



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:57 am BST

PDB ID : 4JI2
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 : 3.64 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

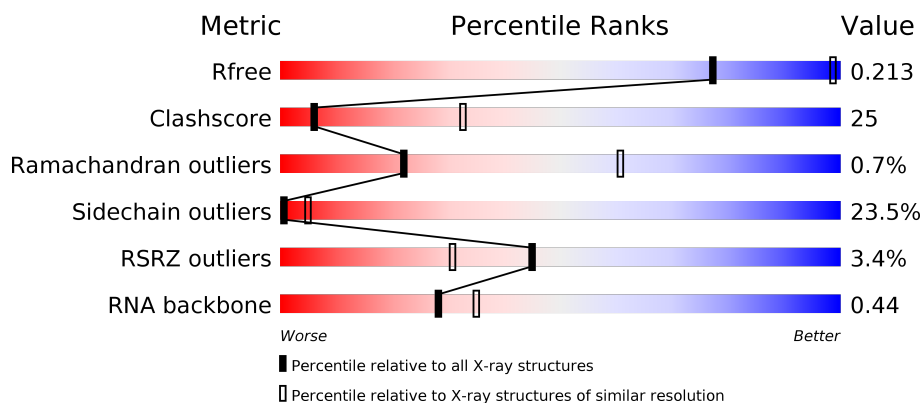
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 Å.

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





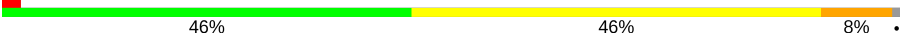
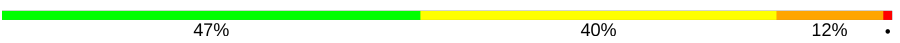


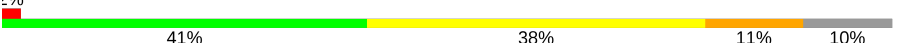
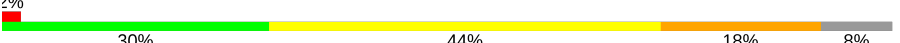
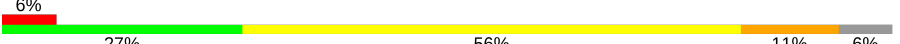

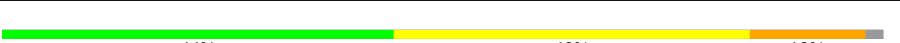
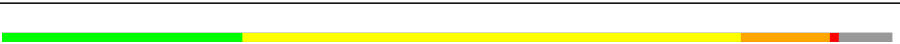
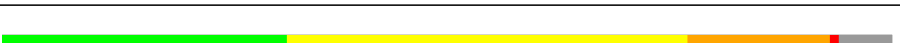
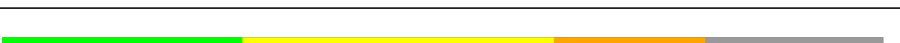

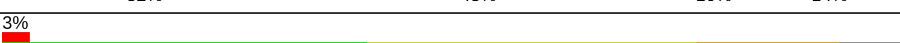
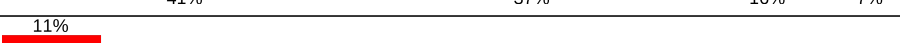
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)
RNA backbone	3102	1019 (4.26-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>2%</div> <div>16% 41% 33% 9%</div> </div>
2	B	256	<div> <div>%</div> <div>37% 40% 13% 9%</div> </div>
3	C	239	<div> <div>6%</div> <div>27% 44% 14% 14%</div> </div>
4	D	209	<div> <div>2%</div> <div>35% 49% 14%</div> </div>

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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
1	PSU	A	1540	-	-	-	X
1	5MC	A	967	-	-	X	-
22	MG	A	1601	-	-	-	X
22	MG	A	1683	-	-	-	X
22	MG	A	1704	-	-	-	X
22	MG	A	1715	-	-	-	X
22	MG	A	1720	-	-	-	X
22	MG	A	1735	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1749	-	-	-	X
22	MG	A	1751	-	-	-	X
22	MG	A	1766	-	-	-	X
22	MG	A	1769	-	-	-	X
22	MG	A	1770	-	-	-	X
22	MG	A	1777	-	-	-	X
22	MG	A	1780	-	-	-	X
22	MG	A	1781	-	-	-	X
22	MG	A	1782	-	-	-	X
22	MG	A	1794	-	-	-	X
22	MG	A	1796	-	-	-	X
22	MG	A	1826	-	-	-	X
22	MG	A	1830	-	-	-	X
22	MG	A	1835	-	-	-	X
22	MG	A	1838	-	-	-	X
22	MG	A	1839	-	-	-	X
22	MG	A	1842	-	-	-	X
22	MG	A	1845	-	-	-	X
22	MG	A	1847	-	-	-	X
22	MG	A	1853	-	-	-	X
22	MG	A	1857	-	-	-	X
22	MG	A	1858	-	-	-	X
22	MG	A	1866	-	-	-	X
22	MG	C	301	-	-	-	X
22	MG	H	201	-	-	-	X
22	MG	P	102	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52307 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	1512	Total	C	N	O	P	0	6	0
			32644	14540	6039	10547	1518			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

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

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	2	Total	Mg	0	0
			2	2		
22	J	1	Total	Mg	0	0
			1	1		
22	Q	1	Total	Mg	0	0
			1	1		
22	D	3	Total	Mg	0	0
			3	3		
22	E	1	Total	Mg	0	0
			1	1		
22	H	1	Total	Mg	0	0
			1	1		
22	B	3	Total	Mg	0	0
			3	3		
22	I	1	Total	Mg	0	0
			1	1		
22	C	2	Total	Mg	0	0
			2	2		
22	A	276	Total	Mg	0	0
			276	276		
22	N	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		

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

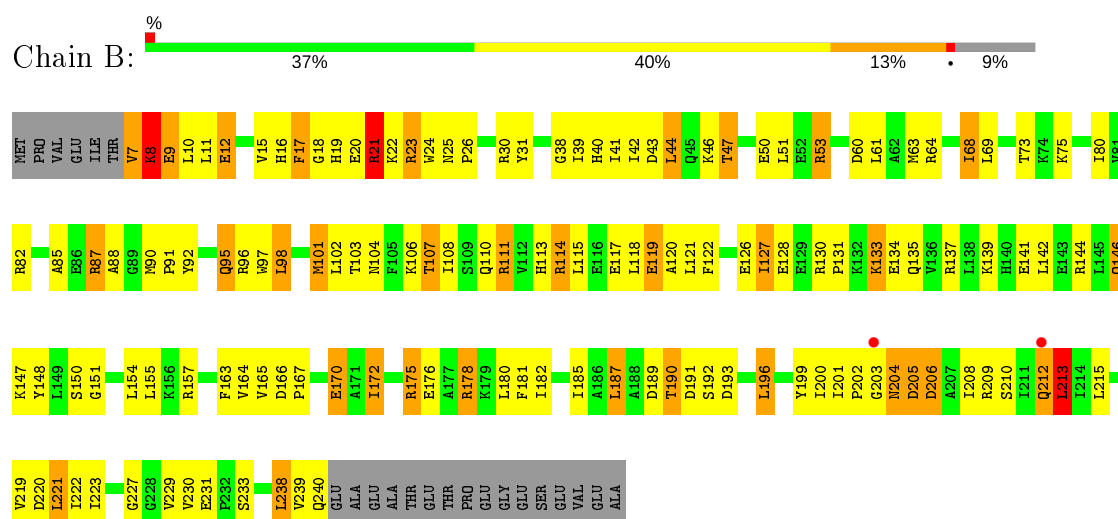
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	D	1	Total 1	Zn 1	0	0
23	N	1	Total 1	Zn 1	0	0

- Molecule 24 is water.

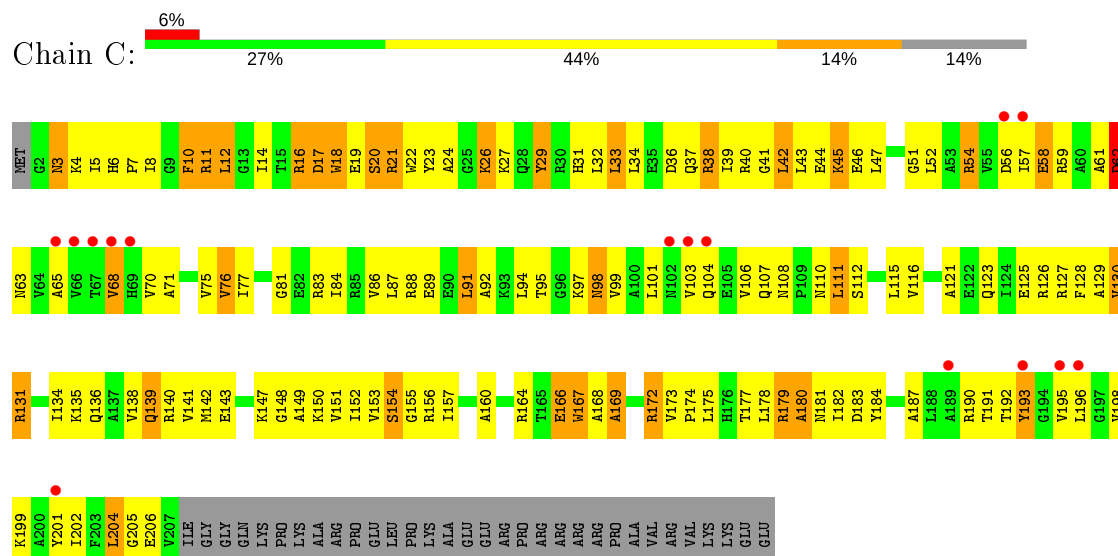
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	266	Total 266	O 266	0	0
24	E	3	Total 3	O 3	0	0
24	K	1	Total 1	O 1	0	0
24	L	1	Total 1	O 1	0	0
24	Q	2	Total 2	O 2	0	0
24	T	2	Total 2	O 2	0	0

U1532	C1397	G1338	G1276	G1214	G1149	U1078	U1020	U960	G998	C832	G770	C707
C1533	A1398	A1339	C1277	G1215	U1150	G1079	G1021	U961	C899	U833	G771	C708
A	C1399	A1340	U1278	G1216	A1151	A1080	G1022	G982	A900	U834	G772	
C	U1341	U1342	A1279	G1217	A1152	G1081	G1023	G983	A901	U835	G773	A712
U	G1401	G1343	A1280	C1218	C1153	G1084	G1024	A984	G902	G836	G774	G713
C	C1402	G1344	U1281	U1219	G1085	U1086	U1025	A965	G903	G837	G775	G714
C1539	C1403	U1345	G1282	G1220	A1187	U1088	G1026	G966	C904	U838	A777	A715
	C1404	U1346	G1283	G1221	C1158	U1089	C1027	G967		U839	A778	A716
	C1405	A1347	C1284	G1222	U1159	U1090	C1028	A968	A907	C840	C779	C717
	U1406	G1348	A1287	C1223	G1160	U1091	G1030A	A969	A908	U841	A780	G718
	C1407	A1349	U1288	G1224	C1161	U1092	G1030B	A970	A909	U842	A781	G719
	A1408	A1350	A1289	G1225	C1162	A1093	G1030C	G971	C910	C849	A782	C720
		U1351	A1290	C1226	G1164	G1094	A1030D	C972	C911	U850	C783	G721
		C1352	G1291	A1227	U1167	U1095	G1031	G973	C912	G851	C784	A722
		G1353	U1292	C1228	A1167	U1096	G1032	A974	A913	G852	C785	A723
		C1354	G1293	A1229	U1178	C1097	G1033	A975	A914	G853	C786	G724
		G1355	G1294	U1232	A1169	U1098	G1034	G976	A915	G854	A787	G725
		G1356	G1295	G1233	G1171	U1099	A1035	A977	G916	G855	U788	C726
		A1357	C1296	G1234	C1172	C1100	G1036	G978	G917	C856	U789	G727
		U1358	C1297	C1235	G1173	A1101	C1037	G979	A918	C857	A790	A728
		C1359	A1298	A1236	G1174	A1102	C1038	U980	A919	G858	A791	A729
		A1360	G1299	C1237	G1175	C1103		U981	U920	A859	A792	G730
		G1361	U1300	A1238	A1176	G1104	A1041	A983	U921	A860	U793	G731
		C1361A	U1301	U1239	G1177		G1042	U984	G922	G861	A794	C732
		C1362	U1302	U1240	G1178		G1043	C985	A923	C862	A795	C733
		A1363	G1303	G1241	U1179	G1108	C1043	A986	C924	U863	C796	G734
		U1364	C1304	C1242	A1180	C1109	A1044		G925	A864	C797	C735
		G1365	G1305	C1243	G1181	A1110	C1045		G926	A865	C798	C736
		C1366	A1306	G1244	G1182	A1111	A1046		G927	A866	A737	C737
		C1367	U1307	A1245	A1183	C1112	G1047		G928	G867	C738	A738
		G1368	U1308	C1246	G1184	C1113	G1048		G929	C868	C739	
		C1369	G1309	U1249	G1185		U1049		C930	U869	U740	
		G1370	G1310	C1249	U1186	G1117	G1050		C931	U870	U804	G741
		C1371	G1311	A1250	G1187	C1118	U1051		C932	U871	C805	G742
		U1372	G1312	A1251	U1188	C1119	U1052		C933	A872	C806	U743
		G1373	U1313	A1252	A1189	A1123	G1053		C934	A873	A807	C744
		A1374	C1314	G1253	C1189	U1124	A1054		C935	G874	C808	C745
		U1375	U1315	G1254	G1190	U1125	A1055		C936	C875	G809	A746
		C1376	G1316	G1255	A1191	U1126	U1056		A937	U876	C810	C747
		A1377	C1317	A1256	C1192	U1127	U1057		A938	C877	C811	C748
		C1378	A1318	U1257	G1193	C1128	G1058		G939	G878	C812	C749
		U1379	C1319	G1258	U1194	C1129	C1059		C940	C879	U813	G750
		C1380	C1320	C1259	G1195	A1130	G1060		G941	C880	A814	U751
		U1381	G1321	C1260	U1196	C1131	G1061		G942	C881	A815	C752
		C1382	A1322	A1261	G1198	C1132	U1062		U943	C882	A816	A753
		C1383	G1323	C1262	U1199		G1063		G944	C883	C817	C754
		C1384	A1324	G1263	C1200	U1135	G1064		A945	G884	G818	G755
		G1385	C1325	C1264	A1201	G1136	U1065		A946	G885	A819	C756
		U1386	G1326	G1265	G1202	C1137	C1066		G947	G886	U820	U757
		C1387	C1327	G1266	C1203	G1138	A1067		C948	G887	G821	G758
		G1388	C1328	G1267	A1204	C1139	G1068		A949	C888	C822	A759
		C1389	U1330	C1268	U1205	C1140	C1069		U950	A889	G823	G760
		U1390	G1331	A1269	G1206	C1141	U1070		G951	G890	C824	G761
		C1391	A1332	C1270	G1207	G1142	C1071		U952	U891	G825	C762
		U1392	C1333	G1271	C1208	G1143	U1072		G953	A892	C826	
		G1393	G1334	G1272	U1211	C1144	U1073		G954	C893	U827	G765
		A1394	C1335	G1273	A1146	C1145	G1074		U955	G894	A828	A766
		C1395	G1336	G1274	U1212	C1147	C1075		U956	G895	G829	A767
		A1396	G1337	A1275	A1213	U1148	G1077		A959	C896	G830	G769

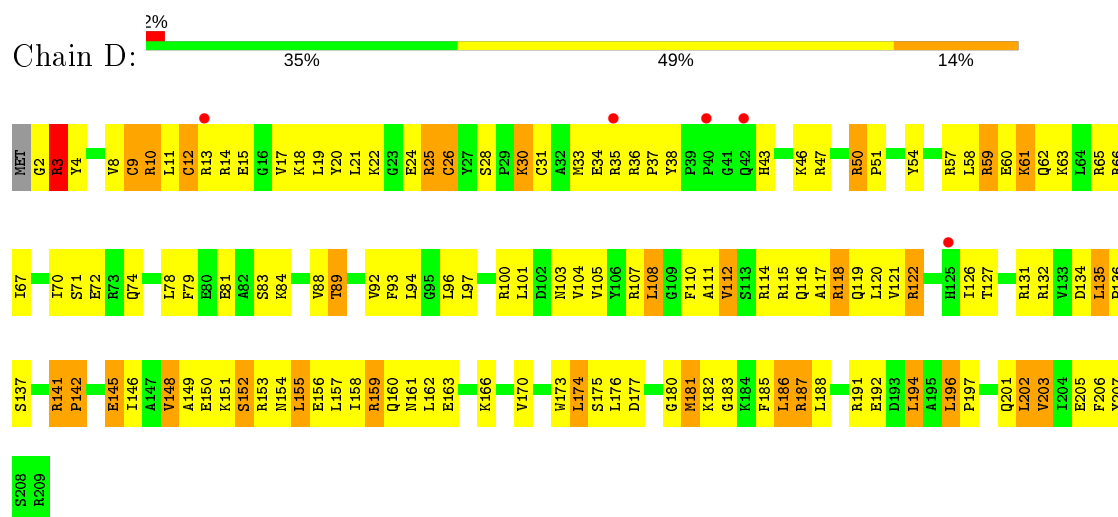
• Molecule 2: RIBOSOMAL PROTEIN S2



• Molecule 3: RIBOSOMAL PROTEIN S3

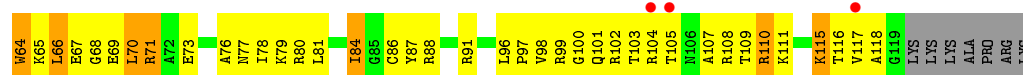


• Molecule 4: RIBOSOMAL PROTEIN S4

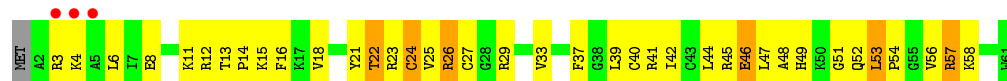


• Molecule 5: RIBOSOMAL PROTEIN S5

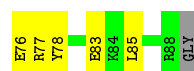
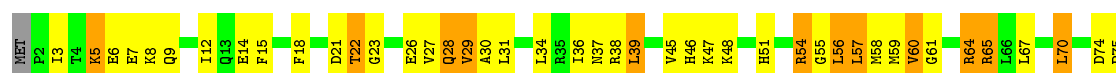




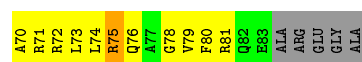
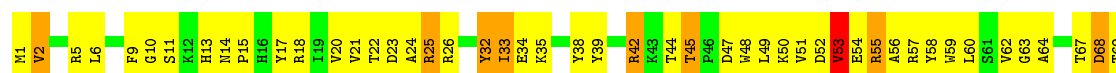
• Molecule 14: RIBOSOMAL PROTEIN S14



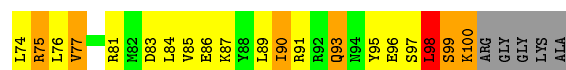
• Molecule 15: RIBOSOMAL PROTEIN S15



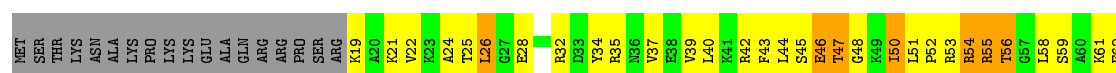
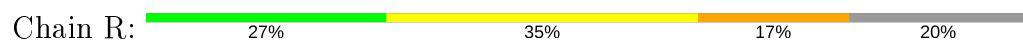
• Molecule 16: RIBOSOMAL PROTEIN S16



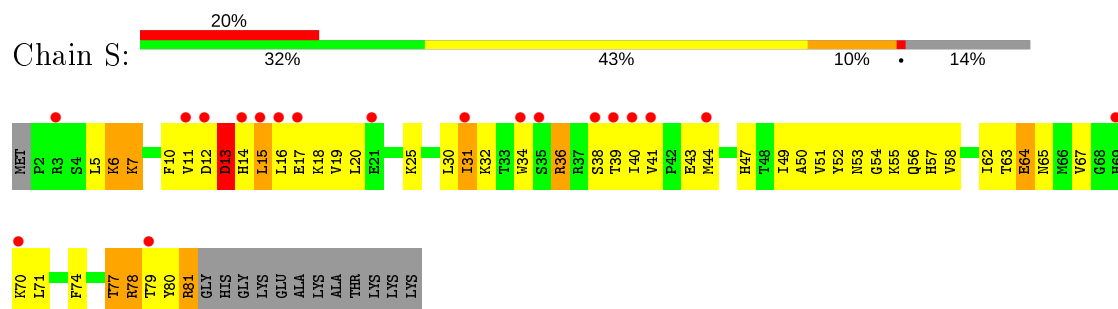
• Molecule 17: RIBOSOMAL PROTEIN S17



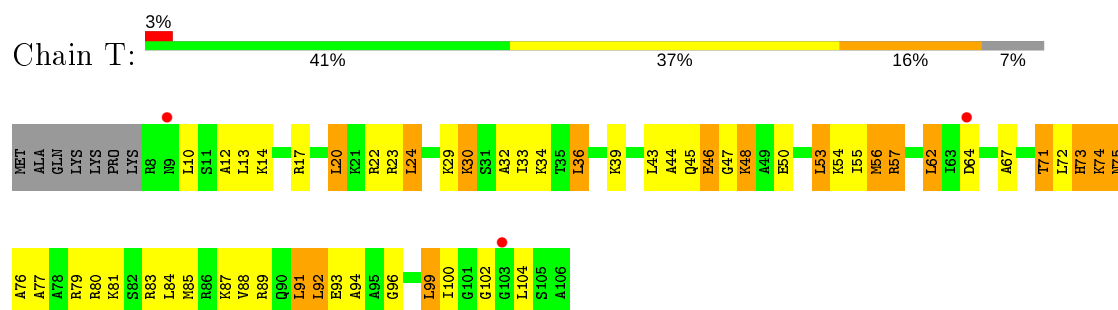
• Molecule 18: RIBOSOMAL PROTEIN S18



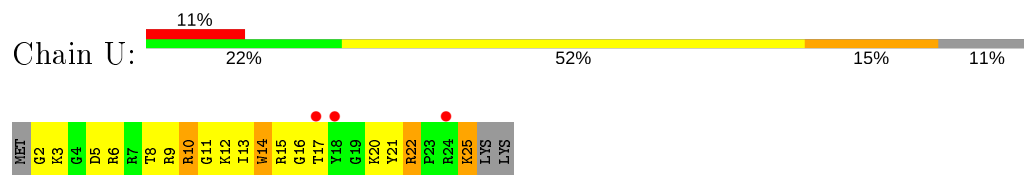
- Molecule 19: RIBOSOMAL PROTEIN S19



- Molecule 20: RIBOSOMAL PROTEIN S20



- Molecule 21: RIBOSOMAL PROTEIN THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.45Å 402.45Å 174.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 3.64 49.57 – 3.64	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.34-3.64) 98.9 (49.57-3.64)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.67Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.155 , 0.211 0.158 , 0.213	Depositor DCC
R_{free} test set	7893 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	120.3	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 134.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52307	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, 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	1.21	178/36139 (0.5%)	2.00	1849/56396 (3.3%)
2	B	0.71	0/1935	0.91	3/2609 (0.1%)
3	C	0.58	1/1636 (0.1%)	0.84	1/2205 (0.0%)
4	D	0.75	1/1733 (0.1%)	0.89	3/2318 (0.1%)
5	E	0.99	0/1162	1.13	2/1564 (0.1%)
6	F	0.61	0/856	0.81	0/1154
7	G	0.58	0/1276	0.78	0/1709
8	H	1.07	2/1136 (0.2%)	1.15	2/1527 (0.1%)
9	I	0.57	0/1029	0.79	0/1379
10	J	0.53	0/805	0.83	1/1082 (0.1%)
11	K	0.69	0/879	0.92	1/1187 (0.1%)
12	L	0.79	0/994	0.98	0/1331
13	M	0.64	0/947	0.87	0/1270
14	N	0.55	0/501	0.77	0/664
15	O	0.79	0/740	0.96	0/987
16	P	0.84	0/716	1.01	3/963 (0.3%)
17	Q	1.02	1/836 (0.1%)	1.14	2/1117 (0.2%)
18	R	0.75	0/579	0.98	1/768 (0.1%)
19	S	0.52	0/661	0.80	0/890
20	T	0.73	0/765	0.99	2/1007 (0.2%)
21	U	0.64	0/212	0.76	0/277
All	All	1.07	183/55537 (0.3%)	1.74	1870/82404 (2.3%)

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	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
7	G	0	1
8	H	0	2
10	J	0	2
12	L	0	2
13	M	0	1
18	R	0	1
19	S	0	1
20	T	0	2
All	All	0	18

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-13.71	1.29	1.37
1	A	279	A	N3-C4	-13.61	1.26	1.34
1	A	279	A	N7-C5	-11.36	1.32	1.39
1	A	817	C	N1-C6	-10.06	1.31	1.37
1	A	793	U	C2-N3	9.46	1.44	1.37
1	A	722	A	C5-C6	-9.32	1.32	1.41
1	A	915	A	N9-C4	-8.68	1.32	1.37
1	A	882	C	N3-C4	-8.61	1.27	1.33
1	A	729	A	N9-C4	-8.47	1.32	1.37
1	A	566	G	N7-C5	-8.30	1.34	1.39
1	A	1509	C	N3-C4	-8.22	1.28	1.33
1	A	1504	G	N7-C5	-8.21	1.34	1.39
1	A	793	U	N3-C4	8.11	1.45	1.38
1	A	574	A	C5-C4	-8.01	1.33	1.38
1	A	1502	A	C5-C6	-7.88	1.33	1.41
1	A	824	C	N1-C6	-7.80	1.32	1.37
1	A	779	C	N1-C6	-7.77	1.32	1.37
1	A	814	A	N9-C4	-7.69	1.33	1.37
1	A	1377	A	N9-C4	-7.65	1.33	1.37
1	A	860	A	N3-C4	-7.65	1.30	1.34
1	A	852	G	C6-O6	7.61	1.31	1.24
1	A	122	G	C2-N3	-7.57	1.26	1.32
4	D	12	CYS	CB-SG	7.56	1.95	1.82
1	A	1514	C	N3-C4	-7.51	1.28	1.33
1	A	882	C	N1-C6	-7.37	1.32	1.37
1	A	1514	C	N1-C6	-7.33	1.32	1.37
1	A	1077	G	N9-C8	-7.32	1.32	1.37
1	A	722	A	N7-C5	-7.30	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	A	N9-C4	-7.21	1.33	1.37
1	A	574	A	N7-C5	-7.21	1.34	1.39
1	A	1509	C	N1-C6	-7.18	1.32	1.37
1	A	266	G	N7-C5	-7.01	1.35	1.39
1	A	1504	G	N9-C8	-6.92	1.33	1.37
1	A	715	A	N9-C4	-6.89	1.33	1.37
1	A	1502	A	N9-C4	-6.87	1.33	1.37
1	A	228	A	N9-C4	-6.81	1.33	1.37
1	A	122	G	C5-C6	-6.74	1.35	1.42
1	A	576	G	N3-C4	-6.73	1.30	1.35
1	A	298	A	N3-C4	-6.72	1.30	1.34
1	A	569	C	N3-C4	-6.71	1.29	1.33
1	A	727	G	C6-N1	-6.70	1.34	1.39
1	A	728	A	N9-C4	-6.69	1.33	1.37
1	A	16	A	N9-C4	-6.68	1.33	1.37
1	A	787	A	N9-C4	-6.55	1.33	1.37
1	A	574	A	N9-C8	-6.52	1.32	1.37
1	A	703	G	C6-O6	6.40	1.29	1.24
1	A	1502	A	N7-C5	-6.39	1.35	1.39
1	A	828	A	N9-C4	-6.38	1.34	1.37
1	A	295	C	N3-C4	-6.35	1.29	1.33
1	A	236	G	N7-C5	-6.31	1.35	1.39
1	A	1094	G	C6-N1	-6.29	1.35	1.39
1	A	1499	A	N9-C4	-6.27	1.34	1.37
1	A	574	A	N3-C4	-6.25	1.31	1.34
1	A	568	G	C6-N1	-6.24	1.35	1.39
1	A	263	A	N9-C4	-6.23	1.34	1.37
1	A	558	G	C5-C6	-6.22	1.36	1.42
1	A	573	A	N7-C5	-6.20	1.35	1.39
1	A	119	A	N9-C4	-6.19	1.34	1.37
1	A	122	G	N3-C4	-6.19	1.31	1.35
1	A	279	A	C5-C6	-6.16	1.35	1.41
1	A	298	A	N9-C4	-6.13	1.34	1.37
1	A	1079	G	N7-C5	-6.09	1.35	1.39
1	A	329	A	C5-C6	-6.07	1.35	1.41
1	A	865	A	C5-C4	-6.07	1.34	1.38
1	A	797	C	N1-C6	-6.06	1.33	1.37
1	A	130	A	N3-C4	-6.05	1.31	1.34
8	H	135	CYS	CB-SG	-6.03	1.72	1.82
1	A	915	A	N3-C4	-6.02	1.31	1.34
1	A	876	G	C6-N1	-5.99	1.35	1.39
1	A	1064	G	N3-C4	-5.98	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1394	A	C5-C6	-5.98	1.35	1.41
1	A	646	U	C4-O4	5.98	1.28	1.23
1	A	753	A	N3-C4	-5.94	1.31	1.34
1	A	124	G	C6-N1	-5.93	1.35	1.39
1	A	1502	A	N3-C4	-5.93	1.31	1.34
1	A	1076	C	N1-C6	-5.91	1.33	1.37
1	A	246	A	C5-C4	-5.89	1.34	1.38
1	A	635	G	C6-O6	5.89	1.29	1.24
1	A	828	A	N3-C4	-5.88	1.31	1.34
1	A	938	A	N9-C4	-5.88	1.34	1.37
1	A	727	G	N7-C5	-5.87	1.35	1.39
1	A	248	C	N1-C6	-5.87	1.33	1.37
3	C	169	ALA	CA-CB	-5.86	1.40	1.52
1	A	570	G	C5-C4	-5.85	1.34	1.38
1	A	589	C	N1-C6	-5.84	1.33	1.37
1	A	703	G	C5-C6	5.84	1.48	1.42
1	A	873	A	C6-N1	-5.80	1.31	1.35
1	A	288	A	N9-C4	-5.78	1.34	1.37
1	A	909	A	N9-C4	-5.78	1.34	1.37
1	A	325	A	N9-C4	-5.77	1.34	1.37
1	A	1499	A	N3-C4	-5.75	1.31	1.34
1	A	923	A	C5-C6	-5.74	1.35	1.41
1	A	1401	G	C6-N1	-5.73	1.35	1.39
1	A	1386	G	N9-C8	-5.73	1.33	1.37
1	A	574	A	N9-C4	-5.73	1.34	1.37
1	A	1504	G	C5-C4	-5.71	1.34	1.38
1	A	569	C	N1-C6	-5.71	1.33	1.37
1	A	561	U	N1-C6	-5.71	1.32	1.38
1	A	266	G	C2-N3	5.70	1.37	1.32
1	A	873	A	C6-N6	-5.69	1.29	1.33
1	A	855	G	N3-C4	-5.67	1.31	1.35
1	A	803	G	C5-C4	-5.66	1.34	1.38
1	A	298	A	C5-C4	-5.65	1.34	1.38
1	A	1232	U	N1-C2	-5.65	1.33	1.38
1	A	836	G	C6-O6	5.64	1.29	1.24
1	A	236	G	C5-C4	-5.63	1.34	1.38
1	A	130	A	N9-C4	-5.59	1.34	1.37
1	A	828	A	N7-C5	-5.57	1.35	1.39
1	A	1507	A	N9-C4	-5.56	1.34	1.37
1	A	856	C	N1-C6	-5.56	1.33	1.37
1	A	918	A	C5-C4	-5.54	1.34	1.38
1	A	877	C	N3-C4	-5.53	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1500	A	N3-C4	-5.52	1.31	1.34
1	A	861	G	N3-C4	-5.51	1.31	1.35
1	A	803	G	N1-C2	-5.50	1.33	1.37
1	A	291	C	N1-C6	-5.48	1.33	1.37
1	A	570	G	N1-C2	-5.46	1.33	1.37
1	A	553	A	N9-C4	-5.45	1.34	1.37
1	A	722	A	N9-C4	-5.44	1.34	1.37
1	A	269	C	N3-C4	-5.44	1.30	1.33
1	A	817	C	N3-C4	-5.43	1.30	1.33
1	A	739	C	N3-C4	-5.42	1.30	1.33
1	A	1525	G	N3-C4	-5.41	1.31	1.35
1	A	482	A	N7-C5	-5.39	1.36	1.39
1	A	856	C	N1-C2	-5.38	1.34	1.40
1	A	896	C	N3-C4	-5.36	1.30	1.33
1	A	852	G	C5-C4	5.36	1.42	1.38
1	A	807	A	C6-N1	-5.36	1.31	1.35
1	A	861	G	N7-C5	-5.35	1.36	1.39
1	A	1526	G	C5-C6	-5.33	1.37	1.42
1	A	634	C	N3-C4	-5.32	1.30	1.33
1	A	109	A	N9-C4	-5.32	1.34	1.37
1	A	329	A	N7-C5	-5.32	1.36	1.39
1	A	733	A	N9-C4	-5.32	1.34	1.37
1	A	150	C	N1-C6	-5.31	1.33	1.37
1	A	1513	A	N9-C4	-5.31	1.34	1.37
1	A	814	A	N3-C4	-5.30	1.31	1.34
1	A	570	G	C6-N1	-5.29	1.35	1.39
1	A	632	A	N3-C4	-5.29	1.31	1.34
1	A	862	C	C4-N4	-5.29	1.29	1.33
1	A	882	C	C2-N3	-5.29	1.31	1.35
1	A	1080	A	N3-C4	-5.28	1.31	1.34
1	A	120	A	N9-C4	-5.27	1.34	1.37
1	A	862	C	C4-C5	-5.26	1.38	1.43
1	A	448	A	N7-C5	-5.25	1.36	1.39
1	A	308	C	N1-C6	-5.24	1.34	1.37
1	A	568	G	C5-C4	-5.23	1.34	1.38
1	A	807	A	N9-C4	-5.22	1.34	1.37
1	A	559	A	N7-C5	-5.22	1.36	1.39
17	Q	32	TYR	CD1-CE1	5.21	1.47	1.39
1	A	125	U	C2-N3	-5.19	1.34	1.37
1	A	1487	G	C6-N1	-5.19	1.35	1.39
1	A	306	G	C6-N1	5.19	1.43	1.39
1	A	881	G	N3-C4	-5.18	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	A	N9-C4	-5.17	1.34	1.37
1	A	861	G	C5-C6	-5.16	1.37	1.42
1	A	931	C	N1-C6	-5.15	1.34	1.37
1	A	753	A	N9-C4	-5.14	1.34	1.37
1	A	852	G	C6-N1	5.14	1.43	1.39
1	A	798	G	N3-C4	-5.13	1.31	1.35
8	H	49	GLU	CG-CD	5.13	1.59	1.51
1	A	802	A	C5-C6	-5.13	1.36	1.41
1	A	860	A	N9-C4	-5.12	1.34	1.37
1	A	855	G	C5-C4	-5.11	1.34	1.38
1	A	1066	C	N1-C6	-5.11	1.34	1.37
1	A	1078	U	C4-C5	-5.11	1.39	1.43
1	A	820	U	C4-O4	-5.11	1.19	1.23
1	A	828	A	C5-C4	-5.10	1.35	1.38
1	A	563	A	N3-C4	-5.09	1.31	1.34
1	A	1052	U	C2-N3	5.09	1.41	1.37
1	A	825	G	C5-C4	-5.08	1.34	1.38
1	A	151	A	N9-C4	-5.07	1.34	1.37
1	A	640	A	N3-C4	-5.06	1.31	1.34
1	A	655	A	C6-N6	-5.05	1.29	1.33
1	A	821	G	C5-C6	-5.05	1.37	1.42
1	A	874	G	N9-C8	-5.04	1.34	1.37
1	A	576	G	C6-N1	-5.04	1.36	1.39
1	A	564	C	N3-C4	-5.03	1.30	1.33
1	A	1064	G	N9-C4	-5.03	1.33	1.38
1	A	119	A	N3-C4	-5.02	1.31	1.34
1	A	771	G	N9-C8	-5.02	1.34	1.37
1	A	712	A	N9-C4	-5.01	1.34	1.37
1	A	1513	A	N3-C4	-5.01	1.31	1.34

