CE1	2.47	0.49
19:S:72:GLY:C	19:S:74:PHE:H	2.13	0.49
3:C:94:LEU:HD22	3:C:95:THR:HG23	1.93	0.49
5:E:151:LEU:HB3	8:H:79:VAL:HG22	1.94	0.49
1:A:1287:A:H2'	1:A:1288:A:C8	2.47	0.49
2:B:18:GLY:O	2:B:19:HIS:HB3	2.12	0.49
15:O:39:LEU:HD22	15:O:43:LEU:HG	1.94	0.49
17:Q:87:LYS:HA	17:Q:90:ILE:HD12	1.93	0.49
1:A:1213:A:C4	1:A:1215:G:C8	3.01	0.49
1:A:426:G:OP1	4:D:38:TYR:OH	2.19	0.49
7:G:5:ARG:HG3	7:G:7:ALA:N	2.28	0.49
1:A:975:A:H4'	1:A:976:G:H5''	1.93	0.49
1:A:148:G:H2'	1:A:149:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:G:P	24:A:2008:HOH:O	2.69	0.49
3:C:91:LEU:HG	3:C:99:VAL:HG21	1.95	0.49
8:H:62:TYR:N	8:H:62:TYR:CD2	2.81	0.49
1:A:1491:G:H2'	1:A:1492:A:C8	2.47	0.49
1:A:1036:G:N2	1:A:1037:C:C2	2.81	0.49
1:A:1127:G:H22	1:A:1145:C:H42	1.59	0.49
1:A:1435:G:H2'	1:A:1436:U:H6	1.72	0.49
8:H:87:SER:HA	8:H:93:VAL:HG22	1.93	0.49
1:A:1324:A:H2'	1:A:1325:C:O4'	2.11	0.49
1:A:1129:C:N4	1:A:1135:U:O4	2.44	0.49
1:A:807:A:H2'	1:A:808:C:C6	2.48	0.49
1:A:7:G:H5'	1:A:298:A:O4'	2.13	0.49
17:Q:84:LEU:O	17:Q:87:LYS:HB3	2.13	0.49
1:A:90:U:H2'	1:A:91:C:C6	2.47	0.49
1:A:781:A:H2'	1:A:782:A:H5'	1.94	0.49
2:B:61:LEU:HD22	2:B:68:ILE:HD11	1.95	0.49
1:A:1138:G:N3	1:A:1138:G:H3'	2.28	0.49
1:A:1127:G:C8	1:A:1127:G:H3'	2.47	0.49
15:O:26:GLU:HG3	15:O:81:LEU:HD12	1.94	0.49
1:A:1451:A:H5'	1:A:1452:C:C5	2.40	0.49
16:P:39:TYR:HA	16:P:48:TRP:O	2.13	0.49
1:A:1409:C:H3'	1:A:1409:C:C6	2.47	0.49
1:A:1288:A:H2'	1:A:1289:A:C8	2.47	0.49
6:F:8:ILE:HD13	6:F:88:VAL:HG22	1.94	0.49
1:A:299:G:C6	1:A:300:A:N1	2.81	0.49
1:A:510:A:H5''	1:A:511:C:OP2	2.13	0.49
1:A:64:G:H4'	1:A:65:U:H3'	1.95	0.49
11:K:120:ARG:HB3	11:K:120:ARG:NH1	2.07	0.49
3:C:6:HIS:CD2	3:C:9:GLY:H	2.28	0.49
10:J:6:ILE:HG13	10:J:72:VAL:CB	2.43	0.49
1:A:1054:C:H4'	1:A:1054:C:OP2	2.11	0.49
1:A:758:G:C6	24:A:3191:HOH:O	2.65	0.49
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.43	0.49
3:C:139:GLN:HA	3:C:139:GLN:OE1	2.13	0.49
1:A:1121:U:H2'	1:A:1122:U:C6	2.48	0.49
12:L:7:ILE:O	12:L:10:LEU:N	2.45	0.49
12:L:59:ARG:HG3	12:L:60:LEU:N	2.28	0.49
7:G:120:ILE:HD13	7:G:120:ILE:N	2.27	0.49
3:C:34:LEU:CD2	3:C:38:ARG:HE	2.25	0.49
4:D:25:ARG:HA	4:D:28:SER:HB3	1.94	0.49
1:A:254:G:H2'	1:A:255:G:H8	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:61:LEU:HD22	6:F:63:TYR:CE1	2.48	0.49
7:G:22:LEU:HD12	7:G:22:LEU:O	2.13	0.49
1:A:1257:U:H2'	1:A:1257:U:O2	2.13	0.49
18:R:59:SER:H	18:R:62:GLU:HB2	1.77	0.49
3:C:40:ARG:HG3	3:C:40:ARG:HH11	1.77	0.49
11:K:65:ALA:HB1	11:K:98:LEU:HD21	1.94	0.49
1:A:1118:C:H42	1:A:1155:G:H1	1.61	0.49
1:A:996:A:H2'	1:A:997:U:C6	2.48	0.49
1:A:921:U:H2'	1:A:922:G:O4'	2.11	0.49
19:S:39:THR:HG22	19:S:70:LYS:HD3	1.95	0.49
7:G:146:GLU:HA	7:G:149:ARG:HB2	1.94	0.49
11:K:48:ILE:HG22	11:K:49:GLY:N	2.25	0.49
7:G:27:ILE:O	7:G:30:ILE:HB	2.13	0.49
8:H:124:ALA:O	8:H:128:GLY:N	2.39	0.49
9:I:55:ALA:O	9:I:56:LEU:HB2	2.11	0.49
6:F:62:TRP:CZ2	6:F:64:GLN:HB2	2.48	0.49
11:K:40:ILE:HG23	11:K:41:THR:HG22	1.95	0.49
7:G:91:VAL:HG11	7:G:96:GLN:HG3	1.95	0.49
1:A:838:G:H1	1:A:848:C:H42	1.59	0.49
1:A:1070:U:H2'	1:A:1071:C:H6	1.78	0.49
1:A:1116:C:O2'	1:A:1117:G:H5'	2.11	0.49
1:A:715:A:H2'	1:A:716:A:C8	2.48	0.49
1:A:67:C:H2'	1:A:68:G:C8	2.48	0.49
13:M:108:ARG:O	13:M:109:THR:C	2.51	0.48
4:D:176:LEU:HD12	4:D:177:ASP:N	2.27	0.48
1:A:1517[B]:G:H2'	1:A:1518[B]:MA6:H8	1.94	0.48
13:M:19:LEU:HD23	13:M:22:ILE:CD1	2.43	0.48
1:A:264:U:H2'	1:A:265:G:C8	2.48	0.48
3:C:14:ILE:C	3:C:16:ARG:H	2.15	0.48
7:G:46:ALA:HB1	7:G:121:ALA:HB2	1.93	0.48
5:E:153:LYS:HD3	5:E:154:GLY:O	2.13	0.48
2:B:70:PHE:CD2	2:B:163:PHE:HB3	2.48	0.48
1:A:676:A:O2'	11:K:115:PRO:HG3	2.13	0.48
4:D:13:ARG:HD2	4:D:36:ARG:O	2.12	0.48
1:A:260:G:H2'	1:A:261:U:C6	2.49	0.48
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.13	0.48
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.95	0.48
1:A:1367:C:H5'	10:J:60:ARG:HH21	1.78	0.48
1:A:1057:G:H2'	1:A:1058:G:O4'	2.13	0.48
1:A:1171:G:H2'	1:A:1172:C:C6	2.48	0.48
6:F:57:GLN:HG2	6:F:57:GLN:H	1.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1350:A:H2'	1:A:1351:U:C6	2.48	0.48
8:H:138:TRP:O	8:H:138:TRP:CE3	2.66	0.48
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.96	0.48
17:Q:87:LYS:NZ	17:Q:88:TYR:HB2	2.28	0.48
1:A:389:A:H2'	1:A:390:C:H5'	1.94	0.48
19:S:20:LEU:HD23	19:S:23:ASN:HD22	1.78	0.48
6:F:51:PRO:HB3	6:F:54:LYS:HA	1.94	0.48
12:L:80:HIS:N	12:L:80:HIS:ND1	2.61	0.48
1:A:260:G:C5	1:A:261:U:C5	3.01	0.48
14:N:9:LYS:HD3	14:N:10:ALA:N	2.28	0.48
13:M:70:LEU:O	13:M:74:VAL:HG23	2.13	0.48
1:A:1135:U:H2'	1:A:1137:C:C4	2.49	0.48
2:B:149:LEU:HA	2:B:149:LEU:HD23	1.52	0.48
1:A:515:G:H2'	1:A:516:PSU:O4'	2.13	0.48
1:A:109:A:H2'	1:A:326:G:N2	2.28	0.48
3:C:53:ALA:HB2	3:C:115:LEU:HG	1.95	0.48
1:A:679:C:H42	1:A:711:G:H1	1.62	0.48
6:F:52:ILE:O	6:F:55:ASP:HB2	2.13	0.48
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.77	0.48
1:A:501:C:H2'	1:A:502:G:H8	1.78	0.48
10:J:32:ALA:HB3	10:J:75:ILE:CD1	2.43	0.48
1:A:1516[B]:G:H2'	1:A:1517[B]:G:C5'	2.44	0.48
15:O:8:LYS:HD2	15:O:31:LEU:HD21	1.96	0.48
7:G:85:TYR:HD1	7:G:154:TYR:HE1	1.58	0.48
1:A:1146:A:H2'	1:A:1147:C:O4'	2.14	0.48
1:A:1237:C:H5''	1:A:1238:A:O4'	2.13	0.48
1:A:920:U:H2'	1:A:921:U:C6	2.48	0.48
1:A:1061:G:C5	1:A:1062:U:C5	3.02	0.48
5:E:51:VAL:N	5:E:52:PRO:HD2	2.28	0.48
5:E:53:LEU:HA	5:E:53:LEU:HD23	1.57	0.48
13:M:33:ALA:O	13:M:37:THR:HG23	2.13	0.48
1:A:756:C:C2	1:A:757:U:C6	3.02	0.48
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.14	0.48
1:A:1426:C:H2'	1:A:1427:U:H6	1.79	0.48
1:A:659:U:OP2	15:O:8:LYS:NZ	2.41	0.48
3:C:150:LYS:HA	3:C:169:ALA:CB	2.43	0.48
1:A:1276:G:H2'	1:A:1277:C:H6	1.78	0.48
6:F:43:LEU:N	6:F:43:LEU:HD13	2.29	0.48
1:A:377:G:OP1	16:P:5:ARG:HD3	2.13	0.48
3:C:115:LEU:HD23	3:C:118:GLN:OE1	2.14	0.48
1:A:74:C:C2	1:A:97:G:N2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LYS:HB3	3:C:203:PHE:CE2	2.49	0.48
9:I:41:VAL:O	9:I:43:ALA:N	2.47	0.48
1:A:180:U:H2'	1:A:181:G:H5'	1.95	0.48
1:A:1101:A:H62	2:B:175:ARG:NH1	2.11	0.48
1:A:314:C:C2'	1:A:315:A:H5'	2.43	0.48
4:D:98:GLU:HG3	4:D:194:LEU:HD11	1.95	0.48
3:C:7:PRO:HD2	3:C:8:ILE:H	1.78	0.48
5:E:98:THR:N	5:E:117:ASP:OD1	2.45	0.48
1:A:1218:C:H2'	1:A:1219:U:C6	2.49	0.48
1:A:349:A:H2'	1:A:350:G:H5''	1.95	0.48
1:A:392:G:H2'	1:A:393:A:H8	1.77	0.48
1:A:1211:U:O2'	1:A:1213:A:N3	2.44	0.48
13:M:29:ARG:O	13:M:32:GLU:HB3	2.14	0.48
12:L:85:ILE:HG23	12:L:85:ILE:HD12	1.65	0.48
1:A:1033:G:N3	1:A:1033:G:H2'	2.27	0.48
1:A:362:G:C8	24:A:2487:HOH:O	2.67	0.48
1:A:674:G:H2'	1:A:675:A:H8	1.78	0.48
18:R:31:LEU:HD22	18:R:66:LEU:HD13	1.96	0.48
9:I:118:LYS:C	9:I:120:ARG:H	2.16	0.48
10:J:51:ARG:HG2	14:N:45:ARG:NH2	2.29	0.48
1:A:355:C:C4	1:A:356:A:N7	2.81	0.48
9:I:2:GLU:OE1	9:I:3:GLN:HB2	2.12	0.48
7:G:136:LYS:O	7:G:139:GLU:HB2	2.13	0.48
1:A:435:C:H1'	24:A:2525:HOH:O	2.13	0.48
1:A:1423:G:N2	1:A:1477:C:N3	2.56	0.48
4:D:150:GLU:N	4:D:150:GLU:CD	2.67	0.48
1:A:642:A:C4	8:H:114:THR:O	2.67	0.48
4:D:176:LEU:HD12	4:D:177:ASP:H	1.79	0.48
13:M:46:LYS:HG3	13:M:46:LYS:H	1.24	0.48
1:A:1005:A:C5	1:A:1025:U:O2'	2.66	0.48
13:M:50:GLU:OE2	13:M:53:VAL:HB	2.14	0.48
14:N:9:LYS:HG2	14:N:12:ARG:NH1	2.28	0.48
1:A:1102:A:C5	1:A:1103:C:C5	3.02	0.48
1:A:344:A:H5''	1:A:345:C:C5	2.42	0.48
5:E:95:ALA:O	5:E:98:THR:OG1	2.26	0.48
4:D:158:ILE:O	4:D:162:LEU:HB2	2.14	0.48
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.96	0.48
3:C:119:ARG:O	3:C:122:GLU:HB3	2.14	0.48
1:A:1317:C:N3	19:S:37:ARG:NH2	2.58	0.47
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:C2	2.44	0.47
7:G:5:ARG:HG3	7:G:7:ALA:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:76:LEU:HD23	17:Q:78:GLU:H	1.79	0.47
1:A:1011:G:H2'	1:A:1012:U:O4'	2.14	0.47
2:B:83:MET:SD	2:B:238:LEU:HD11	2.54	0.47
6:F:29:ALA:HA	6:F:32:ASN:HB2	1.96	0.47
1:A:1095:U:N3	1:A:1096:C:C4	2.82	0.47
1:A:52:G:H3'	24:A:2941:HOH:O	2.13	0.47
1:A:1036:G:H21	1:A:1037:C:H1'	1.79	0.47
1:A:1144:G:C2	1:A:1145:C:C4	3.02	0.47
13:M:4:ILE:H	13:M:8:GLU:CG	2.27	0.47
1:A:1378:C:N4	1:A:1379:G:N3	2.62	0.47
20:T:45:GLN:HB2	20:T:91:LEU:HD21	1.95	0.47
1:A:1172:C:C2'	1:A:1173:G:H5'	2.44	0.47
1:A:1304:G:C6	1:A:1305:G:N1	2.82	0.47
1:A:538:G:H5''	12:L:114:LYS:HB2	1.96	0.47
1:A:79:G:C2	1:A:80:G:C8	3.02	0.47
7:G:153:HIS:CE1	7:G:154:TYR:HE2	2.32	0.47
8:H:123:GLU:O	8:H:127:LEU:HB2	2.13	0.47
6:F:48:LEU:HA	6:F:48:LEU:HD23	1.76	0.47
2:B:84:GLU:O	2:B:219:VAL:HG21	2.14	0.47
16:P:67:THR:O	16:P:70:ALA:HB3	2.15	0.47
15:O:33:THR:HG23	15:O:63:ARG:CZ	2.44	0.47
1:A:558:G:OP1	24:A:2123:HOH:O	2.20	0.47
3:C:43:LEU:CD1	3:C:47:LEU:HD22	2.44	0.47
20:T:75:ASN:C	20:T:77:ALA:N	2.64	0.47
1:A:1110:A:H8	1:A:1110:A:OP2	1.97	0.47
1:A:265:G:C4	1:A:267:C:C5	3.02	0.47
1:A:321:A:N7	1:A:328:C:O2'	2.42	0.47
8:H:51:VAL:HG21	8:H:60:ARG:NH2	2.28	0.47
20:T:10:LEU:O	20:T:13:LEU:HD23	2.15	0.47
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.96	0.47
11:K:17:GLY:O	11:K:80:VAL:HA	2.14	0.47
21:U:7:ARG:O	21:U:21:TYR:CD2	2.67	0.47
1:A:1388:C:H2'	1:A:1389:C:H6	1.79	0.47
3:C:45:LYS:CE	3:C:45:LYS:HA	2.44	0.47
3:C:45:LYS:HA	3:C:45:LYS:NZ	2.29	0.47
1:A:502:G:H2'	1:A:503:C:O4'	2.14	0.47
1:A:362:G:H5''	12:L:61:THR:CG2	2.44	0.47
18:R:37:VAL:HG21	18:R:78:LEU:HB2	1.97	0.47
19:S:18:LYS:CE	19:S:31:ILE:HG12	2.44	0.47
1:A:1277:C:H2'	1:A:1277:C:O2	2.14	0.47
11:K:52:GLY:H	11:K:54:ARG:HH22	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:C:H2'	1:A:313:A:H8	1.79	0.47
13:M:32:GLU:O	13:M:36:LYS:HB2	2.14	0.47
18:R:75:ILE:HG22	18:R:76:LEU:N	2.29	0.47
1:A:562:C:H4'	1:A:563:A:O5'	2.15	0.47
1:A:289:G:N2	1:A:290:C:C2	2.82	0.47
1:A:118:U:H3'	1:A:288:A:H61	1.79	0.47
19:S:13:ASP:N	19:S:13:ASP:OD2	2.47	0.47
13:M:8:GLU:OE2	13:M:8:GLU:N	2.47	0.47
1:A:261:U:H2'	1:A:263:A:OP2	2.14	0.47
6:F:11:ASN:HB3	6:F:14:LEU:HG	1.95	0.47
1:A:411:A:C1'	1:A:413:G:HO2'	2.28	0.47
1:A:858:G:O6	1:A:869:G:H3'	2.14	0.47
10:J:98:ILE:HG22	10:J:99:LYS:N	2.29	0.47
1:A:1197:G:H8	1:A:1197:G:H5'	1.79	0.47
1:A:572:A:N3	1:A:917:G:H1'	2.29	0.47
2:B:162:ILE:O	2:B:185:ILE:N	2.47	0.47
7:G:71:PRO:HG3	7:G:99:LEU:HD12	1.96	0.47
11:K:94:ALA:O	11:K:98:LEU:HG	2.13	0.47
9:I:44:VAL:O	9:I:47:LEU:HD12	2.15	0.47
1:A:1239:A:H62	1:A:1299:A:H62	1.62	0.47
1:A:1539:C:C5	1:A:1540:PSU:C6	3.02	0.47
1:A:1220:G:H21	19:S:54:GLY:CA	2.28	0.47
1:A:260:G:C4	1:A:261:U:C5	3.03	0.47
20:T:56:MET:HE1	20:T:85:MET:CG	2.40	0.47
18:R:25:THR:O	18:R:26:LEU:HD13	2.15	0.47
4:D:67:ILE:HG22	4:D:68:TYR:CD1	2.50	0.47
1:A:236:G:H1'	17:Q:4:LYS:NZ	2.30	0.47
1:A:1332:A:N3	1:A:1333:A:C8	2.82	0.47
1:A:1358:U:H3'	1:A:1359:C:H6	1.80	0.47
7:G:125:MET:HE2	7:G:125:MET:HB3	1.81	0.47
14:N:17:LYS:O	14:N:20:ALA:N	2.43	0.47
1:A:1223:C:P	19:S:78:ARG:HH21	2.37	0.47
9:I:96:LEU:O	9:I:102:LEU:HD11	2.15	0.47
1:A:628:G:H2'	1:A:629:G:O4'	2.14	0.47
2:B:38:GLY:O	2:B:39:ILE:HG13	2.14	0.47
1:A:404:U:O2'	1:A:405:U:H5'	2.14	0.47
1:A:538:G:OP1	12:L:113:ARG:HD3	2.14	0.47
1:A:998:G:C4	1:A:1044:A:C2	3.03	0.47
1:A:1126:U:C4	1:A:1127:G:C2	3.03	0.47
13:M:22:ILE:HG21	13:M:66:LEU:HD13	1.97	0.47
1:A:750:G:H1'	15:O:23:GLY:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:C:N4	1:A:1273:G:H1	2.09	0.47
15:O:15:PHE:CZ	15:O:85:LEU:HD21	2.49	0.47
9:I:86:VAL:HA	9:I:89:ASN:O	2.15	0.47
1:A:975:A:H5'	1:A:975:A:C8	2.50	0.47
1:A:167:G:C2'	1:A:168:G:H5'	2.45	0.47
5:E:43:LEU:HD21	5:E:132:ALA:HB1	1.97	0.47
19:S:62:ILE:HD12	19:S:66:MET:SD	2.55	0.47
1:A:91:C:O2'	1:A:92:C:H5'	2.14	0.47
21:U:7:ARG:HG2	21:U:21:TYR:CZ	2.50	0.47
1:A:890:G:O2'	1:A:906:G:O6	2.19	0.47
1:A:42:G:H1	1:A:400:C:H42	1.62	0.47
1:A:42:G:N2	1:A:43:C:O2	2.48	0.47
4:D:62:GLN:HA	4:D:62:GLN:OE1	2.15	0.47
8:H:8:ASP:O	8:H:12:ARG:HG3	2.15	0.47
19:S:42:PRO:HA	19:S:45:VAL:HG23	1.95	0.47
1:A:1303:C:N4	1:A:1304:G:C6	2.83	0.47
7:G:51:GLN:HG2	7:G:58:PRO:HD3	1.96	0.47
15:O:51:HIS:O	15:O:54:ARG:HB3	2.14	0.47
1:A:1288:A:H2'	1:A:1289:A:O4'	2.15	0.47
1:A:109:A:C4	1:A:327:A:C2	3.03	0.47
11:K:32:ILE:HD11	11:K:68:ALA:HB1	1.96	0.47
10:J:88:LEU:HD22	10:J:88:LEU:N	2.30	0.47
1:A:538:G:P	12:L:115:LYS:HB2	2.55	0.47
1:A:1327:C:OP1	21:U:20:LYS:N	2.41	0.47
15:O:31:LEU:O	15:O:35:ARG:HG3	2.14	0.47
15:O:5:LYS:CE	15:O:5:LYS:H	2.27	0.47
10:J:5:ARG:HG3	10:J:99:LYS:N	2.28	0.47
1:A:235:C:C2'	1:A:236:G:H5'	2.45	0.47
12:L:53:ARG:HG3	12:L:93:LEU:HD22	1.96	0.47
1:A:849:C:O2'	1:A:850:U:H5'	2.15	0.47
1:A:736:C:O2'	1:A:737:A:H5'	2.14	0.47
6:F:4:TYR:HB3	6:F:91:VAL:O	2.14	0.47
5:E:6:PHE:HE2	5:E:36:ASP:HB3	1.79	0.47
18:R:53:ARG:HH12	18:R:59:SER:CA	2.28	0.47
4:D:57:ARG:HH11	4:D:57:ARG:HG2	1.79	0.47
3:C:122:GLU:OE1	3:C:126:ARG:HG3	2.14	0.47
1:A:1118:C:OP1	9:I:104:ARG:NE	2.45	0.47
1:A:995:C:O2'	1:A:996:A:H5'	2.15	0.47
15:O:63:ARG:HH12	15:O:87:ILE:HG21	1.79	0.47
3:C:108:ASN:HD21	3:C:144:SER:HB3	1.80	0.47
1:A:665:A:H5'	1:A:666:G:OP2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:G:C2	1:A:267:C:H6	2.33	0.46
1:A:874:G:O2'	1:A:875:C:H5'	2.15	0.46
19:S:47:HIS:HB3	19:S:49:ILE:HD11	1.97	0.46
13:M:101:GLN:OE1	13:M:101:GLN:N	2.48	0.46
19:S:5:LEU:O	19:S:6:LYS:HD2	2.14	0.46
1:A:501:C:H2'	1:A:502:G:C8	2.51	0.46
1:A:504:C:H6	1:A:504:C:C5'	2.29	0.46
1:A:49:U:O2	1:A:362:G:H1'	2.15	0.46
15:O:15:PHE:HE2	15:O:84:LYS:HG2	1.80	0.46
1:A:674:G:H2'	1:A:675:A:C8	2.50	0.46
1:A:1057:G:H5''	3:C:154:SER:HB3	1.97	0.46
1:A:1128:C:O2'	1:A:1130:A:C8	2.68	0.46
1:A:667:G:H4'	15:O:51:HIS:CE1	2.50	0.46
8:H:137:VAL:HG12	8:H:138:TRP:N	2.28	0.46
1:A:91:C:H2'	1:A:92:C:H6	1.80	0.46
1:A:280:C:H4'	1:A:281:G:OP2	2.16	0.46
1:A:1003:G:O3'	1:A:1003(A):G:C8	2.68	0.46
4:D:38:TYR:CD1	4:D:45:GLN:HG3	2.49	0.46
12:L:27:LEU:C	12:L:29:GLY:N	2.65	0.46
18:R:38:GLU:HA	18:R:41:LYS:HE3	1.96	0.46
1:A:1103:C:H4'	2:B:108:ILE:HD11	1.97	0.46
7:G:151:TYR:O	7:G:153:HIS:N	2.49	0.46
16:P:26:ARG:HD3	16:P:26:ARG:HA	1.71	0.46
1:A:1347:G:C4	9:I:107:ARG:HD2	2.50	0.46
1:A:1339:A:H2'	1:A:1340:A:O4'	2.16	0.46
1:A:725:G:C4	1:A:726:C:C5	3.04	0.46
1:A:724:G:C2	1:A:725:G:C8	3.03	0.46
1:A:203:U:C6	1:A:203:U:H5'	2.50	0.46
1:A:180:U:C2'	1:A:181:G:H5'	2.46	0.46
1:A:294:U:O4	1:A:295:C:N4	2.48	0.46
20:T:8:ARG:HB3	20:T:9:ASN:H	1.60	0.46
20:T:104:LEU:HD23	20:T:104:LEU:HA	1.57	0.46
4:D:107:ARG:HH12	4:D:114:ARG:HH22	1.62	0.46
1:A:1044:A:C5	1:A:1045:C:H1'	2.50	0.46
1:A:258:G:O2'	1:A:259:G:H5'	2.15	0.46
20:T:60:GLU:HG3	20:T:81:LYS:CD	2.45	0.46
7:G:15:ASP:OD2	7:G:18:TYR:N	2.46	0.46
1:A:1486:G:C6	1:A:1487:G:C5	3.04	0.46
5:E:35:GLY:HA3	5:E:112:LEU:HD22	1.96	0.46
1:A:299:G:O6	1:A:300:A:N1	2.49	0.46
10:J:65:LEU:HD23	10:J:65:LEU:C	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:2:ALA:O	13:M:9:ILE:HA	2.15	0.46
1:A:257:G:H2'	1:A:258:G:O4'	2.16	0.46
11:K:16:SER:OG	11:K:79:SER:O	2.29	0.46
1:A:254:G:C2	1:A:255:G:C8	3.04	0.46
17:Q:22:LEU:HD12	17:Q:22:LEU:C	2.35	0.46
1:A:542:G:H2'	1:A:543:C:H6	1.79	0.46
20:T:20:LEU:H	20:T:20:LEU:HD12	1.81	0.46
1:A:8:A:H8	5:E:101:ILE:HG22	1.81	0.46
1:A:803:G:H2'	1:A:804:U:O4'	2.16	0.46
13:M:23:TYR:HB3	13:M:67:GLU:N	2.27	0.46
9:I:9:ARG:HA	9:I:76:ALA:HB1	1.97	0.46
18:R:31:LEU:O	18:R:69:THR:OG1	2.24	0.46
1:A:1236:A:H4'	1:A:1304:G:H4'	1.96	0.46
7:G:135:VAL:O	7:G:139:GLU:HG2	2.15	0.46
1:A:836:G:C6	1:A:851:G:C6	3.03	0.46
1:A:1035:A:N7	1:A:1037:C:C4	2.84	0.46
1:A:427:U:P	4:D:36:ARG:HH22	2.38	0.46
20:T:63:ILE:HD13	20:T:80:ARG:HB3	1.97	0.46
3:C:149:ALA:O	3:C:169:ALA:HB1	2.16	0.46
1:A:1130:A:OP1	1:A:1130:A:H8	1.98	0.46
3:C:120:VAL:HG12	3:C:121:ALA:N	2.30	0.46
16:P:55:ARG:O	16:P:58:TYR:HB3	2.16	0.46
8:H:64:LYS:O	8:H:65:TYR:HD2	1.97	0.46
20:T:16:HIS:CE1	20:T:20:LEU:HD11	2.51	0.46
11:K:21:ILE:HD13	11:K:94:ALA:CB	2.44	0.46
1:A:1014:A:C2	19:S:34:TRP:CE2	3.04	0.46
2:B:15:VAL:HG22	2:B:209:ARG:HH12	1.81	0.46
1:A:939:G:C6	1:A:940:C:N4	2.83	0.46
1:A:691:G:H2'	1:A:692:U:C6	2.50	0.46
19:S:74:PHE:N	19:S:74:PHE:CD1	2.83	0.46
1:A:756:C:H2'	1:A:757:U:O4'	2.16	0.46
15:O:70:LEU:C	15:O:72:ARG:N	2.65	0.46
1:A:1318:A:H4'	19:S:10:PHE:CD2	2.50	0.46
4:D:135:LEU:HA	4:D:136:PRO:HD3	1.64	0.46
12:L:83:VAL:CG2	12:L:100:ILE:HD13	2.39	0.46
1:A:190(E):U:C5	17:Q:72:ARG:NH2	2.83	0.46
2:B:9:GLU:OE1	2:B:12:GLU:N	2.42	0.46
12:L:25:PRO:CA	12:L:27:LEU:H	2.29	0.46
1:A:134:A:C6	1:A:135:C:N3	2.83	0.46
6:F:15:ASP:OD2	6:F:15:ASP:C	2.53	0.46
15:O:6:GLU:CD	15:O:6:GLU:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:6:ILE:HG23	10:J:98:ILE:HG12	1.97	0.46
13:M:7:VAL:HG23	13:M:67:GLU:HG2	1.98	0.46
1:A:184:G:N2	1:A:193:C:N3	2.52	0.46
7:G:20:ASP:OD2	7:G:22:LEU:N	2.47	0.46
12:L:45:PRO:HG2	12:L:49:ASN:O	2.16	0.46
9:I:11:LYS:O	9:I:12:GLU:HB2	2.14	0.46
4:D:153:ARG:NH1	4:D:180:GLY:O	2.49	0.46
1:A:922:G:H1	1:A:1395:C:H42	1.64	0.46
4:D:196:LEU:CD2	4:D:196:LEU:N	2.75	0.46
1:A:346:G:H2'	1:A:347:G:O4'	2.15	0.46
3:C:73:PRO:O	3:C:77:ILE:HG12	2.15	0.46
1:A:138:G:H1'	24:A:2627:HOH:O	2.14	0.46
9:I:90:PRO:O	9:I:93:ARG:HG3	2.16	0.46
11:K:15:ALA:O	11:K:77:MET:HA	2.15	0.46
16:P:73:LEU:HD23	16:P:73:LEU:HA	1.72	0.46
1:A:1127:G:H1	1:A:1145:C:N4	2.08	0.46
1:A:677:U:H3	1:A:713:G:N2	2.07	0.46
11:K:42:TRP:O	11:K:71:LYS:NZ	2.36	0.46
10:J:5:ARG:C	10:J:6:ILE:HG12	2.36	0.46
13:M:96:LEU:HB3	13:M:97:PRO:CD	2.41	0.46
1:A:1053:G:O5'	1:A:1054:C:H5'	2.16	0.46
2:B:34:ALA:O	2:B:41:ILE:HG12	2.15	0.46
8:H:119:LEU:HB2	8:H:123:GLU:HB2	1.97	0.46
4:D:174:LEU:C	4:D:186:LEU:HD21	2.37	0.46
10:J:8:LEU:O	10:J:69:ASN:HA	2.16	0.46
11:K:48:ILE:HD11	11:K:64:ALA:HA	1.97	0.46
6:F:67:MET:HB2	6:F:68:PRO:CD	2.45	0.46
17:Q:20:THR:CG2	17:Q:41:LYS:HG2	2.46	0.46
3:C:95:THR:O	3:C:97:LYS:N	2.48	0.46
1:A:793:U:O4	1:A:1517[A]:G:H5''	2.16	0.46
2:B:10:LEU:C	2:B:10:LEU:HD13	2.37	0.46
1:A:1221:G:C4	1:A:1222:G:C8	3.04	0.46
1:A:874:G:C2'	1:A:875:C:H5'	2.45	0.46
10:J:71:LEU:HA	10:J:71:LEU:HD12	1.64	0.46
15:O:4:THR:HA	15:O:5:LYS:NZ	2.31	0.46
15:O:4:THR:OG1	15:O:6:GLU:HG2	2.16	0.46
3:C:11:ARG:O	3:C:14:ILE:O	2.33	0.46
1:A:1308:U:H3'	13:M:99:ARG:HH21	1.80	0.46
5:E:108:ALA:O	5:E:112:LEU:HB2	2.16	0.46
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.15	0.46
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:G:OP2	1:A:351:G:O2'	2.34	0.46
1:A:24:U:O2'	1:A:25:C:H5'	2.16	0.46
2:B:165:VAL:HG13	2:B:166:ASP:N	2.31	0.46
1:A:910:C:H2'	1:A:911:U:H6	1.81	0.46
1:A:310:G:H2'	1:A:311:C:H6	1.80	0.46
1:A:1162:C:C4	1:A:1175:G:N2	2.84	0.45
11:K:40:ILE:HA	11:K:40:ILE:HD12	1.49	0.45
13:M:81:LEU:HD13	13:M:86:CYS:SG	2.55	0.45
17:Q:40:LYS:HE2	17:Q:42:TYR:CZ	2.51	0.45
1:A:758:G:C5	24:A:3191:HOH:O	2.67	0.45
8:H:121:ASP:OD2	8:H:122:ARG:HD2	2.16	0.45
13:M:39:ILE:HD12	13:M:55:ARG:HH21	1.80	0.45
16:P:4:ILE:HG13	16:P:66:PRO:HA	1.99	0.45
12:L:32:PHE:CB	12:L:84:LEU:HD21	2.45	0.45
8:H:34:GLU:HG2	8:H:118:VAL:HB	1.98	0.45
1:A:1511:G:H2'	1:A:1512:U:O4'	2.15	0.45
9:I:100:GLY:C	9:I:102:LEU:H	2.18	0.45
9:I:100:GLY:HA2	9:I:102:LEU:HD12	1.97	0.45
1:A:835:U:H3	1:A:851:G:H1	1.63	0.45
1:A:304:U:O4	24:A:3017:HOH:O	2.20	0.45
1:A:50:A:O5'	1:A:50:A:H2'	2.15	0.45
13:M:114:ARG:NE	24:M:202:HOH:O	2.49	0.45
1:A:1162:C:H2'	1:A:1163:C:H5'	1.98	0.45
1:A:1143:G:H2'	1:A:1144:G:C8	2.49	0.45
13:M:19:LEU:O	13:M:22:ILE:HD13	2.17	0.45
21:U:18:TYR:HA	21:U:22:ARG:HB3	1.99	0.45
9:I:89:ASN:HB3	9:I:92:TYR:HD1	1.75	0.45
18:R:87:ARG:NH1	18:R:87:ARG:HB2	2.31	0.45
6:F:97:PHE:HB3	18:R:32:ARG:HG3	1.97	0.45
3:C:188:LEU:HD21	3:C:195:VAL:CG2	2.44	0.45
1:A:1476:G:H2'	1:A:1477:C:C6	2.47	0.45
5:E:43:LEU:HD12	5:E:43:LEU:HA	1.47	0.45
19:S:34:TRP:CD1	19:S:52:TYR:CD2	3.04	0.45
