



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:58 PM GMT

PDB ID : 4DR7  
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with codon, crystallographically disordered near-cognate transfer RNA anticodon stem-loop mismatched at the second codon position, and streptomycin bound  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2012-02-16  
Resolution : 3.75 Å(reported)

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

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

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

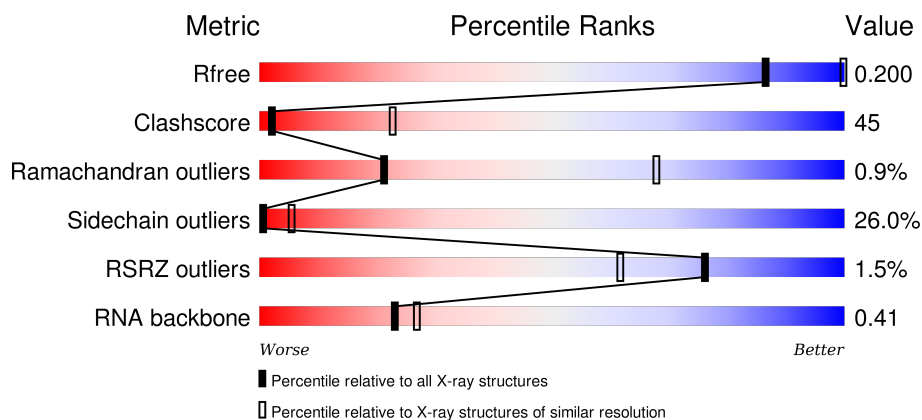
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1268 (4.02-3.50)
Clashscore	102246	1407 (4.02-3.50)
Ramachandran outliers	100387	1346 (4.02-3.50)
Sidechain outliers	100360	1342 (4.02-3.50)
RSRZ outliers	91569	1276 (4.02-3.50)
RNA backbone	2183	1069 (4.70-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	4	
23	W	11	
24	a	8	
25	b	3	

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	2MG	A	1207	-	-	X	-
1	5MC	A	1407	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	UR3	A	1498	-	-	X	-
1	MA6	A	1518[A]	-	-	X	-
1	MA6	A	1518[B]	-	-	X	-
1	MA6	A	1519[A]	-	-	X	-
1	MA6	A	1519[B]	-	-	X	-
26	MG	A	1621	-	-	-	X
26	MG	A	1637	-	-	-	X
26	MG	A	1655	-	-	-	X
26	MG	A	1656	-	-	-	X
26	MG	A	1659	-	-	-	X
26	MG	A	1665	-	-	-	X
26	MG	A	1670	-	-	-	X
26	MG	A	1701	-	-	-	X
26	MG	A	1708	-	-	-	X
26	MG	A	1709	-	-	-	X
26	MG	A	1715	-	-	-	X
26	MG	A	1721	-	-	-	X
26	MG	A	1723	-	-	-	X
26	MG	A	1728	-	-	-	X
26	MG	A	1732	-	-	-	X
26	MG	A	1733	-	-	-	X
26	MG	A	1740	-	-	-	X
26	MG	A	1741	-	-	-	X
26	MG	A	1743	-	-	-	X
26	MG	A	1759	-	-	-	X
26	MG	A	1761	-	-	-	X
26	MG	A	1763	-	-	-	X
26	MG	A	1764	-	-	-	X
26	MG	A	1768	-	-	-	X
26	MG	A	1784	-	-	-	X
26	MG	A	1804	-	-	-	X
26	MG	A	1812	-	-	-	X
26	MG	A	1834	-	-	-	X
26	MG	A	1869	-	-	-	X
26	MG	A	1870	-	-	-	X
26	MG	A	1888	-	-	-	X
26	MG	A	1900	-	-	-	X
26	MG	A	1904	-	-	-	X
26	MG	E	201	-	-	-	X
26	MG	E	204	-	-	-	X
26	MG	N	102	-	-	-	X
26	MG	Q	201	-	-	-	X

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 53659 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	1513	Total	C	N	O	P	0	8	0
			32707	14570	6056	10561	1520			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1896	1211	337	343	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S 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 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S 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 30S 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 30S 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 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			973	612	196	163	2			

- Molecule 13 is a protein called 30S 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 30S 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 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	156	142	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	CONFLICT	UNP Q5SHP7

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	71	Total	C	N	O		0	0	0
			585	373	116	96				

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called 30S 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 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called 5'-R(\*UP\*UP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 23 is a RNA chain called 5'-R(\*GP\*CP\*CP\*UP\*GP\*GP\*AP\*AP\*AP\*GP\*(PSU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	11	Total	C	N	O	P	0	0	0
			235	106	45	74	10			

- Molecule 24 is a RNA chain called 5'-R(P\*UP\*GP\*GP\*AP\*AP\*AP\*GP\*(PSU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	a	8	Total	C	N	O	P	0	0	0
			175	78	34	55	8			

- Molecule 25 is a RNA chain called 5'-R(P\*UP\*UP\*U)-3'.

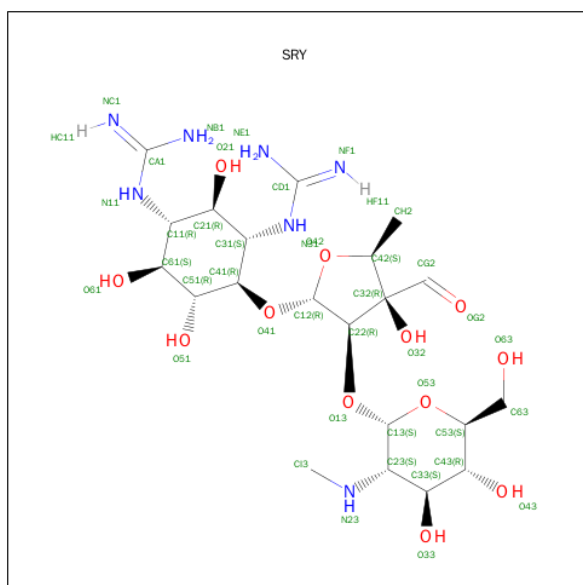
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	b	3	Total	C	N	O	P	0	0	0
			60	27	6	24	3			

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	P	3	Total Mg 3 3	0	0
26	G	1	Total Mg 1 1	0	0
26	J	1	Total Mg 1 1	0	0
26	Q	1	Total Mg 1 1	0	0
26	D	3	Total Mg 3 3	0	0
26	E	4	Total Mg 4 4	0	0
26	H	1	Total Mg 1 1	0	0
26	A	326	Total Mg 326 326	0	0
26	N	1	Total Mg 1 1	0	0
26	S	2	Total Mg 2 2	0	0
26	F	1	Total Mg 1 1	0	0

- Molecule 27 is STREPTOMYCIN (three-letter code: SRY) (formula:  $C_{21}H_{39}N_7O_{12}$ ).



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

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

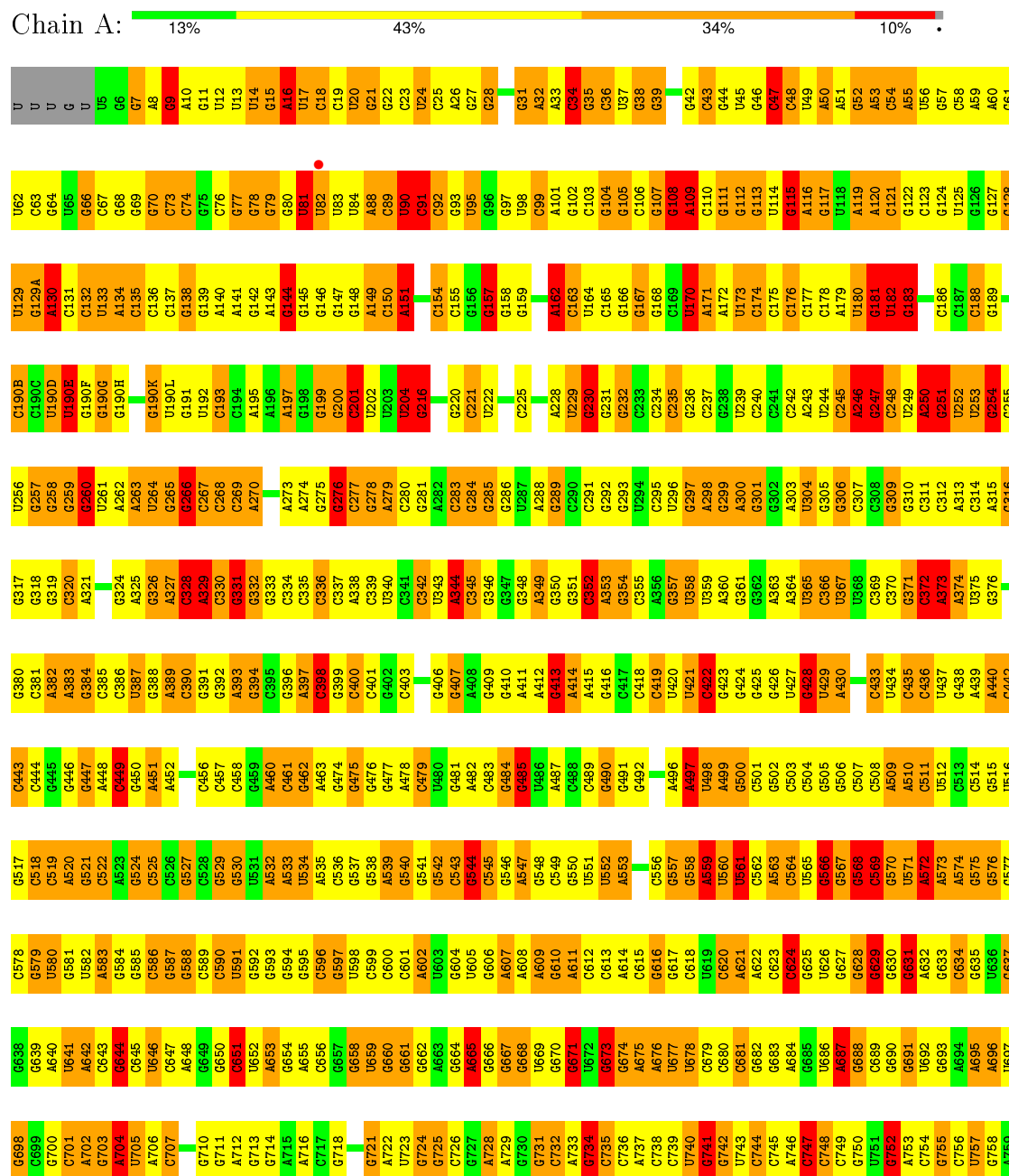
- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	866	Total	O	0	0
			866	866		
29	C	1	Total	O	0	0
			1	1		
29	D	7	Total	O	0	0
			7	7		
29	E	5	Total	O	0	0
			5	5		
29	L	1	Total	O	0	0
			1	1		
29	N	1	Total	O	0	0
			1	1		
29	P	1	Total	O	0	0
			1	1		
29	Q	2	Total	O	0	0
			2	2		
29	T	3	Total	O	0	0
			3	3		
29	U	4	Total	O	0	0
			4	4		
29	W	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

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

- Molecule 1: 16S rRNA

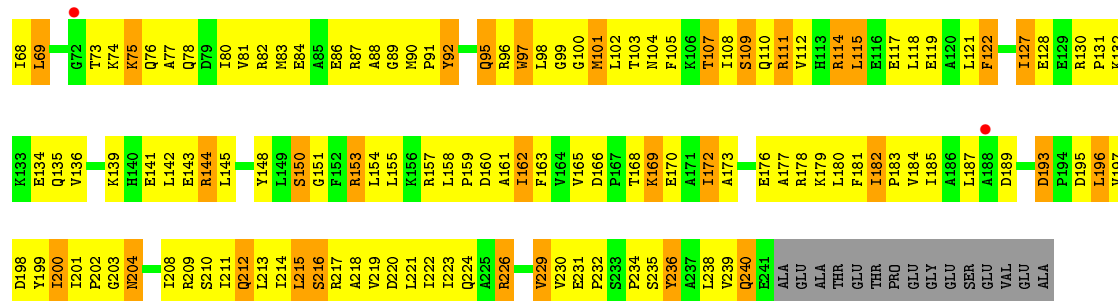


U1510	G1442	A1375	G1316	A1250	G1189	U1125	G1064	G1008	A949	G888	C822	G760
U1511	G1443	U1376	C1317	A1251	G1190	U1126	U1065	G1009	U950	A889	G823	G761
U1512	A1446	A1377	A1318	A1252	A1191	C1127	A1066	G1010	G890	A890	G824	C762
A1513	G1447	C1378	A1319	G1253	G1192	G1128	A1067	G1011	G891	U891	G825	C763
C1514	C1448	G1379	C1320	G1254	G1193	C1129	G1068	U1012	G892	A892	C826	G764
C1515	C1449	U1380	C1321	G1255	U1194	A1130	G1069	G1013	G893	C893	U827	G765
G1516	U1450	U1381	G1322	A1256	G1195	U1070	U1070	A1014	U855	C894	A828	A766
G1517	A1451	C1382	G1323	U1257	U1196	C1132	C1072	A1015	U856	G895	A829	A767
A1518	C1452	C1383	A1324	U1258	G1197	G1133	G1071	A1016	U857	C896	G830	A768
A1519	G1385	G1386	C1325	C1259	G1198	U1134	U1073	G1017	A958	C897	U831	G769
G1520	G1453	G1386	C1326	C1259	U1199	U1135	G1074	C1018	A959	G898	C832	C770
G1521	G1454	G1387	C1327	C1263	G1200	U1136	C1075	C1019	U960	C899	U833	G771
G1522	G1455	G1388	C1328	C1264	A1201	C1137	C1076	U1020	U961	A900	C834	G772
G1523	G1456	C1389	A1329	C1264	G1202	G1138	G1077	G1021	C962	A901	U835	G774
C1524	A1460	C1390	U1330	C1267	C1203	U1078	U1078	G1022	G963	G902	U836	G775
G1525	C1465	U1391	G1331	A1268	A1204	G1109	A1080	G1023	A964	G903	G837	A777
G1526	G1466	G1392	A1332	A1269	U1205	C1141	U1081	G1024	A965	C904	G838	G778
G1527	G1467	U1393	A1333	C1270	G1206	G1142	U1082	U1025	G966	U905	U839	C779
U1528	A1468	A1394	G1334	G1271	G1207	G1143	G1083	G1026	C967	U906	C840	A780
G1529	G1469	C1395	C1335	G1272	C1208	G1144	U1084	C1027	A968	A907	U841	A781
G1530	G1470	A1396	C1336	G1273	C1209	C1145	U1085	G1028	A969	A908	C848	A782
U1531	G1471	C1397	G1337	C1274	C1210	A1146	U1086	C1029	C970	A909	C849	C783
U1532	G1472	A1398	G1338	C1275	U1211	C1147	U1087	C1030	G971	C910	U850	C784
C1533	A1473	C1399	A1339	G1276	U1212	U1148	G1088	G1030A	C972	U911	G851	G785
G1534	G1474	C1400	A1340	U1277	C1213	C1149	G1089	C1030B	G973	C912	G852	G786
A1535	G1475	G1401	U1341	A1278	C1214	U1150	G1090	G1030C	A974	A913	G853	A787
C1536	G1476	C1402	C1342	U1279	G1215	A1151	U1091	C1030D	A975	U788	G854	U789
U1537	C1477	C1403	G1343	U1280	A1152	A1152	U1092	G1031	G976	G855	C856	A790
C1538	G1478	C1404	C1344	C1282	C1153	C1153	A1092	G1032	A977	C913	C857	G791
G1539	C1479	G1405	U1345	G1283	C1218	C1154	A1093	G1033	A978	A918	G858	A792
U1540	G1480	U1406	A1346	C1284	U1219	G1157	G1094	G1034	C979	A919	A859	U793
PSU	U1481	C1407	G1347	A1285	G1221	C1158	U1095	A1035	C980	U920	A860	A794
C	G1482	A1408	U1348	U1286	C1222	U1159	C1096	G1036	U981	U921	G861	C795
U	A1483	A1409	A1349	C1287	G1223	G1160	C1097	C1037	U982	G922	C862	C796
C	G1484	G1410	A1350	A1288	C1161	C1098	C1098	C1038	A983	A923	U863	C797
G1541	U1485	C1411	U1351	G1290	G1162	G1163	G1099	C1039	C984	G924	A864	G798
G1542	C1412	C1152	C1352	G1291	C1226	C1164	C1100	U1040	C985	G925	A865	G799
A1413	U1413	G1486	G1353	U1292	A1227	G1164	A1101	A1041	A986	G926	C866	G800
U1414	G1487	U1414	C1354	U1293	C1228	C1165	A1102	G1042	G987	G927	C867	U801
G1415	G1488	G1415	G1355	G1294	A1229	G1166	C1103	C1043	G988	G928	C868	A802
G1416	C1416	G1416	G1356	G1295	G1167	A1167	G1104	A1044	C989	C930	G869	G803
G1417	G1417	G1417	A1357	C1296	G1231	A1168	C1045	C1045	U991	C931	U870	U804
A1418	A1418	G1418	U1358	G1297	U1232	A1169	G1046	A1046	U992	C932	C805	C806
G1419	G1419	C1420	C1359	C1298	G1233	G1171	G1047	G1047	G993	G933	A872	A807
C1420	G1494	C1421	A1360	A1299	C1234	C1172	G1048	G1048	A994	C934	A873	C808
G1421	C1421	U1301	C1361	U1300	U1235	G1173	A1110	U1049	C995	A935	G874	G809
C1422	U1422	U1302	C1362	U1302	C1237	G1174	C1112	C1051	A996	C936	C875	C810
U1423	G1423	G1303	A1363	G1303	C1238	C1175	C1113	U1052	U997	A937	G876	C811
U1424	U1424	U1304	C1364	G1304	A1239	C1178	C1114	G1053	G998	A938	C877	C812
A1425	C1425	G1305	G1365	G1305	U1240	A1179	C1115	C1054	C999	G939	G878	C813
C1426	C1426	U1307	C1366	U1307	G1241	A1180	C1116	A1055	U1000	U813	C879	A814
A1433	A1433	G1308	C1367	U1308	C1242	G1181	G1117	U1056	A1001	G941	C880	A815
A1503	G1435	G1368	G1368	C1243	C1243	G1182	C1118	G1057	G1002	G942	G881	A816
G1504	U1436	C1369	C1369	C1244	A1183	G1183	C1119	G1058	G1003	U943	C882	A817
G1505	C1437	G1370	G1370	G1311	A1184	G1184	G1120	C1059	G1003A	G944	C883	C817
U1506	G1438	G1371	G1371	G1312	C1246	G1185	U1121	G1060	A1004	G945	U884	G818
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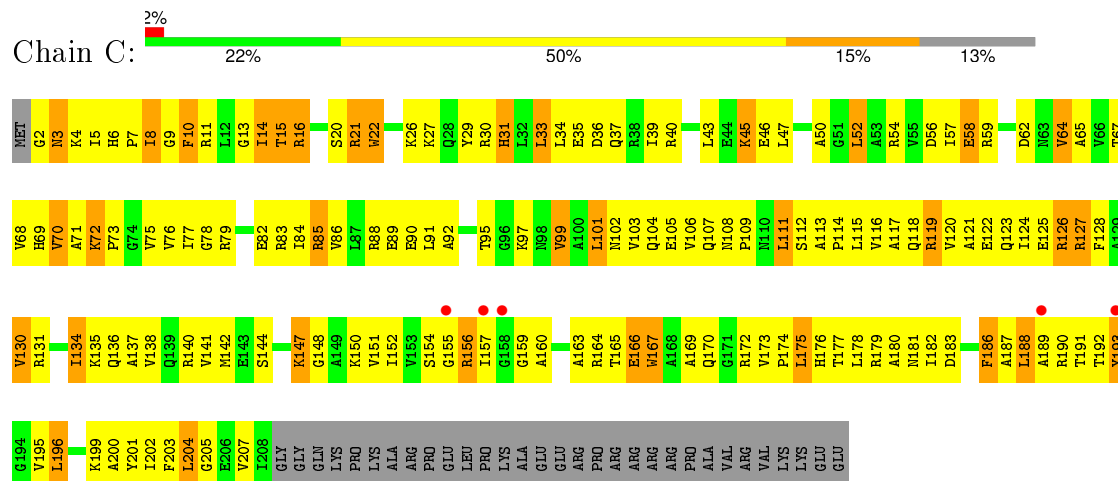
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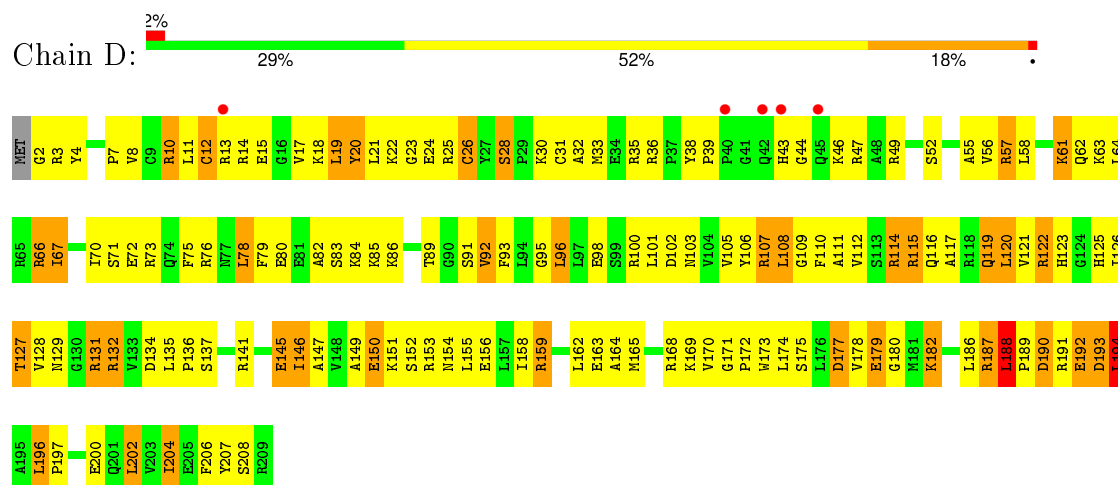
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• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

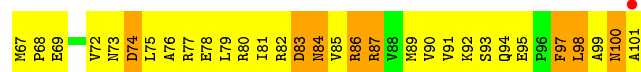


• Molecule 5: 30S ribosomal protein S5

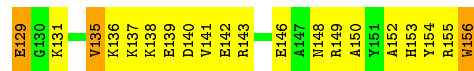
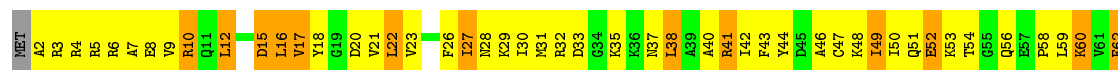




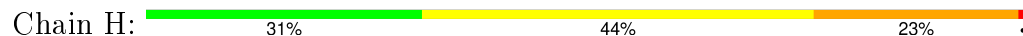
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7



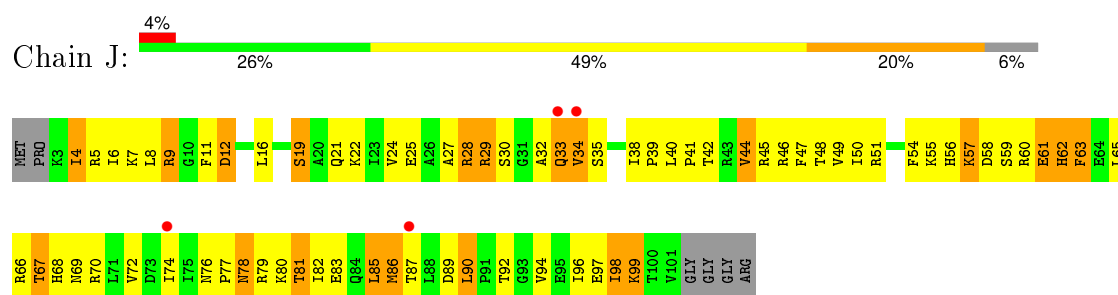
• Molecule 8: 30S ribosomal protein S8



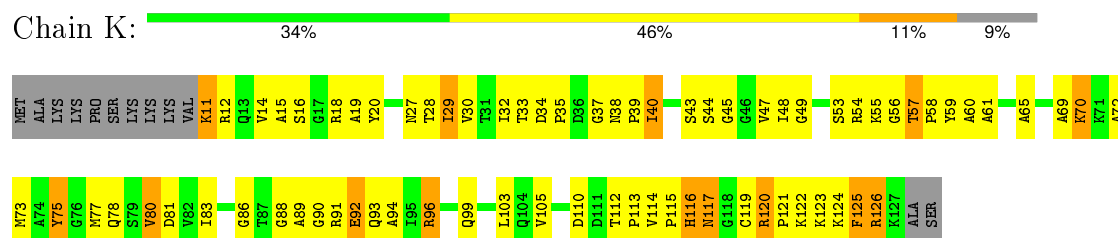
• Molecule 9: 30S ribosomal protein S9



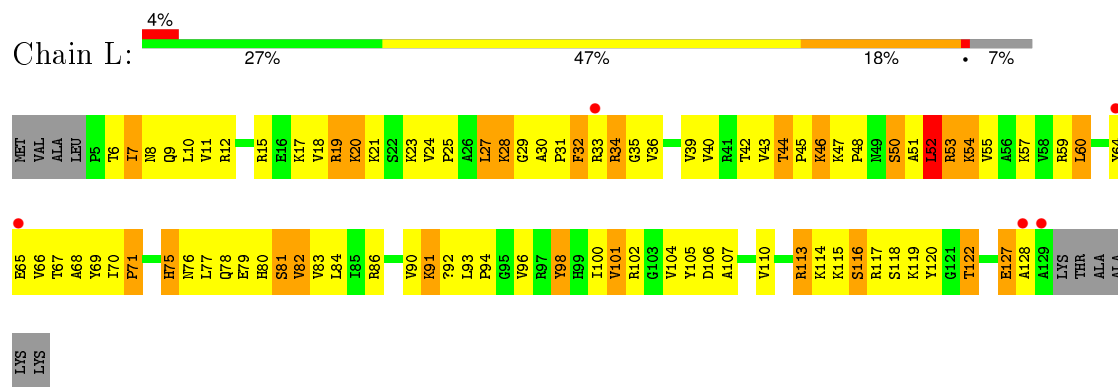
• Molecule 10: 30S ribosomal protein S10