All (1870) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	G	C6-C5-N7	-17.70	119.78	130.40
1	A	735	C	C6-N1-C2	16.27	126.81	120.30
1	A	117	G	N1-C6-O6	15.58	129.25	119.90
1	A	1516[A]	G	C8-N9-C4	-14.80	100.48	106.40
1	A	1516[B]	G	C8-N9-C4	-14.80	100.48	106.40
1	A	635	G	C5-C6-N1	-14.69	104.16	111.50
1	A	117	G	C6-C5-N7	-14.54	121.67	130.40
1	A	770	C	O5'-P-OP2	-14.03	93.08	105.70
1	A	722	A	N1-C6-N6	13.90	126.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	G	N1-C6-O6	13.37	127.92	119.90
1	A	558	G	C4-C5-N7	13.37	116.15	110.80
1	A	242	C	C6-N1-C2	13.32	125.63	120.30
1	A	793	U	C5-C6-N1	13.23	129.31	122.70
1	A	852	G	C5-C6-N1	-13.22	104.89	111.50
1	A	232	G	N9-C4-C5	-12.93	100.23	105.40
1	A	1532	U	C5-C6-N1	12.85	129.13	122.70
1	A	279	A	C2-N3-C4	-12.72	104.24	110.60
1	A	481	G	N3-C4-N9	12.71	133.62	126.00
1	A	873	A	N1-C6-N6	-12.70	110.98	118.60
1	A	266	G	N7-C8-N9	12.63	119.42	113.10
1	A	266	G	C5-N7-C8	-12.57	98.01	104.30
1	A	919	A	O5'-P-OP2	-12.55	94.40	105.70
1	A	279	A	C4-C5-C6	12.54	123.27	117.00
1	A	232	G	N1-C6-O6	12.46	127.38	119.90
1	A	774	G	N1-C6-O6	12.43	127.36	119.90
1	A	122	G	N1-C6-O6	12.42	127.35	119.90
1	A	266	G	C4-C5-N7	12.34	115.73	110.80
1	A	279	A	C6-C5-N7	-12.16	123.78	132.30
1	A	117	G	C5-C6-N1	-12.08	105.46	111.50
1	A	279	A	N7-C8-N9	12.07	119.83	113.80
1	A	366	C	N1-C2-O2	12.02	126.11	118.90
1	A	722	A	C2-N3-C4	-11.93	104.64	110.60
1	A	573	A	C8-N9-C4	-11.85	101.06	105.80
1	A	266	G	N1-C6-O6	11.81	126.98	119.90
1	A	279	A	C5-N7-C8	-11.79	98.00	103.90
1	A	117	G	C4-C5-C6	11.78	125.86	118.80
1	A	722	A	C6-C5-N7	-11.69	124.12	132.30
1	A	245	C	C5-C4-N4	-11.62	112.07	120.20
1	A	279	A	C8-N9-C4	-11.56	101.18	105.80
1	A	266	G	C4-N9-C1'	11.51	141.47	126.50
1	A	279	A	N1-C2-N3	11.48	135.04	129.30
1	A	1370	G	C8-N9-C4	-11.46	101.81	106.40
1	A	884	U	C5-C6-N1	-11.43	116.99	122.70
1	A	1502	A	C2-N3-C4	-11.41	104.89	110.60
1	A	1386	G	C8-N9-C4	11.35	110.94	106.40
1	A	835	U	C5-C4-O4	11.32	132.69	125.90
1	A	277	C	N3-C4-C5	11.28	126.41	121.90
1	A	805	C	C6-N1-C2	11.25	124.80	120.30
1	A	301	G	O5'-P-OP2	-11.23	95.59	105.70
1	A	635	G	C2-N3-C4	-11.19	106.31	111.90
1	A	277	C	C6-N1-C2	11.18	124.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	873	A	C5-C6-N1	11.15	123.28	117.70
1	A	1516[A]	G	N9-C4-C5	11.12	109.85	105.40
1	A	1516[B]	G	N9-C4-C5	11.12	109.85	105.40
1	A	570	G	N1-C6-O6	-11.10	113.24	119.90
1	A	948	C	C6-N1-C2	11.09	124.73	120.30
1	A	117	G	C2-N3-C4	-11.06	106.37	111.90
1	A	817	C	C5-C6-N1	-10.96	115.52	121.00
1	A	722	A	C4-C5-N7	10.92	116.16	110.70
1	A	1344	C	C6-N1-C2	10.87	124.65	120.30
1	A	703	G	C4-C5-N7	-10.84	106.46	110.80
1	A	1190	G	C6-C5-N7	-10.79	123.92	130.40
1	A	283	C	N3-C4-C5	-10.79	117.58	121.90
1	A	245	C	N3-C4-N4	10.74	125.52	118.00
1	A	1395	C	O5'-P-OP2	-10.74	96.03	105.70
1	A	1436	U	N3-C2-O2	-10.63	114.76	122.20
1	A	117	G	C8-N9-C1'	-10.63	113.19	127.00
1	A	836	G	C5-C6-N1	-10.59	106.20	111.50
1	A	825	G	C8-N9-C4	10.58	110.63	106.40
1	A	1346	A	O5'-P-OP2	-10.58	96.18	105.70
1	A	525	C	C6-N1-C2	10.57	124.53	120.30
1	A	814	A	C2-N3-C4	-10.56	105.32	110.60
1	A	875	C	C6-N1-C2	10.56	124.52	120.30
1	A	824	C	C6-N1-C2	10.55	124.52	120.30
1	A	16	A	C8-N9-C4	10.55	110.02	105.80
1	A	283	C	C6-N1-C2	-10.53	116.09	120.30
1	A	1502	A	C6-C5-N7	-10.51	124.95	132.30
1	A	1190	G	C4-N9-C1'	10.50	140.16	126.50
1	A	882	C	C5-C6-N1	-10.48	115.76	121.00
1	A	1528	U	O5'-P-OP2	-10.48	96.26	105.70
1	A	635	G	N1-C6-O6	10.47	126.18	119.90
1	A	1158	C	C6-N1-C2	-10.44	116.12	120.30
1	A	1369	C	C6-N1-C2	-10.44	116.12	120.30
1	A	875	C	C5-C6-N1	-10.42	115.79	121.00
1	A	125	U	C5-C6-N1	-10.42	117.49	122.70
1	A	558	G	C5-N7-C8	-10.40	99.10	104.30
1	A	1374	A	O5'-P-OP2	-10.39	96.35	105.70
1	A	865	A	C5-C6-N1	10.38	122.89	117.70
1	A	1502	A	C5-N7-C8	-10.33	98.74	103.90
1	A	1502	A	N1-C6-N6	10.31	124.79	118.60
1	A	731	G	N1-C6-O6	10.30	126.08	119.90
1	A	558	G	C6-C5-N7	-10.30	124.22	130.40
1	A	481	G	C5-C6-O6	-10.29	122.43	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1526	G	N1-C6-O6	10.27	126.06	119.90
1	A	15	G	N1-C6-O6	10.23	126.04	119.90
1	A	703	G	C5-C6-O6	10.23	134.74	128.60
1	A	232	G	C4-C5-N7	10.21	114.88	110.80
1	A	745	C	N3-C4-C5	10.19	125.98	121.90
1	A	481	G	N3-C4-C5	-10.18	123.51	128.60
1	A	1200	C	C2-N1-C1'	10.16	129.97	118.80
1	A	856	C	N1-C2-O2	-10.14	112.82	118.90
1	A	329	A	C2-N3-C4	-10.09	105.56	110.60
1	A	1227	A	N1-C6-N6	10.08	124.65	118.60
1	A	570	G	C2-N3-C4	10.07	116.94	111.90
1	A	568	G	O5'-P-OP2	-10.07	96.64	105.70
1	A	836	G	N1-C6-O6	10.05	125.93	119.90
1	A	283	C	C5-C6-N1	10.04	126.02	121.00
1	A	817	C	C4-C5-C6	9.85	122.32	117.40
1	A	511	C	C5-C6-N1	-9.84	116.08	121.00
1	A	117	G	C4-N9-C1'	9.82	139.27	126.50
1	A	812	C	N3-C4-C5	-9.79	117.98	121.90
1	A	774	G	C4-C5-N7	9.78	114.71	110.80
1	A	871	U	O5'-P-OP1	-9.77	96.91	105.70
1	A	144	G	N1-C6-O6	9.74	125.75	119.90
1	A	933	G	N1-C6-O6	9.73	125.74	119.90
1	A	122	G	N3-C4-C5	9.68	133.44	128.60
1	A	745	C	C6-N1-C2	9.67	124.17	120.30
1	A	1052	U	C5-C6-N1	9.66	127.53	122.70
1	A	252	U	C5-C6-N1	-9.59	117.91	122.70
1	A	600	C	C2-N3-C4	-9.53	115.13	119.90
1	A	558	G	N1-C6-O6	9.52	125.61	119.90
1	A	860	A	N1-C2-N3	9.52	134.06	129.30
1	A	317	G	C6-C5-N7	-9.51	124.70	130.40
1	A	519	C	C6-N1-C2	9.51	124.10	120.30
1	A	1530	G	C8-N9-C4	9.49	110.20	106.40
1	A	266	G	C4-C5-C6	9.48	124.48	118.80
1	A	317	G	C4-C5-N7	9.46	114.58	110.80
1	A	600	C	N3-C4-C5	9.44	125.68	121.90
1	A	853	G	C5-C6-N1	-9.42	106.79	111.50
1	A	1347	G	N3-C4-C5	-9.41	123.89	128.60
1	A	266	G	C8-N9-C1'	-9.41	114.76	127.00
1	A	774	G	C5-C6-O6	-9.41	122.95	128.60
1	A	1502	A	C4-C5-N7	9.41	115.41	110.70
1	A	366	C	N3-C2-O2	-9.39	115.33	121.90
1	A	379	C	C6-N1-C2	9.38	124.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1200	C	C5-C6-N1	9.37	125.69	121.00
1	A	1528	U	O5'-P-OP1	9.37	121.94	110.70
1	A	862	C	N3-C4-C5	9.37	125.65	121.90
1	A	742	G	N1-C6-O6	9.36	125.52	119.90
1	A	280	C	OP1-P-OP2	9.35	133.63	119.60
1	A	559	A	C8-N9-C4	-9.35	102.06	105.80
1	A	835	U	N1-C2-N3	9.34	120.50	114.90
1	A	314	C	C6-N1-C2	9.31	124.03	120.30
1	A	722	A	C5-N7-C8	-9.30	99.25	103.90
1	A	1490	C	C4-C5-C6	-9.27	112.76	117.40
1	A	1190	G	C8-N9-C1'	-9.27	114.95	127.00
1	A	721	G	C4-N9-C1'	9.26	138.54	126.50
1	A	389	A	N9-C4-C5	9.26	109.50	105.80
1	A	1200	C	N1-C2-O2	9.26	124.45	118.90
1	A	793	U	N1-C2-N3	-9.25	109.35	114.90
1	A	615	C	C6-N1-C2	-9.23	116.61	120.30
1	A	1227	A	C5-N7-C8	-9.20	99.30	103.90
1	A	900	A	C2-N3-C4	-9.19	106.00	110.60
1	A	1344	C	C5-C6-N1	-9.17	116.42	121.00
1	A	51	A	C8-N9-C4	-9.16	102.14	105.80
1	A	721	G	C8-N9-C1'	-9.14	115.12	127.00
1	A	816	A	C8-N9-C4	9.11	109.44	105.80
1	A	389	A	N1-C2-N3	9.08	133.84	129.30
1	A	835	U	N3-C4-C5	-9.07	109.16	114.60
1	A	1532	U	C4-C5-C6	-9.07	114.26	119.70
1	A	852	G	C2-N3-C4	-9.07	107.37	111.90
1	A	1516[A]	G	N7-C8-N9	9.06	117.63	113.10
1	A	1516[B]	G	N7-C8-N9	9.06	117.63	113.10
1	A	1383	C	C6-N1-C2	-9.05	116.68	120.30
1	A	1526	G	C5-C6-O6	-9.04	123.17	128.60
1	A	774	G	C6-C5-N7	-9.02	124.99	130.40
1	A	120	A	C2-N3-C4	-8.99	106.11	110.60
1	A	232	G	C6-C5-N7	-8.98	125.01	130.40
1	A	599	C	C6-N1-C2	8.98	123.89	120.30
1	A	793	U	N3-C4-O4	8.98	125.69	119.40
1	A	1233	G	N1-C6-O6	8.98	125.29	119.90
1	A	235	C	C6-N1-C2	8.96	123.88	120.30
1	A	239	U	O5'-P-OP1	-8.96	97.64	105.70
1	A	864	A	N1-C6-N6	-8.96	113.23	118.60
1	A	647	C	C6-N1-C2	8.96	123.88	120.30
1	A	16	A	N7-C8-N9	-8.94	109.33	113.80
1	A	579	G	C5-C6-O6	-8.93	123.25	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1347	G	P-O3'-C3'	8.92	130.40	119.70
1	A	872	A	N1-C6-N6	8.91	123.95	118.60
1	A	920	U	C5-C4-O4	8.90	131.24	125.90
1	A	945	G	C5-C6-O6	-8.89	123.27	128.60
1	A	242	C	O5'-P-OP2	-8.89	97.70	105.70
1	A	933	G	C5-C6-O6	-8.88	123.27	128.60
1	A	1347	G	N3-C4-N9	8.89	131.33	126.00
1	A	570	G	C5-C6-N1	8.86	115.93	111.50
1	A	309	G	N9-C4-C5	-8.84	101.86	105.40
1	A	1181	G	C8-N9-C4	8.84	109.94	106.40
1	A	1394	A	N1-C6-N6	8.83	123.90	118.60
1	A	481	G	C2-N3-C4	8.81	116.31	111.90
1	A	666	G	C5-C6-N1	-8.81	107.09	111.50
1	A	279	A	C5-C6-N1	-8.80	113.30	117.70
1	A	882	C	N3-C2-O2	-8.80	115.74	121.90
1	A	529	G	C6-C5-N7	-8.79	125.13	130.40
1	A	626	U	C6-N1-C2	-8.79	115.73	121.00
1	A	867	G	N3-C4-N9	8.78	131.27	126.00
1	A	637	G	C8-N9-C4	8.78	109.91	106.40
1	A	126	G	C5-C6-N1	-8.77	107.12	111.50
1	A	511	C	C6-N1-C2	8.76	123.80	120.30
1	A	654	G	N3-C2-N2	-8.76	113.77	119.90
1	A	805	C	N3-C4-C5	8.76	125.40	121.90
1	A	1483	A	C8-N9-C4	8.76	109.30	105.80
1	A	864	A	C5-C6-N6	8.74	130.69	123.70
1	A	279	A	N1-C6-N6	8.74	123.84	118.60
1	A	570	G	N3-C4-C5	-8.73	124.23	128.60
1	A	232	G	C8-N9-C4	8.73	109.89	106.40
1	A	29	G	C2-N3-C4	-8.72	107.54	111.90
1	A	600	C	C5-C6-N1	-8.72	116.64	121.00
1	A	856	C	N3-C4-C5	-8.72	118.41	121.90
1	A	1490	C	N1-C2-O2	8.72	124.13	118.90
1	A	128	G	N1-C6-O6	8.71	125.12	119.90
1	A	1504	G	O5'-P-OP1	-8.70	97.87	105.70
1	A	167	G	C8-N9-C1'	-8.67	115.72	127.00
1	A	823	G	N1-C2-N3	8.67	129.10	123.90
1	A	824	C	C5-C6-N1	-8.67	116.66	121.00
1	A	874	G	O5'-P-OP2	-8.66	97.90	105.70
1	A	588	G	O5'-P-OP2	-8.64	97.92	105.70
1	A	1448	C	C6-N1-C2	8.62	123.75	120.30
1	A	389	A	C4-C5-N7	-8.61	106.40	110.70
1	A	569	C	C5-C6-N1	-8.60	116.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	A	C8-N9-C4	-8.59	102.36	105.80
1	A	1365	G	C8-N9-C4	-8.59	102.96	106.40
1	A	817	C	C6-N1-C2	8.59	123.74	120.30
1	A	721	G	N3-C4-N9	8.59	131.15	126.00
1	A	774	G	N9-C4-C5	-8.57	101.97	105.40
1	A	110	C	N3-C2-O2	8.57	127.90	121.90
1	A	7	G	N3-C4-N9	8.56	131.14	126.00
1	A	933	G	C6-C5-N7	-8.56	125.26	130.40
1	A	309	G	C2-N3-C4	-8.56	107.62	111.90
1	A	353	A	N1-C6-N6	-8.56	113.46	118.60
1	A	1073	U	C5-C6-N1	-8.54	118.43	122.70
17	Q	98	LEU	CA-CB-CG	8.53	134.91	115.30
1	A	1227	A	C4-C5-N7	8.50	114.95	110.70
1	A	703	G	C5-C6-N1	-8.50	107.25	111.50
1	A	167	G	N3-C4-N9	8.49	131.10	126.00
1	A	131	C	C5-C6-N1	-8.49	116.75	121.00
1	A	793	U	N3-C2-O2	8.49	128.14	122.20
1	A	232	G	C5-C6-O6	-8.48	123.51	128.60
1	A	579	G	N1-C6-O6	8.47	124.98	119.90
1	A	815	A	N1-C6-N6	8.47	123.68	118.60
1	A	289	G	C5-C6-O6	-8.46	123.53	128.60
3	C	179	ARG	N-CA-C	-8.45	88.17	111.00
1	A	1529	G	O5'-P-OP1	-8.45	98.10	105.70
1	A	858	G	N1-C6-O6	8.44	124.97	119.90
1	A	867	G	C8-N9-C1'	-8.44	116.03	127.00
1	A	293	G	C5-C6-N1	-8.42	107.29	111.50
1	A	931	C	C5-C6-N1	-8.42	116.79	121.00
1	A	1531	A	N7-C8-N9	8.40	118.00	113.80
1	A	117	G	N1-C2-N3	8.40	128.94	123.90
1	A	286	G	N1-C6-O6	8.40	124.94	119.90
1	A	1501	C	C6-N1-C2	8.39	123.66	120.30
1	A	248	C	C5-C6-N1	-8.36	116.82	121.00
1	A	1414	U	N3-C2-O2	-8.35	116.36	122.20
1	A	874	G	C8-N9-C4	8.33	109.73	106.40
1	A	329	A	N1-C6-N6	8.32	123.59	118.60
1	A	228	A	C2-N3-C4	-8.32	106.44	110.60
1	A	1521	G	N1-C6-O6	-8.32	114.91	119.90
1	A	573	A	N9-C4-C5	8.31	109.12	105.80
1	A	614	A	C8-N9-C4	-8.31	102.48	105.80
1	A	1505	G	C8-N9-C4	-8.31	103.08	106.40
1	A	970	C	N1-C2-O2	8.30	123.88	118.90
1	A	835	U	C6-N1-C2	-8.29	116.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	G	C8-N9-C4	-8.28	103.09	106.40
1	A	251	G	C6-C5-N7	-8.27	125.44	130.40
1	A	659	U	C5-C6-N1	-8.27	118.57	122.70
1	A	1129	C	C6-N1-C2	-8.27	116.99	120.30
1	A	246	A	C5-C6-N1	8.26	121.83	117.70
1	A	1052	U	C6-N1-C2	-8.25	116.05	121.00
1	A	526	C	O5'-P-OP2	-8.25	98.28	105.70
1	A	814	A	N1-C2-N3	8.25	133.42	129.30
1	A	739	C	N3-C4-C5	8.24	125.19	121.90
1	A	1232	U	O5'-P-OP1	-8.23	98.29	105.70
1	A	1108	G	N3-C4-C5	-8.22	124.49	128.60
1	A	793	U	C2-N3-C4	8.22	131.93	127.00
1	A	731	G	C5-C6-O6	-8.21	123.67	128.60
1	A	317	G	C5-C6-O6	-8.21	123.67	128.60
1	A	731	G	C8-N9-C4	8.21	109.68	106.40
1	A	529	G	N1-C6-O6	8.21	124.82	119.90
1	A	276	G	C8-N9-C4	8.20	109.68	106.40
1	A	1052	U	N3-C4-O4	8.20	125.14	119.40
1	A	80	G	N3-C2-N2	-8.20	114.16	119.90
1	A	283	C	C2-N3-C4	8.18	123.99	119.90
1	A	314	C	C5-C6-N1	-8.18	116.91	121.00
1	A	354	G	O5'-P-OP1	-8.17	98.35	105.70
1	A	1490	C	N3-C4-C5	8.17	125.17	121.90
1	A	125	U	N1-C2-N3	8.16	119.80	114.90
1	A	1092	A	N1-C6-N6	8.15	123.49	118.60
1	A	936	C	C6-N1-C2	8.14	123.56	120.30
1	A	389	A	N1-C6-N6	-8.13	113.72	118.60
1	A	524	G	C5-C6-O6	-8.13	123.72	128.60
1	A	736	C	N3-C2-O2	-8.12	116.22	121.90
1	A	560	U	N1-C2-O2	8.12	128.48	122.80
1	A	328	C	N3-C4-N4	-8.11	112.32	118.00
1	A	929	G	N1-C6-O6	8.10	124.76	119.90
1	A	50	A	C8-N9-C4	8.09	109.04	105.80
1	A	733	A	C2-N3-C4	-8.09	106.56	110.60
1	A	126	G	C2-N3-C4	-8.08	107.86	111.90
1	A	285	G	C2-N3-C4	-8.06	107.87	111.90
1	A	802	A	N9-C4-C5	-8.05	102.58	105.80
1	A	269	C	C5-C6-N1	-8.04	116.98	121.00
1	A	139	G	N1-C6-O6	8.04	124.72	119.90
1	A	825	G	N7-C8-N9	-8.03	109.08	113.10
1	A	1195	C	N1-C2-O2	-8.03	114.08	118.90
1	A	938	A	C8-N9-C4	8.02	109.01	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1516[A]	G	N3-C4-N9	-8.02	121.19	126.00
1	A	1516[B]	G	N3-C4-N9	-8.02	121.19	126.00
1	A	302	G	C5-C6-O6	-8.02	123.79	128.60
1	A	8	A	N9-C4-C5	8.02	109.01	105.80
1	A	293	G	N3-C2-N2	-8.01	114.29	119.90
1	A	900	A	N1-C2-N3	8.01	133.30	129.30
1	A	266	G	C5-C6-O6	-8.00	123.80	128.60
1	A	823	G	C2-N3-C4	-8.00	107.90	111.90
1	A	289	G	N1-C6-O6	7.99	124.70	119.90
1	A	1485	U	C6-N1-C2	-7.99	116.21	121.00
1	A	122	G	C2-N3-C4	-7.97	107.91	111.90
1	A	579	G	C4-C5-N7	7.97	113.99	110.80
1	A	122	G	C5-C6-N1	-7.96	107.52	111.50
1	A	522	C	O5'-P-OP2	-7.94	98.55	105.70
1	A	167	G	N9-C4-C5	-7.94	102.22	105.40
1	A	600	C	C6-N1-C2	7.94	123.47	120.30
1	A	306	G	N3-C2-N2	-7.93	114.35	119.90
1	A	1232	U	O5'-P-OP2	7.93	120.22	110.70
1	A	266	G	O4'-C1'-N9	-7.92	101.86	108.20
1	A	366	C	C2-N1-C1'	7.92	127.51	118.80
1	A	593	G	C5-C6-N1	-7.91	107.55	111.50
1	A	882	C	C2-N3-C4	-7.91	115.94	119.90
1	A	1347	G	C8-N9-C1'	-7.91	116.72	127.00
1	A	281	G	C4-C5-N7	7.90	113.96	110.80
1	A	321	A	O5'-P-OP2	-7.90	98.59	105.70
1	A	1525	G	C2-N3-C4	-7.90	107.95	111.90
1	A	821	G	O5'-P-OP1	-7.89	98.60	105.70
1	A	1442	G	N3-C4-N9	7.88	130.73	126.00
1	A	835	U	C4-C5-C6	7.88	124.43	119.70
1	A	675	A	C2-N3-C4	-7.87	106.66	110.60
1	A	21	G	C8-N9-C4	7.87	109.55	106.40
1	A	853	G	C4-C5-C6	7.86	123.52	118.80
1	A	1153	C	C6-N1-C2	7.86	123.44	120.30
1	A	295	C	C5-C6-N1	-7.86	117.07	121.00
1	A	413	G	O4'-C1'-N9	7.84	114.47	108.20
1	A	295	C	N3-C4-C5	7.84	125.04	121.90
1	A	947	G	N9-C4-C5	-7.84	102.27	105.40
1	A	609	A	C2-N3-C4	-7.82	106.69	110.60
1	A	853	G	C6-C5-N7	-7.81	125.71	130.40
1	A	913	A	P-O3'-C3'	7.81	129.07	119.70
1	A	642	A	O5'-P-OP2	-7.81	98.67	105.70
1	A	1386	G	N7-C8-N9	-7.80	109.20	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	G	O4'-C1'-N9	7.80	114.44	108.20
1	A	371	G	O5'-P-OP1	-7.80	98.68	105.70
1	A	588	G	N9-C4-C5	-7.79	102.28	105.40
1	A	723	U	N1-C2-O2	7.79	128.25	122.80
1	A	1078	U	C5-C4-O4	-7.79	121.23	125.90
1	A	279	A	O4'-C1'-N9	-7.78	101.98	108.20
1	A	779	C	C5-C6-N1	-7.76	117.12	121.00
1	A	947	G	N1-C6-O6	7.76	124.56	119.90
1	A	89	C	C6-N1-C2	-7.75	117.20	120.30
1	A	624	C	C6-N1-C2	7.75	123.40	120.30
1	A	865	A	C6-N1-C2	-7.75	113.95	118.60
1	A	1395	C	C6-N1-C2	7.74	123.40	120.30
1	A	1436	U	N1-C2-O2	7.74	128.22	122.80
1	A	1483	A	N9-C4-C5	-7.73	102.71	105.80
1	A	129	U	N3-C4-C5	-7.71	109.97	114.60
1	A	529	G	C4-C5-C6	7.71	123.43	118.80
1	A	654	G	C5-C6-O6	-7.71	123.97	128.60
1	A	739	C	N3-C4-N4	-7.71	112.60	118.00
1	A	1527	C	OP2-P-O3'	7.69	122.11	105.20
1	A	281	G	C5-C6-O6	-7.69	123.99	128.60
1	A	885	G	O5'-P-OP1	-7.69	98.78	105.70
1	A	550	G	C2-N3-C4	-7.69	108.06	111.90
1	A	331	G	C5-C6-N1	-7.68	107.66	111.50
1	A	367	U	O5'-P-OP1	-7.68	98.78	105.70
1	A	760	G	C2-N3-C4	-7.68	108.06	111.90
1	A	875	C	C2-N3-C4	-7.68	116.06	119.90
1	A	947	G	N3-C4-N9	7.68	130.61	126.00
1	A	880	C	C2-N3-C4	-7.68	116.06	119.90
1	A	651	C	C6-N1-C2	7.67	123.37	120.30
1	A	859	A	N1-C6-N6	7.67	123.20	118.60
1	A	1531	A	N1-C6-N6	7.67	123.20	118.60
1	A	1532	U	C5-C4-O4	-7.67	121.30	125.90
1	A	1366	C	C6-N1-C2	-7.67	117.23	120.30
1	A	721	G	C6-C5-N7	-7.67	125.80	130.40
1	A	666	G	N1-C2-N3	7.66	128.50	123.90
1	A	1347	G	C4-N9-C1'	7.65	136.45	126.50
1	A	280	C	O5'-P-OP2	-7.65	98.81	105.70
1	A	331	G	N1-C6-O6	7.65	124.49	119.90
1	A	1417	G	C8-N9-C4	-7.64	103.34	106.40
1	A	29	G	N1-C2-N3	7.64	128.48	123.90
1	A	1403	C	C5-C4-N4	-7.63	114.86	120.20
1	A	1370	G	N7-C8-N9	7.63	116.92	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	753	A	N9-C4-C5	7.62	108.85	105.80
1	A	1158	C	N3-C2-O2	-7.59	116.59	121.90
1	A	1399	C	N1-C2-O2	-7.59	114.35	118.90
1	A	89	C	C5-C6-N1	7.59	124.79	121.00
1	A	524	G	C6-C5-N7	-7.58	125.85	130.40
1	A	858	G	C6-C5-N7	-7.58	125.85	130.40
1	A	1067	A	P-O3'-C3'	7.57	128.79	119.70
1	A	558	G	N7-C8-N9	7.57	116.89	113.10
1	A	787	A	C5-N7-C8	-7.57	100.12	103.90
1	A	735	C	C5-C6-N1	-7.56	117.22	121.00
1	A	928	G	N1-C6-O6	7.55	124.43	119.90
1	A	566	G	C6-C5-N7	-7.55	125.87	130.40
1	A	117	G	N9-C4-C5	-7.54	102.38	105.40
1	A	712	A	C2-N3-C4	-7.54	106.83	110.60
1	A	799	G	C5-C6-O6	-7.53	124.08	128.60
1	A	838	G	C8-N9-C4	7.53	109.41	106.40
1	A	1417	G	N9-C4-C5	7.53	108.41	105.40
1	A	666	G	C2-N3-C4	-7.53	108.14	111.90
1	A	722	A	N9-C4-C5	-7.53	102.79	105.80
1	A	242	C	C5-C6-N1	-7.51	117.25	121.00
1	A	723	U	C2-N1-C1'	7.51	126.71	117.70
1	A	1108	G	C8-N9-C4	-7.50	103.40	106.40
1	A	635	G	C8-N9-C4	7.49	109.39	106.40
1	A	1516[A]	G	C5-C6-O6	7.49	133.09	128.60
1	A	1516[B]	G	C5-C6-O6	7.49	133.09	128.60
1	A	392	G	C5-C6-O6	-7.48	124.11	128.60
1	A	976	G	C4-C5-N7	-7.48	107.81	110.80
1	A	316	G	N1-C6-O6	7.48	124.39	119.90
1	A	1232	U	N1-C2-O2	-7.48	117.57	122.80
1	A	295	C	C6-N1-C2	7.47	123.29	120.30
1	A	577	G	C8-N9-C4	7.47	109.39	106.40
1	A	7	G	C6-N1-C2	-7.47	120.62	125.10
1	A	1373	G	N3-C4-N9	7.47	130.48	126.00
1	A	481	G	N1-C6-O6	7.46	124.38	119.90
1	A	762	C	C5-C4-N4	-7.46	114.98	120.20
1	A	738	C	N3-C4-N4	-7.46	112.78	118.00
1	A	721	G	C4-C5-C6	7.46	123.27	118.80
1	A	228	A	C5-N7-C8	-7.45	100.17	103.90
1	A	126	G	N1-C6-O6	7.45	124.37	119.90
1	A	701	C	N1-C2-O2	7.44	123.37	118.90
1	A	1384	C	N3-C4-C5	7.44	124.88	121.90
1	A	445	G	N1-C6-O6	7.43	124.36	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	G	C4-N9-C1'	7.42	136.15	126.50
1	A	445	G	C6-C5-N7	-7.42	125.95	130.40
1	A	635	G	N1-C2-N3	7.42	128.35	123.90
1	A	933	G	C4-C5-N7	7.42	113.77	110.80
1	A	103	C	N3-C4-C5	-7.42	118.93	121.90
1	A	309	G	C4-C5-N7	7.42	113.77	110.80
1	A	295	C	N3-C4-N4	-7.41	112.81	118.00
1	A	246	A	C2-N3-C4	7.40	114.30	110.60
1	A	1417	G	C4-C5-N7	-7.40	107.84	110.80
1	A	327	A	C5-C6-N1	7.40	121.40	117.70
1	A	593	G	C2-N3-C4	-7.40	108.20	111.90
20	T	94	ALA	N-CA-C	-7.40	91.02	111.00
1	A	598	U	C5-C6-N1	-7.39	119.00	122.70
1	A	569	C	C2-N3-C4	-7.39	116.21	119.90
1	A	1108	G	C4-C5-C6	7.38	123.23	118.80
1	A	1149	C	C6-N1-C2	-7.38	117.35	120.30
1	A	51	A	N7-C8-N9	7.37	117.48	113.80
1	A	183	G	O5'-P-OP1	-7.37	99.07	105.70
1	A	392	G	N1-C6-O6	7.37	124.32	119.90
1	A	250	A	C5-C6-N1	-7.36	114.02	117.70
1	A	1307	U	N3-C2-O2	-7.36	117.05	122.20
1	A	309	G	N1-C2-N2	-7.34	109.59	116.20
1	A	1530	G	N3-C4-C5	7.34	132.27	128.60
1	A	481	G	C8-N9-C1'	-7.34	117.46	127.00
1	A	850	U	C5-C4-O4	7.33	130.30	125.90
1	A	550	G	N1-C2-N3	7.33	128.30	123.90
1	A	1354	C	C6-N1-C2	-7.33	117.37	120.30
1	A	125	U	C4-C5-C6	7.33	124.09	119.70
1	A	812	C	C4-C5-C6	7.32	121.06	117.40
1	A	1525	G	N1-C2-N3	7.32	128.29	123.90
1	A	389	A	C5-C6-N6	7.31	129.55	123.70
1	A	328	C	N1-C2-O2	7.31	123.28	118.90
1	A	591	U	C5-C6-N1	-7.30	119.05	122.70
1	A	293	G	C2-N3-C4	-7.29	108.25	111.90
1	A	278	G	O5'-P-OP2	-7.29	99.14	105.70
1	A	839	U	C2-N1-C1'	7.29	126.44	117.70
1	A	283	C	C2-N1-C1'	7.28	126.81	118.80
1	A	1442	G	N3-C4-C5	-7.28	124.96	128.60
1	A	746	A	N1-C2-N3	7.28	132.94	129.30
1	A	526	C	C5-C6-N1	-7.28	117.36	121.00
1	A	719	C	C6-N1-C2	7.26	123.20	120.30
1	A	92	C	N1-C2-O2	7.26	123.25	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	831	U	N1-C2-O2	-7.25	117.72	122.80
1	A	919	A	C5-C6-N1	7.25	121.32	117.70
1	A	121	C	C6-N1-C2	7.24	123.20	120.30
1	A	1442	G	C4-N9-C1'	7.24	135.91	126.50
1	A	1502	A	N7-C8-N9	7.23	117.42	113.80
1	A	597	G	O5'-P-OP1	-7.22	99.20	105.70
1	A	248	C	C4-C5-C6	7.22	121.01	117.40
1	A	739	C	C5-C6-N1	-7.21	117.40	121.00
1	A	793	U	C5-C4-O4	-7.21	121.58	125.90
1	A	947	G	C5-C6-O6	-7.21	124.28	128.60
1	A	901	A	C2-N3-C4	-7.20	107.00	110.60
1	A	1305	G	P-O3'-C3'	7.19	128.33	119.70
1	A	661	G	N1-C6-O6	7.19	124.22	119.90
1	A	89	C	C2-N1-C1'	7.19	126.70	118.80
1	A	1108	G	C6-C5-N7	-7.18	126.09	130.40
1	A	119	A	C2-N3-C4	-7.18	107.01	110.60
1	A	880	C	O5'-P-OP1	-7.17	99.24	105.70
1	A	1304	G	O5'-P-OP1	-7.17	99.25	105.70
1	A	648	A	C8-N9-C4	7.16	108.66	105.80
1	A	919	A	C8-N9-C4	7.16	108.66	105.80
1	A	106	C	C6-N1-C2	-7.15	117.44	120.30
1	A	1334	G	C8-N9-C4	7.15	109.26	106.40
1	A	813	U	C5-C4-O4	-7.15	121.61	125.90
1	A	266	G	C8-N9-C4	-7.15	103.54	106.40
1	A	867	G	C4-N9-C1'	7.15	135.79	126.50
1	A	562	C	C6-N1-C2	7.15	123.16	120.30
1	A	29	G	N1-C6-O6	7.14	124.18	119.90
1	A	1524	C	N1-C2-O2	-7.14	114.62	118.90
1	A	305	G	C2-N3-C4	-7.13	108.33	111.90
1	A	376	G	C5-C6-N1	-7.13	107.93	111.50
1	A	1103	C	C5-C6-N1	-7.13	117.43	121.00
1	A	873	A	N9-C4-C5	7.13	108.65	105.80
1	A	939	G	C5-C6-O6	-7.12	124.33	128.60
1	A	558	G	C5-C6-O6	-7.12	124.33	128.60
1	A	721	G	N3-C4-C5	-7.12	125.04	128.60
1	A	821	G	C5-C6-O6	-7.11	124.33	128.60
1	A	802	A	N1-C6-N6	7.10	122.86	118.60
1	A	851	G	N1-C6-O6	7.10	124.16	119.90
1	A	328	C	N3-C2-O2	-7.10	116.93	121.90
1	A	1092	A	C4-C5-N7	7.10	114.25	110.70
1	A	797	C	C6-N1-C2	7.09	123.14	120.30
1	A	1227	A	C6-C5-N7	-7.08	127.34	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	G	N1-C6-O6	7.08	124.15	119.90
1	A	1073	U	C6-N1-C2	7.08	125.25	121.00
1	A	658	G	C8-N9-C1'	-7.08	117.79	127.00
1	A	286	G	C8-N9-C4	-7.07	103.57	106.40
1	A	235	C	C5-C6-N1	-7.07	117.46	121.00
1	A	947	G	C6-C5-N7	-7.07	126.16	130.40
1	A	874	G	C8-N9-C1'	-7.06	117.82	127.00
1	A	7	G	N3-C4-C5	-7.06	125.07	128.60
1	A	645	C	C2-N1-C1'	7.06	126.57	118.80
1	A	312	C	N3-C4-C5	7.05	124.72	121.90
1	A	658	G	N9-C4-C5	-7.05	102.58	105.40
1	A	1153	C	C5-C6-N1	-7.05	117.48	121.00
1	A	252	U	C2-N3-C4	-7.04	122.77	127.00
1	A	626	U	N3-C2-O2	-7.03	117.28	122.20
1	A	580	U	N3-C4-C5	-7.03	110.38	114.60
1	A	1158	C	N1-C2-O2	7.03	123.12	118.90
1	A	1158	C	C2-N1-C1'	7.03	126.53	118.80
1	A	971	G	C8-N9-C4	7.03	109.21	106.40
1	A	1366	C	C5-C6-N1	7.02	124.51	121.00
1	A	131	C	C6-N1-C2	7.02	123.11	120.30
1	A	524	G	N1-C6-O6	7.01	124.11	119.90
1	A	877	C	C2-N3-C4	-7.01	116.39	119.90
1	A	248	C	C6-N1-C2	7.00	123.10	120.30
1	A	626	U	N1-C2-N3	7.00	119.10	114.90
4	D	12	CYS	CA-CB-SG	7.00	126.60	114.00
1	A	1200	C	C6-N1-C2	-7.00	117.50	120.30
1	A	658	G	C6-C5-N7	-6.99	126.20	130.40
1	A	822	C	C6-N1-C2	6.99	123.10	120.30
1	A	588	G	C8-N9-C4	6.99	109.19	106.40
1	A	118	U	C5-C4-O4	6.98	130.09	125.90
1	A	864	A	N9-C4-C5	6.98	108.59	105.80
1	A	723	U	C5-C6-N1	6.98	126.19	122.70
1	A	1483	A	N1-C6-N6	6.98	122.79	118.60
1	A	1394	A	C5-C6-N6	-6.98	118.12	123.70
1	A	1200	C	C6-N1-C1'	-6.97	112.43	120.80
1	A	761	G	C2-N3-C4	-6.97	108.42	111.90
1	A	769	G	O5'-P-OP2	-6.96	99.43	105.70
1	A	555	C	C6-N1-C2	-6.96	117.52	120.30
1	A	907	A	O5'-P-OP1	-6.96	99.44	105.70
1	A	945	G	C5-C6-N1	6.96	114.98	111.50
1	A	111	G	O5'-P-OP1	-6.95	99.44	105.70
1	A	939	G	N1-C6-O6	6.95	124.07	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	920	U	C6-N1-C1'	6.94	130.92	121.20
1	A	312	C	C6-N1-C2	6.94	123.08	120.30
1	A	366	C	C6-N1-C1'	-6.94	112.47	120.80
1	A	227	G	C2-N3-C4	-6.94	108.43	111.90
1	A	583	A	N1-C2-N3	6.94	132.77	129.30
1	A	882	C	C4-C5-C6	6.94	120.87	117.40
1	A	742	G	C6-C5-N7	-6.93	126.24	130.40
1	A	757	U	C5-C6-N1	-6.93	119.23	122.70
1	A	309	G	C8-N9-C4	6.93	109.17	106.40
1	A	579	G	C5-N7-C8	-6.93	100.84	104.30
1	A	1147	C	C6-N1-C2	-6.92	117.53	120.30
1	A	167	G	C4-N9-C1'	6.92	135.50	126.50
1	A	1058	G	C5-C6-O6	6.91	132.75	128.60
1	A	379	C	O5'-P-OP2	-6.91	99.48	105.70
1	A	21	G	N1-C2-N2	-6.91	109.98	116.20
1	A	122	G	C4-C5-N7	6.90	113.56	110.80
1	A	573	A	C4-C5-C6	6.90	120.45	117.00
1	A	901	A	N1-C2-N3	6.89	132.75	129.30
1	A	940	C	C6-N1-C2	6.89	123.06	120.30
1	A	285	G	N1-C6-O6	6.88	124.03	119.90
1	A	1373	G	C6-C5-N7	-6.88	126.27	130.40
1	A	62	U	N3-C4-C5	-6.88	110.47	114.60
1	A	89	C	N1-C2-O2	6.88	123.03	118.90
1	A	608	A	C2-N3-C4	-6.88	107.16	110.60
1	A	703	G	N9-C4-C5	6.87	108.15	105.40
1	A	893	C	N1-C2-O2	6.87	123.02	118.90
1	A	90	U	OP1-P-O3'	6.87	120.31	105.20
1	A	808	C	C6-N1-C2	6.86	123.04	120.30
1	A	333	G	C8-N9-C4	6.86	109.14	106.40
1	A	872	A	N9-C4-C5	-6.85	103.06	105.80
1	A	1344	C	O5'-P-OP2	-6.85	99.53	105.70
1	A	1532	U	N1-C2-N3	-6.85	110.79	114.90
1	A	667	G	N1-C6-O6	6.84	124.01	119.90
1	A	853	G	C8-N9-C1'	-6.84	118.10	127.00
1	A	238	G	C2-N3-C4	-6.84	108.48	111.90
1	A	1190	G	N7-C8-N9	6.84	116.52	113.10
1	A	1530	G	N9-C4-C5	-6.83	102.67	105.40
1	A	882	C	N3-C4-N4	-6.83	113.22	118.00
1	A	1529	G	N3-C4-C5	-6.82	125.19	128.60
1	A	1416	G	N1-C6-O6	6.82	123.99	119.90
1	A	1523	G	N1-C6-O6	6.82	123.99	119.90
1	A	1190	G	N3-C4-N9	6.80	130.08	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	G	C5-C6-N1	-6.79	108.10	111.50
1	A	597	G	N3-C4-C5	-6.79	125.20	128.60
1	A	1441	G	C5-C6-N1	-6.79	108.10	111.50
1	A	76	C	N1-C2-O2	-6.79	114.83	118.90
1	A	122	G	N3-C4-N9	-6.79	121.93	126.00
1	A	654	G	N3-C4-N9	-6.79	121.93	126.00
1	A	860	A	C6-N1-C2	-6.78	114.53	118.60
1	A	745	C	C5-C6-N1	-6.77	117.62	121.00
1	A	824	C	O5'-P-OP2	-6.77	99.61	105.70
1	A	903	G	N1-C2-N3	6.77	127.96	123.90
1	A	646	U	N3-C4-C5	-6.77	110.54	114.60
1	A	1515[A]	C	O5'-P-OP2	-6.77	99.61	105.70
1	A	1515[B]	C	O5'-P-OP2	-6.77	99.61	105.70
1	A	722	A	C5-C6-N6	-6.77	118.29	123.70
1	A	317	G	C2-N3-C4	-6.76	108.52	111.90
1	A	676	A	C8-N9-C4	6.76	108.50	105.80
1	A	121	C	N3-C2-O2	6.76	126.63	121.90
1	A	21	G	C8-N9-C1'	-6.75	118.22	127.00
1	A	867	G	C6-C5-N7	-6.75	126.35	130.40
1	A	1108	G	C4-N9-C1'	6.75	135.28	126.50
1	A	32	A	N1-C2-N3	6.75	132.68	129.30
1	A	318	G	N3-C2-N2	-6.75	115.17	119.90
1	A	770	C	C6-N1-C2	6.75	123.00	120.30
1	A	33	A	C5-C6-N1	6.75	121.07	117.70
1	A	1109	C	O5'-P-OP1	-6.74	99.63	105.70
1	A	827	U	C2-N3-C4	-6.74	122.95	127.00
1	A	1197	G	O5'-P-OP1	-6.74	99.63	105.70
1	A	228	A	C4-C5-N7	6.74	114.07	110.70
1	A	658	G	N3-C4-N9	6.74	130.04	126.00
1	A	1373	G	N1-C6-O6	6.74	123.94	119.90
1	A	243	A	N1-C6-N6	6.74	122.64	118.60
1	A	738	C	N3-C4-C5	6.74	124.59	121.90
1	A	284	G	N1-C6-O6	6.73	123.94	119.90
1	A	687	A	P-O3'-C3'	6.72	127.77	119.70
1	A	29	G	C8-N9-C4	6.72	109.09	106.40
1	A	5	U	P-O3'-C3'	6.72	127.76	119.70
1	A	1479	C	C6-N1-C2	-6.71	117.62	120.30
1	A	597	G	N3-C4-N9	6.71	130.03	126.00
1	A	671	G	C8-N9-C4	6.71	109.08	106.40
1	A	1403	C	N3-C4-N4	6.71	122.69	118.00
1	A	26	A	C2-N3-C4	-6.70	107.25	110.60
1	A	859	A	O5'-P-OP2	6.70	118.74	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1367	C	C5-C6-N1	6.70	124.35	121.00
1	A	745	C	C2-N3-C4	-6.70	116.55	119.90
1	A	593	G	C6-C5-N7	-6.69	126.38	130.40
1	A	116	A	C2-N3-C4	-6.69	107.25	110.60
1	A	806	C	C6-N1-C2	6.69	122.98	120.30
1	A	1112	C	C5-C6-N1	-6.69	117.66	121.00
1	A	406	G	N1-C6-O6	6.68	123.91	119.90
1	A	833	U	N3-C2-O2	-6.68	117.52	122.20
1	A	862	C	C5-C4-N4	-6.68	115.53	120.20
1	A	1181	G	N7-C8-N9	-6.67	109.76	113.10
1	A	128	G	C5-C6-O6	-6.67	124.60	128.60
1	A	277	C	C5-C6-N1	-6.67	117.67	121.00
1	A	262	A	N1-C6-N6	-6.67	114.60	118.60
1	A	753	A	N1-C2-N3	6.67	132.63	129.30
1	A	1227	A	N7-C8-N9	6.67	117.13	113.80
1	A	59	A	O5'-P-OP2	-6.66	99.70	105.70
1	A	106	C	OP2-P-O3'	6.66	119.85	105.20
1	A	289	G	C4-C5-N7	6.66	113.46	110.80
1	A	304	U	O5'-P-OP2	6.66	118.69	110.70
1	A	648	A	C6-N1-C2	-6.66	114.61	118.60
1	A	7	G	C8-N9-C1'	-6.65	118.35	127.00
1	A	945	G	C4-C5-N7	6.65	113.46	110.80
1	A	176	C	C6-N1-C2	6.65	122.96	120.30
1	A	653	A	N1-C6-N6	-6.65	114.61	118.60
1	A	835	U	N3-C2-O2	-6.65	117.55	122.20
1	A	856	C	C2-N1-C1'	-6.65	111.49	118.80
1	A	884	U	C6-N1-C2	6.65	124.99	121.00
1	A	576	G	N1-C2-N3	6.64	127.88	123.90
1	A	1505	G	P-O3'-C3'	6.64	127.67	119.70
1	A	655	A	C5-C6-N1	6.63	121.02	117.70
1	A	1512	U	N3-C4-C5	-6.63	110.62	114.60
1	A	1527	C	C2-N1-C1'	6.62	126.09	118.80
1	A	39	G	C5-C6-N1	6.62	114.81	111.50
1	A	1058	G	C4-C5-N7	-6.62	108.15	110.80
1	A	400	C	N3-C4-C5	6.61	124.54	121.90
1	A	127	G	N1-C6-O6	6.60	123.86	119.90
1	A	269	C	C2-N3-C4	-6.60	116.60	119.90
1	A	63	C	N1-C2-O2	-6.60	114.94	118.90
1	A	731	G	N3-C4-C5	6.60	131.90	128.60
1	A	654	G	C5-N7-C8	-6.59	101.00	104.30
1	A	1075	C	N3-C4-C5	6.59	124.53	121.90
1	A	746	A	C6-N1-C2	-6.58	114.65	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	789	U	C5-C4-O4	6.58	129.84	125.90
1	A	873	A	C8-N9-C4	-6.58	103.17	105.80
1	A	111	G	N3-C4-N9	-6.57	122.06	126.00
1	A	874	G	N9-C4-C5	-6.57	102.77	105.40
1	A	269	C	N3-C4-N4	-6.57	113.40	118.00
1	A	931	C	C2-N3-C4	-6.57	116.62	119.90
1	A	577	G	N1-C6-O6	6.56	123.84	119.90
1	A	770	C	C5-C6-N1	-6.56	117.72	121.00
1	A	1099	G	N3-C4-N9	-6.56	122.06	126.00
1	A	1225	A	C8-N9-C4	-6.56	103.18	105.80
1	A	230	G	C8-N9-C1'	-6.56	118.47	127.00
1	A	297	G	C6-C5-N7	-6.56	126.47	130.40
1	A	403	C	C5-C6-N1	-6.55	117.72	121.00
1	A	579	G	C6-C5-N7	-6.55	126.47	130.40
1	A	877	C	C5-C6-N1	-6.55	117.72	121.00
1	A	663	A	N1-C6-N6	-6.55	114.67	118.60
1	A	581	G	O5'-P-OP2	-6.55	99.81	105.70
1	A	62	U	C4-C5-C6	6.54	123.63	119.70
1	A	959	A	N1-C6-N6	6.54	122.53	118.60
1	A	1077	G	N1-C2-N2	-6.54	110.31	116.20
1	A	150	C	N3-C4-C5	-6.53	119.29	121.90
1	A	10	A	N1-C2-N3	6.53	132.56	129.30
1	A	10	A	C2-N3-C4	-6.53	107.34	110.60
1	A	715	A	C2-N3-C4	-6.53	107.34	110.60
1	A	742	G	C5-C6-O6	-6.53	124.69	128.60
1	A	1090	U	N3-C4-C5	-6.53	110.69	114.60
1	A	733	A	O5'-P-OP1	-6.52	99.83	105.70
1	A	839	U	N1-C2-O2	6.52	127.37	122.80
1	A	291	C	C2-N3-C4	-6.52	116.64	119.90
1	A	279	A	C4-N9-C1'	6.51	138.01	126.30
1	A	285	G	C5-C6-N1	-6.51	108.25	111.50
1	A	250	A	N1-C6-N6	6.50	122.50	118.60
1	A	129(A)	G	C4-N9-C1'	6.50	134.95	126.50
1	A	293	G	N1-C6-O6	6.50	123.80	119.90
1	A	1190	G	C4-C5-C6	6.50	122.70	118.80
1	A	129	U	C4-C5-C6	6.49	123.59	119.70
1	A	118	U	N1-C2-N3	6.49	118.79	114.90
1	A	1339	A	N1-C6-N6	-6.49	114.71	118.60
1	A	24	U	C6-N1-C2	6.49	124.89	121.00
1	A	572	A	N1-C6-N6	-6.48	114.71	118.60
1	A	29	G	C6-C5-N7	-6.48	126.51	130.40
1	A	813	U	C2-N1-C1'	6.48	125.47	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	582	U	C5-C6-N1	-6.47	119.46	122.70
1	A	1531	A	C5-C6-N1	-6.47	114.46	117.70
1	A	703	G	C5-N7-C8	6.47	107.53	104.30
1	A	1215	G	C6-C5-N7	-6.47	126.52	130.40
1	A	122	G	N3-C2-N2	-6.47	115.37	119.90
1	A	403	C	C4-C5-C6	6.47	120.63	117.40
1	A	814	A	N1-C6-N6	6.47	122.48	118.60
1	A	31	G	N1-C6-O6	-6.46	116.02	119.90
1	A	107	G	C4-C5-N7	6.46	113.39	110.80
1	A	1441	G	C4-C5-N7	-6.46	108.21	110.80
1	A	33	A	C6-N1-C2	-6.46	114.72	118.60
1	A	242	C	N3-C4-C5	6.46	124.48	121.90
1	A	1227	A	C5-C6-N6	-6.46	118.54	123.70
1	A	854	G	N1-C2-N3	6.45	127.77	123.90
1	A	251	G	N1-C6-O6	6.45	123.77	119.90
1	A	507	C	N3-C4-C5	6.45	124.48	121.90
1	A	1405	G	O5'-P-OP2	-6.45	99.89	105.70
1	A	237	C	N3-C4-C5	-6.45	119.32	121.90
1	A	588	G	C2-N3-C4	-6.45	108.68	111.90
1	A	303	A	N1-C6-N6	6.44	122.47	118.60
1	A	559	A	C6-N1-C2	-6.44	114.73	118.60
1	A	1053	G	C8-N9-C4	6.44	108.98	106.40
1	A	1419	G	C8-N9-C4	-6.44	103.82	106.40
1	A	1190	G	C4-C5-N7	6.44	113.38	110.80
1	A	580	U	C6-N1-C2	-6.43	117.14	121.00
1	A	922	G	N3-C4-C5	-6.43	125.38	128.60
1	A	965	A	C8-N9-C4	6.43	108.37	105.80
1	A	762	C	O5'-P-OP2	6.43	118.41	110.70
1	A	799	G	C4-C5-N7	6.43	113.37	110.80
1	A	1342	C	N1-C2-O2	-6.43	115.04	118.90
1	A	645	C	C5-C6-N1	6.42	124.21	121.00
1	A	1193	G	N1-C6-O6	6.42	123.75	119.90
1	A	653	A	N9-C4-C5	6.42	108.37	105.80
1	A	772	U	N1-C2-O2	-6.42	118.31	122.80
1	A	317	G	C5-N7-C8	-6.42	101.09	104.30
1	A	17	U	C2-N3-C4	-6.41	123.15	127.00
18	R	78	LEU	CA-CB-CG	-6.41	100.55	115.30
1	A	875	C	N3-C4-C5	6.41	124.46	121.90
1	A	1452	C	N1-C2-O2	6.41	122.75	118.90
1	A	333	G	OP2-P-O3'	6.41	119.29	105.20
1	A	105	G	O5'-P-OP2	-6.40	99.94	105.70
1	A	228	A	N1-C6-N6	6.40	122.44	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	880	C	N3-C4-C5	6.40	124.46	121.90
1	A	582	U	C2-N3-C4	-6.40	123.16	127.00
1	A	856	C	C4-C5-C6	6.40	120.60	117.40
1	A	873	A	C4-C5-C6	-6.40	113.80	117.00
1	A	78	G	N1-C6-O6	6.39	123.74	119.90
1	A	867	G	N9-C4-C5	-6.39	102.84	105.40
1	A	855	G	N1-C6-O6	6.39	123.73	119.90
1	A	1215	G	C4-C5-N7	6.38	113.35	110.80
1	A	388	G	N3-C4-C5	-6.38	125.41	128.60
1	A	1414	U	C6-N1-C2	-6.38	117.17	121.00
1	A	90	U	O5'-P-OP2	6.38	118.35	110.70
1	A	586	C	C5-C6-N1	-6.38	117.81	121.00
1	A	802	A	C8-N9-C4	6.38	108.35	105.80
1	A	853	G	N1-C2-N3	6.37	127.72	123.90
1	A	9	G	O5'-P-OP1	6.37	118.35	110.70
1	A	481	G	N9-C4-C5	-6.37	102.85	105.40
1	A	768	A	OP2-P-O3'	6.37	119.22	105.20
1	A	121	C	N1-C2-O2	-6.36	115.08	118.90
1	A	852	G	N1-C6-O6	6.36	123.72	119.90
1	A	281	G	N9-C4-C5	-6.36	102.86	105.40
1	A	553	A	C2-N3-C4	-6.36	107.42	110.60
1	A	524	G	C8-N9-C1'	-6.36	118.74	127.00
1	A	1167	A	C8-N9-C4	-6.36	103.26	105.80
1	A	317	G	N9-C4-C5	-6.35	102.86	105.40
1	A	529	G	C5-C6-N1	-6.35	108.32	111.50
1	A	370	C	O5'-P-OP1	-6.35	99.98	105.70
1	A	572	A	N9-C4-C5	6.35	108.34	105.80
1	A	1197	G	C4-N9-C1'	6.35	134.75	126.50
1	A	1542	U	C6-N1-C2	6.35	124.81	121.00
1	A	117	G	O5'-P-OP2	-6.34	99.99	105.70
1	A	21	G	N3-C4-N9	6.34	129.80	126.00
1	A	131	C	C2-N3-C4	-6.34	116.73	119.90
1	A	138	G	C8-N9-C4	6.34	108.94	106.40
1	A	1351	U	N3-C2-O2	-6.34	117.76	122.20
1	A	22	G	O5'-P-OP2	-6.33	100.00	105.70
1	A	329	A	C5-C6-N1	-6.33	114.53	117.70
1	A	1181	G	C4-N9-C1'	-6.33	118.27	126.50
1	A	851	G	C6-C5-N7	-6.33	126.60	130.40
1	A	310	G	N1-C6-O6	6.33	123.70	119.90
1	A	590	C	OP2-P-O3'	6.32	119.11	105.20
1	A	309	G	C6-C5-N7	-6.32	126.61	130.40
1	A	890	G	C4-C5-N7	-6.32	108.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	C	C2-N3-C4	-6.32	116.74	119.90
1	A	1322	C	C6-N1-C2	-6.32	117.77	120.30
1	A	407	G	C8-N9-C4	6.31	108.92	106.40
1	A	718	G	N1-C6-O6	6.31	123.69	119.90
1	A	1529	G	C4-N9-C1'	6.31	134.71	126.50
1	A	1350	A	C8-N9-C4	-6.31	103.28	105.80
1	A	836	G	C2-N3-C4	-6.31	108.75	111.90
1	A	814	A	C8-N9-C4	6.31	108.32	105.80
1	A	345	C	C6-N1-C2	-6.30	117.78	120.30
1	A	1301	U	P-O3'-C3'	6.30	127.26	119.70
1	A	353	A	C5-C6-N6	6.30	128.74	123.70
1	A	350	G	N7-C8-N9	6.30	116.25	113.10
1	A	21	G	N3-C2-N2	6.30	124.31	119.90
1	A	112	G	C2-N3-C4	-6.30	108.75	111.90
1	A	625	G	C5-C6-N1	6.30	114.65	111.50
1	A	803	G	OP2-P-O3'	6.30	119.05	105.20
1	A	920	U	C2-N1-C1'	-6.30	110.14	117.70
1	A	1268	A	N1-C6-N6	-6.30	114.82	118.60
1	A	730	G	N9-C4-C5	6.29	107.92	105.40
1	A	664	G	C4-C5-N7	-6.29	108.28	110.80
1	A	774	G	C2-N3-C4	-6.29	108.75	111.90
1	A	1051	C	C2-N1-C1'	6.29	125.72	118.80
1	A	734	G	N9-C4-C5	-6.29	102.89	105.40
1	A	661	G	N3-C4-C5	6.29	131.74	128.60
1	A	1442	G	C8-N9-C1'	-6.29	118.83	127.00
1	A	144	G	N3-C2-N2	-6.28	115.50	119.90
1	A	190(I)	G	C8-N9-C4	6.28	108.91	106.40
1	A	326	G	C4-C5-N7	-6.28	108.29	110.80
1	A	862	C	C6-N1-C2	6.28	122.81	120.30
1	A	395	C	C6-N1-C2	6.28	122.81	120.30
1	A	877	C	N3-C4-N4	-6.28	113.61	118.00
1	A	788	U	N3-C4-C5	-6.28	110.83	114.60
1	A	809	G	C5-C6-O6	-6.28	124.83	128.60
1	A	1452	C	C6-N1-C2	6.28	122.81	120.30
1	A	228	A	N3-C4-C5	6.28	131.19	126.80
1	A	168	G	N1-C6-O6	6.27	123.66	119.90
1	A	654	G	C5-C6-N1	6.27	114.64	111.50
1	A	615	C	C2-N1-C1'	6.27	125.69	118.80
1	A	302	G	C8-N9-C4	6.26	108.91	106.40
1	A	677	U	N1-C2-O2	-6.26	118.42	122.80
1	A	144	G	N3-C4-C5	6.26	131.73	128.60
1	A	286	G	C6-C5-N7	-6.26	126.64	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	746	A	C8-N9-C4	6.26	108.30	105.80
1	A	1512	U	N1-C2-O2	-6.25	118.42	122.80
1	A	1117	G	N3-C4-C5	6.25	131.73	128.60
1	A	80	G	N1-C2-N2	6.25	121.83	116.20
1	A	1103	C	C2-N3-C4	-6.25	116.78	119.90
1	A	1190	G	P-O3'-C3'	6.25	127.20	119.70
1	A	1306	A	C8-N9-C4	6.25	108.30	105.80
1	A	856	C	C6-N1-C1'	6.25	128.30	120.80
1	A	878	G	OP1-P-O3'	6.25	118.94	105.20
1	A	1452	C	N1-C2-N3	-6.25	114.83	119.20
1	A	1098	C	C6-N1-C2	6.25	122.80	120.30
1	A	1240	U	C5-C6-N1	-6.24	119.58	122.70
1	A	129(A)	G	C8-N9-C1'	-6.24	118.89	127.00
1	A	14	U	C6-N1-C2	-6.23	117.26	121.00
1	A	1190	G	N1-C6-O6	6.23	123.64	119.90
1	A	32	A	OP1-P-O3'	6.23	118.91	105.20
1	A	1523	G	N3-C2-N2	-6.23	115.54	119.90
1	A	962	C	N1-C2-O2	6.23	122.64	118.90
1	A	1527	C	C5-C4-N4	-6.23	115.84	120.20
1	A	400	C	C6-N1-C2	6.22	122.79	120.30
1	A	243	A	OP1-P-O3'	6.22	118.89	105.20
1	A	329	A	N3-C4-C5	6.22	131.16	126.80
1	A	130	A	C4-C5-C6	6.22	120.11	117.00
1	A	874	G	N1-C6-O6	6.22	123.63	119.90
1	A	1390	U	N3-C4-C5	-6.22	110.87	114.60
1	A	1388	C	O5'-P-OP1	6.22	118.16	110.70
1	A	283	C	N3-C4-N4	6.21	122.35	118.00
1	A	730	G	C4-C5-N7	-6.21	108.32	110.80
1	A	185	A	O5'-P-OP2	-6.21	100.12	105.70
1	A	806	C	C2-N3-C4	-6.20	116.80	119.90
1	A	560	U	N3-C2-O2	-6.20	117.86	122.20
1	A	648	A	N7-C8-N9	-6.20	110.70	113.80
1	A	940	C	C5-C6-N1	-6.20	117.90	121.00
1	A	518	C	C5-C4-N4	6.20	124.54	120.20
1	A	254	G	O5'-P-OP1	-6.20	100.12	105.70
1	A	900	A	C8-N9-C4	-6.20	103.32	105.80
1	A	1051	C	N1-C2-O2	6.19	122.62	118.90
1	A	524	G	C4-N9-C1'	6.19	134.55	126.50
1	A	599	C	C5-C6-N1	-6.19	117.90	121.00
1	A	662	G	C8-N9-C4	6.19	108.88	106.40
1	A	317	G	C5-C6-N1	-6.19	108.41	111.50
1	A	583	A	C2-N3-C4	-6.19	107.51	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1501	C	C5-C6-N1	-6.19	117.91	121.00
1	A	723	U	N3-C2-O2	-6.18	117.87	122.20
1	A	289	G	C5-N7-C8	-6.18	101.21	104.30
1	A	1403	C	C2-N1-C1'	6.18	125.60	118.80
1	A	600	C	N3-C4-N4	-6.18	113.67	118.00
1	A	874	G	N3-C4-N9	6.18	129.71	126.00
1	A	79	G	N3-C4-C5	-6.17	125.51	128.60
1	A	385	C	N3-C4-C5	6.17	124.37	121.90
1	A	106	C	O5'-P-OP1	-6.17	100.15	105.70
1	A	570	G	C8-N9-C4	-6.17	103.93	106.40
1	A	872	A	C5-C6-N6	-6.17	118.77	123.70
1	A	450	G	C8-N9-C4	6.17	108.87	106.40
1	A	1436	U	C2-N1-C1'	6.17	125.10	117.70
1	A	29	G	N9-C4-C5	-6.16	102.94	105.40
1	A	168	G	C4-C5-N7	6.16	113.27	110.80
1	A	795	C	N1-C2-O2	-6.16	115.20	118.90
1	A	558	G	O5'-P-OP1	6.16	118.09	110.70
1	A	1526	G	N3-C2-N2	-6.16	115.59	119.90
1	A	873	A	C2-N3-C4	6.16	113.68	110.60
1	A	739	C	C6-N1-C2	6.16	122.76	120.30
1	A	448	A	N7-C8-N9	6.16	116.88	113.80
1	A	1301	U	N3-C4-O4	6.16	123.71	119.40
1	A	1052	U	N3-C4-C5	-6.15	110.91	114.60
1	A	779	C	C4-C5-C6	6.15	120.48	117.40
1	A	802	A	C4-C5-N7	6.15	113.78	110.70
1	A	859	A	C6-C5-N7	-6.15	128.00	132.30
1	A	780	A	N1-C2-N3	6.15	132.37	129.30
1	A	230	G	C8-N9-C4	6.15	108.86	106.40
1	A	1509	C	C5-C6-N1	-6.15	117.93	121.00
1	A	308	C	N3-C2-O2	-6.14	117.60	121.90
1	A	448	A	C6-C5-N7	-6.14	128.00	132.30
1	A	812	C	C5-C4-N4	6.14	124.50	120.20
1	A	1399	C	N3-C4-C5	-6.14	119.44	121.90
1	A	1062	U	C5-C4-O4	6.14	129.58	125.90
1	A	232	G	C8-N9-C1'	-6.14	119.02	127.00
1	A	310	G	C5-C6-O6	-6.14	124.92	128.60
1	A	129(A)	G	N3-C4-N9	6.14	129.68	126.00
1	A	721	G	N1-C2-N2	-6.14	110.68	116.20
1	A	21	G	N9-C4-C5	-6.13	102.95	105.40
1	A	576	G	C8-N9-C1'	-6.13	119.02	127.00
1	A	168	G	C6-C5-N7	-6.13	126.72	130.40
1	A	1236	A	C5-C6-N6	-6.13	118.80	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	U	N3-C2-O2	-6.13	117.91	122.20
1	A	876	G	C6-N1-C2	-6.13	121.42	125.10