1:A:1360:A:C2'	1:A:1361:G:H5'	2.47	0.45
1:A:622:A:C8	1:A:623:C:C5	3.04	0.45
1:A:183:G:H5'	1:A:183:G:H8	1.82	0.45
1:A:932:C:OP1	7:G:4:ARG:HB3	2.16	0.45
7:G:97:GLN:O	7:G:100:ALA:HB3	2.16	0.45
3:C:173:VAL:N	3:C:174:PRO:HD3	2.30	0.45
1:A:598:U:H4'	8:H:94:TYR:CD1	2.51	0.45
1:A:1005:A:C8	1:A:1025:U:O2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:ASN:N	8:H:15:ASN:ND2	2.58	0.45
18:R:41:LYS:HZ2	18:R:42:ARG:HH12	1.63	0.45
18:R:69:THR:O	18:R:72:ARG:N	2.49	0.45
5:E:76:ILE:HG22	5:E:78:HIS:O	2.16	0.45
7:G:92:SER:HB3	7:G:95:ARG:HB3	1.97	0.45
1:A:93:G:H2'	1:A:95:U:C6	2.51	0.45
1:A:539:A:N6	1:A:540:G:O6	2.49	0.45
13:M:27:LYS:O	13:M:30:ALA:HB3	2.16	0.45
8:H:82:HIS:C	8:H:82:HIS:ND1	2.70	0.45
17:Q:51:TYR:N	17:Q:51:TYR:CD1	2.85	0.45
1:A:827:U:H2'	1:A:870:U:O4	2.16	0.45
1:A:936:C:H2'	1:A:937:A:O4'	2.17	0.45
1:A:1092:A:N3	1:A:1183:A:N6	2.64	0.45
1:A:858:G:N7	24:A:3092:HOH:O	2.35	0.45
6:F:30:LEU:O	6:F:35:ALA:HB3	2.16	0.45
5:E:131:ILE:O	5:E:135:THR:OG1	2.35	0.45
1:A:1525:G:C8	1:A:1525:G:H5''	2.45	0.45
1:A:1409:C:C6	1:A:1409:C:C3'	2.99	0.45
1:A:544:G:OP1	4:D:59:ARG:NH2	2.48	0.45
17:Q:31:LEU:HG	17:Q:31:LEU:O	2.14	0.45
5:E:30:ALA:HB3	5:E:58:ALA:HB2	1.98	0.45
1:A:238:G:C6	1:A:239:U:C4	3.04	0.45
1:A:1216:G:H5''	14:N:5:ALA:CB	2.46	0.45
1:A:1112:C:C4	3:C:178:LEU:HD12	2.51	0.45
6:F:82:ARG:HB2	6:F:85:VAL:HG23	1.99	0.45
1:A:403:C:OP1	4:D:136:PRO:HD2	2.17	0.45
1:A:1379:G:N7	7:G:2:ALA:HB3	2.30	0.45
1:A:657:G:N2	1:A:750:G:C5	2.85	0.45
19:S:51:VAL:HG21	19:S:71:LEU:HD22	1.97	0.45
1:A:948:C:O2'	1:A:949:A:H5'	2.17	0.45
1:A:837:G:C2'	1:A:838:G:H5'	2.46	0.45
1:A:1466:C:H2'	1:A:1467:G:O4'	2.16	0.45
1:A:1050:G:H4'	24:A:2313:HOH:O	2.15	0.45
1:A:1250:A:H4'	9:I:68:GLY:N	2.31	0.45
1:A:1105:A:H1'	24:A:2416:HOH:O	2.16	0.45
1:A:1405:G:O2'	1:A:1406:U:H5'	2.17	0.45
1:A:1127:G:N2	1:A:1145:C:H42	2.15	0.45
1:A:265:G:O2'	1:A:266:G:H5'	2.17	0.45
1:A:826:C:H5'	8:H:12:ARG:NH2	2.32	0.45
7:G:5:ARG:HD3	7:G:7:ALA:HA	1.99	0.45
1:A:489:C:H2'	1:A:490:G:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:15:PHE:HB3	15:O:26:GLU:HB3	1.99	0.45
1:A:17:U:C2	1:A:18:C:C5	3.04	0.45
2:B:162:ILE:CG2	2:B:184:VAL:HG12	2.47	0.45
8:H:119:LEU:N	8:H:119:LEU:HD12	2.30	0.45
7:G:92:SER:HA	7:G:93:PRO:HD2	1.67	0.45
4:D:57:ARG:NH1	4:D:57:ARG:HG2	2.31	0.45
17:Q:8:GLY:O	17:Q:56:VAL:HA	2.17	0.45
19:S:15:LEU:HG	19:S:16:LEU:N	2.32	0.45
2:B:20:GLU:HA	2:B:23:ARG:NH1	2.31	0.45
7:G:45:ASP:O	7:G:48:LYS:HB2	2.16	0.45
1:A:474:G:O2'	1:A:475:G:H5'	2.17	0.45
7:G:32:ARG:HB3	7:G:33:ASP:OD2	2.16	0.45
4:D:8:VAL:HG11	4:D:21:LEU:CB	2.46	0.45
7:G:20:ASP:OD2	7:G:21:VAL:N	2.50	0.45
19:S:30:LEU:HB2	19:S:31:ILE:H	1.53	0.45
13:M:90:LEU:HD11	13:M:94:ARG:HE	1.81	0.45
6:F:46:ARG:HA	6:F:46:ARG:HD3	1.84	0.45
16:P:65:GLN:OE1	16:P:65:GLN:HA	2.15	0.45
1:A:911:U:H2'	1:A:911:U:O2	2.17	0.45
5:E:20:GLN:HG3	5:E:21:ALA:N	2.31	0.45
1:A:162:A:H5''	1:A:163:C:OP2	2.16	0.45
1:A:633:G:H2'	1:A:634:C:C6	2.51	0.45
2:B:179:LYS:HA	8:H:72:PRO:HD3	1.98	0.45
5:E:147:ASP:HA	5:E:150:ARG:HG2	1.99	0.45
4:D:36:ARG:CB	4:D:38:TYR:HE2	2.27	0.45
1:A:33:A:O2'	1:A:363:A:H1'	2.17	0.45
5:E:11:ILE:HA	5:E:11:ILE:HD13	1.38	0.45
3:C:9:GLY:HA2	3:C:12:LEU:HD12	1.99	0.45
1:A:1150:U:H2'	1:A:1151:A:H5'	1.99	0.45
1:A:236:G:OP1	17:Q:40:LYS:NZ	2.44	0.45
17:Q:38:ARG:NH1	17:Q:38:ARG:HG3	2.31	0.45
1:A:1480:G:C6	1:A:1481:U:C4	3.05	0.45
7:G:57:GLU:HA	7:G:58:PRO:HD3	1.85	0.45
1:A:867:G:H5''	1:A:867:G:C8	2.52	0.45
14:N:39:LEU:HA	14:N:39:LEU:HD23	1.43	0.45
1:A:194:C:OP1	20:T:61:SER:OG	2.34	0.45
1:A:579:G:H5'	1:A:728:A:C1'	2.37	0.45
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.69	0.45
1:A:657:G:C2	1:A:750:G:C5	3.04	0.45
2:B:152:PHE:CE1	2:B:155:LEU:HD12	2.52	0.45
6:F:42:GLU:HG3	6:F:61:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:G:H5'	6:F:87:ARG:NH1	2.32	0.45
5:E:64:ARG:NE	5:E:65:ASN:HB2	2.30	0.45
1:A:4:U:C6	1:A:4:U:H5'	2.48	0.45
7:G:70:LYS:HE3	7:G:96:GLN:HB3	1.99	0.45
17:Q:84:LEU:HG	17:Q:84:LEU:H	1.44	0.45
3:C:126:ARG:O	3:C:127:ARG:HB2	2.17	0.45
1:A:62:U:H2'	1:A:63:C:H6	1.81	0.45
1:A:179:A:H2'	1:A:180:U:H6	1.81	0.45
10:J:46:ARG:HB2	10:J:46:ARG:NH1	2.32	0.45
4:D:94:LEU:HD23	4:D:94:LEU:HA	1.70	0.45
13:M:11:ARG:HD3	13:M:45:VAL:HG11	1.99	0.45
13:M:4:ILE:HD12	13:M:8:GLU:HG3	1.98	0.45
1:A:253:U:OP1	17:Q:67:LYS:HE3	2.17	0.45
1:A:1381:U:C6	7:G:156:TRP:CZ2	3.05	0.45
1:A:447:G:H8	1:A:447:G:O5'	2.00	0.45
1:A:646:U:H2'	1:A:647:C:H6	1.82	0.45
8:H:63:LEU:HD12	8:H:63:LEU:HA	1.47	0.45
16:P:4:ILE:HG13	16:P:66:PRO:CA	2.47	0.45
6:F:78:GLU:O	6:F:81:ILE:HG13	2.16	0.45
2:B:24:TRP:HA	2:B:190:THR:O	2.17	0.45
1:A:622:A:H3'	1:A:623:C:H6	1.82	0.45
3:C:66:VAL:O	3:C:101:LEU:HD23	2.17	0.45
20:T:15:ARG:HA	20:T:18:GLN:HG3	1.99	0.45
17:Q:54:GLY:HA2	17:Q:85:VAL:HG21	1.99	0.45
1:A:868:C:O4'	1:A:873:A:C2	2.69	0.45
15:O:21:ASP:OD2	15:O:21:ASP:C	2.55	0.45
1:A:1523:G:H2'	1:A:1524:C:H5'	1.99	0.44
14:N:32:SER:CB	14:N:41:ARG:HB3	2.47	0.44
20:T:30:LYS:HB3	20:T:34:LYS:HE3	1.98	0.44
1:A:435:C:O2	1:A:436:C:C6	2.70	0.44
1:A:408:A:H2'	1:A:409:G:O5'	2.18	0.44
11:K:27:ASN:OD1	11:K:55:LYS:HB3	2.17	0.44
5:E:78:HIS:HA	8:H:105:ARG:HB2	1.99	0.44
8:H:26:VAL:HA	8:H:27:PRO:HD2	1.59	0.44
1:A:1417:G:HO2'	1:A:1418:A:H8	1.64	0.44
2:B:182:ILE:HA	2:B:183:PRO:HD3	1.79	0.44
16:P:36:ILE:HG21	16:P:36:ILE:HD13	1.59	0.44
1:A:665:A:H2'	1:A:732:C:O2	2.17	0.44
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.32	0.44
1:A:547:A:H4'	1:A:548:G:O5'	2.16	0.44
1:A:749:C:O2'	1:A:750:G:H5'	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:GLU:HG2	4:D:25:ARG:H	1.82	0.44
8:H:104:ARG:O	8:H:107:LEU:HB2	2.16	0.44
1:A:1256:A:H1'	1:A:1258:G:C6	2.52	0.44
1:A:1374:A:C4	1:A:1375:A:C8	3.05	0.44
20:T:39:LYS:O	20:T:42:GLN:HB3	2.17	0.44
1:A:370:C:O2'	1:A:371:G:H5'	2.17	0.44
1:A:1000:U:H5''	1:A:1000:U:H6	1.82	0.44
19:S:72:GLY:C	19:S:74:PHE:N	2.65	0.44
9:I:71:SER:O	9:I:74:ILE:HB	2.17	0.44
5:E:109:ILE:HD13	5:E:109:ILE:HG21	1.80	0.44
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.99	0.44
1:A:956:U:C2	1:A:1225:A:C2	3.05	0.44
2:B:213:LEU:HD12	2:B:213:LEU:HA	1.71	0.44
19:S:7:LYS:N	19:S:7:LYS:HD3	2.08	0.44
1:A:740:U:C2'	1:A:741:G:H5'	2.47	0.44
1:A:1127:G:C8	1:A:1127:G:C3'	3.01	0.44
1:A:182:U:OP2	1:A:182:U:H6	2.00	0.44
12:L:30:ALA:HA	12:L:31:PRO:HD2	1.38	0.44
1:A:429:U:H1'	1:A:430:A:H5''	2.00	0.44
1:A:1487:G:C2	1:A:1488:G:C8	3.05	0.44
1:A:1332:A:C2	1:A:1333:A:C5	3.05	0.44
2:B:162:ILE:HG21	2:B:184:VAL:HG12	1.99	0.44
1:A:1309:G:N2	1:A:1329:A:H1'	2.33	0.44
2:B:233:SER:HA	2:B:234:PRO:HD3	1.79	0.44
1:A:1179:A:H3'	1:A:1180:A:H8	1.82	0.44
2:B:164:VAL:HG13	2:B:186:ALA:HB2	1.99	0.44
17:Q:49:GLU:HG2	24:Q:305:HOH:O	2.17	0.44
1:A:990:C:N3	1:A:991:U:C5	2.86	0.44
17:Q:59:ILE:CD1	17:Q:73:VAL:HA	2.47	0.44
1:A:1124:G:H21	1:A:1126:U:H3	1.66	0.44
1:A:1152:A:H2'	1:A:1153:C:C6	2.53	0.44
1:A:254:G:N3	1:A:255:G:C8	2.85	0.44
1:A:1367:C:C2	1:A:1368:G:C8	3.05	0.44
19:S:18:LYS:HE2	19:S:18:LYS:HB3	1.68	0.44
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.99	0.44
16:P:23:ASP:OD2	16:P:25:ARG:HG3	2.17	0.44
8:H:49:GLU:HB3	8:H:60:ARG:HB3	1.98	0.44
15:O:38:ARG:O	15:O:39:LEU:C	2.54	0.44
4:D:145:GLU:OE1	4:D:182:LYS:HB2	2.17	0.44
1:A:90:U:H2'	1:A:91:C:H6	1.82	0.44
1:A:1213:A:H4'	1:A:1214:C:OP1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:14:ARG:HA	13:M:44:ARG:HA	1.99	0.44
1:A:200:G:H2'	1:A:201:C:O4'	2.17	0.44
1:A:840:C:O2'	1:A:841:U:OP2	2.31	0.44
2:B:193:ASP:OD1	2:B:194:PRO:HD2	2.18	0.44
16:P:18:ARG:O	16:P:20:VAL:HG23	2.18	0.44
3:C:69:HIS:N	3:C:69:HIS:ND1	2.66	0.44
10:J:3:LYS:HB2	10:J:3:LYS:NZ	2.32	0.44
12:L:102:ARG:HB3	12:L:102:ARG:HE	1.69	0.44
15:O:71:GLN:O	15:O:75:PRO:HG3	2.17	0.44
1:A:1517[B]:G:H2'	1:A:1518[B]:MA6:C8	2.48	0.44
4:D:58:LEU:O	4:D:58:LEU:HD12	2.18	0.44
18:R:38:GLU:O	18:R:41:LYS:HD2	2.17	0.44
5:E:110:LEU:HD13	5:E:118:ILE:HD13	1.98	0.44
1:A:7:G:C6	1:A:298:A:C2	3.05	0.44
1:A:1497:G:H2'	1:A:1498:UR3:H5'	2.00	0.44
1:A:42:G:C2	1:A:43:C:C2	3.05	0.44
6:F:95:GLU:OE2	6:F:96:PRO:HD3	2.17	0.44
2:B:231:GLU:HG3	2:B:232:PRO:HD2	2.00	0.44
18:R:36:ASN:O	18:R:40:LEU:HG	2.17	0.44
2:B:158:LEU:HD22	2:B:159:PRO:HD2	1.99	0.44
5:E:81:GLU:HB3	5:E:88:LYS:NZ	2.32	0.44
1:A:763:G:H2'	1:A:764:C:H6	1.82	0.44
2:B:187:LEU:HA	2:B:187:LEU:HD23	1.27	0.44
1:A:1003:G:H1'	1:A:1004:A:C2	2.53	0.44
1:A:260:G:C6	1:A:261:U:O4	2.71	0.44
1:A:362:G:OP1	12:L:61:THR:HG22	2.17	0.44
4:D:108:LEU:HA	4:D:108:LEU:HD23	1.46	0.44
1:A:937:A:H5''	1:A:938:A:OP2	2.18	0.44
1:A:1434:A:H2'	1:A:1435:G:O4'	2.18	0.44
18:R:73:ALA:CB	18:R:79:LEU:HD12	2.48	0.44
5:E:110:LEU:HA	5:E:110:LEU:HD23	1.78	0.44
1:A:1347:G:N9	9:I:107:ARG:HD2	2.32	0.44
3:C:156:ARG:H	3:C:163:ALA:HA	1.82	0.44
17:Q:91:ARG:O	17:Q:94:ASN:HB2	2.18	0.44
20:T:72:LEU:O	20:T:74:LYS:HG2	2.18	0.44
1:A:951:G:OP2	13:M:102:ARG:NH2	2.51	0.44
1:A:747:C:H3'	1:A:748:C:C5	2.53	0.44
2:B:74:LYS:HE3	2:B:74:LYS:HB3	1.53	0.44
2:B:154:LEU:H	2:B:154:LEU:HG	1.16	0.44
1:A:190(L):U:O2	20:T:105:SER:HB3	2.17	0.44
19:S:69:HIS:HB3	19:S:73:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:74:LEU:HA	17:Q:74:LEU:HD12	1.70	0.44
4:D:98:GLU:CD	4:D:103:ASN:HD21	2.21	0.44
14:N:9:LYS:O	14:N:9:LYS:HG2	2.17	0.44
10:J:91:PRO:HB3	10:J:94:VAL:HB	2.00	0.44
15:O:15:PHE:CE2	15:O:84:LYS:HG2	2.51	0.44
1:A:1502:A:C2	1:A:1504:G:C2	3.06	0.44
18:R:29:PHE:HZ	18:R:43:PHE:HE1	1.65	0.44
2:B:185:ILE:HG12	2:B:199:TYR:HB2	1.99	0.44
13:M:90:LEU:HD11	13:M:94:ARG:NE	2.32	0.44
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.52	0.44
1:A:199:G:O2'	1:A:200:G:H5'	2.17	0.44
1:A:686:U:O4	1:A:703:G:H1'	2.18	0.44
11:K:13:GLN:HA	11:K:13:GLN:OE1	2.18	0.44
1:A:455:C:H6	1:A:455:C:O5'	2.00	0.44
4:D:38:TYR:HB2	4:D:44:GLY:O	2.18	0.44
13:M:4:ILE:CD1	13:M:8:GLU:HG3	2.47	0.44
1:A:1053:G:N7	1:A:1200:C:H5'	2.32	0.44
6:F:41:GLU:HB3	6:F:43:LEU:CD1	2.47	0.44
13:M:107:ALA:HB3	13:M:111:LYS:HD3	1.98	0.44
8:H:34:GLU:O	8:H:35:ILE:C	2.56	0.44
1:A:950:U:H2'	1:A:951:G:H8	1.82	0.44
16:P:53:VAL:HG23	16:P:54:GLU:H	1.82	0.44
1:A:1193:G:N2	1:A:1194:U:C2	2.86	0.44
2:B:60:ASP:OD2	2:B:64:ARG:NH1	2.50	0.44
1:A:1136:U:H2'	1:A:1136:U:H6	1.60	0.44
1:A:401:C:H2'	1:A:402:G:H8	1.83	0.44
1:A:1499:A:H2'	1:A:1500:A:H8	1.82	0.44
1:A:1518[B]:MA6:O2'	1:A:1519[B]:MA6:OP1	2.35	0.44
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.91	0.44
1:A:1443:G:H5''	1:A:1446:A:O5'	2.18	0.44
1:A:523:A:N1	12:L:92:OTD:H6	2.33	0.44
1:A:160:A:H1'	1:A:344:A:C5	2.53	0.44
1:A:1276:G:H2'	1:A:1277:C:C6	2.53	0.44
1:A:1494:G:H3'	1:A:1494:G:OP1	2.17	0.44
1:A:318:G:N7	24:A:3048:HOH:O	2.50	0.44
18:R:58:LEU:HB3	18:R:62:GLU:HB3	2.00	0.44
1:A:1008:C:H2'	1:A:1009:G:H8	1.82	0.44
1:A:783:C:H2'	1:A:784:C:H6	1.83	0.44
6:F:29:ALA:C	6:F:32:ASN:H	2.21	0.44
1:A:289:G:P	24:A:2005:HOH:O	2.75	0.44
1:A:910:C:C4	1:A:911:U:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:110:VAL:CG2	12:L:120:TYR:HB3	2.47	0.44
1:A:1495:U:H2'	1:A:1496:C:C6	2.52	0.44
1:A:998:G:C2	1:A:999:C:N3	2.86	0.43
12:L:97:ARG:HB2	12:L:98:TYR:CE1	2.53	0.43
15:O:17:ARG:HD3	15:O:77:ARG:NH1	2.33	0.43
2:B:40:HIS:C	2:B:41:ILE:HD13	2.38	0.43
1:A:1504:G:C4'	1:A:1505:G:H5'	2.48	0.43
10:J:50:ILE:HD13	10:J:50:ILE:HA	1.57	0.43
18:R:66:LEU:HD12	18:R:66:LEU:HA	1.73	0.43
1:A:1141:C:H2'	1:A:1142:G:O4'	2.18	0.43
4:D:174:LEU:HD23	4:D:185:PHE:HA	2.00	0.43
8:H:23:SER:HB2	8:H:61:VAL:O	2.18	0.43
1:A:767:A:O5'	1:A:767:A:H8	2.01	0.43
1:A:991:U:O4	1:A:1212:U:O2'	2.28	0.43
2:B:151:GLY:C	2:B:153:ARG:H	2.21	0.43
1:A:1495:U:C4	1:A:1496:C:N4	2.85	0.43
2:B:196:LEU:HD23	2:B:196:LEU:N	2.33	0.43
9:I:19:LEU:HG	9:I:84:ALA:HB1	2.00	0.43
1:A:1034:G:C4	1:A:1035:A:C2	3.06	0.43
13:M:11:ARG:HD2	13:M:12:ASN:N	2.33	0.43
1:A:1451:A:H8	1:A:1451:A:O5'	2.01	0.43
2:B:31:TYR:CE2	2:B:202:PRO:HG3	2.53	0.43
9:I:63:ILE:HD12	9:I:77:ILE:HD13	2.00	0.43
1:A:1130:A:OP1	1:A:1130:A:C8	2.71	0.43
18:R:44:LEU:CD1	18:R:79:LEU:HD22	2.45	0.43
1:A:1231:G:H2'	1:A:1232:U:C6	2.47	0.43
7:G:101:LEU:HA	7:G:101:LEU:HD23	1.43	0.43
5:E:44:GLY:HA3	5:E:62:ALA:HB2	2.00	0.43
1:A:1481:U:H2'	1:A:1482:G:C8	2.52	0.43
5:E:79:GLU:CD	5:E:79:GLU:H	2.22	0.43
1:A:1014:A:H3'	1:A:1015:A:C8	2.54	0.43
1:A:1252:A:O5'	1:A:1252:A:H8	2.01	0.43
1:A:767:A:H3'	24:A:2041:HOH:O	2.17	0.43
2:B:134:GLU:O	2:B:137:ARG:N	2.50	0.43
5:E:41:VAL:O	5:E:67:VAL:HG23	2.19	0.43
12:L:117:ARG:HB3	12:L:122:THR:OG1	2.17	0.43
3:C:114:PRO:HD2	3:C:183:ASP:OD1	2.18	0.43
14:N:6:LEU:HD23	14:N:6:LEU:HA	1.46	0.43
19:S:6:LYS:HB2	19:S:7:LYS:HD3	2.00	0.43
1:A:403:C:O2'	1:A:404:U:H5'	2.18	0.43
13:M:57:ARG:HB3	13:M:58:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1378:C:C5	1:A:1379:G:N9	2.87	0.43
1:A:856:C:C2'	1:A:857:C:H5''	2.42	0.43
3:C:11:ARG:HB2	3:C:11:ARG:HE	1.32	0.43
19:S:41:VAL:CG1	19:S:42:PRO:HD2	2.44	0.43
14:N:15:LYS:HG2	14:N:16:PHE:CD1	2.53	0.43
1:A:1057:G:O3'	3:C:197:GLY:HA3	2.18	0.43
2:B:184:VAL:O	2:B:198:ASP:HB2	2.17	0.43
13:M:16:ASP:OD2	13:M:17:VAL:N	2.51	0.43
1:A:622:A:C8	1:A:623:C:C6	3.07	0.43
1:A:1343:G:H4'	9:I:122:ALA:HB3	2.00	0.43
13:M:31:LYS:HE3	13:M:35:GLU:OE1	2.18	0.43
1:A:595:G:H1'	1:A:596:C:H5	1.83	0.43
13:M:22:ILE:N	13:M:22:ILE:HD12	2.33	0.43
10:J:37:PRO:HA	10:J:71:LEU:O	2.18	0.43
1:A:1168:A:H2'	1:A:1169:A:O4'	2.19	0.43
5:E:106:PRO:O	5:E:110:LEU:HG	2.19	0.43
1:A:457:C:O2'	1:A:458:C:H5'	2.18	0.43
16:P:51:VAL:O	16:P:52:ASP:HB3	2.18	0.43
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.53	0.43
4:D:57:ARG:HA	4:D:202:LEU:HD12	2.00	0.43
2:B:18:GLY:HA2	2:B:42:ILE:HG12	1.99	0.43
1:A:439:A:C6	1:A:497:A:H1'	2.53	0.43
1:A:913:A:H4'	1:A:914:A:O5'	2.18	0.43
1:A:1214:C:H1'	24:A:2314:HOH:O	2.18	0.43
1:A:716:A:H1'	11:K:118:GLY:HA2	2.01	0.43
1:A:1541:PSU:H5''	1:A:1542:U:OP1	2.19	0.43
15:O:57:LEU:HD13	15:O:57:LEU:HA	1.56	0.43
16:P:68:ASP:OD1	16:P:68:ASP:N	2.50	0.43
7:G:12:LEU:H	7:G:12:LEU:HD12	1.83	0.43
10:J:70:ARG:NH1	10:J:70:ARG:HG3	2.33	0.43
15:O:70:LEU:O	15:O:71:GLN:C	2.57	0.43
10:J:34:VAL:O	10:J:36:GLY:N	2.52	0.43
1:A:1491:G:C8	1:A:1492:A:N7	2.86	0.43
4:D:35:ARG:HA	4:D:37:PRO:HD3	2.01	0.43
17:Q:62:SER:HB3	17:Q:72:ARG:NE	2.33	0.43
1:A:414:A:H3'	24:A:2633:HOH:O	2.18	0.43
1:A:1146:A:C5	1:A:1147:C:C5	3.05	0.43
7:G:47:CYS:HB3	7:G:58:PRO:HB2	2.00	0.43
1:A:1009:G:H1	1:A:1020:U:H3	1.67	0.43
1:A:609:A:H5''	1:A:610:G:OP2	2.17	0.43
1:A:150:C:H5''	24:A:3041:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:SER:O	3:C:115:LEU:N	2.51	0.43
11:K:19:ALA:O	11:K:82:VAL:HA	2.19	0.43
10:J:54:PHE:O	10:J:55:LYS:HG2	2.19	0.43
5:E:60:TYR:C	5:E:60:TYR:CD1	2.91	0.43
4:D:8:VAL:HG11	4:D:21:LEU:HB2	2.01	0.43
1:A:257:G:H1	1:A:269:C:N4	2.14	0.43
1:A:413:G:H8	1:A:428:G:N2	2.14	0.43
19:S:22:LEU:HD12	19:S:47:HIS:CE1	2.47	0.43
1:A:1368:G:H5'	9:I:112:LYS:HB3	2.00	0.43
1:A:1230:C:O2'	1:A:1231:G:H5'	2.17	0.43
5:E:98:THR:HB	5:E:117:ASP:HB3	2.00	0.43
8:H:122:ARG:HD2	8:H:122:ARG:H	1.84	0.43
4:D:180:GLY:O	4:D:181:MET:HB2	2.18	0.43
1:A:1278:U:H5''	1:A:1279:A:O4'	2.18	0.43
8:H:51:VAL:HG12	8:H:58:TYR:HB2	1.99	0.43
8:H:27:PRO:HA	8:H:58:TYR:HD2	1.81	0.43
3:C:40:ARG:HG3	3:C:40:ARG:NH1	2.33	0.43
4:D:146:ILE:HD12	4:D:146:ILE:N	2.33	0.43
1:A:1211:U:O2'	1:A:1213:A:C4	2.69	0.43
1:A:1198:G:H2'	1:A:1199:U:C6	2.53	0.43
1:A:278:G:C6	17:Q:95:TYR:CD2	3.07	0.43
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.82	0.43
4:D:11:LEU:O	4:D:12:CYS:C	2.56	0.43
1:A:1499:A:C1'	1:A:1520[A]:G:H5'	2.48	0.43
7:G:20:ASP:O	7:G:24:THR:HG23	2.19	0.43
1:A:1231:G:C5	1:A:1232:U:C5	3.07	0.43
1:A:1347:G:O2'	1:A:1348:U:OP2	2.36	0.43
1:A:1329:A:O2'	1:A:1330:U:H5'	2.18	0.43
2:B:84:GLU:OE2	2:B:235:SER:HB2	2.19	0.43
3:C:108:ASN:ND2	3:C:111:LEU:HD23	2.34	0.43
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	2.00	0.43
10:J:48:THR:HG23	10:J:62:HIS:ND1	2.34	0.43
9:I:22:GLY:HA3	9:I:60:ASP:N	2.33	0.43
5:E:90:VAL:O	5:E:91:LEU:HD23	2.19	0.43
1:A:1108:G:H2'	1:A:1109:C:H5'	2.00	0.43
7:G:68:ASN:ND2	7:G:128:ALA:HA	2.34	0.43
1:A:353:A:H5'	1:A:353:A:H8	1.84	0.43
5:E:139:LEU:N	5:E:139:LEU:HD23	2.34	0.43
3:C:32:LEU:O	3:C:35:GLU:N	2.52	0.43
3:C:23:TYR:HD1	10:J:11:PHE:CE2	2.36	0.43
1:A:1367:C:H5'	10:J:60:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:12:PRO:CB	6:F:57:GLN:HG3	2.49	0.43
1:A:160:A:OP1	1:A:160:A:H8	2.01	0.43
8:H:45:ILE:HG12	8:H:45:ILE:O	2.18	0.43
15:O:45:VAL:HA	15:O:47:LYS:HZ2	1.82	0.43
7:G:30:ILE:HG22	7:G:31:MET:N	2.33	0.43
1:A:1112:C:C6	1:A:1112:C:H3'	2.54	0.43
20:T:18:GLN:HA	20:T:21:LYS:HD2	2.01	0.43
17:Q:6:LEU:O	17:Q:58:GLU:HA	2.19	0.43
12:L:77:LEU:HD21	12:L:107:ALA:HA	2.01	0.43
4:D:14:ARG:HD3	4:D:14:ARG:HA	1.53	0.43
1:A:743:U:O2'	1:A:744:C:H5'	2.19	0.43
1:A:1516[B]:G:H2'	1:A:1517[B]:G:H5''	1.99	0.43
9:I:55:ALA:HB1	9:I:59:PHE:HB2	2.01	0.43
13:M:3:ARG:HB2	13:M:3:ARG:HH11	1.84	0.43
2:B:98:LEU:H	2:B:101:MET:HE3	1.84	0.43
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.30	0.43
1:A:924:C:O2'	1:A:1502:A:N6	2.52	0.43
1:A:723:U:H5'	1:A:724:G:OP2	2.19	0.43
1:A:708:C:O2'	1:A:709:G:H5'	2.19	0.43
17:Q:91:ARG:O	17:Q:94:ASN:N	2.48	0.43
2:B:36:ARG:O	2:B:39:ILE:HD12	2.19	0.43
1:A:187:C:N3	20:T:105:SER:OG	2.34	0.43
14:N:8:GLU:O	14:N:11:LYS:HB3	2.18	0.43
1:A:1023:G:N2	1:A:1024:G:H4'	2.34	0.43
4:D:58:LEU:C	4:D:58:LEU:HD12	2.39	0.43
1:A:1378:C:H3'	1:A:1379:G:H5''	2.01	0.43
12:L:47:LYS:HE2	12:L:92:0TD:H3	2.01	0.43
9:I:15:ALA:HA	9:I:65:VAL:HA	2.01	0.43
9:I:29:ASN:HD21	9:I:65:VAL:HG12	1.83	0.43
18:R:79:LEU:HD23	18:R:80:PRO:CD	2.47	0.43
1:A:1307:U:H2'	1:A:1308:U:O4'	2.18	0.43
1:A:1257:U:HO2'	1:A:1258:G:P	2.42	0.43
1:A:1079:G:C6	1:A:1080:A:N6	2.87	0.43
1:A:1514:C:H5'	24:A:2441:HOH:O	2.18	0.43
12:L:79:GLU:HB3	12:L:80:HIS:ND1	2.33	0.43
1:A:310:G:C5	1:A:311:C:C5	3.07	0.43
1:A:521:G:OP1	12:L:54:LYS:HE2	2.18	0.43
13:M:113:PRO:O	13:M:115:LYS:HE3	2.19	0.43
4:D:11:LEU:HD13	4:D:66:ARG:HG3	2.01	0.42
1:A:1030:C:N4	1:A:1031:G:N7	2.67	0.42
1:A:411:A:H1'	1:A:413:G:HO2'	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:LEU:HB2	2:B:101:MET:HE2	2.01	0.42
5:E:118:ILE:O	5:E:119:LEU:HD23	2.19	0.42
5:E:43:LEU:N	5:E:136:MET:HE1	2.33	0.42
12:L:111:LYS:HD2	12:L:112:ASP:N	2.33	0.42
2:B:129:GLU:CG	2:B:130:ARG:HH21	2.32	0.42
3:C:191:THR:HG21	3:C:193:TYR:CE2	2.54	0.42
4:D:94:LEU:H	4:D:94:LEU:HG	1.62	0.42
3:C:164:ARG:HG3	3:C:165:THR:N	2.33	0.42
8:H:1:MET:HG2	8:H:2:LEU:H	1.84	0.42
1:A:503:C:C2'	1:A:504:C:H5'	2.49	0.42
3:C:34:LEU:HD13	3:C:35:GLU:N	2.34	0.42
1:A:258:G:H2'	1:A:259:G:H8	1.84	0.42
4:D:58:LEU:HD12	4:D:62:GLN:HG2	2.00	0.42
18:R:81:PHE:HD2	18:R:81:PHE:HA	1.67	0.42
5:E:103:GLY:O	5:E:107:ARG:HB3	2.19	0.42
19:S:53:ASN:ND2	19:S:56:GLN:HG3	2.31	0.42
1:A:1030(C):G:N3	1:A:1030(D):A:N6	2.66	0.42
1:A:1068:G:N2	1:A:1191:A:N3	2.65	0.42
17:Q:76:LEU:HD23	17:Q:78:GLU:N	2.34	0.42
20:T:72:LEU:HD23	20:T:72:LEU:HA	1.75	0.42
1:A:951:G:C6	1:A:952:U:C5	3.07	0.42
1:A:768:A:P	24:A:2041:HOH:O	2.76	0.42
1:A:505:G:H2'	1:A:506:G:C8	2.54	0.42
1:A:1095:U:C4	1:A:1096:C:N4	2.87	0.42
1:A:558:G:H3'	1:A:559:A:H3'	2.00	0.42
1:A:851:G:C2'	1:A:852:G:H5'	2.50	0.42
17:Q:15:MET:CB	17:Q:18:THR:HB	2.50	0.42
1:A:380:G:N7	24:A:2369:HOH:O	2.37	0.42
3:C:170:GLN:HG2	3:C:171:GLY:N	2.35	0.42
20:T:49:ALA:O	20:T:53:LEU:HB2	2.19	0.42
1:A:500:G:C6	1:A:501:C:C4	3.08	0.42
1:A:1003(A):G:OP1	1:A:1003(A):G:H8	2.01	0.42
13:M:19:LEU:HA	13:M:22:ILE:HD13	2.02	0.42
2:B:10:LEU:C	2:B:12:GLU:N	2.73	0.42
7:G:5:ARG:HG3	7:G:7:ALA:CA	2.49	0.42