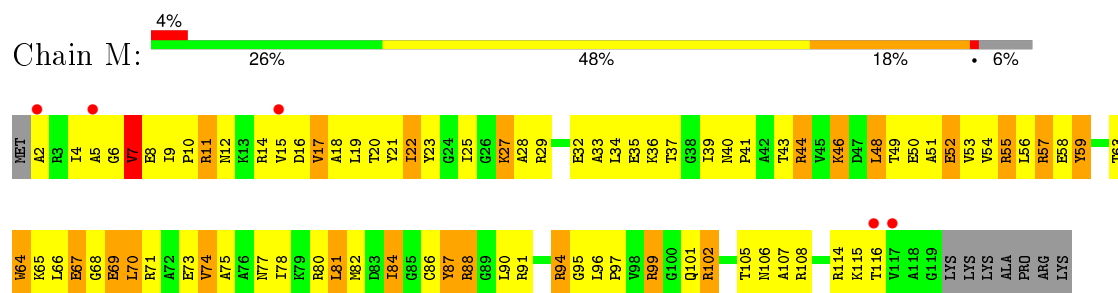
- Molecule 11: 30S ribosomal protein S11



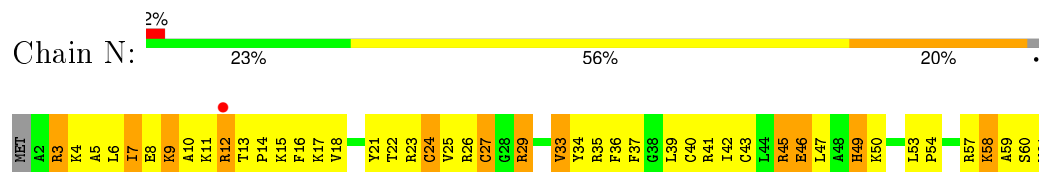
- Molecule 12: 30S ribosomal protein S12



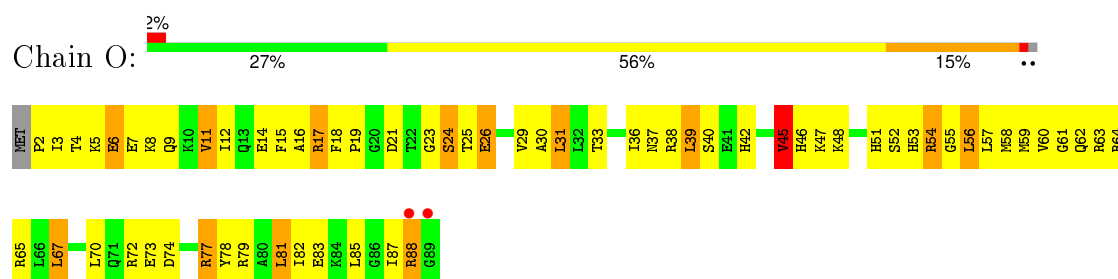
- Molecule 13: 30S ribosomal protein S13



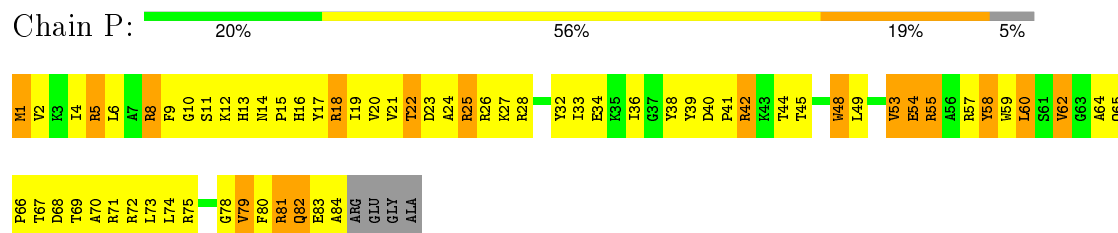
- Molecule 14: 30S ribosomal protein S14



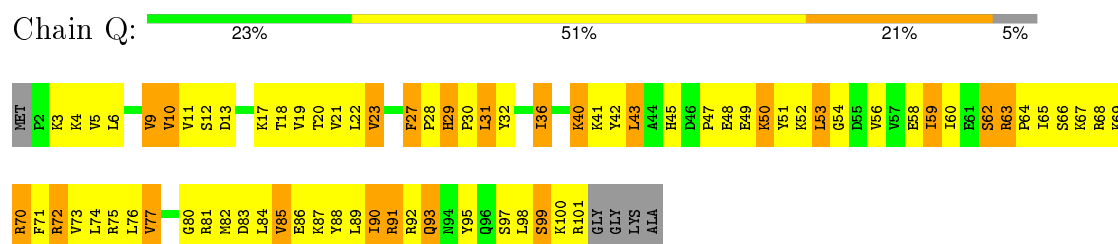
- Molecule 15: 30S ribosomal protein S15



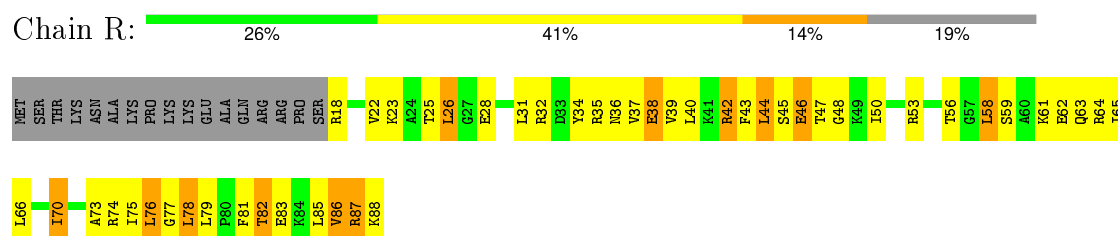
- Molecule 16: 30S ribosomal protein S16



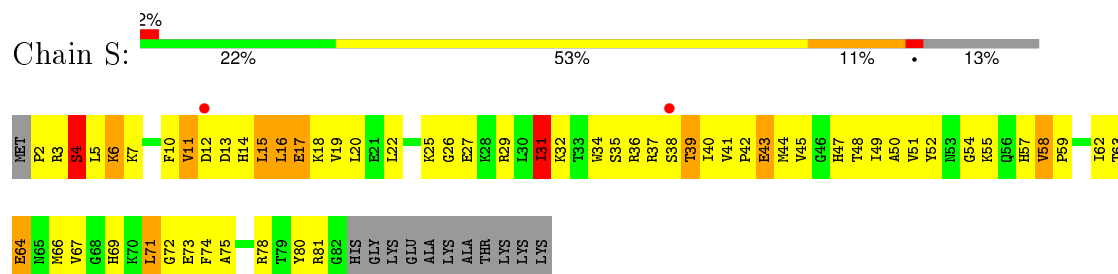
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



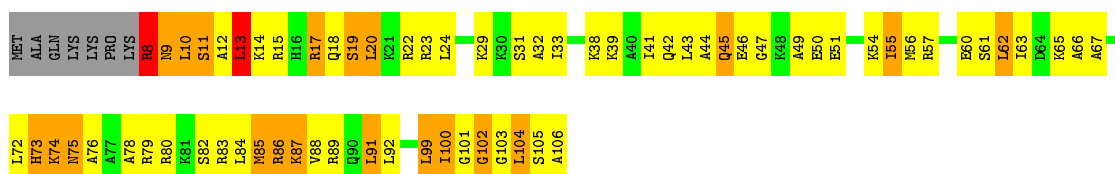
- Molecule 19: 30S ribosomal protein S19



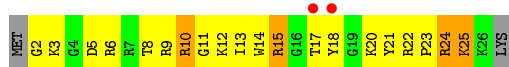
- Molecule 20: 30S ribosomal protein S20







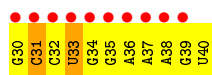
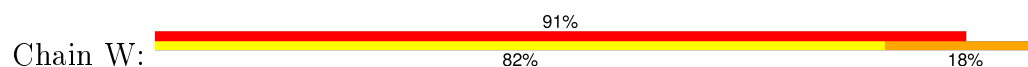
- Molecule 21: 30S ribosomal protein THX



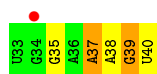
- Molecule 22: 5'-R(\*UP\*UP\*UP\*U)-3'



- Molecule 23: 5'-R(\*GP\*CP\*CP\*UP\*GP\*GP\*AP\*AP\*AP\*GP\*(PSU))-3'



- Molecule 24: 5'-R(P\*UP\*GP\*GP\*AP\*AP\*AP\*GP\*(PSU))-3'



- Molecule 25: 5'-R(P\*UP\*UP\*U)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.49 Å   402.49 Å   174.79 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.91 – 3.75 49.65 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.91-3.75) 100.0 (49.65-3.75)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 3.77 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, $R_{free}$	0.148 , 0.201 0.151 , 0.200	Depositor DCC
$R_{free}$ test set	7304 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	130.7	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 102.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 146049 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	53659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.21	135/36234 (0.4%)	1.90	1769/56547 (3.1%)
2	B	0.74	0/1931	0.93	2/2607 (0.1%)
3	C	0.62	0/1637	0.83	0/2207
4	D	0.73	1/1733 (0.1%)	0.93	4/2318 (0.2%)
5	E	1.04	1/1163 (0.1%)	1.17	3/1566 (0.2%)
6	F	0.65	0/856	0.86	0/1154
7	G	0.68	0/1276	0.87	0/1709
8	H	1.11	2/1136 (0.2%)	1.18	4/1527 (0.3%)
9	I	0.65	0/1029	0.88	2/1379 (0.1%)
10	J	0.71	1/806 (0.1%)	0.95	2/1084 (0.2%)
11	K	0.76	0/888	0.97	0/1198
12	L	0.90	0/978	1.08	3/1308 (0.2%)
13	M	0.68	0/947	0.94	0/1270
14	N	0.68	0/501	0.85	1/664 (0.2%)
15	O	0.86	0/745	1.02	3/992 (0.3%)
16	P	0.93	0/717	1.08	3/965 (0.3%)
17	Q	1.08	1/847 (0.1%)	1.25	4/1131 (0.4%)
18	R	0.76	0/590	1.00	1/782 (0.1%)
19	S	0.57	0/662	0.77	0/892
20	T	0.87	0/765	1.18	4/1007 (0.4%)
21	U	0.69	0/213	0.87	0/279
22	V	0.53	0/84	0.98	0/128
23	W	0.62	0/241	0.92	0/375
24	a	0.85	0/174	1.89	10/270 (3.7%)
25	b	0.76	0/65	1.31	2/98 (2.0%)
All	All	1.08	141/56218 (0.3%)	1.66	1817/83457 (2.2%)

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	3
3	C	0	2
4	D	0	1
8	H	0	2
9	I	0	1
10	J	0	2
12	L	0	2
16	P	0	1
19	S	0	1
20	T	0	2
21	U	0	1
All	All	0	18

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	828	A	N9-C4	-10.24	1.31	1.37
1	A	1513	A	N9-C4	-9.49	1.32	1.37
1	A	266	G	N7-C5	-9.34	1.33	1.39
1	A	573	A	N7-C5	-9.28	1.33	1.39
8	H	135	CYS	CB-SG	-9.04	1.66	1.82
1	A	1227	A	N9-C4	-8.41	1.32	1.37
1	A	1502	A	N3-C4	-8.37	1.29	1.34
1	A	860	A	N3-C4	-8.21	1.29	1.34
1	A	1502	A	N9-C4	-8.06	1.33	1.37
1	A	788	U	C2-N3	7.67	1.43	1.37
1	A	151	A	N9-C4	-7.36	1.33	1.37
1	A	868	C	N1-C6	-7.28	1.32	1.37
1	A	1509	C	N3-C4	-7.25	1.28	1.33
1	A	814	A	N9-C4	-7.15	1.33	1.37
1	A	1066	C	N1-C6	-7.12	1.32	1.37
1	A	787	A	N9-C4	-6.99	1.33	1.37
1	A	109	A	N9-C4	-6.97	1.33	1.37
1	A	130	A	N9-C4	-6.87	1.33	1.37
1	A	563	A	N3-C4	-6.87	1.30	1.34
1	A	366	C	N1-C2	6.81	1.47	1.40
1	A	1502	A	C5-C6	-6.80	1.34	1.41
1	A	1079	G	N7-C5	-6.78	1.35	1.39
1	A	920	U	C4-O4	6.69	1.28	1.23
1	A	868	C	C4-C5	-6.67	1.37	1.43
1	A	1080	A	N3-C4	-6.54	1.30	1.34
1	A	1525	G	C6-N1	-6.52	1.34	1.39
1	A	266	G	C5-C6	-6.52	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	882	C	N3-C4	-6.52	1.29	1.33
1	A	926	G	N9-C4	6.47	1.43	1.38
1	A	691	G	N7-C5	-6.45	1.35	1.39
1	A	298	A	N3-C4	-6.38	1.31	1.34
1	A	767	A	N3-C4	-6.38	1.31	1.34
1	A	26	A	N9-C4	-6.38	1.34	1.37
1	A	1076	C	N1-C6	-6.37	1.33	1.37
1	A	279	A	N9-C4	-6.36	1.34	1.37
1	A	780	A	N9-C4	-6.34	1.34	1.37
1	A	828	A	N7-C5	-6.34	1.35	1.39
1	A	798	G	C5-C4	-6.32	1.33	1.38
1	A	600	C	N1-C6	-6.28	1.33	1.37
1	A	858	G	C6-O6	6.28	1.29	1.24
1	A	26	A	N3-C4	-6.27	1.31	1.34
1	A	574	A	C5-C4	-6.22	1.34	1.38
1	A	1500	A	C6-N1	-6.16	1.31	1.35
1	A	892	A	N9-C4	-6.00	1.34	1.37
1	A	1487	G	N3-C4	-5.98	1.31	1.35
1	A	572	A	C5-C4	-5.97	1.34	1.38
1	A	938	A	N9-C4	-5.97	1.34	1.37
1	A	144	G	N1-C2	5.91	1.42	1.37
1	A	1340	A	N9-C4	-5.88	1.34	1.37
1	A	1239	A	N9-C4	-5.86	1.34	1.37
1	A	1513	A	N3-C4	-5.85	1.31	1.34
1	A	1500	A	N3-C4	-5.85	1.31	1.34
17	Q	9	VAL	CA-CB	-5.85	1.42	1.54
1	A	722	A	C5-C6	-5.84	1.35	1.41
1	A	242	C	N1-C6	-5.82	1.33	1.37
1	A	1528	U	C3'-O3'	5.81	1.50	1.42
1	A	934	C	C2-O2	5.79	1.29	1.24
1	A	644	G	N1-C2	-5.79	1.33	1.37
1	A	913	A	C3'-O3'	5.76	1.50	1.42
1	A	266	G	C3'-C2'	5.75	1.59	1.52
1	A	817	C	N1-C6	-5.75	1.33	1.37
1	A	1487	G	N7-C5	-5.75	1.35	1.39
1	A	1527	C	C4-C5	-5.73	1.38	1.43
1	A	1064	G	N3-C4	-5.73	1.31	1.35
1	A	807	A	N3-C4	-5.72	1.31	1.34
1	A	567	G	C5-C4	-5.71	1.34	1.38
1	A	572	A	C6-N1	-5.69	1.31	1.35
1	A	246	A	C5-C4	-5.67	1.34	1.38
4	D	12	CYS	CB-SG	5.67	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	C	N3-C4	-5.67	1.29	1.33
8	H	137	VAL	CB-CG2	-5.65	1.41	1.52
1	A	325	A	N3-C4	-5.62	1.31	1.34
1	A	698	G	N7-C5	-5.60	1.35	1.39
1	A	868	C	N3-C4	-5.57	1.30	1.33
1	A	1103	C	N1-C6	-5.57	1.33	1.37
1	A	863	U	N1-C2	-5.55	1.33	1.38
1	A	926	G	C5-C6	5.53	1.47	1.42
1	A	609	A	N9-C4	-5.52	1.34	1.37
1	A	298	A	N9-C4	-5.52	1.34	1.37
1	A	320	C	N1-C6	-5.50	1.33	1.37
1	A	915	A	N7-C5	-5.50	1.35	1.39
1	A	566	G	N7-C5	-5.47	1.35	1.39
1	A	577	G	N9-C4	-5.46	1.33	1.38
1	A	144	G	C5-C4	5.46	1.42	1.38
1	A	602	A	N3-C4	-5.46	1.31	1.34
1	A	1377	A	N9-C4	-5.43	1.34	1.37
1	A	107	G	C5-C6	-5.42	1.36	1.42
1	A	601	C	N1-C6	-5.42	1.33	1.37
1	A	1078	U	C4-O4	-5.42	1.19	1.23
1	A	642	A	N9-C4	-5.41	1.34	1.37
1	A	1530	G	C2-N3	-5.41	1.28	1.32
1	A	599	C	N1-C6	-5.41	1.33	1.37
1	A	81	U	N1-C2	5.40	1.43	1.38
1	A	611	A	N9-C4	-5.39	1.34	1.37
1	A	858	G	N3-C4	-5.36	1.31	1.35
1	A	1507	A	C6-N1	-5.34	1.31	1.35
1	A	881	G	N9-C8	-5.33	1.34	1.37
1	A	655	A	N9-C4	-5.33	1.34	1.37
1	A	1487	G	N9-C8	-5.31	1.34	1.37
1	A	1514	C	N3-C4	-5.29	1.30	1.33
5	E	90	VAL	CB-CG1	-5.29	1.41	1.52
1	A	574	A	C6-N1	-5.27	1.31	1.35
1	A	1512	U	C4-O4	5.26	1.27	1.23
1	A	1350	A	N7-C5	-5.25	1.36	1.39
1	A	926	G	C5-C4	5.23	1.42	1.38
1	A	1507	A	N3-C4	-5.22	1.31	1.34
1	A	1513	A	C5-C4	-5.22	1.35	1.38
1	A	266	G	C2-N3	5.22	1.36	1.32
1	A	811	C	N1-C6	-5.22	1.34	1.37
1	A	1502	A	N7-C5	-5.20	1.36	1.39
1	A	704	A	N3-C4	-5.19	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	A	N9-C4	5.18	1.41	1.37
1	A	327	A	C5-C6	-5.18	1.36	1.41
1	A	1053	G	N7-C5	5.15	1.42	1.39
1	A	574	A	N3-C4	-5.15	1.31	1.34
1	A	1080	A	C6-N1	-5.12	1.31	1.35
1	A	1375	A	C6-N6	-5.12	1.29	1.33
1	A	134	A	N3-C4	-5.12	1.31	1.34
1	A	1084	G	C5-C6	5.12	1.47	1.42
1	A	855	G	N3-C4	-5.12	1.31	1.35
1	A	819	A	N3-C4	-5.11	1.31	1.34
1	A	813	U	N1-C6	-5.10	1.33	1.38
1	A	325	A	N9-C4	-5.09	1.34	1.37
1	A	828	A	N3-C4	-5.08	1.31	1.34
1	A	853	G	N7-C5	-5.08	1.36	1.39
1	A	117	G	N1-C2	5.07	1.41	1.37
1	A	640	A	N3-C4	-5.05	1.31	1.34
1	A	823	G	N3-C4	-5.05	1.31	1.35
1	A	117	G	C5-C4	5.05	1.41	1.38
1	A	781	A	N7-C5	-5.05	1.36	1.39
1	A	926	G	C2-N3	5.04	1.36	1.32
1	A	741	G	N9-C4	-5.04	1.33	1.38
1	A	120	A	C6-N1	-5.02	1.32	1.35
1	A	568	G	P-O5'	-5.01	1.54	1.59
1	A	1488	G	N9-C8	-5.01	1.34	1.37
1	A	1350	A	C5-C6	-5.01	1.36	1.41
1	A	239	U	C4-O4	-5.00	1.19	1.23
1	A	640	A	C6-N1	-5.00	1.32	1.35
1	A	74	C	N1-C6	5.00	1.40	1.37
1	A	654	G	C6-N1	-5.00	1.36	1.39
10	J	57	LYS	CB-CG	5.00	1.66	1.52