1	A	909	A	C6-N1-C2	-6.13	114.92	118.60
1	A	908	A	C8-N9-C4	6.13	108.25	105.80
1	A	266	G	N3-C4-N9	6.13	129.68	126.00
1	A	750	G	O5'-P-OP1	-6.13	100.19	105.70
1	A	1092	A	N9-C4-C5	-6.12	103.35	105.80
1	A	864	A	N3-C4-N9	-6.12	122.50	127.40
1	A	1499	A	C6-N1-C2	-6.12	114.93	118.60
1	A	812	C	P-O3'-C3'	6.12	127.04	119.70
1	A	780	A	C6-N1-C2	-6.12	114.93	118.60
1	A	726	C	C2-N3-C4	-6.11	116.84	119.90
1	A	167	G	C6-C5-N7	-6.11	126.73	130.40
1	A	259	G	C5-C6-N1	-6.11	108.44	111.50
1	A	1197	G	C8-N9-C1'	-6.11	119.06	127.00
1	A	280	C	C5-C6-N1	-6.11	117.94	121.00
1	A	1224	G	C8-N9-C4	6.11	108.84	106.40
1	A	1064	G	N3-C4-N9	-6.11	122.34	126.00
1	A	838	G	N9-C4-C5	-6.11	102.96	105.40
1	A	1512	U	N3-C4-O4	6.10	123.67	119.40
1	A	667	G	C6-C5-N7	-6.10	126.74	130.40
1	A	816	A	C2-N3-C4	-6.10	107.55	110.60
1	A	1478	C	C6-N1-C2	-6.10	117.86	120.30
1	A	720	C	N3-C4-C5	6.10	124.34	121.90
1	A	1397	C	C6-N1-C2	6.10	122.74	120.30
1	A	975	A	O4'-C1'-N9	-6.09	103.33	108.20
1	A	1315	U	N3-C2-O2	-6.09	117.93	122.20
1	A	1355	G	C8-N9-C4	-6.09	103.96	106.40
1	A	1477	C	C6-N1-C2	-6.09	117.86	120.30
1	A	884	U	C4-C5-C6	6.09	123.36	119.70
1	A	1232	U	N3-C2-O2	6.09	126.46	122.20
1	A	716	A	O5'-P-OP1	-6.09	100.22	105.70
1	A	1344	C	C2-N1-C1'	-6.09	112.11	118.80
1	A	130	A	N1-C2-N3	6.08	132.34	129.30
1	A	827	U	C5-C6-N1	-6.08	119.66	122.70
1	A	931	C	C6-N1-C2	6.08	122.73	120.30
1	A	916	G	C5-C6-O6	-6.08	124.95	128.60
1	A	799	G	C5-N7-C8	-6.08	101.26	104.30
1	A	300	A	C6-N1-C2	-6.08	114.95	118.60
1	A	760	G	C5-C6-N1	-6.08	108.46	111.50
1	A	316	G	C5-C6-O6	-6.07	124.96	128.60
1	A	806	C	C5-C6-N1	-6.07	117.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	C	N1-C2-O2	-6.07	115.26	118.90
1	A	373	A	N1-C2-N3	6.06	132.33	129.30
1	A	118	U	N3-C4-O4	-6.06	115.16	119.40
1	A	774	G	C5-N7-C8	-6.06	101.27	104.30
1	A	1531	A	C6-C5-N7	-6.06	128.06	132.30
1	A	331	G	C6-C5-N7	-6.05	126.77	130.40
1	A	1441	G	N3-C2-N2	-6.05	115.66	119.90
1	A	8	A	N1-C6-N6	-6.05	114.97	118.60
1	A	1514	C	C2-N3-C4	-6.05	116.88	119.90
1	A	947	G	C8-N9-C1'	-6.04	119.14	127.00
1	A	1514	C	C5-C6-N1	-6.04	117.98	121.00
1	A	1441	G	N9-C4-C5	6.04	107.82	105.40
1	A	1380	U	N3-C4-O4	-6.04	115.17	119.40
1	A	1442	G	C6-C5-N7	-6.04	126.78	130.40
1	A	593	G	N1-C6-O6	6.04	123.52	119.90
1	A	916	G	N3-C4-N9	6.04	129.62	126.00
1	A	7	G	C5-C6-O6	-6.03	124.98	128.60
1	A	729	A	C5-N7-C8	-6.03	100.88	103.90
1	A	728	A	N3-C4-N9	-6.03	122.58	127.40
1	A	309	G	O5'-P-OP2	-6.03	100.28	105.70
1	A	559	A	N7-C8-N9	6.03	116.81	113.80
1	A	1282	C	C6-N1-C2	-6.03	117.89	120.30
1	A	372	C	C4-C5-C6	6.02	120.41	117.40
1	A	820	U	O4'-C1'-N1	6.02	113.02	108.20
1	A	824	C	N1-C2-O2	-6.02	115.29	118.90
1	A	976	G	N3-C4-C5	-6.02	125.59	128.60
1	A	1234	C	C6-N1-C2	6.02	122.71	120.30
1	A	118	U	C5-C6-N1	-6.02	119.69	122.70
1	A	353	A	N9-C4-C5	6.02	108.21	105.80
1	A	614	A	N1-C2-N3	6.02	132.31	129.30
1	A	379	C	C2-N1-C1'	-6.01	112.19	118.80
1	A	945	G	C4-C5-C6	-6.01	115.19	118.80
1	A	103	C	C4-C5-C6	6.01	120.41	117.40
1	A	112	G	N3-C4-C5	6.01	131.61	128.60
1	A	888	G	C4-N9-C1'	6.01	134.32	126.50
1	A	1401	G	N1-C6-O6	-6.01	116.29	119.90
1	A	79	G	C2-N3-C4	6.01	114.90	111.90
1	A	618	C	N1-C2-N3	-6.01	114.99	119.20
1	A	1530	G	OP1-P-OP2	6.00	128.61	119.60
1	A	522	C	C5-C6-N1	-6.00	118.00	121.00
1	A	448	A	C8-N9-C4	-6.00	103.40	105.80
1	A	898	G	N1-C2-N2	-6.00	110.80	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1497	G	N3-C4-C5	-6.00	125.60	128.60
1	A	96	G	C8-N9-C4	-5.99	104.00	106.40
1	A	288	A	C2-N3-C4	-5.99	107.60	110.60
1	A	656	C	N3-C4-C5	5.99	124.30	121.90
1	A	1304	G	C5-C6-N1	-5.99	108.50	111.50
1	A	1295	G	C8-N9-C4	-5.99	104.00	106.40
1	A	329	A	C4-C5-N7	5.99	113.69	110.70
1	A	858	G	C4-C5-C6	5.99	122.39	118.80
1	A	753	A	C4-C5-N7	-5.98	107.71	110.70
1	A	802	A	C5-C6-N6	-5.98	118.91	123.70
1	A	747	C	C5-C6-N1	-5.98	118.01	121.00
1	A	605	U	N3-C4-O4	5.97	123.58	119.40
1	A	1351	U	C6-N1-C2	-5.97	117.42	121.00
1	A	481	G	C4-N9-C1'	5.96	134.25	126.50
1	A	130	A	C6-C5-N7	-5.96	128.13	132.30
1	A	238	G	C5-C6-N1	-5.96	108.52	111.50
1	A	739	C	C2-N3-C4	-5.96	116.92	119.90
1	A	1334	G	OP1-P-OP2	5.96	128.54	119.60
1	A	1373	G	C5-C6-O6	-5.96	125.02	128.60
1	A	10	A	C8-N9-C4	5.96	108.19	105.80
1	A	738	C	C5-C6-N1	-5.96	118.02	121.00
1	A	783	C	N1-C2-O2	-5.96	115.32	118.90
1	A	833	U	N3-C4-C5	-5.96	111.02	114.60
1	A	855	G	C8-N9-C4	5.96	108.78	106.40
1	A	651	C	C5-C6-N1	-5.96	118.02	121.00
1	A	1346	A	N1-C6-N6	-5.95	115.03	118.60
1	A	562	C	N1-C2-O2	5.95	122.47	118.90
1	A	886	G	N1-C6-O6	5.95	123.47	119.90
1	A	188	C	C6-N1-C2	5.95	122.68	120.30
1	A	1380	U	P-O3'-C3'	5.95	126.83	119.70
1	A	835	U	C6-N1-C1'	5.94	129.52	121.20
1	A	529	G	C8-N9-C1'	-5.94	119.28	127.00
1	A	337	C	C5-C6-N1	-5.94	118.03	121.00
1	A	389	A	C8-N9-C4	-5.94	103.42	105.80
1	A	747	C	C6-N1-C2	5.94	122.67	120.30
1	A	1077	G	N3-C2-N2	5.94	124.06	119.90
1	A	1268	A	N9-C4-C5	5.94	108.17	105.80
1	A	793	U	C4-C5-C6	-5.93	116.14	119.70
1	A	922	G	C4-N9-C1'	5.93	134.21	126.50
1	A	117	G	N3-C4-N9	5.93	129.56	126.00
1	A	727	G	N3-C2-N2	5.93	124.05	119.90
1	A	1307	U	N1-C2-O2	5.93	126.95	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	G	N1-C6-O6	5.93	123.46	119.90
1	A	1502	A	N1-C2-N3	5.93	132.26	129.30
1	A	15	G	C5-C6-N1	-5.92	108.54	111.50
1	A	386	C	C2-N1-C1'	5.92	125.32	118.80
1	A	1100	C	OP2-P-O3'	5.92	118.23	105.20
1	A	923	A	C4-C5-N7	5.92	113.66	110.70
1	A	167	G	C8-N9-C4	5.92	108.77	106.40
1	A	617	G	C8-N9-C4	5.92	108.77	106.40
1	A	403	C	C2-N3-C4	-5.92	116.94	119.90
1	A	1345	U	O5'-P-OP1	-5.92	100.38	105.70
1	A	1531	A	C5-N7-C8	-5.92	100.94	103.90
1	A	640	A	C4-C5-C6	5.92	119.96	117.00
1	A	1394	A	C6-C5-N7	-5.92	128.16	132.30
16	P	26	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	A	298	A	C6-N1-C2	-5.91	115.05	118.60
1	A	481	G	C6-C5-N7	-5.91	126.85	130.40
1	A	893	C	N3-C2-O2	-5.91	117.76	121.90
1	A	560	U	C2-N1-C1'	5.91	124.79	117.70
1	A	655	A	N7-C8-N9	-5.91	110.85	113.80
1	A	1330	U	C5-C4-O4	-5.91	122.36	125.90
1	A	830	G	C5-C6-O6	5.90	132.14	128.60
1	A	981	U	C6-N1-C2	-5.90	117.46	121.00
1	A	1263	C	C6-N1-C2	5.90	122.66	120.30
1	A	122	G	C6-C5-N7	-5.90	126.86	130.40
1	A	285	G	N3-C2-N2	-5.90	115.77	119.90
1	A	334	C	C6-N1-C2	5.90	122.66	120.30
1	A	1108	G	N7-C8-N9	5.90	116.05	113.10
1	A	1186	G	N1-C6-O6	5.89	123.44	119.90
5	E	12	LEU	CA-CB-CG	5.89	128.86	115.30
8	H	85	ARG	NE-CZ-NH1	-5.89	117.36	120.30
1	A	827	U	N3-C2-O2	-5.89	118.08	122.20
1	A	859	A	C5-C6-N6	-5.89	118.99	123.70
1	A	80	G	C8-N9-C4	-5.88	104.05	106.40
1	A	115	G	C5-C6-N1	5.88	114.44	111.50
1	A	250	A	C8-N9-C4	5.88	108.15	105.80
1	A	727	G	N1-C2-N2	-5.88	110.91	116.20
1	A	1279	A	N7-C8-N9	5.88	116.74	113.80
1	A	112	G	C5-C6-N1	-5.87	108.56	111.50
1	A	456	C	C6-N1-C2	5.87	122.65	120.30
1	A	658	G	N1-C6-O6	5.87	123.42	119.90
1	A	720	C	C6-N1-C2	5.87	122.65	120.30
17	Q	99	SER	N-CA-C	5.87	126.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	U	N3-C4-C5	-5.87	111.08	114.60
1	A	924	C	OP2-P-O3'	5.86	118.10	105.20
1	A	1527	C	C6-N1-C2	-5.86	117.95	120.30
1	A	1112	C	C2-N3-C4	-5.86	116.97	119.90
1	A	585	G	O5'-P-OP2	-5.86	100.43	105.70
1	A	1197	G	N3-C4-N9	5.86	129.51	126.00
1	A	1501	C	N3-C4-C5	5.86	124.24	121.90
1	A	190(D)	U	C6-N1-C2	5.85	124.51	121.00
1	A	722	A	C5-C6-N1	-5.85	114.77	117.70
1	A	190(G)	G	C5-C6-N1	-5.85	108.57	111.50
1	A	108	G	C8-N9-C4	-5.85	104.06	106.40
1	A	1515[A]	C	O5'-P-OP1	5.85	117.72	110.70
1	A	1515[B]	C	O5'-P-OP1	5.85	117.72	110.70
1	A	1302	U	OP2-P-O3'	5.85	118.07	105.20
1	A	389	A	C4-C5-C6	5.84	119.92	117.00
1	A	618	C	C6-N1-C2	5.84	122.64	120.30
1	A	884	U	O5'-P-OP1	-5.84	100.44	105.70
1	A	232	G	N3-C4-N9	5.84	129.50	126.00
1	A	779	C	C2-N3-C4	-5.84	116.98	119.90
1	A	888	G	C8-N9-C1'	-5.84	119.41	127.00
1	A	260	G	N9-C4-C5	5.84	107.74	105.40
1	A	948	C	N3-C4-C5	5.84	124.24	121.90
1	A	872	A	OP2-P-O3'	5.83	118.04	105.20
1	A	872	A	C2-N3-C4	-5.83	107.68	110.60
1	A	326	G	C5-C6-N1	-5.83	108.58	111.50
1	A	626	U	O5'-P-OP1	-5.83	100.45	105.70
1	A	919	A	C4-C5-C6	-5.83	114.08	117.00
1	A	1305	G	C8-N9-C4	-5.83	104.07	106.40
1	A	852	G	N3-C4-C5	5.83	131.51	128.60
1	A	921	U	N3-C4-C5	-5.82	111.11	114.60
1	A	168	G	C5-C6-O6	-5.82	125.11	128.60
1	A	1279	A	C8-N9-C4	-5.82	103.47	105.80
1	A	1502	A	OP1-P-O3'	5.82	118.01	105.20
1	A	48	C	N1-C2-O2	-5.82	115.41	118.90
1	A	808	C	N3-C4-C5	5.82	124.23	121.90
1	A	1139	G	P-O3'-C3'	5.82	126.68	119.70
1	A	461	C	N1-C2-O2	5.81	122.39	118.90
1	A	1072	G	OP2-P-O3'	5.81	117.99	105.20
1	A	125	U	C2-N3-C4	-5.81	123.51	127.00
1	A	830	G	N1-C6-O6	-5.81	116.41	119.90
1	A	250	A	C2-N3-C4	-5.81	107.69	110.60
1	A	665	A	C5-C6-N1	5.81	120.61	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	G	C8-N9-C4	-5.81	104.08	106.40
1	A	821	G	C4-C5-N7	5.81	113.12	110.80
1	A	23	C	C4-C5-C6	5.80	120.30	117.40
1	A	833	U	C5-C4-O4	5.80	129.38	125.90
1	A	1237	C	C4-C5-C6	5.80	120.30	117.40
1	A	129(A)	G	C6-C5-N7	-5.80	126.92	130.40
1	A	173	U	N3-C2-O2	-5.80	118.14	122.20
1	A	570	G	C6-N1-C2	-5.80	121.62	125.10
1	A	635	G	C4-C5-C6	5.80	122.28	118.80
1	A	637	G	N7-C8-N9	-5.80	110.20	113.10
1	A	648	A	N1-C2-N3	5.80	132.20	129.30
1	A	122	G	C5-C6-O6	-5.80	125.12	128.60
1	A	293	G	N1-C2-N3	5.80	127.38	123.90
1	A	306	G	C5-C6-N1	-5.80	108.60	111.50
1	A	416	G	C6-C5-N7	-5.80	126.92	130.40
1	A	572	A	C5-C6-N1	5.80	120.60	117.70
1	A	1447	G	C4-C5-N7	5.80	113.12	110.80
1	A	876	G	C5-C6-N1	5.79	114.40	111.50
1	A	309	G	N1-C2-N3	5.79	127.38	123.90
1	A	484	G	C8-N9-C1'	-5.79	119.47	127.00
1	A	328	C	N3-C4-C5	5.79	124.22	121.90
1	A	733	A	N1-C2-N3	5.79	132.19	129.30
1	A	412	A	C8-N9-C4	5.79	108.11	105.80
1	A	511	C	C2-N1-C1'	-5.79	112.44	118.80
1	A	947	G	C8-N9-C4	5.79	108.71	106.40
1	A	1502	A	C5-C6-N1	-5.79	114.81	117.70
1	A	251	G	N3-C4-N9	5.78	129.47	126.00
1	A	569	C	C4-C5-C6	5.78	120.29	117.40
1	A	697	U	OP2-P-O3'	5.78	117.92	105.20
1	A	932	C	N3-C4-C5	5.78	124.21	121.90
1	A	888	G	C4-C5-C6	5.78	122.27	118.80
1	A	1531	A	C8-N9-C4	-5.78	103.49	105.80
1	A	190(G)	G	C6-C5-N7	-5.78	126.94	130.40
1	A	262	A	C5-C6-N6	5.78	128.32	123.70
1	A	659	U	N1-C2-N3	5.78	118.37	114.90
1	A	667	G	C8-N9-C1'	-5.78	119.49	127.00
1	A	658	G	N1-C2-N3	5.77	127.36	123.90
1	A	1470	G	N7-C8-N9	-5.77	110.21	113.10
1	A	731	G	N9-C4-C5	-5.77	103.09	105.40
1	A	477	G	C5-C6-N1	-5.77	108.61	111.50
1	A	573	A	N7-C8-N9	5.77	116.69	113.80
1	A	605	U	N3-C4-C5	-5.77	111.14	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	G	P-O3'-C3'	5.77	126.62	119.70
1	A	1319	A	N1-C6-N6	5.77	122.06	118.60
1	A	170	U	N1-C2-O2	-5.76	118.77	122.80
1	A	1200	C	C4-C5-C6	-5.76	114.52	117.40
1	A	733	A	OP1-P-OP2	5.76	128.24	119.60
1	A	1277	C	C6-N1-C2	-5.76	118.00	120.30
1	A	1527	C	OP1-P-O3'	-5.76	92.53	105.20
1	A	333	G	N1-C6-O6	5.75	123.35	119.90
1	A	1300	G	OP2-P-O3'	5.75	117.85	105.20
1	A	364	A	C4-C5-C6	5.75	119.88	117.00
1	A	745	C	N3-C4-N4	-5.75	113.97	118.00
1	A	1092	A	O4'-C1'-N9	-5.75	103.60	108.20
1	A	511	C	C2-N3-C4	-5.75	117.03	119.90
1	A	235	C	N3-C4-N4	-5.75	113.98	118.00
1	A	1092	A	C5-C6-N6	-5.75	119.10	123.70
1	A	605	U	C4-C5-C6	5.74	123.14	119.70
1	A	1217	C	C6-N1-C2	-5.73	118.01	120.30
1	A	934	C	N3-C4-C5	5.73	124.19	121.90
1	A	1211	U	C2-N1-C1'	5.73	124.58	117.70
1	A	1401	G	N3-C4-C5	-5.73	125.73	128.60
1	A	333	G	N3-C2-N2	-5.73	115.89	119.90
1	A	815	A	C8-N9-C4	5.73	108.09	105.80
1	A	1235	U	N1-C2-N3	5.73	118.34	114.90
1	A	770	C	N3-C4-C5	5.73	124.19	121.90
1	A	237	C	N1-C2-N3	5.72	123.21	119.20
1	A	640	A	N1-C6-N6	5.72	122.03	118.60
1	A	654	G	N1-C2-N2	5.72	121.35	116.20
16	P	58	TYR	CB-CA-C	-5.72	98.95	110.40
1	A	109	A	C2-N3-C4	-5.72	107.74	110.60
1	A	580	U	N1-C2-N3	5.72	118.33	114.90
1	A	1276	G	N1-C6-O6	5.72	123.33	119.90
1	A	529	G	C4-N9-C1'	5.71	133.93	126.50
1	A	976	G	O4'-C1'-N9	5.71	112.77	108.20
1	A	379	C	C5-C6-N1	-5.71	118.14	121.00
1	A	1383	C	C5-C6-N1	5.71	123.86	121.00
1	A	1490	C	C5-C6-N1	5.71	123.86	121.00
1	A	124	G	N1-C2-N2	-5.70	111.07	116.20
1	A	792	A	N1-C6-N6	5.70	122.02	118.60
1	A	1529	G	C4-C5-C6	5.70	122.22	118.80
1	A	386	C	C6-N1-C1'	-5.70	113.96	120.80
1	A	193	C	C6-N1-C2	5.70	122.58	120.30
1	A	827	U	N1-C2-N3	5.70	118.32	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	C	N3-C2-O2	-5.70	117.91	121.90
1	A	277	C	N3-C4-N4	-5.70	114.01	118.00
1	A	365	U	N3-C4-O4	5.70	123.39	119.40
1	A	1233	G	C5-C6-N1	-5.70	108.65	111.50
1	A	576	G	C4-N9-C1'	5.69	133.90	126.50
1	A	1441	G	N3-C4-N9	-5.69	122.58	126.00
1	A	35	G	N1-C6-O6	5.69	123.32	119.90
1	A	240	C	N1-C2-O2	-5.69	115.48	118.90
1	A	428	G	P-O3'-C3'	5.69	126.53	119.70
1	A	1508	G	C5-C6-N1	5.69	114.34	111.50
1	A	444	C	N3-C4-C5	5.69	124.17	121.90
1	A	1108	G	N3-C4-N9	5.68	129.41	126.00
1	A	392	G	C6-C5-N7	-5.68	126.99	130.40
1	A	1149	C	C2-N1-C1'	5.68	125.05	118.80
1	A	583	A	C6-N1-C2	-5.68	115.19	118.60
1	A	577	G	C2-N3-C4	-5.68	109.06	111.90
1	A	787	A	N7-C8-N9	5.68	116.64	113.80
1	A	1068	G	O5'-P-OP1	-5.67	100.59	105.70
1	A	1336	C	C2-N1-C1'	5.67	125.04	118.80
1	A	1367	C	C6-N1-C2	-5.67	118.03	120.30
1	A	816	A	N7-C8-N9	-5.66	110.97	113.80
1	A	329	A	C6-C5-N7	-5.66	128.34	132.30
1	A	832	C	C5-C4-N4	-5.66	116.24	120.20
1	A	17	U	C5-C6-N1	-5.66	119.87	122.70
1	A	654	G	C8-N9-C1'	5.66	134.35	127.00
1	A	742	G	N3-C2-N2	-5.65	115.94	119.90
1	A	1394	A	N9-C4-C5	-5.65	103.54	105.80
1	A	475	G	C5-C6-N1	-5.65	108.67	111.50
1	A	820	U	C2-N1-C1'	-5.65	110.92	117.70
1	A	93	G	OP1-P-O3'	5.65	117.62	105.20
1	A	448	A	C5-N7-C8	-5.64	101.08	103.90
1	A	620	C	OP1-P-O3'	5.64	117.62	105.20
1	A	1074	G	C5-C6-N1	-5.64	108.68	111.50
1	A	144	G	C5-C6-O6	-5.64	125.22	128.60
1	A	655	A	C8-N9-C4	5.64	108.06	105.80
1	A	1347	G	OP2-P-O3'	5.64	117.61	105.20
1	A	1373	G	C8-N9-C1'	-5.64	119.67	127.00
1	A	1092	A	C5-N7-C8	-5.64	101.08	103.90
1	A	1246	C	C2-N1-C1'	-5.64	112.60	118.80
1	A	27	G	C4-C5-N7	5.64	113.06	110.80
1	A	139	G	C5-C6-O6	-5.64	125.22	128.60
1	A	805	C	C5-C4-N4	-5.64	116.25	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	A	N7-C8-N9	-5.63	110.98	113.80
1	A	1350	A	C5-N7-C8	-5.63	101.08	103.90
1	A	898	G	C5-C6-O6	5.63	131.98	128.60
1	A	909	A	C5-C6-N6	-5.63	119.19	123.70
1	A	1433	A	C8-N9-C4	-5.63	103.55	105.80
1	A	827	U	OP2-P-O3'	5.63	117.58	105.20
1	A	659	U	C2-N3-C4	-5.62	123.62	127.00
1	A	568	G	N1-C6-O6	-5.62	116.53	119.90
1	A	365	U	C6-N1-C1'	-5.62	113.33	121.20
1	A	1232	U	N3-C4-O4	5.62	123.33	119.40
1	A	21	G	N7-C8-N9	-5.62	110.29	113.10
1	A	703	G	C4-C5-C6	5.62	122.17	118.80
1	A	793	U	OP2-P-O3'	5.62	117.56	105.20
1	A	507	C	C5-C4-N4	-5.62	116.27	120.20
1	A	912	C	C5-C4-N4	-5.62	116.27	120.20
1	A	1469	G	N1-C6-O6	5.62	123.27	119.90
1	A	318	G	N1-C6-O6	5.62	123.27	119.90
1	A	1305	G	C5-C6-N1	-5.62	108.69	111.50
1	A	324	G	C5-C6-N1	-5.61	108.69	111.50
1	A	791	G	N1-C6-O6	5.61	123.27	119.90
1	A	806	C	N3-C4-C5	5.61	124.15	121.90
1	A	927	G	C5-C6-N1	-5.61	108.69	111.50
1	A	1074	G	C2-N3-C4	-5.61	109.09	111.90
1	A	1093	A	P-O3'-C3'	5.61	126.43	119.70
1	A	260	G	N7-C8-N9	5.61	115.90	113.10
1	A	424	G	N1-C6-O6	5.61	123.27	119.90
1	A	945	G	N1-C2-N2	5.61	121.25	116.20
1	A	566	G	N1-C6-O6	5.61	123.27	119.90
1	A	731	G	C2-N3-C4	-5.61	109.10	111.90
1	A	1447	G	C6-C5-N7	-5.61	127.03	130.40
1	A	861	G	C6-C5-N7	-5.61	127.04	130.40
1	A	911	U	C5-C6-N1	-5.61	119.90	122.70
1	A	286	G	N7-C8-N9	5.60	115.90	113.10
1	A	695	A	C5-N7-C8	-5.60	101.10	103.90
1	A	744	C	C6-N1-C2	5.60	122.54	120.30
1	A	852	G	N1-C2-N3	5.60	127.26	123.90
1	A	948	C	C5-C6-N1	-5.60	118.20	121.00
1	A	121	C	O5'-P-OP2	-5.60	100.66	105.70
1	A	350	G	C5-N7-C8	-5.60	101.50	104.30
1	A	27	G	C5-C6-O6	-5.59	125.24	128.60
1	A	658	G	C5-C6-O6	-5.59	125.24	128.60
1	A	19	C	C2-N3-C4	-5.59	117.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	754	C	C2-N3-C4	-5.59	117.11	119.90
1	A	116	A	C5-C6-N1	-5.58	114.91	117.70
1	A	246	A	C6-N1-C2	-5.58	115.25	118.60
1	A	1526	G	C4-C5-N7	5.58	113.03	110.80
1	A	121	C	O5'-P-OP1	5.58	117.40	110.70
1	A	576	G	C6-N1-C2	-5.58	121.75	125.10
1	A	522	C	C2-N1-C1'	-5.58	112.66	118.80
1	A	637	G	N9-C4-C5	-5.58	103.17	105.40
1	A	921	U	C6-N1-C2	-5.58	117.65	121.00
1	A	326	G	C5-C6-O6	5.58	131.94	128.60
1	A	129	U	N1-C2-O2	-5.57	118.90	122.80
1	A	795	C	N3-C2-O2	5.57	125.80	121.90
1	A	799	G	C6-C5-N7	-5.57	127.06	130.40
1	A	259	G	C2-N3-C4	-5.56	109.12	111.90
1	A	248	C	C2-N3-C4	-5.56	117.12	119.90
1	A	832	C	N3-C2-O2	-5.56	118.01	121.90
1	A	839	U	C6-N1-C1'	-5.56	113.42	121.20
1	A	301	G	OP1-P-OP2	5.56	127.94	119.60
1	A	5	U	OP2-P-O3'	5.56	117.42	105.20
1	A	475	G	N1-C2-N3	5.56	127.23	123.90
4	D	196	LEU	CA-CB-CG	-5.56	102.52	115.30
1	A	571	U	N3-C4-C5	5.56	117.93	114.60
1	A	949	A	C8-N9-C4	5.56	108.02	105.80
1	A	110	C	N1-C2-O2	-5.55	115.57	118.90
1	A	119	A	N1-C2-N3	5.55	132.08	129.30
1	A	725	G	C5-C6-O6	-5.55	125.27	128.60
1	A	586	C	C4-C5-C6	5.55	120.18	117.40
1	A	189	G	N3-C4-C5	-5.55	125.82	128.60
1	A	357	G	C8-N9-C4	5.55	108.62	106.40
1	A	482	A	N7-C8-N9	5.55	116.58	113.80
1	A	575	G	OP1-P-OP2	5.55	127.93	119.60
1	A	1187	G	C4-N9-C1'	5.55	133.72	126.50
1	A	308	C	N1-C2-O2	5.55	122.23	118.90
1	A	712	A	N1-C6-N6	5.55	121.93	118.60
1	A	1448	C	N3-C4-C5	5.55	124.12	121.90
1	A	132	C	N3-C2-O2	-5.55	118.02	121.90
1	A	505	G	N1-C6-O6	-5.55	116.57	119.90
1	A	1149	C	C5-C6-N1	5.55	123.77	121.00
1	A	138	G	N7-C8-N9	-5.54	110.33	113.10
1	A	874	G	OP1-P-OP2	5.54	127.91	119.60
1	A	16	A	O5'-P-OP1	5.54	117.34	110.70
1	A	353	A	C4-C5-N7	-5.53	107.93	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	G	C4-C5-N7	-5.53	108.59	110.80
1	A	716	A	C5-C6-N6	-5.53	119.27	123.70
1	A	852	G	C6-N1-C2	5.53	128.42	125.10
1	A	237	C	C6-N1-C2	-5.53	118.09	120.30
1	A	117	G	C5-C6-O6	-5.53	125.28	128.60
1	A	279	A	N9-C4-C5	5.53	108.01	105.80
1	A	731	G	N3-C2-N2	-5.53	116.03	119.90
1	A	655	A	N1-C6-N6	-5.53	115.28	118.60
1	A	1200	C	O5'-P-OP2	5.53	117.33	110.70
1	A	823	G	C5-C6-O6	-5.52	125.29	128.60
1	A	560	U	C6-N1-C1'	-5.52	113.47	121.20
1	A	658	G	C4-N9-C1'	5.52	133.68	126.50
1	A	896	C	C2-N3-C4	-5.52	117.14	119.90
1	A	1514	C	C4-C5-C6	5.52	120.16	117.40
1	A	1305	G	N7-C8-N9	5.52	115.86	113.10
1	A	1287	A	C5-C6-N6	5.51	128.11	123.70
1	A	558	G	C8-N9-C4	-5.51	104.19	106.40
1	A	1542	U	C5-C6-N1	-5.51	119.94	122.70
1	A	76	C	C2-N1-C1'	-5.51	112.74	118.80
1	A	787	A	C2-N3-C4	-5.51	107.84	110.60
1	A	1416	G	N3-C2-N2	-5.51	116.04	119.90
1	A	524	G	C4-C5-N7	5.51	113.00	110.80
1	A	445	G	N7-C8-N9	5.51	115.85	113.10
1	A	771	G	C8-N9-C1'	-5.51	119.84	127.00
1	A	877	C	N1-C2-O2	-5.51	115.60	118.90
1	A	280	C	N3-C4-N4	-5.50	114.15	118.00
1	A	863	U	N3-C4-C5	-5.50	111.30	114.60
1	A	823	G	N1-C6-O6	5.50	123.20	119.90
1	A	1079	G	C8-N9-C4	-5.50	104.20	106.40
1	A	1403	C	C6-N1-C1'	-5.50	114.20	120.80
1	A	872	A	C6-C5-N7	-5.50	128.45	132.30
1	A	614	A	C6-N1-C2	-5.50	115.30	118.60
1	A	1336	C	P-O3'-C3'	-5.50	113.11	119.70
1	A	599	C	C2-N3-C4	-5.49	117.16	119.90
1	A	895	G	C8-N9-C4	-5.49	104.20	106.40
1	A	1242	C	C2-N1-C1'	5.49	124.84	118.80
1	A	297	G	OP1-P-OP2	-5.49	111.37	119.60
1	A	300	A	C5-C6-N1	5.49	120.44	117.70
1	A	1078	U	C5-C6-N1	5.49	125.44	122.70
1	A	1341	U	C2-N1-C1'	-5.49	111.11	117.70
1	A	821	G	C6-C5-N7	-5.49	127.11	130.40
1	A	111	G	N9-C4-C5	5.49	107.59	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	G	C2-N3-C4	-5.48	109.16	111.90
1	A	1526	G	C6-C5-N7	-5.48	127.11	130.40
1	A	592	G	C5-C6-N1	-5.48	108.76	111.50
1	A	892	A	N1-C2-N3	5.48	132.04	129.30
1	A	720	C	N1-C2-O2	5.47	122.19	118.90
1	A	736	C	C2-N3-C4	-5.47	117.16	119.90
1	A	894	G	N1-C6-O6	5.47	123.19	119.90
10	J	40	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	104	G	N1-C6-O6	5.47	123.18	119.90
1	A	1167	A	N7-C8-N9	5.47	116.54	113.80
1	A	1336	C	C6-N1-C1'	-5.47	114.24	120.80
1	A	1318	A	C8-N9-C4	5.47	107.99	105.80
1	A	635	G	N3-C4-C5	5.47	131.33	128.60
2	B	61	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	124	G	N1-C2-N3	5.46	127.18	123.90
1	A	579	G	C2-N3-C4	-5.46	109.17	111.90
1	A	653	A	OP2-P-O3'	5.46	117.22	105.20
1	A	657	G	C8-N9-C4	5.46	108.58	106.40
1	A	805	C	N1-C2-N3	-5.46	115.38	119.20
1	A	854	G	C8-N9-C1'	-5.46	119.90	127.00
1	A	245	C	C2-N1-C1'	5.46	124.81	118.80
1	A	250	A	N9-C4-C5	-5.46	103.62	105.80
1	A	1336	C	N1-C2-O2	5.46	122.17	118.90
1	A	1049	U	P-O3'-C3'	5.46	126.25	119.70
1	A	235	C	C2-N1-C1'	-5.45	112.80	118.80
1	A	1431	C	N1-C2-O2	-5.45	115.63	118.90
1	A	645	C	C6-N1-C2	-5.45	118.12	120.30
1	A	667	G	C8-N9-C4	5.45	108.58	106.40
1	A	819	A	OP2-P-O3'	5.45	117.19	105.20
1	A	202	U	N3-C2-O2	5.45	126.01	122.20
1	A	251	G	C8-N9-C1'	-5.45	119.92	127.00
1	A	276	G	N7-C8-N9	-5.45	110.38	113.10
1	A	342	C	N3-C4-C5	-5.45	119.72	121.90
1	A	1395	C	OP2-P-O3'	5.45	117.19	105.20
1	A	1414	U	C5-C4-O4	5.45	129.17	125.90
1	A	70	G	N3-C4-N9	-5.45	122.73	126.00
1	A	295	C	C2-N3-C4	-5.45	117.18	119.90
1	A	722	A	C4-C5-C6	5.44	119.72	117.00
1	A	770	C	C2-N3-C4	-5.44	117.18	119.90
1	A	570	G	C4-N9-C1'	5.44	133.57	126.50
1	A	867	G	N3-C4-C5	-5.44	125.88	128.60
1	A	562	C	C5-C6-N1	-5.44	118.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1416	G	OP2-P-O3'	5.44	117.17	105.20
1	A	823	G	OP2-P-O3'	5.44	117.16	105.20
1	A	18	C	C6-N1-C2	5.43	122.47	120.30
1	A	413	G	C8-N9-C4	-5.43	104.23	106.40
1	A	577	G	N9-C4-C5	-5.43	103.23	105.40
1	A	765	G	C5-C6-N1	-5.43	108.78	111.50
11	K	125	PHE	N-CA-C	5.43	125.66	111.00
1	A	303	A	C5-C6-N6	-5.43	119.36	123.70
1	A	747	C	C2-N3-C4	-5.43	117.19	119.90
1	A	63	C	N3-C2-O2	5.42	125.70	121.90
1	A	126	G	N3-C2-N2	-5.42	116.10	119.90
1	A	876	G	N3-C4-C5	-5.42	125.89	128.60
1	A	181	G	C4-N9-C1'	5.42	133.55	126.50
1	A	554	C	C6-N1-C2	5.42	122.47	120.30
1	A	584	G	OP2-P-O3'	5.42	117.13	105.20
1	A	59	A	N1-C6-N6	-5.42	115.35	118.60
1	A	482	A	C4-C5-C6	5.42	119.71	117.00
1	A	483	C	C4-C5-C6	5.42	120.11	117.40
1	A	938	A	N7-C8-N9	-5.42	111.09	113.80
1	A	1394	A	C4-C5-N7	5.42	113.41	110.70
1	A	1063	C	N3-C4-C5	5.42	124.07	121.90
1	A	1469	G	C5-C6-O6	-5.42	125.35	128.60
1	A	644	G	C5-C6-O6	-5.41	125.35	128.60
1	A	934	C	C6-N1-C2	5.41	122.46	120.30
1	A	867	G	C5-C6-O6	-5.41	125.36	128.60
1	A	1055	A	C5-C6-N1	5.41	120.40	117.70
1	A	70	G	C5-C6-N1	-5.40	108.80	111.50
1	A	181	G	N3-C4-N9	5.40	129.24	126.00
1	A	972	C	O5'-P-OP2	-5.40	100.84	105.70
1	A	1347	G	N1-C2-N2	-5.40	111.34	116.20
1	A	840	C	N1-C2-O2	5.40	122.14	118.90
1	A	872	A	C4-C5-N7	5.40	113.40	110.70
1	A	522	C	N1-C2-O2	-5.40	115.66	118.90
1	A	605	U	N1-C2-N3	5.40	118.14	114.90
1	A	799	G	N1-C6-O6	5.39	123.14	119.90
1	A	920	U	N1-C2-O2	-5.39	119.03	122.80
1	A	1078	U	N3-C4-O4	5.39	123.17	119.40
1	A	9	G	O5'-P-OP2	-5.39	100.85	105.70
1	A	617	G	N7-C8-N9	-5.39	110.41	113.10
1	A	170	U	N1-C2-N3	5.39	118.13	114.90
1	A	824	C	C2-N3-C4	-5.39	117.21	119.90
1	A	941	G	C5-N7-C8	-5.39	101.61	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1414	U	N1-C2-O2	5.39	126.57	122.80
1	A	146	G	N3-C2-N2	-5.38	116.13	119.90
1	A	564	C	OP2-P-O3'	5.38	117.04	105.20
1	A	851	G	C5-C6-O6	-5.38	125.37	128.60
1	A	1527	C	N3-C2-O2	-5.38	118.13	121.90
1	A	771	G	N3-C4-N9	5.38	129.23	126.00
1	A	1238	A	N9-C4-C5	5.38	107.95	105.80
1	A	614	A	N7-C8-N9	5.38	116.49	113.80
1	A	716	A	N9-C4-C5	-5.38	103.65	105.80
1	A	1182	G	P-O3'-C3'	5.38	126.15	119.70
1	A	1310	G	N3-C4-C5	-5.37	125.91	128.60
1	A	484	G	C4-N9-C1'	5.37	133.48	126.50
1	A	12	U	O5'-P-OP2	-5.37	100.87	105.70
1	A	1543	C	N1-C2-O2	5.37	122.12	118.90
1	A	365	U	C2-N1-C1'	5.37	124.14	117.70
1	A	623	C	C6-N1-C2	5.37	122.45	120.30
1	A	831	U	N3-C2-O2	5.37	125.96	122.20
1	A	1078	U	C2-N1-C1'	5.36	124.13	117.70
1	A	1373	G	N9-C4-C5	-5.36	103.26	105.40
1	A	518	C	P-O3'-C3'	5.36	126.13	119.70
1	A	1200	C	C5-C4-N4	-5.36	116.45	120.20
1	A	1211	U	N1-C2-O2	5.36	126.55	122.80
1	A	576	G	N3-C4-C5	-5.35	125.92	128.60
1	A	266	G	N9-C4-C5	-5.35	103.26	105.40
1	A	394	G	C4-C5-N7	-5.35	108.66	110.80
1	A	890	G	C5-C6-N1	-5.35	108.83	111.50
1	A	47	C	C5-C4-N4	-5.35	116.46	120.20
1	A	484	G	N1-C2-N2	-5.35	111.39	116.20
1	A	771	G	C6-C5-N7	-5.35	127.19	130.40
1	A	1153	C	N3-C4-N4	-5.35	114.26	118.00
1	A	1512	U	C4-C5-C6	5.35	122.91	119.70
1	A	445	G	C8-N9-C4	-5.35	104.26	106.40
1	A	1350	A	N7-C8-N9	5.35	116.47	113.80
1	A	712	A	C8-N9-C4	5.34	107.94	105.80
1	A	885	G	OP1-P-OP2	5.34	127.62	119.60
1	A	919	A	N7-C8-N9	-5.34	111.13	113.80
1	A	390	C	O5'-P-OP2	-5.34	100.89	105.70
1	A	1283	G	C8-N9-C4	-5.34	104.26	106.40
1	A	909	A	C5-C6-N1	5.34	120.37	117.70
1	A	284	G	C2-N3-C4	-5.34	109.23	111.90
1	A	615	C	C5-C6-N1	5.34	123.67	121.00
1	A	9	G	C2-N3-C4	-5.34	109.23	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	A	C8-N9-C4	5.34	107.94	105.80
1	A	130	A	N1-C6-N6	5.33	121.80	118.60
1	A	190	C	C5-C6-N1	-5.33	118.33	121.00
1	A	66	G	C8-N9-C4	-5.33	104.27	106.40
1	A	661	G	C2-N3-C4	-5.33	109.24	111.90
1	A	782	A	C2-N3-C4	-5.33	107.94	110.60
1	A	251	G	C4-C5-C6	5.32	121.99	118.80
1	A	1469	G	N3-C2-N2	-5.32	116.17	119.90
1	A	145	G	N1-C6-O6	5.32	123.09	119.90
1	A	291	C	C4-C5-C6	5.32	120.06	117.40
1	A	485	G	C8-N9-C4	5.32	108.53	106.40
1	A	581	G	C2-N3-C4	-5.32	109.24	111.90
1	A	723	U	C6-N1-C2	-5.32	117.81	121.00
1	A	224	C	C5-C6-N1	-5.32	118.34	121.00
1	A	524	G	N3-C4-N9	5.32	129.19	126.00
1	A	920	U	N3-C4-C5	-5.32	111.41	114.60
1	A	923	A	N9-C4-C5	-5.32	103.67	105.80
1	A	1200	C	N3-C2-O2	-5.32	118.18	121.90
1	A	643	C	N3-C4-C5	5.32	124.03	121.90
1	A	448	A	N1-C6-N6	5.31	121.79	118.60
1	A	645	C	N3-C4-N4	5.31	121.72	118.00
1	A	686	U	C4-C5-C6	5.31	122.89	119.70
1	A	48	C	N3-C2-O2	5.31	125.62	121.90
1	A	126	G	N1-C2-N3	5.31	127.09	123.90
1	A	144	G	N1-C2-N2	5.31	120.98	116.20
1	A	251	G	C4-N9-C1'	5.31	133.40	126.50
1	A	642	A	C6-N1-C2	-5.31	115.42	118.60
1	A	127	G	C5-C6-O6	-5.31	125.42	128.60
1	A	15	G	C5-C6-O6	-5.30	125.42	128.60
1	A	50	A	N9-C4-C5	-5.30	103.68	105.80
1	A	320	C	C5-C6-N1	-5.30	118.35	121.00
1	A	864	A	OP2-P-O3'	5.30	116.87	105.20
1	A	863	U	C5-C4-O4	5.30	129.08	125.90
1	A	1130	A	C8-N9-C4	-5.30	103.68	105.80
1	A	79	G	C8-N9-C4	-5.30	104.28	106.40
1	A	484	G	N3-C4-N9	5.30	129.18	126.00
1	A	32	A	C4-C5-C6	5.30	119.65	117.00
1	A	322	C	N3-C4-C5	5.30	124.02	121.90
1	A	328	C	C2-N1-C1'	5.30	124.63	118.80
1	A	1436	U	C6-N1-C2	-5.30	117.82	121.00
1	A	1485	U	C2-N1-C1'	5.30	124.06	117.70
1	A	831	U	O5'-P-OP2	5.29	117.05	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	G	N1-C2-N3	5.29	127.08	123.90
1	A	929	G	C2-N3-C4	-5.29	109.25	111.90
1	A	1158	C	C5-C4-N4	5.29	123.91	120.20
1	A	1470	G	C4-C5-N7	-5.29	108.68	110.80
1	A	1529	G	C8-N9-C1'	-5.29	120.12	127.00
1	A	1190	G	N1-C2-N2	-5.29	111.44	116.20
1	A	1447	G	N1-C6-O6	5.29	123.08	119.90
1	A	746	A	O5'-P-OP1	5.29	117.05	110.70
1	A	943	U	O5'-P-OP2	-5.29	100.94	105.70
1	A	1502	A	C4-C5-C6	5.29	119.64	117.00
20	T	62	LEU	CB-CG-CD1	-5.29	102.01	111.00
1	A	48	C	C2-N1-C1'	-5.29	112.99	118.80
1	A	729	A	OP2-P-O3'	5.29	116.83	105.20
1	A	43	C	C5-C6-N1	-5.28	118.36	121.00
1	A	330	C	OP2-P-O3'	5.28	116.82	105.20
1	A	1485	U	C5-C6-N1	5.28	125.34	122.70
1	A	817	C	O4'-C1'-N1	-5.27	103.98	108.20
1	A	167	G	N1-C2-N2	-5.27	111.46	116.20
1	A	239	U	OP1-P-OP2	5.27	127.51	119.60
1	A	47	C	C6-N1-C1'	-5.27	114.48	120.80
1	A	580	U	C5-C4-O4	5.27	129.06	125.90
1	A	634	C	N3-C2-O2	-5.27	118.21	121.90
1	A	1370	G	N1-C6-O6	-5.27	116.74	119.90
1	A	767	A	O5'-P-OP2	-5.27	100.96	105.70
1	A	232	G	C6-N1-C2	5.26	128.26	125.10
1	A	735	C	N1-C2-N3	-5.26	115.52	119.20
1	A	753	A	C5-C6-N6	5.26	127.91	123.70
1	A	365	U	C5-C4-O4	-5.26	122.74	125.90
1	A	617	G	C5-N7-C8	5.26	106.93	104.30
1	A	1053	G	N7-C8-N9	-5.26	110.47	113.10
1	A	1342	C	N3-C2-O2	5.26	125.58	121.90
1	A	238	G	N1-C6-O6	5.26	123.05	119.90
1	A	402	G	C5-C6-O6	-5.26	125.45	128.60
1	A	879	C	N3-C4-C5	5.26	124.00	121.90
1	A	1236	A	OP2-P-O3'	5.26	116.77	105.20
1	A	1341	U	C6-N1-C2	5.25	124.15	121.00
1	A	873	A	C6-C5-N7	5.25	135.98	132.30
1	A	1447	G	C5-N7-C8	-5.25	101.67	104.30
1	A	393	A	C8-N9-C4	5.25	107.90	105.80
1	A	862	C	N3-C2-O2	5.25	125.57	121.90
1	A	176	C	OP1-P-OP2	5.25	127.47	119.60
1	A	313	A	C8-N9-C4	5.25	107.90	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	C	C5-C6-N1	-5.25	118.38	121.00
1	A	646	U	C5-C4-O4	5.25	129.05	125.90
1	A	736	C	N1-C2-O2	5.25	122.05	118.90
2	B	68	ILE	CB-CA-C	-5.25	101.11	111.60
1	A	1099	G	N3-C4-C5	5.25	131.22	128.60
1	A	941	G	C4-C5-N7	5.24	112.90	110.80
1	A	1341	U	C5-C6-N1	-5.24	120.08	122.70
1	A	770	C	O5'-P-OP1	5.24	116.98	110.70
1	A	970	C	N3-C2-O2	-5.24	118.24	121.90
1	A	788	U	N3-C4-O4	5.23	123.06	119.40
1	A	934	C	C2-N1-C1'	-5.23	113.04	118.80
1	A	742	G	C4-C5-C6	5.23	121.94	118.80
1	A	1526	G	C5-N7-C8	-5.23	101.68	104.30
1	A	243	A	O4'-C1'-N9	5.23	112.38	108.20
1	A	302	G	N9-C4-C5	-5.23	103.31	105.40
1	A	47	C	C6-N1-C2	5.23	122.39	120.30
1	A	252	U	N1-C2-N3	5.23	118.04	114.90
1	A	1361(A)	C	C5-C6-N1	5.23	123.61	121.00
1	A	70	G	N3-C4-C5	5.23	131.21	128.60
1	A	808	C	OP2-P-O3'	5.23	116.70	105.20
1	A	939	G	C6-C5-N7	-5.23	127.26	130.40
1	A	360	A	C5-N7-C8	-5.22	101.29	103.90
1	A	557	G	O5'-P-OP1	5.22	116.97	110.70
1	A	853	G	N1-C2-N2	-5.22	111.50	116.20
1	A	1509	C	C4-C5-C6	5.22	120.01	117.40
1	A	7	G	C4-C5-C6	5.22	121.93	118.80
1	A	190(B)	C	C5-C6-N1	5.22	123.61	121.00
1	A	555	C	C2-N1-C1'	5.22	124.54	118.80
1	A	792	A	P-O3'-C3'	5.22	125.96	119.70
1	A	860	A	C4-C5-C6	5.22	119.61	117.00
1	A	881	G	C6-N1-C2	-5.22	121.97	125.10
1	A	167	G	N1-C6-O6	5.22	123.03	119.90
1	A	1527	C	N3-C4-N4	5.22	121.65	118.00
1	A	323	U	C5-C6-N1	-5.21	120.09	122.70
1	A	644	G	C5-C6-N1	5.21	114.11	111.50
1	A	1365	G	N3-C4-C5	-5.21	125.99	128.60
1	A	1389	C	O5'-P-OP1	5.21	116.95	110.70
1	A	190(G)	G	N1-C6-O6	5.21	123.03	119.90
1	A	971	G	N7-C8-N9	-5.21	110.50	113.10
1	A	181	G	C6-C5-N7	-5.21	127.28	130.40
1	A	771	G	C8-N9-C4	5.21	108.48	106.40
1	A	1085	U	O5'-P-OP2	-5.21	101.01	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1508	G	O5'-P-OP2	5.21	116.95	110.70
1	A	460	A	N3-C4-C5	-5.21	123.16	126.80
1	A	1461	G	C8-N9-C4	5.20	108.48	106.40
1	A	518	C	N3-C4-N4	-5.20	114.36	118.00
1	A	793	U	OP1-P-OP2	-5.20	111.80	119.60
1	A	1317	C	C6-N1-C2	5.20	122.38	120.30
1	A	460	A	C6-N1-C2	-5.20	115.48	118.60
1	A	771	G	N9-C4-C5	-5.20	103.32	105.40
1	A	942	G	O5'-P-OP1	5.20	116.94	110.70
1	A	604	G	C8-N9-C4	5.20	108.48	106.40
1	A	833	U	C4-C5-C6	5.20	122.82	119.70
1	A	1355	G	N3-C4-C5	-5.20	126.00	128.60
1	A	1416	G	C5-C6-N1	-5.20	108.90	111.50
1	A	77	G	N3-C4-N9	5.20	129.12	126.00
1	A	1055	A	C2-N3-C4	5.20	113.20	110.60
1	A	851	G	C4-N9-C1'	5.19	133.25	126.50
1	A	874	G	N1-C2-N3	5.19	127.02	123.90
1	A	923	A	N1-C6-N6	5.19	121.72	118.60
1	A	1058	G	N1-C6-O6	-5.19	116.78	119.90
1	A	221	C	N3-C4-N4	-5.19	114.37	118.00
1	A	604	G	N7-C8-N9	-5.19	110.50	113.10
1	A	302	G	C5-C6-N1	5.19	114.09	111.50
1	A	874	G	C5-C6-O6	-5.19	125.49	128.60
1	A	1399	C	C6-N1-C2	-5.19	118.22	120.30
1	A	962	C	OP2-P-O3'	5.18	116.61	105.20
1	A	1064	G	N3-C2-N2	-5.18	116.27	119.90
1	A	1212	U	O4'-C1'-N1	5.18	112.35	108.20
1	A	1497	G	N3-C4-N9	5.18	129.11	126.00
1	A	314	C	O5'-P-OP2	-5.18	101.04	105.70
1	A	1532	U	N3-C2-O2	5.18	125.83	122.20
1	A	841	U	C5-C6-N1	5.18	125.29	122.70
1	A	721	G	N1-C2-N3	5.18	127.01	123.90
1	A	907	A	N7-C8-N9	-5.18	111.21	113.80
1	A	522	C	C6-N1-C2	5.17	122.37	120.30
1	A	599	C	C5-C4-N4	-5.17	116.58	120.20
1	A	1516[A]	G	N1-C6-O6	-5.17	116.80	119.90
1	A	1516[B]	G	N1-C6-O6	-5.17	116.80	119.90
1	A	759	A	OP2-P-O3'	5.17	116.58	105.20
1	A	818	G	C8-N9-C4	-5.17	104.33	106.40
1	A	991	U	P-O3'-C3'	5.17	125.91	119.70
2	B	213	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	43	C	C6-N1-C2	5.17	122.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	A	O4'-C1'-N9	-5.17	104.06	108.20
1	A	922	G	N3-C4-N9	5.17	129.10	126.00
1	A	1414	U	C2-N1-C1'	5.17	123.90	117.70
1	A	391	G	N3-C4-N9	5.17	129.10	126.00
1	A	910	C	C6-N1-C2	5.17	122.37	120.30
1	A	1081	G	O5'-P-OP2	-5.17	101.05	105.70
1	A	7	G	C6-C5-N7	-5.16	127.30	130.40
1	A	193	C	O5'-P-OP1	5.16	116.89	110.70
1	A	306	G	N1-C2-N2	5.16	120.84	116.20
1	A	500	G	C4-C5-N7	5.16	112.86	110.80
1	A	735	C	C2-N1-C1'	-5.16	113.12	118.80
1	A	969	A	N1-C6-N6	5.16	121.70	118.60
4	D	94	LEU	CA-CB-CG	-5.16	103.43	115.30
1	A	278	G	OP1-P-OP2	5.16	127.34	119.60
1	A	666	G	C4-C5-C6	5.16	121.89	118.80
1	A	836	G	C6-C5-N7	-5.16	127.31	130.40
1	A	646	U	C2-N3-C4	5.15	130.09	127.00
1	A	1341	U	N3-C2-O2	5.15	125.81	122.20
1	A	230	G	N1-C2-N2	-5.15	111.56	116.20
1	A	738	C	C2-N3-C4	-5.15	117.33	119.90
1	A	826	C	C6-N1-C2	5.15	122.36	120.30
1	A	509	A	C3'-C2'-C1'	-5.15	97.38	101.50
1	A	964	A	C8-N9-C4	-5.15	103.74	105.80
1	A	331	G	C4-C5-C6	5.14	121.89	118.80
1	A	485	G	N7-C8-N9	-5.14	110.53	113.10
1	A	1294	G	N3-C4-N9	-5.14	122.91	126.00
1	A	667	G	N9-C4-C5	-5.14	103.34	105.40
1	A	856	C	N1-C2-N3	5.14	122.80	119.20
1	A	1390	U	C4-C5-C6	5.14	122.78	119.70
1	A	154	C	C6-N1-C2	5.14	122.36	120.30
1	A	833	U	O4'-C1'-N1	5.14	112.31	108.20
1	A	858	G	C2-N3-C4	-5.14	109.33	111.90
1	A	1280	A	O5'-P-OP1	-5.14	101.07	105.70
1	A	370	C	OP2-P-O3'	5.14	116.51	105.20
1	A	681	C	C6-N1-C2	5.14	122.36	120.30
1	A	1385	G	C8-N9-C4	5.14	108.45	106.40
1	A	871	U	OP1-P-OP2	5.14	127.31	119.60
1	A	364	A	N1-C2-N3	5.14	131.87	129.30
1	A	836	G	O4'-C1'-N9	-5.14	104.09	108.20
1	A	246	A	OP1-P-O3'	5.13	116.50	105.20
1	A	653	A	C8-N9-C4	-5.13	103.75	105.80
1	A	734	G	C4-C5-N7	5.13	112.85	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	A	C8-N9-C4	5.13	107.85	105.80
1	A	858	G	C4-N9-C1'	5.13	133.17	126.50
1	A	595	G	C5-C6-N1	-5.13	108.94	111.50
1	A	491	G	N1-C6-O6	5.12	122.97	119.90
1	A	254	G	C2-N3-C4	-5.12	109.34	111.90
1	A	930	C	C2-N3-C4	-5.12	117.34	119.90
1	A	632	A	N1-C2-N3	5.12	131.86	129.30
1	A	484	G	P-O3'-C3'	5.12	125.84	119.70
1	A	1215	G	N1-C6-O6	5.12	122.97	119.90
1	A	394	G	C5-C6-O6	5.12	131.67	128.60
1	A	22	G	P-O3'-C3'	5.12	125.84	119.70
1	A	304	U	N3-C4-O4	-5.12	115.82	119.40
1	A	1135	U	C2-N1-C1'	5.12	123.84	117.70
1	A	945	G	C5-N7-C8	-5.11	101.74	104.30
1	A	1528	U	C6-N1-C1'	-5.11	114.05	121.20
1	A	59	A	C5-C6-N1	5.11	120.25	117.70
1	A	131	C	C4-C5-C6	5.11	119.95	117.40
1	A	1383	C	N3-C4-C5	-5.11	119.86	121.90
1	A	975	A	C5-C6-N1	-5.11	115.15	117.70
1	A	1530	G	C2-N3-C4	-5.11	109.35	111.90
16	P	60	LEU	CA-CB-CG	-5.11	103.56	115.30
1	A	698	G	C4-N9-C1'	5.10	133.13	126.50
1	A	732	C	N3-C4-C5	5.10	123.94	121.90
1	A	757	U	C2-N1-C1'	-5.10	111.58	117.70
1	A	975	A	N1-C6-N6	5.10	121.66	118.60
1	A	976	G	C5-C6-O6	5.10	131.66	128.60
1	A	28	G	C2-N3-C4	-5.10	109.35	111.90
1	A	482	A	C8-N9-C4	-5.10	103.76	105.80
1	A	658	G	N1-C2-N2	-5.10	111.61	116.20
1	A	1065	U	P-O3'-C3'	5.10	125.82	119.70
1	A	1373	G	C4-N9-C1'	5.10	133.13	126.50
1	A	1425	U	O4'-C1'-N1	5.10	112.28	108.20
1	A	668	G	C8-N9-C4	5.10	108.44	106.40
1	A	777	A	C6-N1-C2	-5.10	115.54	118.60
1	A	78	G	OP1-P-O3'	5.09	116.41	105.20
1	A	247	G	O5'-P-OP1	5.09	116.81	110.70
1	A	281	G	N1-C6-O6	5.09	122.96	119.90
1	A	1215	G	C5-N7-C8	-5.09	101.75	104.30
1	A	1380	U	C5-C4-O4	5.09	128.96	125.90
1	A	107	G	C6-C5-N7	-5.09	127.35	130.40
1	A	485	G	C4-C5-N7	-5.09	108.76	110.80
1	A	395	C	C5-C6-N1	-5.09	118.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	817	C	OP1-P-O3'	5.09	116.39	105.20
1	A	68	G	C4-N9-C1'	-5.09	119.89	126.50
1	A	932	C	C2-N3-C4	-5.09	117.36	119.90
1	A	1342	C	N3-C4-N4	5.09	121.56	118.00
1	A	606	G	C5-C6-N1	-5.09	108.96	111.50
1	A	1153	C	N3-C4-C5	5.09	123.93	121.90
1	A	21	G	C5-N7-C8	5.08	106.84	104.30
1	A	551	U	C5-C4-O4	-5.08	122.85	125.90
1	A	384	G	C8-N9-C4	5.08	108.43	106.40
1	A	1243	C	C2-N1-C1'	-5.08	113.22	118.80
1	A	902	G	O5'-P-OP2	-5.08	101.13	105.70
1	A	807	A	N1-C6-N6	-5.08	115.55	118.60
1	A	576	G	C4-C5-C6	5.07	121.84	118.80
1	A	1333	A	C6-N1-C2	-5.07	115.56	118.60
1	A	697	U	C5-C6-N1	-5.07	120.16	122.70
1	A	1161	C	C6-N1-C2	5.07	122.33	120.30
1	A	789	U	N1-C2-N3	5.07	117.94	114.90
1	A	1414	U	OP1-P-O3'	5.07	116.35	105.20
1	A	1417	G	N3-C2-N2	-5.07	116.35	119.90
1	A	189	G	N3-C4-N9	5.07	129.04	126.00
1	A	305	G	N3-C4-C5	5.07	131.13	128.60
1	A	807	A	N7-C8-N9	-5.07	111.27	113.80
1	A	869	G	O5'-P-OP1	-5.06	101.14	105.70
1	A	181	G	P-O3'-C3'	5.06	125.77	119.70
1	A	267	C	N3-C4-C5	5.06	123.92	121.90
1	A	529	G	N3-C4-N9	5.06	129.04	126.00
1	A	1092	A	C6-C5-N7	-5.06	128.76	132.30
1	A	762	C	N3-C4-N4	5.06	121.54	118.00
1	A	240	C	N3-C4-C5	5.06	123.92	121.90
1	A	448	A	C4-C5-N7	5.06	113.23	110.70
5	E	41	VAL	CB-CA-C	-5.06	101.79	111.40
1	A	21	G	OP2-P-O3'	5.06	116.33	105.20
1	A	183	G	C6-C5-N7	-5.06	127.36	130.40
1	A	959	A	C5-C6-N6	-5.06	119.65	123.70
1	A	787	A	C8-N9-C4	-5.05	103.78	105.80
1	A	559	A	P-O3'-C3'	5.05	125.76	119.70
1	A	882	C	N1-C2-O2	5.05	121.93	118.90
1	A	992	U	P-O3'-C3'	5.05	125.76	119.70
1	A	26	A	C5-C6-N6	5.05	127.74	123.70
1	A	647	C	N1-C2-O2	5.05	121.93	118.90
1	A	596	C	OP1-P-O3'	5.05	116.31	105.20
1	A	622	A	C4-C5-N7	5.05	113.22	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	728	A	C2-N3-C4	-5.05	108.08	110.60
1	A	259	G	N1-C2-N3	5.05	126.93	123.90
1	A	135	C	N3-C2-O2	5.05	125.43	121.90
1	A	823	G	C6-N1-C2	-5.04	122.07	125.10
1	A	1383	C	C2-N1-C1'	5.04	124.35	118.80
1	A	640	A	C6-C5-N7	-5.04	128.77	132.30
1	A	289	G	C6-C5-N7	-5.04	127.38	130.40
1	A	724	G	N9-C1'-C2'	-5.04	106.46	112.00
1	A	1190	G	C5-N7-C8	-5.04	101.78	104.30
1	A	389	A	C5-N7-C8	5.04	106.42	103.90
1	A	898	G	N1-C2-N3	5.03	126.92	123.90
1	A	1129	C	O4'-C1'-N1	5.03	112.22	108.20
1	A	1200	C	OP1-P-OP2	-5.03	112.05	119.60
1	A	590	C	C4-C5-C6	5.03	119.91	117.40
1	A	702	A	OP1-P-OP2	-5.03	112.06	119.60
1	A	908	A	C4-C5-C6	-5.03	114.49	117.00
1	A	122	G	O5'-P-OP1	-5.03	101.17	105.70
1	A	644	G	C4-C5-N7	5.03	112.81	110.80
1	A	887	G	O5'-P-OP1	5.03	116.73	110.70
1	A	1074	G	C6-C5-N7	-5.03	127.39	130.40
1	A	1334	G	C8-N9-C1'	-5.03	120.47	127.00
1	A	50	A	N7-C8-N9	-5.02	111.29	113.80
1	A	588	G	N1-C6-O6	5.02	122.91	119.90
1	A	1197	G	N3-C4-C5	-5.02	126.09	128.60
1	A	32	A	OP2-P-O3'	-5.02	94.15	105.20
1	A	676	A	N7-C8-N9	-5.02	111.29	113.80
1	A	25	C	C4-C5-C6	5.02	119.91	117.40
1	A	309	G	C5-C6-O6	-5.02	125.59	128.60
1	A	919	A	N1-C2-N3	-5.02	126.79	129.30
1	A	1188	A	O5'-P-OP1	-5.02	101.18	105.70
1	A	1243	C	C6-N1-C1'	5.02	126.82	120.80
1	A	15	G	N3-C2-N2	-5.02	116.39	119.90
1	A	500	G	N3-C4-C5	5.02	131.11	128.60
1	A	1084	G	N1-C2-N3	5.02	126.91	123.90
1	A	190(B)	C	N3-C4-N4	5.01	121.51	118.00
1	A	1310	G	N3-C4-N9	5.01	129.01	126.00
1	A	773	G	C5-C6-O6	-5.01	125.59	128.60
1	A	932	C	N3-C2-O2	-5.01	118.39	121.90
1	A	128	G	C4-C5-N7	5.01	112.80	110.80
1	A	599	C	N3-C4-C5	5.01	123.90	121.90
1	A	648	A	C5-C6-N1	5.01	120.20	117.70
1	A	695	A	N7-C8-N9	5.01	116.31	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1246	C	N3-C2-O2	5.01	125.41	121.90
1	A	389	A	C6-N1-C2	-5.01	115.60	118.60
1	A	832	C	C2-N3-C4	-5.01	117.40	119.90
1	A	1190	G	C5-C6-N1	-5.01	109.00	111.50
1	A	1343	G	N3-C4-C5	5.01	131.10	128.60
8	H	105	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	A	664	G	O5'-P-OP2	-5.00	101.19	105.70
1	A	1077	G	C8-N9-C4	5.00	108.40	106.40
1	A	169	C	N1-C2-O2	5.00	121.90	118.90
1	A	1515[A]	C	C6-N1-C2	-5.00	118.30	120.30
1	A	1515[B]	C	C6-N1-C2	-5.00	118.30	120.30
1	A	294	U	C5-C4-O4	-5.00	122.90	125.90
1	A	1530	G	O5'-P-OP2	-5.00	101.20	105.70