3:C:8:ILE:O	3:C:11:ARG:N	2.50	0.42
1:A:418:C:H2'	1:A:419:C:C6	2.46	0.42
1:A:1277:C:H1'	1:A:1282:C:H1'	2.02	0.42
18:R:53:ARG:HA	18:R:56:THR:HG23	2.02	0.42
1:A:15:G:H21	5:E:18:ARG:HA	1.84	0.42
4:D:155:LEU:HA	4:D:155:LEU:HD23	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:155:ARG:HA	7:G:155:ARG:HD3	1.59	0.42
2:B:71:VAL:O	2:B:164:VAL:HA	2.19	0.42
3:C:147:LYS:HB3	3:C:203:PHE:CD2	2.54	0.42
1:A:440:A:H5''	1:A:442:C:OP2	2.20	0.42
1:A:606:G:H1'	1:A:632:A:H61	1.84	0.42
16:P:42:ARG:H	16:P:42:ARG:HG2	1.62	0.42
16:P:74:LEU:HA	16:P:74:LEU:HD23	1.65	0.42
9:I:53:VAL:HG21	9:I:85:LEU:CD2	2.49	0.42
13:M:4:ILE:CG2	13:M:57:ARG:HA	2.50	0.42
1:A:872:A:C2	1:A:874:G:C6	3.08	0.42
6:F:19:LEU:O	6:F:19:LEU:HD12	2.19	0.42
15:O:27:VAL:HG12	15:O:31:LEU:HD13	2.00	0.42
15:O:15:PHE:HZ	15:O:85:LEU:HD21	1.83	0.42
7:G:149:ARG:HH11	7:G:149:ARG:HG2	1.84	0.42
1:A:350:G:C6	1:A:351:G:O6	2.72	0.42
17:Q:87:LYS:HZ3	17:Q:88:TYR:HB2	1.84	0.42
1:A:92:C:H2'	1:A:93:G:O4'	2.19	0.42
1:A:138:G:C2	1:A:226:G:N3	2.88	0.42
17:Q:47:PRO:HG2	17:Q:48:GLU:OE1	2.20	0.42
1:A:374:A:OP1	1:A:452:A:N6	2.41	0.42
1:A:642:A:H2'	1:A:643:C:C6	2.55	0.42
17:Q:5:VAL:HG23	17:Q:59:ILE:O	2.18	0.42
16:P:45:THR:HG22	16:P:46:PRO:HD2	2.02	0.42
1:A:357:G:C2	1:A:358:U:C5	3.07	0.42
9:I:62:TYR:C	9:I:62:TYR:CD1	2.92	0.42
1:A:404:U:C2'	1:A:405:U:H5'	2.50	0.42
1:A:1124:G:H1	1:A:1149:C:N4	2.13	0.42
1:A:265:G:C5	1:A:267:C:H5	2.37	0.42
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.35	0.42
14:N:42:ILE:O	14:N:46:GLU:HG3	2.19	0.42
1:A:428:G:H4'	1:A:429:U:O5'	2.20	0.42
15:O:74:ASP:OD2	15:O:77:ARG:HD3	2.18	0.42
17:Q:40:LYS:HD3	17:Q:42:TYR:OH	2.19	0.42
9:I:65:VAL:O	9:I:66:ARG:HB2	2.20	0.42
10:J:21:GLN:O	10:J:24:VAL:HG12	2.19	0.42
17:Q:84:LEU:HD23	17:Q:84:LEU:HA	1.76	0.42
1:A:623:C:O2	1:A:623:C:H2'	2.19	0.42
2:B:74:LYS:O	2:B:78:GLN:HG3	2.19	0.42
1:A:1342:C:O2'	1:A:1343:G:H5'	2.18	0.42
5:E:68:GLU:OE1	5:E:68:GLU:N	2.53	0.42
12:L:127:GLU:N	12:L:127:GLU:CD	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4:TYR:CD1	4:D:11:LEU:HD11	2.55	0.42
19:S:80:TYR:CD1	19:S:81:ARG:N	2.87	0.42
1:A:1492:A:H2'	1:A:1493:A:O5'	2.19	0.42
1:A:57:G:H2'	1:A:58:C:H6	1.85	0.42
5:E:35:GLY:HA3	5:E:112:LEU:O	2.20	0.42
1:A:773:G:H1	1:A:806:C:N4	2.14	0.42
5:E:18:ARG:O	5:E:18:ARG:HG2	2.19	0.42
16:P:56:ALA:O	16:P:60:LEU:HG	2.19	0.42
2:B:15:VAL:HG22	2:B:209:ARG:NH1	2.34	0.42
1:A:821:G:O2'	1:A:822:C:H5'	2.19	0.42
1:A:303:A:N6	24:A:3017:HOH:O	2.52	0.42
1:A:35:G:O2'	12:L:118:SER:O	2.33	0.42
11:K:84:VAL:HG11	11:K:91:ARG:HH11	1.84	0.42
8:H:44:PHE:O	8:H:80:ILE:HD11	2.20	0.42
1:A:588:G:HO2'	1:A:589:C:P	2.42	0.42
1:A:459:G:H8	1:A:459:G:O5'	2.02	0.42
1:A:283:C:O5'	1:A:283:C:H6	2.02	0.42
2:B:51:LEU:O	2:B:51:LEU:HD23	2.19	0.42
1:A:1327:C:H2'	1:A:1328:C:C6	2.54	0.42
20:T:33:ILE:O	20:T:34:LYS:C	2.58	0.42
8:H:92:ARG:O	8:H:93:VAL:HG13	2.20	0.42
1:A:128:G:O2'	1:A:129:U:H5'	2.19	0.42
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.19	0.42
1:A:693:G:H2'	1:A:694:A:C8	2.54	0.42
1:A:694:A:H2'	1:A:695:A:O4'	2.19	0.42
19:S:28:LYS:NZ	19:S:31:ILE:HA	2.35	0.42
1:A:671:G:H2'	1:A:672:U:C6	2.55	0.42
1:A:737:A:H2'	1:A:738:C:O4'	2.19	0.42
10:J:63:PHE:CD2	14:N:58:LYS:HA	2.55	0.42
2:B:19:HIS:CE1	2:B:206:ASP:HB2	2.55	0.42
1:A:610:G:C5	1:A:611:A:N7	2.88	0.42
1:A:1207:2MG:HM23	1:A:1208:C:C2	2.55	0.42
1:A:643:C:H5'	8:H:31:PHE:CD1	2.54	0.42
1:A:1059:C:OP1	3:C:199:LYS:NZ	2.53	0.42
1:A:161:A:H2'	1:A:162:A:C8	2.54	0.42
16:P:8:ARG:HG2	16:P:9:PHE:N	2.33	0.42
5:E:48:ALA:HB1	5:E:49:PRO:HD2	2.02	0.42
10:J:14:LYS:HE2	10:J:14:LYS:HB3	1.71	0.42
10:J:16:LEU:HD22	10:J:16:LEU:HA	1.90	0.42
15:O:70:LEU:HD13	15:O:70:LEU:HA	1.62	0.42
4:D:104:VAL:O	4:D:108:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:40:CYS:SG	14:N:42:ILE:HB	2.60	0.42
1:A:128:G:OP1	17:Q:2:PRO:HD2	2.20	0.42
1:A:581:G:C8	24:A:3191:HOH:O	2.71	0.42
1:A:582:U:O2'	1:A:583:A:H5'	2.20	0.42
1:A:457:C:H2'	1:A:458:C:C6	2.47	0.42
1:A:1418:A:H5''	1:A:1419:G:OP2	2.20	0.42
1:A:725:G:C5	1:A:726:C:C5	3.08	0.42
1:A:1125:U:H3'	24:A:2985:HOH:O	2.18	0.42
7:G:143:ARG:O	7:G:147:ALA:HB2	2.20	0.42
1:A:393:A:C2	1:A:394:G:C8	3.08	0.42
16:P:28:ARG:NH1	16:P:29:ASP:OD2	2.53	0.42
12:L:59:ARG:HD3	12:L:65:GLU:OE1	2.20	0.42
9:I:41:VAL:C	9:I:43:ALA:H	2.23	0.42
2:B:175:ARG:O	2:B:175:ARG:HG2	2.20	0.42
20:T:65:LYS:O	20:T:68:LYS:HB2	2.19	0.42
1:A:519:C:H2'	1:A:520:A:C8	2.55	0.42
4:D:4:TYR:CE1	4:D:11:LEU:HD11	2.54	0.42
20:T:93:GLU:CD	20:T:93:GLU:N	2.70	0.42
1:A:1517[A]:G:C6	1:A:1518[A]:MA6:C5	3.03	0.42
6:F:14:LEU:HD22	6:F:18:GLN:HB3	2.02	0.42
19:S:51:VAL:O	19:S:58:VAL:HG23	2.20	0.42
1:A:1008:C:H2'	1:A:1009:G:C8	2.54	0.42
2:B:178:ARG:HH21	8:H:74:PRO:HG3	1.84	0.42
7:G:144:MET:O	7:G:147:ALA:HB3	2.20	0.42
2:B:139:LYS:HG2	2:B:140:HIS:N	2.34	0.42
2:B:24:TRP:CH2	2:B:26:PRO:HA	2.55	0.42
2:B:165:VAL:CG1	2:B:166:ASP:N	2.82	0.42
1:A:1234:C:O2'	1:A:1235:U:H5'	2.20	0.42
3:C:42:LEU:O	3:C:42:LEU:HG	2.13	0.42
5:E:123:LEU:HD23	5:E:123:LEU:HA	1.62	0.42
4:D:8:VAL:O	4:D:11:LEU:N	2.45	0.42
16:P:74:LEU:O	16:P:77:ALA:HB3	2.19	0.42
18:R:37:VAL:O	18:R:38:GLU:C	2.57	0.42
13:M:96:LEU:O	13:M:110:ARG:NH1	2.53	0.42
1:A:252:U:H2'	1:A:253:U:C6	2.54	0.42
1:A:1451:A:H2'	1:A:1453:G:O6	2.19	0.42
2:B:41:ILE:HD13	2:B:41:ILE:N	2.34	0.42
7:G:85:TYR:CD1	7:G:154:TYR:HE1	2.36	0.42
9:I:28:VAL:HG12	9:I:29:ASN:OD1	2.19	0.42
1:A:1057:G:H4'	3:C:197:GLY:N	2.30	0.42
1:A:1129:C:H4'	1:A:1130:A:OP1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:80:VAL:CG2	11:K:103:LEU:HB3	2.49	0.42
1:A:449:C:C5	1:A:450:G:C5	3.08	0.42
1:A:1239:A:H62	1:A:1299:A:N6	2.18	0.42
4:D:120:LEU:HB3	4:D:126:ILE:HD11	2.01	0.42
4:D:103:ASN:OD1	4:D:114:ARG:NH2	2.51	0.41
3:C:34:LEU:HD21	3:C:38:ARG:HE	1.84	0.41
3:C:11:ARG:NH1	3:C:177:THR:O	2.53	0.41
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.53	0.41
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.80	0.41
1:A:235:C:O2'	1:A:236:G:H5'	2.20	0.41
3:C:121:ALA:O	3:C:124:ILE:HB	2.19	0.41
8:H:110:ALA:H	8:H:121:ASP:CG	2.23	0.41
1:A:167:G:C2	1:A:168:G:C8	3.08	0.41
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.84	0.41
19:S:34:TRP:HD1	19:S:52:TYR:CD2	2.38	0.41
3:C:142:MET:HA	3:C:146:ALA:HB3	2.02	0.41
9:I:10:ARG:HD3	9:I:75:ASP:CB	2.49	0.41
1:A:183:G:O2'	1:A:224:C:O2'	2.21	0.41
4:D:117:ALA:HA	4:D:120:LEU:HB2	2.01	0.41
5:E:81:GLU:O	5:E:82:VAL:HG23	2.20	0.41
2:B:134:GLU:OE1	2:B:137:ARG:HD2	2.20	0.41
4:D:23:GLY:HA3	4:D:112:VAL:HG12	2.02	0.41
1:A:770:C:H1'	1:A:899:C:H42	1.85	0.41
7:G:52:GLU:OE2	7:G:53:LYS:HG2	2.19	0.41
18:R:21:LYS:HD3	18:R:21:LYS:HA	1.61	0.41
1:A:1228:C:H4'	13:M:116:THR:HA	2.01	0.41
2:B:33:TYR:O	2:B:34:ALA:HB2	2.20	0.41
1:A:184:G:H1	1:A:193:C:N4	2.13	0.41
1:A:317:G:C2'	1:A:318:G:H5'	2.50	0.41
2:B:80:ILE:H	2:B:80:ILE:HD12	1.85	0.41
2:B:127:ILE:H	2:B:127:ILE:HG13	1.51	0.41
3:C:147:LYS:HE2	3:C:203:PHE:CE2	2.55	0.41
1:A:1239:A:H4'	1:A:1240:U:H5''	2.02	0.41
1:A:194:C:H5''	20:T:65:LYS:HG3	2.02	0.41
2:B:153:ARG:HB3	2:B:154:LEU:HD23	2.01	0.41
1:A:1248:A:O2'	9:I:70:LYS:NZ	2.51	0.41
13:M:88:ARG:HH11	13:M:88:ARG:HD3	1.71	0.41
1:A:1316:G:N2	1:A:1319:A:OP2	2.53	0.41
1:A:663:A:O2'	1:A:664:G:H5'	2.20	0.41
6:F:3:ARG:C	6:F:93:SER:HB2	2.41	0.41
10:J:5:ARG:H	10:J:5:ARG:HG2	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:C:O2	1:A:1196:U:C5	2.74	0.41
2:B:43:ASP:OD1	2:B:45:GLN:HG2	2.20	0.41
1:A:1505:G:H3'	1:A:1505:G:C8	2.55	0.41
1:A:758:G:O6	24:A:3191:HOH:O	2.22	0.41
2:B:112:VAL:O	2:B:115:LEU:HB3	2.21	0.41
11:K:51:LYS:H	11:K:54:ARG:HH21	1.68	0.41
1:A:682:G:H1	1:A:708:C:N4	2.17	0.41
1:A:684:A:N3	11:K:39:PRO:HD2	2.35	0.41
17:Q:57:VAL:HA	17:Q:77:VAL:HG23	2.02	0.41
1:A:707:C:H4'	11:K:20:TYR:CD2	2.55	0.41
1:A:314:C:O2'	1:A:315:A:H5'	2.20	0.41
5:E:150:ARG:HE	5:E:150:ARG:HB2	1.61	0.41
1:A:990:C:O2'	1:A:991:U:H5'	2.20	0.41
1:A:655:A:H2'	1:A:656:C:O4'	2.21	0.41
18:R:22:VAL:O	18:R:22:VAL:HG12	2.20	0.41
3:C:35:GLU:HA	3:C:38:ARG:HD2	2.03	0.41
1:A:1033:G:C8	1:A:1034:G:C8	3.09	0.41
20:T:78:ALA:O	20:T:79:ARG:C	2.57	0.41
1:A:363:A:N6	12:L:28:LYS:HD3	2.35	0.41
4:D:30:LYS:C	4:D:32:ALA:H	2.03	0.41
10:J:5:ARG:CD	10:J:99:LYS:HB2	2.44	0.41
1:A:1323:G:C6	1:A:1324:A:C6	3.09	0.41
18:R:29:PHE:HZ	18:R:43:PHE:CE1	2.39	0.41
1:A:1169:A:C5	1:A:1171:G:H1'	2.56	0.41
3:C:198:VAL:HG12	3:C:198:VAL:O	2.20	0.41
1:A:706:A:H1'	11:K:29:ILE:HD11	2.01	0.41
1:A:15:G:H5'	1:A:1396:A:O2'	2.20	0.41
1:A:1190:G:H5'	3:C:176:HIS:NE2	2.35	0.41
1:A:557:G:H2'	1:A:558:G:O4'	2.20	0.41
11:K:19:ALA:HB2	11:K:32:ILE:HG23	2.03	0.41
4:D:128:VAL:O	4:D:129:ASN:HB2	2.21	0.41
1:A:124:G:C5	1:A:125:U:C5	3.09	0.41
1:A:591:U:OP1	8:H:30:ARG:NE	2.53	0.41
1:A:407:G:O2'	4:D:116:GLN:HG3	2.21	0.41
7:G:117:ALA:CA	7:G:120:ILE:HG12	2.36	0.41
2:B:43:ASP:CG	2:B:46:LYS:HG2	2.40	0.41
1:A:127:G:H4'	17:Q:2:PRO:HG2	2.02	0.41
1:A:737:A:H8	1:A:737:A:O5'	2.03	0.41
1:A:1349:A:OP1	9:I:118:LYS:HG3	2.20	0.41
1:A:975:A:H4'	1:A:976:G:C5'	2.51	0.41
16:P:3:LYS:HA	16:P:65:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:58:MET:HG2	15:O:58:MET:H	1.59	0.41
16:P:80:PHE:CD1	16:P:80:PHE:N	2.88	0.41
1:A:179:A:H2'	1:A:180:U:C6	2.55	0.41
1:A:338:A:H2'	1:A:339:C:O4'	2.19	0.41
1:A:158:G:H2'	1:A:159:G:H5'	2.02	0.41
1:A:486:U:H2'	1:A:487:A:H8	1.83	0.41
10:J:64:GLU:HG2	14:N:59:ALA:HB2	2.02	0.41
1:A:509:A:H3'	1:A:509:A:C8	2.55	0.41
2:B:114:ARG:NH1	2:B:117:GLU:OE2	2.53	0.41
19:S:3:ARG:HG2	19:S:4:SER:H	1.84	0.41
1:A:662:G:H2'	1:A:663:A:H8	1.79	0.41
3:C:35:GLU:OE1	3:C:59:ARG:NH1	2.45	0.41
1:A:130:A:OP2	1:A:190(E):U:O2'	2.28	0.41
1:A:981:U:C2	1:A:982:U:C5	3.09	0.41
1:A:251:G:H4'	1:A:252:U:C5'	2.49	0.41
1:A:253:U:H2'	1:A:254:G:C8	2.54	0.41
7:G:111:ARG:NH2	7:G:123:GLU:HA	2.26	0.41
3:C:188:LEU:C	3:C:188:LEU:HD13	2.40	0.41
16:P:23:ASP:O	16:P:26:ARG:HB2	2.20	0.41
1:A:1350:A:H2'	1:A:1351:U:H6	1.85	0.41
11:K:54:ARG:HB2	11:K:54:ARG:CZ	2.44	0.41
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.55	0.41
8:H:97:VAL:O	8:H:100:ILE:HD12	2.20	0.41
4:D:190:ASP:OD2	4:D:192:GLU:N	2.48	0.41
19:S:32:LYS:HZ3	19:S:32:LYS:H	1.66	0.41
3:C:148:GLY:HA3	3:C:172:ARG:H	1.85	0.41
3:C:108:ASN:HA	3:C:109:PRO:HD2	1.89	0.41
10:J:48:THR:HG23	10:J:62:HIS:CE1	2.55	0.41
14:N:11:LYS:O	14:N:13:THR:OG1	2.27	0.41
1:A:229:U:H2'	1:A:230:G:C8	2.55	0.41
3:C:123:GLN:HB3	3:C:128:PHE:HD1	1.85	0.41
1:A:16:A:N1	1:A:919:A:H2	2.18	0.41
1:A:503:C:H2'	1:A:504:C:H5'	2.02	0.41
1:A:538:G:OP2	12:L:115:LYS:HB2	2.21	0.41
1:A:1406:U:H5'	1:A:1518[B]:MA6:O2'	2.20	0.41
1:A:1427:U:H2'	1:A:1428:A:H8	1.84	0.41
14:N:12:ARG:HD3	14:N:12:ARG:HA	1.65	0.41
4:D:100:ARG:O	4:D:104:VAL:HG23	2.21	0.41
1:A:414:A:N3	1:A:415:A:C8	2.89	0.41
2:B:43:ASP:OD1	2:B:44:LEU:N	2.53	0.41
1:A:926:G:H5'	1:A:927:G:O5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:9:ARG:HA	9:I:76:ALA:CB	2.51	0.41
6:F:2:ARG:HB3	6:F:92:LYS:HE3	2.03	0.41
1:A:1238:A:N7	1:A:1303:C:H1'	2.35	0.41
5:E:101:ILE:HG23	5:E:101:ILE:HD12	1.73	0.41
1:A:892:A:C2	1:A:893:C:C2	3.09	0.41
3:C:47:LEU:HD12	3:C:83:ARG:HH22	1.86	0.41
1:A:698:G:N2	24:A:3116:HOH:O	2.38	0.41
1:A:1346:A:C5	7:G:10:ARG:CZ	3.04	0.41
16:P:38:TYR:O	16:P:49:LEU:HD12	2.20	0.41
2:B:240:GLN:OE1	2:B:240:GLN:N	2.53	0.41
14:N:53:LEU:HD23	14:N:53:LEU:HA	1.67	0.41
9:I:85:LEU:HA	9:I:85:LEU:HD12	1.82	0.41
1:A:986:A:H3'	1:A:987:G:H8	1.85	0.41
1:A:986:A:N6	1:A:987:G:C6	2.89	0.41
7:G:108:ALA:O	7:G:111:ARG:HB2	2.20	0.41
1:A:758:G:O2'	1:A:759:A:O5'	2.31	0.41
1:A:1532:U:C6	1:A:1532:U:C3'	3.03	0.41
5:E:17:ALA:HB2	5:E:26:PHE:CD2	2.55	0.41
6:F:80:ARG:NH2	6:F:88:VAL:O	2.53	0.41
7:G:106:GLN:O	7:G:110:GLN:HG3	2.21	0.41
10:J:55:LYS:HG3	10:J:56:HIS:N	2.34	0.41
4:D:127:THR:HA	4:D:131:ARG:O	2.20	0.41
12:L:21:LYS:H	12:L:21:LYS:HG2	1.52	0.41
4:D:12:CYS:SG	4:D:19:LEU:O	2.79	0.41
1:A:742:G:H2'	1:A:743:U:O4'	2.21	0.41
1:A:1492:A:C8	1:A:1492:A:C3'	3.04	0.41
1:A:1518[B]:MA6:O2'	1:A:1519[B]:MA6:P	2.79	0.41
13:M:3:ARG:HA	13:M:8:GLU:HG2	2.03	0.41
2:B:97:TRP:CD2	2:B:173:ALA:HB2	2.55	0.41
18:R:37:VAL:O	18:R:41:LYS:HG3	2.21	0.41
3:C:14:ILE:HB	3:C:15:THR:CG2	2.50	0.41
1:A:254:G:C4	1:A:255:G:C8	3.09	0.41
2:B:44:LEU:HA	2:B:47:THR:HB	2.02	0.41
10:J:11:PHE:CD1	14:N:55:GLY:HA3	2.56	0.41
9:I:15:ALA:HB2	9:I:65:VAL:HG23	2.03	0.41
6:F:69:GLU:O	6:F:72:VAL:HG23	2.20	0.41
2:B:162:ILE:HD13	2:B:162:ILE:HA	1.57	0.41
1:A:417:C:H2'	1:A:418:C:H6	1.85	0.41
2:B:59:GLU:HB2	2:B:221:LEU:HD11	2.03	0.41
12:L:6:THR:HG23	12:L:9:GLN:OE1	2.20	0.41
7:G:70:LYS:HA	7:G:71:PRO:HD2	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:88:TYR:CG	9:I:88:TYR:O	2.74	0.41
1:A:1016:A:H2'	1:A:1017:G:O4'	2.21	0.41
2:B:25:ASN:O	2:B:26:PRO:C	2.56	0.41
1:A:450:G:O5'	1:A:450:G:H8	2.04	0.41
1:A:73:C:O2'	1:A:74:C:H5'	2.21	0.41
1:A:353:A:H5'	1:A:353:A:C8	2.56	0.41
1:A:770:C:N4	24:A:2450:HOH:O	2.37	0.41
4:D:78:LEU:HB3	4:D:93:PHE:HE2	1.85	0.41
1:A:1253:G:H1'	1:A:1355:G:O2'	2.21	0.41
1:A:460:A:O2'	1:A:461:C:H5'	2.20	0.41
1:A:191:G:N2	20:T:103:GLY:O	2.53	0.41
12:L:17:LYS:HG2	12:L:17:LYS:H	1.52	0.41
4:D:97:LEU:HD23	4:D:97:LEU:HA	1.76	0.41
4:D:110:PHE:CD1	4:D:110:PHE:N	2.86	0.41
4:D:11:LEU:HD13	4:D:66:ARG:CG	2.51	0.41
4:D:38:TYR:N	4:D:38:TYR:CD2	2.85	0.41
8:H:11:THR:O	8:H:12:ARG:C	2.57	0.41
7:G:5:ARG:NH1	7:G:6:ARG:HB2	2.36	0.41
13:M:23:TYR:HB2	13:M:67:GLU:OE1	2.20	0.41
13:M:67:GLU:HB3	13:M:68:GLY:H	1.50	0.41
1:A:1501:C:H5''	1:A:1502:A:OP2	2.20	0.41
1:A:184:G:H8	1:A:184:G:O5'	2.04	0.41
2:B:69:LEU:HA	2:B:69:LEU:HD23	1.86	0.41
8:H:107:LEU:HD23	8:H:107:LEU:HA	1.77	0.41
5:E:118:ILE:HG21	5:E:118:ILE:HD13	1.78	0.41
1:A:1347:G:C6	9:I:107:ARG:NH1	2.89	0.41
2:B:129:GLU:H	2:B:129:GLU:HG2	1.64	0.41
19:S:62:ILE:HD12	19:S:62:ILE:HA	1.73	0.41
1:A:138:G:N2	1:A:226:G:H1'	2.36	0.41
16:P:54:GLU:OE1	16:P:54:GLU:HA	2.21	0.41
18:R:76:LEU:HD23	18:R:76:LEU:HA	1.94	0.41
3:C:111:LEU:HD21	3:C:144:SER:O	2.21	0.41
1:A:727:G:C6	1:A:731:G:C6	3.09	0.41
7:G:148:ASN:C	7:G:150:ALA:N	2.74	0.41
2:B:90:MET:HA	2:B:91:PRO:HD3	1.86	0.41
1:A:714:G:N3	1:A:777:A:H1'	2.36	0.41
1:A:811:C:H4'	1:A:900:A:N6	2.36	0.41
5:E:63:ARG:HE	5:E:63:ARG:HB2	1.20	0.41
19:S:10:PHE:CE2	19:S:37:ARG:HD3	2.53	0.40
1:A:1499:A:O4'	1:A:1520[A]:G:H5'	2.21	0.40
1:A:1005:A:H5'	1:A:1037:C:O2'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:A:C2	1:A:1220:G:C2	3.10	0.40
1:A:826:C:H2'	1:A:827:U:C6	2.54	0.40
20:T:33:ILE:CD1	20:T:63:ILE:HA	2.50	0.40
19:S:22:LEU:CD1	19:S:27:GLU:HA	2.49	0.40
19:S:58:VAL:O	19:S:60:VAL:HG23	2.21	0.40
1:A:1442:G:C6	1:A:1446:A:C6	3.09	0.40
15:O:50:HIS:O	15:O:53:HIS:HB3	2.21	0.40
1:A:1371:G:OP1	9:I:12:GLU:HB2	2.22	0.40
3:C:188:LEU:CD1	3:C:190:ARG:HG2	2.51	0.40
1:A:1276:G:C4	1:A:1277:C:C5	3.09	0.40
1:A:1408:A:C6	1:A:1494:G:N2	2.89	0.40
2:B:208:ILE:HG22	2:B:209:ARG:N	2.35	0.40
1:A:860:A:H2'	1:A:861:G:O4'	2.21	0.40
1:A:1466:C:C5	1:A:1467:G:C5	3.09	0.40
2:B:60:ASP:OD2	2:B:64:ARG:HD2	2.21	0.40
1:A:567:G:H2'	1:A:568:G:O4'	2.21	0.40
4:D:163:GLU:O	4:D:166:LYS:HB2	2.20	0.40
6:F:98:LEU:HA	6:F:98:LEU:HD23	1.84	0.40
1:A:1463:C:O5'	1:A:1463:C:H6	2.03	0.40
10:J:32:ALA:O	10:J:34:VAL:HG23	2.21	0.40
1:A:937:A:H1'	1:A:1379:G:H22	1.86	0.40
3:C:11:ARG:HH11	3:C:180:ALA:HB3	1.86	0.40
7:G:78:ARG:HG3	7:G:156:TRP:HE3	1.86	0.40
20:T:50:GLU:CB	20:T:99:LEU:HD13	2.50	0.40
1:A:1217:C:C2	1:A:1218:C:C5	3.08	0.40
2:B:19:HIS:NE2	2:B:206:ASP:HB2	2.36	0.40
14:N:26:ARG:HG3	14:N:26:ARG:NH1	2.35	0.40
6:F:48:LEU:N	6:F:56:PRO:O	2.52	0.40
6:F:53:ALA:O	6:F:54:LYS:HB2	2.21	0.40
1:A:1216:G:H5''	14:N:5:ALA:HB2	2.04	0.40
1:A:1108:G:H5''	1:A:1108:G:H8	1.86	0.40
1:A:1345:U:H3'	24:A:2740:HOH:O	2.22	0.40
12:L:70:ILE:HA	12:L:71:PRO:HD3	1.70	0.40
1:A:526:C:P	12:L:91:LYS:HZ3	2.44	0.40
10:J:75:ILE:HD13	10:J:76:ASN:OD1	2.21	0.40
1:A:1036:G:N2	1:A:1037:C:O2	2.55	0.40
17:Q:27:PHE:CD1	17:Q:27:PHE:O	2.75	0.40
2:B:174:VAL:CG2	2:B:184:VAL:HG11	2.52	0.40
1:A:1030(A):G:H2'	1:A:1030(C):G:OP2	2.21	0.40
1:A:1307:U:H2'	1:A:1308:U:C6	2.56	0.40
1:A:1217:C:H2'	1:A:1218:C:C6	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:43:LEU:HA	15:O:43:LEU:HD23	1.77	0.40
5:E:80:ILE:HG21	5:E:80:ILE:HD13	1.79	0.40
16:P:19:ILE:O	16:P:36:ILE:N	2.54	0.40
1:A:861:G:H2'	1:A:862:C:H6	1.86	0.40
11:K:18:ARG:O	11:K:33:THR:HG22	2.21	0.40
1:A:50:A:N6	1:A:361:G:H4'	2.36	0.40
5:E:33:VAL:HG11	5:E:109:ILE:HA	2.03	0.40
1:A:1198:G:C6	1:A:1199:U:C4	3.10	0.40
5:E:14:ARG:HE	5:E:16:THR:CG2	2.34	0.40
5:E:152:ARG:HE	5:E:152:ARG:HB2	1.51	0.40
1:A:546:G:O2'	1:A:548:G:H4'	2.22	0.40
1:A:1492:A:H8	1:A:1492:A:H3'	1.85	0.40
1:A:981:U:O4	1:A:1222:G:O6	2.39	0.40
15:O:6:GLU:O	15:O:7:GLU:C	2.58	0.40
11:K:41:THR:OG1	11:K:42:TRP:N	2.55	0.40
1:A:1053:G:H4'	1:A:1054:C:H5'	2.03	0.40
1:A:1505:G:H4'	1:A:1506:U:C5'	2.45	0.40
7:G:85:TYR:CD1	7:G:154:TYR:CE1	3.04	0.40
12:L:48:PRO:HD2	12:L:49:ASN:H	1.85	0.40
5:E:119:LEU:HA	5:E:119:LEU:HD23	1.67	0.40
8:H:106:GLY:HA2	8:H:122:ARG:HH22	1.85	0.40
16:P:58:TYR:O	16:P:59:TRP:C	2.56	0.40
12:L:6:THR:CG2	12:L:9:GLN:HG3	2.49	0.40
4:D:145:GLU:HB2	4:D:184:LYS:HD2	2.03	0.40
1:A:1125:U:C5'	24:A:2985:HOH:O	2.68	0.40
1:A:939:G:C4	1:A:940:C:C5	3.09	0.40
14:N:33:VAL:HA	14:N:39:LEU:O	2.21	0.40
19:S:7:LYS:CD	19:S:7:LYS:H	2.17	0.40
1:A:1518[A]:MA6:H2'	1:A:1519[A]:MA6:C8	2.51	0.40
1:A:1515[A]:C:H42	1:A:1520[A]:G:H1	1.69	0.40
1:A:1029:C:H5'	1:A:1033:G:C2	2.57	0.40
1:A:1451:A:H8	1:A:1451:A:C5'	2.35	0.40
1:A:1442:G:N7	1:A:1446:A:C6	2.90	0.40
12:L:53:ARG:NH1	12:L:92:OTD:CG	2.84	0.40
1:A:1256:A:N6	1:A:1277:C:H3'	2.35	0.40
5:E:35:GLY:N	5:E:112:LEU:HD22	2.36	0.40
7:G:91:VAL:CG1	7:G:96:GLN:HG3	2.52	0.40
1:A:1008:C:C2	1:A:1021:G:O6	2.75	0.40
1:A:1021:G:C6	1:A:1022:G:H1'	2.56	0.40
12:L:84:LEU:HB3	12:L:101:VAL:HG23	2.03	0.40
5:E:40:ARG:HB3	5:E:66:MET:CE	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:84:ILE:HD12	19:S:74:PHE:CE2	2.57	0.40
1:A:956:U:C2'	1:A:957:U:H5'	2.52	0.40
17:Q:18:THR:HA	17:Q:44:ALA:O	2.22	0.40
5:E:83:GLU:HA	5:E:87:SER:O	2.21	0.40
12:L:90:VAL:HB	12:L:96:VAL:HG21	2.04	0.40
4:D:101:LEU:HD12	4:D:101:LEU:HA	1.74	0.40
1:A:88:A:C4	1:A:89:C:C6	3.10	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)
18:R:25:THR:OG1	18:R:25:THR:OG1[8_555]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	194 (84%)	32 (14%)	6 (3%)	7	46
3	C	204/239 (85%)	170 (83%)	32 (16%)	2 (1%)	19	66
4	D	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	34	77
5	E	148/162 (91%)	137 (93%)	8 (5%)	3 (2%)	9	53
6	F	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	19	66
7	G	153/156 (98%)	135 (88%)	18 (12%)	0	100	100
8	H	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
9	I	125/128 (98%)	105 (84%)	19 (15%)	1 (1%)	24	69
10	J	96/105 (91%)	77 (80%)	14 (15%)	5 (5%)	2	27
11	K	114/129 (88%)	97 (85%)	16 (14%)	1 (1%)	21	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	121/135 (90%)	101 (84%)	16 (13%)	4 (3%)	5	41
13	M	116/126 (92%)	94 (81%)	20 (17%)	2 (2%)	11	56
14	N	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
15	O	85/89 (96%)	74 (87%)	11 (13%)	0	100	100
16	P	81/88 (92%)	75 (93%)	6 (7%)	0	100	100
17	Q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
18	R	68/88 (77%)	62 (91%)	5 (7%)	1 (2%)	13	58
19	S	78/93 (84%)	72 (92%)	5 (6%)	1 (1%)	15	61
20	T	97/106 (92%)	75 (77%)	20 (21%)	2 (2%)	9	52
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2336/2541 (92%)	2023 (87%)	283 (12%)	30 (1%)	15	61