All (1817) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	G	C6-C5-N7	-19.86	118.48	130.40
1	A	366	C	N1-C2-O2	17.84	129.60	118.90
1	A	117	G	N1-C6-O6	15.21	129.03	119.90
1	A	1200	C	C2-N1-C1'	15.12	135.43	118.80
1	A	573	A	C8-N9-C4	-15.02	99.79	105.80
1	A	266	G	N1-C6-O6	14.91	128.85	119.90
1	A	1403	C	N3-C2-O2	14.11	131.78	121.90
1	A	1200	C	N1-C2-O2	14.05	127.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	858	G	C5-C6-N1	-13.71	104.64	111.50
1	A	366	C	N3-C2-O2	-13.36	112.55	121.90
1	A	1524	C	N3-C4-C5	-13.31	116.58	121.90
1	A	266	G	C5-C6-O6	-12.74	120.95	128.60
1	A	117	G	N9-C4-C5	-12.34	100.46	105.40
1	A	266	G	C4-C5-C6	12.10	126.06	118.80
1	A	1524	C	C6-N1-C2	-12.09	115.46	120.30
1	A	1092	A	N1-C6-N6	12.09	125.85	118.60
1	A	863	U	C2-N1-C1'	-12.03	103.27	117.70
1	A	1403	C	N1-C2-O2	-11.95	111.73	118.90
1	A	366	C	C2-N1-C1'	11.95	131.94	118.80
1	A	481	G	N1-C6-O6	11.95	127.07	119.90
1	A	1281	U	C5-C4-O4	11.94	133.06	125.90
1	A	624	C	C6-N1-C2	11.88	125.05	120.30
1	A	117	G	C6-C5-N7	-11.85	123.29	130.40
1	A	117	G	C2-N3-C4	-11.83	105.98	111.90
1	A	104	G	N1-C6-O6	11.73	126.94	119.90
1	A	144	G	N1-C6-O6	11.73	126.94	119.90
1	A	762	C	C6-N1-C2	11.70	124.98	120.30
1	A	579	G	N1-C6-O6	11.67	126.90	119.90
1	A	266	G	C4-C5-N7	11.64	115.45	110.80
1	A	873	A	C8-N9-C4	-11.51	101.20	105.80
1	A	1200	C	C5-C6-N1	11.48	126.74	121.00
1	A	1234	C	C6-N1-C2	11.42	124.87	120.30
1	A	1084	G	N3-C4-C5	-11.26	122.97	128.60
1	A	1079	G	C8-N9-C4	-11.20	101.92	106.40
1	A	1200	C	C6-N1-C1'	-11.19	107.38	120.80
1	A	586	C	C6-N1-C2	11.14	124.76	120.30
1	A	570	G	N3-C4-C5	-10.99	123.11	128.60
1	A	283	C	C2-N1-C1'	10.97	130.87	118.80
1	A	295	C	C6-N1-C2	10.96	124.68	120.30
1	A	117	G	C8-N9-C1'	-10.95	112.77	127.00
1	A	634	C	C6-N1-C2	-10.87	115.95	120.30
1	A	1084	G	C4-C5-N7	-10.80	106.48	110.80
1	A	788	U	N3-C4-O4	10.76	126.93	119.40
1	A	920	U	N3-C4-C5	-10.65	108.21	114.60
1	A	572	A	N1-C6-N6	-10.62	112.23	118.60
1	A	863	U	C5-C4-O4	10.58	132.25	125.90
1	A	868	C	N1-C2-O2	-10.58	112.55	118.90
1	A	732	C	N3-C4-C5	10.56	126.12	121.90
1	A	144	G	C5-C6-N1	-10.54	106.23	111.50
1	A	266	G	N7-C8-N9	10.54	118.37	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	A	C5-C6-N1	10.33	122.86	117.70
1	A	824	C	C6-N1-C2	10.31	124.42	120.30
1	A	449	C	C6-N1-C2	-10.25	116.20	120.30
1	A	572	A	N9-C4-C5	10.25	109.90	105.80
1	A	1502	A	C2-N3-C4	-10.24	105.48	110.60
1	A	248	C	C5-C6-N1	-10.22	115.89	121.00
1	A	644	G	C4-C5-N7	10.20	114.88	110.80
1	A	873	A	C2-N3-C4	10.20	115.70	110.60
1	A	863	U	C6-N1-C1'	10.18	135.45	121.20
1	A	248	C	C6-N1-C2	10.17	124.37	120.30
1	A	884	U	C5-C6-N1	-10.15	117.62	122.70
1	A	820	U	N1-C2-N3	10.05	120.93	114.90
1	A	1329	A	N1-C6-N6	10.02	124.61	118.60
1	A	860	A	C8-N9-C4	-10.00	101.80	105.80
1	A	703	G	C4-C5-N7	-9.97	106.81	110.80
1	A	176	C	C6-N1-C2	9.96	124.28	120.30
1	A	559	A	C6-N1-C2	-9.95	112.63	118.60
1	A	856	C	N1-C2-O2	-9.94	112.94	118.90
1	A	283	C	C5-C6-N1	9.94	125.97	121.00
1	A	1190	G	C4-N9-C1'	9.93	139.41	126.50
1	A	691	G	C8-N9-C4	-9.92	102.43	106.40
1	A	90	U	C5-C4-O4	9.90	131.84	125.90
1	A	117	G	C5-C6-N1	-9.90	106.55	111.50
1	A	770	C	C5-C6-N1	-9.90	116.05	121.00
1	A	648	A	C8-N9-C4	9.89	109.76	105.80
1	A	859	A	N1-C6-N6	9.89	124.53	118.60
1	A	266	G	C4-N9-C1'	9.87	139.33	126.50
1	A	729	A	N1-C6-N6	9.86	124.51	118.60
1	A	1530	G	N3-C4-C5	9.81	133.50	128.60
1	A	920	U	C5-C4-O4	9.76	131.75	125.90
1	A	866	C	C6-N1-C2	-9.75	116.40	120.30
1	A	1370	G	C8-N9-C4	-9.75	102.50	106.40
1	A	635	G	C2-N3-C4	-9.75	107.03	111.90
1	A	1381	U	N1-C2-O2	9.74	129.62	122.80
1	A	864	A	N1-C6-N6	-9.70	112.78	118.60
1	A	563	A	C8-N9-C4	-9.67	101.93	105.80
1	A	722	A	N1-C6-N6	9.67	124.40	118.60
1	A	825	G	C8-N9-C4	9.67	110.27	106.40
1	A	117	G	C8-N9-C4	9.66	110.26	106.40
1	A	1524	C	N1-C2-O2	-9.61	113.14	118.90
1	A	266	G	N3-C4-N9	9.58	131.75	126.00
1	A	146	G	N1-C6-O6	9.57	125.64	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	529	G	C4-C5-C6	9.54	124.52	118.80
1	A	139	G	C5-C6-N1	-9.53	106.74	111.50
1	A	232	G	C6-C5-N7	-9.51	124.69	130.40
1	A	1335	C	C6-N1-C2	9.51	124.10	120.30
1	A	563	A	N9-C4-C5	9.49	109.59	105.80
1	A	366	C	C6-N1-C1'	-9.48	109.43	120.80
1	A	1232	U	N1-C2-O2	-9.47	116.17	122.80
1	A	1066	C	C6-N1-C1'	-9.47	109.44	120.80
1	A	874	G	N1-C6-O6	9.47	125.58	119.90
1	A	703	G	C5-C6-O6	9.44	134.26	128.60
1	A	1528	U	C2-N1-C1'	9.43	129.02	117.70
1	A	91	C	C2-N1-C1'	9.43	129.17	118.80
1	A	481	G	C6-C5-N7	-9.43	124.75	130.40
1	A	266	G	C5-N7-C8	-9.42	99.59	104.30
1	A	768	A	C8-N9-C4	9.41	109.57	105.80
1	A	283	C	N1-C2-O2	9.40	124.54	118.90
1	A	328	C	N3-C4-N4	-9.38	111.44	118.00
1	A	732	C	C2-N3-C4	-9.36	115.22	119.90
1	A	621	A	C8-N9-C4	-9.32	102.07	105.80
1	A	815	A	C8-N9-C4	9.31	109.53	105.80
1	A	867	G	N1-C6-O6	9.31	125.49	119.90
1	A	1514	C	N1-C2-O2	-9.31	113.31	118.90
1	A	648	A	N7-C8-N9	-9.31	109.15	113.80
1	A	867	G	C8-N9-C1'	-9.30	114.90	127.00
1	A	698	G	C4-N9-C1'	9.29	138.58	126.50
1	A	795	C	N3-C2-O2	9.25	128.38	121.90
1	A	721	G	C6-C5-N7	-9.24	124.86	130.40
1	A	864	A	C5-C6-N6	9.21	131.07	123.70
1	A	90	U	N3-C4-O4	-9.20	112.96	119.40
1	A	1239	A	C8-N9-C4	9.20	109.48	105.80
1	A	529	G	N1-C6-O6	9.17	125.40	119.90
1	A	269	C	C5-C6-N1	-9.13	116.43	121.00
1	A	860	A	N9-C4-C5	9.13	109.45	105.80
1	A	722	A	C2-N3-C4	-9.10	106.05	110.60
1	A	1507	A	N1-C6-N6	-9.09	113.15	118.60
1	A	1200	C	C6-N1-C2	-9.08	116.67	120.30
1	A	559	A	C8-N9-C4	-9.08	102.17	105.80
1	A	644	G	C6-C5-N7	-9.06	124.96	130.40
1	A	577	G	C2-N3-C4	-9.06	107.37	111.90
1	A	940	C	C6-N1-C2	9.04	123.92	120.30
1	A	283	C	C2-N3-C4	9.02	124.41	119.90
1	A	818	G	N1-C6-O6	9.02	125.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	A	C5-N7-C8	-9.02	99.39	103.90
1	A	1381	U	N3-C2-O2	-9.00	115.90	122.20
1	A	635	G	C6-C5-N7	-8.99	125.00	130.40
1	A	481	G	C5-C6-N1	-8.98	107.01	111.50
1	A	1108	G	N3-C4-C5	-8.98	124.11	128.60
1	A	623	C	C6-N1-C2	8.97	123.89	120.30
1	A	1392	G	C6-C5-N7	-8.97	125.02	130.40
1	A	1107	C	C6-N1-C2	-8.96	116.72	120.30
1	A	881	G	C8-N9-C4	8.93	109.97	106.40
1	A	635	G	C5-C6-N1	-8.92	107.04	111.50
1	A	788	U	N3-C2-O2	8.91	128.44	122.20
1	A	975	A	N1-C6-N6	8.86	123.92	118.60
1	A	232	G	N1-C6-O6	8.86	125.22	119.90
1	A	284	G	N1-C6-O6	8.86	125.22	119.90
1	A	1186	G	N3-C4-C5	8.86	133.03	128.60
1	A	1068	G	C8-N9-C4	-8.84	102.86	106.40
1	A	1392	G	N1-C6-O6	8.83	125.20	119.90
1	A	91	C	C6-N1-C2	-8.82	116.77	120.30
1	A	783	C	C6-N1-C2	8.80	123.82	120.30
1	A	885	G	C2-N3-C4	-8.80	107.50	111.90
1	A	570	G	C8-N9-C4	-8.78	102.89	106.40
1	A	1524	C	C4-C5-C6	8.78	121.79	117.40
1	A	909	A	C5-C6-N6	-8.77	116.69	123.70
1	A	651	C	C6-N1-C2	8.73	123.79	120.30
1	A	698	G	C6-C5-N7	-8.73	125.16	130.40
1	A	529	G	C4-N9-C1'	8.73	137.85	126.50
1	A	621	A	N7-C8-N9	8.73	118.17	113.80
1	A	144	G	C2-N3-C4	-8.72	107.54	111.90
1	A	1053	G	C8-N9-C4	8.72	109.89	106.40
1	A	244	U	N1-C2-O2	8.72	128.90	122.80
1	A	91	C	N1-C2-O2	8.71	124.13	118.90
1	A	926	G	N3-C4-C5	-8.71	124.25	128.60
1	A	700	G	C4-C5-N7	8.70	114.28	110.80
1	A	700	G	N3-C4-N9	8.69	131.22	126.00
1	A	1066	C	C6-N1-C2	8.69	123.78	120.30
1	A	259	G	N1-C2-N3	8.68	129.11	123.90
1	A	1228	C	N1-C2-O2	8.68	124.11	118.90
1	A	741	G	N3-C4-N9	-8.68	120.80	126.00
1	A	814	A	C2-N3-C4	-8.67	106.27	110.60
1	A	1186	G	C2-N3-C4	-8.66	107.57	111.90
1	A	529	G	C8-N9-C1'	-8.64	115.77	127.00
1	A	50	A	C8-N9-C4	8.61	109.24	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	G	C5-C6-O6	-8.61	123.44	128.60
1	A	277	C	C6-N1-C2	8.60	123.74	120.30
1	A	1468	A	C8-N9-C4	8.59	109.24	105.80
1	A	795	C	N1-C2-O2	-8.58	113.75	118.90
1	A	1388	C	N3-C2-O2	8.55	127.89	121.90
1	A	266	G	C8-N9-C4	-8.55	102.98	106.40
1	A	868	C	C6-N1-C2	-8.55	116.88	120.30
1	A	618	C	C2-N1-C1'	-8.54	109.41	118.80
1	A	971	G	N1-C6-O6	8.53	125.02	119.90
1	A	909	A	N1-C6-N6	8.53	123.72	118.60
1	A	573	A	C4-C5-C6	8.52	121.26	117.00
1	A	1202	G	N1-C6-O6	-8.52	114.79	119.90
1	A	735	C	C6-N1-C2	8.52	123.71	120.30
1	A	858	G	N1-C6-O6	8.51	125.00	119.90
1	A	525	C	C6-N1-C2	8.50	123.70	120.30
1	A	127	G	C8-N9-C4	8.47	109.79	106.40
1	A	928	G	N1-C6-O6	8.47	124.98	119.90
1	A	232	G	C4-C5-N7	8.46	114.18	110.80
1	A	283	C	C6-N1-C2	-8.46	116.92	120.30
1	A	884	U	C4-C5-C6	8.46	124.77	119.70
1	A	1200	C	N3-C2-O2	-8.45	115.98	121.90
1	A	650	G	C8-N9-C4	8.45	109.78	106.40
1	A	780	A	C8-N9-C4	8.44	109.17	105.80
1	A	1080	A	N1-C6-N6	-8.43	113.54	118.60
1	A	382	A	C8-N9-C4	-8.42	102.43	105.80
1	A	656	C	C6-N1-C2	8.41	123.67	120.30
1	A	268	C	N1-C2-O2	8.40	123.94	118.90
1	A	519	C	N1-C2-O2	8.39	123.94	118.90
1	A	182	U	N3-C2-O2	-8.39	116.33	122.20
1	A	1083	U	N3-C2-O2	8.38	128.07	122.20
1	A	701	C	N1-C2-O2	8.37	123.92	118.90
1	A	721	G	N3-C4-N9	8.37	131.02	126.00
1	A	788	U	C5-C6-N1	8.37	126.88	122.70
1	A	872	A	C2-N3-C4	-8.36	106.42	110.60
1	A	572	A	C8-N9-C4	-8.36	102.46	105.80
1	A	874	G	C8-N9-C4	8.35	109.74	106.40
1	A	1527	C	C5-C4-N4	-8.34	114.36	120.20
1	A	111	G	N3-C4-N9	-8.34	121.00	126.00
1	A	763	G	C8-N9-C4	8.33	109.73	106.40
1	A	1202	G	C5-C6-O6	8.32	133.59	128.60
1	A	573	A	N7-C8-N9	8.32	117.96	113.80
1	A	1058	G	C8-N9-C4	8.31	109.72	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	716	A	N1-C6-N6	-8.29	113.63	118.60
1	A	8	A	C8-N9-C4	-8.28	102.49	105.80
1	A	175	C	C6-N1-C2	8.26	123.60	120.30
1	A	634	C	N3-C4-C5	-8.26	118.60	121.90
1	A	440	A	C2-N3-C4	-8.23	106.48	110.60
1	A	721	G	C4-C5-C6	8.23	123.74	118.80
1	A	810	C	N3-C4-N4	8.23	123.76	118.00
1	A	259	G	N1-C2-N2	-8.22	108.80	116.20
1	A	874	G	N9-C4-C5	-8.22	102.11	105.40
1	A	914	A	C8-N9-C4	-8.20	102.52	105.80
1	A	398	C	C6-N1-C2	8.19	123.58	120.30
1	A	559	A	N3-C4-C5	-8.18	121.08	126.80
1	A	814	A	N1-C2-N3	8.18	133.39	129.30
1	A	871	U	N1-C2-O2	8.18	128.53	122.80
1	A	1365	G	C8-N9-C4	-8.18	103.13	106.40
1	A	1054	C	N1-C2-O2	8.18	123.81	118.90
1	A	965	A	C8-N9-C4	8.17	109.07	105.80
1	A	721	G	C4-N9-C1'	8.16	137.11	126.50
1	A	132	C	C2-N3-C4	-8.15	115.82	119.90
1	A	283	C	N3-C4-C5	-8.14	118.64	121.90
1	A	867	G	C6-C5-N7	-8.12	125.53	130.40
1	A	1390	U	N3-C4-C5	-8.11	109.73	114.60
1	A	829	G	C8-N9-C4	8.11	109.64	106.40
1	A	1186	G	C5-C6-N1	-8.10	107.45	111.50
1	A	1392	G	C5-C6-N1	-8.10	107.45	111.50
1	A	266	G	C8-N9-C1'	-8.09	116.48	127.00
1	A	864	A	N9-C4-C5	8.08	109.03	105.80
1	A	1502	A	C5-N7-C8	-8.07	99.86	103.90
1	A	1512	U	N3-C4-C5	-8.07	109.76	114.60
1	A	873	A	C5-C6-N1	8.07	121.73	117.70
1	A	1190	G	N7-C8-N9	8.06	117.13	113.10
1	A	1530	G	N3-C4-N9	-8.05	121.17	126.00
1	A	816	A	N1-C6-N6	-8.05	113.77	118.60
1	A	1186	G	N3-C4-N9	-8.05	121.17	126.00
1	A	1452	C	N1-C2-O2	8.04	123.72	118.90
1	A	659	U	C5-C6-N1	-8.03	118.68	122.70
1	A	278	G	C4-C5-N7	-8.02	107.59	110.80
1	A	1083	U	C5-C4-O4	-8.02	121.09	125.90
1	A	32	A	C6-N1-C2	-8.01	113.80	118.60
1	A	1500	A	N1-C6-N6	-8.00	113.80	118.60
1	A	288	A	C2-N3-C4	-8.00	106.60	110.60
1	A	867	G	C4-N9-C1'	7.99	136.89	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1227	A	N1-C6-N6	7.99	123.39	118.60
1	A	788	U	N3-C4-C5	-7.99	109.81	114.60
1	A	481	G	C4-C5-C6	7.98	123.59	118.80
1	A	1279	A	C8-N9-C4	-7.98	102.61	105.80
1	A	91	C	N3-C2-O2	-7.97	116.32	121.90
1	A	940	C	C5-C6-N1	-7.97	117.02	121.00
1	A	807	A	N1-C2-N3	7.96	133.28	129.30
1	A	1092	A	N9-C4-C5	-7.96	102.62	105.80
1	A	1190	G	C8-N9-C1'	-7.96	116.66	127.00
1	A	479	C	N3-C4-C5	-7.95	118.72	121.90
1	A	820	U	N1-C2-O2	-7.95	117.23	122.80
1	A	885	G	N3-C4-C5	7.94	132.57	128.60
1	A	944	G	C5-C6-O6	7.94	133.36	128.60
1	A	1488	G	C8-N9-C4	7.94	109.58	106.40
1	A	265	G	N1-C2-N2	-7.93	109.06	116.20
1	A	1507	A	N9-C4-C5	7.93	108.97	105.80
1	A	1235	U	N1-C2-N3	7.93	119.66	114.90
1	A	704	A	C8-N9-C4	-7.93	102.63	105.80
1	A	609	A	C2-N3-C4	-7.92	106.64	110.60
1	A	815	A	N7-C8-N9	-7.92	109.84	113.80
1	A	853	G	C6-C5-N7	-7.92	125.65	130.40
1	A	1322	C	C2-N1-C1'	7.92	127.51	118.80
1	A	674	G	C8-N9-C4	7.92	109.57	106.40
1	A	970	C	N1-C2-O2	7.92	123.65	118.90
1	A	43	C	C6-N1-C2	7.91	123.47	120.30
1	A	299	G	N1-C6-O6	7.91	124.65	119.90
1	A	1528	U	C6-N1-C1'	-7.91	110.13	121.20
1	A	732	C	C5-C6-N1	-7.91	117.05	121.00
1	A	628	G	N3-C4-N9	7.91	130.74	126.00
1	A	721	G	C8-N9-C1'	-7.90	116.73	127.00
1	A	1064	G	N9-C4-C5	7.90	108.56	105.40
1	A	232	G	N9-C4-C5	-7.88	102.25	105.40
1	A	117	G	C4-N9-C1'	7.88	136.74	126.50
9	I	39	GLY	N-CA-C	-7.88	93.41	113.10
1	A	729	A	C5-C6-N6	-7.87	117.40	123.70
1	A	874	G	C5-C6-O6	-7.87	123.88	128.60
1	A	117	G	C4-C5-C6	7.87	123.52	118.80
1	A	852	G	N1-C6-O6	7.85	124.61	119.90
1	A	104	G	C6-C5-N7	-7.85	125.69	130.40
1	A	1344	C	C6-N1-C2	7.85	123.44	120.30
1	A	1493[A]	A	C5-N7-C8	-7.84	99.98	103.90
1	A	1493[B]	A	C5-N7-C8	-7.84	99.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1488	G	N7-C8-N9	-7.84	109.18	113.10
1	A	559	A	C5-C6-N1	7.84	121.62	117.70
1	A	813	U	C2-N1-C1'	7.84	127.10	117.70
24	a	39	G	N1-C6-O6	7.83	124.60	119.90
1	A	487	A	C8-N9-C4	7.83	108.93	105.80
1	A	522	C	C5-C6-N1	-7.83	117.09	121.00
20	T	20	LEU	CA-CB-CG	-7.83	97.30	115.30
1	A	266	G	N3-C4-C5	-7.82	124.69	128.60
1	A	1222	G	C5-C6-N1	-7.81	107.60	111.50
1	A	635	G	N1-C6-O6	7.80	124.58	119.90
1	A	858	G	C4-C5-C6	7.79	123.47	118.80
1	A	529	G	C5-C6-N1	-7.78	107.61	111.50
1	A	819	A	C4-C5-C6	7.78	120.89	117.00
1	A	596	C	C6-N1-C2	7.77	123.41	120.30
1	A	963	G	N1-C6-O6	7.75	124.55	119.90
1	A	135	C	N3-C4-C5	-7.75	118.80	121.90
1	A	383	A	N1-C6-N6	-7.74	113.96	118.60
1	A	580	U	N3-C4-C5	-7.74	109.96	114.60
1	A	570	G	C4-N9-C1'	7.74	136.56	126.50
1	A	400	C	N3-C4-C5	7.73	124.99	121.90
1	A	918	A	N1-C2-N3	7.73	133.16	129.30
1	A	1528	U	P-O3'-C3'	7.73	128.97	119.70
1	A	1092	A	C6-C5-N7	-7.72	126.89	132.30
1	A	190(G)	G	C5-C6-N1	-7.71	107.65	111.50
1	A	1414	U	N3-C2-O2	-7.71	116.81	122.20
1	A	1074	G	C5-C6-N1	-7.71	107.65	111.50
1	A	867	G	N3-C4-N9	7.70	130.62	126.00
1	A	522	C	C2-N1-C1'	-7.70	110.33	118.80
1	A	783	C	N3-C4-C5	7.69	124.98	121.90
1	A	1277	C	C6-N1-C2	-7.69	117.22	120.30
1	A	1099	G	N9-C4-C5	7.69	108.47	105.40
1	A	109	A	C2-N3-C4	-7.68	106.76	110.60
1	A	753	A	N9-C4-C5	7.68	108.87	105.80
1	A	813	U	C5-C4-O4	-7.67	121.30	125.90
1	A	1394	A	C5-C6-N6	-7.67	117.56	123.70
1	A	570	G	C2-N3-C4	7.67	115.74	111.90
1	A	128	G	N1-C6-O6	7.66	124.49	119.90
1	A	805	C	N3-C4-C5	7.66	124.96	121.90
1	A	770	C	C6-N1-C2	7.66	123.36	120.30
1	A	1108	G	C8-N9-C4	-7.66	103.34	106.40
1	A	783	C	N3-C4-N4	-7.65	112.64	118.00
1	A	55	A	N1-C6-N6	-7.63	114.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	G	C8-N9-C4	7.62	109.45	106.40
1	A	700	G	C6-C5-N7	-7.61	125.83	130.40
1	A	779	C	N1-C2-O2	-7.61	114.34	118.90
1	A	1230	C	N3-C4-N4	7.61	123.32	118.00
1	A	946	A	C6-N1-C2	-7.60	114.04	118.60
1	A	1390	U	N1-C2-N3	7.60	119.46	114.90
1	A	529	G	C6-C5-N7	-7.60	125.84	130.40
1	A	591	U	C5-C6-N1	-7.60	118.90	122.70
1	A	1496	C	N3-C4-C5	-7.60	118.86	121.90
1	A	697	U	C5-C6-N1	-7.59	118.90	122.70
1	A	1525	G	N1-C6-O6	-7.59	115.34	119.90
1	A	722	A	C6-C5-N7	-7.59	126.99	132.30
1	A	1353	G	N3-C4-C5	-7.59	124.81	128.60
1	A	1240	U	C5-C4-O4	7.58	130.45	125.90
1	A	1053	G	N7-C8-N9	-7.58	109.31	113.10
1	A	242	C	C4-C5-C6	7.58	121.19	117.40
1	A	326	G	C5-C6-N1	-7.57	107.72	111.50
1	A	858	G	N3-C2-N2	-7.57	114.60	119.90
1	A	32	A	C4-N9-C1'	7.57	139.92	126.30
1	A	572	A	C2-N3-C4	7.57	114.38	110.60
1	A	782	A	C8-N9-C4	-7.56	102.78	105.80
1	A	618	C	N3-C2-O2	7.56	127.19	121.90
1	A	297	G	N3-C4-C5	-7.55	124.82	128.60
1	A	1190	G	C8-N9-C4	-7.54	103.38	106.40
1	A	1403	C	N3-C4-N4	7.53	123.27	118.00
1	A	981	U	N3-C4-O4	7.52	124.67	119.40
1	A	1525	G	C5-C6-N1	7.52	115.26	111.50
1	A	579	G	C4-C5-N7	7.52	113.81	110.80
1	A	782	A	N9-C4-C5	7.52	108.81	105.80
1	A	400	C	N1-C2-O2	7.52	123.41	118.90
1	A	693	G	N1-C6-O6	7.52	124.41	119.90
1	A	1487	G	N3-C4-C5	-7.51	124.84	128.60
1	A	667	G	C2-N3-C4	-7.51	108.15	111.90
1	A	784	C	N3-C2-O2	-7.51	116.65	121.90
1	A	107	G	C4-C5-N7	7.49	113.80	110.80
1	A	928	G	C5-C6-O6	-7.49	124.10	128.60
1	A	1084	G	C5-N7-C8	7.49	108.05	104.30
1	A	1202	G	C4-C5-N7	-7.49	107.80	110.80
1	A	874	G	C8-N9-C1'	-7.49	117.26	127.00
1	A	698	G	C8-N9-C1'	-7.48	117.27	127.00
1	A	16	A	C8-N9-C4	7.48	108.79	105.80
1	A	1055	A	N1-C6-N6	-7.48	114.11	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	C	C6-N1-C2	-7.47	117.31	120.30
1	A	648	A	C5-N7-C8	7.46	107.63	103.90
1	A	27	G	C5-C6-O6	-7.46	124.13	128.60
1	A	893	C	N1-C2-O2	7.45	123.37	118.90
1	A	230	G	C8-N9-C1'	-7.45	117.32	127.00
1	A	859	A	C5-C6-N6	-7.44	117.75	123.70
1	A	881	G	C8-N9-C1'	-7.44	117.33	127.00
1	A	332	G	C5-C6-O6	-7.43	124.14	128.60
1	A	1281	U	N3-C4-O4	-7.42	114.20	119.40
1	A	781	A	C8-N9-C4	-7.42	102.83	105.80
1	A	923	A	C2-N3-C4	-7.42	106.89	110.60
1	A	920	U	C4-C5-C6	7.42	124.15	119.70
1	A	382	A	N9-C4-C5	7.40	108.76	105.80
1	A	628	G	N3-C4-C5	-7.40	124.90	128.60
1	A	637	G	C5-C6-N1	-7.39	107.80	111.50
1	A	698	G	N3-C4-C5	-7.39	124.91	128.60
1	A	1232	U	N3-C2-O2	7.38	127.37	122.20
1	A	760	G	C8-N9-C1'	-7.36	117.43	127.00
1	A	573	A	N9-C4-C5	7.36	108.75	105.80
1	A	1305	G	C5-C6-N1	-7.36	107.82	111.50
1	A	328	C	C5-C4-N4	7.36	125.35	120.20
1	A	1092	A	C5-C6-N6	-7.36	117.81	123.70
1	A	852	G	C5-C6-N1	-7.35	107.82	111.50
1	A	134	A	N1-C2-N3	7.33	132.97	129.30
1	A	745	C	C6-N1-C2	7.33	123.23	120.30
1	A	1094	G	C4-C5-N7	7.33	113.73	110.80
1	A	816	A	C5-C6-N6	7.33	129.56	123.70
1	A	946	A	N1-C6-N6	-7.32	114.21	118.60
1	A	436	C	C6-N1-C2	7.32	123.23	120.30
1	A	1068	G	N7-C8-N9	7.32	116.76	113.10
1	A	1199	U	N3-C2-O2	-7.31	117.08	122.20
1	A	251	G	N1-C2-N2	-7.31	109.62	116.20
1	A	447	G	N3-C4-N9	7.31	130.38	126.00
1	A	1370	G	N7-C8-N9	7.30	116.75	113.10
1	A	1084	G	N1-C6-O6	-7.30	115.52	119.90
1	A	635	G	N1-C2-N3	7.29	128.28	123.90
1	A	1092	A	C4-C5-N7	7.29	114.34	110.70
1	A	139	G	N1-C6-O6	7.29	124.27	119.90
1	A	38	G	N3-C4-N9	-7.28	121.63	126.00
1	A	1193	G	C5-C6-N1	-7.28	107.86	111.50
1	A	27	G	C8-N9-C4	-7.28	103.49	106.40
1	A	1080	A	N9-C4-C5	7.28	108.71	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	C	N3-C4-C5	7.27	124.81	121.90
1	A	823	G	C2-N3-C4	-7.27	108.26	111.90
1	A	1353	G	C8-N9-C4	-7.27	103.49	106.40
1	A	787	A	C5-N7-C8	-7.27	100.27	103.90
1	A	597	G	N3-C4-N9	7.26	130.36	126.00
1	A	1301	U	C6-N1-C2	-7.26	116.64	121.00
1	A	250	A	C5-C6-N1	-7.25	114.08	117.70
1	A	1205	U	N3-C2-O2	-7.24	117.13	122.20
1	A	1447	G	N1-C6-O6	7.24	124.25	119.90
1	A	1350	A	C5-N7-C8	-7.24	100.28	103.90
1	A	830	G	C2-N3-C4	-7.23	108.28	111.90
1	A	1143	G	N1-C6-O6	7.22	124.23	119.90
1	A	7	G	N9-C4-C5	-7.22	102.51	105.40
15	O	67	LEU	CA-CB-CG	-7.22	98.70	115.30
1	A	635	G	C4-C5-C6	7.20	123.12	118.80
1	A	577	G	N3-C4-C5	7.19	132.20	128.60
1	A	867	G	C4-C5-C6	7.19	123.11	118.80
1	A	1403	C	C6-N1-C2	7.19	123.18	120.30
1	A	254	G	C2-N3-C4	-7.19	108.31	111.90
1	A	451	A	C2-N3-C4	-7.19	107.00	110.60
1	A	586	C	C2-N1-C1'	-7.19	110.89	118.80
1	A	929	G	N1-C6-O6	7.18	124.21	119.90
1	A	1231	G	C8-N9-C1'	-7.18	117.66	127.00
1	A	868	C	N3-C4-C5	-7.18	119.03	121.90
1	A	32	A	C8-N9-C1'	-7.18	114.78	127.70
1	A	1530	G	C8-N9-C4	7.18	109.27	106.40