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	20	GLU	Peptide
2	B	8	LYS	Peptide
3	C	166	GLU	Peptide
3	C	3	ASN	Peptide
3	C	89	GLU	Peptide
4	D	3	ARG	Peptide
7	G	154	TYR	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
10	J	50	ILE	Peptide
10	J	90	LEU	Peptide
12	L	25	PRO	Peptide
12	L	90	VAL	Peptide
13	M	62	ASN	Peptide
18	R	86	VAL	Peptide
19	S	13	ASP	Peptide
20	T	48	LYS	Peptide
20	T	93	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32644	0	16503	1058	0
2	B	1900	0	1950	123	0
3	C	1612	0	1676	115	0
4	D	1703	0	1763	132	0
5	E	1146	0	1207	66	0
6	F	843	0	857	38	0
7	G	1257	0	1296	78	0
8	H	1116	0	1177	70	0
9	I	1010	0	1037	78	0
10	J	792	0	835	59	0
11	K	864	0	881	51	0
12	L	977	0	1060	78	0
13	M	937	0	995	72	0
14	N	492	0	529	37	0
15	O	729	0	768	38	0
16	P	700	0	720	45	0
17	Q	823	0	891	59	0
18	R	574	0	644	50	0
19	S	647	0	673	42	0
20	T	763	0	861	44	0
21	U	208	0	221	22	0
22	A	276	0	0	0	0
22	B	3	0	0	0	0
22	C	2	0	0	0	0
22	D	3	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	H	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	N	1	0	0	0	0
22	P	2	0	0	0	0
22	Q	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	266	0	0	7	0
24	E	3	0	0	0	0
24	K	1	0	0	0	0
24	L	1	0	0	0	0
24	Q	2	0	0	0	0
24	T	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	52307	0	36544	2147	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (2147) 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)
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.36	1.05
4:D:3:ARG:HH11	4:D:71:SER:H	1.13	0.94
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.01	0.93
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.51	0.93
1:A:992:U:H3	1:A:1044:A:H62	1.09	0.92
19:S:41:VAL:HG22	19:S:44:MET:HG3	1.53	0.90
1:A:664:G:H22	1:A:741:G:H1	1.20	0.89
14:N:53:LEU:HD12	14:N:56:VAL:HG21	1.55	0.89
1:A:413:G:H8	1:A:428:G:H21	1.20	0.89
18:R:50:ILE:HD11	18:R:70:ILE:HG21	1.55	0.88
1:A:1348:U:H4'	9:I:120:ARG:HD2	1.54	0.88
1:A:912:C:OP1	12:L:46:LYS:NZ	2.07	0.88
1:A:1195:C:H3'	1:A:1196:U:H5''	1.54	0.88
18:R:37:VAL:O	18:R:40:LEU:N	2.07	0.87
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.56	0.87
2:B:15:VAL:HG11	2:B:213:LEU:HD23	1.55	0.86
1:A:76:C:H42	1:A:95:U:H3	1.23	0.86
5:E:144:THR:O	5:E:148:VAL:HG23	1.75	0.86
1:A:130:A:H5'	17:Q:63:ARG:HE	1.40	0.85
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.09	0.85
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.07	0.85
12:L:27:LEU:O	12:L:29:GLY:N	2.09	0.85
1:A:1413:A:H2'	1:A:1414:U:H6	1.41	0.85
1:A:263:A:OP2	20:T:79:ARG:NH1	2.10	0.84
1:A:1349:A:OP1	9:I:118:LYS:NZ	2.10	0.84
1:A:839:U:H5'	1:A:840:C:H5	1.43	0.83
1:A:130:A:OP2	1:A:190(E):U:O2'	1.96	0.83
1:A:132:C:O2	1:A:230:G:N2	2.11	0.83
4:D:103:ASN:OD1	4:D:114:ARG:NH2	2.10	0.83
1:A:1051:C:N4	1:A:1207:2MG:O6	2.11	0.83
3:C:11:ARG:HG3	3:C:178:LEU:HD11	1.59	0.83
5:E:121:LYS:HG2	5:E:123:LEU:HD23	1.61	0.82
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.62	0.82
18:R:55:ARG:HB3	18:R:55:ARG:HH11	1.43	0.81
9:I:86:VAL:HG21	9:I:93:ARG:HG3	1.61	0.81
1:A:79:G:N1	1:A:80:G:N7	2.28	0.81
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.14	0.80
6:F:8:ILE:HB	6:F:61:LEU:HD12	1.63	0.80
4:D:187:ARG:NE	4:D:188:LEU:H	1.79	0.80
1:A:1034:G:H2'	1:A:1035:A:H8	1.46	0.80
1:A:1009:G:H1	1:A:1020:U:H3	1.30	0.80
1:A:35:G:O2'	12:L:118:SER:O	2.00	0.80
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.63	0.79
21:U:10:ARG:HH11	21:U:10:ARG:HB2	1.47	0.79
15:O:6:GLU:OE1	15:O:6:GLU:N	2.12	0.79
1:A:262:A:H5'	20:T:74:LYS:HD3	1.66	0.78
14:N:57:ARG:HB3	14:N:57:ARG:HH11	1.48	0.78
1:A:409:G:H1	1:A:433:C:H42	1.31	0.78
7:G:71:PRO:O	7:G:96:GLN:NE2	2.16	0.78
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.47	0.78
1:A:547:A:OP2	4:D:2:GLY:N	2.15	0.78
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.66	0.78
7:G:87:VAL:HG11	7:G:154:TYR:HB2	1.64	0.78
8:H:87:SER:HA	8:H:93:VAL:HG13	1.66	0.78
1:A:1279:A:OP1	10:J:7:LYS:NZ	2.17	0.78
3:C:139:GLN:O	3:C:143:GLU:N	2.16	0.78
13:M:96:LEU:O	13:M:110:ARG:NH1	2.17	0.78
1:A:1124:G:N2	1:A:1126:U:O4	2.16	0.77
20:T:83:ARG:NH2	24:T:202:HOH:O	2.16	0.77
13:M:68:GLY:HA2	13:M:71:ARG:HD2	1.66	0.77
1:A:1376:U:OP1	7:G:98:SER:OG	2.03	0.77
10:J:50:ILE:HA	10:J:60:ARG:HB3	1.65	0.77
14:N:40:CYS:O	14:N:44:LEU:N	2.14	0.77
1:A:279:A:OP2	17:Q:95:TYR:OH	2.02	0.77
1:A:95:U:H2'	1:A:96:G:H8	1.50	0.77
13:M:49:THR:HB	13:M:52:GLU:H	1.48	0.77
1:A:1422:G:H2'	1:A:1423:G:H8	1.49	0.77
1:A:1263:C:N4	1:A:1272:G:O6	2.17	0.76
1:A:1009:G:N2	1:A:1010:G:N3	2.33	0.76
7:G:86:GLN:HB2	7:G:148:ASN:HD22	1.51	0.76
1:A:103:C:OP1	20:T:17:ARG:NH1	2.19	0.76
1:A:1168:A:H2'	1:A:1169:A:C8	2.19	0.76
1:A:1347:G:H3'	9:I:108:VAL:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:LYS:HA	3:C:169:ALA:CB	2.16	0.76
12:L:25:PRO:C	12:L:27:LEU:H	1.87	0.76
1:A:1347:G:N2	1:A:1373:G:H2'	2.00	0.75
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.66	0.75
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.22	0.75
1:A:1416:G:N2	1:A:1484:C:O2	2.19	0.75
2:B:103:THR:HA	2:B:180:LEU:HD11	1.68	0.75
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.26	0.75
4:D:25:ARG:HG3	4:D:30:LYS:HD3	1.67	0.75
5:E:84:PHE:HB3	5:E:134:ALA:HB2	1.69	0.75
11:K:57:THR:HG23	11:K:60:ALA:H	1.50	0.75
1:A:1367:C:O5'	9:I:112:LYS:NZ	2.20	0.75
1:A:953:G:N7	13:M:104:ARG:NH2	2.35	0.75
3:C:20:SER:HB3	3:C:57:ILE:HB	1.69	0.74
4:D:50:ARG:NH1	4:D:51:PRO:O	2.19	0.74
2:B:21:ARG:HH11	2:B:22:LYS:HB3	1.52	0.74
4:D:154:ASN:O	4:D:159:ARG:NH2	2.19	0.74
1:A:1004:A:H5''	1:A:1025:U:C2	2.22	0.74
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.69	0.74
1:A:1491:G:N2	1:A:1492:A:N7	2.35	0.74
1:A:959:A:O2'	1:A:984:C:O2'	2.04	0.74
14:N:26:ARG:HD2	14:N:47:LEU:HD21	1.69	0.74
1:A:1413:A:H2	1:A:1487:G:H22	1.35	0.74
21:U:10:ARG:NH1	21:U:10:ARG:HB2	2.03	0.74
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.19	0.74
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.23	0.74
1:A:384:G:H2'	1:A:385:C:C6	2.23	0.74
1:A:736:C:H2'	1:A:737:A:C8	2.23	0.74
3:C:84:ILE:HG23	3:C:88:ARG:HH12	1.51	0.74
1:A:1255:G:N2	1:A:1259:C:O2	2.19	0.73
3:C:88:ARG:HH21	3:C:101:LEU:HB2	1.54	0.73
1:A:1125:U:O4	10:J:5:ARG:NH2	2.21	0.73
1:A:989:C:N3	1:A:1216:G:N2	2.35	0.73
2:B:17:PHE:HD1	2:B:18:GLY:H	1.37	0.73
3:C:150:LYS:HB2	3:C:201:TYR:HB2	1.71	0.73
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.20	0.73
1:A:1063:C:H2'	1:A:1064:G:C8	2.24	0.73
14:N:8:GLU:HA	14:N:11:LYS:HD3	1.70	0.73
1:A:95:U:H2'	1:A:96:G:C8	2.24	0.72
11:K:48:ILE:HD12	11:K:63:LEU:HB2	1.70	0.72
1:A:986:A:H1'	19:S:55:LYS:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:83:ASP:OD1	17:Q:84:LEU:N	2.22	0.72
1:A:235:C:N4	24:A:1986:HOH:O	2.22	0.72
4:D:63:LYS:NZ	4:D:197:PRO:O	2.20	0.72
1:A:1305:G:N2	1:A:1331:G:H1'	2.05	0.72
18:R:51:LEU:HD22	18:R:55:ARG:HH12	1.55	0.72
18:R:88:LYS:NZ	18:R:88:LYS:OXT	2.20	0.72
3:C:150:LYS:HA	3:C:169:ALA:HB2	1.69	0.72
1:A:1291:G:OP1	7:G:37:ASN:ND2	2.23	0.71
1:A:1435:G:H2'	1:A:1436:U:H6	1.55	0.71
1:A:436:C:H2'	1:A:437:U:H6	1.53	0.71
2:B:47:THR:OG1	2:B:202:PRO:O	2.06	0.71
18:R:55:ARG:HB3	18:R:55:ARG:NH1	2.05	0.71
1:A:1195:C:H3'	1:A:1196:U:C5'	2.20	0.71
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.54	0.71
20:T:100:ILE:HG22	20:T:102:GLY:H	1.55	0.71
1:A:1316:G:N1	1:A:1319:A:OP2	2.23	0.71
1:A:1175:G:H2'	1:A:1176:A:C8	2.26	0.71
1:A:149:A:H2'	1:A:150:C:H6	1.54	0.71
1:A:677:U:H3	1:A:713:G:H22	1.37	0.71
3:C:88:ARG:HG3	3:C:91:LEU:HD22	1.72	0.71
1:A:144:G:H1	1:A:178:C:H42	1.35	0.70
9:I:91:ASP:N	9:I:91:ASP:OD1	2.22	0.70
12:L:113:ARG:HH11	12:L:116:SER:H	1.37	0.70
1:A:1435:G:H2'	1:A:1436:U:C6	2.26	0.70
1:A:1190:G:H5'	3:C:4:LYS:H	1.57	0.70
2:B:16:HIS:HB3	2:B:210:SER:HB3	1.73	0.70
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.22	0.70
1:A:1298:C:H4'	1:A:1299:A:H5''	1.72	0.70
1:A:144:G:N2	1:A:178:C:N3	2.39	0.70
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.74	0.70
13:M:49:THR:HG22	13:M:51:ALA:H	1.56	0.70
1:A:839:U:H5'	1:A:840:C:C5	2.26	0.70
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.73	0.70
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.24	0.70
1:A:854:G:H3'	1:A:871:U:O4	1.92	0.70
3:C:17:ASP:O	3:C:54:ARG:NH2	2.20	0.70
3:C:147:LYS:HD3	3:C:205:GLY:H	1.56	0.70
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.07	0.70
9:I:48:GLU:OE1	9:I:51:ARG:NH2	2.25	0.70
19:S:18:LYS:HD2	19:S:31:ILE:HG13	1.73	0.70
15:O:39:LEU:HD13	15:O:56:LEU:HG	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.26	0.69
12:L:27:LEU:C	12:L:29:GLY:H	1.93	0.69
16:P:67:THR:HG22	16:P:69:THR:H	1.57	0.69
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.74	0.69
5:E:80:ILE:HG22	8:H:104:ARG:HH21	1.56	0.69
16:P:22:THR:HA	16:P:33:ILE:HG12	1.75	0.69
1:A:1391:U:H2'	1:A:1392:G:C8	2.27	0.69
1:A:501:C:H2'	1:A:502:G:C8	2.26	0.69
1:A:343:U:O2'	1:A:346:G:O6	2.06	0.69
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.73	0.69
1:A:419:C:H42	1:A:424:G:H1	1.41	0.69
1:A:1055:A:N7	1:A:1200:C:N4	2.41	0.69
1:A:279:A:H5''	1:A:281:G:O4'	1.92	0.69
1:A:344:A:H5'	1:A:345:C:C5	2.28	0.69
20:T:45:GLN:HA	20:T:91:LEU:HD12	1.74	0.69
1:A:258:G:H2'	1:A:259:G:H8	1.57	0.69
1:A:324:G:OP1	20:T:22:ARG:NH1	2.26	0.69
2:B:21:ARG:HA	2:B:39:ILE:HG23	1.75	0.68
1:A:1367:C:H5'	10:J:60:ARG:HH11	1.57	0.68
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.74	0.68
17:Q:81:ARG:HB3	17:Q:84:LEU:HD12	1.75	0.68
18:R:58:LEU:HD22	18:R:62:GLU:HB3	1.73	0.68
1:A:966:M2G:H3'	1:A:967:5MC:HM51	1.76	0.68
8:H:2:LEU:HD23	8:H:3:THR:H	1.57	0.68
20:T:39:LYS:HG2	20:T:55:ILE:HD13	1.73	0.68
1:A:1012:U:H2'	1:A:1013:G:C8	2.28	0.68
1:A:1244:C:H42	1:A:1293:G:H1	1.40	0.68
1:A:79:G:C2	1:A:80:G:N7	2.61	0.68
1:A:986:A:N3	19:S:52:TYR:OH	2.24	0.68
1:A:986:A:O2'	19:S:55:LYS:O	2.12	0.68
16:P:21:VAL:HG12	16:P:33:ILE:HG13	1.75	0.68
1:A:1125:U:OP2	1:A:1145:C:N4	2.27	0.68
1:A:1290:G:H2'	1:A:1291:G:C8	2.28	0.68
2:B:102:LEU:HD23	2:B:182:ILE:HD12	1.75	0.68
1:A:1100:C:OP2	2:B:96:ARG:NH1	2.27	0.68
1:A:646:U:H2'	1:A:647:C:C6	2.28	0.68
5:E:15:ARG:HG3	5:E:28:PHE:CE2	2.29	0.68
1:A:1220:G:N2	19:S:54:GLY:O	2.23	0.68
10:J:79:ARG:O	10:J:82:ILE:N	2.27	0.68
14:N:29:ARG:NH1	14:N:40:CYS:SG	2.67	0.68
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:206:PHE:HD2	4:D:207:TYR:CD2	2.12	0.67
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.75	0.67
13:M:76:ALA:HA	13:M:79:LYS:HG3	1.75	0.67
1:A:1226:C:OP2	13:M:91:ARG:NH2	2.27	0.67
7:G:115:ARG:HB3	7:G:118:VAL:HG23	1.75	0.67
4:D:25:ARG:HA	4:D:28:SER:HB2	1.76	0.67
5:E:80:ILE:HG22	8:H:104:ARG:NH2	2.08	0.67
1:A:1047:G:H5'	14:N:4:LYS:HD2	1.76	0.67
1:A:1261:A:H1'	1:A:1283:G:H5'	1.77	0.67
5:E:65:ASN:ND2	5:E:65:ASN:O	2.28	0.67
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.30	0.67
1:A:1309:G:OP2	13:M:99:ARG:NH1	2.27	0.67
1:A:1228:C:H5'	13:M:115:LYS:O	1.95	0.67
4:D:173:TRP:HB2	4:D:187:ARG:O	1.94	0.66
5:E:18:ARG:HG2	5:E:19:MET:N	2.09	0.66
1:A:517:G:N1	1:A:533:A:OP2	2.18	0.66
1:A:793:U:H4'	1:A:794:A:OP2	1.94	0.66
1:A:1257:U:H4'	1:A:1258:G:O5'	1.95	0.66
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.29	0.66
14:N:24:CYS:HB3	14:N:29:ARG:HB3	1.76	0.66
3:C:24:ALA:HB3	3:C:29:TYR:CD1	2.29	0.66
11:K:40:ILE:HG22	11:K:41:THR:HG22	1.77	0.66
1:A:101:A:H2'	1:A:102:G:H8	1.60	0.66
1:A:1426:C:H2'	1:A:1427:U:C6	2.31	0.66
1:A:1515[B]:C:H42	1:A:1520[B]:G:H1	1.41	0.66
1:A:627:G:H2'	1:A:628:G:H8	1.61	0.66
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.78	0.66
8:H:28:ALA:HB2	8:H:59:LEU:HG	1.78	0.66
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.77	0.66
12:L:33:ARG:O	12:L:85:ILE:HG22	1.96	0.66
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.77	0.66
17:Q:62:SER:HB3	17:Q:72:ARG:HD3	1.78	0.66
1:A:1517[A]:G:H2'	1:A:1518[A]:MA6:H8	1.76	0.66
1:A:1034:G:H2'	1:A:1035:A:C8	2.29	0.66
20:T:100:ILE:HG22	20:T:102:GLY:N	2.10	0.66
11:K:41:THR:OG1	11:K:42:TRP:N	2.27	0.65
1:A:1349:A:P	9:I:118:LYS:HZ1	2.20	0.65
1:A:1124:G:H5'	10:J:36:GLY:HA3	1.78	0.65
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.78	0.65
1:A:1347:G:C8	9:I:107:ARG:HB3	2.31	0.65
1:A:1418:A:H2'	1:A:1419:G:O4'	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1387:G:O2'	24:A:2055:HOH:O	2.15	0.65
2:B:107:THR:O	2:B:110:GLN:HB2	1.95	0.65
8:H:95:VAL:HG12	8:H:99:GLU:HB2	1.77	0.65
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.77	0.65
1:A:1020:U:H2'	1:A:1021:G:C8	2.32	0.65
1:A:1179:A:H2'	1:A:1180:A:O4'	1.96	0.65
1:A:964:A:O2'	10:J:55:LYS:NZ	2.24	0.65
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.78	0.65
1:A:831:U:H2'	1:A:832:C:H6	1.61	0.65
9:I:43:ALA:HA	9:I:74:ILE:HD12	1.78	0.65
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.30	0.65
17:Q:59:ILE:HG23	17:Q:71:PHE:HD1	1.61	0.65
3:C:52:LEU:HD11	3:C:68:VAL:HG22	1.79	0.65
1:A:1181:G:O2'	1:A:1182:G:O5'	2.14	0.65
3:C:154:SER:OG	3:C:155:GLY:N	2.28	0.65
2:B:189:ASP:O	2:B:192:SER:OG	2.15	0.65
4:D:149:ALA:O	4:D:152:SER:N	2.31	0.64
13:M:117:VAL:HG12	13:M:118:ALA:H	1.62	0.64
5:E:122:GLU:OE1	5:E:131:ILE:HG13	1.96	0.64
1:A:1014:A:H5'	19:S:14:HIS:CD2	2.32	0.64
2:B:17:PHE:HD1	2:B:18:GLY:N	1.95	0.64
5:E:116:THR:OG1	5:E:117:ASP:OD2	2.15	0.64
1:A:793:U:H5''	24:A:2162:HOH:O	1.98	0.64
1:A:1128:C:O2'	1:A:1130:A:N7	2.30	0.64
2:B:18:GLY:O	2:B:204:ASN:ND2	2.31	0.64
2:B:44:LEU:HA	2:B:47:THR:HB	1.79	0.64
1:A:833:U:H2'	1:A:834:C:C6	2.32	0.64
1:A:967:5MC:H5''	1:A:968:A:H2'	1.78	0.64
1:A:1070:U:H2'	1:A:1071:C:H6	1.61	0.64
1:A:1402:4OC:HM42	1:A:1500:A:H61	1.61	0.64
1:A:668:G:H1	1:A:738:C:H42	1.45	0.64
1:A:75:G:C2	1:A:96:G:C2	2.86	0.64
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.31	0.64
1:A:1443:G:H4'	1:A:1446:A:H5'	1.80	0.64
20:T:10:LEU:HD13	20:T:12:ALA:H	1.62	0.64
21:U:10:ARG:HG3	21:U:13:ILE:HD11	1.79	0.64
1:A:1425:U:H2'	1:A:1426:C:H6	1.63	0.64
1:A:1020:U:H2'	1:A:1021:G:H8	1.63	0.63
2:B:118:LEU:HB2	2:B:142:LEU:HD23	1.80	0.63
1:A:427:U:OP1	4:D:13:ARG:NH2	2.31	0.63
1:A:89:C:H2'	1:A:90:U:C6	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.79	0.63
1:A:1402:4OC:H2'	1:A:1403:C:O4'	1.98	0.63
7:G:108:ALA:O	7:G:119:ARG:HB3	1.98	0.63
10:J:51:ARG:CZ	10:J:61:GLU:HB3	2.28	0.63
16:P:20:VAL:HG11	16:P:32:TYR:CD1	2.34	0.63
21:U:17:THR:O	21:U:22:ARG:NH1	2.32	0.63
1:A:89:C:H2'	1:A:90:U:H6	1.64	0.63
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.80	0.63
1:A:1103:C:H5'	2:B:98:LEU:HD13	1.79	0.63
3:C:131:ARG:HH22	3:C:157:ILE:HG21	1.63	0.63
7:G:84:ASN:OD1	7:G:84:ASN:N	2.31	0.63
1:A:991:U:O4	1:A:1215:G:N1	2.31	0.63
13:M:97:PRO:HG3	13:M:110:ARG:HB3	1.81	0.63
1:A:1202:G:H1'	14:N:42:ILE:HD12	1.81	0.62
1:A:560:U:H5'	1:A:566:G:C2	2.34	0.62
1:A:1152:A:H5''	10:J:13:HIS:CD2	2.34	0.62
13:M:97:PRO:HA	13:M:110:ARG:HD3	1.81	0.62
1:A:258:G:H2'	1:A:259:G:C8	2.33	0.62
2:B:114:ARG:HH11	2:B:118:LEU:HD21	1.64	0.62
2:B:21:ARG:NH1	2:B:22:LYS:HB3	2.13	0.62
7:G:87:VAL:HG12	7:G:88:PRO:HD2	1.82	0.62
8:H:2:LEU:HD23	8:H:3:THR:N	2.14	0.62
1:A:1003:G:H1	1:A:1038:C:H42	1.46	0.62
1:A:1141:C:H2'	1:A:1142:G:C8	2.34	0.62
1:A:989:C:H42	1:A:1216:G:H1	1.47	0.62
1:A:1425:U:H3	1:A:1475:G:H1	1.44	0.62
1:A:350:G:H5''	1:A:350:G:H8	1.64	0.62
1:A:436:C:H2'	1:A:437:U:C6	2.34	0.62
1:A:955:U:H1'	1:A:1227:A:H61	1.65	0.62
12:L:25:PRO:HA	12:L:27:LEU:H	1.64	0.62
1:A:1532:U:H2'	1:A:1533:C:H5''	1.81	0.62
1:A:966:M2G:H2'	1:A:967:5MC:H6	1.63	0.62
2:B:16:HIS:CB	2:B:210:SER:HB3	2.30	0.62
2:B:23:ARG:HA	2:B:23:ARG:NH1	2.14	0.62
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.82	0.62
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.32	0.62
1:A:875:C:O2'	8:H:14:ARG:NH1	2.33	0.62
4:D:187:ARG:HE	4:D:188:LEU:H	1.45	0.62
9:I:64:THR:OG1	9:I:66:ARG:NH1	2.32	0.62
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.80	0.62
13:M:55:ARG:O	13:M:58:GLU:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.35	0.62
17:Q:90:ILE:HD13	17:Q:93:GLN:HB3	1.82	0.62
1:A:538:G:H5''	12:L:114:LYS:HB2	1.82	0.62
9:I:5:TYR:HD1	9:I:6:GLY:N	1.97	0.62
1:A:1139:G:O2'	1:A:1140:C:OP2	2.15	0.62
1:A:828:A:H5''	1:A:859:A:C2	2.35	0.62
1:A:992:U:H3	1:A:1044:A:N6	1.90	0.62
2:B:166:ASP:HB2	2:B:205:ASP:OD2	2.00	0.62
2:B:21:ARG:HB2	2:B:38:GLY:O	2.00	0.62
13:M:5:ALA:HB3	13:M:8:GLU:HG3	1.80	0.62
4:D:25:ARG:NH1	4:D:30:LYS:HB2	2.15	0.62
1:A:1234:C:H1'	1:A:1364:U:O2	2.00	0.61
1:A:1422:G:H2'	1:A:1423:G:C8	2.34	0.61
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	2.00	0.61
1:A:31:G:N2	1:A:48:C:OP1	2.32	0.61
4:D:150:GLU:HA	4:D:153:ARG:HB2	1.82	0.61
10:J:38:ILE:HD11	10:J:71:LEU:HB2	1.80	0.61
13:M:34:LEU:HD21	13:M:41:PRO:HA	1.81	0.61
19:S:77:THR:HG22	19:S:78:ARG:HG2	1.82	0.61
1:A:1510:U:H2'	1:A:1511:G:C8	2.34	0.61
1:A:401:C:O2'	1:A:621:A:N3	2.29	0.61
3:C:21:ARG:HH22	3:C:56:ASP:HB3	1.65	0.61
1:A:9:G:OP2	5:E:121:LYS:NZ	2.31	0.61
10:J:50:ILE:H	14:N:41:ARG:HD2	1.65	0.61
4:D:13:ARG:NH1	4:D:36:ARG:HE	1.97	0.61
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.82	0.61
1:A:143:A:O3'	1:A:144:G:H8	1.83	0.61
1:A:872:A:O2'	1:A:873:A:H5''	2.00	0.61
1:A:835:U:OP1	18:R:64:ARG:NH2	2.33	0.61
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.15	0.61
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.36	0.61
1:A:673:G:H2'	1:A:674:G:C8	2.35	0.61
12:L:25:PRO:C	12:L:27:LEU:N	2.54	0.61
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.41	0.61
17:Q:43:LEU:HG	17:Q:68:ARG:HH12	1.66	0.61
20:T:46:GLU:HG2	20:T:48:LYS:HE3	1.83	0.61
1:A:1356:G:H2'	1:A:1357:A:C8	2.36	0.61
20:T:46:GLU:HB3	20:T:48:LYS:HG3	1.83	0.61
1:A:256:U:H2'	1:A:257:G:C8	2.36	0.61
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.66	0.61
16:P:23:ASP:OD1	16:P:24:ALA:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:150:GLU:N	4:D:150:GLU:OE2	2.31	0.61
7:G:70:LYS:O	7:G:72:ARG:NH1	2.34	0.61
11:K:16:SER:HB2	11:K:106:LYS:HZ3	1.66	0.61
4:D:24:GLU:HG3	4:D:112:VAL:HG11	1.83	0.60
7:G:149:ARG:O	7:G:149:ARG:NH1	2.34	0.60
1:A:633:G:H2'	1:A:634:C:C6	2.36	0.60
2:B:127:ILE:O	2:B:135:GLN:NE2	2.33	0.60
3:C:91:LEU:HD23	3:C:92:ALA:N	2.15	0.60
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.33	0.60
18:R:53:ARG:HG2	18:R:63:GLN:OE1	2.00	0.60
20:T:89:ARG:HH21	20:T:104:LEU:HB3	1.67	0.60
1:A:1441:G:H4'	1:A:1442:G:C5	2.37	0.60
1:A:377:G:N2	1:A:386:C:O2	2.32	0.60
7:G:144:MET:O	7:G:147:ALA:HB3	2.01	0.60
10:J:89:ASP:HB3	10:J:91:PRO:HD3	1.83	0.60
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.37	0.60
2:B:91:PRO:HG3	2:B:155:LEU:HD21	1.84	0.60
13:M:16:ASP:OD1	13:M:16:ASP:N	2.33	0.60
1:A:444:C:H2'	1:A:445:G:C8	2.36	0.60
11:K:121:PRO:HG2	11:K:126:ARG:HG2	1.82	0.60
1:A:1371:G:H2'	1:A:1372:U:H6	1.66	0.60
1:A:103:C:O2'	1:A:172:A:N1	2.25	0.60
1:A:1413:A:H2'	1:A:1414:U:C6	2.31	0.60
12:L:24:VAL:HG12	12:L:26:ALA:H	1.66	0.60
16:P:17:TYR:HB2	16:P:39:TYR:HB3	1.82	0.60
1:A:1229:A:OP1	13:M:116:THR:OG1	2.14	0.60
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.17	0.60
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.37	0.60
1:A:45:U:H2'	1:A:46:G:C8	2.37	0.60
1:A:793:U:H3'	1:A:794:A:H5''	1.84	0.60
2:B:219:VAL:O	2:B:223:ILE:HG13	2.02	0.60
3:C:22:TRP:CH2	3:C:33:LEU:HD13	2.37	0.60
3:C:86:VAL:HG12	3:C:87:LEU:HG	1.82	0.60
10:J:7:LYS:HB3	10:J:97:GLU:HB2	1.82	0.60
13:M:67:GLU:O	13:M:71:ARG:HG3	2.00	0.60
1:A:1130:A:H4'	9:I:3:GLN:HE22	1.66	0.60
1:A:1211:U:H5'	1:A:1212:U:OP1	2.02	0.60
1:A:1255:G:O2'	1:A:1258:G:H1'	2.02	0.60
1:A:1366:C:H2'	1:A:1367:C:H6	1.67	0.60
10:J:55:LYS:HD2	10:J:56:HIS:H	1.67	0.60
1:A:1323:G:H2'	1:A:1324:A:C8	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:A:C6	1:A:263:A:C6	2.90	0.59
1:A:626:U:H2'	1:A:627:G:H8	1.68	0.59
1:A:665:A:N3	1:A:732:C:H2'	2.17	0.59
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.06	0.59
3:C:24:ALA:HB3	3:C:29:TYR:HD1	1.67	0.59
4:D:155:LEU:HD13	4:D:156:GLU:N	2.17	0.59
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.84	0.59
1:A:1260:C:OP1	1:A:1284:C:O2'	2.20	0.59
1:A:1425:U:H2'	1:A:1426:C:C6	2.38	0.59
1:A:202:U:H3'	1:A:203:U:C5'	2.32	0.59
1:A:56:U:H2'	1:A:57:G:C8	2.37	0.59
4:D:3:ARG:HH11	4:D:71:SER:N	1.94	0.59
1:A:1511:G:H2'	1:A:1512:U:O4'	2.03	0.59
1:A:204:U:H5'	1:A:216:G:N9	2.17	0.59
1:A:580:U:H2'	1:A:581:G:O4'	2.02	0.59
2:B:131:PRO:O	2:B:134:GLU:HB3	2.02	0.59
2:B:178:ARG:O	8:H:71:GLY:HA2	2.02	0.59
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.83	0.59
4:D:187:ARG:HH21	4:D:188:LEU:HB2	1.65	0.59
5:E:98:THR:HB	5:E:117:ASP:HB3	1.82	0.59
12:L:19:ARG:HA	12:L:20:LYS:NZ	2.17	0.59
13:M:51:ALA:HA	13:M:54:VAL:HG12	1.83	0.59
15:O:70:LEU:HD13	15:O:78:TYR:CA	2.32	0.59
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.83	0.59
1:A:1424:C:H2'	1:A:1425:U:H6	1.67	0.59
1:A:792:A:H5''	1:A:793:U:C5	2.38	0.59
4:D:187:ARG:HE	4:D:188:LEU:N	2.00	0.59
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.85	0.59
12:L:27:LEU:HD23	12:L:28:LYS:HG2	1.84	0.59
1:A:1058:G:H2'	1:A:1059:C:O4'	2.02	0.59
1:A:297:G:N2	1:A:300:A:OP2	2.34	0.59
1:A:358:U:H2'	1:A:359:U:H6	1.68	0.59
1:A:790:A:H2'	1:A:791:G:C8	2.37	0.59
1:A:1111:A:H61	3:C:177:THR:HA	1.68	0.59
4:D:107:ARG:HH21	4:D:194:LEU:HD11	1.66	0.59
1:A:1064:G:H1'	1:A:1190:G:H21	1.67	0.59
1:A:794:A:C5	1:A:795:C:C4	2.90	0.59
4:D:108:LEU:HD11	4:D:183:GLY:HA3	1.84	0.59
21:U:5:ASP:O	21:U:11:GLY:HA3	2.02	0.59
5:E:86:ALA:HB3	5:E:125:SER:HB3	1.84	0.59
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:121:ALA:O	7:G:124:LEU:HD12	2.03	0.59
1:A:1339:A:H5''	1:A:1340:A:OP2	2.03	0.59
1:A:56:U:H2'	1:A:57:G:H8	1.68	0.59
1:A:836:G:OP1	18:R:61:LYS:NZ	2.27	0.59
9:I:64:THR:HG1	9:I:66:ARG:HH12	1.51	0.59
1:A:881:G:P	12:L:12:ARG:HH22	2.26	0.59
1:A:1222:G:OP1	19:S:77:THR:HG21	2.02	0.59
1:A:953:G:H5'	1:A:965:A:H61	1.68	0.59
2:B:7:VAL:N	2:B:8:LYS:HZ3	2.01	0.59
1:A:1055:A:O2'	3:C:156:ARG:NH2	2.36	0.59
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.38	0.59
12:L:25:PRO:CA	12:L:27:LEU:H	2.15	0.59
16:P:53:VAL:O	16:P:56:ALA:N	2.35	0.59
1:A:1003:G:H2'	1:A:1003(A):G:H5''	1.84	0.58
1:A:1064:G:N2	1:A:1190:G:H2'	2.17	0.58
1:A:539:A:H2'	1:A:540:G:C8	2.38	0.58
1:A:865:A:H2'	1:A:866:C:C6	2.38	0.58
3:C:130:VAL:HG23	3:C:131:ARG:NH1	2.17	0.58
5:E:101:ILE:O	5:E:120:THR:HB	2.02	0.58
17:Q:40:LYS:HE2	17:Q:42:TYR:CZ	2.37	0.58
1:A:401:C:H2'	1:A:402:G:C8	2.38	0.58
1:A:551:U:H2'	1:A:552:U:C6	2.38	0.58
1:A:939:G:H5''	7:G:102:ARG:NH1	2.19	0.58
1:A:1440:C:H2'	1:A:1441:G:O4'	2.03	0.58
1:A:382:A:H2'	1:A:383:A:C8	2.38	0.58
1:A:411:A:N9	1:A:413:G:H1'	2.18	0.58
1:A:627:G:H2'	1:A:628:G:C8	2.37	0.58
1:A:895:G:H2'	1:A:896:C:C6	2.38	0.58
8:H:10:LEU:HD13	8:H:83:ILE:HD13	1.86	0.58
8:H:14:ARG:HE	8:H:83:ILE:HG22	1.69	0.58
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.19	0.58
8:H:82:HIS:NE2	8:H:84:ARG:HD3	2.18	0.58
11:K:117:ASN:N	11:K:117:ASN:OD1	2.36	0.58
12:L:41:ARG:HG2	12:L:42:THR:H	1.68	0.58
13:M:16:ASP:HB3	13:M:34:LEU:HD23	1.85	0.58
1:A:1287:A:H2'	1:A:1288:A:C8	2.38	0.58
1:A:1366:C:H2'	1:A:1367:C:C6	2.39	0.58
9:I:48:GLU:N	9:I:49:PRO:HD2	2.17	0.58
21:U:13:ILE:O	21:U:16:GLY:N	2.25	0.58
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.35	0.58
1:A:1475:G:H2'	1:A:1476:G:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:G:N2	1:A:382:A:H3'	2.18	0.58
1:A:403:C:OP2	4:D:74:GLN:NE2	2.37	0.58
9:I:88:TYR:HD2	9:I:89:ASN:HB2	1.69	0.58
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.85	0.58
1:A:149:A:H2'	1:A:150:C:C6	2.38	0.58
1:A:390:C:H2'	1:A:391:G:C8	2.39	0.58
1:A:973:G:H3'	1:A:974:A:H5''	1.86	0.58
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.18	0.58
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.86	0.58
1:A:359:U:H2'	1:A:360:A:C8	2.39	0.58
7:G:69:VAL:HG11	7:G:104:LEU:HD21	1.86	0.58
1:A:202:U:H3'	1:A:203:U:H5'	1.83	0.58
1:A:79:G:C2	1:A:80:G:C8	2.92	0.58
1:A:827:U:H5''	1:A:828:A:OP2	2.04	0.58
6:F:94:GLN:HB3	18:R:32:ARG:HD3	1.84	0.58
1:A:1373:G:H5''	7:G:36:LYS:HD2	1.85	0.58
8:H:116:LYS:HD2	8:H:129:VAL:HG11	1.85	0.58
17:Q:29:HIS:CE1	17:Q:32:TYR:H	2.22	0.58
21:U:10:ARG:HA	21:U:13:ILE:HG12	1.85	0.58
1:A:36:C:N4	24:A:2134:HOH:O	2.37	0.57
1:A:540:G:H2'	1:A:541:G:O4'	2.03	0.57
1:A:1131:G:H2'	1:A:1132:C:C6	2.39	0.57
3:C:150:LYS:CB	3:C:201:TYR:HB2	2.34	0.57
9:I:86:VAL:HG22	9:I:90:PRO:HA	1.86	0.57
18:R:87:ARG:HB2	18:R:87:ARG:HH11	1.68	0.57
1:A:1296:C:H4'	1:A:1302:U:C5	2.39	0.57
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.04	0.57
17:Q:97:SER:OG	17:Q:98:LEU:HD23	2.03	0.57
1:A:1243:C:OP1	21:U:10:ARG:NH1	2.37	0.57
1:A:269:C:H2'	1:A:270:A:C8	2.38	0.57
1:A:1143:G:H2'	1:A:1144:G:C8	2.39	0.57
1:A:90:U:O2'	1:A:91:C:O5'	2.19	0.57
1:A:673:G:H5''	6:F:87:ARG:NH1	2.19	0.57
7:G:17:VAL:HB	7:G:44:TYR:OH	2.04	0.57
10:J:7:LYS:HZ3	10:J:9:ARG:HH21	1.53	0.57
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.85	0.57
7:G:27:ILE:HD13	7:G:40:ALA:HA	1.86	0.57
9:I:9:ARG:HD3	9:I:14:VAL:HG22	1.87	0.57
10:J:49:VAL:HG23	10:J:62:HIS:HA	1.86	0.57
16:P:6:LEU:HD11	16:P:73:LEU:HD12	1.86	0.57
1:A:1092:A:N3	1:A:1183:A:N6	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:U:H4'	10:J:41:PRO:HG3	1.87	0.57
1:A:667:G:H4'	15:O:51:HIS:CE1	2.40	0.57
1:A:142:G:H2'	1:A:143:A:H8	1.70	0.57
1:A:895:G:H2'	1:A:896:C:H6	1.69	0.57
2:B:19:HIS:ND1	2:B:189:ASP:OD2	2.36	0.57
3:C:26:LYS:HG2	3:C:27:LYS:HG3	1.85	0.57
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.87	0.57
1:A:1181:G:C2	1:A:1182:G:N2	2.72	0.57
1:A:243:A:H4'	1:A:244:U:H5''	1.87	0.57
1:A:300:A:H8	1:A:300:A:O5'	1.87	0.57
1:A:401:C:H2'	1:A:402:G:H8	1.70	0.57
4:D:104:VAL:HG11	4:D:146:ILE:HG13	1.87	0.57
18:R:59:SER:H	18:R:62:GLU:HB2	1.69	0.57
1:A:1090:U:H2'	1:A:1091:U:H6	1.70	0.57
13:M:65:LYS:O	13:M:70:LEU:HG	2.05	0.57
1:A:141:A:H1'	1:A:182:U:O2	2.05	0.56
1:A:620:C:H2'	1:A:621:A:C8	2.39	0.56
1:A:1007:C:H42	1:A:1022:G:H1	1.53	0.56
1:A:960:U:H1'	1:A:1223:C:H5'	1.87	0.56
1:A:1474:G:H2'	1:A:1475:G:C8	2.40	0.56
1:A:298:A:N6	24:A:2052:HOH:O	2.01	0.56
2:B:15:VAL:HG13	2:B:209:ARG:HG3	1.86	0.56
4:D:11:LEU:HD13	4:D:66:ARG:HD3	1.87	0.56
11:K:121:PRO:HB2	11:K:125:PHE:HB2	1.87	0.56
18:R:50:ILE:HD11	18:R:70:ILE:CG2	2.32	0.56
1:A:551:U:H2'	1:A:552:U:H6	1.70	0.56
4:D:9:CYS:O	4:D:12:CYS:HB2	2.03	0.56
7:G:111:ARG:HD3	7:G:113:GLU:HG3	1.87	0.56
16:P:74:LEU:O	16:P:79:VAL:HG23	2.05	0.56
19:S:11:VAL:HA	19:S:38:SER:HB3	1.87	0.56
1:A:686:U:HO2'	1:A:687:A:H8	1.53	0.56
1:A:827:U:O2'	8:H:19:VAL:HG11	2.06	0.56
10:J:87:THR:HA	10:J:89:ASP:OD2	2.05	0.56
11:K:33:THR:HA	11:K:39:PRO:HA	1.88	0.56
1:A:344:A:H4'	1:A:345:C:OP2	2.05	0.56
4:D:175:SER:N	4:D:186:LEU:HD21	2.21	0.56
1:A:998:G:N2	1:A:1043:C:O2	2.24	0.56
1:A:1274:G:H2'	1:A:1275:A:H8	1.70	0.56
1:A:89:C:H2'	1:A:90:U:O4'	2.06	0.56
7:G:151:TYR:O	7:G:155:ARG:NH2	2.38	0.56
20:T:20:LEU:O	20:T:23:ARG:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:C:O2	8:H:3:THR:HG21	2.05	0.56
4:D:61:LYS:HA	4:D:203:VAL:HG13	1.87	0.56
1:A:1200:C:O2	1:A:1205:U:N3	2.25	0.56
2:B:91:PRO:HG3	2:B:155:LEU:CD2	2.35	0.56
3:C:88:ARG:HA	3:C:91:LEU:HB3	1.88	0.56
1:A:407:G:OP1	4:D:115:ARG:NH2	2.39	0.56
13:M:52:GLU:HG2	13:M:55:ARG:NH2	2.21	0.56
19:S:55:LYS:NZ	19:S:56:GLN:HB2	2.21	0.56
1:A:795:C:H5''	1:A:796:C:OP2	2.06	0.56
1:A:981:U:H2'	1:A:982:U:H5	1.71	0.56
4:D:206:PHE:HD2	4:D:207:TYR:CE2	2.24	0.56
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.41	0.56
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.88	0.56
18:R:34:TYR:CE1	18:R:35:ARG:HG3	2.40	0.56
18:R:22:VAL:HG23	18:R:56:THR:HA	1.87	0.56
1:A:103:C:P	20:T:17:ARG:HH12	2.28	0.56
1:A:1329:A:P	13:M:28:ALA:HB3	2.46	0.56
1:A:908:A:C2	1:A:909:A:C4	2.94	0.56
2:B:118:LEU:HD11	2:B:141:GLU:OE1	2.05	0.56
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.71	0.56
13:M:56:LEU:O	13:M:60:VAL:HG23	2.05	0.56
1:A:902:G:H2'	1:A:903:G:H8	1.71	0.55
1:A:528:C:H41	12:L:49:ASN:ND2	2.04	0.55
1:A:659:U:OP2	15:O:8:LYS:HE2	2.06	0.55
16:P:68:ASP:OD1	16:P:68:ASP:N	2.39	0.55
20:T:54:LYS:HA	20:T:57:ARG:HD3	1.88	0.55
1:A:1199:U:H5''	1:A:1200:C:OP2	2.06	0.55
1:A:179:A:H2'	1:A:180:U:C6	2.41	0.55
1:A:390:C:H2'	1:A:391:G:H8	1.71	0.55
1:A:419:C:N4	1:A:424:G:H1	2.04	0.55
6:F:27:GLN:O	6:F:31:GLU:HG3	2.06	0.55
7:G:92:SER:HB3	7:G:95:ARG:H	1.70	0.55
8:H:86:ILE:HG22	8:H:87:SER:N	2.21	0.55
12:L:83:VAL:HG21	12:L:100:ILE:HG13	1.87	0.55
16:P:71:ARG:HG3	16:P:80:PHE:HE1	1.71	0.55
21:U:9:ARG:HG3	21:U:22:ARG:HG2	1.88	0.55
1:A:1497:G:O2'	1:A:1518[A]:MA6:H92	2.06	0.55
1:A:626:U:H2'	1:A:627:G:C8	2.42	0.55
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.42	0.55
7:G:80:VAL:HG11	7:G:154:TYR:HE1	1.71	0.55
13:M:91:ARG:HB3	13:M:98:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:8:GLU:HA	14:N:11:LYS:HB2	1.89	0.55
1:A:939:G:H1	1:A:1344:C:H42	1.55	0.55
1:A:978:A:OP1	1:A:978:A:H8	1.89	0.55
3:C:41:GLY:O	3:C:45:LYS:HB2	2.06	0.55
11:K:98:LEU:HA	11:K:101:SER:HB3	1.87	0.55
12:L:47:LYS:H	12:L:47:LYS:HD2	1.71	0.55
21:U:14:TRP:CZ3	21:U:15:ARG:HG3	2.42	0.55
4:D:31:CYS:C	4:D:33:MET:H	2.10	0.55
12:L:41:ARG:HH21	12:L:43:VAL:HG13	1.71	0.55
13:M:25:ILE:HG12	13:M:66:LEU:HD13	1.88	0.55
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.88	0.55
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.88	0.55
20:T:89:ARG:HE	20:T:104:LEU:HD13	1.71	0.55
1:A:21:G:H2'	1:A:22:G:C8	2.41	0.55
1:A:445:G:H1	1:A:489:C:H42	1.54	0.55
1:A:647:C:H2'	1:A:648:A:H8	1.71	0.55
1:A:666:G:H5'	1:A:726:C:H1'	1.89	0.55
3:C:179:ARG:HD2	3:C:206:GLU:HG2	1.89	0.55
3:C:58:GLU:H	3:C:65:ALA:HB3	1.72	0.55
8:H:87:SER:CA	8:H:93:VAL:HG13	2.36	0.55
10:J:10:GLY:HA3	10:J:16:LEU:HD21	1.89	0.55
11:K:32:ILE:O	11:K:40:ILE:N	2.36	0.55
1:A:1228:C:H4'	13:M:116:THR:HA	1.88	0.55
1:A:1415:G:H3'	1:A:1416:G:H8	1.71	0.55
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.89	0.55
4:D:57:ARG:HG3	4:D:202:LEU:HD12	1.89	0.55
1:A:337:C:H2'	1:A:338:A:H8	1.71	0.55
1:A:481:G:O2'	1:A:482:A:H8	1.90	0.55
1:A:77:G:C6	1:A:93:G:N1	2.75	0.55
4:D:107:ARG:HH21	4:D:194:LEU:CD1	2.20	0.55
16:P:6:LEU:HD23	16:P:17:TYR:CD1	2.42	0.55
1:A:765:G:C6	1:A:812:C:C2	2.95	0.55
12:L:27:LEU:HG	12:L:28:LYS:H	1.72	0.55
20:T:50:GLU:HB3	20:T:99:LEU:HB2	1.89	0.55
1:A:106:C:O2	1:A:379:C:H4'	2.07	0.55
1:A:1241:G:H2'	1:A:1242:C:H6	1.72	0.55
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.07	0.55
1:A:1487:G:H2'	1:A:1488:G:O4'	2.07	0.55
1:A:40:C:H2'	1:A:41:G:C8	2.42	0.55
1:A:792:A:H1'	1:A:793:U:OP2	2.07	0.55
10:J:51:ARG:HG3	10:J:59:SER:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:G:N7	1:A:1446:A:N6	2.55	0.54
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.89	0.54
7:G:61:VAL:HG22	7:G:128:ALA:HB1	1.90	0.54
1:A:1259:C:H42	1:A:1276:G:H1	1.53	0.54
1:A:1484:C:H2'	1:A:1485:U:O4'	2.06	0.54
2:B:21:ARG:NH1	2:B:22:LYS:O	2.40	0.54
3:C:130:VAL:HG11	3:C:153:VAL:HG21	1.88	0.54
4:D:101:LEU:O	4:D:105:VAL:HG23	2.07	0.54
1:A:1006:C:H2'	1:A:1007:C:C6	2.43	0.54
1:A:1539:C:H2'	1:A:1540:PSU:O4'	2.07	0.54
1:A:17:U:H2'	1:A:18:C:C6	2.42	0.54
1:A:7:G:H5'	1:A:298:A:H5'	1.89	0.54
1:A:373:A:H2'	1:A:374:A:H8	1.73	0.54
14:N:23:ARG:HD3	14:N:29:ARG:O	2.07	0.54
16:P:20:VAL:HG12	16:P:35:LYS:HA	1.88	0.54
1:A:1238:A:OP1	1:A:1336:C:N4	2.39	0.54
1:A:129(A):G:H1'	1:A:190(E):U:H2'	1.90	0.54
3:C:149:ALA:O	3:C:169:ALA:HB1	2.07	0.54
1:A:1191:A:OP1	3:C:4:LYS:NZ	2.29	0.54
1:A:1414:U:H2'	1:A:1415:G:C8	2.42	0.54
1:A:509:A:H3'	1:A:509:A:C8	2.42	0.54
1:A:859:A:H2'	1:A:860:A:O4'	2.08	0.54
7:G:26:PHE:HA	7:G:101:LEU:HD13	1.88	0.54
12:L:59:ARG:CZ	12:L:65:GLU:HG2	2.38	0.54
1:A:1147:C:H2'	1:A:1148:U:C6	2.43	0.54
1:A:579:G:O3'	15:O:54:ARG:NH2	2.41	0.54
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.71	0.54
12:L:34:ARG:HB2	12:L:105:TYR:HE1	1.73	0.54
16:P:67:THR:HB	16:P:70:ALA:H	1.72	0.54
1:A:345:C:OP2	1:A:345:C:H6	1.91	0.54
5:E:118:ILE:HG12	5:E:119:LEU:N	2.22	0.54
8:H:86:ILE:HG21	8:H:133:LEU:HD22	1.89	0.54
14:N:37:PHE:C	14:N:39:LEU:H	2.09	0.54
18:R:53:ARG:NH1	18:R:59:SER:HA	2.22	0.54
1:A:949:A:C2	1:A:1233:G:N3	2.76	0.54
1:A:1329:A:O2'	1:A:1330:U:H5'	2.08	0.54
1:A:731:G:OP1	1:A:766:A:H1'	2.08	0.54
1:A:831:U:H2'	1:A:832:C:C6	2.42	0.54
2:B:16:HIS:HB2	2:B:204:ASN:HB2	1.90	0.54
12:L:86:ARG:HH11	12:L:86:ARG:HG2	1.73	0.54
20:T:44:ALA:HB1	20:T:91:LEU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:C:OP2	20:T:14:LYS:HD2	2.08	0.54
1:A:1391:U:H2'	1:A:1392:G:H8	1.73	0.54
1:A:1414:U:H5''	1:A:1415:G:OP2	2.08	0.54
1:A:270:A:H2'	1:A:271:C:C6	2.43	0.54
1:A:376:G:C4	1:A:389:A:C2	2.96	0.54
15:O:26:GLU:OE2	15:O:77:ARG:NH1	2.41	0.54
16:P:67:THR:HG22	16:P:68:ASP:N	2.23	0.54
1:A:1051:C:H3'	1:A:1052:U:C6	2.43	0.54
1:A:1058:G:C2	1:A:1059:C:H1'	2.43	0.54
1:A:1059:C:H2'	1:A:1060:C:C6	2.43	0.54
1:A:1113:C:H42	1:A:1187:G:H1	1.54	0.54
1:A:946:A:H2'	1:A:947:G:C8	2.43	0.54
3:C:136:GLN:O	3:C:140:ARG:HG3	2.08	0.54
1:A:1147:C:O2	9:I:16:ARG:NH2	2.40	0.54
1:A:1354:C:H2'	1:A:1355:G:H8	1.72	0.53
1:A:1426:C:H2'	1:A:1427:U:H6	1.72	0.53
1:A:1502:A:H2	1:A:1505:G:H1	1.56	0.53
2:B:21:ARG:HD2	2:B:22:LYS:H	1.72	0.53
4:D:57:ARG:CG	4:D:202:LEU:HD12	2.38	0.53
16:P:57:ARG:HG3	16:P:79:VAL:HG12	1.88	0.53
1:A:204:U:H5'	1:A:216:G:C8	2.43	0.53
1:A:587:G:H3'	24:A:1962:HOH:O	2.09	0.53
2:B:87:ARG:HH21	2:B:233:SER:HA	1.73	0.53
12:L:67:THR:HB	12:L:96:VAL:HG13	1.90	0.53
16:P:53:VAL:O	16:P:55:ARG:N	2.42	0.53
1:A:1222:G:N2	1:A:1223:C:O2	2.41	0.53
1:A:1493:A:H2'	1:A:1494:G:H8	1.73	0.53
1:A:373:A:H1'	1:A:481:G:N3	2.23	0.53
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.91	0.53
21:U:13:ILE:HG22	21:U:22:ARG:CZ	2.39	0.53
21:U:13:ILE:HG22	21:U:22:ARG:NH2	2.23	0.53
1:A:1392:G:H21	1:A:1502:A:H8	1.56	0.53
1:A:858:G:C6	1:A:869:G:C8	2.97	0.53
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.72	0.53
10:J:54:PHE:O	10:J:55:LYS:HG3	2.08	0.53
17:Q:60:ILE:O	17:Q:62:SER:OG	2.24	0.53
1:A:1328:C:OP1	21:U:20:LYS:NZ	2.36	0.53
1:A:1346:A:OP1	9:I:120:ARG:NH1	2.41	0.53
1:A:383:A:C6	1:A:384:G:H1'	2.44	0.53
9:I:118:LYS:O	9:I:120:ARG:N	2.34	0.53
1:A:1009:G:H21	1:A:1010:G:H1'	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:G:O2'	1:A:1199:U:H5	1.91	0.53
1:A:174:C:H2'	1:A:175:C:H6	1.74	0.53
1:A:204:U:H4'	1:A:216:G:O5'	2.07	0.53
1:A:679:C:H2'	1:A:680:C:H6	1.74	0.53
1:A:828:A:H2'	1:A:829:G:O4'	2.09	0.53
1:A:853:G:C2	1:A:854:G:C8	2.97	0.53
2:B:172:ILE:H	2:B:172:ILE:HD12	1.74	0.53
1:A:1225:A:H3'	13:M:103:THR:OG1	2.09	0.53
1:A:236:G:H2'	1:A:237:C:O4'	2.08	0.53
2:B:23:ARG:HA	2:B:23:ARG:CZ	2.38	0.53
5:E:5:ASP:OD2	5:E:6:PHE:HB2	2.08	0.53
1:A:1474:G:H2'	1:A:1475:G:H8	1.71	0.53
1:A:426:G:OP1	4:D:38:TYR:OH	2.20	0.53
4:D:78:LEU:O	4:D:81:GLU:HB3	2.08	0.53
7:G:113:GLU:O	7:G:119:ARG:HD3	2.08	0.53
7:G:146:GLU:OE2	7:G:149:ARG:HG3	2.09	0.53
8:H:112:LEU:HD23	8:H:112:LEU:N	2.23	0.53
9:I:78:LYS:HD2	9:I:101:PHE:CE2	2.44	0.53
1:A:1318:A:H4'	19:S:10:PHE:CE2	2.44	0.53
1:A:115:G:H1'	1:A:116:A:N7	2.23	0.53
1:A:1053:G:HO2'	1:A:1199:U:H5	1.57	0.53
1:A:152:A:N6	1:A:170:U:C2	2.77	0.53
1:A:184:G:H2'	1:A:185:A:H8	1.74	0.53
1:A:190(C):C:H2'	1:A:190(D):U:O4'	2.09	0.53
1:A:517:G:H5'	1:A:519:C:C2	2.43	0.53
1:A:88:A:H2'	1:A:89:C:O4'	2.08	0.53
16:P:34:GLU:OE2	16:P:55:ARG:HD2	2.08	0.53
17:Q:62:SER:CB	17:Q:72:ARG:HD3	2.38	0.53
1:A:1118:C:H1'	1:A:1179:A:C4	2.43	0.53
1:A:679:C:H2'	1:A:680:C:C6	2.43	0.53
13:M:40:ASN:HD22	13:M:43:THR:HG23	1.73	0.53
1:A:1006:C:OP1	1:A:1037:C:O2'	2.26	0.52
1:A:1070:U:H2'	1:A:1071:C:C6	2.43	0.52
1:A:1389:C:H2'	1:A:1390:U:O4'	2.09	0.52
1:A:1465:C:H2'	1:A:1466:C:O4'	2.09	0.52
1:A:342:C:H2'	1:A:343:U:O4'	2.09	0.52
1:A:802:A:H8	1:A:802:A:O5'	1.93	0.52
6:F:11:ASN:ND2	6:F:13:ASN:OD1	2.41	0.52
7:G:73:MET:HB2	7:G:89:MET:O	2.09	0.52
9:I:90:PRO:O	9:I:93:ARG:HB2	2.07	0.52
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:86:ARG:N	12:L:99:HIS:O	2.41	0.52
1:A:192:U:H2'	1:A:193:C:C6	2.44	0.52
1:A:399:G:H2'	1:A:400:C:H6	1.74	0.52
4:D:20:TYR:HA	4:D:26:CYS:SG	2.49	0.52
11:K:12:ARG:HB3	11:K:14:VAL:HG13	1.91	0.52
11:K:50:TYR:CD2	11:K:54:ARG:HB3	2.45	0.52
16:P:13:HIS:O	16:P:42:ARG:NH1	2.43	0.52
20:T:64:ASP:O	20:T:67:ALA:HB3	2.09	0.52
1:A:1049:U:H4'	1:A:1050:G:O5'	2.09	0.52
1:A:1226:C:OP2	13:M:103:THR:HG21	2.08	0.52
1:A:1417:G:O2'	1:A:1483:A:N6	2.38	0.52
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.91	0.52
1:A:77:G:N2	1:A:78:G:N3	2.57	0.52
1:A:241:C:H4'	12:L:19:ARG:NH2	2.24	0.52
1:A:1216:G:H2'	1:A:1217:C:C6	2.44	0.52
4:D:180:GLY:C	4:D:182:LYS:H	2.12	0.52
10:J:26:ALA:HB3	10:J:85:LEU:HD11	1.92	0.52
17:Q:3:LYS:HB3	17:Q:60:ILE:HD11	1.90	0.52
1:A:1026:G:O6	1:A:1036:G:N1	2.38	0.52
1:A:643:C:C2'	1:A:644:G:H5'	2.38	0.52
1:A:851:G:H5''	1:A:851:G:H8	1.74	0.52
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.92	0.52
13:M:101:GLN:OE1	13:M:101:GLN:N	2.43	0.52
16:P:22:THR:HA	16:P:33:ILE:CG1	2.40	0.52
19:S:5:LEU:HD22	19:S:70:LYS:NZ	2.24	0.52
1:A:1437:C:H2'	1:A:1438:G:H8	1.75	0.52
1:A:80:G:H2'	1:A:81:U:H5'	1.91	0.52
1:A:922:G:C2	1:A:1396:A:C6	2.98	0.52
2:B:104:ASN:OD1	2:B:107:THR:OG1	2.27	0.52
2:B:187:LEU:HD12	2:B:205:ASP:HA	1.92	0.52
2:B:19:HIS:CE1	2:B:206:ASP:H	2.27	0.52
7:G:18:TYR:CD2	7:G:59:LEU:HD13	2.44	0.52
1:A:474:G:H5''	16:P:81:ARG:HG2	1.92	0.52
1:A:268:C:H2'	1:A:269:C:H6	1.74	0.52
1:A:299:G:C6	1:A:300:A:C6	2.98	0.52
1:A:448:A:P	1:A:485:G:H22	2.32	0.52
1:A:836:G:H8	1:A:836:G:H5''	1.74	0.52
6:F:36:ARG:NH1	6:F:38:GLU:OE1	2.43	0.52
12:L:7:ILE:O	12:L:10:LEU:N	2.42	0.52
17:Q:89:LEU:O	17:Q:93:GLN:HB2	2.09	0.52
1:A:1150:U:O4	1:A:1151:A:N6	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1514:C:H2'	1:A:1515[A]:C:O4'	2.09	0.52
3:C:18:TRP:HZ2	14:N:56:VAL:O	1.93	0.52
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.92	0.52
6:F:2:ARG:O	6:F:66:GLU:HA	2.09	0.52
14:N:53:LEU:HD23	14:N:53:LEU:H	1.75	0.52
1:A:191:G:O2'	20:T:102:GLY:O	2.13	0.52
1:A:1006:C:H42	1:A:1024:G:N2	2.07	0.52
1:A:115:G:O2'	1:A:116:A:OP2	2.26	0.52
1:A:217:C:H2'	1:A:218:C:H6	1.75	0.52
1:A:707:C:H2'	1:A:708:C:C6	2.45	0.52
3:C:36:ASP:O	3:C:40:ARG:HG2	2.09	0.52
5:E:82:VAL:HB	5:E:89:ILE:HG22	1.91	0.52
10:J:48:THR:OG1	10:J:62:HIS:ND1	2.42	0.52
1:A:1417:G:C2'	1:A:1483:A:H61	2.23	0.52
1:A:349:A:H2'	1:A:350:G:H5''	1.92	0.52
3:C:108:ASN:HB3	3:C:111:LEU:HB2	1.92	0.52
1:A:692:U:OP2	11:K:26:ASN:ND2	2.42	0.52
13:M:4:ILE:HD12	13:M:57:ARG:HB2	1.91	0.52
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:H2	2.39	0.51
1:A:1509:C:H42	1:A:1526:G:H1	1.57	0.51
1:A:383:A:C5	1:A:384:G:H1'	2.44	0.51
1:A:77:G:C2	1:A:78:G:C4	2.98	0.51
5:E:80:ILE:HD11	5:E:138:ALA:HB1	1.92	0.51
11:K:29:ILE:HG12	11:K:30:VAL:N	2.24	0.51
13:M:39:ILE:HG13	13:M:55:ARG:HH21	1.75	0.51
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.44	0.51
1:A:131:C:H2'	1:A:132:C:C6	2.45	0.51
1:A:229:U:O2'	1:A:230:G:H5'	2.10	0.51
1:A:869:G:N7	24:A:2102:HOH:O	2.34	0.51
3:C:129:ALA:HB1	3:C:131:ARG:HH11	1.75	0.51
17:Q:66:SER:H	17:Q:69:LYS:HB2	1.76	0.51
1:A:1382:C:H2'	1:A:1383:C:H6	1.76	0.51
1:A:16:A:O2'	1:A:17:U:H5'	2.10	0.51
1:A:981:U:H2'	1:A:982:U:C5	2.45	0.51
3:C:40:ARG:HB3	3:C:44:GLU:OE2	2.11	0.51
4:D:93:PHE:CE1	4:D:97:LEU:HD11	2.46	0.51
1:A:932:C:H4'	7:G:4:ARG:HH21	1.74	0.51
1:A:1030(D):A:C8	1:A:1031:G:H1'	2.45	0.51
1:A:112:G:O2'	1:A:113:G:H5'	2.10	0.51
1:A:933:G:N2	1:A:1384:C:O2	2.38	0.51
1:A:1415:G:H3'	1:A:1416:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:G:H1'	1:A:262:A:N1	2.26	0.51
1:A:358:U:H2'	1:A:359:U:C6	2.45	0.51
1:A:579:G:H2'	1:A:580:U:C6	2.46	0.51
4:D:201:GLN:O	4:D:205:GLU:HB2	2.11	0.51
8:H:27:PRO:HB3	8:H:58:TYR:CE2	2.45	0.51
9:I:105:ASP:OD1	9:I:107:ARG:HG3	2.10	0.51
17:Q:93:GLN:NE2	17:Q:96:GLU:OE2	2.41	0.51
19:S:11:VAL:HG21	19:S:16:LEU:HD13	1.93	0.51
1:A:1190:G:OP1	3:C:4:LYS:HA	2.10	0.51
1:A:1228:C:H2'	1:A:1229:A:H8	1.76	0.51
1:A:1504:G:H4'	1:A:1505:G:H5'	1.91	0.51
1:A:512:U:H2'	1:A:513:C:C6	2.46	0.51
1:A:97:G:H2'	1:A:98:U:O4'	2.11	0.51
3:C:38:ARG:CZ	3:C:38:ARG:HB2	2.40	0.51
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.93	0.51
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.92	0.51
11:K:92:GLU:HB3	11:K:96:ARG:HH22	1.73	0.51
12:L:36:VAL:HG12	12:L:82:VAL:HB	1.92	0.51
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.45	0.51
2:B:127:ILE:HG22	2:B:135:GLN:HG2	1.92	0.51
5:E:86:ALA:CB	5:E:125:SER:HB3	2.41	0.51
11:K:33:THR:HG22	11:K:39:PRO:HA	1.92	0.51
11:K:60:ALA:HA	11:K:63:LEU:HD12	1.92	0.51
1:A:853:G:C2'	1:A:854:G:H5'	2.41	0.51
9:I:27:THR:HG22	9:I:62:TYR:HA	1.93	0.51
3:C:58:GLU:HB3	10:J:92:THR:HG23	1.92	0.51
18:R:46:GLU:CD	18:R:46:GLU:H	2.14	0.51
18:R:87:ARG:O	18:R:88:LYS:HB2	2.11	0.51
1:A:99:C:H2'	1:A:101:A:C8	2.45	0.51
1:A:1355:G:H1	1:A:1367:C:H42	1.58	0.51
1:A:21:G:C2	1:A:22:G:C6	2.99	0.51
1:A:603:U:H3	1:A:635:G:H1	1.59	0.51
9:I:69:GLY:O	9:I:73:GLN:HG3	2.10	0.51
12:L:66:VAL:HG11	12:L:98:TYR:HE1	1.76	0.51
1:A:1505:G:H3'	1:A:1505:G:C8	2.46	0.51
1:A:463:A:H2'	1:A:474:G:O4'	2.11	0.51
1:A:496:A:C2	1:A:497:A:C5	2.99	0.51
15:O:3:ILE:HA	15:O:7:GLU:OE1	2.11	0.51
1:A:184:G:H2'	1:A:185:A:C8	2.46	0.51
1:A:757:U:H2'	1:A:758:G:O4'	2.11	0.51
1:A:909:A:H2'	1:A:910:C:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:M2G:H2'	1:A:967:5MC:C6	2.44	0.51
5:E:90:VAL:C	5:E:91:LEU:HD23	2.31	0.51
8:H:11:THR:O	8:H:14:ARG:N	2.43	0.51
1:A:1347:G:H21	1:A:1373:G:H2'	1.71	0.50
1:A:1346:A:O2'	1:A:1347:G:OP2	2.28	0.50
1:A:135:C:O2	16:P:1:MET:HB2	2.12	0.50
1:A:144:G:H1	1:A:178:C:N4	2.07	0.50
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.11	0.50
1:A:372:C:H4'	1:A:373:A:O5'	2.11	0.50
1:A:502:G:P	12:L:118:SER:HG	2.34	0.50
1:A:782:A:OP1	1:A:1521:G:N2	2.41	0.50
1:A:1057:G:N2	1:A:1203:C:O2	2.43	0.50
1:A:1112:C:H1'	3:C:179:ARG:NH1	2.26	0.50
1:A:1328:C:H2'	1:A:1329:A:C8	2.47	0.50
1:A:283:C:C2	1:A:284:G:C8	2.99	0.50
1:A:976:G:OP2	1:A:1358:U:O2'	2.18	0.50
13:M:86:CYS:SG	13:M:87:TYR:N	2.85	0.50
1:A:1338:G:H2'	1:A:1339:A:C8	2.46	0.50
1:A:1489:G:H2'	1:A:1490:C:C6	2.46	0.50
1:A:164:U:H2'	1:A:165:C:C6	2.46	0.50
1:A:521:G:OP1	12:L:54:LYS:HE2	2.11	0.50
1:A:647:C:H2'	1:A:648:A:C8	2.46	0.50
1:A:79:G:C4	1:A:91:C:O2	2.64	0.50
2:B:181:PHE:CE2	8:H:70:GLN:HB3	2.47	0.50
20:T:45:GLN:HA	20:T:91:LEU:CD1	2.40	0.50
1:A:1074:G:C6	1:A:1075:C:C4	3.00	0.50
1:A:1172:C:H2'	1:A:1173:G:H8	1.76	0.50
1:A:1221:G:H4'	19:S:53:ASN:O	2.10	0.50
1:A:256:U:H2'	1:A:257:G:H8	1.77	0.50
1:A:385:C:H2'	1:A:386:C:H6	1.77	0.50
3:C:139:GLN:O	3:C:142:MET:N	2.45	0.50
8:H:46:LYS:HD3	8:H:64:LYS:HG3	1.93	0.50
12:L:76:ASN:OD1	12:L:77:LEU:HD23	2.12	0.50
19:S:40:ILE:HB	19:S:67:VAL:O	2.12	0.50
1:A:1007:C:N3	1:A:1022:G:N2	2.59	0.50
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.94	0.50
2:B:40:HIS:HB2	2:B:190:THR:HG21	1.92	0.50
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.26	0.50
5:E:75:THR:HB	5:E:117:ASP:O	2.11	0.50
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.46	0.50
7:G:111:ARG:HD3	7:G:113:GLU:CG	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:G:O2'	1:A:1191:A:O5'	2.29	0.50
3:C:106:VAL:HG11	3:C:115:LEU:HD11	1.94	0.50
3:C:121:ALA:O	3:C:125:GLU:HG3	2.12	0.50
1:A:933:G:OP2	7:G:3:ARG:HB3	2.12	0.50
12:L:39:VAL:HG12	12:L:41:ARG:HB2	1.93	0.50
12:L:33:ARG:O	12:L:84:LEU:HD12	2.12	0.50
16:P:10:GLY:HA3	16:P:14:ASN:O	2.11	0.50
17:Q:5:VAL:O	17:Q:6:LEU:HD23	2.11	0.50
1:A:644:G:C5	1:A:645:C:C5	3.00	0.50
2:B:114:ARG:HD2	2:B:118:LEU:HG	1.93	0.50
6:F:14:LEU:HD22	6:F:18:GLN:OE1	2.12	0.50
1:A:1057:G:H2'	1:A:1058:G:O4'	2.11	0.50
1:A:1442:G:C5	1:A:1446:A:C6	3.00	0.50
1:A:285:G:C2	1:A:286:G:C8	3.00	0.50
1:A:994:A:O2'	14:N:11:LYS:HG2	2.12	0.50
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.25	0.50
3:C:19:GLU:HB2	14:N:52:GLN:HA	1.94	0.50
5:E:79:GLU:HB3	5:E:92:LYS:HA	1.92	0.50
10:J:21:GLN:HA	10:J:24:VAL:HG12	1.93	0.50
12:L:8:ASN:HB2	17:Q:34:LYS:HZ3	1.76	0.50
1:A:397:A:H5'	1:A:398:C:OP1	2.12	0.50
1:A:92:C:H2'	1:A:92:C:O2	2.11	0.50
5:E:76:ILE:HD11	5:E:118:ILE:HD12	1.94	0.50
6:F:91:VAL:HG11	18:R:72:ARG:HH12	1.77	0.50
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.45	0.50
14:N:22:THR:HB	14:N:33:VAL:HB	1.93	0.50
1:A:1441:G:H21	1:A:1460:A:H62	1.59	0.49
1:A:1516[A]:G:N1	1:A:1519[A]:MA6:OP2	2.39	0.49
1:A:250:A:H4'	1:A:251:G:O5'	2.11	0.49
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.94	0.49
1:A:645:C:H2'	1:A:645:C:O2	2.12	0.49
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.94	0.49
10:J:66:ARG:HB3	10:J:66:ARG:NH1	2.27	0.49
14:N:48:ALA:HB2	14:N:53:LEU:HD11	1.94	0.49
1:A:1402:4OC:HM42	1:A:1500:A:N6	2.26	0.49
1:A:266:G:H5''	1:A:266:G:H8	1.76	0.49
1:A:299:G:H2'	1:A:300:A:C8	2.47	0.49
1:A:474:G:H2'	1:A:475:G:O4'	2.12	0.49
1:A:665:A:C2	1:A:732:C:C2	3.00	0.49
1:A:76:C:N4	1:A:93:G:H1	2.09	0.49
1:A:779:C:H2'	1:A:780:A:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:G:C3'	1:A:839:U:H5''	2.42	0.49
4:D:3:ARG:NH1	4:D:71:SER:H	1.95	0.49
7:G:18:TYR:CD2	7:G:59:LEU:HD22	2.47	0.49
1:A:112:G:C2'	1:A:113:G:H5'	2.43	0.49
1:A:391:G:C6	1:A:392:G:C5	2.99	0.49
1:A:788:U:H2'	1:A:789:U:C6	2.47	0.49
1:A:78:G:N1	1:A:92:C:N4	2.60	0.49
3:C:127:ARG:HG2	3:C:193:TYR:OH	2.13	0.49
3:C:7:PRO:HG2	3:C:184:TYR:CD1	2.47	0.49
4:D:206:PHE:CD2	4:D:207:TYR:CE2	3.00	0.49
4:D:15:GLU:HB3	4:D:63:LYS:HG3	1.95	0.49
5:E:71:LEU:HD21	5:E:113:ALA:O	2.13	0.49
12:L:46:LYS:N	12:L:92:ASP:O	2.43	0.49
13:M:52:GLU:HG2	13:M:55:ARG:HH22	1.76	0.49
1:A:1032:G:H2'	1:A:1033:G:C8	2.47	0.49
1:A:1228:C:H2'	1:A:1229:A:C8	2.48	0.49
3:C:42:LEU:HD23	3:C:43:LEU:HD22	1.94	0.49
11:K:58:PRO:O	11:K:61:ALA:HB3	2.12	0.49
13:M:34:LEU:CD2	13:M:41:PRO:HA	2.42	0.49
1:A:1142:G:H2'	1:A:1143:G:O4'	2.11	0.49
1:A:142:G:H2'	1:A:143:A:C8	2.48	0.49
1:A:1520[B]:G:H2'	1:A:1521:G:H8	1.76	0.49
1:A:330:C:H2'	1:A:331:G:H5'	1.93	0.49
1:A:459:G:H1'	1:A:463:A:H61	1.78	0.49
1:A:475:G:H2'	1:A:476:G:O4'	2.13	0.49
1:A:836:G:C6	1:A:851:G:C6	3.00	0.49
7:G:122:HIS:O	7:G:126:ASP:HB2	2.12	0.49
12:L:55:VAL:CG2	12:L:67:THR:HG22	2.42	0.49
17:Q:68:ARG:HB3	17:Q:68:ARG:HH11	1.76	0.49
21:U:14:TRP:HZ3	21:U:15:ARG:HG3	1.78	0.49
1:A:1382:C:H2'	1:A:1383:C:C6	2.48	0.49
1:A:1407:5MC:O2'	1:A:1408:A:H5'	2.13	0.49
1:A:279:A:H8	1:A:279:A:H5'	1.78	0.49
1:A:316:G:H2'	1:A:317:G:H8	1.76	0.49
4:D:111:ALA:HA	4:D:161:ASN:HD22	1.78	0.49
5:E:105:VAL:HG23	5:E:106:PRO:HD3	1.94	0.49
1:A:825:G:H21	8:H:11:THR:HG21	1.77	0.49
8:H:85:ARG:NE	8:H:87:SER:O	2.46	0.49
15:O:36:ILE:CD1	15:O:60:VAL:HG23	2.43	0.49
18:R:59:SER:N	18:R:62:GLU:OE1	2.45	0.49
1:A:714:G:H2'	1:A:715:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:C:O2'	1:A:901:A:N1	2.40	0.49
2:B:189:ASP:HB3	2:B:203:GLY:O	2.13	0.49
12:L:58:VAL:O	12:L:65:GLU:HA	2.11	0.49
13:M:17:VAL:O	13:M:20:THR:HG22	2.13	0.49
13:M:91:ARG:HH22	13:M:103:THR:HG21	1.77	0.49
16:P:52:ASP:O	16:P:55:ARG:HB2	2.13	0.49
1:A:966:M2G:CM1	1:A:967:5MC:H1'	2.43	0.49
2:B:17:PHE:CD1	2:B:18:GLY:N	2.74	0.49
3:C:123:GLN:O	3:C:128:PHE:HD1	1.96	0.49
1:A:1501:C:N4	1:A:1504:G:C2	2.81	0.49
1:A:253:U:H2'	1:A:254:G:C8	2.48	0.49
1:A:381:C:H2'	1:A:382:A:O4'	2.12	0.49
1:A:866:C:C2	1:A:867:G:H1'	2.48	0.49
4:D:21:LEU:HD23	4:D:115:ARG:HD2	1.94	0.49
7:G:62:PHE:CD2	7:G:62:PHE:C	2.86	0.49
18:R:25:THR:OG1	18:R:42:ARG:NH2	2.46	0.49
1:A:1063:C:H2'	1:A:1064:G:H8	1.75	0.48
1:A:1223:C:OP1	19:S:78:ARG:NH2	2.45	0.48
1:A:129:U:O3'	1:A:129(A):G:H3'	2.12	0.48
1:A:1306:A:H2'	1:A:1307:U:O4'	2.12	0.48
1:A:1348:U:OP2	1:A:1373:G:N2	2.43	0.48
6:F:14:LEU:CD1	6:F:18:GLN:HB3	2.27	0.48
12:L:22:SER:C	12:L:24:VAL:H	2.16	0.48
12:L:30:ALA:HB1	12:L:31:PRO:HD2	1.94	0.48
20:T:29:LYS:O	20:T:32:ALA:HB3	2.13	0.48
20:T:71:THR:O	20:T:72:LEU:HD23	2.12	0.48
1:A:109:A:C6	1:A:326:G:C6	3.01	0.48
1:A:451:A:N6	1:A:481:G:C4	2.81	0.48
1:A:737:A:H2'	1:A:738:C:C6	2.47	0.48
1:A:750:G:H1'	15:O:23:GLY:H	1.77	0.48
1:A:854:G:N2	1:A:855:G:C4	2.81	0.48
2:B:185:ILE:HA	2:B:199:TYR:O	2.13	0.48
2:B:68:ILE:HD12	2:B:222:ILE:HD11	1.95	0.48
5:E:99:GLY:H	5:E:117:ASP:CG	2.17	0.48