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
10	J	35	SER
12	L	28	LYS
2	B	9	GLU
2	B	11	LEU
2	B	101	MET
3	C	15	THR
3	C	62	ASP
5	E	118	ILE
6	F	96	PRO
19	S	31	ILE
4	D	31	CYS
12	L	25	PRO
18	R	60	ALA
20	T	77	ALA
5	E	16	THR
5	E	70	PRO
10	J	54	PHE
12	L	79	GLU
20	T	13	LEU
9	I	119	ALA
10	J	34	VAL
10	J	60	ARG

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Mol	Chain	Res	Type
12	L	46	LYS
13	M	23	TYR
10	J	18	ALA
2	B	25	ASN
2	B	211	ILE
13	M	7	VAL
11	K	95	ILE

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%)	144 (71%)	58 (29%)	0	4
3	C	160/188 (85%)	108 (68%)	52 (32%)	0	2
4	D	180/181 (99%)	135 (75%)	45 (25%)	1	6
5	E	115/123 (94%)	81 (70%)	34 (30%)	0	3
6	F	90/90 (100%)	75 (83%)	15 (17%)	3	18
7	G	126/127 (99%)	94 (75%)	32 (25%)	1	5
8	H	119/119 (100%)	83 (70%)	36 (30%)	0	3
9	I	98/99 (99%)	71 (72%)	27 (28%)	0	4
10	J	87/92 (95%)	64 (74%)	23 (26%)	0	5
11	K	88/99 (89%)	66 (75%)	22 (25%)	1	6
12	L	103/110 (94%)	68 (66%)	35 (34%)	0	2
13	M	94/101 (93%)	64 (68%)	30 (32%)	0	3
14	N	49/50 (98%)	35 (71%)	14 (29%)	0	4
15	O	79/80 (99%)	50 (63%)	29 (37%)	0	1
16	P	72/74 (97%)	58 (81%)	14 (19%)	2	12
17	Q	94/97 (97%)	67 (71%)	27 (29%)	0	4
18	R	61/77 (79%)	43 (70%)	18 (30%)	0	3
19	S	71/80 (89%)	51 (72%)	20 (28%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	76/82 (93%)	53 (70%)	23 (30%)	0	3
21	U	19/22 (86%)	14 (74%)	5 (26%)	0	5
All	All	1983/2111 (94%)	1424 (72%)	559 (28%)	0	4