1	A	760	G	C6-C5-N7	-7.17	126.10	130.40
1	A	854	G	N1-C2-N2	-7.17	109.75	116.20
1	A	722	A	C4-C5-N7	7.16	114.28	110.70
1	A	197	A	N1-C6-N6	-7.16	114.30	118.60
1	A	1338	G	C5-C6-O6	7.16	132.90	128.60
1	A	109	A	N3-C4-N9	-7.16	121.67	127.40
1	A	522	C	C6-N1-C2	7.16	123.16	120.30
1	A	703	G	N9-C4-C5	7.16	108.26	105.40
1	A	732	C	C6-N1-C2	7.16	123.16	120.30
1	A	283	C	C6-N1-C1'	-7.15	112.22	120.80
1	A	20	U	C5-C6-N1	-7.15	119.12	122.70
1	A	783	C	C2-N1-C1'	-7.14	110.94	118.80
1	A	1399	C	C5-C4-N4	-7.14	115.20	120.20
1	A	183	G	C8-N9-C4	-7.14	103.54	106.40
1	A	583	A	N1-C6-N6	7.14	122.89	118.60
24	a	38	A	C5-C6-N1	-7.13	114.13	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	G	N1-C6-O6	7.13	124.18	119.90
1	A	718	G	N1-C6-O6	7.12	124.17	119.90
1	A	1230	C	C5-C4-N4	-7.11	115.22	120.20
1	A	813	U	N3-C4-O4	7.11	124.37	119.40
1	A	1227	A	C5-N7-C8	-7.10	100.35	103.90
1	A	365	U	C2-N1-C1'	7.10	126.22	117.70
1	A	1230	C	N3-C2-O2	7.10	126.87	121.90
1	A	50	A	N1-C2-N3	-7.10	125.75	129.30
1	A	1375	A	C5-C6-N1	7.10	121.25	117.70
1	A	729	A	C4-C5-N7	7.09	114.25	110.70
1	A	1310	G	C8-N9-C1'	-7.09	117.78	127.00
1	A	1276	G	N1-C6-O6	7.09	124.15	119.90
1	A	68	G	C8-N9-C4	7.08	109.23	106.40
1	A	91	C	C5-C6-N1	7.08	124.54	121.00
1	A	371	G	N1-C6-O6	-7.08	115.65	119.90
1	A	934	C	N1-C2-N3	-7.08	114.25	119.20
1	A	828	A	C2-N3-C4	-7.08	107.06	110.60
1	A	701	C	N3-C2-O2	-7.07	116.95	121.90
1	A	8	A	N9-C4-C5	7.07	108.63	105.80
1	A	856	C	N3-C4-C5	-7.07	119.07	121.90
1	A	698	G	N3-C4-N9	7.07	130.24	126.00
1	A	1190	G	C6-C5-N7	-7.07	126.16	130.40
1	A	120	A	N1-C6-N6	-7.06	114.36	118.60
1	A	895	G	C8-N9-C4	-7.06	103.58	106.40
1	A	945	G	C5-C6-N1	7.06	115.03	111.50
1	A	36	C	N3-C2-O2	-7.06	116.96	121.90
1	A	1388	C	C6-N1-C2	7.06	123.12	120.30
1	A	1507	A	C8-N9-C4	-7.05	102.98	105.80
1	A	365	U	N3-C4-O4	7.05	124.34	119.40
1	A	259	G	C2-N3-C4	-7.05	108.38	111.90
1	A	912	C	N3-C4-C5	7.05	124.72	121.90
1	A	1061	G	C2-N3-C4	-7.04	108.38	111.90
1	A	1380	U	N3-C2-O2	-7.04	117.27	122.20
1	A	269	C	C2-N3-C4	-7.04	116.38	119.90
1	A	1341	U	C5-C4-O4	7.04	130.12	125.90
1	A	799	G	N1-C6-O6	7.03	124.12	119.90
1	A	700	G	C5-C6-O6	-7.03	124.38	128.60
1	A	621	A	C5-N7-C8	-7.02	100.39	103.90
1	A	975	A	C4-C5-N7	7.01	114.21	110.70
1	A	681	C	C6-N1-C2	-7.01	117.50	120.30
1	A	190(G)	G	N1-C6-O6	7.01	124.11	119.90
1	A	104	G	C5-C6-N1	-7.01	108.00	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	G	C8-N9-C4	7.01	109.20	106.40
1	A	1322	C	N3-C4-C5	-7.01	119.10	121.90
1	A	250	A	C2-N3-C4	-7.00	107.10	110.60
1	A	1061	G	C5-C6-N1	-7.00	108.00	111.50
1	A	181	G	C4-N9-C1'	6.99	135.59	126.50
1	A	774	G	N1-C6-O6	6.99	124.09	119.90
1	A	940	C	C2-N3-C4	-6.99	116.41	119.90
1	A	552	U	C2-N3-C4	-6.98	122.81	127.00
1	A	1438	G	N1-C6-O6	6.98	124.09	119.90
1	A	1047	G	C8-N9-C4	6.98	109.19	106.40
1	A	117	G	C5-C6-O6	-6.98	124.41	128.60
1	A	316	G	N1-C6-O6	-6.98	115.71	119.90
1	A	329	A	C2-N3-C4	-6.98	107.11	110.60
1	A	1399	C	N3-C4-N4	6.97	122.88	118.00
1	A	674	G	N9-C4-C5	-6.97	102.61	105.40
1	A	278	G	N9-C4-C5	6.96	108.19	105.40
1	A	590	C	C6-N1-C2	6.96	123.09	120.30
1	A	817	C	C6-N1-C1'	-6.96	112.44	120.80
1	A	753	A	N1-C6-N6	-6.96	114.42	118.60
1	A	1403	C	C5-C4-N4	-6.96	115.33	120.20
1	A	552	U	N3-C2-O2	-6.96	117.33	122.20
1	A	854	G	C8-N9-C1'	-6.96	117.95	127.00
1	A	127	G	N1-C6-O6	6.96	124.07	119.90
1	A	447	G	C8-N9-C1'	-6.95	117.96	127.00
1	A	580	U	C5-C4-O4	6.95	130.07	125.90
1	A	722	A	C5-N7-C8	-6.95	100.42	103.90
1	A	1493[A]	A	N7-C8-N9	6.95	117.28	113.80
1	A	1493[B]	A	N7-C8-N9	6.95	117.28	113.80
1	A	27	G	C4-C5-N7	6.95	113.58	110.80
4	D	202	LEU	CA-CB-CG	-6.94	99.34	115.30
1	A	703	G	N1-C6-O6	-6.94	115.74	119.90
1	A	1421	G	C8-N9-C4	-6.94	103.62	106.40
1	A	686	U	C5-C4-O4	6.93	130.06	125.90
1	A	235	C	C6-N1-C2	6.93	123.07	120.30
1	A	946	A	C8-N9-C4	-6.93	103.03	105.80
1	A	1373	G	N9-C4-C5	6.93	108.17	105.40
1	A	295	C	C5-C6-N1	-6.92	117.54	121.00
1	A	755	G	C5-C6-O6	-6.92	124.45	128.60
10	J	58	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	A	182	U	N1-C2-O2	6.91	127.64	122.80
1	A	824	C	N3-C4-C5	6.91	124.66	121.90
1	A	549	C	C6-N1-C2	6.91	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	863	U	N3-C4-O4	-6.91	114.57	119.40
1	A	260	G	C5-C6-N1	-6.90	108.05	111.50
1	A	1442	G	C8-N9-C1'	-6.89	118.04	127.00
1	A	1525	G	N9-C4-C5	6.89	108.16	105.40
1	A	635	G	C8-N9-C1'	-6.89	118.04	127.00
1	A	1228	C	C2-N1-C1'	6.89	126.38	118.80
1	A	246	A	C2-N3-C4	6.88	114.04	110.60
1	A	975	A	C5-N7-C8	-6.88	100.46	103.90
1	A	1530	G	N7-C8-N9	-6.88	109.66	113.10
1	A	487	A	N7-C8-N9	-6.88	110.36	113.80
1	A	113	G	N1-C6-O6	6.87	124.02	119.90
1	A	758	G	C2-N3-C4	-6.87	108.46	111.90
1	A	1066	C	N1-C2-O2	6.86	123.02	118.90
1	A	919	A	N1-C6-N6	6.86	122.71	118.60
1	A	1323	G	C2-N3-C4	-6.86	108.47	111.90
1	A	167	G	C5-C6-N1	6.85	114.92	111.50
1	A	90	U	C2-N1-C1'	-6.85	109.48	117.70
1	A	700	G	N3-C2-N2	6.85	124.69	119.90
1	A	830	G	N1-C2-N3	6.85	128.01	123.90
1	A	787	A	C2-N3-C4	-6.85	107.18	110.60
1	A	1336	C	N3-C4-C5	-6.84	119.16	121.90
1	A	357	G	C4-C5-N7	-6.84	108.06	110.80
1	A	741	G	C4-N9-C1'	-6.84	117.61	126.50
1	A	852	G	C2-N3-C4	-6.84	108.48	111.90
24	a	39	G	C5-C6-O6	-6.84	124.50	128.60
1	A	729	A	C6-C5-N7	-6.83	127.52	132.30
1	A	884	U	N3-C2-O2	-6.83	117.42	122.20
1	A	1202	G	N3-C4-C5	-6.83	125.19	128.60
1	A	874	G	C6-C5-N7	-6.83	126.31	130.40
1	A	857	C	C6-N1-C2	6.82	123.03	120.30
1	A	881	G	N9-C4-C5	-6.82	102.67	105.40
1	A	104	G	C2-N3-C4	-6.82	108.49	111.90
1	A	188	C	N3-C4-C5	-6.82	119.17	121.90
1	A	1178	G	C8-N9-C4	-6.81	103.68	106.40
1	A	398	C	N3-C4-C5	6.81	124.62	121.90
1	A	1200	C	C2-N3-C4	6.80	123.30	119.90
1	A	1337	G	C5-C6-N1	-6.80	108.10	111.50
1	A	1338	G	N1-C6-O6	-6.79	115.83	119.90
1	A	193	C	C5-C6-N1	-6.78	117.61	121.00
25	b	3	U	N1-C2-O2	6.78	127.55	122.80
1	A	644	G	N3-C2-N2	6.78	124.64	119.90
1	A	1292	U	N3-C2-O2	6.78	126.94	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	39	G	N9-C4-C5	-6.78	102.69	105.40
1	A	947	G	C4-C5-N7	6.77	113.51	110.80
1	A	788	U	N1-C2-O2	-6.77	118.06	122.80
1	A	1310	G	N3-C4-N9	6.77	130.06	126.00
1	A	1343	G	C6-C5-N7	-6.77	126.34	130.40
1	A	1447	G	C4-C5-N7	6.77	113.51	110.80
1	A	677	U	N1-C2-N3	6.76	118.96	114.90
1	A	168	G	C5-C6-N1	-6.76	108.12	111.50
1	A	765	G	N1-C6-O6	6.75	123.95	119.90
1	A	285	G	N3-C4-C5	6.75	131.98	128.60
1	A	706	A	C2-N3-C4	-6.75	107.22	110.60
1	A	1195	C	N3-C4-N4	6.75	122.72	118.00
1	A	1249	C	C6-N1-C2	-6.75	117.60	120.30
1	A	133	U	C5-C4-O4	6.75	129.95	125.90
1	A	1202	G	N9-C4-C5	6.75	108.10	105.40
1	A	677	U	N3-C2-O2	-6.74	117.48	122.20
1	A	973	G	C8-N9-C4	6.74	109.10	106.40
1	A	1054	C	C2-N3-C4	6.74	123.27	119.90
1	A	32	A	N3-C4-C5	-6.73	122.09	126.80
1	A	563	A	N1-C6-N6	-6.73	114.56	118.60
1	A	27	G	C5-N7-C8	-6.73	100.94	104.30
1	A	1338	G	N9-C4-C5	6.72	108.09	105.40
1	A	383	A	N9-C4-C5	6.72	108.49	105.80
1	A	1329	A	C5-C6-N6	-6.71	118.33	123.70
1	A	400	C	N3-C4-N4	-6.71	113.30	118.00
1	A	662	G	N1-C6-O6	6.71	123.92	119.90
17	Q	63	ARG	NE-CZ-NH1	-6.71	116.95	120.30
1	A	73	C	C5-C6-N1	6.70	124.35	121.00
1	A	644	G	N1-C2-N2	-6.70	110.17	116.20
1	A	964	A	C8-N9-C4	-6.70	103.12	105.80
1	A	1066	C	N1-C2-N3	-6.70	114.51	119.20
1	A	623	C	C5-C6-N1	-6.70	117.65	121.00
1	A	157	G	N1-C6-O6	6.69	123.92	119.90
1	A	615	C	C6-N1-C2	-6.69	117.62	120.30
1	A	824	C	C5-C6-N1	-6.68	117.66	121.00
1	A	1442	G	C4-N9-C1'	6.68	135.18	126.50
1	A	762	C	N3-C4-C5	6.68	124.57	121.90
1	A	64	G	N1-C6-O6	6.67	123.91	119.90
1	A	885	G	N1-C6-O6	6.67	123.90	119.90
1	A	275	G	N9-C4-C5	-6.67	102.73	105.40
24	a	39	G	C4-C5-N7	6.67	113.47	110.80
1	A	1447	G	C5-C6-O6	-6.67	124.60	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	G	N7-C8-N9	6.66	116.43	113.10
1	A	747	C	C6-N1-C2	6.66	122.96	120.30
1	A	975	A	N9-C4-C5	-6.66	103.14	105.80
1	A	285	G	C2-N3-C4	-6.66	108.57	111.90
1	A	586	C	C5-C6-N1	-6.66	117.67	121.00
1	A	687	A	P-O3'-C3'	6.66	127.69	119.70
1	A	1077	G	C6-C5-N7	-6.66	126.41	130.40
1	A	28	G	N9-C4-C5	6.65	108.06	105.40
1	A	1405	G	N3-C4-C5	6.65	131.93	128.60
1	A	729	A	N7-C8-N9	6.65	117.12	113.80
1	A	16	A	C2-N3-C4	-6.64	107.28	110.60
1	A	1234	C	N1-C2-N3	-6.64	114.55	119.20
1	A	14	U	C6-N1-C2	-6.64	117.02	121.00
1	A	275	G	C8-N9-C1'	-6.64	118.37	127.00
1	A	795	C	N3-C4-C5	-6.64	119.24	121.90
1	A	782	A	N1-C2-N3	6.64	132.62	129.30
1	A	18	C	C6-N1-C2	6.64	122.95	120.30
1	A	109	A	N9-C4-C5	6.64	108.45	105.80
1	A	828	A	C5-N7-C8	-6.64	100.58	103.90
1	A	1282	C	C6-N1-C2	-6.63	117.65	120.30
1	A	171	A	N1-C6-N6	-6.62	114.63	118.60
1	A	873	A	N7-C8-N9	6.62	117.11	113.80
1	A	247	G	C8-N9-C4	6.62	109.05	106.40
1	A	873	A	N3-C4-C5	-6.62	122.17	126.80
1	A	117	G	N1-C2-N3	6.61	127.87	123.90
1	A	529	G	N3-C4-N9	6.61	129.97	126.00
1	A	1483	A	N1-C6-N6	-6.61	114.63	118.60
17	Q	9	VAL	CB-CA-C	-6.61	98.85	111.40
1	A	275	G	C8-N9-C4	6.60	109.04	106.40
1	A	47	C	N3-C4-C5	6.59	124.54	121.90
1	A	700	G	N9-C4-C5	-6.59	102.76	105.40
1	A	1073	U	C5-C6-N1	-6.59	119.41	122.70
1	A	1107	C	C5-C6-N1	6.59	124.29	121.00
1	A	818	G	N3-C2-N2	-6.58	115.29	119.90
1	A	1226	C	C6-N1-C2	6.58	122.93	120.30
1	A	529	G	N3-C4-C5	-6.58	125.31	128.60
1	A	934	C	N1-C2-O2	6.58	122.85	118.90
1	A	784	C	C6-N1-C2	-6.58	117.67	120.30
1	A	824	C	C2-N1-C1'	-6.57	111.57	118.80
1	A	130	A	C2-N3-C4	-6.57	107.31	110.60
1	A	620	C	N1-C2-O2	6.57	122.84	118.90
1	A	1322	C	N3-C4-N4	6.57	122.60	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	G	N1-C2-N2	6.57	122.11	116.20
1	A	1079	G	N7-C8-N9	6.57	116.38	113.10
1	A	449	C	N3-C4-N4	6.56	122.59	118.00
1	A	543	C	C6-N1-C2	-6.56	117.67	120.30
1	A	644	G	C5-N7-C8	-6.56	101.02	104.30
1	A	7	G	N3-C4-N9	6.56	129.94	126.00
1	A	818	G	C5-C6-N1	-6.56	108.22	111.50
1	A	559	A	N1-C2-N3	6.56	132.58	129.30
1	A	563	A	C2-N3-C4	6.56	113.88	110.60
1	A	1227	A	C4-C5-N7	6.56	113.98	110.70
1	A	1227	A	C2-N3-C4	-6.56	107.32	110.60
1	A	521	G	N1-C6-O6	-6.56	115.97	119.90
1	A	784	C	N3-C4-C5	-6.56	119.28	121.90
1	A	1524	C	N3-C4-N4	6.55	122.59	118.00
1	A	734	G	N1-C6-O6	6.55	123.83	119.90
1	A	365	U	C5-C4-O4	-6.55	121.97	125.90
1	A	251	G	N3-C4-N9	6.55	129.93	126.00
1	A	676	A	C8-N9-C4	6.55	108.42	105.80
1	A	525	C	N3-C2-O2	6.55	126.48	121.90
1	A	1094	G	N9-C4-C5	-6.55	102.78	105.40
1	A	170	U	C5-C6-N1	-6.54	119.43	122.70
1	A	265	G	C2-N3-C4	-6.54	108.63	111.90
1	A	1033	G	C8-N9-C4	-6.54	103.78	106.40
1	A	1414	U	C5-C6-N1	-6.54	119.43	122.70
1	A	403	C	C5-C6-N1	-6.54	117.73	121.00
1	A	1500	A	N9-C4-C5	6.54	108.42	105.80
1	A	620	C	C6-N1-C2	6.53	122.91	120.30
1	A	854	G	C6-C5-N7	-6.53	126.48	130.40
1	A	1249	C	N3-C4-C5	-6.53	119.29	121.90
1	A	1341	U	C2-N1-C1'	-6.53	109.86	117.70
1	A	372	C	C6-N1-C1'	-6.53	112.97	120.80
1	A	1058	G	N7-C8-N9	-6.53	109.84	113.10
1	A	971	G	C5-C6-N1	-6.52	108.24	111.50
1	A	32	A	N3-C4-N9	6.52	132.62	127.40
1	A	770	C	C2-N3-C4	-6.52	116.64	119.90
1	A	742	G	N3-C4-N9	-6.52	122.09	126.00
1	A	859	A	N9-C4-C5	-6.51	103.19	105.80
1	A	1060	C	C2-N1-C1'	6.51	125.97	118.80
1	A	745	C	N3-C4-C5	6.51	124.50	121.90
1	A	1502	A	C4-C5-N7	6.51	113.96	110.70
1	A	885	G	C5-C6-N1	-6.51	108.25	111.50
1	A	365	U	C6-N1-C1'	-6.51	112.09	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	A	C5-N7-C8	-6.51	100.65	103.90
1	A	651	C	N3-C2-O2	6.51	126.45	121.90
1	A	889	A	N1-C2-N3	6.50	132.55	129.30
1	A	918	A	C6-N1-C2	-6.50	114.70	118.60
1	A	698	G	C4-C5-C6	6.50	122.70	118.80
1	A	229	U	N1-C2-O2	-6.50	118.25	122.80
1	A	1084	G	C6-N1-C2	-6.49	121.20	125.10
1	A	1051	C	N3-C4-C5	-6.49	119.30	121.90
1	A	1390	U	C4-C5-C6	6.48	123.59	119.70
1	A	963	G	C5-C6-N1	-6.48	108.26	111.50
1	A	268	C	C6-N1-C2	6.48	122.89	120.30
1	A	1053	G	C5-N7-C8	6.47	107.54	104.30
1	A	534	U	N3-C2-O2	6.47	126.73	122.20
1	A	760	G	C4-N9-C1'	6.47	134.91	126.50
1	A	111	G	N3-C4-C5	6.46	131.83	128.60
1	A	774	G	N9-C4-C5	-6.46	102.81	105.40
1	A	13	U	N3-C4-O4	6.46	123.92	119.40
1	A	181	G	N3-C4-C5	-6.46	125.37	128.60
1	A	276	G	N1-C6-O6	-6.46	116.03	119.90
1	A	1341	U	N3-C4-O4	-6.46	114.88	119.40
1	A	725	G	C5-C6-N1	6.45	114.73	111.50
1	A	693	G	C5-C6-O6	-6.45	124.73	128.60
1	A	1301	U	N3-C4-C5	-6.45	110.73	114.60
1	A	597	G	N1-C2-N2	-6.44	110.40	116.20
1	A	108	G	N1-C6-O6	6.44	123.76	119.90
1	A	258	G	N1-C6-O6	6.44	123.76	119.90
1	A	644	G	C4-N9-C1'	6.43	134.87	126.50
1	A	77	G	N3-C4-N9	6.43	129.86	126.00
1	A	761	G	C2-N3-C4	-6.43	108.69	111.90
1	A	867	G	N9-C4-C5	-6.42	102.83	105.40
1	A	867	G	N1-C2-N3	6.42	127.75	123.90
1	A	654	G	N1-C2-N2	-6.42	110.42	116.20
1	A	798	G	N1-C2-N2	6.42	121.98	116.20
1	A	825	G	N7-C8-N9	-6.42	109.89	113.10
1	A	561	U	N3-C4-O4	6.42	123.89	119.40
1	A	789	U	C5-C6-N1	6.42	125.91	122.70
1	A	248	C	C2-N3-C4	-6.41	116.69	119.90
1	A	1350	A	C8-N9-C4	-6.41	103.23	105.80
1	A	204	U	C2-N1-C1'	6.41	125.39	117.70
1	A	522	C	N3-C4-N4	-6.41	113.51	118.00
1	A	15	G	N1-C6-O6	6.41	123.74	119.90
1	A	1199	U	C6-N1-C2	-6.40	117.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1390	U	C6-N1-C2	-6.40	117.16	121.00
1	A	92	C	C6-N1-C1'	-6.39	113.13	120.80
1	A	1433	A	N1-C2-N3	6.39	132.50	129.30
1	A	635	G	N9-C4-C5	-6.39	102.84	105.40
1	A	807	A	N7-C8-N9	-6.39	110.61	113.80
1	A	1092	A	C5-N7-C8	-6.39	100.71	103.90
1	A	868	C	N3-C4-N4	6.39	122.47	118.00
1	A	870	U	C5-C6-N1	-6.38	119.51	122.70
1	A	721	G	N1-C2-N2	-6.38	110.46	116.20
1	A	1183	A	N1-C6-N6	6.38	122.43	118.60
1	A	390	C	N3-C4-N4	6.38	122.47	118.00
1	A	1099	G	C4-C5-N7	-6.38	108.25	110.80
1	A	32	A	C4-C5-C6	6.38	120.19	117.00
1	A	90	U	C6-N1-C1'	6.38	130.13	121.20
1	A	679	C	N1-C2-O2	-6.38	115.07	118.90
1	A	297	G	C8-N9-C4	-6.38	103.85	106.40
1	A	866	C	N1-C2-N3	6.37	123.66	119.20
1	A	1340	A	C2-N3-C4	-6.37	107.42	110.60
1	A	123	C	N3-C4-C5	-6.37	119.35	121.90
1	A	928	G	C6-C5-N7	-6.37	126.58	130.40
1	A	9	G	C4-C5-N7	6.36	113.34	110.80
1	A	129	U	N1-C2-N3	6.36	118.72	114.90
1	A	618	C	C6-N1-C2	6.36	122.84	120.30
1	A	946	A	N9-C4-C5	6.36	108.34	105.80
1	A	1073	U	C6-N1-C2	6.36	124.82	121.00
1	A	1107	C	N3-C4-C5	-6.36	119.36	121.90
1	A	447	G	N9-C4-C5	-6.36	102.86	105.40
1	A	77	G	C4-C5-N7	6.36	113.34	110.80
1	A	524	G	C5-C6-N1	-6.36	108.32	111.50
1	A	789	U	C6-N1-C2	-6.35	117.19	121.00
1	A	902	G	C8-N9-C4	6.35	108.94	106.40
1	A	639	G	C5-C6-O6	-6.35	124.79	128.60
1	A	269	C	C4-C5-C6	6.34	120.57	117.40
1	A	703	G	C5-N7-C8	6.34	107.47	104.30
1	A	230	G	C4-N9-C1'	6.34	134.74	126.50
1	A	1237	C	C4-C5-C6	6.33	120.57	117.40
1	A	960	U	N1-C2-O2	6.33	127.23	122.80
1	A	28	G	C4-C5-N7	-6.33	108.27	110.80
1	A	671	G	C5-C6-N1	-6.33	108.34	111.50
1	A	839	U	N1-C2-O2	6.33	127.23	122.80
1	A	579	G	C5-N7-C8	-6.32	101.14	104.30
1	A	874	G	C4-C5-N7	6.32	113.33	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	194	LEU	CA-CB-CG	6.32	129.84	115.30
1	A	721	G	C5-C6-N1	-6.32	108.34	111.50
9	I	47	LEU	CA-CB-CG	-6.32	100.77	115.30
1	A	924	C	N3-C2-O2	6.32	126.32	121.90
1	A	407	G	C2-N3-C4	-6.31	108.75	111.90
1	A	962	C	C6-N1-C2	6.31	122.82	120.30
1	A	616	G	C5-C6-N1	-6.31	108.35	111.50
1	A	741	G	N3-C4-C5	6.31	131.75	128.60
1	A	154	C	C5-C4-N4	-6.30	115.79	120.20
1	A	830	G	N1-C6-O6	6.30	123.68	119.90
1	A	881	G	N3-C4-N9	6.30	129.78	126.00
1	A	1487	G	C8-N9-C4	-6.30	103.88	106.40
1	A	1497	G	N3-C4-N9	6.29	129.78	126.00
1	A	372	C	C6-N1-C2	6.29	122.82	120.30
1	A	428	G	C8-N9-C4	-6.29	103.88	106.40
1	A	91	C	N3-C4-N4	6.29	122.40	118.00
1	A	342	C	C6-N1-C2	-6.29	117.79	120.30
1	A	1279	A	N7-C8-N9	6.29	116.94	113.80
1	A	1205	U	C2-N1-C1'	6.28	125.24	117.70
1	A	597	G	C6-C5-N7	-6.28	126.63	130.40
1	A	1530	G	C5-C6-N1	-6.28	108.36	111.50
1	A	77	G	N9-C4-C5	-6.28	102.89	105.40
1	A	557	G	N9-C4-C5	6.28	107.91	105.40
1	A	810	C	C5-C4-N4	-6.28	115.81	120.20
1	A	1389	C	C6-N1-C2	6.28	122.81	120.30
1	A	1350	A	N7-C8-N9	6.27	116.94	113.80
1	A	250	A	C8-N9-C4	6.27	108.31	105.80
1	A	297	G	C4-N9-C1'	6.27	134.65	126.50
1	A	721	G	N3-C4-C5	-6.27	125.46	128.60
1	A	774	G	C4-C5-N7	6.27	113.31	110.80
1	A	1074	G	C2-N3-C4	-6.27	108.77	111.90
1	A	1362	C	C6-N1-C2	-6.27	117.79	120.30
1	A	91	C	C5-C4-N4	-6.26	115.81	120.20
1	A	691	G	N7-C8-N9	6.26	116.23	113.10
1	A	788	U	C2-N3-C4	6.26	130.76	127.00
1	A	927	G	N1-C6-O6	6.26	123.66	119.90
1	A	285	G	C5-C6-N1	-6.26	108.37	111.50
1	A	246	A	N1-C2-N3	-6.26	126.17	129.30
1	A	1342	C	N1-C2-O2	-6.26	115.15	118.90
1	A	125	U	N1-C2-N3	6.25	118.65	114.90
1	A	1531	A	N7-C8-N9	6.25	116.92	113.80
1	A	637	G	N1-C6-O6	6.25	123.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	C	C2-N1-C1'	6.24	125.67	118.80
1	A	795	C	C6-N1-C2	6.24	122.80	120.30
1	A	252	U	C5-C6-N1	-6.24	119.58	122.70
1	A	1327	C	C4-C5-C6	6.24	120.52	117.40
1	A	32	A	C5-C6-N6	-6.23	118.71	123.70
1	A	947	G	N9-C4-C5	-6.23	102.91	105.40
1	A	1068	G	N3-C4-C5	-6.23	125.49	128.60
1	A	1281	U	N1-C2-N3	6.23	118.64	114.90
1	A	981	U	C5-C6-N1	6.22	125.81	122.70
1	A	665	A	C5-N7-C8	-6.22	100.79	103.90
1	A	969	A	N1-C6-N6	6.22	122.33	118.60
1	A	1310	G	C4-N9-C1'	6.22	134.59	126.50
1	A	598	U	N1-C2-O2	-6.22	118.45	122.80
1	A	260	G	N1-C2-N3	6.22	127.63	123.90
1	A	928	G	C4-C5-N7	6.21	113.28	110.80
1	A	1329	A	C6-C5-N7	-6.21	127.95	132.30
1	A	162	A	C8-N9-C4	-6.21	103.32	105.80
1	A	1157	A	C5-C6-N6	6.21	128.67	123.70
1	A	1228	C	C6-N1-C1'	-6.21	113.35	120.80
1	A	1338	G	C4-C5-N7	-6.21	108.32	110.80
1	A	199	G	C2-N3-C4	-6.20	108.80	111.90
1	A	828	A	N1-C6-N6	6.20	122.32	118.60
1	A	1178	G	N9-C4-C5	6.20	107.88	105.40
1	A	1512	U	C4-C5-C6	6.19	123.42	119.70
1	A	201	C	C2-N1-C1'	6.19	125.61	118.80
1	A	1157	A	N1-C6-N6	-6.19	114.89	118.60
1	A	232	G	C5-N7-C8	-6.18	101.21	104.30
1	A	400	C	N3-C2-O2	-6.18	117.57	121.90
1	A	7	G	C8-N9-C1'	-6.18	118.97	127.00
1	A	242	C	C5-C6-N1	-6.18	117.91	121.00
1	A	246	A	N7-C8-N9	-6.18	110.71	113.80
1	A	50	A	C4-C5-C6	-6.18	113.91	117.00
1	A	640	A	N1-C2-N3	6.17	132.39	129.30
1	A	884	U	N1-C2-O2	6.17	127.12	122.80
1	A	558	G	C4-C5-N7	6.16	113.27	110.80
1	A	887	G	N1-C2-N3	6.16	127.60	123.90
1	A	1066	C	C2-N1-C1'	6.16	125.58	118.80
1	A	859	A	C8-N9-C4	6.16	108.27	105.80
1	A	862	C	N3-C4-C5	6.16	124.36	121.90
1	A	673	G	C5-C6-O6	-6.16	124.90	128.60
1	A	1209	C	C6-N1-C2	-6.16	117.84	120.30
1	A	912	C	C4-C5-C6	-6.15	114.32	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190(E)	U	C2-N3-C4	-6.15	123.31	127.00
1	A	1064	G	N3-C2-N2	-6.15	115.59	119.90
1	A	1231	G	N3-C4-N9	6.15	129.69	126.00
24	a	39	G	C8-N9-C4	6.15	108.86	106.40
1	A	284	G	C6-C5-N7	-6.15	126.71	130.40
1	A	1235	U	N1-C2-O2	-6.15	118.50	122.80
1	A	898	G	N1-C2-N3	6.14	127.59	123.90
1	A	848	C	C5-C6-N1	6.14	124.07	121.00
1	A	1442	G	N3-C4-C5	-6.14	125.53	128.60
1	A	285	G	N1-C6-O6	6.14	123.58	119.90
1	A	897	C	N3-C4-C5	6.13	124.35	121.90
1	A	1103	C	C5-C6-N1	-6.13	117.93	121.00
1	A	1487	G	N9-C4-C5	6.13	107.85	105.40
1	A	109	A	C8-N9-C4	-6.13	103.35	105.80
1	A	181	G	C4-C5-C6	6.13	122.48	118.80
1	A	755	G	N1-C6-O6	6.13	123.58	119.90
1	A	900	A	C2-N3-C4	-6.13	107.54	110.60
1	A	257	G	C8-N9-C4	6.12	108.85	106.40
1	A	1493[A]	A	C3'-C2'-C1'	-6.12	96.60	101.50
1	A	1493[B]	A	C3'-C2'-C1'	-6.12	96.60	101.50