6:F:1:MET:HB3	6:F:66:GLU:HG2	1.95	0.48
1:A:737:A:H1'	6:F:73:ASN:OD1	2.14	0.48
11:K:59:TYR:CE2	11:K:63:LEU:HD11	2.48	0.48
1:A:1188:A:O2'	14:N:58:LYS:HE2	2.14	0.48
19:S:32:LYS:HB3	19:S:34:TRP:CZ3	2.47	0.48
20:T:92:LEU:O	20:T:96:GLY:HA3	2.13	0.48
1:A:1336:C:H5"	1:A:1336:C:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:C:H2'	1:A:1421:G:H8	1.79	0.48
1:A:1484:C:H2'	1:A:1485:U:C1'	2.42	0.48
1:A:960:U:H2'	1:A:1225:A:H62	1.77	0.48
5:E:84:PHE:CB	5:E:134:ALA:HB2	2.42	0.48
7:G:136:LYS:HE3	7:G:140:ASP:OD2	2.12	0.48
8:H:56:LYS:N	8:H:56:LYS:HD3	2.27	0.48
1:A:1290:G:O2'	1:A:1291:G:H5'	2.13	0.48
1:A:435:C:H2'	1:A:436:C:C6	2.48	0.48
1:A:918:A:H2'	1:A:919:A:C8	2.49	0.48
3:C:46:GLU:HG2	3:C:83:ARG:HH21	1.78	0.48
1:A:1228:C:O3'	13:M:116:THR:HG23	2.14	0.48
1:A:981:U:H5'	14:N:21:TYR:CE1	2.49	0.48
15:O:9:GLN:HA	15:O:12:ILE:HD12	1.95	0.48
17:Q:53:LEU:HD21	17:Q:85:VAL:HG11	1.94	0.48
1:A:1260:C:O5'	1:A:1284:C:H4'	2.13	0.48
1:A:411:A:C8	1:A:413:G:H1'	2.48	0.48
1:A:645:C:H5''	1:A:646:U:OP2	2.13	0.48
1:A:960:U:H4'	1:A:961:U:C5'	2.43	0.48
2:B:106:LYS:O	2:B:110:GLN:HG3	2.14	0.48
8:H:82:HIS:ND1	8:H:138:TRP:CE2	2.75	0.48
17:Q:24:GLU:OE2	17:Q:37:LYS:HD2	2.13	0.48
1:A:1011:G:H2'	1:A:1011:G:N3	2.28	0.48
1:A:1392:G:N2	1:A:1502:A:H8	2.11	0.48
1:A:253:U:H2'	1:A:254:G:H8	1.77	0.48
1:A:509:A:H5'	4:D:54:TYR:HD2	1.78	0.48
1:A:512:U:H2'	1:A:513:C:H6	1.76	0.48
1:A:643:C:H2'	1:A:644:G:H5'	1.95	0.48
4:D:174:LEU:O	4:D:186:LEU:HD11	2.13	0.48
2:B:178:ARG:NH2	8:H:68:ARG:HH22	2.11	0.48
1:A:1152:A:H5''	10:J:13:HIS:CG	2.48	0.48
16:P:2:VAL:O	16:P:64:ALA:HA	2.14	0.48
20:T:77:ALA:O	20:T:81:LYS:HG3	2.13	0.48
1:A:1305:G:H22	1:A:1331:G:H1'	1.75	0.48
1:A:1505:G:H8	1:A:1505:G:H3'	1.79	0.48
1:A:1406:U:HO2'	1:A:1517[B]:G:N2	2.12	0.48
1:A:865:A:H2'	1:A:866:C:H6	1.77	0.48
2:B:12:GLU:HG2	2:B:15:VAL:HB	1.96	0.48
3:C:148:GLY:HA3	3:C:172:ARG:O	2.14	0.48
4:D:196:LEU:HA	4:D:196:LEU:HD23	1.60	0.48
4:D:20:TYR:HB3	4:D:26:CYS:HB3	1.96	0.48
5:E:149:GLU:O	5:E:153:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.95	0.48
18:R:22:VAL:HG13	18:R:42:ARG:NH1	2.28	0.48
19:S:55:LYS:HZ3	19:S:56:GLN:HB2	1.77	0.48
1:A:1005:A:H2	1:A:1026:G:H1'	1.78	0.48
1:A:1047:G:C2'	1:A:1048:G:H5'	2.44	0.48
1:A:1086:U:H3	1:A:1099:G:H22	1.60	0.48
1:A:1244:C:H5''	1:A:1245:A:OP2	2.14	0.48
1:A:1297:C:O2'	1:A:1298:C:OP2	2.30	0.48
1:A:502:G:C2	1:A:503:C:C2	3.01	0.48
1:A:781:A:H2'	1:A:782:A:H5'	1.95	0.48
4:D:170:VAL:HG13	4:D:174:LEU:HD12	1.95	0.48
5:E:11:ILE:HG22	5:E:12:LEU:N	2.29	0.48
15:O:36:ILE:HD12	15:O:60:VAL:HG23	1.95	0.48
20:T:84:LEU:HA	20:T:87:LYS:HZ2	1.79	0.48
1:A:1094:G:O2'	1:A:1108:G:N2	2.47	0.48
1:A:1157:A:H4'	1:A:1158:C:O5'	2.14	0.48
1:A:1296:C:H4'	1:A:1302:U:H5	1.77	0.48
3:C:156:ARG:HG2	3:C:160:ALA:O	2.14	0.48
3:C:81:GLY:O	3:C:84:ILE:HB	2.14	0.48
4:D:158:ILE:HA	4:D:158:ILE:HD13	1.64	0.48
7:G:154:TYR:H	7:G:155:ARG:HH21	1.61	0.48
10:J:6:ILE:HD12	10:J:98:ILE:HG12	1.95	0.48
1:A:1004:A:H5''	1:A:1025:U:N3	2.27	0.48
1:A:1077:G:N2	1:A:1080:A:OP2	2.45	0.48
1:A:1101:A:H4'	1:A:1102:A:O5'	2.14	0.48
1:A:1355:G:H2'	1:A:1356:G:H8	1.78	0.48
1:A:1416:G:N2	1:A:1484:C:C2	2.82	0.48
1:A:1488:G:H2'	1:A:1489:G:C8	2.48	0.48
1:A:179:A:H2'	1:A:180:U:H6	1.79	0.48
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.14	0.48
1:A:216:G:C2	1:A:217:C:C4	3.01	0.48
1:A:268:C:H2'	1:A:269:C:C6	2.48	0.48
1:A:337:C:H2'	1:A:338:A:C8	2.48	0.48
1:A:434:U:H2'	1:A:435:C:C6	2.49	0.48
1:A:581:G:O3'	15:O:64:ARG:NH2	2.47	0.48
1:A:642:A:H2'	1:A:643:C:O4'	2.14	0.48
1:A:77:G:C4	1:A:93:G:N2	2.82	0.48
1:A:78:G:C2	1:A:92:C:C4	3.01	0.48
9:I:28:VAL:HG12	9:I:29:ASN:HB2	1.95	0.48
20:T:89:ARG:NH2	20:T:104:LEU:HB3	2.28	0.48
1:A:1451:A:H5''	1:A:1452:C:H5	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:G:H2'	1:A:692:U:C6	2.48	0.47
2:B:21:ARG:CG	2:B:22:LYS:H	2.26	0.47
3:C:98:ASN:N	3:C:98:ASN:OD1	2.47	0.47
7:G:113:GLU:HG2	7:G:113:GLU:H	1.40	0.47
1:A:161:A:H2'	1:A:162:A:C8	2.49	0.47
1:A:376:G:N3	1:A:389:A:C2	2.82	0.47
1:A:518:C:C5	1:A:529:G:N7	2.82	0.47
1:A:620:C:C2	4:D:135:LEU:HD13	2.49	0.47
3:C:131:ARG:O	3:C:135:LYS:HG2	2.13	0.47
8:H:1:MET:HG2	8:H:2:LEU:N	2.29	0.47
8:H:48:TYR:HA	8:H:60:ARG:O	2.15	0.47
9:I:26:VAL:HG12	9:I:61:ALA:HB3	1.94	0.47
14:N:14:PRO:HB2	14:N:16:PHE:O	2.14	0.47
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.14	0.47
1:A:76:C:H2'	1:A:77:G:H8	1.78	0.47
1:A:830:G:C6	1:A:831:U:C4	3.02	0.47
1:A:858:G:C6	1:A:869:G:N7	2.82	0.47
3:C:138:VAL:HG13	3:C:149:ALA:HB3	1.96	0.47
4:D:141:ARG:NH1	4:D:141:ARG:HB2	2.29	0.47
8:H:26:VAL:HG23	8:H:27:PRO:HD2	1.95	0.47
13:M:2:ALA:O	13:M:10:PRO:HD2	2.15	0.47
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.95	0.47
1:A:1144:G:H21	1:A:1146:A:H62	1.63	0.47
1:A:1184:G:H2'	1:A:1185:G:H8	1.79	0.47
1:A:404:U:H2'	1:A:405:U:H6	1.78	0.47
1:A:60:A:H4'	1:A:61:G:O5'	2.15	0.47
1:A:618:C:N3	1:A:622:A:N6	2.62	0.47
2:B:178:ARG:NH2	8:H:74:PRO:HG3	2.29	0.47
3:C:10:PHE:CD2	3:C:178:LEU:HD12	2.49	0.47
4:D:111:ALA:HB1	4:D:116:GLN:HG2	1.97	0.47
7:G:59:LEU:HD11	7:G:63:LYS:HE3	1.96	0.47
1:A:826:C:H5'	8:H:12:ARG:NH1	2.29	0.47
4:D:24:GLU:O	4:D:25:ARG:HB3	2.14	0.47
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.95	0.47
11:K:29:ILE:HB	11:K:44:SER:CB	2.45	0.47
20:T:64:ASP:OD2	20:T:81:LYS:NZ	2.44	0.47
1:A:1130:A:OP2	1:A:1130:A:H8	1.98	0.47
1:A:176:C:O2'	1:A:177:C:H5'	2.15	0.47
1:A:820:U:H4'	1:A:821:G:OP2	2.15	0.47
1:A:866:C:N3	1:A:867:G:H1'	2.30	0.47
2:B:167:PRO:HG2	2:B:192:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:ARG:HD2	4:D:71:SER:N	2.30	0.47
5:E:48:ALA:HB2	5:E:57:LYS:HE2	1.97	0.47
6:F:98:LEU:HD13	18:R:28:GLU:HG3	1.96	0.47
20:T:50:GLU:H	20:T:99:LEU:HD12	1.80	0.47
1:A:1201:A:H4'	1:A:1202:G:H5''	1.96	0.47
1:A:1415:G:C6	1:A:1416:G:C6	3.03	0.47
1:A:943:U:H1'	9:I:124:GLN:HE22	1.79	0.47
1:A:978:A:C6	1:A:1318:A:C6	3.02	0.47
4:D:92:VAL:O	4:D:96:LEU:HD13	2.13	0.47
1:A:19:C:H5''	5:E:86:ALA:HB2	1.97	0.47
7:G:18:TYR:HD2	7:G:59:LEU:HD13	1.79	0.47
9:I:112:LYS:HG3	9:I:118:LYS:HA	1.97	0.47
10:J:32:ALA:O	10:J:34:VAL:HG23	2.15	0.47
17:Q:29:HIS:HB2	17:Q:36:ILE:HD12	1.97	0.47
18:R:44:LEU:HD13	18:R:48:GLY:O	2.15	0.47
19:S:74:PHE:N	19:S:74:PHE:CD1	2.82	0.47
1:A:1112:C:H42	3:C:178:LEU:H	1.62	0.47
1:A:1243:C:H2'	1:A:1244:C:H6	1.80	0.47
1:A:935:A:O2'	1:A:1383:C:O2	2.33	0.47
1:A:1406:U:H2'	1:A:1407:5MC:C6	2.49	0.47
1:A:1481:U:H2'	1:A:1482:G:O4'	2.15	0.47
1:A:399:G:H2'	1:A:400:C:C6	2.49	0.47
1:A:860:A:N6	1:A:861:G:C2	2.83	0.47
2:B:175:ARG:HG3	2:B:175:ARG:HH11	1.79	0.47
2:B:189:ASP:CG	2:B:205:ASP:HB3	2.35	0.47
3:C:22:TRP:HB3	3:C:59:ARG:HB2	1.95	0.47
7:G:62:PHE:HD2	7:G:62:PHE:C	2.18	0.47
8:H:107:LEU:HD23	8:H:107:LEU:N	2.30	0.47
8:H:95:VAL:HG12	8:H:99:GLU:CB	2.45	0.47
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.96	0.47
13:M:32:GLU:HG2	13:M:64:TRP:HZ2	1.80	0.47
16:P:38:TYR:HE2	16:P:50:LYS:HE2	1.78	0.47
1:A:376:G:H5''	16:P:5:ARG:HD2	1.96	0.47
16:P:75:ARG:C	16:P:78:GLY:H	2.18	0.47
19:S:13:ASP:O	19:S:17:GLU:HG3	2.15	0.47
19:S:25:LYS:HE2	19:S:25:LYS:HB3	1.67	0.47
1:A:1301:U:O2'	1:A:1302:U:H3'	2.14	0.47
1:A:1419:G:C6	1:A:1420:C:C4	3.03	0.47
1:A:78:G:C6	1:A:79:G:C8	3.02	0.47
1:A:860:A:H2'	1:A:861:G:O4'	2.15	0.47
2:B:8:LYS:HB2	2:B:8:LYS:HE2	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:LEU:HD13	3:C:47:LEU:HD13	1.97	0.47
4:D:157:LEU:O	4:D:160:GLN:HB3	2.15	0.47
8:H:118:VAL:C	8:H:119:LEU:HD23	2.34	0.47
1:A:1491:G:H5''	12:L:47:LYS:HE3	1.96	0.47
1:A:280:C:C4	17:Q:91:ARG:NH1	2.83	0.47
18:R:43:PHE:HB3	18:R:66:LEU:HD21	1.97	0.47
1:A:102:G:H2'	1:A:103:C:H6	1.79	0.47
1:A:1069:C:O2'	1:A:1192:C:H1'	2.15	0.47
1:A:1112:C:O2	3:C:179:ARG:HG3	2.15	0.47
1:A:352:C:H6	1:A:352:C:H5''	1.80	0.47
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.97	0.47
9:I:49:PRO:HD3	9:I:101:PHE:CE2	2.50	0.47
9:I:53:VAL:HB	9:I:92:TYR:CZ	2.50	0.47
19:S:32:LYS:HB3	19:S:34:TRP:HZ3	1.79	0.47
1:A:1250:A:C6	1:A:1251:A:N1	2.83	0.47
1:A:303:A:H2'	1:A:304:U:O4'	2.15	0.47
1:A:443:C:H42	1:A:491:G:H1	1.63	0.47
1:A:501:C:H2'	1:A:502:G:H8	1.74	0.47
1:A:520:A:H61	1:A:529:G:H1'	1.79	0.47
1:A:6:G:H2'	5:E:119:LEU:HD11	1.97	0.47
1:A:953:G:C5'	1:A:965:A:H61	2.27	0.47
3:C:43:LEU:HD12	3:C:47:LEU:HD22	1.96	0.47
12:L:87:GLY:H	12:L:99:HIS:H	1.62	0.47
18:R:21:LYS:O	18:R:24:ALA:HB3	2.15	0.47
1:A:1255:G:H2'	1:A:1279:A:N6	2.29	0.46
1:A:325:A:H2'	1:A:326:G:O4'	2.15	0.46
1:A:858:G:H3'	1:A:869:G:O6	2.15	0.46
2:B:21:ARG:CD	2:B:22:LYS:H	2.28	0.46
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.45	0.46
9:I:85:LEU:O	9:I:88:TYR:HB3	2.14	0.46
17:Q:65:ILE:HG21	17:Q:69:LYS:HZ3	1.80	0.46
1:A:1032:G:H2'	1:A:1033:G:H8	1.79	0.46
1:A:1078:U:H5''	1:A:1079:G:OP2	2.16	0.46
1:A:1130:A:OP2	1:A:1130:A:C8	2.68	0.46
1:A:284:G:H2'	1:A:285:G:C8	2.50	0.46
1:A:485:G:O2'	1:A:486:U:P	2.73	0.46
1:A:511:C:O2	4:D:43:HIS:NE2	2.46	0.46
1:A:602:A:H2'	1:A:603:U:O4'	2.15	0.46
2:B:31:TYR:CD2	2:B:31:TYR:N	2.83	0.46
4:D:187:ARG:NE	4:D:188:LEU:N	2.54	0.46
6:F:25:ILE:HD12	6:F:28:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:LEU:O	6:F:79:LEU:HD13	2.16	0.46
9:I:97:LYS:HB2	9:I:98:PRO:HD3	1.97	0.46
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.97	0.46
17:Q:65:ILE:HB	17:Q:69:LYS:HB2	1.96	0.46
1:A:110:C:H2'	1:A:111:G:O4'	2.15	0.46
1:A:1195:C:C4	1:A:1197:G:C8	3.03	0.46
1:A:1347:G:H1'	1:A:1348:U:H5	1.79	0.46
1:A:1399:C:C2	1:A:1502:A:N6	2.84	0.46
1:A:284:G:H2'	1:A:285:G:H8	1.81	0.46
1:A:357:G:C2	1:A:358:U:C5	3.03	0.46
2:B:170:GLU:HA	2:B:170:GLU:OE2	2.14	0.46
3:C:167:TRP:CG	3:C:168:ALA:N	2.84	0.46
4:D:59:ARG:HE	4:D:59:ARG:HB3	1.66	0.46
6:F:69:GLU:N	6:F:69:GLU:OE1	2.47	0.46
1:A:1381:U:C1'	7:G:156:TRP:HH2	2.28	0.46
17:Q:29:HIS:HE1	17:Q:31:LEU:HB3	1.80	0.46
18:R:37:VAL:O	18:R:39:VAL:N	2.48	0.46
18:R:43:PHE:C	18:R:51:LEU:HD12	2.35	0.46
1:A:1250:A:C6	1:A:1251:A:C6	3.04	0.46
1:A:1327:C:H2'	1:A:1328:C:C6	2.50	0.46
1:A:1330:U:H2'	1:A:1331:G:H5'	1.96	0.46
1:A:442:C:H2'	1:A:443:C:C6	2.51	0.46
1:A:951:G:OP2	13:M:102:ARG:NH2	2.37	0.46
2:B:223:ILE:HB	2:B:230:VAL:HG22	1.98	0.46
7:G:152:ALA:O	7:G:155:ARG:NE	2.48	0.46
8:H:104:ARG:HD2	8:H:138:TRP:CD2	2.50	0.46
8:H:127:LEU:HA	8:H:127:LEU:HD13	1.66	0.46
9:I:97:LYS:HE3	9:I:97:LYS:HB3	1.76	0.46
11:K:19:ALA:HB2	11:K:80:VAL:HG11	1.97	0.46
13:M:99:ARG:HB2	13:M:101:GLN:NE2	2.30	0.46
1:A:1241:G:C4	1:A:1242:C:C5	3.03	0.46
1:A:1355:G:H2'	1:A:1356:G:C8	2.50	0.46
1:A:166:G:C6	1:A:167:G:C6	3.03	0.46
1:A:279:A:C8	1:A:279:A:H5'	2.50	0.46
1:A:451:A:H8	1:A:451:A:O5'	1.99	0.46
1:A:707:C:H2'	1:A:708:C:H6	1.80	0.46
1:A:924:C:H5'	1:A:1399:C:OP2	2.16	0.46
2:B:18:GLY:HA2	2:B:42:ILE:HD12	1.98	0.46
1:A:437:U:H1'	4:D:119:GLN:NE2	2.31	0.46
4:D:59:ARG:HA	4:D:62:GLN:HB2	1.96	0.46
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:12:ILE:C	15:O:14:GLU:N	2.68	0.46
17:Q:90:ILE:HA	17:Q:93:GLN:HB2	1.98	0.46
1:A:1006:C:N3	1:A:1007:C:N4	2.63	0.46
1:A:1063:C:H3'	1:A:1064:G:H2'	1.98	0.46
1:A:1196:U:H3'	1:A:1197:G:H5'	1.96	0.46
1:A:142:G:N3	1:A:196:A:H2	2.13	0.46
1:A:247:G:OP2	17:Q:100:LYS:HD2	2.16	0.46
1:A:375:U:H2'	1:A:376:G:O4'	2.16	0.46
1:A:513:C:H2'	1:A:514:C:C6	2.50	0.46
1:A:691:G:H2'	1:A:692:U:H6	1.80	0.46
1:A:837:G:H1	1:A:849:C:H42	1.62	0.46
4:D:148:VAL:HG12	4:D:153:ARG:NH1	2.30	0.46
1:A:437:U:H5'	4:D:155:LEU:HD11	1.98	0.46
4:D:79:PHE:HA	4:D:93:PHE:CE2	2.51	0.46
7:G:44:TYR:O	7:G:48:LYS:HD3	2.15	0.46
8:H:124:ALA:O	8:H:128:GLY:N	2.39	0.46
10:J:15:THR:HG22	10:J:94:VAL:HG13	1.97	0.46
16:P:51:VAL:HG12	16:P:53:VAL:N	2.31	0.46
16:P:78:GLY:C	16:P:80:PHE:N	2.69	0.46
1:A:1095:U:H2'	1:A:1096:C:O4'	2.15	0.46
1:A:1130:A:OP1	1:A:1131:G:H8	1.98	0.46
1:A:1218:C:H2'	1:A:1219:U:C6	2.51	0.46
1:A:132:C:O2'	1:A:133:U:H5'	2.16	0.46
1:A:1493:A:O2'	1:A:1494:G:O4'	2.30	0.46
1:A:1402:4OC:O2	1:A:1500:A:N1	2.49	0.46
2:B:131:PRO:HB3	2:B:133:LYS:NZ	2.31	0.46
3:C:174:PRO:HB2	3:C:177:THR:OG1	2.16	0.46
9:I:125:TYR:CD2	9:I:125:TYR:N	2.84	0.46
11:K:13:GLN:N	11:K:13:GLN:OE1	2.49	0.46
12:L:5:PRO:HG2	12:L:10:LEU:HD21	1.97	0.46
17:Q:56:VAL:O	17:Q:77:VAL:HG23	2.16	0.46
1:A:1163:C:H2'	1:A:1164:G:C8	2.51	0.46
1:A:1418:A:H3'	1:A:1418:A:OP2	2.16	0.46
1:A:183:G:HO2'	1:A:224:C:HO2'	1.63	0.46
1:A:22:G:H2'	1:A:23:C:C6	2.50	0.46
1:A:243:A:C2	1:A:245:C:H2'	2.51	0.46
1:A:413:G:H8	1:A:428:G:N2	1.99	0.46
1:A:571:U:H5''	1:A:572:A:OP2	2.16	0.46
1:A:56:U:O2'	1:A:57:G:H5'	2.15	0.46
1:A:663:A:H2'	1:A:664:G:O4'	2.16	0.46
1:A:939:G:H5''	7:G:102:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:A:O3'	1:A:980:C:N4	2.48	0.46
2:B:122:PHE:HE2	2:B:139:LYS:HD2	1.81	0.46
4:D:118:ARG:O	4:D:122:ARG:HB2	2.16	0.46
4:D:43:HIS:HB3	4:D:46:LYS:HD2	1.98	0.46
8:H:64:LYS:HB3	8:H:79:VAL:HG21	1.96	0.46
9:I:46:ALA:HB1	9:I:77:ILE:CG2	2.46	0.46
10:J:17:ASP:O	10:J:21:GLN:HB2	2.16	0.46
10:J:42:THR:HG23	10:J:67:THR:O	2.15	0.46
10:J:48:THR:HA	10:J:62:HIS:HB3	1.97	0.46
19:S:16:LEU:O	19:S:20:LEU:HG	2.15	0.46
1:A:1007:C:N4	1:A:1022:G:H1	2.14	0.46
1:A:1053:G:H4'	1:A:1054:C:H5'	1.98	0.46
1:A:1201:A:H4'	1:A:1202:G:O5'	2.15	0.46
1:A:1232:U:P	9:I:126:SER:HB2	2.56	0.46
1:A:1385:G:H2'	1:A:1386:G:O4'	2.15	0.46
1:A:1416:G:H3'	1:A:1417:G:H8	1.81	0.46
1:A:229:U:H2'	1:A:230:G:H8	1.81	0.46
1:A:53:A:N6	1:A:54:C:C4	2.84	0.46
1:A:544:G:C5	1:A:545:C:C5	3.04	0.46
1:A:695:A:H61	1:A:797:C:H1'	1.80	0.46
3:C:8:ILE:O	3:C:12:LEU:N	2.49	0.46
5:E:109:ILE:HG22	5:E:110:LEU:N	2.31	0.46
5:E:151:LEU:O	5:E:151:LEU:HD22	2.16	0.46
10:J:51:ARG:NE	10:J:61:GLU:HB3	2.30	0.46
11:K:20:TYR:CE2	11:K:83:ILE:HD13	2.50	0.46
11:K:40:ILE:CG2	11:K:41:THR:HG22	2.43	0.46
11:K:51:LYS:HD3	11:K:51:LYS:HA	1.57	0.46
13:M:81:LEU:HA	13:M:84:ILE:HD11	1.97	0.46
16:P:23:ASP:OD1	16:P:25:ARG:HG3	2.16	0.46
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.51	0.46
19:S:56:GLN:HG2	19:S:57:HIS:H	1.81	0.46
1:A:1240:U:N3	7:G:32:ARG:HD2	2.31	0.46
1:A:1258:G:H2'	1:A:1259:C:C6	2.51	0.46
1:A:222:U:H2'	1:A:223:U:C6	2.50	0.46
1:A:392:G:H2'	1:A:393:A:C8	2.51	0.46
1:A:902:G:H2'	1:A:903:G:C8	2.50	0.46
2:B:223:ILE:O	2:B:227:GLY:N	2.45	0.46
3:C:21:ARG:NH2	3:C:56:ASP:HB3	2.30	0.46
9:I:16:ARG:HB2	9:I:64:THR:HG23	1.97	0.46
18:R:55:ARG:HD2	18:R:55:ARG:O	2.15	0.46
1:A:113:G:H2'	1:A:114:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:G:H2'	1:A:634:C:H6	1.81	0.45
1:A:689:C:O2'	1:A:705:U:O2'	2.25	0.45
2:B:21:ARG:HD2	2:B:22:LYS:N	2.31	0.45
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.51	0.45
1:A:620:C:N1	4:D:135:LEU:HD13	2.31	0.45
4:D:108:LEU:CD1	4:D:183:GLY:HA3	2.46	0.45
6:F:82:ARG:HD2	6:F:82:ARG:HA	1.77	0.45
8:H:86:ILE:HG22	8:H:133:LEU:O	2.16	0.45
9:I:32:ASP:OD1	9:I:33:PHE:N	2.49	0.45
15:O:37:ASN:O	15:O:38:ARG:C	2.55	0.45
18:R:32:ARG:C	18:R:69:THR:HG21	2.37	0.45
18:R:53:ARG:HH11	18:R:59:SER:HA	1.80	0.45
1:A:1067:A:H4'	1:A:1068:G:O5'	2.16	0.45
1:A:1201:A:H4'	1:A:1202:G:C5'	2.46	0.45
1:A:1437:C:H2'	1:A:1438:G:C8	2.51	0.45
3:C:22:TRP:CE3	3:C:32:LEU:HD23	2.50	0.45
1:A:659:U:OP1	15:O:8:LYS:HD3	2.15	0.45
20:T:20:LEU:O	20:T:24:LEU:HD13	2.16	0.45
1:A:1009:G:N2	1:A:1010:G:H1'	2.31	0.45
1:A:1329:A:C5'	13:M:29:ARG:HD2	2.46	0.45
1:A:1332:A:H2'	1:A:1333:A:C8	2.52	0.45
1:A:1395:C:O2'	1:A:1396:A:H5'	2.15	0.45
1:A:802:A:H2'	1:A:803:G:O4'	2.16	0.45
2:B:9:GLU:OE2	2:B:12:GLU:N	2.49	0.45
2:B:30:ARG:HD2	2:B:31:TYR:CE2	2.51	0.45
3:C:62:ASP:O	3:C:97:LYS:HD2	2.15	0.45
4:D:18:LYS:HD3	4:D:20:TYR:HE2	1.81	0.45
5:E:68:GLU:HG3	5:E:68:GLU:O	2.16	0.45
7:G:156:TRP:CD1	7:G:156:TRP:O	2.70	0.45
8:H:11:THR:O	8:H:12:ARG:C	2.53	0.45
11:K:16:SER:HB2	11:K:106:LYS:NZ	2.31	0.45
1:A:1179:A:O3'	9:I:103:THR:HG23	2.16	0.45
1:A:1375:A:OP1	7:G:12:LEU:HD21	2.16	0.45
1:A:858:G:O6	1:A:869:G:C8	2.69	0.45
2:B:193:ASP:O	2:B:196:LEU:HD12	2.17	0.45
4:D:112:VAL:HG23	4:D:116:GLN:OE1	2.17	0.45
5:E:135:THR:O	5:E:138:ALA:HB3	2.17	0.45
10:J:66:ARG:HB3	10:J:66:ARG:HH11	1.82	0.45
20:T:14:LYS:HB2	20:T:17:ARG:NH2	2.32	0.45
1:A:299:G:O5'	1:A:299:G:H8	2.00	0.45
1:A:413:G:H2'	1:A:428:G:N2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:G:C6	1:A:546:G:C2	3.04	0.45
1:A:600:C:N3	1:A:638:G:N2	2.62	0.45
2:B:130:ARG:NH1	2:B:134:GLU:OE1	2.50	0.45
2:B:80:ILE:HG22	2:B:215:LEU:HD12	1.98	0.45
3:C:22:TRP:CH2	3:C:32:LEU:HB3	2.52	0.45
7:G:113:GLU:HG3	7:G:119:ARG:HA	1.99	0.45
9:I:78:LYS:HD2	9:I:101:PHE:HE2	1.81	0.45
1:A:1068:G:OP2	1:A:1094:G:H8	1.99	0.45
1:A:1253:G:O2'	1:A:1356:G:H4'	2.16	0.45
1:A:192:U:H2'	1:A:193:C:H6	1.81	0.45
1:A:452:A:O4'	16:P:72:ARG:NH1	2.50	0.45
1:A:514:C:H2'	1:A:515:G:C8	2.51	0.45
2:B:117:GLU:O	2:B:120:ALA:HB3	2.17	0.45
2:B:187:LEU:HD22	2:B:187:LEU:HA	1.46	0.45
4:D:194:LEU:HD13	4:D:194:LEU:HA	1.55	0.45
4:D:43:HIS:HA	4:D:46:LYS:HE3	1.99	0.45
13:M:40:ASN:ND2	13:M:43:THR:HG23	2.31	0.45
13:M:78:ILE:HA	13:M:78:ILE:HD13	1.64	0.45
15:O:46:HIS:C	15:O:48:LYS:H	2.18	0.45
15:O:55:GLY:O	15:O:59:MET:HG3	2.17	0.45
1:A:1015:A:C5	1:A:1016:A:C5	3.05	0.45
1:A:1027:C:H42	1:A:1035:A:N6	2.15	0.45
1:A:1041:A:H2'	1:A:1042:G:O4'	2.17	0.45
1:A:340:U:H2'	1:A:341:C:H6	1.81	0.45
1:A:554:C:H2'	1:A:555:C:C6	2.51	0.45
3:C:10:PHE:O	3:C:10:PHE:HD2	2.00	0.45
4:D:126:ILE:HD13	4:D:126:ILE:HA	1.66	0.45
4:D:186:LEU:HG	4:D:186:LEU:H	1.46	0.45
4:D:83:SER:HA	4:D:89:THR:HG23	1.98	0.45
8:H:113:SER:HB3	8:H:134:ILE:HD11	1.98	0.45
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.98	0.45
17:Q:21:VAL:O	17:Q:41:LYS:HA	2.17	0.45
1:A:1141:C:H2'	1:A:1142:G:H8	1.80	0.45
1:A:35:G:H2'	1:A:36:C:C6	2.52	0.45
2:B:118:LEU:CB	2:B:142:LEU:HD23	2.46	0.45
2:B:80:ILE:HD13	2:B:212:GLN:HG2	1.99	0.45
3:C:151:VAL:H	3:C:169:ALA:HB2	1.82	0.45
3:C:155:GLY:HA2	3:C:164:ARG:O	2.16	0.45
3:C:31:HIS:HA	3:C:34:LEU:HB2	1.99	0.45
4:D:63:LYS:O	4:D:67:ILE:HG12	2.16	0.45
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:59:LEU:O	7:G:62:PHE:HB3	2.16	0.45
8:H:15:ASN:OD1	8:H:15:ASN:N	2.50	0.45
10:J:48:THR:HG1	10:J:62:HIS:HD1	1.63	0.45
19:S:40:ILE:HD13	19:S:62:ILE:HD11	1.98	0.45
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.97	0.45
1:A:1098:C:H2'	1:A:1099:G:O4'	2.17	0.45
1:A:538:G:P	12:L:115:LYS:HB2	2.57	0.45
1:A:935:A:H2'	1:A:936:C:O4'	2.17	0.45
4:D:176:LEU:HD12	4:D:177:ASP:N	2.31	0.45
8:H:100:ILE:HA	8:H:101:PRO:HD2	1.37	0.45
9:I:3:GLN:HG3	9:I:20:ARG:HG2	1.99	0.45
10:J:36:GLY:HA2	10:J:37:PRO:HD3	1.75	0.45
1:A:1492:A:H2'	1:A:1492:A:N3	2.32	0.45
1:A:35:G:C6	1:A:36:C:N4	2.84	0.45
1:A:429:U:H1'	1:A:430:A:H5''	1.99	0.45
1:A:510:A:H5''	1:A:511:C:OP2	2.17	0.45
1:A:735:C:H2'	1:A:736:C:H6	1.81	0.45
1:A:901:A:N7	1:A:902:G:H1'	2.32	0.45
1:A:953:G:C6	1:A:954:G:C4	3.05	0.45
1:A:953:G:H2'	1:A:954:G:O4'	2.16	0.45
3:C:173:VAL:HG12	3:C:175:LEU:HD21	1.99	0.45
3:C:83:ARG:HG2	3:C:87:LEU:HD12	1.98	0.45
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.98	0.45
8:H:49:GLU:O	8:H:59:LEU:HA	2.17	0.45
2:B:178:ARG:HH21	8:H:68:ARG:HH22	1.63	0.45
12:L:19:ARG:HA	12:L:20:LYS:HZ1	1.82	0.45
13:M:48:LEU:HB3	13:M:53:VAL:HG23	1.99	0.45
19:S:18:LYS:HZ1	19:S:32:LYS:H	1.65	0.45
1:A:1128:C:N4	1:A:1139:G:N3	2.66	0.44
1:A:200:G:C6	1:A:201:C:C4	3.05	0.44
1:A:217:C:H2'	1:A:218:C:C6	2.52	0.44
1:A:474:G:C2	1:A:475:G:C4	3.05	0.44
1:A:877:C:O2'	8:H:3:THR:HG23	2.17	0.44
1:A:888:G:H5''	1:A:889:A:O5'	2.16	0.44
7:G:73:MET:HA	7:G:91:VAL:HG23	1.98	0.44
12:L:76:ASN:ND2	12:L:108:ALA:H	2.15	0.44
14:N:29:ARG:NH1	14:N:42:ILE:HG13	2.32	0.44
14:N:3:ARG:HB2	14:N:6:LEU:HB2	1.99	0.44
17:Q:59:ILE:HA	17:Q:59:ILE:HD12	1.69	0.44
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.83	0.44
1:A:254:G:OP1	17:Q:67:LYS:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:A:OP1	1:A:280:C:O2'	2.27	0.44
1:A:532:A:H2'	1:A:533:A:OP1	2.17	0.44
1:A:1347:G:O6	9:I:10:ARG:NH2	2.50	0.44
10:J:7:LYS:HG2	10:J:9:ARG:HG2	1.98	0.44
1:A:1347:G:N2	1:A:1374:A:OP2	2.28	0.44
1:A:1424:C:H2'	1:A:1425:U:C6	2.48	0.44
1:A:600:C:N4	1:A:638:G:H1	2.16	0.44
1:A:840:C:H5'	1:A:848:C:O2	2.17	0.44
2:B:134:GLU:O	2:B:137:ARG:HG2	2.18	0.44
2:B:220:ASP:HA	2:B:230:VAL:HG21	1.99	0.44
4:D:148:VAL:HB	4:D:181:MET:HB3	2.00	0.44
4:D:155:LEU:HD13	4:D:156:GLU:H	1.80	0.44
5:E:61:TYR:O	5:E:64:ARG:O	2.35	0.44
8:H:10:LEU:N	8:H:10:LEU:HD23	2.31	0.44
11:K:40:ILE:HG13	11:K:75:TYR:CD1	2.52	0.44
19:S:15:LEU:HD12	19:S:16:LEU:H	1.83	0.44
19:S:5:LEU:HD22	19:S:70:LYS:HZ1	1.82	0.44
1:A:1000:U:C4	1:A:1042:G:C6	3.06	0.44
1:A:1255:G:O2'	1:A:1258:G:O2'	2.35	0.44
1:A:656:C:O2'	15:O:28:GLN:NE2	2.51	0.44
1:A:76:C:N4	1:A:93:G:N1	2.66	0.44
1:A:76:C:N4	1:A:95:U:H3	2.04	0.44
3:C:23:TYR:CD1	10:J:10:GLY:HA2	2.52	0.44
4:D:207:TYR:CD2	4:D:207:TYR:N	2.84	0.44
5:E:64:ARG:H	5:E:64:ARG:HG2	1.66	0.44
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.18	0.44
12:L:51:ALA:O	12:L:52:LEU:HD23	2.17	0.44
13:M:22:ILE:HD12	13:M:25:ILE:HG13	2.00	0.44
14:N:24:CYS:CB	14:N:40:CYS:HB3	2.47	0.44
15:O:14:GLU:HB3	15:O:15:PHE:HD1	1.82	0.44
1:A:1221:G:C4	1:A:1222:G:C8	3.05	0.44
1:A:1310:G:H5'	13:M:77:ASN:HD21	1.81	0.44
1:A:1328:C:H2'	1:A:1329:A:H8	1.81	0.44
1:A:1486:G:C6	1:A:1487:G:C6	3.06	0.44
1:A:736:C:H2'	1:A:737:A:H8	1.78	0.44
1:A:778:G:H2'	1:A:779:C:O4'	2.17	0.44
2:B:95:GLN:HG2	2:B:148:TYR:HD2	1.82	0.44
1:A:409:G:OP1	4:D:24:GLU:O	2.35	0.44
4:D:15:GLU:HB3	4:D:63:LYS:CG	2.48	0.44
1:A:923:A:OP1	5:E:21:ALA:HB2	2.17	0.44
8:H:102:ARG:O	8:H:102:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:G:H4'	9:I:122:ALA:HB3	1.99	0.44
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.17	0.44
13:M:20:THR:OG1	13:M:20:THR:O	2.33	0.44
16:P:11:SER:N	16:P:14:ASN:O	2.49	0.44
1:A:1245:A:N1	1:A:1293:G:C2	2.85	0.44
1:A:178:C:H2'	1:A:179:A:H5'	1.99	0.44
1:A:374:A:H2'	1:A:374:A:N3	2.33	0.44
1:A:500:G:C5	1:A:546:G:N2	2.86	0.44
1:A:537:G:H2'	1:A:538:G:C8	2.52	0.44
1:A:613:C:OP1	4:D:84:LYS:HE3	2.17	0.44
1:A:813:U:H6	1:A:813:U:OP2	2.00	0.44
7:G:145:ALA:C	7:G:147:ALA:H	2.21	0.44
10:J:31:GLY:HA3	10:J:81:THR:OG1	2.17	0.44
12:L:46:LYS:HG2	12:L:94:TRP:CE2	2.53	0.44
13:M:45:VAL:O	13:M:48:LEU:HD23	2.18	0.44
17:Q:75:ARG:HB2	17:Q:75:ARG:HH11	1.83	0.44
18:R:26:LEU:HA	18:R:26:LEU:HD12	1.56	0.44
20:T:29:LYS:O	20:T:33:ILE:HG12	2.18	0.44
1:A:1035:A:C6	1:A:1036:G:C6	3.05	0.44
1:A:581:G:O6	1:A:758:G:C8	2.71	0.44
1:A:619:U:C4	4:D:135:LEU:HD21	2.53	0.44
1:A:620:C:H2'	1:A:621:A:O4'	2.17	0.44
1:A:903:G:O2'	1:A:904:C:H5'	2.18	0.44
1:A:916:G:H2'	1:A:917:G:H8	1.83	0.44
1:A:939:G:C6	1:A:940:C:N4	2.85	0.44
2:B:154:LEU:HA	2:B:154:LEU:HD13	1.56	0.44
7:G:136:LYS:HE2	7:G:136:LYS:HB3	1.58	0.44
12:L:38:THR:HB	12:L:39:VAL:H	1.62	0.44
18:R:45:SER:OG	18:R:47:THR:O	2.31	0.44
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.18	0.44
1:A:614:A:H2'	1:A:615:C:H6	1.83	0.44
1:A:402:G:H4'	1:A:620:C:O2	2.18	0.44
1:A:642:A:H2'	1:A:643:C:C6	2.53	0.44
1:A:664:G:OP1	18:R:64:ARG:HD2	2.17	0.44
4:D:111:ALA:HB3	4:D:117:ALA:HB2	1.99	0.44
17:Q:6:LEU:HB3	17:Q:23:VAL:HG11	1.99	0.44
1:A:1058:G:H22	10:J:53:PRO:HG3	1.83	0.44
1:A:1064:G:OP1	1:A:1386:G:H4'	2.17	0.44
1:A:113:G:H2'	1:A:114:U:H6	1.83	0.44
1:A:1162:C:H2'	1:A:1163:C:C6	2.53	0.44
1:A:392:G:H2'	1:A:393:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:G:H2'	1:A:485:G:N2	2.33	0.44
1:A:960:U:O5'	1:A:961:U:H5''	2.18	0.44
2:B:60:ASP:O	2:B:64:ARG:HG3	2.18	0.44
3:C:39:ILE:HG21	3:C:57:ILE:CD1	2.48	0.44
5:E:78:HIS:CD2	8:H:104:ARG:HG2	2.53	0.44
9:I:31:GLN:HG2	9:I:35:GLU:HB3	1.99	0.44
12:L:19:ARG:HA	12:L:20:LYS:HZ2	1.82	0.44
16:P:45:THR:O	16:P:48:TRP:HD1	2.01	0.44
19:S:64:GLU:HG3	19:S:65:ASN:H	1.82	0.44
1:A:1232:U:H6	1:A:1232:U:O5'	2.01	0.43
1:A:1442:G:C5	1:A:1446:A:N6	2.86	0.43
1:A:384:G:C6	1:A:385:C:N4	2.86	0.43
1:A:819:A:H4'	1:A:820:U:OP2	2.18	0.43
2:B:150:SER:OG	2:B:151:GLY:N	2.50	0.43
2:B:87:ARG:HD2	2:B:219:VAL:HG11	1.99	0.43
2:B:7:VAL:HG11	2:B:221:LEU:CD2	2.48	0.43
5:E:37:ARG:O	5:E:114:GLY:HA3	2.18	0.43
8:H:83:ILE:HG22	8:H:83:ILE:O	2.18	0.43
14:N:37:PHE:C	14:N:39:LEU:N	2.72	0.43
15:O:57:LEU:HA	15:O:57:LEU:HD12	1.74	0.43
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.61	0.43
18:R:42:ARG:NH1	18:R:42:ARG:HB3	2.33	0.43
1:A:1018:C:H2'	1:A:1019:C:O4'	2.18	0.43
1:A:1035:A:H2'	1:A:1036:G:C8	2.53	0.43
1:A:1519[A]:MA6:H3'	1:A:1520[A]:G:C5'	2.49	0.43
1:A:353:A:H5'	1:A:353:A:H8	1.83	0.43
1:A:514:C:H2'	1:A:515:G:H8	1.83	0.43
1:A:922:G:N3	1:A:1398:A:H2	2.16	0.43
2:B:50:GLU:O	2:B:53:ARG:HG3	2.17	0.43
5:E:112:LEU:C	5:E:114:GLY:H	2.18	0.43
12:L:58:VAL:HG12	12:L:59:ARG:N	2.33	0.43
13:M:100:GLY:N	13:M:101:GLN:OE1	2.51	0.43
1:A:1158:C:H42	1:A:1181:G:H1	1.67	0.43
1:A:1264:C:H2'	1:A:1265:G:C8	2.53	0.43
1:A:1349:A:C2	1:A:1374:A:C4	3.06	0.43
1:A:484:G:H8	1:A:484:G:O5'	1.99	0.43
1:A:671:G:H5'	6:F:77:ARG:HH21	1.81	0.43
1:A:78:G:N2	1:A:92:C:C5	2.87	0.43
2:B:172:ILE:H	2:B:172:ILE:CD1	2.28	0.43
2:B:187:LEU:HD22	2:B:201:ILE:O	2.18	0.43
3:C:3:ASN:HB3	3:C:4:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:G:OP1	4:D:10:ARG:NH2	2.51	0.43
4:D:207:TYR:HD2	4:D:207:TYR:N	2.16	0.43
11:K:72:ALA:O	11:K:75:TYR:N	2.43	0.43
13:M:107:ALA:HB3	13:M:111:LYS:HE3	2.00	0.43
17:Q:26:GLN:HG2	17:Q:37:LYS:HB2	2.00	0.43
1:A:736:C:OP2	18:R:68:LYS:HE3	2.19	0.43
19:S:6:LYS:HB2	19:S:6:LYS:HE2	1.52	0.43
20:T:73:HIS:O	20:T:76:ALA:HB3	2.19	0.43
1:A:1050:G:O6	1:A:1208:C:N4	2.50	0.43
1:A:1240:U:C2	7:G:32:ARG:HD2	2.52	0.43
1:A:1354:C:H2'	1:A:1355:G:C8	2.51	0.43
1:A:313:A:H2'	1:A:314:C:C6	2.53	0.43
1:A:378:G:H2'	1:A:379:C:C6	2.54	0.43
1:A:866:C:H2'	1:A:867:G:O4'	2.18	0.43
2:B:180:LEU:O	2:B:181:PHE:HB2	2.18	0.43
3:C:88:ARG:NH2	3:C:101:LEU:HB2	2.29	0.43
4:D:170:VAL:CG1	4:D:174:LEU:HB2	2.48	0.43
5:E:137:GLU:HA	5:E:140:ARG:HH11	1.81	0.43
9:I:62:TYR:HD1	9:I:63:ILE:N	2.17	0.43
11:K:20:TYR:CZ	11:K:83:ILE:HD13	2.52	0.43
12:L:42:THR:HG21	12:L:52:LEU:HB3	1.99	0.43
1:A:1073:U:O2	2:B:104:ASN:ND2	2.51	0.43
1:A:1203:C:H2'	1:A:1204:A:O4'	2.18	0.43
1:A:1212:U:H4'	1:A:1213:A:C8	2.54	0.43
1:A:1328:C:OP1	21:U:21:TYR:OH	2.35	0.43
1:A:1412:C:H42	1:A:1488:G:H1	1.66	0.43
1:A:429:U:H4'	1:A:430:A:O5'	2.17	0.43
1:A:502:G:H2'	1:A:503:C:O4'	2.19	0.43
1:A:675:A:H1'	11:K:116:HIS:CD2	2.53	0.43
1:A:782:A:H2'	1:A:783:C:O4'	2.18	0.43
1:A:925:G:C2	1:A:927:G:C8	3.06	0.43
2:B:113:HIS:H	2:B:113:HIS:HD1	1.65	0.43
2:B:16:HIS:ND1	2:B:17:PHE:O	2.51	0.43
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.79	0.43
2:B:238:LEU:HD22	2:B:238:LEU:HA	1.83	0.43
3:C:47:LEU:HD21	3:C:76:VAL:HG23	1.98	0.43
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.83	0.43
9:I:5:TYR:CD1	9:I:6:GLY:N	2.83	0.43
9:I:73:GLN:O	9:I:77:ILE:HG12	2.18	0.43
12:L:27:LEU:C	12:L:29:GLY:N	2.60	0.43
18:R:51:LEU:HB2	18:R:56:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:78:LEU:HA	18:R:78:LEU:HD23	1.58	0.43
1:A:1065:U:H5'	1:A:1190:G:N2	2.33	0.43
1:A:1189:C:P	10:J:51:ARG:HH22	2.41	0.43
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.69	0.43
9:I:27:THR:HG23	9:I:63:ILE:H	1.83	0.43
11:K:30:VAL:HG21	11:K:65:ALA:HA	2.00	0.43
12:L:113:ARG:HG3	12:L:113:ARG:O	2.17	0.43
1:A:1130:A:OP1	1:A:1131:G:C8	2.71	0.43
1:A:1236:A:OP1	21:U:3:LYS:HG3	2.19	0.43
1:A:11:G:C5	1:A:12:U:C5	3.07	0.43
1:A:1494:G:H2'	1:A:1495:U:H5'	2.01	0.43
1:A:1526:G:H2'	1:A:1527:C:H6	1.83	0.43
1:A:731:G:O2'	1:A:732:C:H5'	2.18	0.43
1:A:894:G:C6	1:A:895:G:C5	3.06	0.43
1:A:95:U:O2'	1:A:96:G:H5'	2.17	0.43
1:A:968:A:C8	1:A:1062:U:H4'	2.54	0.43
2:B:11:LEU:O	2:B:11:LEU:HD23	2.18	0.43
4:D:154:ASN:C	4:D:159:ARG:HH21	2.20	0.43
5:E:69:VAL:HG21	5:E:113:ALA:HB1	2.00	0.43
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.61	0.43
10:J:27:ALA:HA	10:J:81:THR:CG2	2.47	0.43
10:J:7:LYS:HA	10:J:71:LEU:HD12	1.99	0.43
20:T:81:LYS:O	20:T:85:MET:HG3	2.18	0.43
1:A:767:A:H2'	1:A:768:A:O4'	2.18	0.43
2:B:73:THR:HG23	2:B:95:GLN:O	2.19	0.43
4:D:88:VAL:O	4:D:92:VAL:HG23	2.18	0.43
6:F:95:GLU:O	6:F:97:PHE:N	2.52	0.43
7:G:26:PHE:O	7:G:30:ILE:HG13	2.19	0.43
9:I:8:GLY:HA2	9:I:79:LEU:CD1	2.48	0.43
9:I:99:LEU:HB3	9:I:101:PHE:CD1	2.54	0.43
17:Q:15:MET:HE3	17:Q:15:MET:HB2	1.83	0.43
21:U:25:LYS:HA	21:U:25:LYS:HE3	2.00	0.43
1:A:1032:G:C2	1:A:1033:G:C4	3.07	0.43
1:A:1092:A:O5'	1:A:1092:A:H8	2.01	0.43
1:A:1228:C:OP1	13:M:115:LYS:HG2	2.18	0.43
1:A:1269:A:N1	1:A:1312:G:O2'	2.49	0.43
1:A:927:G:H1	1:A:1390:U:H3	1.64	0.43
1:A:1477:C:H2'	1:A:1478:C:C6	2.54	0.43
1:A:193:C:H2'	1:A:194:C:H6	1.84	0.43
8:H:28:ALA:CB	8:H:59:LEU:HG	2.46	0.43
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1147:C:H4'	9:I:5:TYR:HE2	1.83	0.43
11:K:40:ILE:HG23	11:K:75:TYR:HD1	1.84	0.43
12:L:113:ARG:HD3	12:L:115:LYS:H	1.83	0.43
1:A:501:C:O3'	12:L:118:SER:OG	2.36	0.43
19:S:7:LYS:HE3	19:S:7:LYS:HB3	1.91	0.43
20:T:36:LEU:HD22	20:T:36:LEU:HA	1.81	0.43
1:A:1026:G:C8	1:A:1027:C:C6	3.07	0.43
1:A:1283:G:H2'	1:A:1284:C:H6	1.83	0.43
1:A:1517[A]:G:H2'	1:A:1518[A]:MA6:C8	2.46	0.43
1:A:243:A:H2	1:A:245:C:H2'	1.84	0.43
1:A:586:C:O3'	8:H:89:PRO:HB2	2.19	0.43
1:A:728:A:H2'	1:A:729:A:O4'	2.19	0.43
1:A:836:G:C8	1:A:836:G:H5''	2.53	0.43
1:A:827:U:H2'	1:A:859:A:N1	2.34	0.43
1:A:893:C:H2'	1:A:894:G:C8	2.54	0.43
4:D:117:ALA:O	4:D:121:VAL:HG23	2.19	0.43
4:D:4:TYR:CE2	4:D:11:LEU:HD11	2.53	0.43
5:E:11:ILE:HG21	5:E:31:LEU:HD12	2.01	0.43
6:F:11:ASN:OD1	6:F:14:LEU:HD23	2.18	0.43
6:F:53:ALA:C	6:F:55:ASP:H	2.22	0.43
12:L:71:PRO:O	12:L:102:ARG:HD3	2.19	0.43
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.54	0.43
1:A:1368:G:H5'	9:I:112:LYS:O	2.19	0.42
1:A:1416:G:H2'	1:A:1417:G:O4'	2.19	0.42
1:A:407:G:O6	1:A:408:A:N6	2.51	0.42
1:A:409:G:H1	1:A:433:C:N4	2.09	0.42
1:A:414:A:OP2	1:A:428:G:N2	2.21	0.42
1:A:451:A:N7	1:A:481:G:N1	2.67	0.42
1:A:481:G:O2'	1:A:482:A:C8	2.71	0.42
2:B:24:TRP:CG	2:B:25:ASN:N	2.86	0.42
2:B:44:LEU:HD12	2:B:44:LEU:H	1.83	0.42
4:D:60:GLU:HA	4:D:60:GLU:OE1	2.17	0.42
7:G:80:VAL:HG11	7:G:154:TYR:CE1	2.51	0.42
11:K:24:SER:OG	11:K:25:TYR:N	2.52	0.42
1:A:1329:A:H5'	13:M:29:ARG:HD2	2.00	0.42
1:A:1357:A:C5	1:A:1358:U:C4	3.07	0.42
1:A:815:A:N6	1:A:1509:C:H1'	2.34	0.42
1:A:328:C:H4'	1:A:329:A:H5'	2.00	0.42
1:A:448:A:OP2	1:A:485:G:N2	2.44	0.42
1:A:824:C:H2'	1:A:825:G:C8	2.54	0.42
1:A:939:G:H2'	1:A:940:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:ARG:HD3	3:C:126:ARG:HA	1.82	0.42
4:D:3:ARG:HD2	4:D:71:SER:H	1.85	0.42
5:E:12:LEU:HD13	5:E:31:LEU:HB2	2.00	0.42
5:E:80:ILE:CD1	5:E:138:ALA:HB1	2.49	0.42
7:G:151:TYR:N	7:G:151:TYR:CD1	2.85	0.42
8:H:39:LEU:HA	8:H:39:LEU:HD23	1.64	0.42
10:J:40:LEU:HD12	10:J:69:ASN:HB2	2.01	0.42
17:Q:29:HIS:O	17:Q:33:GLY:HA2	2.19	0.42
19:S:19:VAL:HG23	19:S:47:HIS:CE1	2.54	0.42
20:T:75:ASN:N	20:T:75:ASN:OD1	2.51	0.42
1:A:1236:A:O5'	21:U:2:GLY:N	2.52	0.42
1:A:1010:G:H2'	1:A:1011:G:H5''	2.01	0.42
1:A:1315:U:H2'	1:A:1316:G:O4'	2.19	0.42
1:A:634:C:O2'	1:A:635:G:H5'	2.19	0.42
1:A:839:U:O2	1:A:839:U:H2'	2.18	0.42
2:B:88:ALA:HB1	2:B:90:MET:HG2	2.01	0.42
3:C:199:LYS:HB3	3:C:201:TYR:HE1	1.83	0.42
3:C:77:ILE:CG2	3:C:81:GLY:HA2	2.49	0.42
4:D:57:ARG:NH2	5:E:107:ARG:HD3	2.34	0.42
6:F:25:ILE:HD12	6:F:25:ILE:HA	1.88	0.42
8:H:1:MET:HG2	8:H:2:LEU:O	2.18	0.42
10:J:30:SER:OG	10:J:81:THR:HG23	2.18	0.42
11:K:109:VAL:HA	18:R:85:LEU:O	2.19	0.42
1:A:1256:A:H4'	1:A:1257:U:O5'	2.18	0.42
1:A:1355:G:H1	1:A:1367:C:N4	2.17	0.42
1:A:1498:UR3:H1'	1:A:1499:A:N7	2.34	0.42
1:A:439:A:C4	1:A:497:A:C2	3.07	0.42
1:A:768:A:C5	1:A:769:G:C8	3.07	0.42
1:A:691:G:O2'	1:A:797:C:H4'	2.19	0.42
1:A:942:G:H21	9:I:124:GLN:NE2	2.18	0.42
3:C:39:ILE:HG21	3:C:57:ILE:HD12	2.01	0.42
11:K:58:PRO:HD3	11:K:89:ALA:HB1	2.01	0.42
12:L:77:LEU:HD21	12:L:107:ALA:HA	2.02	0.42
12:L:89:ARG:HG2	12:L:97:ARG:HA	2.01	0.42
15:O:65:ARG:HB2	15:O:65:ARG:HE	1.35	0.42
17:Q:90:ILE:O	17:Q:91:ARG:C	2.58	0.42
1:A:1320:C:H42	19:S:36:ARG:HD3	1.84	0.42
1:A:1314:C:O2'	1:A:1315:U:H5'	2.19	0.42
1:A:1332:A:H2'	1:A:1333:A:H8	1.83	0.42
1:A:1478:C:H2'	1:A:1479:C:C6	2.54	0.42
1:A:1515[B]:C:N4	1:A:1520[B]:G:H1	2.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:C:C4	1:A:356:A:N7	2.87	0.42
1:A:444:C:H2'	1:A:445:G:H8	1.82	0.42
1:A:663:A:H61	1:A:742:G:H1	1.65	0.42
1:A:806:C:O2'	1:A:807:A:H5'	2.20	0.42
2:B:23:ARG:HA	2:B:23:ARG:HH11	1.85	0.42
2:B:87:ARG:NH1	2:B:219:VAL:HB	2.35	0.42
2:B:82:ARG:HG3	2:B:92:TYR:CE1	2.55	0.42
4:D:150:GLU:OE1	4:D:151:LYS:HG2	2.18	0.42
1:A:8:A:H5'	5:E:101:ILE:HG22	2.02	0.42
5:E:144:THR:HG22	5:E:145:LYS:N	2.34	0.42
7:G:54:THR:C	7:G:56:GLN:H	2.22	0.42
12:L:46:LYS:HG3	12:L:92:ASP:O	2.20	0.42
16:P:38:TYR:O	16:P:49:LEU:HD12	2.20	0.42
17:Q:62:SER:OG	17:Q:72:ARG:HG2	2.19	0.42
19:S:49:ILE:HG22	19:S:51:VAL:HG22	2.02	0.42
1:A:1064:G:H22	1:A:1190:G:H2'	1.83	0.42
1:A:1198:G:H2'	1:A:1199:U:C6	2.55	0.42
1:A:1279:A:H4'	1:A:1280:A:OP1	2.19	0.42
1:A:1300:G:H5''	1:A:1335:C:N4	2.34	0.42
1:A:1367:C:N3	1:A:1368:G:C8	2.88	0.42
1:A:1520[B]:G:H2'	1:A:1521:G:C8	2.53	0.42
1:A:259:G:O2'	1:A:260:G:H5'	2.20	0.42
1:A:350:G:H8	1:A:350:G:C5'	2.31	0.42
1:A:49:U:O2'	1:A:50:A:H2'	2.20	0.42
1:A:695:A:H2'	1:A:696:A:C8	2.54	0.42
1:A:77:G:N2	1:A:78:G:C4	2.87	0.42
1:A:781:A:C4	1:A:802:A:C2	3.07	0.42
2:B:87:ARG:HH11	2:B:219:VAL:HB	1.83	0.42
3:C:52:LEU:HD11	3:C:68:VAL:CG2	2.47	0.42
4:D:202:LEU:HD13	4:D:202:LEU:HA	1.37	0.42
9:I:127:LYS:O	9:I:128:ARG:C	2.57	0.42
10:J:47:PHE:O	10:J:62:HIS:HB2	2.20	0.42
12:L:34:ARG:HB2	12:L:105:TYR:CE1	2.54	0.42
12:L:60:LEU:HB2	12:L:64:TYR:O	2.19	0.42
15:O:46:HIS:C	15:O:48:LYS:N	2.73	0.42
1:A:1003:G:H22	1:A:1004:A:H1'	1.85	0.42
1:A:1130:A:H5''	9:I:20:ARG:HH21	1.84	0.42
1:A:1266:G:N2	1:A:1269:A:OP2	2.42	0.42
1:A:1518[A]:MA6:H93	1:A:1519[A]:MA6:N6	2.35	0.42
1:A:442:C:H2'	1:A:443:C:H6	1.84	0.42
1:A:824:C:H2'	1:A:825:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:G:N2	1:A:92:C:C4	2.88	0.42
3:C:150:LYS:HE3	3:C:173:VAL:HB	2.02	0.42
6:F:33:TYR:HD2	6:F:71:ARG:HD2	1.84	0.42
10:J:49:VAL:HG23	10:J:61:GLU:O	2.20	0.42
11:K:53:SER:O	11:K:55:LYS:N	2.52	0.42
12:L:22:SER:C	12:L:24:VAL:N	2.73	0.42
14:N:12:ARG:HB3	14:N:13:THR:H	1.65	0.42
17:Q:17:LYS:N	17:Q:49:GLU:OE2	2.42	0.42
20:T:87:LYS:O	20:T:91:LEU:HB2	2.19	0.42
21:U:10:ARG:HG3	21:U:13:ILE:CD1	2.45	0.42
1:A:1258:G:OP2	1:A:1258:G:H8	2.02	0.42
1:A:1421:G:H2'	1:A:1422:G:O4'	2.20	0.42
1:A:243:A:C2	1:A:246:A:C8	3.08	0.42
1:A:162:A:H1'	1:A:348:G:O2'	2.20	0.42
1:A:544:G:C6	1:A:545:C:C4	3.08	0.42
1:A:856:C:H2'	1:A:857:C:H6	1.85	0.42
6:F:33:TYR:HA	6:F:71:ARG:CZ	2.50	0.42
8:H:70:GLN:OE1	8:H:70:GLN:HA	2.20	0.42
8:H:9:MET:HG3	8:H:26:VAL:HG21	2.02	0.42
16:P:75:ARG:HE	16:P:80:PHE:HD1	1.66	0.42
18:R:76:LEU:HA	18:R:76:LEU:HD23	1.57	0.42
19:S:80:TYR:CZ	19:S:81:ARG:HB3	2.55	0.42
1:A:1502:A:C2	1:A:1504:G:C2	3.08	0.42
1:A:1530:G:H2'	1:A:1531:A:C8	2.54	0.42
1:A:359:U:H2'	1:A:360:A:H8	1.81	0.42
1:A:411:A:C4	1:A:413:G:H1'	2.55	0.42
1:A:442:C:H42	1:A:492:G:H1	1.67	0.42
1:A:475:G:C2	1:A:476:G:C5	3.08	0.42
1:A:500:G:C6	1:A:501:C:C4	3.08	0.42
1:A:642:A:H2'	1:A:643:C:H6	1.85	0.42
1:A:794:A:H2'	1:A:795:C:O4'	2.19	0.42
1:A:781:A:C5	1:A:802:A:C2	3.08	0.42
1:A:903:G:H2'	1:A:904:C:H6	1.84	0.42
2:B:43:ASP:OD1	2:B:46:LYS:HG3	2.20	0.42
5:E:81:GLU:HG2	5:E:88:LYS:HE2	2.02	0.42
10:J:50:ILE:HA	10:J:60:ARG:CB	2.43	0.42
12:L:53:ARG:HH11	12:L:93:LEU:HD21	1.85	0.42
18:R:47:THR:HG22	18:R:48:GLY:H	1.85	0.42
1:A:1435:G:O5'	1:A:1435:G:H8	2.03	0.42
1:A:1474:G:N1	1:A:1475:G:O6	2.53	0.42
1:A:1486:G:H2'	1:A:1487:G:C1'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1493:A:HO2'	1:A:1494:G:H8	1.67	0.42
1:A:179:A:O2'	1:A:180:U:H5'	2.20	0.42
1:A:293:G:H1	1:A:304:U:H3	1.68	0.42
1:A:411:A:N7	1:A:413:G:C4	2.88	0.42
1:A:477:G:N2	1:A:478:A:C5	2.88	0.42
1:A:881:G:H2'	1:A:882:C:O4'	2.20	0.42
3:C:131:ARG:O	3:C:134:ILE:HB	2.19	0.42
4:D:36:ARG:N	4:D:37:PRO:HD3	2.35	0.42
7:G:62:PHE:CD2	7:G:63:LYS:HD3	2.55	0.42
13:M:71:ARG:HH11	13:M:71:ARG:HB3	1.85	0.42
13:M:81:LEU:HD11	13:M:88:ARG:NH2	2.34	0.42
14:N:54:PRO:C	14:N:56:VAL:H	2.24	0.42
15:O:22:THR:O	15:O:27:VAL:HG11	2.20	0.42
15:O:5:LYS:O	15:O:8:LYS:N	2.53	0.42
1:A:1003:G:N2	1:A:1038:C:N3	2.67	0.41
1:A:102:G:H2'	1:A:103:C:C6	2.55	0.41
1:A:1199:U:O5'	1:A:1199:U:H6	2.02	0.41
1:A:1493:A:C2'	1:A:1494:G:H8	2.32	0.41
1:A:66:G:N3	1:A:66:G:H2'	2.35	0.41
4:D:116:GLN:NE2	4:D:157:LEU:HD11	2.34	0.41
6:F:25:ILE:HD12	6:F:28:ARG:HH11	1.85	0.41
6:F:91:VAL:HG12	6:F:92:LYS:O	2.19	0.41
7:G:140:ASP:HA	7:G:143:ARG:HB2	2.02	0.41
1:A:1375:A:P	7:G:28:ASN:HD22	2.43	0.41
13:M:88:ARG:HA	13:M:91:ARG:HB2	2.02	0.41
18:R:58:LEU:HA	18:R:58:LEU:HD23	1.83	0.41
19:S:31:ILE:O	19:S:50:ALA:HB3	2.20	0.41
19:S:5:LEU:O	19:S:6:LYS:NZ	2.43	0.41
21:U:13:ILE:HG13	21:U:14:TRP:N	2.35	0.41
1:A:1177:G:H8	1:A:1177:G:OP2	2.04	0.41
1:A:1277:C:O2'	1:A:1279:A:H8	2.03	0.41
1:A:342:C:O5'	1:A:342:C:H6	2.03	0.41
1:A:901:A:C5	1:A:902:G:H1'	2.55	0.41
2:B:142:LEU:O	2:B:146:GLN:HB2	2.20	0.41
3:C:112:SER:HB3	3:C:115:LEU:CD1	2.50	0.41
3:C:187:ALA:HB3	3:C:198:VAL:HB	2.02	0.41
3:C:51:GLY:O	3:C:71:ALA:N	2.39	0.41
4:D:150:GLU:N	4:D:150:GLU:CD	2.74	0.41
4:D:163:GLU:HG3	4:D:166:LYS:CE	2.50	0.41
5:E:57:LYS:O	5:E:61:TYR:HD2	2.03	0.41
7:G:76:ARG:O	7:G:87:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:GLU:HB3	9:I:101:PHE:CZ	2.54	0.41
11:K:40:ILE:HG23	11:K:75:TYR:CD1	2.55	0.41
12:L:65:GLU:OE1	12:L:65:GLU:N	2.53	0.41
13:M:27:LYS:HD3	13:M:27:LYS:HA	1.94	0.41
17:Q:83:ASP:O	17:Q:86:GLU:HB2	2.20	0.41
1:A:1097:C:H2'	1:A:1098:C:C6	2.55	0.41
1:A:120:A:H2'	1:A:122:G:N7	2.35	0.41
1:A:130:A:H1'	1:A:263:A:O2'	2.19	0.41
1:A:567:G:H2'	1:A:568:G:O4'	2.20	0.41
1:A:674:G:H5'	6:F:50:TYR:CE2	2.55	0.41
1:A:686:U:O2'	1:A:687:A:H8	2.03	0.41
1:A:77:G:H1	1:A:92:C:H42	1.69	0.41
1:A:78:G:C2	1:A:79:G:H1'	2.56	0.41
1:A:892:A:C2	1:A:907:A:C4	3.08	0.41
2:B:53:ARG:HB2	2:B:53:ARG:HE	1.73	0.41
2:B:85:ALA:HB3	2:B:92:TYR:HB3	2.01	0.41
3:C:110:ASN:O	3:C:141:VAL:HG22	2.20	0.41
7:G:145:ALA:O	7:G:146:GLU:HB2	2.19	0.41
7:G:17:VAL:HG12	7:G:18:TYR:N	2.34	0.41
11:K:43:SER:OG	11:K:44:SER:N	2.53	0.41
19:S:63:THR:OG1	19:S:65:ASN:OD1	2.37	0.41
1:A:664:G:OP1	18:R:64:ARG:NH1	2.43	0.41
1:A:79:G:N1	1:A:80:G:C5	2.87	0.41
3:C:179:ARG:NE	3:C:206:GLU:OE1	2.53	0.41
3:C:43:LEU:HA	3:C:47:LEU:HD13	2.03	0.41
4:D:25:ARG:O	4:D:25:ARG:HG2	2.20	0.41
6:F:80:ARG:CD	6:F:88:VAL:HB	2.51	0.41
1:A:1346:A:C5	7:G:10:ARG:CZ	3.03	0.41
7:G:12:LEU:HD23	7:G:12:LEU:HA	1.90	0.41
7:G:97:GLN:HE21	7:G:97:GLN:HA	1.84	0.41
9:I:11:LYS:O	9:I:12:GLU:HB3	2.20	0.41
10:J:38:ILE:HD11	10:J:71:LEU:CB	2.47	0.41
10:J:40:LEU:HB2	10:J:69:ASN:O	2.20	0.41
16:P:17:TYR:HD1	16:P:39:TYR:HD2	1.67	0.41
20:T:44:ALA:O	20:T:47:GLY:N	2.46	0.41
1:A:1130:A:P	1:A:1130:A:H3'	2.61	0.41
1:A:216:G:H2'	1:A:217:C:H6	1.84	0.41
1:A:356:A:O2'	1:A:367:U:O2'	2.37	0.41
1:A:407:G:C6	1:A:408:A:C6	3.09	0.41
1:A:600:C:H42	1:A:638:G:H1	1.67	0.41
1:A:632:A:H2'	1:A:633:G:H5'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:C:O2'	1:A:798:G:H5'	2.20	0.41
1:A:893:C:H2'	1:A:894:G:H8	1.86	0.41
4:D:145:GLU:OE1	4:D:182:LYS:HG2	2.20	0.41
8:H:108:GLY:HA3	8:H:138:TRP:HB3	2.02	0.41
11:K:11:LYS:HE2	11:K:11:LYS:HB2	1.64	0.41
13:M:47:ASP:OD2	13:M:47:ASP:N	2.53	0.41
1:A:1124:G:N7	1:A:1145:C:H6	2.18	0.41
1:A:1175:G:H2'	1:A:1176:A:H8	1.81	0.41
1:A:1261:A:H5''	1:A:1262:C:OP2	2.21	0.41
1:A:945:G:C2	1:A:1337:G:C2	3.09	0.41
1:A:137:C:O4'	16:P:63:GLY:HA3	2.20	0.41
1:A:1530:G:H4'	1:A:1530:G:OP1	2.20	0.41
1:A:277:C:OP1	17:Q:68:ARG:NH2	2.54	0.41
1:A:7:G:H5'	1:A:298:A:O4'	2.20	0.41
1:A:60:A:P	1:A:331:G:H22	2.43	0.41
1:A:900:A:H2'	1:A:901:A:O4'	2.21	0.41
1:A:945:G:H2'	1:A:945:G:N3	2.35	0.41
3:C:178:LEU:HA	3:C:178:LEU:HD23	1.84	0.41
3:C:6:HIS:CD2	3:C:8:ILE:H	2.37	0.41
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.41	0.41
4:D:3:ARG:HH12	4:D:70:ILE:HG13	1.86	0.41
5:E:32:VAL:HB	5:E:58:ALA:HB1	2.02	0.41
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.39	0.41
10:J:68:HIS:CD2	10:J:68:HIS:N	2.88	0.41
10:J:8:LEU:HD11	10:J:72:VAL:HG23	2.02	0.41
12:L:100:ILE:HD12	12:L:100:ILE:HA	1.92	0.41
15:O:22:THR:OG1	15:O:23:GLY:N	2.53	0.41
17:Q:45:HIS:H	17:Q:72:ARG:HA	1.86	0.41
1:A:278:G:C6	17:Q:95:TYR:CD2	3.09	0.41
1:A:1148:U:H2'	1:A:1149:C:O4'	2.21	0.41
1:A:1299:A:H2'	1:A:1299:A:N3	2.35	0.41
1:A:1417:G:H8	1:A:1417:G:OP2	2.04	0.41
1:A:1502:A:H2'	1:A:1504:G:N7	2.35	0.41
1:A:602:A:C2	1:A:603:U:C2	3.08	0.41
1:A:833:U:H2'	1:A:834:C:H6	1.79	0.41
1:A:92:C:O2	1:A:93:G:C8	2.74	0.41
1:A:997:U:H3	1:A:1044:A:H2	1.67	0.41
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.76	0.41
9:I:112:LYS:HG2	9:I:113:LYS:N	2.35	0.41
11:K:40:ILE:HA	11:K:40:ILE:HD12	1.78	0.41
13:M:15:VAL:HG21	13:M:48:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:65:LYS:C	13:M:66:LEU:HD23	2.40	0.41
14:N:14:PRO:O	14:N:15:LYS:HB3	2.21	0.41
15:O:18:PHE:CE1	15:O:21:ASP:HB2	2.56	0.41
15:O:36:ILE:HA	15:O:59:MET:CE	2.50	0.41
15:O:30:ALA:HA	15:O:85:LEU:HD11	2.01	0.41
17:Q:47:PRO:HD2	17:Q:48:GLU:H	1.85	0.41
18:R:40:LEU:HD23	18:R:40:LEU:HA	1.57	0.41
1:A:1054:C:OP1	1:A:1197:G:OP1	2.39	0.41
1:A:1110:A:H8	1:A:1110:A:O5'	2.04	0.41
1:A:1297:C:HO2'	1:A:1298:C:P	2.43	0.41
1:A:1422:G:C2	1:A:1423:G:N7	2.88	0.41
1:A:340:U:H2'	1:A:341:C:C6	2.56	0.41
1:A:456:C:N3	1:A:477:G:C2	2.88	0.41
1:A:632:A:C2'	1:A:633:G:H5'	2.50	0.41
1:A:784:C:C2	1:A:799:G:N2	2.89	0.41
1:A:925:G:O4'	1:A:1502:A:C5	2.74	0.41
1:A:1111:A:N1	3:C:177:THR:HB	2.35	0.41
4:D:17:VAL:HG11	4:D:63:LYS:HE2	2.02	0.41
4:D:18:LYS:HG3	4:D:33:MET:HG3	2.03	0.41
8:H:102:ARG:HH11	8:H:105:ARG:HD3	1.86	0.41
10:J:85:LEU:HD13	10:J:85:LEU:HA	1.73	0.41
18:R:22:VAL:O	18:R:25:THR:N	2.50	0.41
1:A:1019:C:H2'	1:A:1020:U:C6	2.56	0.41
1:A:1340:A:H2'	1:A:1341:U:O4'	2.21	0.41
1:A:1369:C:H2'	1:A:1370:G:O4'	2.21	0.41
1:A:204:U:H5'	1:A:216:G:C4	2.55	0.41
1:A:251:G:H4'	1:A:252:U:O5'	2.21	0.41
1:A:74:C:H2'	1:A:75:G:O4'	2.20	0.41
1:A:77:G:O2'	1:A:78:G:H5'	2.20	0.41
1:A:803:G:C6	1:A:804:U:C4	3.09	0.41
1:A:942:G:N2	1:A:943:U:C2	2.89	0.41
2:B:180:LEU:HB2	2:B:182:ILE:HG13	2.03	0.41
4:D:121:VAL:HG11	4:D:136:PRO:HA	2.01	0.41
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.51	0.41
11:K:68:ALA:O	11:K:71:LYS:HB2	2.21	0.41
12:L:57:LYS:HD3	12:L:67:THR:HG23	2.02	0.41
19:S:80:TYR:CG	19:S:81:ARG:N	2.89	0.41
1:A:1128:C:O2	1:A:1143:G:N2	2.47	0.41
1:A:1292:U:H2'	1:A:1293:G:C8	2.55	0.41
1:A:474:G:H4'	16:P:81:ARG:NH2	2.36	0.41
1:A:539:A:H2'	1:A:540:G:H8	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:G:C6	1:A:645:C:C5	3.08	0.41
1:A:687:A:H4'	1:A:688:G:O5'	2.21	0.41
1:A:851:G:H5''	1:A:851:G:C8	2.56	0.41
2:B:191:ASP:OD1	2:B:192:SER:N	2.53	0.41
2:B:240:GLN:OE1	2:B:240:GLN:N	2.53	0.41
3:C:179:ARG:O	3:C:181:ASN:N	2.54	0.41
5:E:80:ILE:HG21	5:E:80:ILE:HD13	1.65	0.41
13:M:46:LYS:HE2	13:M:47:ASP:OD2	2.21	0.41
15:O:12:ILE:CG1	15:O:31:LEU:HD11	2.51	0.41
1:A:1149:C:O2'	1:A:1280:A:N1	2.50	0.41
1:A:1320:C:N3	19:S:36:ARG:HD3	2.35	0.41
1:A:132:C:H2'	1:A:133:U:H6	1.85	0.41
1:A:1372:U:H2'	1:A:1373:G:O4'	2.20	0.41
1:A:37:U:H2'	1:A:38:G:O4'	2.20	0.41
1:A:456:C:H2'	1:A:457:C:C6	2.57	0.41
1:A:730:G:N2	1:A:765:G:H5''	2.36	0.41
3:C:5:ILE:HD13	3:C:10:PHE:HB2	2.03	0.41
3:C:61:ALA:C	3:C:63:ASN:H	2.24	0.41
4:D:14:ARG:HD3	4:D:14:ARG:HA	1.97	0.41
5:E:90:VAL:O	5:E:120:THR:HA	2.21	0.41
6:F:11:ASN:HB2	6:F:86:ARG:NE	2.36	0.41
9:I:103:THR:HG22	9:I:104:ARG:O	2.21	0.41
1:A:1367:C:H3'	9:I:112:LYS:HZ2	1.86	0.41
12:L:28:LYS:C	12:L:30:ALA:H	2.24	0.41
15:O:60:VAL:HG12	15:O:61:GLY:N	2.36	0.41
1:A:238:G:OP1	17:Q:25:ARG:NH2	2.54	0.41
1:A:1281:U:H6	1:A:1281:U:H2'	1.67	0.40
1:A:1417:G:C8	1:A:1417:G:OP2	2.74	0.40
1:A:391:G:C6	1:A:392:G:N7	2.89	0.40
1:A:524:G:H2'	1:A:525:C:C6	2.56	0.40
1:A:886:G:H1	1:A:911:U:H3	1.69	0.40
3:C:16:ARG:NH1	3:C:183:ASP:OD2	2.54	0.40
1:A:619:U:N3	4:D:135:LEU:HD21	2.36	0.40
4:D:65:ARG:NH1	4:D:72:GLU:HB2	2.36	0.40
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.61	0.40
7:G:99:LEU:HA	7:G:99:LEU:HD23	1.48	0.40
11:K:24:SER:OG	11:K:26:ASN:N	2.54	0.40
12:L:46:LYS:HG2	12:L:94:TRP:CZ2	2.56	0.40
13:M:22:ILE:HB	13:M:25:ILE:HB	2.02	0.40
13:M:44:ARG:HB3	13:M:46:LYS:HD3	2.03	0.40
13:M:64:TRP:HE3	13:M:66:LEU:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:46:GLU:O	14:N:49:HIS:HB2	2.21	0.40
17:Q:72:ARG:HG2	17:Q:72:ARG:H	1.70	0.40
18:R:52:PRO:HB2	18:R:54:ARG:HG3	2.03	0.40
1:A:1061:G:C6	1:A:1062:U:N3	2.89	0.40
1:A:1250:A:C5	1:A:1251:A:C6	3.09	0.40
1:A:1368:G:H2'	1:A:1369:C:H5'	2.03	0.40
1:A:1505:G:H4'	1:A:1506:U:H5''	2.02	0.40
1:A:22:G:H2'	1:A:23:C:H6	1.86	0.40
1:A:629:G:H2'	1:A:630:G:H8	1.85	0.40
1:A:78:G:N2	1:A:79:G:H1'	2.36	0.40
1:A:853:G:C4	1:A:854:G:C8	3.09	0.40
1:A:880:C:O5'	1:A:880:C:H6	2.04	0.40
1:A:951:G:C5	1:A:952:U:C5	3.09	0.40
3:C:202:ILE:CG2	3:C:204:LEU:HD23	2.51	0.40
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.50	0.40
8:H:73:ASP:N	8:H:74:PRO:HD3	2.37	0.40
9:I:32:ASP:CG	9:I:33:PHE:H	2.24	0.40
10:J:7:LYS:HE2	10:J:9:ARG:HE	1.86	0.40
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.77	0.40
17:Q:63:ARG:HA	17:Q:64:PRO:HD3	1.82	0.40
18:R:70:ILE:HG22	18:R:71:LYS:N	2.35	0.40
20:T:53:LEU:HA	20:T:53:LEU:HD22	1.78	0.40
20:T:84:LEU:HA	20:T:87:LYS:NZ	2.36	0.40
1:A:1290:G:H2'	1:A:1291:G:H8	1.79	0.40
3:C:5:ILE:CD1	3:C:10:PHE:HB2	2.50	0.40
3:C:150:LYS:HG3	3:C:173:VAL:HG21	2.04	0.40
3:C:34:LEU:HD22	3:C:38:ARG:HH22	1.87	0.40
4:D:191:ARG:HD2	4:D:191:ARG:HA	1.79	0.40
7:G:36:LYS:HZ3	7:G:36:LYS:HG3	1.46	0.40
8:H:4:ASP:C	8:H:4:ASP:OD1	2.59	0.40
9:I:79:LEU:HD13	9:I:83:ARG:HD2	2.03	0.40
13:M:81:LEU:HA	13:M:81:LEU:HD23	1.92	0.40
15:O:74:ASP:HA	15:O:75:PRO:HD2	1.83	0.40
1:A:1071:C:O2'	1:A:1072:G:H5'	2.21	0.40
1:A:1473:A:H2'	1:A:1474:G:C8	2.56	0.40
1:A:200:G:C5	1:A:201:C:C5	3.09	0.40
1:A:316:G:OP2	1:A:351:G:O2'	2.40	0.40
1:A:627:G:O2'	1:A:628:G:H5'	2.21	0.40
1:A:794:A:H2'	1:A:795:C:C6	2.56	0.40
2:B:19:HIS:HE1	2:B:206:ASP:H	1.68	0.40
3:C:130:VAL:HG23	3:C:131:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:ARG:HD2	4:D:118:ARG:HH21	1.74	0.40
4:D:71:SER:HB3	4:D:74:GLN:HG3	2.03	0.40
5:E:137:GLU:O	5:E:137:GLU:HG3	2.21	0.40
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.57	0.40
9:I:125:TYR:CG	9:I:125:TYR:O	2.74	0.40
11:K:115:PRO:C	11:K:117:ASN:H	2.23	0.40
16:P:74:LEU:HA	16:P:74:LEU:HD23	1.70	0.40
1:A:363:A:OP1	12:L:61:THR:OG1	2.31	0.40
1:A:841:U:H5'	1:A:848:C:O4'	2.21	0.40
2:B:119:GLU:HG2	2:B:119:GLU:H	1.67	0.40
2:B:155:LEU:HA	2:B:155:LEU:HD23	1.87	0.40
3:C:150:LYS:HA	3:C:169:ALA:HB1	1.99	0.40
4:D:105:VAL:HG13	4:D:110:PHE:HD2	1.85	0.40
4:D:10:ARG:HG2	4:D:11:LEU:HD23	2.04	0.40
4:D:15:GLU:CD	4:D:59:ARG:HH21	2.25	0.40
6:F:45:LEU:HD22	6:F:46:ARG:N	2.36	0.40
9:I:19:LEU:HD21	9:I:59:PHE:CG	2.56	0.40
12:L:102:ARG:HE	12:L:102:ARG:HB3	1.56	0.40
13:M:65:LYS:H	13:M:65:LYS:HG2	1.52	0.40
16:P:51:VAL:HG12	16:P:52:ASP:C	2.42	0.40
17:Q:48:GLU:HG3	17:Q:50:LYS:HB2	2.02	0.40
19:S:30:LEU:HB3	19:S:31:ILE:H	1.65	0.40
20:T:30:LYS:O	20:T:34:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	211 (91%)	18 (8%)	3 (1%)	12	48
3	C	204/239 (85%)	170 (83%)	32 (16%)	2 (1%)	15	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
5	E	148/162 (91%)	135 (91%)	12 (8%)	1 (1%)	22	61
6	F	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
7	G	153/156 (98%)	138 (90%)	15 (10%)	0	100	100
8	H	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	I	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	58
10	J	96/105 (91%)	79 (82%)	16 (17%)	1 (1%)	15	54
11	K	114/129 (88%)	100 (88%)	14 (12%)	0	100	100
12	L	122/135 (90%)	109 (89%)	12 (10%)	1 (1%)	19	58
13	M	116/126 (92%)	104 (90%)	9 (8%)	3 (3%)	5	34
14	N	58/61 (95%)	47 (81%)	11 (19%)	0	100	100
15	O	85/89 (96%)	71 (84%)	14 (16%)	0	100	100
16	P	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	13	50
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	R	68/88 (77%)	58 (85%)	10 (15%)	0	100	100
19	S	78/93 (84%)	68 (87%)	8 (10%)	2 (3%)	5	34
20	T	97/106 (92%)	88 (91%)	7 (7%)	2 (2%)	7	39
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2337/2541 (92%)	2077 (89%)	243 (10%)	17 (1%)	22	61