All (559) 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	17	PHE
2	B	19	HIS
2	B	20	GLU
2	B	24	TRP
2	B	30	ARG
2	B	33	TYR
2	B	36	ARG
2	B	47	THR
2	B	48	MET
2	B	50	GLU
2	B	51	LEU
2	B	53	ARG
2	B	60	ASP
2	B	69	LEU
2	B	74	LYS
2	B	76	GLN
2	B	79	ASP
2	B	87	ARG
2	B	90	MET
2	B	102	LEU
2	B	109	SER
2	B	110	GLN
2	B	111	ARG
2	B	121	LEU
2	B	127	ILE
2	B	130	ARG
2	B	132	LYS
2	B	133	LYS
2	B	135	GLN
2	B	137	ARG

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Mol	Chain	Res	Type
2	B	144	ARG
2	B	145	LEU
2	B	154	LEU
2	B	155	LEU
2	B	157	ARG
2	B	162	ILE
2	B	163	PHE
2	B	168	THR
2	B	170	GLU
2	B	172	ILE
2	B	174	VAL
2	B	175	ARG
2	B	178	ARG
2	B	182	ILE
2	B	184	VAL
2	B	194	PRO
2	B	205	ASP
2	B	208	ILE
2	B	209	ARG
2	B	221	LEU
2	B	222	ILE
2	B	226	ARG
2	B	238	LEU
2	B	239	VAL
3	C	4	LYS
3	C	11	ARG
3	C	12	LEU
3	C	14	ILE
3	C	15	THR
3	C	21	ARG
3	C	27	LYS
3	C	30	ARG
3	C	34	LEU
3	C	35	GLU
3	C	37	GLN
3	C	40	ARG
3	C	42	LEU
3	C	43	LEU
3	C	44	GLU
3	C	45	LYS
3	C	46	GLU
3	C	52	LEU