1	A	265	G	N9-C4-C5	-6.12	102.95	105.40
1	A	926	G	N3-C4-N9	6.12	129.67	126.00
1	A	970	C	N3-C2-O2	-6.12	117.62	121.90
1	A	1391	U	C5-C6-N1	-6.12	119.64	122.70
1	A	1500	A	C6-N1-C2	-6.12	114.93	118.60
1	A	524	G	N1-C6-O6	6.11	123.57	119.90
1	A	35	G	N1-C6-O6	6.11	123.56	119.90
1	A	1253	G	C6-C5-N7	-6.11	126.74	130.40
1	A	1300	G	N9-C4-C5	6.10	107.84	105.40
1	A	1487	G	C6-N1-C2	-6.10	121.44	125.10
1	A	540	G	N1-C6-O6	6.10	123.56	119.90
1	A	230	G	N1-C2-N2	-6.10	110.71	116.20
1	A	373	A	C5-C6-N6	6.10	128.58	123.70
1	A	1058	G	C6-C5-N7	6.10	134.06	130.40
1	A	1483	A	C5-N7-C8	6.09	106.95	103.90
1	A	782	A	N1-C6-N6	-6.09	114.94	118.60
1	A	130	A	C5-N7-C8	-6.09	100.86	103.90
1	A	976	G	C2-N3-C4	-6.09	108.86	111.90
1	A	910	C	C2-N3-C4	-6.08	116.86	119.90
1	A	1531	A	C5-C6-N6	-6.08	118.83	123.70
1	A	144	G	C6-C5-N7	-6.08	126.75	130.40
1	A	335	C	C5-C6-N1	-6.08	117.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	C	N3-C4-C5	6.07	124.33	121.90
1	A	768	A	N7-C8-N9	-6.07	110.77	113.80
8	H	38	ILE	CB-CA-C	-6.07	99.46	111.60
1	A	115	G	C5-C6-N1	6.07	114.53	111.50
1	A	654	G	N1-C2-N3	6.07	127.54	123.90
1	A	174	C	C5-C4-N4	-6.06	115.95	120.20
1	A	733	A	C2-N3-C4	-6.06	107.57	110.60
1	A	833	U	N3-C2-O2	-6.05	117.96	122.20
1	A	812	C	C6-N1-C2	-6.05	117.88	120.30
1	A	1488	G	C5-N7-C8	6.05	107.32	104.30
1	A	127	G	N3-C4-C5	6.04	131.62	128.60
1	A	741	G	C4-C5-N7	-6.04	108.38	110.80
1	A	631	G	C4-N9-C1'	6.04	134.35	126.50
1	A	586	C	N3-C4-C5	6.03	124.31	121.90
1	A	1502	A	C6-C5-N7	-6.03	128.08	132.30
1	A	1237	C	N3-C4-C5	-6.03	119.49	121.90
1	A	742	G	N1-C2-N2	6.03	121.63	116.20
1	A	1079	G	N9-C4-C5	6.03	107.81	105.40
1	A	263	A	N1-C6-N6	-6.03	114.98	118.60
1	A	78	G	N1-C6-O6	6.03	123.52	119.90
1	A	1029	C	C6-N1-C2	-6.03	117.89	120.30
8	H	12	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	A	300	A	C4-C5-C6	6.02	120.01	117.00
1	A	868	C	N3-C2-O2	6.02	126.12	121.90
1	A	260	G	C4-C5-C6	6.02	122.41	118.80
1	A	363	A	C2-N3-C4	-6.02	107.59	110.60
1	A	1487	G	C4-N9-C1'	6.02	134.32	126.50
1	A	572	A	C6-N1-C2	-6.01	114.99	118.60
1	A	1505	G	N3-C2-N2	-6.01	115.69	119.90
1	A	1399	C	C6-N1-C2	-6.00	117.90	120.30
1	A	447	G	C6-C5-N7	-6.00	126.80	130.40
1	A	570	G	N9-C4-C5	6.00	107.80	105.40
1	A	1497	G	C8-N9-C1'	-6.00	119.20	127.00
1	A	852	G	C8-N9-C4	6.00	108.80	106.40
1	A	1337	G	N1-C6-O6	5.99	123.50	119.90
1	A	854	G	C2-N3-C4	-5.99	108.91	111.90
1	A	873	A	N9-C4-C5	5.99	108.19	105.80
1	A	1084	G	C5-C6-O6	5.98	132.19	128.60
1	A	79	G	N7-C8-N9	5.98	116.09	113.10
1	A	145	G	N1-C6-O6	5.97	123.48	119.90
1	A	21	G	N3-C4-N9	5.97	129.58	126.00
1	A	607	A	C5-C6-N1	-5.97	114.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	893	C	C2-N3-C4	5.97	122.89	119.90
1	A	896	C	C6-N1-C2	-5.97	117.91	120.30
1	A	1491	G	N3-C2-N2	-5.97	115.72	119.90
1	A	374	A	C8-N9-C4	5.97	108.19	105.80
1	A	1074	G	C4-C5-C6	5.97	122.38	118.80
1	A	1530	G	N3-C2-N2	-5.97	115.72	119.90
1	A	1325	C	C6-N1-C2	-5.97	117.91	120.30
1	A	1353	G	C2-N3-C4	5.96	114.88	111.90
1	A	117	G	C4-C5-N7	5.96	113.19	110.80
1	A	944	G	N1-C6-O6	-5.96	116.32	119.90
1	A	259	G	C4-C5-C6	5.96	122.38	118.80
1	A	786	G	N1-C6-O6	5.96	123.47	119.90
1	A	1531	A	C8-N9-C4	-5.96	103.42	105.80
1	A	768	A	N1-C6-N6	5.96	122.17	118.60
1	A	774	G	C5-C6-O6	-5.95	125.03	128.60
1	A	856	C	C4-C5-C6	5.95	120.38	117.40
1	A	1094	G	C6-C5-N7	-5.95	126.83	130.40
1	A	349	A	N1-C6-N6	-5.95	115.03	118.60
1	A	651	C	N3-C4-C5	5.95	124.28	121.90
1	A	712	A	N1-C2-N3	5.95	132.27	129.30
1	A	767	A	N9-C4-C5	5.95	108.18	105.80
1	A	946	A	C5-C6-N1	5.95	120.67	117.70
1	A	1531	A	C5-N7-C8	-5.95	100.93	103.90
1	A	38	G	C8-N9-C1'	5.94	134.72	127.00
1	A	170	U	N1-C2-O2	-5.94	118.64	122.80
1	A	1089	G	C8-N9-C4	-5.94	104.03	106.40
1	A	1439	C	N3-C4-C5	-5.94	119.53	121.90
1	A	1307	U	N1-C2-O2	5.94	126.95	122.80
17	Q	31	LEU	CA-CB-CG	-5.94	101.65	115.30
1	A	15	G	N9-C4-C5	-5.93	103.03	105.40
1	A	250	A	N1-C6-N6	5.93	122.16	118.60
1	A	654	G	C2-N3-C4	-5.93	108.93	111.90
1	A	853	G	N3-C4-N9	5.93	129.56	126.00
1	A	807	A	C8-N9-C4	5.93	108.17	105.80
8	H	135	CYS	CA-CB-SG	-5.93	103.32	114.00
1	A	1234	C	N3-C4-C5	5.93	124.27	121.90
1	A	265	G	C6-C5-N7	-5.93	126.84	130.40
1	A	898	G	C2-N3-C4	-5.93	108.94	111.90
1	A	190(K)	G	C8-N9-C4	5.92	108.77	106.40
1	A	542	G	N1-C6-O6	-5.92	116.35	119.90
1	A	774	G	C6-C5-N7	-5.92	126.85	130.40
1	A	791	G	C5-C6-N1	-5.92	108.54	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718	G	C5-C6-O6	-5.92	125.05	128.60
1	A	920	U	N1-C2-N3	5.92	118.45	114.90
1	A	618	C	N3-C4-N4	-5.92	113.86	118.00
1	A	674	G	C2-N3-C4	-5.92	108.94	111.90
1	A	1529	G	N3-C2-N2	-5.91	115.76	119.90
1	A	711	G	C2-N3-C4	-5.91	108.94	111.90
1	A	1084	G	N1-C2-N3	5.91	127.45	123.90
1	A	136	C	C6-N1-C2	-5.91	117.94	120.30
1	A	931	C	C5-C6-N1	-5.91	118.05	121.00
1	A	1335	C	N1-C2-N3	-5.91	115.06	119.20
1	A	1507	A	N1-C2-N3	5.91	132.25	129.30
1	A	38	G	C4-N9-C1'	-5.91	118.82	126.50
1	A	144	G	N3-C2-N2	-5.91	115.77	119.90
1	A	553	A	C8-N9-C4	5.91	108.16	105.80
1	A	1300	G	C4-C5-N7	-5.91	108.44	110.80
1	A	328	C	P-O3'-C3'	5.90	126.78	119.70
1	A	317	G	C2-N3-C4	-5.90	108.95	111.90
1	A	1529	G	N1-C2-N3	5.90	127.44	123.90
1	A	1530	G	N1-C2-N2	5.90	121.51	116.20
24	a	37	A	C2-N3-C4	-5.90	107.65	110.60
2	B	7	VAL	N-CA-C	5.90	126.93	111.00
1	A	447	G	C4-N9-C1'	5.90	134.17	126.50
1	A	610	G	N1-C6-O6	-5.90	116.36	119.90
1	A	799	G	C4-C5-N7	5.90	113.16	110.80
1	A	1301	U	N3-C4-O4	5.90	123.53	119.40
1	A	924	C	N3-C4-C5	-5.89	119.54	121.90
1	A	104	G	C5-C6-O6	-5.89	125.06	128.60
1	A	854	G	C4-N9-C1'	5.89	134.15	126.50
1	A	1214	C	C2-N1-C1'	5.88	125.27	118.80
24	a	37	A	C5-C6-N1	-5.88	114.76	117.70
1	A	1099	G	C8-N9-C4	-5.88	104.05	106.40
8	H	136	GLU	N-CA-C	-5.88	95.13	111.00
1	A	284	G	C2-N3-C4	-5.88	108.96	111.90
1	A	686	U	C5-C6-N1	-5.88	119.76	122.70
1	A	1534	C	N1-C2-O2	5.88	122.42	118.90
1	A	1530	G	C4-N9-C1'	-5.87	118.86	126.50
1	A	650	G	N1-C6-O6	5.87	123.42	119.90
1	A	963	G	C6-C5-N7	-5.87	126.88	130.40
1	A	1253	G	N1-C6-O6	5.87	123.42	119.90
1	A	1467	G	C8-N9-C4	-5.87	104.05	106.40
1	A	90	U	N3-C2-O2	-5.87	118.09	122.20
1	A	1502	A	N3-C4-C5	5.87	130.91	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	G	N1-C6-O6	5.86	123.42	119.90
1	A	400	C	C6-N1-C2	5.86	122.65	120.30
1	A	53	A	C6-N1-C2	-5.86	115.08	118.60
1	A	449	C	C2-N1-C1'	5.86	125.25	118.80
1	A	599	C	C2-N3-C4	-5.86	116.97	119.90
1	A	875	C	C2-N3-C4	-5.86	116.97	119.90
1	A	552	U	N3-C4-O4	-5.86	115.30	119.40
1	A	880	C	C6-N1-C2	5.85	122.64	120.30
1	A	1062	U	C5-C4-O4	5.85	129.41	125.90
1	A	1452	C	C6-N1-C2	5.85	122.64	120.30
1	A	658	G	N1-C2-N3	5.85	127.41	123.90
1	A	1310	G	N1-C2-N2	-5.85	110.93	116.20
1	A	1064	G	C6-N1-C2	-5.85	121.59	125.10
1	A	251	G	N3-C4-C5	-5.85	125.68	128.60
1	A	1414	U	C4-C5-C6	5.85	123.21	119.70
1	A	607	A	C6-N1-C2	5.84	122.11	118.60
1	A	1108	G	C4-N9-C1'	5.84	134.10	126.50
1	A	1527	C	N3-C4-N4	5.84	122.09	118.00
1	A	579	G	C6-C5-N7	-5.84	126.89	130.40
1	A	975	A	C6-N1-C2	5.84	122.10	118.60
1	A	796	C	C4-C5-C6	5.84	120.32	117.40
1	A	481	G	C4-N9-C1'	5.84	134.09	126.50
1	A	741	G	C6-C5-N7	5.84	133.90	130.40
1	A	1335	C	C5-C4-N4	-5.84	116.11	120.20
1	A	1483	A	C2-N3-C4	5.84	113.52	110.60
20	T	13	LEU	CB-CA-C	-5.84	99.11	110.20
1	A	1438	G	C8-N9-C4	5.83	108.73	106.40
1	A	1523	G	N3-C2-N2	-5.83	115.82	119.90
1	A	1487	G	C4-C5-C6	5.83	122.30	118.80
1	A	1190	G	C4-C5-C6	5.82	122.30	118.80
1	A	864	A	C4-C5-N7	-5.82	107.79	110.70
1	A	656	C	N3-C4-C5	5.82	124.23	121.90
1	A	852	G	N9-C4-C5	-5.82	103.07	105.40
1	A	190(G)	G	C4-C5-C6	5.82	122.29	118.80
1	A	679	C	C5-C6-N1	-5.82	118.09	121.00
1	A	1249	C	C5-C6-N1	5.82	123.91	121.00
1	A	1482	G	C8-N9-C1'	-5.82	119.44	127.00
1	A	1510	U	N1-C2-O2	5.82	126.87	122.80
1	A	129	U	C5-C4-O4	5.82	129.39	125.90
1	A	865	A	C5-C6-N1	5.82	120.61	117.70
1	A	344	A	N7-C8-N9	5.81	116.71	113.80
1	A	693	G	C6-C5-N7	-5.81	126.91	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	G	N9-C4-C5	-5.81	103.08	105.40
1	A	854	G	N1-C2-N3	5.81	127.39	123.90
1	A	297	G	C5-C6-O6	5.80	132.08	128.60
1	A	707	C	C2-N1-C1'	-5.80	112.42	118.80
1	A	38	G	N3-C4-C5	5.80	131.50	128.60
1	A	235	C	C5-C6-N1	-5.80	118.10	121.00
1	A	242	C	C6-N1-C2	5.80	122.62	120.30
1	A	259	G	C5-C6-N1	-5.80	108.60	111.50
1	A	565	U	C6-N1-C2	5.80	124.48	121.00
1	A	676	A	N7-C8-N9	-5.80	110.90	113.80
1	A	925	G	N3-C4-C5	-5.80	125.70	128.60
1	A	860	A	N1-C2-N3	5.79	132.20	129.30
1	A	1200	C	N3-C4-N4	5.79	122.06	118.00
1	A	142	G	N3-C4-C5	-5.79	125.70	128.60
1	A	251	G	C8-N9-C1'	-5.79	119.47	127.00
1	A	1303	C	N3-C4-N4	-5.79	113.95	118.00
1	A	925	G	N3-C4-N9	5.79	129.47	126.00
1	A	519	C	C6-N1-C2	5.78	122.61	120.30
1	A	944	G	N9-C4-C5	5.78	107.71	105.40
1	A	1281	U	C6-N1-C1'	5.78	129.29	121.20
1	A	597	G	C8-N9-C1'	-5.78	119.49	127.00
1	A	760	G	C4-C5-C6	5.78	122.27	118.80
1	A	258	G	C2-N3-C4	-5.78	109.01	111.90
1	A	332	G	C4-C5-N7	5.78	113.11	110.80
1	A	566	G	N3-C4-N9	5.78	129.47	126.00
1	A	552	U	N1-C2-N3	5.77	118.36	114.90
1	A	644	G	N7-C8-N9	5.77	115.99	113.10
1	A	831	U	C5-C4-O4	5.77	129.36	125.90
1	A	629	G	N3-C4-C5	-5.77	125.72	128.60
1	A	716	A	C5-C6-N1	5.77	120.58	117.70
1	A	779	C	C2-N3-C4	-5.77	117.02	119.90
1	A	945	G	C4-C5-C6	-5.77	115.34	118.80
1	A	1153	C	C6-N1-C2	5.77	122.61	120.30
1	A	910	C	C5-C6-N1	-5.76	118.12	121.00
1	A	180	U	C5-C4-O4	-5.76	122.44	125.90
1	A	259	G	C8-N9-C4	-5.76	104.10	106.40
1	A	68	G	N7-C8-N9	-5.76	110.22	113.10
1	A	752	G	N1-C6-O6	5.76	123.35	119.90
1	A	1231	G	C4-N9-C1'	5.75	133.98	126.50
1	A	73	C	C2-N3-C4	5.75	122.78	119.90
1	A	618	C	C6-N1-C1'	5.75	127.70	120.80
1	A	414	A	N1-C2-N3	5.75	132.17	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	799	G	C5-C6-O6	-5.74	125.15	128.60
1	A	1227	A	N3-C4-C5	5.74	130.82	126.80
1	A	15	G	C8-N9-C4	5.74	108.70	106.40
1	A	1129	C	C5-C6-N1	5.74	123.87	121.00
1	A	130	A	N1-C6-N6	5.74	122.04	118.60
1	A	181	G	C8-N9-C1'	-5.74	119.54	127.00
1	A	292	G	N1-C6-O6	5.74	123.34	119.90
1	A	725	G	C5-C6-O6	-5.73	125.16	128.60
1	A	251	G	N3-C2-N2	5.73	123.91	119.90
1	A	1373	G	C8-N9-C4	-5.73	104.11	106.40
1	A	265	G	C8-N9-C1'	-5.73	119.55	127.00
1	A	637	G	C8-N9-C1'	-5.73	119.55	127.00
1	A	1055	A	C2-N3-C4	5.73	113.46	110.60
1	A	50	A	N7-C8-N9	-5.73	110.94	113.80
1	A	911	U	C2-N1-C1'	-5.73	110.83	117.70
1	A	635	G	N1-C2-N2	-5.72	111.05	116.20
1	A	875	C	C5-C6-N1	-5.72	118.14	121.00
1	A	905	U	C4-C5-C6	5.72	123.13	119.70
1	A	154	C	C6-N1-C1'	-5.72	113.94	120.80
1	A	558	G	C6-C5-N7	-5.72	126.97	130.40
1	A	693	G	N9-C4-C5	-5.72	103.11	105.40
1	A	745	C	C2-N3-C4	-5.72	117.04	119.90
1	A	326	G	N3-C4-N9	-5.72	122.57	126.00
1	A	21	G	C8-N9-C1'	-5.71	119.57	127.00
1	A	125	U	N3-C2-O2	-5.71	118.20	122.20
1	A	32	A	C6-C5-N7	-5.71	128.30	132.30
1	A	373	A	N1-C6-N6	-5.71	115.17	118.60
1	A	674	G	N1-C6-O6	5.71	123.32	119.90
1	A	698	G	C8-N9-C4	-5.71	104.12	106.40
1	A	1221	G	C5-C6-N1	-5.71	108.65	111.50
1	A	1531	A	C4-C5-N7	5.71	113.55	110.70
1	A	711	G	C5-N7-C8	-5.70	101.45	104.30
1	A	540	G	C5-C6-O6	-5.70	125.18	128.60
1	A	127	G	C5-C6-O6	-5.70	125.18	128.60
1	A	704	A	N7-C8-N9	5.70	116.65	113.80
1	A	963	G	N7-C8-N9	5.70	115.95	113.10
1	A	631	G	N7-C8-N9	5.70	115.95	113.10
1	A	779	C	C6-N1-C2	5.70	122.58	120.30
1	A	407	G	N3-C4-C5	5.70	131.45	128.60
1	A	1134	G	C8-N9-C4	-5.70	104.12	106.40
1	A	144	G	N3-C4-C5	5.70	131.45	128.60
1	A	232	G	C8-N9-C1'	-5.70	119.59	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	677	U	C6-N1-C2	-5.69	117.58	121.00
1	A	920	U	C6-N1-C2	-5.69	117.58	121.00
1	A	240	C	C6-N1-C2	5.69	122.58	120.30
1	A	279	A	C2-N3-C4	-5.69	107.75	110.60
1	A	1415	G	C8-N9-C4	5.69	108.68	106.40
1	A	1062	U	C6-N1-C2	-5.69	117.59	121.00
1	A	673	G	C4-C5-N7	5.68	113.07	110.80
1	A	856	C	N1-C2-N3	5.68	123.18	119.20
1	A	440	A	N1-C2-N3	5.68	132.14	129.30
1	A	1092	A	C8-N9-C1'	-5.68	117.48	127.70
1	A	91	C	C6-N1-C1'	-5.67	113.99	120.80
1	A	1084	G	N9-C4-C5	5.67	107.67	105.40
1	A	1329	A	N9-C4-C5	-5.67	103.53	105.80
1	A	1504	G	N3-C4-N9	5.67	129.40	126.00
1	A	753	A	C4-C5-N7	-5.67	107.86	110.70
1	A	858	G	C4-C5-N7	-5.67	108.53	110.80
1	A	1364	U	C6-N1-C2	5.67	124.40	121.00
1	A	1310	G	C6-C5-N7	-5.66	127.00	130.40
1	A	1381	U	C2-N1-C1'	5.66	124.50	117.70
1	A	204	U	C5-C6-N1	5.66	125.53	122.70
1	A	121	C	C6-N1-C2	5.66	122.56	120.30
1	A	1074	G	N1-C6-O6	5.66	123.30	119.90
15	O	77	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	A	1388	C	N1-C2-O2	-5.66	115.51	118.90
1	A	597	G	C4-N9-C1'	5.66	133.85	126.50
1	A	1074	G	C6-C5-N7	-5.66	127.01	130.40
1	A	1524	C	N1-C2-N3	5.66	123.16	119.20
1	A	1058	G	C4-C5-N7	-5.65	108.54	110.80
1	A	637	G	C6-C5-N7	-5.65	127.01	130.40
1	A	971	G	C2-N3-C4	-5.65	109.08	111.90
1	A	1143	G	C4-C5-N7	5.65	113.06	110.80
1	A	830	G	N3-C2-N2	-5.65	115.95	119.90
1	A	21	G	N9-C4-C5	-5.65	103.14	105.40
1	A	330	C	N1-C2-O2	-5.65	115.51	118.90
1	A	1394	A	C5-C6-N1	5.64	120.52	117.70
1	A	1433	A	C6-N1-C2	-5.64	115.21	118.60
5	E	63	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	1442	G	N3-C4-N9	5.64	129.38	126.00
1	A	1505	G	C4-C5-N7	-5.64	108.55	110.80
1	A	902	G	N7-C8-N9	-5.64	110.28	113.10
1	A	1120	G	N3-C4-C5	-5.64	125.78	128.60
1	A	1286	A	C8-N9-C4	-5.63	103.55	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1438	G	C5-C6-O6	-5.63	125.22	128.60
1	A	111	G	C8-N9-C1'	5.63	134.32	127.00
1	A	393	A	C2-N3-C4	-5.62	107.79	110.60
1	A	1190	G	N3-C4-C5	-5.62	125.79	128.60
1	A	125	U	C4-C5-C6	5.62	123.07	119.70
1	A	435	C	N3-C4-C5	-5.62	119.65	121.90
1	A	933	G	C6-C5-N7	-5.62	127.03	130.40
1	A	1301	U	N1-C2-N3	5.62	118.27	114.90
1	A	1527	C	C2-N1-C1'	5.62	124.98	118.80
1	A	383	A	C8-N9-C4	-5.62	103.55	105.80
1	A	497	A	N1-C6-N6	-5.62	115.23	118.60
1	A	656	C	C5-C4-N4	-5.62	116.27	120.20
1	A	216	G	N1-C6-O6	-5.62	116.53	119.90
1	A	1077	G	C4-C5-C6	5.61	122.17	118.80
1	A	162	A	N1-C6-N6	-5.61	115.23	118.60
1	A	816	A	N7-C8-N9	-5.61	111.00	113.80
1	A	1531	A	C5-C6-N1	5.61	120.50	117.70
1	A	270	A	N1-C6-N6	5.61	121.96	118.60
1	A	190(G)	G	C6-C5-N7	-5.60	127.04	130.40
1	A	787	A	N7-C8-N9	5.60	116.60	113.80
1	A	588	G	C8-N9-C4	5.60	108.64	106.40
1	A	816	A	N3-C4-N9	-5.60	122.92	127.40
1	A	559	A	N7-C8-N9	5.60	116.60	113.80
1	A	1220	G	N1-C6-O6	5.60	123.26	119.90
1	A	1392	G	C4-C5-N7	5.60	113.04	110.80
1	A	21	G	N7-C8-N9	-5.59	110.30	113.10
1	A	120	A	N7-C8-N9	-5.59	111.00	113.80
1	A	1392	G	C4-N9-C1'	5.59	133.77	126.50
1	A	1343	G	C4-C5-N7	5.59	113.04	110.80
1	A	204	U	C6-N1-C1'	-5.59	113.38	121.20
24	a	39	G	N3-C4-C5	5.59	131.40	128.60
1	A	38	G	C5-C6-N1	-5.59	108.71	111.50
1	A	831	U	N3-C2-O2	-5.59	118.29	122.20
1	A	122	G	C2-N3-C4	-5.59	109.11	111.90
1	A	497	A	C4-C5-N7	-5.59	107.91	110.70
1	A	675	A	C2-N3-C4	-5.59	107.81	110.60
1	A	767	A	N1-C6-N6	-5.58	115.25	118.60
1	A	113	G	C6-C5-N7	-5.58	127.05	130.40
1	A	146	G	C5-C6-O6	-5.58	125.25	128.60
1	A	741	G	C8-N9-C1'	5.58	134.26	127.00
1	A	1186	G	N1-C6-O6	5.58	123.25	119.90
1	A	634	C	C5-C4-N4	5.58	124.11	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	G	C4-C5-C6	5.58	122.15	118.80
1	A	190(B)	C	C6-N1-C2	-5.58	118.07	120.30
17	Q	99	SER	N-CA-C	5.58	126.06	111.00
1	A	1075	C	C6-N1-C2	5.57	122.53	120.30
1	A	761	G	C6-C5-N7	-5.57	127.06	130.40
1	A	644	G	N3-C4-N9	5.57	129.34	126.00
1	A	696	A	N1-C6-N6	5.57	121.94	118.60
1	A	1112	C	N3-C2-O2	-5.57	118.00	121.90
1	A	79	G	C8-N9-C4	-5.56	104.17	106.40
1	A	265	G	N1-C2-N3	5.56	127.24	123.90
1	A	1253	G	C8-N9-C4	-5.56	104.18	106.40
1	A	332	G	N3-C2-N2	-5.56	116.01	119.90
1	A	373	A	N1-C2-N3	5.56	132.08	129.30
1	A	1425	U	C5-C4-O4	5.56	129.23	125.90
1	A	252	U	C4-C5-C6	5.55	123.03	119.70
1	A	1068	G	C6-C5-N7	-5.55	127.07	130.40
1	A	863	U	N1-C2-O2	-5.55	118.92	122.80
1	A	931	C	C2-N3-C4	-5.55	117.12	119.90
1	A	201	C	N1-C2-O2	5.55	122.23	118.90
1	A	52	G	N1-C2-N2	-5.55	111.21	116.20
1	A	55	A	C6-N1-C2	-5.55	115.27	118.60
1	A	580	U	C4-C5-C6	5.55	123.03	119.70
1	A	1500	A	C8-N9-C4	-5.54	103.58	105.80
1	A	389	A	C4-C5-C6	5.54	119.77	117.00
1	A	577	G	C8-N9-C4	5.54	108.62	106.40
1	A	811	C	C6-N1-C1'	-5.54	114.15	120.80
1	A	881	G	N7-C8-N9	-5.54	110.33	113.10
20	T	13	LEU	CB-CG-CD1	5.54	120.42	111.00
1	A	1415	G	C8-N9-C1'	-5.54	119.80	127.00
1	A	747	C	N1-C2-O2	-5.54	115.58	118.90
1	A	1322	C	C6-N1-C2	-5.54	118.08	120.30
1	A	9	G	N9-C4-C5	-5.54	103.19	105.40
1	A	422	C	N1-C2-N3	-5.54	115.32	119.20
1	A	1322	C	C6-N1-C1'	-5.54	114.16	120.80
1	A	232	G	N3-C4-N9	5.54	129.32	126.00
1	A	893	C	N1-C2-N3	-5.54	115.33	119.20
1	A	190(B)	C	C5-C6-N1	5.53	123.77	121.00
1	A	650	G	N7-C8-N9	-5.53	110.33	113.10
1	A	811	C	C5-C4-N4	-5.53	116.33	120.20
1	A	1293	G	N3-C4-N9	-5.53	122.68	126.00
1	A	924	C	C2-N3-C4	5.53	122.67	119.90
1	A	1529	G	C4-N9-C1'	5.53	133.69	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	A	N1-C2-N3	5.53	132.06	129.30
1	A	926	G	C4-C5-N7	-5.53	108.59	110.80
1	A	829	G	N9-C4-C5	-5.53	103.19	105.40
1	A	1157	A	N9-C4-C5	5.53	108.01	105.80
1	A	27	G	N1-C6-O6	5.53	123.22	119.90
1	A	135	C	C2-N1-C1'	-5.53	112.72	118.80
1	A	889	A	C8-N9-C4	-5.53	103.59	105.80
1	A	1394	A	N1-C6-N6	5.53	121.92	118.60
1	A	1084	G	N3-C4-N9	5.52	129.31	126.00
1	A	628	G	C4-N9-C1'	5.52	133.68	126.50
1	A	283	C	N3-C4-N4	5.52	121.86	118.00
1	A	357	G	C5-C6-O6	5.52	131.91	128.60
1	A	650	G	C2-N3-C4	-5.52	109.14	111.90
1	A	711	G	C8-N9-C4	-5.52	104.19	106.40
1	A	864	A	C8-N9-C4	-5.52	103.59	105.80
1	A	867	G	C5-C6-N1	-5.51	108.74	111.50
1	A	245	C	C5-C4-N4	-5.51	116.34	120.20
1	A	761	G	N1-C2-N3	5.51	127.21	123.90
1	A	962	C	N3-C4-C5	5.51	124.10	121.90
1	A	969	A	C6-C5-N7	-5.51	128.44	132.30
1	A	281	G	C4-C5-N7	5.51	113.00	110.80
1	A	778	G	N1-C2-N3	-5.51	120.60	123.90
1	A	1249	C	N3-C4-N4	5.51	121.85	118.00
1	A	142	G	C5-C6-N1	5.50	114.25	111.50
1	A	767	A	C5-C6-N6	5.50	128.10	123.70
1	A	1280	A	N9-C4-C5	5.50	108.00	105.80
1	A	117	G	N3-C4-N9	5.50	129.30	126.00
16	P	58	TYR	CB-CA-C	-5.50	99.40	110.40
1	A	145	G	C5-C6-N1	-5.50	108.75	111.50
1	A	973	G	N7-C8-N9	-5.50	110.35	113.10
1	A	264	U	C5-C4-O4	5.50	129.20	125.90
1	A	1392	G	C8-N9-C1'	-5.49	119.86	127.00
1	A	1140	C	C6-N1-C2	-5.49	118.10	120.30
1	A	107	G	N1-C6-O6	5.49	123.19	119.90
1	A	583	A	C8-N9-C4	5.49	108.00	105.80
1	A	583	A	C2-N3-C4	-5.49	107.85	110.60
1	A	175	C	C5-C6-N1	-5.49	118.26	121.00
1	A	1083	U	C6-N1-C2	5.49	124.29	121.00
1	A	372	C	N3-C4-N4	5.49	121.84	118.00
1	A	1322	C	C5-C6-N1	5.49	123.74	121.00
1	A	976	G	N3-C4-N9	-5.49	122.71	126.00
1	A	1417	G	N3-C4-C5	-5.49	125.86	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	675	A	C5-C6-N6	5.48	128.09	123.70
1	A	77	G	C5-C6-O6	-5.48	125.31	128.60
1	A	279	A	N1-C2-N3	5.48	132.04	129.30
1	A	301	G	C4-N9-C1'	5.48	133.62	126.50
1	A	20	U	C4-C5-C6	5.48	122.99	119.70
1	A	1373	G	C4-C5-N7	-5.48	108.61	110.80
1	A	1083	U	N3-C4-O4	5.47	123.23	119.40
1	A	73	C	N3-C2-O2	5.47	125.73	121.90
1	A	1235	U	C6-N1-C2	-5.47	117.72	121.00
1	A	1374	A	C8-N9-C4	-5.47	103.61	105.80
1	A	570	G	C6-N1-C2	-5.47	121.82	125.10
1	A	686	U	C4-C5-C6	5.47	122.98	119.70