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
9	I	119	ALA
12	L	28	LYS
3	C	180	ALA
19	S	31	ILE
20	T	73	HIS
2	B	95	GLN
13	M	23	TYR
19	S	13	ASP
3	C	62	ASP
5	E	70	PRO
20	T	99	LEU
10	J	34	VAL

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Mol	Chain	Res	Type
13	M	84	ILE
2	B	229	VAL
13	M	7	VAL
16	P	53	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	148 (73%)	54 (27%)	0	3
3	C	160/188 (85%)	113 (71%)	47 (29%)	0	2
4	D	180/181 (99%)	139 (77%)	41 (23%)	1	5
5	E	115/123 (94%)	80 (70%)	35 (30%)	0	2
6	F	90/90 (100%)	68 (76%)	22 (24%)	0	4
7	G	126/127 (99%)	104 (82%)	22 (18%)	2	12
8	H	119/119 (100%)	95 (80%)	24 (20%)	1	8
9	I	98/99 (99%)	77 (79%)	21 (21%)	1	6
10	J	87/92 (95%)	65 (75%)	22 (25%)	0	4
11	K	88/99 (89%)	72 (82%)	16 (18%)	1	10
12	L	104/111 (94%)	74 (71%)	30 (29%)	0	2
13	M	94/101 (93%)	71 (76%)	23 (24%)	0	4
14	N	49/50 (98%)	42 (86%)	7 (14%)	3	21
15	O	79/80 (99%)	62 (78%)	17 (22%)	1	6
16	P	72/74 (97%)	57 (79%)	15 (21%)	1	7
17	Q	94/97 (97%)	74 (79%)	20 (21%)	1	7
18	R	61/77 (79%)	46 (75%)	15 (25%)	0	4
19	S	71/80 (89%)	57 (80%)	14 (20%)	1	8
20	T	76/82 (93%)	59 (78%)	17 (22%)	1	6
21	U	19/22 (86%)	14 (74%)	5 (26%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1984/2112 (94%)	1517 (76%)	467 (24%)	1 5