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Mol	Chain	Res	Type
3	C	62	ASP
3	C	67	THR
3	C	82	GLU
3	C	84	ILE
3	C	89	GLU
3	C	94	LEU
3	C	97	LYS
3	C	101	LEU
3	C	102	ASN
3	C	111	LEU
3	C	112	SER
3	C	120	VAL
3	C	122	GLU
3	C	131	ARG
3	C	132	ARG
3	C	134	ILE
3	C	135	LYS
3	C	138	VAL
3	C	144	SER
3	C	153	VAL
3	C	156	ARG
3	C	157	ILE
3	C	162	GLN
3	C	165	THR
3	C	167	TRP
3	C	172	ARG
3	C	173	VAL
3	C	175	LEU
3	C	178	LEU
3	C	191	THR
3	C	192	THR
3	C	195	VAL
3	C	199	LYS
3	C	204	LEU
4	D	3	ARG
4	D	5	ILE
4	D	17	VAL
4	D	24	GLU
4	D	25	ARG
4	D	26	CYS
4	D	28	SER
4	D	35	ARG

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Mol	Chain	Res	Type
4	D	38	TYR
4	D	39	PRO
4	D	47	ARG
4	D	49	ARG
4	D	57	ARG
4	D	58	LEU
4	D	64	LEU
4	D	66	ARG
4	D	70	ILE
4	D	71	SER
4	D	73	ARG
4	D	74	GLN
4	D	76	ARG
4	D	78	LEU
4	D	84	LYS
4	D	107	ARG
4	D	118	ARG
4	D	122	ARG
4	D	126	ILE
4	D	132	ARG
4	D	135	LEU
4	D	137	SER
4	D	157	LEU
4	D	162	LEU
4	D	166	LYS
4	D	169	LYS
4	D	170	VAL
4	D	178	VAL
4	D	181	MET
4	D	182	LYS
4	D	184	LYS
4	D	186	LEU
4	D	187	ARG
4	D	190	ASP
4	D	191	ARG
4	D	194	LEU
4	D	202	LEU
5	E	6	PHE
5	E	11	ILE
5	E	12	LEU
5	E	13	ILE
5	E	15	ARG

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Mol	Chain	Res	Type
5	E	18	ARG
5	E	24	ARG
5	E	25	ARG
5	E	26	PHE
5	E	27	ARG
5	E	31	LEU
5	E	41	VAL
5	E	47	LYS
5	E	50	GLU
5	E	55	VAL
5	E	56	GLN
5	E	60	TYR
5	E	63	ARG
5	E	64	ARG
5	E	67	VAL
5	E	78	HIS
5	E	79	GLU
5	E	81	GLU
5	E	87	SER
5	E	100	VAL
5	E	105	VAL
5	E	107	ARG
5	E	111	GLU
5	E	112	LEU
5	E	117	ASP
5	E	126	ARG
5	E	144	THR
5	E	150	ARG
5	E	153	LYS
6	F	10	LEU
6	F	21	LEU
6	F	27	GLN
6	F	30	LEU
6	F	32	ASN
6	F	38	GLU
6	F	42	GLU
6	F	43	LEU
6	F	54	LYS
6	F	66	GLU
6	F	73	ASN
6	F	74	ASP
6	F	82	ARG

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Mol	Chain	Res	Type
6	F	83	ASP
6	F	93	SER
7	G	5	ARG
7	G	9	VAL
7	G	12	LEU
7	G	21	VAL
7	G	22	LEU
7	G	37	ASN
7	G	38	LEU
7	G	48	LYS
7	G	49	ILE
7	G	51	GLN
7	G	54	THR
7	G	59	LEU
7	G	70	LYS
7	G	75	VAL
7	G	84	ASN
7	G	94	ARG
7	G	106	GLN
7	G	109	ASN
7	G	113	GLU
7	G	115	ARG
7	G	118	VAL
7	G	125	MET
7	G	126	ASP
7	G	129	GLU
7	G	131	LYS
7	G	135	VAL
7	G	140	ASP
7	G	141	VAL
7	G	143	ARG
7	G	146	GLU
7	G	155	ARG
7	G	156	TRP
8	H	3	THR
8	H	5	PRO
8	H	8	ASP
8	H	15	ASN
8	H	18	ARG
8	H	24	THR
8	H	25	ASP
8	H	26	VAL

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Mol	Chain	Res	Type
8	H	35	ILE
8	H	36	LEU
8	H	37	ARG
8	H	39	LEU
8	H	45	ILE
8	H	51	VAL
8	H	53	VAL
8	H	56	LYS
8	H	62	TYR
8	H	64	LYS
8	H	69	ARG
8	H	76	PRO
8	H	80	ILE
8	H	82	HIS
8	H	84	ARG
8	H	85	ARG
8	H	87	SER
8	H	91	ARG
8	H	93	VAL
8	H	102	ARG
8	H	104	ARG
8	H	105	ARG
8	H	116	LYS
8	H	119	LEU
8	H	121	ASP
8	H	127	LEU
8	H	129	VAL
8	H	133	LEU
9	I	2	GLU
9	I	9	ARG
9	I	11	LYS
9	I	23	ASN
9	I	29	ASN
9	I	34	ASN
9	I	38	GLN
9	I	42	ARG
9	I	47	LEU
9	I	56	LEU
9	I	58	HIS
9	I	62	TYR
9	I	64	THR
9	I	71	SER

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Mol	Chain	Res	Type
9	I	75	ASP
9	I	79	LEU
9	I	85	LEU
9	I	91	ASP
9	I	99	LEU
9	I	102	LEU
9	I	107	ARG
9	I	108	VAL
9	I	111	ARG
9	I	112	LYS
9	I	116	LYS
9	I	121	ARG
9	I	124	GLN
10	J	5	ARG
10	J	6	ILE
10	J	12	ASP
10	J	15	THR
10	J	16	LEU
10	J	30	SER
10	J	38	ILE
10	J	46	ARG
10	J	48	THR
10	J	60	ARG
10	J	65	LEU
10	J	66	ARG
10	J	67	THR
10	J	69	ASN
10	J	70	ARG
10	J	73	ASP
10	J	76	ASN
10	J	81	THR
10	J	85	LEU
10	J	87	THR
10	J	88	LEU
10	J	90	LEU
10	J	95	GLU
11	K	11	LYS
11	K	12	ARG
11	K	18	ARG
11	K	29	ILE
11	K	30	VAL
11	K	36	ASP

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Mol	Chain	Res	Type
11	K	38	ASN
11	K	40	ILE
11	K	41	THR
11	K	58	PRO
11	K	62	GLN
11	K	70	LYS
11	K	80	VAL
11	K	84	VAL
11	K	87	THR
11	K	108	ILE
11	K	111	ASP
11	K	116	HIS
11	K	117	ASN
11	K	120	ARG
11	K	123	LYS
11	K	126	ARG
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	23	LYS
12	L	24	VAL
12	L	28	LYS
12	L	33	ARG
12	L	38	THR
12	L	39	VAL
12	L	42	THR
12	L	43	VAL
12	L	44	THR
12	L	47	LYS
12	L	60	LEU
12	L	61	THR
12	L	78	GLN
12	L	79	GLU
12	L	80	HIS
12	L	82	VAL
12	L	89	ARG
12	L	93	LEU
12	L	94	LEU
12	L	97	ARG

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Mol	Chain	Res	Type
12	L	100	ILE
12	L	101	VAL
12	L	111	LYS
12	L	113	ARG
12	L	114	LYS
12	L	116	SER
12	L	118	SER
12	L	126	LYS
12	L	127	GLU
13	M	4	ILE
13	M	9	ILE
13	M	14	ARG
13	M	27	LYS
13	M	29	ARG
13	M	32	GLU
13	M	36	LYS
13	M	39	ILE
13	M	46	LYS
13	M	47	ASP
13	M	49	THR
13	M	56	LEU
13	M	58	GLU
13	M	62	ASN
13	M	63	THR
13	M	64	TRP
13	M	66	LEU
13	M	69	GLU
13	M	70	LEU
13	M	71	ARG
13	M	81	LEU
13	M	90	LEU
13	M	92	HIS
13	M	98	VAL
13	M	108	ARG
13	M	109	THR
13	M	110	ARG
13	M	115	LYS
13	M	116	THR
13	M	117	VAL
14	N	7	ILE
14	N	8	GLU
14	N	9	LYS

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Mol	Chain	Res	Type
14	N	11	LYS
14	N	21	TYR
14	N	26	ARG
14	N	29	ARG
14	N	33	VAL
14	N	41	ARG
14	N	44	LEU
14	N	45	ARG
14	N	47	LEU
14	N	52	GLN
14	N	58	LYS
15	O	5	LYS
15	O	6	GLU
15	O	8	LYS
15	O	9	GLN
15	O	10	LYS
15	O	13	GLN
15	O	14	GLU
15	O	21	ASP
15	O	22	THR
15	O	29	VAL
15	O	32	LEU
15	O	33	THR
15	O	34	LEU
15	O	36	ILE
15	O	39	LEU
15	O	45	VAL
15	O	47	LYS
15	O	54	ARG
15	O	56	LEU
15	O	57	LEU
15	O	58	MET
15	O	64	ARG
15	O	68	ARG
15	O	70	LEU
15	O	73	GLU
15	O	76	GLU
15	O	77	ARG
15	O	84	LYS
15	O	87	ILE
16	P	1	MET
16	P	4	ILE

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Mol	Chain	Res	Type
16	P	26	ARG
16	P	42	ARG
16	P	45	THR
16	P	48	TRP
16	P	50	LYS
16	P	52	ASP
16	P	57	ARG
16	P	67	THR
16	P	68	ASP
16	P	72	ARG
16	P	76	GLN
16	P	83	GLU
17	Q	5	VAL
17	Q	6	LEU
17	Q	7	THR
17	Q	9	VAL
17	Q	11	VAL
17	Q	17	LYS
17	Q	22	LEU
17	Q	34	LYS
17	Q	35	VAL
17	Q	36	ILE
17	Q	43	LEU
17	Q	48	GLU
17	Q	57	VAL
17	Q	59	ILE
17	Q	60	ILE
17	Q	62	SER
17	Q	63	ARG
17	Q	68	ARG
17	Q	69	LYS
17	Q	72	ARG
17	Q	79	SER
17	Q	87	LYS
17	Q	88	TYR
17	Q	89	LEU
17	Q	92	ARG
17	Q	98	LEU
17	Q	100	LYS
18	R	26	LEU
18	R	28	GLU
18	R	39	VAL

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Mol	Chain	Res	Type
18	R	41	LYS
18	R	47	THR
18	R	53	ARG
18	R	54	ARG
18	R	55	ARG
18	R	56	THR
18	R	65	ILE
18	R	68	LYS
18	R	69	THR
18	R	75	ILE
18	R	78	LEU
18	R	83	GLU
18	R	86	VAL
18	R	87	ARG
18	R	88	LYS
19	S	4	SER
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	12	ASP
19	S	13	ASP
19	S	15	LEU
19	S	18	LYS
19	S	29	ARG
19	S	31	ILE
19	S	32	LYS
19	S	35	SER
19	S	36	ARG
19	S	37	ARG
19	S	41	VAL
19	S	43	GLU
19	S	61	TYR
19	S	71	LEU
19	S	78	ARG
19	S	79	THR
20	T	14	LYS
20	T	18	GLN
20	T	24	LEU
20	T	25	ARG
20	T	29	LYS
20	T	36	LEU
20	T	41	ILE

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Mol	Chain	Res	Type
20	T	45	GLN
20	T	50	GLU
20	T	51	GLU
20	T	53	LEU
20	T	54	LYS
20	T	56	MET
20	T	62	LEU
20	T	71	THR
20	T	72	LEU
20	T	73	HIS
20	T	75	ASN
20	T	80	ARG
20	T	81	LYS
20	T	84	LEU
20	T	89	ARG
20	T	93	GLU
21	U	6	ARG
21	U	8	THR
21	U	15	ARG
21	U	17	THR
21	U	22	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
3	C	6	HIS
5	E	65	ASN
8	H	15	ASN
9	I	29	ASN
17	Q	94	ASN
19	S	23	ASN
19	S	47	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	418 (27%)	46 (3%)

All (418) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	9	G
1	A	12	U
1	A	15	G
1	A	16	A
1	A	30	U
1	A	31	G
1	A	32	A
1	A	39	G
1	A	43	C
1	A	45	U
1	A	47	C
1	A	48	C
1	A	49	U
1	A	51	A
1	A	54	C
1	A	55	A
1	A	58	C
1	A	77	G
1	A	81	U
1	A	82	U
1	A	101	A
1	A	109	A
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	138	G
1	A	145	G
1	A	151	A
1	A	158	G
1	A	163	C
1	A	174	C
1	A	176	C
1	A	181	G
1	A	182	U
1	A	190(E)	U
1	A	190(H)	G
1	A	191	G
1	A	195	A

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Mol	Chain	Res	Type
1	A	197	A
1	A	198	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	224	C
1	A	225	C
1	A	231	G
1	A	236	G
1	A	240	C
1	A	245	C
1	A	247	G
1	A	250	A
1	A	251	G
1	A	253	U
1	A	264	U
1	A	266	G
1	A	267	C
1	A	272	C
1	A	279	A
1	A	280	C
1	A	289	G
1	A	293	G
1	A	298	A
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	331	G
1	A	344	A
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

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Mol	Chain	Res	Type
1	A	365	U
1	A	366	C
1	A	367	U
1	A	369	C
1	A	373	A
1	A	384	G
1	A	390	C
1	A	398	C
1	A	406	G
1	A	409	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	415	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	440	A
1	A	446	G
1	A	452	A
1	A	456	C
1	A	461	C
1	A	462	G
1	A	477	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
1	A	503	C
1	A	504	C
1	A	507	C
1	A	509	A
1	A	510	A
1	A	511	C
1	A	514	C
1	A	515	G
1	A	518	C

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Mol	Chain	Res	Type
1	A	519	C
1	A	524	G
1	A	526	C
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	536	C
1	A	537	G
1	A	539	A
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	581	G
1	A	587	G
1	A	588	G
1	A	589	C
1	A	609	A
1	A	618	C
1	A	625	G
1	A	642	A
1	A	653	A
1	A	665	A
1	A	666	G
1	A	670	G
1	A	672	U
1	A	674	G
1	A	686	U
1	A	687	A
1	A	689	C
1	A	692	U
1	A	695	A

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Mol	Chain	Res	Type
1	A	702	A
1	A	703	G
1	A	705	U
1	A	716	A
1	A	719	C
1	A	720	C
1	A	721	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	729	A
1	A	731	G
1	A	734	G
1	A	741	G
1	A	744	C
1	A	747	C
1	A	748	C
1	A	749	C
1	A	753	A
1	A	755	G
1	A	759	A
1	A	764	C
1	A	766	A
1	A	774	G
1	A	777	A
1	A	780	A
1	A	781	A
1	A	793	U
1	A	794	A
1	A	804	U
1	A	807	A
1	A	815	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	820	U
1	A	822	C
1	A	827	U
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U

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Mol	Chain	Res	Type
1	A	848	C
1	A	855	G
1	A	857	C
1	A	870	U
1	A	872	A
1	A	873	A
1	A	889	A
1	A	902	G
1	A	917	G
1	A	920	U
1	A	922	G
1	A	926	G
1	A	927	G
1	A	931	C
1	A	933	G
1	A	934	C
1	A	935	A
1	A	937	A
1	A	939	G
1	A	942	G
1	A	952	U
1	A	954	G
1	A	960	U
1	A	964	A
1	A	965	A
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	986	A
1	A	992	U
1	A	993	G
1	A	997	U
1	A	1002	G
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A

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Mol	Chain	Res	Type
1	A	1007	C
1	A	1009	G
1	A	1010	G
1	A	1011	G
1	A	1012	U
1	A	1021	G
1	A	1022	G
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1029	C
1	A	1030	C
1	A	1030(A)	G
1	A	1030(B)	C
1	A	1030(C)	G
1	A	1031	G
1	A	1033	G
1	A	1034	G
1	A	1035	A
1	A	1038	C
1	A	1039	C
1	A	1045	C
1	A	1046	A
1	A	1053	G
1	A	1054	C
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1070	U
1	A	1077	G
1	A	1094	G
1	A	1095	U
1	A	1100	C
1	A	1101	A
1	A	1104	G
1	A	1108	G
1	A	1109	C
1	A	1110	A
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C

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Mol	Chain	Res	Type
1	A	1130	A
1	A	1131	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	1151	A
1	A	1152	A
1	A	1153	C
1	A	1154	G
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1162	C
1	A	1163	C
1	A	1171	G
1	A	1173	G
1	A	1175	G
1	A	1179	A
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1209	C
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1225	A
1	A	1226	C
1	A	1233	G
1	A	1238	A
1	A	1240	U

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Mol	Chain	Res	Type
1	A	1241	G
1	A	1247	U
1	A	1249	C
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1277	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1298	C
1	A	1300	G
1	A	1302	U
1	A	1304	G
1	A	1310	G
1	A	1312	G
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1332	A
1	A	1336	C
1	A	1338	G
1	A	1341	U
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1356	G
1	A	1363	A
1	A	1364	U
1	A	1370	G
1	A	1376	U
1	A	1377	A
1	A	1378	C
1	A	1379	G
1	A	1380	U
1	A	1381	U

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Mol	Chain	Res	Type
1	A	1393	U
1	A	1394	A
1	A	1401	G
1	A	1403	C
1	A	1407	5MC
1	A	1408	A
1	A	1410	G
1	A	1413	A
1	A	1414	U
1	A	1418	A
1	A	1440	C
1	A	1442	G
1	A	1446	A
1	A	1451	A
1	A	1452	C
1	A	1460	A
1	A	1474	G
1	A	1476	G
1	A	1487	G
1	A	1489	G
1	A	1490	C
1	A	1491	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1495	U
1	A	1496	C
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	1507	A
1	A	1508	G
1	A	1529	G
1	A	1530	G
1	A	1531	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	243	A
1	A	250	A
1	A	328	C
1	A	329	A
1	A	350	G
1	A	353	A
1	A	372	C
1	A	428	G
1	A	429	U
1	A	509	A
1	A	518	C
1	A	531	U
1	A	532	A
1	A	559	A
1	A	588	G
1	A	609	A
1	A	748	C
1	A	758	G
1	A	780	A
1	A	793	U
1	A	817	C
1	A	832	C
1	A	890	G
1	A	919	A
1	A	992	U
1	A	1054	C
1	A	1065	U
1	A	1093	A
1	A	1125	U
1	A	1201	A
1	A	1225	A
1	A	1226	C
1	A	1256	A
1	A	1257	U
1	A	1319	A
1	A	1346	A
1	A	1380	U
1	A	1490	C
1	A	1491	G
1	A	1493	A

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Mol	Chain	Res	Type
1	A	1505	G
1	A	1529	G
1	A	1530	G

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

17 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	2MG	A	1207	1,22	17,26,27	1.07	1 (5%)	21,38,41	2.42	7 (33%)
1	5MC	A	1400	1	13,22,23	4.47	4 (30%)	15,32,35	2.54	4 (26%)
1	4OC	A	1402	1	13,23,24	1.78	1 (7%)	18,32,35	0.72	0
1	5MC	A	1404	1	13,22,23	1.35	3 (23%)	15,32,35	0.95	1 (6%)
1	5MC	A	1407	1	13,22,23	1.28	1 (7%)	15,32,35	1.30	3 (20%)
1	UR3	A	1498	1	12,22,23	2.28	4 (33%)	16,32,35	1.58	4 (25%)
1	MA6	A	1518[A]	1	16,26,27	1.13	2 (12%)	18,38,41	0.93	2 (11%)
1	MA6	A	1518[B]	1	16,26,27	1.33	2 (12%)	18,38,41	1.07	2 (11%)
1	MA6	A	1519[A]	1	16,26,27	1.50	3 (18%)	18,38,41	1.43	4 (22%)
1	MA6	A	1519[B]	1	16,26,27	1.69	5 (31%)	18,38,41	1.00	2 (11%)
1	PSU	A	1540	1	13,21,22	1.06	1 (7%)	18,30,33	3.78	5 (27%)
1	PSU	A	1541	1	13,21,22	1.15	2 (15%)	18,30,33	4.24	5 (27%)
1	PSU	A	516	1,22	13,21,22	1.25	2 (15%)	18,30,33	5.32	5 (27%)
1	7MG	A	527	1	19,26,27	2.05	6 (31%)	24,39,42	2.41	7 (29%)
1	M2G	A	966	1	17,27,28	1.36	4 (23%)	22,40,43	2.58	4 (18%)
1	5MC	A	967	1	13,22,23	1.29	1 (7%)	15,32,35	1.08	1 (6%)
12	0TD	L	92	12	4,9,10	1.16	0	4,11,13	4.78	2 (50%)