1	A	260	G	C2-N3-C4	-5.47	109.17	111.90
1	A	678	U	C5-C4-O4	-5.47	122.62	125.90
1	A	132	C	C5-C6-N1	-5.46	118.27	121.00
1	A	1199	U	N1-C2-N3	5.46	118.18	114.90
1	A	300	A	C8-N9-C4	-5.46	103.61	105.80
1	A	745	C	C5-C6-N1	-5.46	118.27	121.00
1	A	816	A	C2-N3-C4	-5.46	107.87	110.60
1	A	860	A	C4-C5-C6	5.46	119.73	117.00
1	A	335	C	C6-N1-C2	5.46	122.48	120.30
1	A	734	G	N7-C8-N9	5.46	115.83	113.10
1	A	59	A	C5-C6-N1	5.46	120.43	117.70
1	A	419	C	C6-N1-C2	5.45	122.48	120.30
1	A	1368	G	N3-C4-C5	-5.45	125.87	128.60
1	A	174	C	C2-N1-C1'	5.45	124.80	118.80
1	A	180	U	C6-N1-C1'	-5.45	113.57	121.20
1	A	366	C	C6-N1-C2	-5.45	118.12	120.30
1	A	853	G	C4-N9-C1'	5.45	133.59	126.50
4	D	12	CYS	CA-CB-SG	5.45	123.81	114.00
1	A	34	C	N1-C2-O2	-5.45	115.63	118.90
1	A	43	C	C5-C6-N1	-5.45	118.28	121.00
1	A	1434	A	C8-N9-C4	5.45	107.98	105.80
1	A	32	A	N1-C6-N6	5.45	121.87	118.60
1	A	232	G	C4-N9-C1'	5.45	133.58	126.50
1	A	280	C	N3-C4-N4	-5.45	114.19	118.00
1	A	1098	C	C6-N1-C2	5.45	122.48	120.30
1	A	1240	U	N3-C2-O2	-5.45	118.39	122.20
1	A	1354	C	C6-N1-C2	-5.45	118.12	120.30
1	A	1494	G	N3-C4-N9	5.45	129.27	126.00
1	A	70	G	N3-C4-C5	5.45	131.32	128.60
1	A	394	G	C5-C6-O6	5.44	131.87	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	953	G	N9-C4-C5	-5.44	103.22	105.40
1	A	1323	G	C5-C6-N1	-5.44	108.78	111.50
1	A	1506	U	C5-C4-O4	-5.44	122.64	125.90
1	A	26	A	N1-C2-N3	5.44	132.02	129.30
1	A	265	G	N3-C2-N2	5.43	123.70	119.90
1	A	1055	A	N9-C4-C5	5.43	107.97	105.80
1	A	1527	C	C6-N1-C1'	-5.43	114.28	120.80
1	A	111	G	N3-C2-N2	-5.43	116.10	119.90
1	A	1493[A]	A	C4-C5-N7	5.43	113.41	110.70
1	A	1493[B]	A	C4-C5-N7	5.43	113.41	110.70
1	A	552	U	N3-C4-C5	5.43	117.86	114.60
1	A	250	A	N9-C4-C5	-5.42	103.63	105.80
1	A	278	G	C5-C6-O6	5.42	131.85	128.60
1	A	1502	A	N3-C4-N9	-5.42	123.06	127.40
1	A	608	A	C2-N3-C4	-5.42	107.89	110.60
1	A	648	A	C6-N1-C2	-5.42	115.35	118.60
1	A	724	G	N1-C6-O6	5.42	123.15	119.90
1	A	924	C	N1-C2-O2	-5.42	115.65	118.90
1	A	120	A	C5-N7-C8	5.42	106.61	103.90
1	A	317	G	N3-C4-C5	5.42	131.31	128.60
1	A	628	G	C8-N9-C1'	-5.42	119.96	127.00
1	A	675	A	C5-C6-N1	-5.42	114.99	117.70
1	A	230	G	N3-C4-N9	5.42	129.25	126.00
1	A	530	G	N1-C6-O6	-5.42	116.65	119.90
1	A	1343	G	N7-C8-N9	5.42	115.81	113.10
1	A	1405	G	N3-C4-N9	-5.42	122.75	126.00
1	A	107	G	C6-C5-N7	-5.42	127.15	130.40
18	R	76	LEU	CA-CB-CG	-5.41	102.85	115.30
1	A	259	G	C4-N9-C1'	5.41	133.53	126.50
1	A	874	G	C2-N3-C4	-5.41	109.19	111.90
1	A	881	G	N1-C6-O6	5.41	123.15	119.90
1	A	400	C	C5-C6-N1	-5.41	118.30	121.00
1	A	671	G	N1-C6-O6	5.41	123.14	119.90
1	A	1125	U	N3-C2-O2	5.41	125.99	122.20
1	A	107	G	N9-C4-C5	-5.41	103.24	105.40
1	A	283	C	N3-C2-O2	-5.41	118.12	121.90
1	A	817	C	C2-N1-C1'	5.41	124.75	118.80
1	A	589	C	C2-N3-C4	-5.40	117.20	119.90
1	A	1242	C	N3-C4-C5	5.40	124.06	121.90
1	A	304	U	C5-C6-N1	-5.40	120.00	122.70
1	A	16	A	N7-C8-N9	-5.39	111.10	113.80
1	A	124	G	N1-C2-N3	5.39	127.14	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1202	G	C8-N9-C4	-5.39	104.24	106.40
1	A	641	U	N1-C2-N3	5.38	118.13	114.90
1	A	826	C	N3-C4-N4	5.38	121.77	118.00
1	A	20	U	C2-N3-C4	-5.38	123.77	127.00
1	A	1143	G	C5-C6-O6	-5.38	125.37	128.60
1	A	1276	G	C6-C5-N7	-5.38	127.17	130.40
1	A	1395	C	N1-C2-O2	-5.38	115.67	118.90
1	A	1413	A	N1-C2-N3	5.38	131.99	129.30
1	A	1231	G	N9-C4-C5	-5.38	103.25	105.40
16	P	60	LEU	CA-CB-CG	-5.38	102.93	115.30
1	A	631	G	C8-N9-C4	-5.37	104.25	106.40
1	A	1375	A	N1-C6-N6	-5.37	115.38	118.60
1	A	197	A	C5-C6-N6	5.37	128.00	123.70
1	A	264	U	N1-C2-N3	5.37	118.12	114.90
1	A	413	G	C4-C5-N7	-5.37	108.65	110.80
1	A	490	G	C5-C6-O6	-5.37	125.38	128.60
5	E	69	VAL	CB-CA-C	-5.37	101.20	111.40
1	A	931	C	N3-C4-C5	5.37	124.05	121.90
1	A	1023	G	N3-C4-C5	-5.37	125.92	128.60
1	A	1332	A	C5-C6-N6	5.37	127.99	123.70
1	A	1053	G	C4-C5-N7	-5.37	108.65	110.80
1	A	1108	G	N3-C4-N9	5.37	129.22	126.00
1	A	92	C	C5-C4-N4	-5.36	116.44	120.20
1	A	279	A	C4-C5-C6	5.36	119.68	117.00
1	A	497	A	N9-C4-C5	5.36	107.95	105.80
1	A	1054	C	C5-C6-N1	5.36	123.68	121.00
1	A	1206	G	C5-C6-N1	-5.36	108.82	111.50
1	A	1350	A	C4-C5-N7	5.36	113.38	110.70
1	A	566	G	C6-C5-N7	-5.36	127.19	130.40
1	A	200	G	C5-C6-N1	-5.36	108.82	111.50
1	A	800	G	C4-N9-C1'	5.36	133.46	126.50
1	A	854	G	N9-C4-C5	-5.35	103.26	105.40
1	A	524	G	N3-C2-N2	-5.35	116.15	119.90
1	A	779	C	C5-C6-N1	-5.35	118.32	121.00
1	A	1304	G	C8-N9-C4	-5.35	104.26	106.40
1	A	1338	G	N1-C2-N3	5.35	127.11	123.90
1	A	1460	A	N1-C6-N6	5.35	121.81	118.60
1	A	10	A	N1-C2-N3	5.35	131.97	129.30
1	A	358	U	N1-C2-N3	5.35	118.11	114.90
1	A	1165	C	C6-N1-C2	-5.35	118.16	120.30
1	A	1399	C	N1-C2-O2	-5.35	115.69	118.90
1	A	204	U	N1-C2-N3	-5.35	111.69	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	934	C	C2-N3-C4	5.35	122.57	119.90
1	A	1125	U	C5-C4-O4	-5.35	122.69	125.90
1	A	1080	A	C5-C6-N6	5.35	127.98	123.70
1	A	558	G	N1-C6-O6	5.34	123.11	119.90
4	D	188	LEU	CB-CG-CD1	5.34	120.08	111.00
1	A	77	G	C6-C5-N7	-5.34	127.19	130.40
1	A	277	C	C5-C6-N1	-5.34	118.33	121.00
1	A	291	C	N3-C4-C5	5.34	124.04	121.90
1	A	1068	G	C4-N9-C1'	5.34	133.44	126.50
1	A	1433	A	N1-C6-N6	-5.34	115.39	118.60
1	A	786	G	C5-C6-N1	-5.34	108.83	111.50
1	A	1530	G	N1-C6-O6	5.34	123.10	119.90
1	A	483	C	C2-N1-C1'	-5.34	112.93	118.80
1	A	644	G	C8-N9-C1'	-5.34	120.06	127.00
1	A	1246	C	C2-N1-C1'	-5.34	112.93	118.80
1	A	55	A	C5-C6-N1	5.33	120.37	117.70
1	A	281	G	C5-N7-C8	-5.33	101.64	104.30
1	A	767	A	C4-C5-N7	-5.33	108.03	110.70
1	A	871	U	N3-C2-O2	-5.33	118.47	122.20
1	A	1167	A	C8-N9-C4	-5.33	103.67	105.80
20	T	102	GLY	N-CA-C	-5.33	99.78	113.10
1	A	635	G	C4-N9-C1'	5.33	133.43	126.50
1	A	557	G	C4-C5-N7	-5.33	108.67	110.80
1	A	351	G	N1-C2-N3	5.32	127.09	123.90
1	A	403	C	C4-C5-C6	5.32	120.06	117.40
1	A	288	A	N1-C6-N6	5.32	121.79	118.60
1	A	1055	A	C5-C6-N1	5.32	120.36	117.70
1	A	1286	A	N7-C8-N9	5.32	116.46	113.80
1	A	780	A	N7-C8-N9	-5.32	111.14	113.80
1	A	1092	A	C4-N9-C1'	5.32	135.87	126.30
1	A	317	G	N1-C6-O6	5.31	123.09	119.90
1	A	1324	A	C8-N9-C4	-5.31	103.67	105.80
1	A	423	G	N3-C4-N9	5.31	129.19	126.00
1	A	479	C	C2-N3-C4	5.31	122.55	119.90
1	A	876	G	C5-N7-C8	-5.31	101.64	104.30
1	A	1480	G	C5-C6-N1	-5.31	108.84	111.50
1	A	980	C	C5-C4-N4	-5.31	116.48	120.20
1	A	936	C	C5-C6-N1	-5.30	118.35	121.00
1	A	1481	U	C5-C4-O4	5.30	129.08	125.90
2	B	25	ASN	C-N-CD	5.30	139.54	128.40
1	A	17	U	N1-C2-N3	5.30	118.08	114.90
1	A	70	G	N1-C6-O6	5.29	123.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	783	C	C5-C6-N1	-5.29	118.35	121.00
1	A	895	G	N7-C8-N9	5.29	115.75	113.10
1	A	963	G	C8-N9-C4	-5.29	104.28	106.40
1	A	1415	G	N9-C4-C5	-5.29	103.28	105.40
1	A	607	A	N1-C6-N6	5.29	121.77	118.60
1	A	69	G	C8-N9-C4	5.29	108.52	106.40
1	A	389	A	N1-C2-N3	5.29	131.94	129.30
1	A	732	C	N3-C2-O2	-5.29	118.20	121.90
1	A	752	G	C8-N9-C4	5.29	108.52	106.40
1	A	822	C	C2-N3-C4	-5.29	117.26	119.90
1	A	947	G	C6-C5-N7	-5.29	127.23	130.40
1	A	1091	U	N3-C4-C5	-5.29	111.43	114.60
1	A	534	U	C6-N1-C2	5.29	124.17	121.00
1	A	820	U	C6-N1-C1'	5.29	128.60	121.20
1	A	947	G	N3-C2-N2	5.29	123.60	119.90
1	A	705	U	C5-C6-N1	-5.28	120.06	122.70
1	A	1295	G	C8-N9-C4	-5.28	104.29	106.40
1	A	861	G	C5-C6-N1	5.28	114.14	111.50
1	A	920	U	C6-N1-C1'	5.28	128.59	121.20
1	A	1201	A	N3-C4-C5	-5.28	123.11	126.80
1	A	259	G	C6-C5-N7	-5.27	127.24	130.40
14	N	10	ALA	N-CA-C	-5.27	96.76	111.00
1	A	577	G	N1-C2-N3	5.27	127.06	123.90
1	A	721	G	N3-C2-N2	5.27	123.59	119.90
1	A	1350	A	C6-C5-N7	-5.27	128.61	132.30
1	A	820	U	C2-N3-C4	-5.27	123.84	127.00
1	A	934	C	C6-N1-C2	5.27	122.41	120.30
1	A	827	U	C2-N1-C1'	5.27	124.02	117.70
1	A	54	C	C2-N3-C4	-5.26	117.27	119.90
1	A	635	G	C8-N9-C4	5.26	108.51	106.40
1	A	644	G	N9-C4-C5	-5.26	103.29	105.40
1	A	800	G	C6-C5-N7	-5.26	127.24	130.40
1	A	819	A	N1-C2-N3	5.26	131.93	129.30
12	L	66	VAL	CB-CA-C	-5.26	101.40	111.40
1	A	919	A	C5-C6-N6	-5.26	119.49	123.70
1	A	1077	G	N1-C2-N2	-5.26	111.46	116.20
1	A	1380	U	C5-C4-O4	5.26	129.06	125.90
10	J	58	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	1033	G	N9-C4-C5	5.26	107.50	105.40
1	A	1281	U	N3-C2-O2	-5.26	118.52	122.20
1	A	221	C	C5-C6-N1	-5.25	118.37	121.00
1	A	565	U	N1-C2-N3	-5.25	111.75	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	964	A	C2-N3-C4	-5.25	107.97	110.60
1	A	1505	G	N9-C4-C5	5.25	107.50	105.40
1	A	1512	U	N1-C2-N3	5.25	118.05	114.90
1	A	1487	G	N3-C2-N2	-5.25	116.22	119.90
1	A	1494	G	C6-C5-N7	-5.25	127.25	130.40
1	A	248	C	C4-C5-C6	5.25	120.03	117.40
1	A	1249	C	C2-N1-C1'	5.25	124.58	118.80
1	A	112	G	C8-N9-C4	5.25	108.50	106.40
1	A	119	A	N1-C6-N6	5.25	121.75	118.60
1	A	244	U	N1-C2-N3	-5.24	111.75	114.90
1	A	1058	G	N3-C4-C5	5.24	131.22	128.60
15	O	45	VAL	CB-CA-C	-5.24	101.44	111.40
1	A	573	A	C6-C5-N7	-5.24	128.63	132.30
1	A	1392	G	C4-C5-C6	5.24	121.94	118.80
1	A	711	G	N7-C8-N9	5.24	115.72	113.10
1	A	740	U	C5-C6-N1	-5.24	120.08	122.70
1	A	1099	G	N3-C4-N9	-5.24	122.86	126.00
1	A	440	A	C5-C6-N1	-5.23	115.08	117.70
1	A	1200	C	C5-C4-N4	-5.23	116.54	120.20
1	A	801	U	N3-C4-C5	5.23	117.74	114.60
1	A	831	U	N1-C2-N3	5.23	118.04	114.90
1	A	946	A	N1-C2-N3	5.23	131.92	129.30
1	A	149	A	N1-C6-N6	-5.23	115.46	118.60
1	A	650	G	N3-C2-N2	-5.23	116.24	119.90
1	A	668	G	C8-N9-C4	5.23	108.49	106.40
1	A	489	C	C6-N1-C2	5.23	122.39	120.30
1	A	1497	G	N3-C4-C5	-5.22	125.99	128.60
1	A	309	G	C4-C5-N7	5.22	112.89	110.80
1	A	544	G	N3-C4-C5	-5.22	125.99	128.60
1	A	816	A	N3-C4-C5	5.22	130.46	126.80
1	A	122	G	N3-C4-C5	5.22	131.21	128.60
1	A	352	C	N1-C2-O2	-5.22	115.77	118.90
1	A	965	A	N9-C4-C5	-5.22	103.71	105.80
1	A	1096	C	C6-N1-C2	-5.22	118.21	120.30
1	A	975	A	C2-N3-C4	-5.22	107.99	110.60
1	A	1305	G	C4-C5-C6	5.22	121.93	118.80
1	A	641	U	C2-N3-C4	-5.21	123.87	127.00
1	A	1027	C	N3-C4-C5	-5.21	119.81	121.90
1	A	1525	G	C6-N1-C2	-5.21	121.97	125.10
1	A	744	C	C5-C6-N1	-5.21	118.39	121.00
1	A	823	G	N1-C2-N3	5.21	127.03	123.90
1	A	190(E)	U	N1-C2-N3	5.21	118.03	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	931	C	N3-C4-N4	-5.21	114.35	118.00
1	A	1507	A	C5-C6-N6	5.21	127.87	123.70
1	A	1134	G	N9-C4-C5	5.21	107.48	105.40
1	A	331	G	C8-N9-C1'	-5.21	120.23	127.00
1	A	1484	C	N1-C2-O2	-5.21	115.78	118.90
1	A	15	G	C4-C5-N7	5.20	112.88	110.80
1	A	781	A	N7-C8-N9	5.20	116.40	113.80
1	A	781	A	C4-C5-C6	5.20	119.60	117.00
1	A	782	A	C5-C6-N6	5.20	127.86	123.70
1	A	953	G	N1-C6-O6	5.20	123.02	119.90
1	A	1421	G	N7-C8-N9	5.20	115.70	113.10
1	A	900	A	N1-C2-N3	5.20	131.90	129.30
1	A	679	C	C6-N1-C2	5.20	122.38	120.30
1	A	964	A	N7-C8-N9	5.19	116.40	113.80
1	A	436	C	C2-N1-C1'	-5.19	113.09	118.80
1	A	830	G	C5-C6-N1	-5.19	108.90	111.50
1	A	1049	U	C2-N1-C1'	5.19	123.93	117.70
12	L	17	LYS	CD-CE-NZ	5.19	123.64	111.70
1	A	25	C	C6-N1-C2	5.19	122.38	120.30
1	A	104	G	C4-C5-C6	5.19	121.91	118.80
1	A	481	G	C8-N9-C1'	-5.19	120.25	127.00
1	A	1108	G	C4-C5-C6	5.19	121.91	118.80
1	A	540	G	C4-C5-N7	5.19	112.88	110.80
1	A	804	U	C4-C5-C6	5.19	122.81	119.70
1	A	1037	C	C6-N1-C2	-5.18	118.23	120.30
1	A	882	C	N1-C2-N3	5.18	122.83	119.20
5	E	63	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	760	G	N9-C4-C5	-5.18	103.33	105.40
1	A	497	A	C5-C6-N6	5.18	127.84	123.70
1	A	1322	C	C2-N3-C4	5.18	122.49	119.90
1	A	1293	G	N3-C4-C5	5.18	131.19	128.60
1	A	1272	G	N3-C4-C5	-5.18	126.01	128.60
1	A	232	G	C5-C6-N1	-5.17	108.91	111.50
1	A	691	G	C6-C5-N7	-5.17	127.30	130.40
1	A	311	C	C5-C6-N1	-5.17	118.42	121.00
1	A	969	A	C5-N7-C8	-5.17	101.31	103.90
1	A	1030(C)	G	C8-N9-C4	-5.17	104.33	106.40
1	A	816	A	C6-C5-N7	5.17	135.92	132.30
1	A	558	G	C5-N7-C8	-5.17	101.72	104.30
1	A	811	C	C2-N3-C4	-5.17	117.32	119.90
1	A	816	A	C8-N9-C4	5.17	107.87	105.80
1	A	134	A	C2-N3-C4	-5.16	108.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	G	C5-C6-O6	-5.16	125.50	128.60
1	A	190(H)	G	C4-C5-N7	-5.16	108.74	110.80
1	A	648	A	C4-C5-N7	-5.16	108.12	110.70
1	A	1253	G	C4-N9-C1'	5.16	133.21	126.50
1	A	700	G	N3-C4-C5	-5.16	126.02	128.60
1	A	1493[A]	A	N1-C6-N6	5.16	121.69	118.60
1	A	1493[B]	A	N1-C6-N6	5.16	121.69	118.60
1	A	824	C	C2-N3-C4	-5.16	117.32	119.90
1	A	190(B)	C	C2-N1-C1'	5.16	124.47	118.80
1	A	667	G	N3-C4-C5	5.16	131.18	128.60
1	A	566	G	N3-C4-C5	-5.15	126.02	128.60
1	A	280	C	C5-C6-N1	-5.15	118.42	121.00
1	A	701	C	N3-C4-N4	-5.15	114.39	118.00
1	A	705	U	N1-C2-N3	5.15	117.99	114.90
1	A	976	G	N3-C2-N2	-5.15	116.30	119.90
1	A	1390	U	C5-C4-O4	5.15	128.99	125.90
1	A	97	G	C8-N9-C4	-5.15	104.34	106.40
1	A	596	C	N3-C2-O2	5.15	125.50	121.90
1	A	193	C	C6-N1-C2	5.15	122.36	120.30
1	A	1052	U	C6-N1-C2	-5.14	117.91	121.00
1	A	596	C	C2-N1-C1'	-5.14	113.14	118.80
1	A	220	G	N1-C6-O6	5.14	122.98	119.90
1	A	306	G	N3-C4-C5	5.14	131.17	128.60
1	A	785	G	C8-N9-C4	5.14	108.46	106.40
1	A	1377	A	N1-C6-N6	-5.14	115.52	118.60
1	A	1395	C	C5-C4-N4	5.14	123.80	120.20
1	A	612	C	C5-C6-N1	-5.14	118.43	121.00
1	A	1484	C	N3-C2-O2	5.14	125.50	121.90
1	A	109	A	C5-C6-N6	5.13	127.81	123.70
1	A	357	G	N9-C4-C5	5.13	107.45	105.40
1	A	246	A	C8-N9-C4	5.13	107.85	105.80
1	A	881	G	C6-C5-N7	-5.13	127.32	130.40
1	A	558	G	C5-C6-O6	-5.13	125.52	128.60
1	A	796	C	C5-C6-N1	-5.13	118.44	121.00
1	A	1186	G	N3-C2-N2	-5.13	116.31	119.90
1	A	618	C	C5-C4-N4	5.13	123.79	120.20
1	A	120	A	C5-C6-N6	5.13	127.80	123.70
1	A	435	C	C6-N1-C2	-5.13	118.25	120.30
1	A	805	C	C4-C5-C6	-5.13	114.84	117.40
12	L	52	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	683	G	C8-N9-C4	-5.12	104.35	106.40
1	A	390	C	N3-C4-C5	-5.12	119.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	758	G	N1-C2-N3	5.12	126.97	123.90
1	A	1030(C)	G	N3-C4-C5	-5.12	126.04	128.60
1	A	1365	G	N9-C4-C5	5.12	107.45	105.40
1	A	201	C	C6-N1-C1'	-5.12	114.65	120.80
1	A	539	A	C2-N3-C4	5.12	113.16	110.60
1	A	570	G	N3-C4-N9	5.12	129.07	126.00
1	A	812	C	N3-C2-O2	-5.12	118.31	121.90
1	A	889	A	C4-C5-C6	5.12	119.56	117.00
1	A	1332	A	C8-N9-C4	-5.12	103.75	105.80
1	A	1077	G	N1-C2-N3	5.12	126.97	123.90
1	A	828	A	C6-C5-N7	-5.12	128.72	132.30
1	A	109	A	N1-C2-N3	5.12	131.86	129.30
1	A	1139	G	N3-C4-C5	-5.12	126.04	128.60
1	A	317	G	C4-C5-N7	5.11	112.84	110.80
1	A	621	A	C6-C5-N7	-5.11	128.72	132.30
1	A	910	C	N1-C2-N3	5.11	122.78	119.20
1	A	919	A	C4-C5-N7	5.11	113.26	110.70
1	A	1370	G	C4-N9-C1'	5.11	133.14	126.50
1	A	47	C	C6-N1-C2	5.11	122.34	120.30
1	A	316	G	C6-C5-N7	5.11	133.46	130.40
1	A	803	G	N1-C2-N2	-5.11	111.60	116.20
1	A	823	G	C6-C5-N7	-5.11	127.33	130.40
1	A	10	A	N1-C6-N6	-5.11	115.54	118.60
1	A	530	G	N3-C2-N2	5.11	123.47	119.90
1	A	120	A	C4-C5-N7	-5.10	108.15	110.70
1	A	266	G	N9-C4-C5	-5.10	103.36	105.40
1	A	284	G	C5-C6-N1	-5.10	108.95	111.50
1	A	521	G	C6-C5-N7	5.10	133.46	130.40
1	A	660	G	N9-C4-C5	-5.10	103.36	105.40
1	A	1344	C	C5-C6-N1	-5.10	118.45	121.00
1	A	181	G	N3-C4-N9	5.10	129.06	126.00
1	A	66	G	C2-N3-C4	-5.10	109.35	111.90
1	A	485	G	C5-C6-N1	-5.10	108.95	111.50
1	A	741	G	N9-C4-C5	5.10	107.44	105.40
1	A	1341	U	C6-N1-C1'	5.10	128.34	121.20
1	A	757	U	N1-C2-O2	-5.10	119.23	122.80
1	A	253	U	N1-C2-O2	-5.09	119.23	122.80
1	A	930	C	C2-N3-C4	-5.09	117.35	119.90
1	A	1084	G	C4-C5-C6	5.09	121.86	118.80
1	A	1504	G	N9-C4-C5	-5.09	103.36	105.40
1	A	190(F)	G	C4-C5-N7	-5.09	108.76	110.80
1	A	259	G	N7-C8-N9	5.09	115.64	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	G	C8-N9-C1'	-5.09	120.39	127.00
1	A	1078	U	C4-C5-C6	-5.09	116.65	119.70
1	A	1222	G	N1-C6-O6	5.09	122.95	119.90
1	A	796	C	N3-C4-C5	-5.09	119.86	121.90
1	A	306	G	N1-C6-O6	5.09	122.95	119.90
1	A	853	G	N7-C8-N9	5.09	115.64	113.10
1	A	909	A	C4-C5-N7	5.09	113.24	110.70
1	A	1277	C	N3-C2-O2	-5.09	118.34	121.90
1	A	1012	U	C6-N1-C2	-5.08	117.95	121.00
1	A	947	G	N1-C2-N2	-5.08	111.62	116.20
1	A	1310	G	N9-C4-C5	-5.08	103.37	105.40
24	a	37	A	N1-C2-N3	5.08	131.84	129.30
1	A	336	C	N3-C4-N4	5.08	121.56	118.00
1	A	903	G	N9-C4-C5	5.08	107.43	105.40
1	A	1195	C	C5-C4-N4	-5.08	116.64	120.20
1	A	1236	A	C5-C6-N6	-5.08	119.64	123.70
1	A	393	A	N1-C6-N6	5.08	121.65	118.60
1	A	814	A	C8-N9-C4	5.07	107.83	105.80
1	A	597	G	N1-C2-N3	5.07	126.94	123.90
1	A	933	G	C4-C5-N7	5.07	112.83	110.80
1	A	977	A	N3-C4-C5	-5.07	123.25	126.80
1	A	1405	G	C4-N9-C1'	-5.07	119.91	126.50
1	A	1494	G	C4-C5-N7	5.07	112.83	110.80
1	A	92	C	N1-C2-O2	5.07	121.94	118.90
1	A	344	A	C5-N7-C8	-5.07	101.37	103.90
1	A	183	G	N7-C8-N9	5.06	115.63	113.10
1	A	544	G	C4-N9-C1'	5.06	133.08	126.50
1	A	579	G	N3-C4-C5	5.06	131.13	128.60
1	A	190(D)	U	N3-C2-O2	-5.06	118.66	122.20
1	A	292	G	C8-N9-C4	5.06	108.42	106.40
1	A	794	A	N1-C2-N3	-5.06	126.77	129.30
1	A	795	C	C2-N1-C1'	-5.06	113.23	118.80
1	A	1127	G	N1-C6-O6	-5.06	116.86	119.90
1	A	858	G	C4-N9-C1'	5.06	133.08	126.50
1	A	886	G	C5-C6-N1	-5.06	108.97	111.50
1	A	433	C	N3-C2-O2	-5.05	118.36	121.90
1	A	50	A	C6-N1-C2	5.05	121.63	118.60
1	A	149	A	N1-C2-N3	5.05	131.83	129.30
1	A	642	A	N1-C2-N3	5.05	131.83	129.30
1	A	600	C	C4-C5-C6	5.05	119.92	117.40
1	A	658	G	N1-C2-N2	-5.05	111.66	116.20
1	A	1356	G	C8-N9-C4	-5.05	104.38	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	U	C2-N3-C4	-5.05	123.97	127.00
1	A	903	G	N1-C6-O6	-5.05	116.87	119.90
1	A	1324	A	N1-C6-N6	5.05	121.63	118.60
1	A	403	C	C2-N1-C1'	-5.04	113.25	118.80
1	A	1232	U	C2-N3-C4	-5.04	123.97	127.00
1	A	16	A	C5-C6-N1	-5.04	115.18	117.70
1	A	288	A	N3-C4-C5	5.04	130.33	126.80
1	A	447	G	N3-C2-N2	5.04	123.43	119.90
1	A	910	C	C4-C5-C6	5.04	119.92	117.40
1	A	1279	A	C4-C5-C6	5.04	119.52	117.00
1	A	637	G	C4-N9-C1'	5.04	133.05	126.50
1	A	1434	A	C5-C6-N6	-5.04	119.67	123.70
1	A	1476	G	C8-N9-C4	-5.04	104.38	106.40
1	A	521	G	C4-C5-N7	-5.03	108.79	110.80
1	A	964	A	N9-C4-C5	5.03	107.81	105.80
25	b	3	U	N3-C2-O2	-5.03	118.68	122.20
1	A	64	G	C6-C5-N7	-5.03	127.38	130.40
1	A	646	U	C5-C4-O4	5.03	128.92	125.90
1	A	330	C	N3-C4-C5	-5.03	119.89	121.90
1	A	800	G	N1-C6-O6	5.03	122.92	119.90
1	A	899	C	C2-N1-C1'	5.03	124.33	118.80
1	A	250	A	C6-N1-C2	5.03	121.62	118.60
1	A	558	G	C8-N9-C4	-5.03	104.39	106.40
1	A	1488	G	C4-C5-N7	-5.03	108.79	110.80
1	A	142	G	C2-N3-C4	5.03	114.41	111.90
1	A	826	C	C2-N1-C1'	5.03	124.33	118.80
1	A	135	C	C6-N1-C1'	5.02	126.83	120.80
1	A	1055	A	C4-C5-N7	-5.02	108.19	110.70
1	A	828	A	C4-C5-N7	5.02	113.21	110.70
1	A	1099	G	N3-C2-N2	-5.02	116.39	119.90
1	A	1303	C	N3-C4-C5	5.02	123.91	121.90
1	A	712	A	C2-N3-C4	-5.02	108.09	110.60
1	A	651	C	N1-C2-O2	-5.02	115.89	118.90
1	A	859	A	N3-C4-N9	5.02	131.41	127.40
1	A	357	G	N1-C6-O6	-5.02	116.89	119.90
1	A	21	G	N3-C2-N2	5.01	123.41	119.90
16	P	5	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	276	G	C5-C6-O6	5.01	131.60	128.60
1	A	611	A	N1-C6-N6	5.01	121.61	118.60
1	A	786	G	N3-C4-C5	5.01	131.10	128.60
1	A	125	U	C5-C6-N1	-5.01	120.20	122.70
1	A	673	G	N1-C6-O6	5.01	122.90	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1303	C	C6-N1-C2	5.00	122.30	120.30
1	A	266	G	P-O3'-C3'	5.00	125.70	119.70
1	A	1179	A	N1-C6-N6	-5.00	115.60	118.60