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

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	9	GLU
2	B	10	LEU
2	B	12	GLU
2	B	17	PHE
2	B	21	ARG
2	B	23	ARG
2	B	44	LEU
2	B	47	THR
2	B	51	LEU
2	B	53	ARG
2	B	63	MET
2	B	69	LEU
2	B	75	LYS
2	B	87	ARG
2	B	98	LEU
2	B	101	MET
2	B	107	THR
2	B	108	ILE
2	B	111	ARG
2	B	114	ARG
2	B	115	LEU
2	B	119	GLU
2	B	121	LEU
2	B	126	GLU
2	B	127	ILE
2	B	128	GLU
2	B	133	LYS
2	B	144	ARG
2	B	146	GLN
2	B	147	LYS
2	B	157	ARG
2	B	163	PHE
2	B	164	VAL
2	B	165	VAL
2	B	170	GLU

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Mol	Chain	Res	Type
2	B	172	ILE
2	B	175	ARG
2	B	178	ARG
2	B	187	LEU
2	B	190	THR
2	B	196	LEU
2	B	200	ILE
2	B	204	ASN
2	B	205	ASP
2	B	206	ASP
2	B	208	ILE
2	B	212	GLN
2	B	213	LEU
2	B	221	LEU
2	B	231	GLU
2	B	238	LEU
2	B	239	VAL
3	C	10	PHE
3	C	11	ARG
3	C	12	LEU
3	C	14	ILE
3	C	16	ARG
3	C	17	ASP
3	C	18	TRP
3	C	20	SER
3	C	21	ARG
3	C	26	LYS
3	C	29	TYR
3	C	33	LEU
3	C	37	GLN
3	C	38	ARG
3	C	42	LEU
3	C	45	LYS
3	C	54	ARG
3	C	58	GLU
3	C	62	ASP
3	C	68	VAL
3	C	70	VAL
3	C	75	VAL
3	C	76	VAL
3	C	91	LEU
3	C	94	LEU

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Mol	Chain	Res	Type
3	C	95	THR
3	C	98	ASN
3	C	103	VAL
3	C	104	GLN
3	C	107	GLN
3	C	111	LEU
3	C	116	VAL
3	C	130	VAL
3	C	131	ARG
3	C	139	GLN
3	C	152	ILE
3	C	154	SER
3	C	166	GLU
3	C	167	TRP
3	C	172	ARG
3	C	190	ARG
3	C	191	THR
3	C	192	THR
3	C	193	TYR
3	C	195	VAL
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	8	VAL
4	D	9	CYS
4	D	10	ARG
4	D	19	LEU
4	D	25	ARG
4	D	26	CYS
4	D	30	LYS
4	D	34	GLU
4	D	35	ARG
4	D	47	ARG
4	D	50	ARG
4	D	58	LEU
4	D	59	ARG
4	D	61	LYS
4	D	89	THR
4	D	108	LEU
4	D	112	VAL
4	D	118	ARG
4	D	122	ARG

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Mol	Chain	Res	Type
4	D	127	THR
4	D	131	ARG
4	D	132	ARG
4	D	134	ASP
4	D	135	LEU
4	D	141	ARG
4	D	142	PRO
4	D	145	GLU
4	D	148	VAL
4	D	152	SER
4	D	155	LEU
4	D	159	ARG
4	D	162	LEU
4	D	174	LEU
4	D	181	MET
4	D	186	LEU
4	D	187	ARG
4	D	192	GLU
4	D	194	LEU
4	D	202	LEU
4	D	203	VAL
5	E	6	PHE
5	E	12	LEU
5	E	14	ARG
5	E	18	ARG
5	E	19	MET
5	E	25	ARG
5	E	26	PHE
5	E	31	LEU
5	E	32	VAL
5	E	38	GLN
5	E	41	VAL
5	E	43	LEU
5	E	45	PHE
5	E	47	LYS
5	E	53	LEU
5	E	55	VAL
5	E	60	TYR
5	E	64	ARG
5	E	68	GLU
5	E	71	LEU
5	E	75	THR

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Mol	Chain	Res	Type
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	116	THR
5	E	118	ILE
5	E	120	THR
5	E	123	LEU
5	E	125	SER
5	E	131	ILE
5	E	151	LEU
5	E	152	ARG
6	F	7	ASN
6	F	9	VAL
6	F	10	LEU
6	F	14	LEU
6	F	15	ASP
6	F	19	LEU
6	F	21	LEU
6	F	24	GLU
6	F	25	ILE
6	F	30	LEU
6	F	32	ASN
6	F	37	VAL
6	F	40	VAL
6	F	43	LEU
6	F	61	LEU
6	F	69	GLU
6	F	70	ASP
6	F	80	ARG
6	F	83	ASP
6	F	86	ARG
6	F	91	VAL
6	F	92	LYS
7	G	5	ARG
7	G	6	ARG
7	G	21	VAL
7	G	41	ARG
7	G	45	ASP
7	G	50	ILE

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Mol	Chain	Res	Type
7	G	62	PHE
7	G	64	GLN
7	G	67	GLU
7	G	74	GLU
7	G	75	VAL
7	G	84	ASN
7	G	87	VAL
7	G	97	GLN
7	G	98	SER
7	G	113	GLU
7	G	122	HIS
7	G	124	LEU
7	G	126	ASP
7	G	129	GLU
7	G	136	LYS
7	G	155	ARG
8	H	2	LEU
8	H	5	PRO
8	H	11	THR
8	H	14	ARG
8	H	18	ARG
8	H	19	VAL
8	H	21	LYS
8	H	23	SER
8	H	56	LYS
8	H	63	LEU
8	H	83	ILE
8	H	85	ARG
8	H	86	ILE
8	H	91	ARG
8	H	92	ARG
8	H	95	VAL
8	H	98	LYS
8	H	102	ARG
8	H	104	ARG
8	H	109	ILE
8	H	113	SER
8	H	119	LEU
8	H	121	ASP
8	H	127	LEU
9	I	5	TYR
9	I	12	GLU

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Mol	Chain	Res	Type
9	I	16	ARG
9	I	26	VAL
9	I	29	ASN
9	I	51	ARG
9	I	53	VAL
9	I	54	ASP
9	I	62	TYR
9	I	64	THR
9	I	79	LEU
9	I	86	VAL
9	I	87	GLN
9	I	91	ASP
9	I	95	LYS
9	I	96	LEU
9	I	102	LEU
9	I	111	ARG
9	I	118	LYS
9	I	121	ARG
9	I	126	SER
10	J	5	ARG
10	J	9	ARG
10	J	16	LEU
10	J	44	VAL
10	J	48	THR
10	J	49	VAL
10	J	55	LYS
10	J	62	HIS
10	J	67	THR
10	J	68	HIS
10	J	69	ASN
10	J	71	LEU
10	J	73	ASP
10	J	74	ILE
10	J	78	ASN
10	J	79	ARG
10	J	80	LYS
10	J	82	ILE
10	J	87	THR
10	J	90	LEU
10	J	94	VAL
10	J	95	GLU
11	K	11	LYS