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	2MG	A	1207	1,22	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	0/3/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/3/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[B]	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	0/7/37/38	0/3/3/3
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	5MC	A	967	1	-	0/3/25/26	0/2/2/2
12	0TD	L	92	12	-	0/2/12/14	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1400	5MC	C4-N3	-7.53	1.23	1.35
1	A	1402	4OC	C6-N1	-5.32	1.28	1.35
1	A	1498	UR3	C4-N3	-5.24	1.30	1.38
1	A	527	7MG	C8-N9	-4.85	1.38	1.45
1	A	527	7MG	C2-N1	-3.98	1.28	1.35
1	A	967	5MC	C6-C5	-3.40	1.31	1.40
1	A	1407	5MC	C6-C5	-3.36	1.31	1.40
1	A	1498	UR3	O4-C4	-3.33	1.16	1.24
1	A	527	7MG	C6-N1	-3.00	1.27	1.33
1	A	1498	UR3	C6-C5	-2.98	1.31	1.38
1	A	1498	UR3	C3U-N3	-2.91	1.41	1.47
1	A	966	M2G	C4-N3	-2.87	1.31	1.35
1	A	527	7MG	CM7-N7	-2.86	1.41	1.46
1	A	1519[A]	MA6	C10-N6	-2.67	1.39	1.45
1	A	1404	5MC	CM5-C5	-2.62	1.45	1.51
1	A	1518[A]	MA6	C10-N6	-2.41	1.39	1.45
1	A	1541	PSU	O4'-C1'	-2.39	1.40	1.44
1	A	527	7MG	C2-N3	-2.34	1.31	1.35
1	A	516	PSU	O4'-C1'	-2.25	1.40	1.44
1	A	966	M2G	C2-N2	-2.05	1.31	1.34
1	A	1404	5MC	C4-N3	-2.04	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C2-N2	2.06	1.38	1.34
1	A	966	M2G	CM1-N2	2.13	1.50	1.45
1	A	1400	5MC	C6-C5	2.25	1.46	1.40
1	A	1519[B]	MA6	C4-N3	2.25	1.38	1.35
1	A	1518[B]	MA6	C5-C4	2.36	1.45	1.40
1	A	1404	5MC	C4-N4	2.37	1.40	1.34
1	A	966	M2G	C6-C5	2.41	1.46	1.41
1	A	1518[A]	MA6	C2-N1	2.43	1.38	1.33
1	A	1519[B]	MA6	C5-C4	2.55	1.46	1.40
1	A	1519[A]	MA6	C5-C4	2.64	1.46	1.40
1	A	1519[B]	MA6	C2-N3	2.66	1.36	1.32
1	A	1541	PSU	C4-N3	2.82	1.38	1.33
1	A	1519[B]	MA6	C2-N1	2.96	1.39	1.33
1	A	516	PSU	C4-N3	3.07	1.38	1.33
1	A	1518[B]	MA6	C6-N1	3.22	1.38	1.34
1	A	1540	PSU	C4-N3	3.26	1.39	1.33
1	A	1207	2MG	C6-N1	3.42	1.39	1.33
1	A	1519[A]	MA6	C2-N1	3.49	1.40	1.33
1	A	1519[B]	MA6	C6-N1	4.02	1.39	1.34
1	A	1400	5MC	CM5-C5	8.38	1.68	1.51
1	A	1400	5MC	C5-C4	11.21	1.58	1.41

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-19.17	116.10	128.33
1	A	1541	PSU	N1-C2-N3	-15.54	118.42	128.33
1	A	1540	PSU	N1-C2-N3	-13.39	119.79	128.33
12	L	92	0TD	CSB-SB-CB	-9.01	84.54	101.54
1	A	966	M2G	C5-C6-N1	-8.84	111.50	123.59
1	A	527	7MG	C5-C4-N3	-8.64	118.40	126.82
1	A	1400	5MC	N4-C4-N3	-7.65	105.86	116.95
1	A	1207	2MG	C5-C6-N1	-7.35	113.55	123.59
1	A	966	M2G	N1-C2-N2	-5.90	110.51	117.16
1	A	1207	2MG	CM2-N2-C2	-4.99	117.44	123.07
1	A	516	PSU	C5-C1'-C2'	-3.76	108.83	115.52
1	A	966	M2G	CM2-N2-C2	-3.38	117.87	121.34
1	A	527	7MG	C5-C6-N1	-3.20	118.54	123.46
1	A	1407	5MC	N4-C4-N3	-2.83	112.84	116.95
1	A	527	7MG	N2-C2-N1	-2.77	112.61	117.20
12	L	92	0TD	O-C-CA	-2.47	118.90	125.44
1	A	1519[A]	MA6	C4-C5-N7	-2.46	107.22	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C2-N3-C4	-2.44	112.15	115.09
1	A	1400	5MC	O4'-C1'-N1	-2.43	102.97	108.08
1	A	1207	2MG	C2'-C1'-N9	-2.36	110.69	114.29
1	A	1207	2MG	N2-C2-N1	-2.19	114.39	116.94
1	A	1519[A]	MA6	C2'-C1'-N9	-2.10	111.09	114.29
1	A	1518[A]	MA6	N3-C2-N1	2.02	130.44	128.89
1	A	527	7MG	O5'-C5'-C4'	2.09	116.78	109.12
1	A	527	7MG	C6-N1-C2	2.13	118.89	115.94
1	A	1407	5MC	CM5-C5-C6	2.19	123.03	118.62
1	A	967	5MC	C5-C4-N3	2.19	124.94	121.27
1	A	1519[B]	MA6	N3-C2-N1	2.27	130.63	128.89
1	A	966	M2G	N3-C2-N2	2.29	119.75	117.16
1	A	1404	5MC	CM5-C5-C6	2.30	123.24	118.62
1	A	1498	UR3	C4'-O4'-C1'	2.31	112.25	109.72
1	A	1498	UR3	C6-C5-C4	2.37	121.72	117.28
1	A	1407	5MC	C5-C4-N3	2.39	125.26	121.27
1	A	1207	2MG	C4-C5-N7	2.42	111.71	109.48
1	A	1498	UR3	O2'-C2'-C3'	2.49	119.94	111.83
1	A	1518[A]	MA6	C2-N1-C6	2.50	116.74	111.43
1	A	1519[B]	MA6	C2-N1-C6	2.50	116.75	111.43
1	A	1518[B]	MA6	C2-N1-C6	2.53	116.81	111.43
1	A	1540	PSU	C6-N1-C2	2.57	119.60	115.47
1	A	1400	5MC	C5-C4-N3	2.62	125.65	121.27
1	A	1541	PSU	O4'-C1'-C2'	2.74	107.52	104.73
1	A	1519[A]	MA6	C2-N1-C6	2.76	117.31	111.43
1	A	1518[B]	MA6	N3-C2-N1	2.78	131.02	128.89
1	A	527	7MG	CM7-N7-C8	2.81	128.49	120.52
1	A	1540	PSU	C4-C5-C1'	2.99	126.70	121.23
1	A	1540	PSU	O4'-C1'-C2'	3.01	107.80	104.73
1	A	1541	PSU	C5-C1'-C2'	3.05	120.94	115.52
1	A	516	PSU	C6-N1-C2	3.11	120.46	115.47
1	A	1519[A]	MA6	N3-C2-N1	3.13	131.29	128.89
1	A	1541	PSU	C6-N1-C2	3.31	120.79	115.47
1	A	1207	2MG	C6-N1-C2	3.57	120.50	115.31
1	A	1498	UR3	O3'-C3'-C2'	3.64	123.67	111.83
1	A	516	PSU	O4'-C1'-C2'	3.73	108.53	104.73
1	A	527	7MG	N3-C4-N9	3.97	132.71	126.75
1	A	1400	5MC	C5-C4-N4	4.27	128.48	122.20
1	A	1541	PSU	C4-N3-C2	6.46	120.83	115.25
1	A	1540	PSU	C4-N3-C2	6.90	121.22	115.25
1	A	516	PSU	C4-N3-C2	9.64	123.58	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	2	0
1	A	1402	4OC	1	0
1	A	1407	5MC	1	0
1	A	1498	UR3	3	0
1	A	1518[A]	MA6	5	0
1	A	1518[B]	MA6	8	0
1	A	1519[A]	MA6	3	0
1	A	1519[B]	MA6	5	0
1	A	1540	PSU	1	0
1	A	1541	PSU	1	0
1	A	516	PSU	1	0
1	A	527	7MG	1	0
1	A	966	M2G	2	0
1	A	967	5MC	3	0
12	L	92	0TD	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 403 ligands modelled in this entry, 403 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1500/1522 (98%)	-0.34	7 (0%) 91 88	90, 130, 210, 340	0
2	B	234/256 (91%)	-0.34	3 (1%) 79 71	106, 148, 236, 282	0
3	C	206/239 (86%)	-0.48	0 100 100	100, 136, 182, 210	0
4	D	208/209 (99%)	-0.37	0 100 100	89, 127, 172, 212	0
5	E	150/162 (92%)	-0.41	0 100 100	80, 112, 151, 188	0
6	F	101/101 (100%)	-0.34	1 (0%) 84 77	118, 147, 181, 236	0
7	G	155/156 (99%)	-0.27	0 100 100	130, 166, 208, 238	0
8	H	138/138 (100%)	-0.46	0 100 100	95, 120, 158, 192	0
9	I	127/128 (99%)	-0.17	5 (3%) 43 35	126, 167, 207, 227	0
10	J	98/105 (93%)	-0.16	0 100 100	113, 164, 199, 261	0
11	K	116/129 (89%)	-0.23	0 100 100	106, 145, 192, 209	0
12	L	123/135 (91%)	-0.29	1 (0%) 87 81	87, 117, 145, 197	0
13	M	118/126 (93%)	-0.04	4 (3%) 49 39	129, 173, 210, 242	0
14	N	60/61 (98%)	-0.32	0 100 100	110, 139, 199, 221	0
15	O	87/89 (97%)	-0.31	0 100 100	115, 143, 171, 203	0
16	P	83/88 (94%)	-0.09	0 100 100	97, 128, 160, 186	0
17	Q	99/105 (94%)	-0.27	0 100 100	98, 124, 161, 168	0
18	R	70/88 (79%)	-0.09	1 (1%) 78 69	124, 162, 232, 270	0
19	S	80/93 (86%)	-0.24	1 (1%) 79 71	140, 175, 218, 249	0
20	T	99/106 (93%)	-0.34	0 100 100	107, 133, 184, 208	0
21	U	24/27 (88%)	0.31	1 (4%) 40 32	149, 172, 193, 207	0
All	All	3876/4063 (95%)	-0.31	24 (0%) 90 85	80, 138, 201, 340	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1030(D)	A	6.1
1	A	1030(C)	G	3.4
9	I	15	ALA	3.4
12	L	128	ALA	3.1
2	B	235	SER	3.1
1	A	1031	G	3.0
2	B	238	LEU	3.0
13	M	2	ALA	3.0
9	I	16	ARG	2.8
1	A	1129	C	2.8
6	F	101	ALA	2.6
1	A	1027	C	2.5
9	I	8	GLY	2.5
9	I	64	THR	2.3
1	A	1003	G	2.3
18	R	88	LYS	2.3
21	U	18	TYR	2.3
1	A	81	U	2.3
9	I	65	VAL	2.2
13	M	4	ILE	2.2
13	M	7	VAL	2.2
2	B	125	PRO	2.1
19	S	2	PRO	2.1
13	M	117	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	5MC	A	1404	21/22	0.90	0.28	-	103,111,130,135	0
1	5MC	A	1407	21/22	0.96	0.12	-	109,123,133,135	0
1	5MC	A	967	21/22	0.97	0.15	-	121,129,135,138	0
1	4OC	A	1402	22/23	0.93	0.27	-	114,119,123,133	0
1	UR3	A	1498	21/22	0.94	0.23	-	94,108,123,134	0
1	7MG	A	527	24/25	0.96	0.18	-	105,113,130,135	0
1	MA6	A	1518[A]	24/25	0.89	0.26	-	96,104,114,119	24
1	PSU	A	516	20/21	0.96	0.12	-	114,123,141,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	M2G	A	966	25/26	0.96	0.17	-	121,130,137,138	0
1	5MC	A	1400	21/22	0.96	0.17	-	92,111,126,132	0
1	MA6	A	1519[B]	24/25	0.93	0.29	-	90,96,98,106	24
12	0TD	L	92	10/11	0.98	0.48	-	81,121,135,281	0
1	PSU	A	1540	20/21	0.80	0.40	-	244,249,261,261	0
1	MA6	A	1518[B]	24/25	0.89	0.26	-	101,105,117,119	24
1	PSU	A	1541	20/21	0.85	0.20	-	211,223,230,234	0
1	2MG	A	1207	24/25	0.97	0.09	-	115,127,139,142	0
1	MA6	A	1519[A]	24/25	0.93	0.29	-	91,97,106,109	24