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
2	B	75	LYS	Peptide
2	B	89	GLY	Peptide
3	C	166	GLU	Peptide
3	C	2	GLY	Peptide
4	D	154	ASN	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
9	I	38	GLN	Peptide
10	J	61	GLU	Peptide
10	J	85	LEU	Peptide
12	L	46	LYS	Peptide
12	L	91	LYS	Peptide
16	P	82	GLN	Peptide
19	S	4	SER	Peptide
20	T	12	ALA	Peptide
20	T	8	ARG	Peptide
21	U	24	ARG	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32707	0	16542	1874	1
2	B	1896	0	1936	217	0
3	C	1613	0	1677	201	0
4	D	1703	0	1763	203	0
5	E	1147	0	1207	135	1
6	F	843	0	857	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1257	0	1296	146	0
8	H	1116	0	1177	118	0
9	I	1010	0	1037	144	0
10	J	793	0	835	125	0
11	K	873	0	894	76	0
12	L	973	0	1058	109	0
13	M	937	0	995	134	0
14	N	492	0	529	85	0
15	O	734	0	771	101	0
16	P	701	0	720	73	0
17	Q	834	0	906	115	0
18	R	585	0	657	80	0
19	S	648	0	673	83	0
20	T	763	0	861	101	0
21	U	209	0	221	43	0
22	V	77	0	42	1	0
23	W	235	0	121	34	0
24	a	175	0	87	0	0
25	b	60	0	31	0	0
26	A	326	0	0	0	0
26	D	3	0	0	0	0
26	E	4	0	0	0	0
26	F	1	0	0	0	0
26	G	1	0	0	0	0
26	H	1	0	0	0	0
26	J	1	0	0	0	0
26	N	1	0	0	0	0
26	P	3	0	0	0	0
26	Q	1	0	0	0	0
26	S	2	0	0	0	0
27	A	40	0	38	14	0
28	D	1	0	0	0	0
28	N	1	0	0	0	0
29	A	866	0	0	97	0
29	C	1	0	0	0	0
29	D	7	0	0	1	0
29	E	5	0	0	0	0
29	L	1	0	0	0	0
29	N	1	0	0	0	0
29	P	1	0	0	0	0
29	Q	2	0	0	0	0
29	T	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	U	4	0	0	0	0
29	W	1	0	0	0	0
All	All	53659	0	36931	3978	2