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Mol	Chain	Res	Type
11	K	12	ARG
11	K	13	GLN
11	K	24	SER
11	K	29	ILE
11	K	40	ILE
11	K	41	THR
11	K	63	LEU
11	K	75	TYR
11	K	77	MET
11	K	81	ASP
11	K	91	ARG
11	K	99	GLN
11	K	114	VAL
11	K	117	ASN
11	K	126	ARG
12	L	6	THR
12	L	7	ILE
12	L	10	LEU
12	L	18	VAL
12	L	20	LYS
12	L	33	ARG
12	L	41	ARG
12	L	42	THR
12	L	43	VAL
12	L	44	THR
12	L	54	LYS
12	L	55	VAL
12	L	59	ARG
12	L	61	THR
12	L	62	SER
12	L	64	TYR
12	L	66	VAL
12	L	67	THR
12	L	75	HIS
12	L	79	GLU
12	L	82	VAL
12	L	90	VAL
12	L	96	VAL
12	L	97	ARG
12	L	100	ILE
12	L	111	LYS
12	L	113	ARG

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Mol	Chain	Res	Type
12	L	116	SER
12	L	122	THR
12	L	126	LYS
13	M	12	ASN
13	M	14	ARG
13	M	27	LYS
13	M	34	LEU
13	M	35	GLU
13	M	46	LYS
13	M	48	LEU
13	M	50	GLU
13	M	56	LEU
13	M	57	ARG
13	M	59	TYR
13	M	64	TRP
13	M	66	LEU
13	M	69	GLU
13	M	70	LEU
13	M	71	ARG
13	M	73	GLU
13	M	80	ARG
13	M	105	THR
13	M	108	ARG
13	M	109	THR
13	M	110	ARG
13	M	115	LYS
14	N	22	THR
14	N	24	CYS
14	N	25	VAL
14	N	26	ARG
14	N	46	GLU
14	N	53	LEU
14	N	57	ARG
15	O	5	LYS
15	O	22	THR
15	O	28	GLN
15	O	29	VAL
15	O	34	LEU
15	O	39	LEU
15	O	45	VAL
15	O	47	LYS
15	O	54	ARG

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Mol	Chain	Res	Type
15	O	56	LEU
15	O	57	LEU
15	O	60	VAL
15	O	64	ARG
15	O	65	ARG
15	O	70	LEU
15	O	76	GLU
15	O	83	GLU
16	P	2	VAL
16	P	25	ARG
16	P	32	TYR
16	P	33	ILE
16	P	42	ARG
16	P	44	THR
16	P	45	THR
16	P	47	ASP
16	P	53	VAL
16	P	54	GLU
16	P	55	ARG
16	P	62	VAL
16	P	68	ASP
16	P	75	ARG
16	P	76	GLN
17	Q	3	LYS
17	Q	23	VAL
17	Q	25	ARG
17	Q	35	VAL
17	Q	36	ILE
17	Q	40	LYS
17	Q	43	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	68	ARG
17	Q	72	ARG
17	Q	74	LEU
17	Q	75	ARG
17	Q	76	LEU
17	Q	77	VAL
17	Q	90	ILE
17	Q	93	GLN
17	Q	98	LEU
17	Q	99	SER

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Mol	Chain	Res	Type
17	Q	100	LYS
18	R	19	LYS
18	R	26	LEU
18	R	46	GLU
18	R	47	THR
18	R	50	ILE
18	R	54	ARG
18	R	55	ARG
18	R	56	THR
18	R	64	ARG
18	R	68	LYS
18	R	69	THR
18	R	70	ILE
18	R	86	VAL
18	R	87	ARG
18	R	88	LYS
19	S	6	LYS
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	36	ARG
19	S	39	THR
19	S	43	GLU
19	S	58	VAL
19	S	64	GLU
19	S	71	LEU
19	S	77	THR
19	S	78	ARG
19	S	79	THR
19	S	81	ARG
20	T	13	LEU
20	T	20	LEU
20	T	24	LEU
20	T	30	LYS
20	T	36	LEU
20	T	43	LEU
20	T	46	GLU
20	T	53	LEU
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	71	THR

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Mol	Chain	Res	Type
20	T	74	LYS
20	T	75	ASN
20	T	80	ARG
20	T	91	LEU
20	T	92	LEU
21	U	6	ARG
21	U	10	ARG
21	U	14	TRP
21	U	22	ARG
21	U	25	LYS

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

Mol	Chain	Res	Type
3	C	6	HIS
4	D	62	GLN
4	D	119	GLN
5	E	65	ASN
7	G	148	ASN
9	I	73	GLN
9	I	124	GLN
11	K	116	HIS
12	L	49	ASN
15	O	28	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	377 (25%)	59 (3%)

All (377) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C

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Mol	Chain	Res	Type
1	A	48	C
1	A	51	A
1	A	54	C
1	A	67	C
1	A	74	C
1	A	80	G
1	A	81	U
1	A	82	U
1	A	92	C
1	A	93	G
1	A	98	U
1	A	108	G
1	A	109	A
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	145	G
1	A	151	A
1	A	159	G
1	A	160	A
1	A	163	C
1	A	182	U
1	A	183	G
1	A	188	C
1	A	190(D)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	226	G
1	A	231	G
1	A	243	A
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G

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Mol	Chain	Res	Type
1	A	267	C
1	A	289	G
1	A	299	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	347	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	369	C
1	A	373	A
1	A	374	A
1	A	382	A
1	A	384	G
1	A	387	U
1	A	388	G
1	A	390	C
1	A	391	G
1	A	392	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	419	C
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	452	A
1	A	453	A
1	A	460	A
1	A	461	C

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Mol	Chain	Res	Type
1	A	475	G
1	A	476	G
1	A	478	A
1	A	479	C
1	A	481	G
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	499	A
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	521	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	538	G
1	A	547	A
1	A	549	C
1	A	558	G
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	588	G
1	A	596	C
1	A	620	C
1	A	624	C
1	A	644	G
1	A	645	C

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Mol	Chain	Res	Type
1	A	646	U
1	A	653	A
1	A	665	A
1	A	670	G
1	A	671	G
1	A	686	U
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	721	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	728	A
1	A	731	G
1	A	733	A
1	A	734	G
1	A	737	A
1	A	741	G
1	A	749	C
1	A	752	G
1	A	755	G
1	A	777	A
1	A	780	A
1	A	781	A
1	A	782	A
1	A	783	C
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	812	C
1	A	813	U
1	A	814	A
1	A	817	C
1	A	818	G
1	A	826	C
1	A	827	U
1	A	828	A

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Mol	Chain	Res	Type
1	A	829	G
1	A	838	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	870	U
1	A	872	A
1	A	873	A
1	A	888	G
1	A	889	A
1	A	902	G
1	A	914	A
1	A	916	G
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	937	A
1	A	940	C
1	A	941	G
1	A	950	U
1	A	956	U
1	A	961	U
1	A	962	C
1	A	964	A
1	A	966	M2G
1	A	967	5MC
1	A	968	A
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	978	A
1	A	984	C
1	A	985	C

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Mol	Chain	Res	Type
1	A	986	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1011	G
1	A	1012	U
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1028	C
1	A	1030(B)	C
1	A	1030(C)	G
1	A	1031	G
1	A	1042	G
1	A	1043	C
1	A	1045	C
1	A	1046	A
1	A	1048	G
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1060	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1103	C
1	A	1104	G
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	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1142	G
1	A	1146	A
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1164	G
1	A	1171	G
1	A	1177	G
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1216	G
1	A	1222	G
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1241	G
1	A	1243	C
1	A	1244	C
1	A	1252	A

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Mol	Chain	Res	Type
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1261	A
1	A	1270	C
1	A	1278	U
1	A	1280	A
1	A	1287	A
1	A	1288	A
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1306	A
1	A	1310	G
1	A	1317	C
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1336	C
1	A	1339	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1360	A
1	A	1363	A
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1390	U
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1406	U
1	A	1411	C

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Mol	Chain	Res	Type
1	A	1414	U
1	A	1417	G
1	A	1418	A
1	A	1421	G
1	A	1424	C
1	A	1437	C
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1453	G
1	A	1473	A
1	A	1474	G
1	A	1475	G
1	A	1477	C
1	A	1480	G
1	A	1485	U
1	A	1486	G
1	A	1487	G
1	A	1490	C
1	A	1492	A
1	A	1493	A
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1533	C

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	91	C
1	A	115	G
1	A	129(A)	G

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Mol	Chain	Res	Type
1	A	181	G
1	A	243	A
1	A	250	A
1	A	251	G
1	A	350	G
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	509	A
1	A	510	A
1	A	518	C
1	A	532	A
1	A	559	A
1	A	575	G
1	A	587	G
1	A	686	U
1	A	687	A
1	A	701	C
1	A	733	A
1	A	748	C
1	A	792	A
1	A	812	C
1	A	828	A
1	A	840	C
1	A	870	U
1	A	913	A
1	A	960	U
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1139	G
1	A	1145	C
1	A	1181	G
1	A	1182	G
1	A	1190	G
1	A	1201	A

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Mol	Chain	Res	Type
1	A	1225	A
1	A	1256	A
1	A	1257	U
1	A	1279	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1335	C
1	A	1347	G
1	A	1380	U
1	A	1496	C
1	A	1504	G
1	A	1505	G

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

16 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	MA6	A	1519[B]	1	19,26,27	1.31	4 (21%)	18,38,41	0.55	0
1	4OC	A	1402	1	16,23,24	1.01	0	17,32,35	0.93	1 (5%)
1	5MC	A	1404	1	15,22,23	1.79	2 (13%)	19,32,35	1.43	3 (15%)
1	PSU	A	516	1	17,21,22	0.99	1 (5%)	20,30,33	2.94	7 (35%)
1	5MC	A	1400	1	15,22,23	0.88	0	19,32,35	1.52	3 (15%)
1	MA6	A	1519[A]	1	19,26,27	0.86	1 (5%)	18,38,41	0.75	1 (5%)
1	M2G	A	966	1	20,27,28	1.32	2 (10%)	22,40,43	2.28	2 (9%)
1	MA6	A	1518[B]	1	19,26,27	1.32	3 (15%)	18,38,41	1.12	2 (11%)
1	5MC	A	967	1	15,22,23	0.86	0	19,32,35	1.32	2 (10%)
1	MA6	A	1518[A]	1	19,26,27	1.08	2 (10%)	18,38,41	0.73	0
1	PSU	A	1540	1	17,21,22	1.01	1 (5%)	20,30,33	3.03	5 (25%)
1	UR3	A	1498	1,22	14,22,23	1.35	2 (14%)	15,32,35	1.43	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1407	1	15,22,23	1.54	3 (20%)	19,32,35	1.22	1 (5%)
1	7MG	A	527	1,22	22,26,27	2.17	7 (31%)	28,39,42	1.55	8 (28%)
1	2MG	A	1207	1	19,26,27	2.79	5 (26%)	21,38,41	2.01	3 (14%)
1	PSU	A	1541	1	17,21,22	0.96	2 (11%)	20,30,33	3.12	6 (30%)

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	MA6	A	1519[B]	1	-	3/7/29/30	0/3/3/3
1	4OC	A	1402	1	-	4/9/29/30	0/2/2/2
1	5MC	A	1404	1	-	1/5/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	MA6	A	1519[A]	1	-	5/7/29/30	0/3/3/3
1	M2G	A	966	1	-	6/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	2/7/29/30	0/3/3/3
1	5MC	A	967	1	-	3/5/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	2/7/25/26	0/2/2/2
1	UR3	A	1498	1,22	-	2/5/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	7MG	A	527	1,22	-	2/7/37/38	0/3/3/3
1	2MG	A	1207	1	-	4/5/27/28	0/3/3/3
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	8.85	1.41	1.34
1	A	1207	2MG	C6-N1	6.67	1.44	1.33
1	A	1404	5MC	C5-C4	5.89	1.50	1.41
1	A	527	7MG	C2-N2	4.50	1.42	1.33
1	A	527	7MG	C4-N3	4.48	1.40	1.34
1	A	1407	5MC	C5-C4	4.43	1.48	1.41
1	A	527	7MG	C8-N9	-4.41	1.35	1.45
1	A	966	M2G	C6-N1	4.30	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	C6-N1	-3.52	1.31	1.35
1	A	527	7MG	C5-N7	3.34	1.45	1.39
1	A	1541	PSU	C4-N3	3.21	1.38	1.33
1	A	1540	PSU	C4-N3	3.16	1.38	1.33
1	A	527	7MG	C6-C5	3.00	1.45	1.41
1	A	1518[B]	MA6	C6-N1	2.91	1.37	1.33
1	A	516	PSU	C4-N3	2.81	1.37	1.33
1	A	1519[B]	MA6	C2-N3	2.80	1.36	1.32
1	A	1207	2MG	C4-N3	2.68	1.39	1.35
1	A	1498	UR3	C4-N3	-2.66	1.34	1.38
1	A	1519[B]	MA6	C4-N3	2.59	1.39	1.35
1	A	1519[A]	MA6	C2-N1	2.53	1.38	1.33
1	A	1518[B]	MA6	C4-N3	2.50	1.39	1.35
1	A	1207	2MG	C2-N1	2.48	1.42	1.34
1	A	1519[B]	MA6	C2-N1	2.46	1.38	1.33
1	A	1519[B]	MA6	C6-N1	2.44	1.36	1.33
1	A	1407	5MC	C4-N3	-2.44	1.31	1.35
1	A	1404	5MC	C6-C5	-2.37	1.33	1.40
1	A	1518[A]	MA6	C6-N1	2.34	1.36	1.33
1	A	527	7MG	O6-C6	-2.31	1.18	1.24
1	A	527	7MG	C2-N3	-2.28	1.31	1.35
1	A	1518[B]	MA6	C2-N1	2.24	1.38	1.33
1	A	1207	2MG	CM2-N2	2.15	1.48	1.45
1	A	966	M2G	C4-N3	2.10	1.38	1.35
1	A	1518[A]	MA6	C4-N3	2.10	1.38	1.35
1	A	1541	PSU	O4'-C1'	-2.03	1.41	1.44
1	A	1407	5MC	C6-C5	-2.00	1.34	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	N1-C2-N3	-10.54	120.05	128.43
1	A	1541	PSU	N1-C2-N3	-10.51	120.08	128.43
1	A	516	PSU	N1-C2-N3	-9.57	120.82	128.43
1	A	966	M2G	C5-C6-N1	-8.12	112.33	123.43
1	A	1207	2MG	C5-C6-N1	-7.20	113.58	123.43
1	A	966	M2G	C6-N1-C2	6.04	123.38	116.18
1	A	1541	PSU	C4-N3-C2	5.79	120.03	115.14
1	A	1540	PSU	C4-N3-C2	5.58	119.85	115.14
1	A	516	PSU	C4-N3-C2	5.50	119.78	115.14
1	A	1541	PSU	C5-C4-N3	-4.50	119.56	125.36
1	A	1404	5MC	N4-C4-N3	-4.30	110.95	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	C5-C4-N3	-4.24	119.90	125.36
1	A	1400	5MC	CM5-C5-C4	-4.03	117.64	121.72
1	A	1540	PSU	C5-C4-N3	-4.02	120.19	125.36
1	A	1407	5MC	N4-C4-N3	-3.87	111.57	117.03
1	A	1207	2MG	C6-N1-C2	3.67	121.75	115.18
1	A	516	PSU	C5-C6-N1	-3.51	120.12	124.44
1	A	967	5MC	C2-N3-C4	3.47	120.21	116.02
1	A	527	7MG	C5-C4-N3	-3.44	120.87	126.49
1	A	1400	5MC	CM5-C5-C6	3.21	125.45	118.68
1	A	527	7MG	C4-N9-C1'	-3.16	119.10	126.60
1	A	1541	PSU	C6-N1-C2	3.06	120.40	115.36
1	A	1540	PSU	C6-N1-C2	3.05	120.39	115.36
1	A	1402	4OC	CM4-N4-C4	-2.95	120.43	122.97
1	A	1498	UR3	O3'-C3'-C2'	2.90	121.21	111.82
1	A	1540	PSU	C5-C6-N1	-2.87	120.92	124.44
1	A	527	7MG	N3-C4-N9	2.85	130.58	126.91
1	A	1518[B]	MA6	N1-C6-N6	-2.84	114.06	117.06
1	A	1400	5MC	C2-N3-C4	2.79	119.39	116.02
1	A	516	PSU	C6-N1-C2	2.77	119.94	115.36
1	A	1541	PSU	C5-C6-N1	-2.54	121.31	124.44
1	A	527	7MG	C2-N3-C4	2.53	120.89	113.89
1	A	1207	2MG	C4-C5-N7	2.49	111.99	109.40
1	A	527	7MG	N7-C8-N9	2.42	106.84	103.38
1	A	1498	UR3	C3'-C2'-C1'	2.38	104.56	100.98
1	A	967	5MC	CM5-C5-C6	2.33	123.60	118.68
1	A	1518[B]	MA6	C1'-N9-C4	-2.32	122.56	126.64
1	A	516	PSU	C5-C1'-C2'	-2.30	111.22	115.32
1	A	527	7MG	C6-N1-C2	2.26	119.52	115.93
1	A	1404	5MC	C5-C4-N3	2.25	124.82	121.26
1	A	1541	PSU	O4'-C1'-C5	-2.24	106.46	109.93
1	A	527	7MG	N2-C2-N1	2.22	120.70	117.25
1	A	516	PSU	O4'-C1'-C2'	2.21	108.25	104.66
1	A	527	7MG	N1-C2-N3	-2.11	122.12	125.42
1	A	1404	5MC	CM5-C5-C4	2.05	123.80	121.72
1	A	1519[A]	MA6	N3-C2-N1	2.01	131.83	128.68

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	N1-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1402	4OC	N3-C4-N4-CM4
1	A	1402	4OC	C5-C4-N4-CM4
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	967	5MC	C2'-C1'-N1-C6
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1207	2MG	N1-C2-N2-CM2
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1540	PSU	O4'-C4'-C5'-O5'
1	A	1540	PSU	C3'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1518[B]	MA6	O4'-C4'-C5'-O5'
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C10
1	A	1519[A]	MA6	C5-C6-N6-C10
1	A	966	M2G	N3-C2-N2-CM2
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N1-C2-N2-CM2
1	A	966	M2G	N3-C2-N2-CM1
1	A	1404	5MC	O4'-C4'-C5'-O5'
1	A	1518[B]	MA6	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	N1-C6-N6-C9

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	4	0
1	A	1404	5MC	1	0
1	A	1400	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519[A]	MA6	5	0
1	A	966	M2G	6	0
1	A	967	5MC	7	0
1	A	1518[A]	MA6	5	0
1	A	1540	PSU	1	0
1	A	1498	UR3	5	0
1	A	1407	5MC	2	0
1	A	1207	2MG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 295 ligands modelled in this entry, 295 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.20	28 (1%) 66 52	74, 136, 280, 374	0
2	B	234/256 (91%)	-0.20	2 (0%) 84 73	104, 156, 254, 272	0
3	C	206/239 (86%)	0.01	15 (7%) 15 9	171, 215, 243, 274	0
4	D	208/209 (99%)	-0.23	5 (2%) 59 43	86, 137, 190, 243	0
5	E	150/162 (92%)	-0.36	0 100 100	70, 106, 151, 203	0
6	F	101/101 (100%)	-0.41	1 (0%) 82 71	117, 157, 185, 213	0
7	G	155/156 (99%)	-0.06	3 (1%) 66 52	136, 185, 233, 255	0
8	H	138/138 (100%)	-0.53	0 100 100	71, 98, 135, 168	0
9	I	127/128 (99%)	0.41	15 (11%) 4 3	139, 201, 245, 269	0
10	J	98/105 (93%)	0.69	20 (20%) 1 0	150, 241, 295, 344	0
11	K	116/129 (89%)	-0.14	3 (2%) 56 40	100, 131, 170, 192	0
12	L	124/135 (91%)	-0.07	3 (2%) 59 43	82, 134, 167, 216	0
13	M	118/126 (93%)	0.17	7 (5%) 22 13	125, 162, 214, 232	0
14	N	60/61 (98%)	0.10	3 (5%) 28 18	179, 215, 270, 292	0
15	O	87/89 (97%)	-0.41	0 100 100	84, 119, 159, 179	0
16	P	83/88 (94%)	-0.09	0 100 100	95, 134, 164, 208	0
17	Q	99/105 (94%)	-0.30	0 100 100	75, 110, 148, 162	0
18	R	70/88 (79%)	-0.56	0 100 100	95, 135, 187, 215	0
19	S	80/93 (86%)	0.88	19 (23%) 0 0	176, 219, 255, 273	0
20	T	99/106 (93%)	-0.18	3 (3%) 50 34	106, 136, 194, 226	0
21	U	24/27 (88%)	0.52	3 (12%) 3 3	131, 183, 201, 209	0
All	All	3875/4063 (95%)	-0.13	130 (3%) 45 31	70, 146, 250, 374	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1003(A)	G	7.6
19	S	38	SER	7.4
1	A	993	G	7.1
1	A	1006	C	7.1
3	C	66	VAL	5.3
1	A	1018	C	5.0
1	A	1017	G	4.9
1	A	995	C	4.7
1	A	994	A	4.6
13	M	2	ALA	4.6
9	I	15	ALA	4.6
1	A	1005	A	4.4
14	N	3	ARG	4.3
19	S	12	ASP	4.2
1	A	1037	C	4.2
9	I	65	VAL	4.2
10	J	10	GLY	4.1
10	J	90	LEU	4.0
14	N	5	ALA	4.0
9	I	8	GLY	3.9
19	S	41	VAL	3.8
21	U	18	TYR	3.8
19	S	39	THR	3.8
13	M	43	THR	3.8
9	I	66	ARG	3.7
3	C	65	ALA	3.7
9	I	9	ARG	3.5
1	A	1024	G	3.5
10	J	89	ASP	3.5
19	S	35	SER	3.5
1	A	1224	G	3.5
3	C	67	THR	3.5
7	G	2	ALA	3.4
10	J	71	LEU	3.3
1	A	1019	C	3.3
10	J	93	GLY	3.2
1	A	1539	C	3.2
19	S	40	ILE	3.2
1	A	990	C	3.1
3	C	68	VAL	3.1
10	J	97	GLU	3.1
9	I	64	THR	3.1
1	A	1007	C	3.0

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Mol	Chain	Res	Type	RSRZ
10	J	94	VAL	3.0
19	S	31	ILE	3.0
1	A	1023	G	3.0
1	A	1036	G	3.0
1	A	81	U	3.0
9	I	67	GLY	3.0
9	I	14	VAL	3.0
1	A	1004	A	3.0
21	U	24	ARG	2.9
1	A	1129	C	2.9
4	D	40	PRO	2.9
1	A	1025	U	2.9
3	C	201	TYR	2.9
9	I	43	ALA	2.8
21	U	17	THR	2.8
9	I	63	ILE	2.8
13	M	105	THR	2.8
12	L	114	LYS	2.8
1	A	1002	G	2.8
13	M	117	VAL	2.8
10	J	96	ILE	2.7
3	C	189	ALA	2.7
4	D	42	GLN	2.7
7	G	62	PHE	2.7
10	J	91	PRO	2.6
13	M	104	ARG	2.6
10	J	34	VAL	2.6
9	I	17	VAL	2.6
4	D	125	HIS	2.6
4	D	35	ARG	2.6
10	J	7	LYS	2.6
1	A	1032	G	2.6
2	B	212	GLN	2.6
3	C	102	ASN	2.6
13	M	45	VAL	2.5
2	B	203	GLY	2.5
1	A	1038	C	2.5
10	J	98	ILE	2.5
1	A	1542	U	2.5
3	C	196	LEU	2.5
9	I	19	LEU	2.5
9	I	16	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
11	K	19	ALA	2.4
10	J	65	LEU	2.4
9	I	4	TYR	2.4
7	G	4	ARG	2.4
10	J	40	LEU	2.4
19	S	16	LEU	2.4
3	C	104	GLN	2.4
19	S	14	HIS	2.4
11	K	21	ILE	2.4
20	T	103	GLY	2.4
9	I	7	THR	2.3
10	J	6	ILE	2.3
19	S	69	HIS	2.3
20	T	64	ASP	2.3
19	S	21	GLU	2.3
11	K	30	VAL	2.3
10	J	63	PHE	2.3
10	J	70	ARG	2.3
3	C	193	TYR	2.2
19	S	70	LYS	2.2
19	S	17	GLU	2.2
1	A	1026	G	2.2
3	C	195	VAL	2.2
1	A	1276	G	2.2
3	C	103	VAL	2.2
19	S	34	TRP	2.1
3	C	56	ASP	2.1
19	S	11	VAL	2.1
3	C	69	HIS	2.1
4	D	13	ARG	2.1
1	A	706	A	2.1
20	T	9	ASN	2.1
14	N	4	LYS	2.0
19	S	79	THR	2.0
19	S	15	LEU	2.0
10	J	23	ILE	2.0
10	J	8	LEU	2.0
19	S	3	ARG	2.0
6	F	63	TYR	2.0
12	L	113	ARG	2.0
19	S	44	MET	2.0
10	J	39	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
12	L	72	GLY	2.0
3	C	57	ILE	2.0
13	M	44	ARG	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. 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	B-factors(Å ²)	Q<0.9
1	PSU	A	1540	20/21	0.66	0.71	296,308,331,333	0
1	PSU	A	1541	20/21	0.85	0.65	285,299,307,307	0
1	4OC	A	1402	22/23	0.92	0.23	108,116,134,137	0
1	MA6	A	1518[B]	24/25	0.93	0.22	111,120,133,136	24
1	7MG	A	527	24/25	0.93	0.22	103,120,142,145	0
1	MA6	A	1518[A]	24/25	0.93	0.22	107,118,124,124	24
1	2MG	A	1207	24/25	0.94	0.16	195,204,278,284	0
1	5MC	A	1400	21/22	0.95	0.19	103,123,130,131	0
1	5MC	A	1407	21/22	0.95	0.12	136,163,172,178	0
1	MA6	A	1519[A]	24/25	0.95	0.28	100,107,112,116	24
1	MA6	A	1519[B]	24/25	0.95	0.28	102,107,118,119	24
1	PSU	A	516	20/21	0.95	0.10	133,147,164,166	0
1	5MC	A	1404	21/22	0.96	0.16	99,108,151,155	0
1	UR3	A	1498	21/22	0.96	0.29	105,120,144,147	0
1	M2G	A	966	25/26	0.96	0.15	136,150,159,160	0
1	5MC	A	967	21/22	0.97	0.13	125,144,150,153	0

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. 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	B-factors(\AA^2)	Q<0.9
22	MG	A	1838	1/1	0.20	0.87	121,121,121,121	0
22	MG	A	1847	1/1	0.30	0.90	127,127,127,127	0
22	MG	A	1858	1/1	0.34	0.63	125,125,125,125	0
22	MG	A	1766	1/1	0.37	1.26	100,100,100,100	0
22	MG	A	1776	1/1	0.44	0.15	110,110,110,110	0
22	MG	A	1642	1/1	0.46	0.15	88,88,88,88	0
22	MG	A	1810	1/1	0.47	0.39	102,102,102,102	0
22	MG	A	1731	1/1	0.49	0.38	107,107,107,107	0
22	MG	A	1716	1/1	0.53	0.40	137,137,137,137	0
22	MG	P	102	1/1	0.53	0.45	124,124,124,124	0
22	MG	A	1849	1/1	0.55	0.28	126,126,126,126	0
22	MG	A	1704	1/1	0.56	0.44	126,126,126,126	0
22	MG	A	1753	1/1	0.56	0.37	109,109,109,109	0
22	MG	A	1826	1/1	0.59	0.76	134,134,134,134	0
22	MG	A	1751	1/1	0.59	0.93	143,143,143,143	0
22	MG	A	1829	1/1	0.60	0.37	463,463,463,463	0
22	MG	A	1682	1/1	0.61	0.32	82,82,82,82	0
22	MG	A	1781	1/1	0.61	0.64	130,130,130,130	0
22	MG	A	1842	1/1	0.62	1.15	119,119,119,119	0
22	MG	A	1822	1/1	0.63	0.22	116,116,116,116	0
22	MG	A	1777	1/1	0.65	1.28	144,144,144,144	0
22	MG	A	1794	1/1	0.66	0.91	132,132,132,132	0
22	MG	A	1830	1/1	0.68	0.66	91,91,91,91	0
22	MG	A	1811	1/1	0.68	0.25	147,147,147,147	0
22	MG	A	1601	1/1	0.69	0.43	132,132,132,132	0
22	MG	A	1763	1/1	0.70	0.29	137,137,137,137	0
22	MG	A	1833	1/1	0.70	0.26	122,122,122,122	0
22	MG	A	1845	1/1	0.70	0.92	110,110,110,110	0
22	MG	A	1846	1/1	0.71	0.21	142,142,142,142	0
22	MG	A	1866	1/1	0.71	0.49	124,124,124,124	0
22	MG	A	1672	1/1	0.71	0.14	139,139,139,139	0
22	MG	A	1770	1/1	0.71	0.97	99,99,99,99	0
22	MG	A	1735	1/1	0.71	0.51	81,81,81,81	0
22	MG	A	1809	1/1	0.72	0.37	109,109,109,109	0
22	MG	H	201	1/1	0.72	0.64	118,118,118,118	0
22	MG	A	1782	1/1	0.72	0.55	118,118,118,118	0
22	MG	A	1749	1/1	0.72	0.41	121,121,121,121	0
22	MG	A	1839	1/1	0.73	0.58	133,133,133,133	0
22	MG	A	1625	1/1	0.73	0.31	122,122,122,122	0
22	MG	A	1796	1/1	0.74	0.56	92,92,92,92	0
22	MG	A	1853	1/1	0.74	0.41	116,116,116,116	0
22	MG	A	1665	1/1	0.75	0.31	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1769	1/1	0.75	0.41	118,118,118,118	0
22	MG	A	1660	1/1	0.75	0.14	113,113,113,113	0
22	MG	C	301	1/1	0.75	0.44	133,133,133,133	0
22	MG	A	1857	1/1	0.76	0.54	133,133,133,133	0
22	MG	A	1662	1/1	0.76	0.37	78,78,78,78	0
22	MG	A	1720	1/1	0.77	0.77	98,98,98,98	0
22	MG	A	1808	1/1	0.77	0.11	163,163,163,163	0
22	MG	A	1715	1/1	0.77	0.52	137,137,137,137	0
22	MG	A	1872	1/1	0.78	0.13	407,407,407,407	0
22	MG	A	1703	1/1	0.79	0.39	153,153,153,153	0
22	MG	A	1761	1/1	0.79	0.34	107,107,107,107	0
22	MG	A	1780	1/1	0.79	0.50	61,61,61,61	0
22	MG	A	1683	1/1	0.79	0.65	98,98,98,98	0
22	MG	A	1835	1/1	0.79	0.55	98,98,98,98	0
22	MG	A	1834	1/1	0.79	0.35	118,118,118,118	0
22	MG	A	1841	1/1	0.80	0.78	118,118,118,118	0
22	MG	Q	201	1/1	0.80	0.21	126,126,126,126	0
22	MG	A	1787	1/1	0.80	0.12	141,141,141,141	0
22	MG	A	1854	1/1	0.80	0.45	137,137,137,137	0
22	MG	A	1868	1/1	0.80	0.36	99,99,99,99	0
22	MG	A	1824	1/1	0.80	0.20	133,133,133,133	0
22	MG	A	1843	1/1	0.81	0.80	106,106,106,106	0
22	MG	A	1832	1/1	0.82	0.77	89,89,89,89	0
22	MG	A	1622	1/1	0.83	0.23	148,148,148,148	0
22	MG	A	1729	1/1	0.83	0.32	85,85,85,85	0
22	MG	A	1736	1/1	0.84	0.22	114,114,114,114	0
22	MG	A	1684	1/1	0.84	0.33	127,127,127,127	0
22	MG	A	1783	1/1	0.84	0.41	129,129,129,129	0
22	MG	A	1865	1/1	0.84	0.21	134,134,134,134	0
22	MG	A	1679	1/1	0.84	0.47	146,146,146,146	0
22	MG	A	1677	1/1	0.84	0.14	299,299,299,299	0
22	MG	A	1605	1/1	0.84	0.80	85,85,85,85	0
22	MG	A	1759	1/1	0.84	0.26	107,107,107,107	0
22	MG	A	1836	1/1	0.85	0.42	120,120,120,120	0
22	MG	A	1798	1/1	0.85	0.20	148,148,148,148	0
22	MG	A	1851	1/1	0.85	0.28	132,132,132,132	0
22	MG	A	1687	1/1	0.85	0.25	117,117,117,117	0
22	MG	A	1633	1/1	0.85	1.02	100,100,100,100	0
22	MG	A	1711	1/1	0.85	0.33	149,149,149,149	0
22	MG	A	1815	1/1	0.85	0.46	115,115,115,115	0
22	MG	A	1791	1/1	0.86	0.46	99,99,99,99	0
22	MG	A	1821	1/1	0.86	0.34	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1745	1/1	0.86	0.18	107,107,107,107	0
22	MG	A	1856	1/1	0.86	0.28	127,127,127,127	0
22	MG	P	101	1/1	0.86	0.22	115,115,115,115	0
22	MG	A	1867	1/1	0.86	0.55	118,118,118,118	0
22	MG	A	1850	1/1	0.86	0.36	125,125,125,125	0
22	MG	A	1855	1/1	0.87	0.87	128,128,128,128	0
22	MG	A	1799	1/1	0.87	0.26	84,84,84,84	0
22	MG	A	1767	1/1	0.87	0.23	107,107,107,107	0
22	MG	A	1712	1/1	0.87	0.34	149,149,149,149	0
22	MG	A	1629	1/1	0.87	0.52	121,121,121,121	0
22	MG	A	1797	1/1	0.87	0.54	116,116,116,116	0
22	MG	A	1755	1/1	0.88	0.38	122,122,122,122	0
22	MG	A	1718	1/1	0.88	0.16	92,92,92,92	0
22	MG	A	1696	1/1	0.88	0.35	128,128,128,128	0
22	MG	A	1874	1/1	0.88	0.20	431,431,431,431	0
22	MG	D	304	1/1	0.88	0.56	110,110,110,110	0
22	MG	A	1661	1/1	0.88	0.45	87,87,87,87	0
22	MG	J	201	1/1	0.88	0.34	105,105,105,105	0
22	MG	A	1674	1/1	0.88	0.46	124,124,124,124	0
22	MG	A	1754	1/1	0.88	0.10	156,156,156,156	0
22	MG	D	303	1/1	0.88	0.22	88,88,88,88	0
22	MG	A	1701	1/1	0.88	0.32	138,138,138,138	0
22	MG	A	1806	1/1	0.88	0.29	414,414,414,414	0
22	MG	A	1772	1/1	0.88	1.46	120,120,120,120	0
22	MG	A	1638	1/1	0.88	0.33	97,97,97,97	0
22	MG	A	1848	1/1	0.89	0.41	94,94,94,94	0
22	MG	A	1619	1/1	0.89	0.63	106,106,106,106	0
22	MG	A	1733	1/1	0.89	0.33	116,116,116,116	0
22	MG	A	1778	1/1	0.89	0.15	157,157,157,157	0
22	MG	A	1852	1/1	0.89	0.50	108,108,108,108	0
22	MG	A	1644	1/1	0.89	0.34	82,82,82,82	0
22	MG	C	302	1/1	0.89	0.12	129,129,129,129	0
22	MG	A	1823	1/1	0.89	0.20	146,146,146,146	0
22	MG	I	201	1/1	0.89	0.81	136,136,136,136	0
22	MG	A	1785	1/1	0.90	0.21	127,127,127,127	0
22	MG	A	1837	1/1	0.90	0.96	123,123,123,123	0
22	MG	A	1802	1/1	0.90	0.50	148,148,148,148	0
22	MG	A	1694	1/1	0.90	0.34	76,76,76,76	0
22	MG	A	1790	1/1	0.90	0.73	146,146,146,146	0
22	MG	A	1859	1/1	0.90	0.81	123,123,123,123	0
22	MG	A	1626	1/1	0.90	0.29	147,147,147,147	0
22	MG	A	1817	1/1	0.90	0.93	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1819	1/1	0.90	0.18	103,103,103,103	0
22	MG	A	1725	1/1	0.90	0.80	119,119,119,119	0
22	MG	A	1671	1/1	0.90	0.24	140,140,140,140	0
22	MG	A	1685	1/1	0.90	0.10	236,236,236,236	0
22	MG	A	1756	1/1	0.90	0.26	109,109,109,109	0
22	MG	A	1873	1/1	0.90	0.10	437,437,437,437	0
22	MG	A	1871	1/1	0.90	0.47	148,148,148,148	0
22	MG	A	1686	1/1	0.90	0.13	226,226,226,226	0
22	MG	A	1789	1/1	0.91	0.11	96,96,96,96	0
22	MG	A	1705	1/1	0.91	0.18	369,369,369,369	0
22	MG	A	1773	1/1	0.91	0.43	120,120,120,120	0
22	MG	A	1673	1/1	0.91	0.10	120,120,120,120	0
22	MG	A	1800	1/1	0.91	0.09	132,132,132,132	0
22	MG	A	1863	1/1	0.91	0.31	101,101,101,101	0
22	MG	A	1803	1/1	0.91	0.47	250,250,250,250	0
23	ZN	N	101	1/1	0.91	0.14	214,214,214,214	0
22	MG	A	1827	1/1	0.91	0.98	147,147,147,147	0
22	MG	E	201	1/1	0.91	0.12	121,121,121,121	0
22	MG	A	1631	1/1	0.91	0.32	109,109,109,109	0
22	MG	A	1699	1/1	0.91	0.39	97,97,97,97	0
22	MG	A	1666	1/1	0.91	0.21	123,123,123,123	0
22	MG	B	302	1/1	0.91	0.15	111,111,111,111	0
22	MG	A	1740	1/1	0.91	0.40	125,125,125,125	0
22	MG	D	302	1/1	0.92	0.19	103,103,103,103	0
22	MG	A	1639	1/1	0.92	0.31	216,216,216,216	0
22	MG	A	1814	1/1	0.92	0.56	131,131,131,131	0
22	MG	A	1743	1/1	0.92	0.19	104,104,104,104	0
22	MG	A	1774	1/1	0.92	0.51	112,112,112,112	0
22	MG	A	1739	1/1	0.92	0.49	74,74,74,74	0
22	MG	A	1758	1/1	0.92	0.28	109,109,109,109	0
22	MG	A	1689	1/1	0.92	0.76	170,170,170,170	0
22	MG	A	1678	1/1	0.92	0.44	106,106,106,106	0
22	MG	A	1765	1/1	0.92	0.76	90,90,90,90	0
22	MG	A	1784	1/1	0.92	0.20	120,120,120,120	0
22	MG	A	1768	1/1	0.92	0.13	147,147,147,147	0
22	MG	A	1700	1/1	0.92	0.17	184,184,184,184	0
22	MG	A	1738	1/1	0.92	0.54	100,100,100,100	0
22	MG	A	1864	1/1	0.92	0.43	122,122,122,122	0
22	MG	A	1786	1/1	0.92	0.18	153,153,153,153	0
22	MG	A	1748	1/1	0.92	0.32	120,120,120,120	0
22	MG	A	1667	1/1	0.92	0.27	115,115,115,115	0
22	MG	A	1752	1/1	0.92	0.50	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1764	1/1	0.93	0.25	101,101,101,101	0
22	MG	A	1779	1/1	0.93	0.20	129,129,129,129	0
22	MG	A	1653	1/1	0.93	0.17	113,113,113,113	0
22	MG	A	1676	1/1	0.93	0.24	113,113,113,113	0
22	MG	A	1608	1/1	0.93	0.11	143,143,143,143	0
22	MG	A	1664	1/1	0.93	0.44	101,101,101,101	0
22	MG	A	1732	1/1	0.93	0.33	136,136,136,136	0
22	MG	A	1688	1/1	0.93	0.13	144,144,144,144	0
22	MG	F	201	1/1	0.93	0.16	107,107,107,107	0
22	MG	A	1844	1/1	0.93	0.18	100,100,100,100	0
22	MG	A	1793	1/1	0.94	0.25	80,80,80,80	0
22	MG	A	1681	1/1	0.94	0.35	132,132,132,132	0
22	MG	A	1669	1/1	0.94	0.19	152,152,152,152	0
22	MG	A	1801	1/1	0.94	0.18	154,154,154,154	0
22	MG	A	1628	1/1	0.94	0.78	85,85,85,85	0
22	MG	A	1825	1/1	0.94	0.35	110,110,110,110	0
22	MG	A	1870	1/1	0.94	0.58	85,85,85,85	0
22	MG	A	1652	1/1	0.94	0.13	98,98,98,98	0
22	MG	A	1744	1/1	0.94	0.32	117,117,117,117	0
22	MG	A	1818	1/1	0.94	0.97	100,100,100,100	0
22	MG	A	1737	1/1	0.94	0.24	99,99,99,99	0
22	MG	A	1861	1/1	0.94	0.11	89,89,89,89	0
22	MG	A	1610	1/1	0.94	0.24	124,124,124,124	0
22	MG	A	1840	1/1	0.94	0.22	104,104,104,104	0
22	MG	A	1702	1/1	0.94	0.21	184,184,184,184	0
22	MG	A	1657	1/1	0.94	0.15	98,98,98,98	0
22	MG	A	1690	1/1	0.94	0.06	136,136,136,136	0
22	MG	A	1727	1/1	0.95	0.74	140,140,140,140	0
22	MG	A	1816	1/1	0.95	0.41	105,105,105,105	0
22	MG	A	1649	1/1	0.95	0.48	116,116,116,116	0
22	MG	A	1722	1/1	0.95	0.24	155,155,155,155	0
22	MG	A	1635	1/1	0.95	0.12	99,99,99,99	0
22	MG	A	1831	1/1	0.95	0.33	52,52,52,52	0
22	MG	A	1714	1/1	0.95	0.21	219,219,219,219	0
22	MG	A	1728	1/1	0.95	0.05	214,214,214,214	0
22	MG	A	1692	1/1	0.95	0.27	150,150,150,150	0
22	MG	A	1646	1/1	0.95	0.40	91,91,91,91	0
22	MG	A	1650	1/1	0.95	0.24	90,90,90,90	0
22	MG	A	1723	1/1	0.95	0.16	102,102,102,102	0
22	MG	A	1862	1/1	0.95	0.32	127,127,127,127	0
22	MG	A	1710	1/1	0.95	0.41	114,114,114,114	0
22	MG	A	1828	1/1	0.95	0.28	447,447,447,447	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	B	301	1/1	0.95	0.20	99,99,99,99	0
22	MG	A	1792	1/1	0.96	0.13	97,97,97,97	0
22	MG	A	1675	1/1	0.96	0.21	116,116,116,116	0
22	MG	A	1659	1/1	0.96	0.12	121,121,121,121	0
22	MG	A	1624	1/1	0.96	0.25	117,117,117,117	0
22	MG	A	1697	1/1	0.96	0.33	127,127,127,127	0
22	MG	A	1647	1/1	0.96	0.44	182,182,182,182	0
22	MG	A	1645	1/1	0.96	0.06	91,91,91,91	0
22	MG	A	1643	1/1	0.96	0.15	90,90,90,90	0
22	MG	A	1869	1/1	0.96	0.19	106,106,106,106	0
22	MG	A	1612	1/1	0.96	0.12	164,164,164,164	0
22	MG	A	1603	1/1	0.96	0.23	84,84,84,84	0
22	MG	A	1805	1/1	0.96	0.12	203,203,203,203	0
22	MG	A	1648	1/1	0.96	0.14	164,164,164,164	0
22	MG	A	1726	1/1	0.96	0.41	134,134,134,134	0
22	MG	A	1742	1/1	0.96	0.31	116,116,116,116	0
22	MG	A	1741	1/1	0.96	0.17	76,76,76,76	0
22	MG	A	1807	1/1	0.96	0.12	278,278,278,278	0
22	MG	A	1795	1/1	0.96	0.52	117,117,117,117	0
22	MG	A	1875	1/1	0.96	0.07	228,228,228,228	0
22	MG	A	1813	1/1	0.96	0.19	122,122,122,122	0
22	MG	A	1707	1/1	0.97	0.07	167,167,167,167	0
22	MG	A	1820	1/1	0.97	0.06	91,91,91,91	0
22	MG	A	1621	1/1	0.97	0.31	123,123,123,123	0
22	MG	A	1730	1/1	0.97	0.26	110,110,110,110	0
22	MG	A	1654	1/1	0.97	0.10	49,49,49,49	0
22	MG	A	1747	1/1	0.97	0.07	105,105,105,105	0
22	MG	A	1771	1/1	0.97	0.67	83,83,83,83	0
22	MG	A	1734	1/1	0.97	0.26	129,129,129,129	0
22	MG	A	1804	1/1	0.97	0.11	194,194,194,194	0
22	MG	A	1615	1/1	0.97	0.12	99,99,99,99	0
22	MG	A	1706	1/1	0.98	0.36	97,97,97,97	0
22	MG	A	1616	1/1	0.98	0.18	66,66,66,66	0
22	MG	A	1876	1/1	0.98	0.24	399,399,399,399	0
22	MG	A	1724	1/1	0.98	0.37	92,92,92,92	0
22	MG	A	1860	1/1	0.98	0.56	123,123,123,123	0
22	MG	A	1695	1/1	0.98	0.11	81,81,81,81	0
22	MG	A	1614	1/1	0.98	0.18	135,135,135,135	0
22	MG	A	1691	1/1	0.98	0.38	155,155,155,155	0
22	MG	A	1656	1/1	0.98	0.14	178,178,178,178	0
22	MG	A	1668	1/1	0.98	0.12	136,136,136,136	0
22	MG	A	1604	1/1	0.98	0.12	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1609	1/1	0.98	0.18	94,94,94,94	0
22	MG	A	1680	1/1	0.98	0.29	136,136,136,136	0
23	ZN	D	301	1/1	0.98	0.28	122,122,122,122	0
22	MG	A	1670	1/1	0.98	0.10	140,140,140,140	0
22	MG	A	1658	1/1	0.98	0.18	130,130,130,130	0
22	MG	A	1618	1/1	0.98	0.35	94,94,94,94	0
22	MG	A	1713	1/1	0.98	0.32	431,431,431,431	0
22	MG	N	102	1/1	0.98	0.30	225,225,225,225	0
22	MG	A	1762	1/1	0.98	0.30	83,83,83,83	0
22	MG	A	1617	1/1	0.98	0.29	56,56,56,56	0
22	MG	A	1788	1/1	0.98	0.51	77,77,77,77	0
22	MG	A	1602	1/1	0.98	0.21	130,130,130,130	0
22	MG	A	1627	1/1	0.98	0.83	79,79,79,79	0
22	MG	A	1760	1/1	0.98	0.20	98,98,98,98	0
22	MG	A	1613	1/1	0.98	0.21	121,121,121,121	0
22	MG	A	1717	1/1	0.98	0.24	94,94,94,94	0
22	MG	A	1746	1/1	0.99	0.17	101,101,101,101	0
22	MG	A	1708	1/1	0.99	0.18	120,120,120,120	0
22	MG	A	1636	1/1	0.99	0.12	69,69,69,69	0
22	MG	A	1812	1/1	0.99	0.16	99,99,99,99	0
22	MG	A	1634	1/1	0.99	0.20	235,235,235,235	0
22	MG	A	1693	1/1	0.99	0.15	133,133,133,133	0
22	MG	A	1640	1/1	0.99	0.16	72,72,72,72	0
22	MG	A	1637	1/1	0.99	0.37	85,85,85,85	0
22	MG	A	1620	1/1	0.99	0.10	83,83,83,83	0
22	MG	A	1623	1/1	0.99	0.14	135,135,135,135	0
22	MG	A	1632	1/1	0.99	0.14	128,128,128,128	0
22	MG	B	303	1/1	0.99	0.18	184,184,184,184	0
22	MG	A	1641	1/1	0.99	0.12	99,99,99,99	0
22	MG	A	1757	1/1	0.99	0.09	80,80,80,80	0
22	MG	A	1719	1/1	0.99	0.19	139,139,139,139	0
22	MG	A	1709	1/1	0.99	0.11	140,140,140,140	0
22	MG	A	1651	1/1	0.99	0.15	61,61,61,61	0
22	MG	A	1775	1/1	0.99	0.12	121,121,121,121	0
22	MG	A	1698	1/1	0.99	0.36	182,182,182,182	0
22	MG	A	1630	1/1	0.99	0.24	83,83,83,83	0
22	MG	A	1750	1/1	0.99	0.23	123,123,123,123	0
22	MG	A	1611	1/1	0.99	0.12	92,92,92,92	0
22	MG	A	1606	1/1	0.99	0.11	96,96,96,96	0
22	MG	A	1655	1/1	0.99	0.14	131,131,131,131	0
22	MG	A	1607	1/1	0.99	0.20	91,91,91,91	0
22	MG	A	1663	1/1	1.00	0.09	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1721	1/1	1.00	0.20	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.