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1806	1/1	0.96	1.19	22.90	412,412,412,412	0
22	MG	A	1892	1/1	0.69	0.80	22.02	400,400,400,400	0
22	MG	A	1815	1/1	0.92	0.69	21.68	515,515,515,515	0
22	MG	A	1657	1/1	0.92	1.11	16.84	148,148,148,148	0
22	MG	A	1746	1/1	0.56	0.44	16.14	132,132,132,132	0
22	MG	A	1926	1/1	0.99	0.30	12.46	462,462,462,462	0
22	MG	A	1767	1/1	0.79	0.38	11.29	548,548,548,548	0
22	MG	A	1722	1/1	0.66	0.36	9.09	120,120,120,120	0
22	MG	A	1921	1/1	0.99	0.42	8.68	349,349,349,349	0
22	MG	A	1691	1/1	0.84	0.36	8.46	91,91,91,91	0
22	MG	N	102	1/1	0.85	0.74	8.13	116,116,116,116	0
22	MG	A	1676	1/1	0.95	0.33	7.90	93,93,93,93	0
22	MG	A	1715	1/1	0.92	0.28	6.42	125,125,125,125	0
22	MG	A	1724	1/1	0.88	0.42	6.26	93,93,93,93	0
22	MG	A	1865	1/1	0.91	0.35	5.09	474,474,474,474	0
22	MG	A	1704	1/1	0.95	0.41	4.99	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1971	1/1	0.78	0.23	4.98	116,116,116,116	0
22	MG	A	1931	1/1	0.98	0.24	4.22	232,232,232,232	0
22	MG	A	1614	1/1	0.83	0.29	4.07	120,120,120,120	0
22	MG	A	1666	1/1	0.92	0.25	3.89	81,81,81,81	0
22	MG	A	1893	1/1	0.94	0.17	3.63	406,406,406,406	0
22	MG	A	1686	1/1	0.98	0.28	3.62	225,225,225,225	0
22	MG	A	1721	1/1	0.93	0.37	3.42	97,97,97,97	0
22	MG	A	1711	1/1	0.99	0.59	3.34	106,106,106,106	0
22	MG	A	1687	1/1	0.99	0.20	2.81	99,99,99,99	0
22	MG	A	1975	1/1	0.83	0.20	2.69	108,108,108,108	0
22	MG	A	1665	1/1	0.99	0.20	2.66	158,158,158,158	0
22	MG	A	1628	1/1	0.87	0.21	2.64	203,203,203,203	0
22	MG	A	1692	1/1	0.97	0.26	2.10	95,95,95,95	0
22	MG	A	1627	1/1	0.99	0.23	1.73	98,98,98,98	0
22	MG	A	1803	1/1	0.99	0.18	1.43	129,129,129,129	0
22	MG	A	1680	1/1	0.93	0.22	1.42	116,116,116,116	0
22	MG	A	1718	1/1	0.94	0.24	1.27	87,87,87,87	0
22	MG	D	303	1/1	0.88	0.24	1.09	127,127,127,127	0
22	MG	B	301	1/1	0.92	0.33	1.04	141,141,141,141	0
22	MG	A	1647	1/1	0.83	0.17	1.00	201,201,201,201	0
22	MG	A	1699	1/1	0.92	0.23	0.85	112,112,112,112	0
22	MG	A	1843	1/1	0.97	0.22	0.82	456,456,456,456	0
22	MG	A	1834	1/1	0.92	0.16	0.64	349,349,349,349	0
22	MG	A	1883	1/1	0.96	0.15	0.38	500,500,500,500	0
23	ZN	D	301	1/1	1.00	0.31	0.32	119,119,119,119	0
22	MG	A	1641	1/1	0.99	0.17	0.08	158,158,158,158	0
22	MG	A	1961	1/1	0.87	0.19	0.04	126,126,126,126	0
22	MG	A	1710	1/1	0.75	0.14	0.03	105,105,105,105	0
22	MG	A	1629	1/1	0.96	0.19	-0.11	145,145,145,145	0
22	MG	A	1642	1/1	0.94	0.15	-0.20	96,96,96,96	0
22	MG	A	1673	1/1	0.98	0.21	-0.27	109,109,109,109	0
22	MG	A	1611	1/1	0.94	0.22	-0.27	148,148,148,148	0
23	ZN	N	101	1/1	0.99	0.18	-0.30	114,114,114,114	0
22	MG	A	1615	1/1	0.97	0.15	-0.47	98,98,98,98	0
22	MG	A	1863	1/1	0.96	0.10	-0.57	472,472,472,472	0
22	MG	A	1636	1/1	0.91	0.14	-0.77	79,79,79,79	0
22	MG	A	1678	1/1	0.98	0.16	-0.93	132,132,132,132	0
22	MG	A	1735	1/1	0.96	0.10	-0.94	87,87,87,87	0
22	MG	A	1701	1/1	0.99	0.15	-1.23	60,60,60,60	0
22	MG	A	1610	1/1	0.95	0.17	-1.33	123,123,123,123	0
22	MG	A	1743	1/1	0.99	0.23	-1.37	104,104,104,104	0
22	MG	A	1643	1/1	0.96	0.16	-1.44	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1830	1/1	0.97	0.09	-1.58	395,395,395,395	0
22	MG	A	1944	1/1	0.88	0.13	-2.12	153,153,153,153	0
22	MG	A	1605	1/1	0.99	0.13	-2.15	89,89,89,89	0
22	MG	A	1697	1/1	0.98	0.05	-2.48	87,87,87,87	0
22	MG	A	1839	1/1	0.98	0.11	-2.52	271,271,271,271	0
22	MG	B	302	1/1	0.84	0.06	-3.31	116,116,116,116	0
22	MG	A	1901	1/1	0.95	0.11	-3.49	212,212,212,212	0
22	MG	A	1632	1/1	0.99	0.07	-3.70	82,82,82,82	0
22	MG	A	1616	1/1	0.99	0.14	-4.78	88,88,88,88	0
22	MG	A	1664	1/1	0.93	0.09	-5.63	126,126,126,126	0
22	MG	A	1726	1/1	0.94	0.08	-9.37	104,104,104,104	0
22	MG	A	1941	1/1	0.97	0.24	-	132,132,132,132	0
22	MG	A	1809	1/1	0.88	0.42	-	485,485,485,485	0
22	MG	A	1656	1/1	0.94	0.26	-	166,166,166,166	0
22	MG	A	1916	1/1	0.91	1.28	-	290,290,290,290	0
22	MG	A	1651	1/1	0.68	0.86	-	131,131,131,131	0
22	MG	A	1776	1/1	0.93	0.19	-	523,523,523,523	0
22	MG	A	1951	1/1	0.52	0.52	-	131,131,131,131	0
22	MG	A	1848	1/1	0.85	1.23	-	550,550,550,550	0
22	MG	A	1875	1/1	0.78	0.32	-	447,447,447,447	0
22	MG	A	1671	1/1	0.94	0.30	-	121,121,121,121	0
22	MG	A	1874	1/1	0.89	0.25	-	437,437,437,437	0
22	MG	A	1728	1/1	0.86	0.17	-	140,140,140,140	0
22	MG	A	1797	1/1	0.91	0.23	-	431,431,431,431	0
22	MG	A	1972	1/1	0.85	0.17	-	135,135,135,135	0
22	MG	A	1935	1/1	0.76	0.40	-	102,102,102,102	0
22	MG	A	1620	1/1	0.96	0.87	-	82,82,82,82	0
22	MG	A	1919	1/1	0.80	0.41	-	401,401,401,401	0
22	MG	A	1750	1/1	0.97	0.09	-	96,96,96,96	0
22	MG	A	1617	1/1	0.92	1.04	-	107,107,107,107	0
22	MG	A	1654	1/1	0.85	0.50	-	113,113,113,113	0
22	MG	A	1626	1/1	0.97	0.10	-	169,169,169,169	0
22	MG	A	1741	1/1	0.97	0.10	-	137,137,137,137	0
22	MG	A	1959	1/1	0.81	0.42	-	133,133,133,133	0
22	MG	A	1733	1/1	0.88	0.09	-	116,116,116,116	0
22	MG	A	1713	1/1	0.98	0.26	-	107,107,107,107	0
22	MG	A	1677	1/1	0.98	0.07	-	191,191,191,191	0
22	MG	Q	201	1/1	0.71	0.44	-	99,99,99,99	0
22	MG	A	1872	1/1	0.91	0.21	-	389,389,389,389	0
22	MG	A	1974	1/1	0.83	0.33	-	137,137,137,137	0
22	MG	A	1660	1/1	0.84	0.14	-	132,132,132,132	0
22	MG	A	1818	1/1	0.74	0.25	-	478,478,478,478	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1842	1/1	0.95	0.09	-	151,151,151,151	0
22	MG	A	1716	1/1	0.96	0.49	-	132,132,132,132	0
22	MG	A	1930	1/1	0.96	0.09	-	156,156,156,156	0
22	MG	A	1922	1/1	0.74	0.39	-	446,446,446,446	0
22	MG	A	1640	1/1	0.97	0.32	-	143,143,143,143	0
22	MG	A	1925	1/1	0.99	0.12	-	262,262,262,262	0
22	MG	A	1706	1/1	0.94	0.36	-	110,110,110,110	0
22	MG	A	1734	1/1	0.96	0.65	-	91,91,91,91	0
22	MG	A	1822	1/1	0.97	0.28	-	443,443,443,443	0
22	MG	A	1789	1/1	0.83	0.09	-	529,529,529,529	0
22	MG	A	1645	1/1	0.83	0.29	-	144,144,144,144	0
22	MG	A	1679	1/1	0.99	0.18	-	107,107,107,107	0
22	MG	A	1933	1/1	0.88	0.34	-	483,483,483,483	0
22	MG	A	1790	1/1	0.85	0.42	-	504,504,504,504	0
22	MG	A	1672	1/1	0.88	0.13	-	144,144,144,144	0
22	MG	A	1738	1/1	0.94	0.21	-	114,114,114,114	0
22	MG	A	1751	1/1	0.64	0.30	-	130,130,130,130	0
22	MG	A	1852	1/1	0.97	0.26	-	480,480,480,480	0
22	MG	O	1000	1/1	0.71	0.37	-	242,242,242,242	0
22	MG	A	1754	1/1	0.76	0.41	-	170,170,170,170	0
22	MG	A	1784	1/1	0.72	0.54	-	486,486,486,486	0
22	MG	A	1787	1/1	0.97	0.24	-	430,430,430,430	0
22	MG	A	1634	1/1	0.97	0.31	-	154,154,154,154	0
22	MG	G	201	1/1	0.22	0.25	-	550,550,550,550	0
22	MG	A	1964	1/1	0.93	0.43	-	124,124,124,124	0
22	MG	A	1745	1/1	0.98	0.45	-	236,236,236,236	0
22	MG	A	1886	1/1	0.97	0.30	-	490,490,490,490	0
22	MG	A	1777	1/1	0.80	0.32	-	481,481,481,481	0
22	MG	A	1824	1/1	0.75	1.22	-	484,484,484,484	0
22	MG	A	1770	1/1	0.92	0.14	-	532,532,532,532	0
22	MG	A	1845	1/1	0.91	0.28	-	395,395,395,395	0
22	MG	D	304	1/1	0.94	0.12	-	470,470,470,470	0
22	MG	A	1762	1/1	0.97	0.09	-	137,137,137,137	0
22	MG	A	1652	1/1	0.98	0.17	-	95,95,95,95	0
22	MG	C	301	1/1	0.94	0.18	-	111,111,111,111	0
22	MG	A	1855	1/1	0.75	0.19	-	466,466,466,466	0
22	MG	N	103	1/1	0.93	0.06	-	333,333,333,333	0
22	MG	A	1889	1/1	0.93	0.21	-	456,456,456,456	0
22	MG	A	1820	1/1	0.74	0.39	-	448,448,448,448	0
22	MG	A	1700	1/1	0.91	0.77	-	142,142,142,142	0
22	MG	A	1914	1/1	0.85	0.41	-	439,439,439,439	0
22	MG	A	1690	1/1	0.94	0.05	-	190,190,190,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1653	1/1	0.95	0.08	-	228,228,228,228	0
22	MG	A	1693	1/1	0.92	0.50	-	131,131,131,131	0
22	MG	A	1955	1/1	0.79	0.12	-	132,132,132,132	0
22	MG	A	1621	1/1	0.50	0.66	-	178,178,178,178	0
22	MG	A	1851	1/1	0.90	0.22	-	481,481,481,481	0
22	MG	A	1956	1/1	0.83	0.26	-	156,156,156,156	0
22	MG	A	1828	1/1	0.84	0.56	-	467,467,467,467	0
22	MG	A	1823	1/1	0.94	0.10	-	496,496,496,496	0
22	MG	A	1674	1/1	0.88	0.19	-	189,189,189,189	0
22	MG	A	1604	1/1	0.88	0.35	-	93,93,93,93	0
22	MG	A	1917	1/1	0.67	0.65	-	456,456,456,456	0
22	MG	A	1887	1/1	0.98	0.49	-	191,191,191,191	0
22	MG	A	1891	1/1	0.88	1.05	-	496,496,496,496	0
22	MG	A	1965	1/1	0.94	0.23	-	101,101,101,101	0
22	MG	A	1912	1/1	1.00	0.17	-	46,46,46,46	0
22	MG	A	1811	1/1	0.98	0.29	-	436,436,436,436	0
22	MG	A	1736	1/1	0.81	0.63	-	118,118,118,118	0
22	MG	A	1768	1/1	0.63	0.23	-	501,501,501,501	0
22	MG	A	1759	1/1	0.89	0.41	-	496,496,496,496	0
22	MG	A	1783	1/1	0.80	0.20	-	535,535,535,535	0
22	MG	A	1744	1/1	0.85	0.06	-	237,237,237,237	0
22	MG	A	1939	1/1	0.70	0.49	-	103,103,103,103	0
22	MG	A	1832	1/1	0.91	0.22	-	312,312,312,312	0
22	MG	A	1758	1/1	0.91	0.53	-	481,481,481,481	0
22	MG	A	1897	1/1	0.94	0.49	-	428,428,428,428	0
22	MG	A	1903	1/1	0.98	0.16	-	223,223,223,223	0
22	MG	A	1847	1/1	0.93	0.48	-	453,453,453,453	0
22	MG	A	1833	1/1	0.95	0.19	-	319,319,319,319	0
22	MG	A	1607	1/1	0.96	0.14	-	121,121,121,121	0
22	MG	A	1877	1/1	0.98	0.23	-	460,460,460,460	0
22	MG	A	1766	1/1	0.74	0.28	-	549,549,549,549	0
22	MG	A	1708	1/1	0.61	0.69	-	129,129,129,129	0
22	MG	A	1771	1/1	0.94	0.37	-	519,519,519,519	0
22	MG	A	1739	1/1	0.89	0.31	-	83,83,83,83	0
22	MG	A	1749	1/1	0.96	0.05	-	122,122,122,122	0
22	MG	A	1946	1/1	0.74	0.45	-	155,155,155,155	0
22	MG	A	1633	1/1	0.92	0.39	-	101,101,101,101	0
22	MG	A	1689	1/1	0.82	0.61	-	125,125,125,125	0
22	MG	A	1960	1/1	0.56	0.27	-	136,136,136,136	0
22	MG	A	1603	1/1	0.95	0.04	-	157,157,157,157	0
22	MG	A	1819	1/1	0.96	0.57	-	360,360,360,360	0
22	MG	A	1963	1/1	0.90	0.31	-	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1850	1/1	0.95	0.26	-	233,233,233,233	0
22	MG	A	1904	1/1	0.98	0.29	-	217,217,217,217	0
22	MG	A	1829	1/1	0.90	0.42	-	507,507,507,507	0
22	MG	A	1853	1/1	0.97	0.43	-	264,264,264,264	0
22	MG	D	305	1/1	0.58	0.57	-	103,103,103,103	0
22	MG	A	1772	1/1	0.94	0.19	-	274,274,274,274	0
22	MG	A	1702	1/1	0.97	0.22	-	122,122,122,122	0
22	MG	A	1793	1/1	0.88	0.38	-	550,550,550,550	0
22	MG	A	1967	1/1	0.11	0.85	-	144,144,144,144	0
22	MG	A	1966	1/1	0.77	0.17	-	138,138,138,138	0
22	MG	A	1950	1/1	0.70	0.45	-	126,126,126,126	0
22	MG	A	1723	1/1	0.72	0.42	-	126,126,126,126	0
22	MG	A	1601	1/1	0.98	0.04	-	145,145,145,145	0
22	MG	A	1870	1/1	0.98	0.24	-	444,444,444,444	0
22	MG	A	1840	1/1	0.75	0.20	-	493,493,493,493	0
22	MG	A	1858	1/1	0.76	0.93	-	429,429,429,429	0
22	MG	A	1663	1/1	0.99	0.38	-	166,166,166,166	0
22	MG	A	1688	1/1	0.78	0.45	-	122,122,122,122	0
22	MG	A	1649	1/1	0.86	0.45	-	137,137,137,137	0
22	MG	A	1927	1/1	0.97	0.15	-	160,160,160,160	0
22	MG	A	1612	1/1	0.99	0.34	-	116,116,116,116	0
22	MG	A	1923	1/1	0.80	0.31	-	424,424,424,424	0
22	MG	A	1608	1/1	0.94	0.11	-	122,122,122,122	0
22	MG	A	1895	1/1	0.97	0.68	-	525,525,525,525	0
22	MG	A	1884	1/1	0.99	0.37	-	428,428,428,428	0
22	MG	A	1748	1/1	0.95	0.30	-	153,153,153,153	0
22	MG	A	1948	1/1	0.64	0.98	-	127,127,127,127	0
22	MG	A	1942	1/1	0.65	0.43	-	122,122,122,122	0
22	MG	A	1742	1/1	0.71	0.51	-	133,133,133,133	0
22	MG	A	1953	1/1	0.68	0.18	-	130,130,130,130	0
22	MG	A	1658	1/1	0.50	0.10	-	207,207,207,207	0
22	MG	A	1813	1/1	0.97	0.13	-	491,491,491,491	0
22	MG	A	1646	1/1	0.97	0.25	-	95,95,95,95	0
22	MG	I	201	1/1	0.73	0.31	-	137,137,137,137	0
22	MG	K	201	1/1	0.79	0.08	-	123,123,123,123	0
22	MG	A	1780	1/1	0.92	0.12	-	432,432,432,432	0
22	MG	A	1796	1/1	0.88	0.42	-	480,480,480,480	0
22	MG	A	1805	1/1	0.92	0.94	-	550,550,550,550	0
22	MG	A	1888	1/1	0.93	0.19	-	470,470,470,470	0
22	MG	A	1624	1/1	0.82	0.30	-	106,106,106,106	0
22	MG	A	1720	1/1	0.93	0.27	-	130,130,130,130	0
22	MG	A	1812	1/1	0.94	0.18	-	474,474,474,474	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1737	1/1	0.59	0.13	-	133,133,133,133	0
22	MG	A	1881	1/1	0.90	0.31	-	525,525,525,525	0
22	MG	A	1764	1/1	0.68	0.29	-	502,502,502,502	0
22	MG	A	1826	1/1	0.96	0.06	-	537,537,537,537	0
22	MG	A	1775	1/1	0.73	0.20	-	538,538,538,538	0
22	MG	A	1683	1/1	0.66	1.00	-	135,135,135,135	0
22	MG	A	1876	1/1	0.68	0.46	-	422,422,422,422	0
22	MG	A	1761	1/1	0.98	0.11	-	458,458,458,458	0
22	MG	A	1622	1/1	0.93	0.21	-	119,119,119,119	0
22	MG	A	1907	1/1	0.99	0.08	-	329,329,329,329	0
22	MG	L	201	1/1	0.92	0.45	-	468,468,468,468	0
22	MG	C	302	1/1	0.53	0.57	-	122,122,122,122	0
22	MG	A	1841	1/1	0.91	0.70	-	462,462,462,462	0
22	MG	A	1860	1/1	0.90	0.39	-	434,434,434,434	0
22	MG	A	1781	1/1	0.68	0.25	-	504,504,504,504	0
22	MG	A	1866	1/1	0.83	0.13	-	497,497,497,497	0
22	MG	A	1808	1/1	0.97	0.11	-	480,480,480,480	0
22	MG	A	1712	1/1	0.80	0.45	-	123,123,123,123	0
22	MG	A	1915	1/1	0.94	0.42	-	419,419,419,419	0
22	MG	A	1864	1/1	0.94	0.29	-	316,316,316,316	0
22	MG	A	1900	1/1	0.96	0.37	-	442,442,442,442	0
22	MG	A	1659	1/1	0.52	0.46	-	131,131,131,131	0
22	MG	A	1769	1/1	0.88	0.07	-	397,397,397,397	0
22	MG	I	202	1/1	0.74	0.20	-	146,146,146,146	0
22	MG	A	1717	1/1	0.96	0.27	-	102,102,102,102	0
22	MG	A	1707	1/1	0.78	0.38	-	100,100,100,100	0
22	MG	A	1740	1/1	0.97	0.10	-	85,85,85,85	0
22	MG	A	1630	1/1	0.93	0.34	-	146,146,146,146	0
22	MG	A	1785	1/1	0.90	0.06	-	353,353,353,353	0
22	MG	A	1976	1/1	0.76	0.14	-	133,133,133,133	0
22	MG	A	1969	1/1	0.92	0.15	-	78,78,78,78	0
22	MG	A	1644	1/1	0.83	0.58	-	141,141,141,141	0
22	MG	A	1755	1/1	0.91	0.20	-	144,144,144,144	0
22	MG	A	1890	1/1	0.94	0.47	-	425,425,425,425	0
22	MG	A	1856	1/1	0.71	0.23	-	484,484,484,484	0
22	MG	A	1827	1/1	0.90	0.42	-	500,500,500,500	0
22	MG	F	201	1/1	0.93	0.10	-	435,435,435,435	0
22	MG	A	1625	1/1	0.75	0.34	-	188,188,188,188	0
22	MG	A	1947	1/1	0.92	0.25	-	116,116,116,116	0
22	MG	A	1732	1/1	0.71	0.32	-	123,123,123,123	0
22	MG	A	1694	1/1	0.91	0.20	-	127,127,127,127	0
22	MG	A	1804	1/1	0.90	0.16	-	318,318,318,318	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1802	1/1	0.90	0.56	-	458,458,458,458	0
22	MG	A	1757	1/1	0.79	0.48	-	550,550,550,550	0
22	MG	A	1936	1/1	0.75	0.46	-	110,110,110,110	0
22	MG	A	1885	1/1	0.87	0.14	-	534,534,534,534	0
22	MG	A	1859	1/1	0.74	0.36	-	495,495,495,495	0
22	MG	A	1831	1/1	0.85	0.36	-	486,486,486,486	0
22	MG	A	1869	1/1	0.78	0.20	-	550,550,550,550	0
22	MG	A	1662	1/1	0.98	0.06	-	110,110,110,110	0
22	MG	A	1871	1/1	0.97	0.14	-	426,426,426,426	0
22	MG	A	1779	1/1	0.91	0.19	-	411,411,411,411	0
22	MG	A	1635	1/1	0.92	0.21	-	74,74,74,74	0
22	MG	A	1857	1/1	0.36	0.39	-	487,487,487,487	0
22	MG	A	1910	1/1	0.96	0.63	-	526,526,526,526	0
22	MG	A	1685	1/1	0.94	0.14	-	141,141,141,141	0
22	MG	A	1613	1/1	0.97	0.17	-	97,97,97,97	0
22	MG	A	1799	1/1	0.88	0.47	-	550,550,550,550	0
22	MG	A	1695	1/1	0.90	0.19	-	118,118,118,118	0
22	MG	H	201	1/1	0.94	0.40	-	421,421,421,421	0
22	MG	A	1623	1/1	0.97	0.10	-	90,90,90,90	0
22	MG	A	1795	1/1	0.90	0.25	-	416,416,416,416	0
22	MG	A	1928	1/1	0.90	0.49	-	126,126,126,126	0
22	MG	A	1905	1/1	0.92	0.17	-	426,426,426,426	0
22	MG	A	1821	1/1	0.85	0.42	-	543,543,543,543	0
22	MG	A	1682	1/1	0.81	0.11	-	218,218,218,218	0
22	MG	A	1940	1/1	0.81	0.69	-	119,119,119,119	0
22	MG	A	1962	1/1	0.97	0.25	-	127,127,127,127	0
22	MG	A	1773	1/1	0.87	0.43	-	550,550,550,550	0
22	MG	A	1913	1/1	0.96	0.20	-	317,317,317,317	0
22	MG	A	1810	1/1	0.97	0.07	-	264,264,264,264	0
22	MG	A	1908	1/1	0.96	0.24	-	345,345,345,345	0
22	MG	D	302	1/1	0.74	0.18	-	92,92,92,92	0
22	MG	C	303	1/1	0.82	0.07	-	144,144,144,144	0
22	MG	A	1817	1/1	0.96	0.28	-	385,385,385,385	0
22	MG	A	1973	1/1	0.70	0.24	-	137,137,137,137	0
22	MG	A	1725	1/1	0.96	0.13	-	120,120,120,120	0
22	MG	A	1639	1/1	0.98	0.12	-	126,126,126,126	0
22	MG	A	1814	1/1	0.86	0.24	-	506,506,506,506	0
22	MG	A	1727	1/1	0.57	0.48	-	122,122,122,122	0
22	MG	A	1945	1/1	0.80	0.17	-	168,168,168,168	0
22	MG	A	1752	1/1	0.96	0.47	-	141,141,141,141	0
22	MG	A	1667	1/1	0.98	0.07	-	112,112,112,112	0
22	MG	A	1763	1/1	0.89	0.15	-	451,451,451,451	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	E	201	1/1	0.84	0.13	-	135,135,135,135	0
22	MG	A	1631	1/1	0.95	0.29	-	99,99,99,99	0
22	MG	A	1937	1/1	0.99	0.06	-	107,107,107,107	0
22	MG	A	1882	1/1	0.87	0.29	-	501,501,501,501	0
22	MG	A	1619	1/1	0.91	0.27	-	132,132,132,132	0
22	MG	A	1730	1/1	0.83	0.32	-	118,118,118,118	0
22	MG	A	1920	1/1	0.96	0.18	-	245,245,245,245	0
22	MG	A	1854	1/1	0.99	0.12	-	126,126,126,126	0
22	MG	A	1760	1/1	0.97	0.33	-	407,407,407,407	0
22	MG	A	1719	1/1	0.72	0.98	-	121,121,121,121	0
22	MG	A	1618	1/1	0.78	0.27	-	107,107,107,107	0
22	MG	A	1765	1/1	0.84	0.32	-	482,482,482,482	0
22	MG	A	1879	1/1	0.98	0.17	-	509,509,509,509	0
22	MG	A	1709	1/1	0.79	0.31	-	112,112,112,112	0
22	MG	A	1837	1/1	0.73	0.16	-	523,523,523,523	0
22	MG	A	1918	1/1	0.89	0.26	-	422,422,422,422	0
22	MG	A	1801	1/1	0.91	0.58	-	480,480,480,480	0
22	MG	A	1878	1/1	0.76	0.29	-	498,498,498,498	0
22	MG	A	1932	1/1	0.99	0.22	-	92,92,92,92	0
22	MG	A	1794	1/1	0.99	0.08	-	393,393,393,393	0
22	MG	A	1747	1/1	0.70	0.26	-	131,131,131,131	0
22	MG	A	1637	1/1	1.00	0.12	-	124,124,124,124	0
22	MG	A	1670	1/1	0.99	0.19	-	87,87,87,87	0
22	MG	A	1703	1/1	0.92	0.30	-	125,125,125,125	0
22	MG	A	1894	1/1	0.99	0.37	-	379,379,379,379	0
22	MG	A	1924	1/1	0.91	0.09	-	322,322,322,322	0
22	MG	A	1698	1/1	0.96	0.33	-	113,113,113,113	0
22	MG	A	1705	1/1	0.98	0.20	-	135,135,135,135	0
22	MG	A	1606	1/1	0.89	0.16	-	183,183,183,183	0
22	MG	A	1696	1/1	0.89	0.30	-	127,127,127,127	0
22	MG	A	1788	1/1	0.71	0.23	-	550,550,550,550	0
22	MG	A	1957	1/1	0.90	0.37	-	105,105,105,105	0
22	MG	A	1868	1/1	0.95	0.06	-	442,442,442,442	0
22	MG	A	1838	1/1	0.92	0.42	-	388,388,388,388	0
22	MG	A	1880	1/1	0.91	0.21	-	431,431,431,431	0
22	MG	A	1792	1/1	0.68	0.42	-	530,530,530,530	0
22	MG	A	1602	1/1	0.99	0.16	-	124,124,124,124	0
22	MG	A	1684	1/1	0.81	0.52	-	121,121,121,121	0
22	MG	A	1970	1/1	0.68	0.17	-	140,140,140,140	0
22	MG	A	1816	1/1	0.90	0.44	-	449,449,449,449	0
22	MG	A	1729	1/1	0.89	0.26	-	125,125,125,125	0
22	MG	A	1929	1/1	0.80	0.77	-	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1798	1/1	0.88	0.29	-	550,550,550,550	0
22	MG	A	1899	1/1	0.92	0.24	-	550,550,550,550	0
22	MG	S	101	1/1	0.84	0.17	-	127,127,127,127	0
22	MG	A	1778	1/1	0.81	0.10	-	232,232,232,232	0
22	MG	A	1638	1/1	0.97	0.28	-	96,96,96,96	0
22	MG	A	1807	1/1	0.83	1.65	-	550,550,550,550	0
22	MG	A	1714	1/1	0.96	0.18	-	76,76,76,76	0
22	MG	A	1675	1/1	0.50	1.31	-	125,125,125,125	0
22	MG	A	1655	1/1	0.90	0.22	-	150,150,150,150	0
22	MG	A	1849	1/1	0.88	0.36	-	512,512,512,512	0
22	MG	A	1934	1/1	0.95	0.21	-	111,111,111,111	0
22	MG	A	1896	1/1	0.78	0.60	-	436,436,436,436	0
22	MG	A	1774	1/1	0.96	0.08	-	402,402,402,402	0
22	MG	A	1731	1/1	0.95	0.45	-	114,114,114,114	0
22	MG	A	1867	1/1	0.92	0.36	-	459,459,459,459	0
22	MG	A	1681	1/1	0.99	0.14	-	247,247,247,247	0
22	MG	A	1668	1/1	0.53	0.24	-	111,111,111,111	0
22	MG	Q	202	1/1	0.94	0.27	-	455,455,455,455	0
22	MG	A	1825	1/1	0.96	0.62	-	490,490,490,490	0
22	MG	A	1836	1/1	0.94	0.11	-	409,409,409,409	0
22	MG	A	1609	1/1	0.96	0.21	-	114,114,114,114	0
22	MG	A	1800	1/1	0.94	0.30	-	441,441,441,441	0
22	MG	A	1786	1/1	0.96	0.08	-	300,300,300,300	0
22	MG	A	1949	1/1	0.56	0.52	-	116,116,116,116	0
22	MG	A	1911	1/1	0.70	0.44	-	502,502,502,502	0
22	MG	A	1791	1/1	0.92	0.72	-	373,373,373,373	0
22	MG	A	1938	1/1	0.91	0.36	-	149,149,149,149	0
22	MG	A	1909	1/1	0.99	0.18	-	149,149,149,149	0
22	MG	A	1661	1/1	0.94	0.64	-	163,163,163,163	0
22	MG	A	1902	1/1	0.87	0.46	-	435,435,435,435	0
22	MG	A	1873	1/1	0.99	0.35	-	390,390,390,390	0
22	MG	A	1954	1/1	0.59	0.43	-	139,139,139,139	0
22	MG	A	1648	1/1	0.97	0.12	-	121,121,121,121	0
22	MG	A	1753	1/1	0.92	0.52	-	117,117,117,117	0
22	MG	A	1906	1/1	0.94	0.23	-	394,394,394,394	0
22	MG	A	1958	1/1	0.80	0.36	-	124,124,124,124	0
22	MG	A	1835	1/1	0.90	0.12	-	363,363,363,363	0
22	MG	A	1756	1/1	0.98	0.64	-	127,127,127,127	0
22	MG	A	1782	1/1	0.78	0.23	-	501,501,501,501	0
22	MG	A	1898	1/1	0.85	0.53	-	463,463,463,463	0
22	MG	P	101	1/1	0.62	0.39	-	111,111,111,111	0
22	MG	A	1861	1/1	0.80	0.65	-	497,497,497,497	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1952	1/1	0.97	0.26	-	93,93,93,93	0
22	MG	A	1862	1/1	0.71	0.17	-	487,487,487,487	0
22	MG	A	1650	1/1	0.97	0.17	-	129,129,129,129	0
22	MG	A	1844	1/1	0.93	0.13	-	369,369,369,369	0
22	MG	A	1669	1/1	0.99	0.18	-	137,137,137,137	0
22	MG	A	1977	1/1	0.92	0.22	-	129,129,129,129	0
22	MG	A	1846	1/1	0.99	0.15	-	484,484,484,484	0
22	MG	A	1943	1/1	0.59	0.62	-	139,139,139,139	0
22	MG	A	1968	1/1	0.82	0.86	-	127,127,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.