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 45.

All (3978) 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)
1:A:451:A:O2'	29:A:2729:HOH:O	1.59	1.20
12:L:70:ILE:HG21	12:L:75:HIS:HD2	1.13	1.14
15:O:88:ARG:HE	15:O:88:ARG:HA	1.10	1.12
1:A:266:G:H5'	1:A:266:G:C8	1.83	1.12
21:U:10:ARG:CB	21:U:10:ARG:HH11	1.62	1.12
7:G:12:LEU:HD12	7:G:12:LEU:H	1.08	1.11
1:A:1054:C:H3'	1:A:1054:C:O2	1.48	1.11
10:J:55:LYS:HG2	10:J:56:HIS:H	0.99	1.11
10:J:30:SER:HB2	10:J:80:LYS:HB2	1.32	1.11
9:I:50:LEU:HD11	9:I:81:ILE:HG21	1.20	1.10
1:A:692:U:OP1	11:K:124:LYS:NZ	1.82	1.10
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.33	1.10
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.33	1.10
1:A:1493[A]:A:H8	1:A:1493[A]:A:H3'	1.10	1.10
2:B:25:ASN:ND2	2:B:193:ASP:HB2	1.67	1.09
1:A:266:G:O2'	1:A:267:C:OP2	1.72	1.08
1:A:538:G:H5''	12:L:114:LYS:HB2	1.35	1.08
1:A:1493[A]:A:H3'	1:A:1493[A]:A:C8	1.86	1.07
4:D:36:ARG:HB3	4:D:38:TYR:CE2	1.87	1.07
14:N:27:CYS:SG	14:N:29:ARG:HB2	1.94	1.07
12:L:127:GLU:CG	12:L:128:ALA:H	1.62	1.07
20:T:57:ARG:HH21	20:T:100:ILE:HD13	1.19	1.07
12:L:127:GLU:HG3	12:L:128:ALA:H	0.93	1.06
1:A:328:C:O2'	1:A:329:A:OP2	1.72	1.06
5:E:126:ARG:HG2	5:E:126:ARG:HH11	1.16	1.06
7:G:50:ILE:HG21	7:G:58:PRO:HA	1.34	1.06
1:A:328:C:H2'	1:A:328:C:O2	1.55	1.06
7:G:5:ARG:HG3	7:G:7:ALA:H	1.17	1.06
2:B:75:LYS:HA	2:B:78:GLN:HG3	1.37	1.06
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.14	1.06
8:H:102:ARG:H	8:H:102:ARG:HD2	1.17	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.14	1.05
12:L:127:GLU:HG3	12:L:128:ALA:N	1.70	1.05
20:T:49:ALA:HB3	20:T:99:LEU:HD21	1.38	1.04
1:A:543:C:C2'	1:A:544:G:H5'	1.87	1.04
1:A:89:C:H5	1:A:90:U:N3	1.54	1.04
1:A:61:G:O2'	29:A:2002:HOH:O	1.76	1.04
4:D:32:ALA:HA	4:D:35:ARG:HB2	1.39	1.04
6:F:12:PRO:HG3	6:F:58:GLY:HA2	1.33	1.03
1:A:1443:G:H4'	1:A:1446:A:H5'	1.41	1.03
21:U:10:ARG:HB2	21:U:10:ARG:HH11	1.21	1.03
1:A:107:G:H2'	1:A:108:G:H5''	1.40	1.03
1:A:89:C:C5	1:A:90:U:N3	2.25	1.02
1:A:858:G:O2'	1:A:859:A:H5'	1.59	1.02
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.37	1.02
6:F:50:TYR:CE1	18:R:77:GLY:HA2	1.95	1.02
7:G:152:ALA:O	7:G:155:ARG:NH1	1.93	1.01
1:A:1026:G:H2'	1:A:1027:C:H5''	1.42	1.01
18:R:87:ARG:HH21	18:R:87:ARG:HG3	1.22	1.01
1:A:1498:UR3:H4'	1:A:1519[A]:MA6:C2	1.91	1.01
10:J:86:MET:HG3	10:J:87:THR:H	1.26	1.00
1:A:1148:U:H2'	1:A:1149:C:O4'	1.61	1.00
1:A:1347:G:H3'	9:I:108:VAL:O	1.59	1.00
18:R:37:VAL:O	18:R:40:LEU:N	1.92	1.00
17:Q:100:LYS:HB2	17:Q:101:ARG:HH11	1.21	1.00
1:A:103:C:OP1	20:T:17:ARG:NH1	1.93	1.00
11:K:15:ALA:HA	11:K:77:MET:HA	1.43	1.00
4:D:150:GLU:OE2	4:D:150:GLU:N	1.92	1.00
1:A:1497:G:C2'	1:A:1498:UR3:H5'	1.91	1.00
1:A:9:G:OP1	5:E:122:GLU:HG3	1.60	0.99
1:A:1328:C:OP1	21:U:20:LYS:NZ	1.96	0.99
13:M:16:ASP:OD2	13:M:17:VAL:N	1.95	0.99
1:A:710:G:H5''	6:F:54:LYS:HE3	1.43	0.99
1:A:746:A:H2'	1:A:747:C:H5'	1.44	0.99
1:A:1316:G:N2	1:A:1319:A:OP2	1.96	0.98
1:A:571:U:H5''	1:A:572:A:OP2	1.63	0.98
1:A:1049:U:H4'	1:A:1050:G:O5'	1.60	0.98
4:D:18:LYS:HE3	4:D:20:TYR:HE2	1.29	0.98
1:A:1404:5MC:H1'	1:A:1499:A:C2	1.99	0.98
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.46	0.98
7:G:16:LEU:HD22	7:G:16:LEU:H	1.29	0.98
1:A:1026:G:O2'	1:A:1027:C:OP1	1.80	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:G:H2'	1:A:868:C:H5'	1.44	0.97
27:A:1928:SRV:HI32	27:A:1928:SRV:H22	1.46	0.97
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.45	0.97
1:A:1435:G:H2'	1:A:1436:U:C6	1.99	0.97
18:R:26:LEU:HD11	18:R:42:ARG:HD3	1.45	0.97
10:J:55:LYS:HG2	10:J:56:HIS:N	1.79	0.96
9:I:9:ARG:HB2	9:I:13:ALA:O	1.63	0.96
7:G:120:ILE:HD13	7:G:120:ILE:N	1.78	0.96
12:L:27:LEU:HG	12:L:28:LYS:H	1.30	0.96
1:A:1532:U:H2'	1:A:1533:C:C6	2.01	0.96
12:L:70:ILE:HG21	12:L:75:HIS:CD2	2.00	0.96
1:A:644:G:H5'	1:A:644:G:H8	1.28	0.95
1:A:914:A:P	27:A:1928:SRV:HI33	2.06	0.95
1:A:1305:G:OP2	21:U:2:GLY:N	1.99	0.95
9:I:108:VAL:HG12	9:I:109:VAL:H	1.31	0.95
6:F:50:TYR:HE1	18:R:77:GLY:HA2	1.30	0.94
1:A:1299:A:C5	1:A:1301:U:O2	2.20	0.94
1:A:792:A:H4'	1:A:793:U:OP1	1.65	0.94
23:W:31:C:N4	23:W:39:G:H1	1.63	0.94
1:A:1068:G:P	29:A:2218:HOH:O	2.25	0.94
1:A:1104:G:O5'	2:B:111:ARG:HD2	1.67	0.94
1:A:372:C:O2'	29:A:2721:HOH:O	1.84	0.94
1:A:707:C:H4'	11:K:20:TYR:CD1	2.01	0.94
10:J:30:SER:CB	10:J:80:LYS:HB2	1.98	0.94
1:A:746:A:C2'	1:A:747:C:H5'	1.96	0.94
6:F:87:ARG:HH11	6:F:87:ARG:HG3	1.33	0.94
1:A:1064:G:H22	1:A:1190:G:H2'	1.31	0.93
10:J:44:VAL:HG13	10:J:66:ARG:HD3	1.50	0.93
13:M:49:THR:HG22	13:M:51:ALA:H	1.32	0.93
15:O:5:LYS:HA	15:O:5:LYS:NZ	1.83	0.93
3:C:188:LEU:HD11	3:C:195:VAL:HG13	1.51	0.93
13:M:49:THR:HB	13:M:52:GLU:HG3	1.50	0.93
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.49	0.93
8:H:54:ASP:OD2	8:H:55:GLY:N	2.02	0.93
17:Q:40:LYS:HD2	17:Q:42:TYR:CE1	2.04	0.93
1:A:1064:G:N2	1:A:1190:G:H2'	1.84	0.93
12:L:20:LYS:HE2	12:L:20:LYS:H	1.34	0.92
1:A:499:A:H4'	1:A:500:G:OP1	1.66	0.92
1:A:1412:C:H2'	1:A:1413:A:C8	2.05	0.92
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.34	0.92
5:E:37:ARG:HG2	5:E:37:ARG:HH11	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:U:C2'	1:A:230:G:H5'	2.00	0.92
4:D:36:ARG:HB3	4:D:38:TYR:HE2	1.30	0.92
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.10	0.92
15:O:79:ARG:HH11	15:O:79:ARG:HG3	1.35	0.92
18:R:87:ARG:CG	18:R:87:ARG:HH21	1.82	0.91
4:D:83:SER:HA	4:D:89:THR:HG23	1.52	0.91
11:K:120:ARG:HG2	11:K:120:ARG:HH11	1.34	0.91
8:H:102:ARG:N	8:H:102:ARG:HD2	1.85	0.91
1:A:1392:G:C2'	1:A:1393:U:H5'	1.99	0.91
1:A:279:A:OP2	17:Q:95:TYR:OH	1.86	0.91
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.52	0.91
1:A:867:G:C2'	1:A:868:C:H5'	2.01	0.91
1:A:1392:G:H2'	1:A:1393:U:H5'	1.49	0.91
1:A:1035:A:H2'	1:A:1036:G:H8	1.34	0.91
15:O:88:ARG:NE	15:O:88:ARG:HA	1.85	0.91
1:A:1381:U:C5	1:A:1382:C:C5	2.58	0.91
5:E:106:PRO:O	5:E:110:LEU:HD12	1.71	0.91
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.54	0.90
12:L:47:LYS:N	12:L:48:PRO:HD2	1.85	0.90
10:J:55:LYS:CG	10:J:56:HIS:H	1.78	0.90
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.35	0.89
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.07	0.89
3:C:127:ARG:HA	3:C:127:ARG:NE	1.85	0.89
12:L:76:ASN:O	12:L:77:LEU:HD23	1.72	0.89
1:A:991:U:O2'	1:A:992:U:O5'	1.90	0.89
2:B:74:LYS:HE3	2:B:166:ASP:HB2	1.54	0.89
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.54	0.89
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.53	0.89
1:A:1538:C:H2'	1:A:1539:C:O4'	1.73	0.89
1:A:192:U:H1'	20:T:103:GLY:HA2	1.55	0.89
16:P:67:THR:HG22	16:P:68:ASP:H	1.36	0.89
10:J:25:GLU:HA	10:J:28:ARG:HB2	1.55	0.89
1:A:791:G:H2'	1:A:792:A:H5'	1.55	0.88
1:A:1442:G:C6	1:A:1446:A:N6	2.41	0.88
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.55	0.88
1:A:500:G:C5	1:A:546:G:N2	2.42	0.88
1:A:484:G:O2'	1:A:485:G:OP2	1.90	0.88
10:J:48:THR:HA	10:J:62:HIS:HB3	1.54	0.88
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.55	0.88
7:G:38:LEU:O	7:G:42:ILE:HG13	1.71	0.88
1:A:1047:G:C2'	1:A:1048:G:H5'	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:88:ARG:CA	15:O:88:ARG:HE	1.83	0.88
1:A:604:G:H2'	1:A:605:U:H5'	1.54	0.88
1:A:543:C:H2'	1:A:544:G:H5'	1.52	0.88
12:L:117:ARG:O	12:L:120:TYR:N	2.06	0.88
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.52	0.88
1:A:1493[A]:A:H2	23:W:36:A:HO2'	1.19	0.88
2:B:236:TYR:O	2:B:239:VAL:HG23	1.73	0.88
7:G:18:TYR:OH	7:G:58:PRO:HG2	1.74	0.87
1:A:1136:U:H5''	1:A:1137:C:OP2	1.74	0.87
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.55	0.87
1:A:353:A:OP1	29:A:2224:HOH:O	1.91	0.87
1:A:1047:G:H5''	14:N:4:LYS:HD3	1.56	0.87
16:P:1:MET:O	16:P:1:MET:HG2	1.75	0.87
1:A:1035:A:H2'	1:A:1036:G:C8	2.09	0.87
16:P:74:LEU:HB3	16:P:79:VAL:HG21	1.54	0.87
15:O:25:THR:O	15:O:29:VAL:HG23	1.75	0.87
1:A:839:U:O2	1:A:839:U:H2'	1.72	0.87
1:A:1256:A:H4'	1:A:1257:U:O5'	1.74	0.86
1:A:974:A:OP2	14:N:41:ARG:NH1	2.09	0.86
1:A:176:C:O2'	1:A:177:C:H5'	1.75	0.86
10:J:82:ILE:HA	10:J:85:LEU:CB	2.05	0.86
20:T:61:SER:OG	20:T:65:LYS:HD2	1.73	0.86
13:M:39:ILE:HG22	13:M:40:ASN:O	1.76	0.86
1:A:1381:U:H5	1:A:1382:C:C5	1.92	0.86
5:E:51:VAL:HG23	5:E:52:PRO:HD3	1.57	0.86
1:A:1493[A]:A:C8	1:A:1493[A]:A:C3'	2.59	0.86
6:F:98:LEU:H	6:F:98:LEU:HD13	1.41	0.85
1:A:1412:C:H2'	1:A:1413:A:H8	1.39	0.85
8:H:112:LEU:N	8:H:112:LEU:HD23	1.91	0.85
10:J:40:LEU:HB2	10:J:69:ASN:HB2	1.58	0.85
13:M:19:LEU:O	13:M:22:ILE:HG12	1.76	0.85
1:A:1004:A:H5''	29:A:2325:HOH:O	1.75	0.85
1:A:54:C:C4	1:A:352:C:C5	2.65	0.85
1:A:284:G:H2'	1:A:285:G:H8	1.41	0.85
13:M:108:ARG:NH2	13:M:114:ARG:HA	1.92	0.85
1:A:1068:G:H8	1:A:1068:G:OP2	1.59	0.85
1:A:192:U:C1'	20:T:103:GLY:HA2	2.05	0.85
1:A:328:C:C2'	1:A:328:C:O2	2.22	0.85
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.56	0.85
1:A:1225:A:H5'	1:A:1226:C:OP2	1.77	0.85
1:A:981:U:H5'	14:N:21:TYR:CE1	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:192:GLU:N	4:D:192:GLU:OE2	2.10	0.85
1:A:393:A:C2	1:A:394:G:C8	2.64	0.85
12:L:27:LEU:C	12:L:29:GLY:H	1.81	0.84
1:A:821:G:H4'	29:A:2105:HOH:O	1.74	0.84
3:C:123:GLN:O	3:C:128:PHE:HB2	1.77	0.84
3:C:16:ARG:HG2	3:C:16:ARG:HH11	1.40	0.84
19:S:15:LEU:O	19:S:19:VAL:HG12	1.77	0.84
3:C:58:GLU:H	3:C:65:ALA:HB3	1.43	0.84
20:T:57:ARG:NH2	20:T:100:ILE:HD13	1.93	0.84
1:A:54:C:C4	1:A:352:C:H5	1.96	0.84
11:K:33:THR:HG22	11:K:39:PRO:HA	1.58	0.84
2:B:61:LEU:HD13	2:B:66:GLY:HA3	1.60	0.84
1:A:304:U:O4	29:A:2495:HOH:O	1.94	0.84
17:Q:10:VAL:HG11	17:Q:52:LYS:O	1.77	0.84
1:A:509:A:O2'	1:A:510:A:OP1	1.93	0.83
1:A:114:U:O2'	1:A:115:G:H5'	1.78	0.83
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.59	0.83
1:A:1321:C:H4'	13:M:87:TYR:HE2	1.42	0.83
1:A:604:G:C2'	1:A:605:U:H5'	2.07	0.83
4:D:98:GLU:OE2	4:D:107:ARG:HD3	1.77	0.83
10:J:34:VAL:HG13	10:J:74:ILE:HG22	1.59	0.83
5:E:90:VAL:O	5:E:91:LEU:HD23	1.77	0.83
16:P:67:THR:HG22	16:P:68:ASP:N	1.91	0.83
1:A:1212:U:H1'	1:A:1213:A:OP2	1.78	0.83
2:B:170:GLU:OE2	2:B:170:GLU:HA	1.79	0.83
18:R:38:GLU:OE2	18:R:38:GLU:N	2.12	0.83
8:H:112:LEU:HD23	8:H:112:LEU:H	1.44	0.83
1:A:1300:G:O2'	1:A:1301:U:P	2.37	0.83
1:A:1281:U:H4'	1:A:1282:C:OP2	1.76	0.83
19:S:18:LYS:HG2	19:S:31:ILE:HD11	1.59	0.83
1:A:448:A:O2'	1:A:449:C:H5'	1.79	0.83
15:O:45:VAL:HB	15:O:46:HIS:ND1	1.92	0.83
10:J:47:PHE:CZ	14:N:37:PHE:HE1	1.97	0.82
4:D:70:ILE:HG22	4:D:71:SER:O	1.79	0.82
2:B:82:ARG:HA	2:B:92:TYR:CE2	2.14	0.82
9:I:32:ASP:OD1	9:I:33:PHE:N	2.12	0.82
1:A:1057:G:H5''	3:C:154:SER:HB2	1.61	0.82
1:A:1435:G:H2'	1:A:1436:U:H6	1.40	0.82
23:W:31:C:H42	23:W:39:G:H1	0.84	0.82
2:B:130:ARG:NH1	2:B:134:GLU:OE1	2.12	0.82
19:S:17:GLU:HA	19:S:20:LEU:HD12	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:VAL:O	3:C:124:ILE:HG13	1.80	0.82
1:A:1399:C:O2	1:A:1401:G:C5	2.32	0.82
9:I:17:VAL:HG13	9:I:63:ILE:HD11	1.62	0.82
15:O:26:GLU:OE2	15:O:77:ARG:NH1	2.12	0.82
1:A:512:U:O2	1:A:540:G:N2	2.13	0.81
5:E:144:THR:O	5:E:148:VAL:CG2	2.28	0.81
1:A:1532:U:C4	1:A:1533:C:N4	2.48	0.81
19:S:10:PHE:O	19:S:39:THR:OG1	1.98	0.81
1:A:107:G:C2'	1:A:108:G:H5''	2.09	0.81
1:A:1314:C:OP2	19:S:6:LYS:HD3	1.80	0.81
4:D:173:TRP:O	4:D:174:LEU:HD23	1.80	0.81
1:A:1054:C:C3'	1:A:1054:C:O2	2.28	0.81
1:A:839:U:H5'	1:A:840:C:H5	1.44	0.81
2:B:131:PRO:O	2:B:134:GLU:HB3	1.80	0.81
17:Q:100:LYS:HB2	17:Q:101:ARG:NH1	1.96	0.81
1:A:117:G:OP2	29:A:2018:HOH:O	1.98	0.81
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.14	0.81
1:A:138:G:H8	1:A:138:G:H5'	1.45	0.81
21:U:10:ARG:CG	21:U:10:ARG:HH11	1.94	0.81
17:Q:40:LYS:HG2	17:Q:41:LYS:N	1.93	0.81
1:A:1532:U:H2'	1:A:1533:C:H6	1.46	0.81
1:A:1399:C:C6	1:A:1502:A:N6	2.48	0.81
7:G:5:ARG:HG3	7:G:7:ALA:N	1.96	0.81
19:S:18:LYS:O	19:S:22:LEU:HG	1.81	0.81
4:D:19:LEU:HD23	4:D:19:LEU:H	1.45	0.80
4:D:120:LEU:HD22	4:D:126:ILE:HD11	1.61	0.80
1:A:673:G:H2'	1:A:674:G:C8	2.15	0.80
1:A:392:G:H2'	1:A:393:A:H8	1.46	0.80
1:A:1057:G:H5''	3:C:154:SER:CB	2.12	0.80
1:A:1300:G:O2'	1:A:1301:U:O5'	1.99	0.80
1:A:303:A:N6	29:A:2495:HOH:O	2.15	0.80
1:A:539:A:H2'	1:A:540:G:C8	2.17	0.80
1:A:415:A:H2'	1:A:416:G:H8	1.44	0.80
1:A:141:A:H1'	1:A:182:U:O2	1.82	0.80
1:A:984:C:H42	1:A:1221:G:H1	1.28	0.80
1:A:250:A:H4'	1:A:251:G:O5'	1.82	0.80
1:A:628:G:C2'	1:A:629:G:H5'	2.12	0.80
1:A:1412:C:OP1	12:L:57:LYS:NZ	2.15	0.80
1:A:1496:C:H2'	1:A:1497:G:C8	2.16	0.80
10:J:16:LEU:HD21	10:J:70:ARG:HG3	1.63	0.80
1:A:853:G:C2'	1:A:854:G:H5'	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:LYS:HE3	4:D:20:TYR:CE2	2.17	0.80
1:A:1356:G:H2'	1:A:1357:A:C8	2.17	0.80
1:A:89:C:H5	1:A:90:U:C4	2.00	0.80
1:A:1054:C:O2	23:W:34:G:H5'	1.81	0.80
13:M:19:LEU:O	13:M:22:ILE:CG1	2.30	0.79
18:R:43:PHE:C	18:R:44:LEU:HD23	2.02	0.79
2:B:87:ARG:HD2	2:B:88:ALA:H	1.47	0.79
13:M:84:ILE:HD12	13:M:86:CYS:HB2	1.64	0.79
1:A:512:U:OP1	4:D:46:LYS:NZ	2.15	0.79
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.63	0.79
17:Q:29:HIS:CE1	17:Q:32:TYR:H	2.01	0.79
19:S:80:TYR:CE1	19:S:81:ARG:HG2	2.16	0.79
1:A:114:U:C2'	1:A:115:G:H5'	2.13	0.79
1:A:1101:A:H4'	1:A:1102:A:O5'	1.82	0.79
15:O:5:LYS:HA	15:O:5:LYS:HZ2	1.43	0.79
4:D:100:ARG:NH1	4:D:137:SER:HA	1.97	0.79
1:A:624:C:H5''	29:A:2767:HOH:O	1.82	0.79
7:G:120:ILE:HD13	7:G:120:ILE:H	1.48	0.79
8:H:55:GLY:HA3	8:H:56:LYS:HE3	1.63	0.79
15:O:9:GLN:OE1	15:O:9:GLN:HA	1.81	0.79
1:A:1515[B]:C:N4	1:A:1520[B]:G:O6	2.14	0.79
1:A:89:C:H5	1:A:90:U:H3	1.16	0.79
1:A:229:U:H2'	1:A:230:G:H5'	1.62	0.79
1:A:777:A:OP1	29:A:2536:HOH:O	2.00	0.79
9:I:50:LEU:CD1	9:I:81:ILE:HG21	2.08	0.79
1:A:542:G:OP1	4:D:10:ARG:NH2	2.16	0.79
20:T:50:GLU:CA	20:T:99:LEU:HD11	2.13	0.79
1:A:924:C:O2'	1:A:1399:C:H6	1.65	0.78
1:A:1272:G:N7	29:A:2695:HOH:O	2.16	0.78
9:I:69:GLY:O	9:I:73:GLN:HG3	1.83	0.78
9:I:43:ALA:HA	9:I:74:ILE:HD12	1.63	0.78
2:B:87:ARG:HE	2:B:219:VAL:HG11	1.48	0.78
1:A:527:7MG:OP2	27:A:1928:SRV:O32	2.01	0.78
1:A:1346:A:C4	7:G:10:ARG:NH1	2.51	0.78
9:I:90:PRO:O	9:I:93:ARG:HG3	1.82	0.78
8:H:10:LEU:HD23	8:H:10:LEU:N	1.97	0.78
20:T:67:ALA:O	20:T:73:HIS:ND1	2.16	0.78
3:C:86:VAL:O	3:C:89:GLU:HB3	1.82	0.78
1:A:643:C:H2'	1:A:644:G:H5''	1.65	0.78
1:A:1033:G:H2'	1:A:1034:G:H5'	1.66	0.78
15:O:85:LEU:HD23	15:O:85:LEU:N	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:LYS:HD2	4:D:62:GLN:N	1.97	0.78
1:A:1147:C:H4'	9:I:5:TYR:HE2	1.47	0.78
5:E:126:ARG:CG	5:E:126:ARG:HH11	1.97	0.78
1:A:352:C:O2'	1:A:354:G:OP1	2.02	0.78
5:E:24:ARG:HG2	5:E:24:ARG:HH11	1.47	0.78
8:H:4:ASP:OD2	8:H:85:ARG:NE	2.15	0.78
4:D:159:ARG:HG2	4:D:159:ARG:HH11	1.48	0.78
1:A:76:C:O2'	1:A:77:G:H5'	1.83	0.78
5:E:48:ALA:HB1	5:E:49:PRO:HD2	1.65	0.78
20:T:10:LEU:CD2	20:T:13:LEU:H	1.96	0.78
1:A:1400:5MC:H3'	1:A:1401:G:C5'	2.14	0.78
1:A:597:G:H1	1:A:643:C:H42	1.29	0.78
1:A:965:A:C2	1:A:969:A:C2	2.72	0.78
1:A:1347:G:O2'	1:A:1348:U:P	2.41	0.78
9:I:31:GLN:NE2	9:I:36:TYR:HD1	1.81	0.78
5:E:144:THR:HG22	5:E:145:LYS:H	1.49	0.78
1:A:643:C:C2'	1:A:644:G:H5''	2.14	0.77
7:G:97:GLN:O	7:G:101:LEU:HD12	1.84	0.77
1:A:1157:A:H4'	1:A:1158:C:O5'	1.83	0.77
6:F:48:LEU:CD1	6:F:52:ILE:HG13	2.14	0.77
4:D:15:GLU:HG3	4:D:63:LYS:HD3	1.65	0.77
3:C:46:GLU:HB3	3:C:47:LEU:HD12	1.66	0.77
1:A:768:A:OP2	29:A:2052:HOH:O	2.02	0.77
9:I:121:ARG:HH11	9:I:121:ARG:HG3	1.48	0.77
21:U:10:ARG:NH1	21:U:10:ARG:CB	2.45	0.77
15:O:74:ASP:OD2	15:O:77:ARG:HG2	1.84	0.77
20:T:54:LYS:HG2	20:T:55:ILE:HD12	1.65	0.77
3:C:179:ARG:HD2	3:C:207:VAL:HG22	1.65	0.77
9:I:108:VAL:HG12	9:I:109:VAL:N	1.99	0.77
1:A:1534:C:N3	1:A:1535:A:C2	2.53	0.77
10:J:29:ARG:N	10:J:29:ARG:HD2	2.00	0.77
19:S:80:TYR:CD1	19:S:81:ARG:N	2.53	0.77
4:D:119:GLN:HG3	4:D:123:HIS:HD1	1.49	0.77
4:D:208:SER:HA	29:D:404:HOH:O	1.85	0.77
2:B:36:ARG:HG3	2:B:41:ILE:HD11	1.66	0.77
18:R:47:THR:HG22	18:R:48:GLY:H	1.50	0.77
1:A:673:G:H5''	6:F:87:ARG:NH1	2.00	0.77
3:C:116:VAL:O	3:C:120:VAL:HG23	1.85	0.77
13:M:11:ARG:HG3	13:M:12:ASN:N	1.99	0.77
1:A:89:C:C2'	1:A:90:U:O5'	2.33	0.77
1:A:201:C:H42	1:A:216:G:H1	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:G:H2'	1:A:1027:C:O2	1.84	0.76
12:L:53:ARG:HD2	12:L:93:LEU:HD21	1.65	0.76
2:B:219:VAL:HA	2:B:222:ILE:HG12	1.66	0.76
4:D:32:ALA:O	4:D:36:ARG:N	2.17	0.76
13:M:51:ALA:O	13:M:54:VAL:HG12	1.85	0.76
27:A:1928:SRV:HI32	27:A:1928:SRV:C22	2.16	0.76
5:E:8:GLU:HB3	5:E:34:VAL:HG12	1.65	0.76
1:A:1245:A:C2	1:A:1293:G:C2	2.74	0.76
1:A:1498:UR3:H4'	1:A:1519[A]:MA6:H2	1.67	0.76
15:O:33:THR:HG23	15:O:63:ARG:NH1	1.99	0.76
1:A:1047:G:N7	29:A:2425:HOH:O	2.19	0.76
14:N:26:ARG:HD3	14:N:47:LEU:HD11	1.66	0.76
6:F:12:PRO:CG	6:F:58:GLY:HA2	2.14	0.76
1:A:247:G:OP2	17:Q:100:LYS:HG2	1.85	0.76
2:B:240:GLN:O	2:B:240:GLN:HG2	1.84	0.76
1:A:137:C:C2'	1:A:138:G:H5''	2.15	0.76
6:F:7:ASN:HD21	18:R:34:TYR:HE1	1.32	0.76
3:C:155:GLY:O	3:C:196:LEU:HD22	1.85	0.76
11:K:48:ILE:HG22	11:K:49:GLY:H	1.48	0.76
1:A:628:G:O2'	1:A:629:G:H5'	1.86	0.76
7:G:64:GLN:O	7:G:68:ASN:ND2	2.18	0.76
2:B:6:THR:HB	2:B:48:MET:HE3	1.67	0.76
1:A:284:G:H2'	1:A:285:G:C8	2.21	0.76
5:E:144:THR:HG22	5:E:145:LYS:N	2.01	0.76
1:A:438:G:H4'	4:D:123:HIS:HD2	1.51	0.76
10:J:42:THR:HG23	10:J:67:THR:O	1.85	0.76
1:A:1268:A:OP1	29:A:2314:HOH:O	2.02	0.76
3:C:11:ARG:NH1	3:C:177:THR:O	2.19	0.76
1:A:677:U:H3	1:A:713:G:H22	1.32	0.76
1:A:1504:G:OP1	1:A:1507:A:H4'	1.86	0.76
1:A:543:C:O2'	1:A:544:G:H5'	1.85	0.76
1:A:1314:C:C5	19:S:6:LYS:HE2	2.21	0.76
18:R:26:LEU:HD11	18:R:42:ARG:CD	2.16	0.76
2:B:16:HIS:CD2	2:B:17:PHE:HD2	2.04	0.76
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.68	0.75
1:A:438:G:H4'	4:D:123:HIS:CD2	2.21	0.75
1:A:1343:G:H1'	9:I:121:ARG:HH12	1.51	0.75
1:A:1034:G:H2'	1:A:1035:A:C8	2.22	0.75
1:A:461:C:OP2	29:A:2254:HOH:O	2.04	0.75
9:I:53:VAL:HG21	9:I:85:LEU:HD11	1.66	0.75
1:A:1407:5MC:C2'	1:A:1408:A:H5'	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:76:ASN:C	10:J:78:ASN:H	1.88	0.75
1:A:1003(A):G:N2	1:A:1038:C:O2	2.19	0.75
20:T:51:GLU:O	20:T:55:ILE:HD13	1.85	0.75
1:A:463:A:H2'	1:A:474:G:H8	1.50	0.75
1:A:1408:A:H2'	1:A:1409:C:H6	1.49	0.75
1:A:731:G:OP1	1:A:766:A:H1'	1.87	0.75
1:A:827:U:H5''	1:A:828:A:OP2	1.85	0.75
10:J:76:ASN:O	10:J:78:ASN:N	2.19	0.75
12:L:117:ARG:O	12:L:119:LYS:N	2.20	0.75
1:A:1225:A:H2'	1:A:1225:A:N3	2.00	0.75
15:O:8:LYS:O	15:O:11:VAL:HG13	1.86	0.75
1:A:853:G:H2'	1:A:854:G:H5'	1.68	0.75
1:A:73:C:N4	1:A:74:C:N4	2.34	0.75
15:O:70:LEU:CD2	15:O:78:TYR:HB2	2.15	0.75
1:A:1006:C:H42	1:A:1023:G:H1	1.34	0.75
5:E:122:GLU:OE1	5:E:131:ILE:HG13	1.86	0.75
13:M:37:THR:O	13:M:55:ARG:HD2	1.86	0.75
1:A:1256:A:N6	1:A:1277:C:C5	2.54	0.75
4:D:173:TRP:HB3	4:D:187:ARG:HH21	1.52	0.75
7:G:90:GLU:HA	7:G:90:GLU:OE1	1.87	0.75
1:A:1005:A:N7	1:A:1026:G:N1	2.30	0.75
1:A:1010:G:N2	1:A:1020:U:H1'	2.02	0.75
7:G:103:TRP:CE2	7:G:137:LYS:HG2	2.21	0.75
1:A:1054:C:OP1	1:A:1197:G:OP2	2.04	0.75
6:F:87:ARG:NH1	6:F:87:ARG:HG3	2.01	0.75
2:B:97:TRP:CE3	2:B:98:LEU:O	2.40	0.75
11:K:18:ARG:NH1	11:K:35:PRO:O	2.19	0.75
21:U:10:ARG:NH1	21:U:10:ARG:HB2	2.00	0.74
10:J:28:ARG:HB3	10:J:29:ARG:HH11	1.52	0.74
5:E:13:ILE:HG22	5:E:14:ARG:N	2.02	0.74
5:E:76:ILE:HG22	5:E:93:PRO:HG3	1.67	0.74
1:A:39:G:N3	1:A:39:G:H2'	2.81	0.74
1:A:427:U:OP1	4:D:13:ARG:NH2	2.20	0.74
15:O:17:ARG:NH1	15:O:17:ARG:HG3	1.91	0.74
1:A:229:U:O2'	1:A:230:G:H5'	1.87	0.74
15:O:15:PHE:CE2	15:O:85:LEU:HD21	2.21	0.74
20:T:44:ALA:HA	20:T:92:LEU:HD21	1.68	0.74
4:D:8:VAL:O	4:D:11:LEU:N	2.17	0.74
1:A:839:U:H5'	1:A:840:C:C5	2.23	0.74
1:A:1212:U:H4'	1:A:1213:A:O5'	1.84	0.74
9:I:48:GLU:HB3	9:I:101:PHE:CZ	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:G:H5'	1:A:644:G:C8	2.18	0.74
1:A:474:G:H4'	16:P:81:ARG:HH21	1.51	0.74
20:T:82:SER:O	20:T:86:ARG:HG3	1.87	0.74
1:A:503:C:OP2	12:L:116:SER:HB3	1.87	0.74
23:W:39:G:N2	23:W:40:PSU:O4	2.21	0.74
3:C:137:ALA:O	3:C:141:VAL:HG23	1.87	0.74
10:J:78:ASN:OD1	10:J:79:ARG:NH1	2.21	0.74
1:A:1404:5MC:H1'	1:A:1499:A:H2	1.52	0.74
1:A:297:G:N7	29:A:2519:HOH:O	2.19	0.74
1:A:348:G:N7	29:A:2636:HOH:O	2.21	0.74
1:A:620:C:C2	4:D:135:LEU:HD22	2.22	0.74
1:A:583:A:OP2	29:A:2103:HOH:O	2.05	0.74
1:A:440:A:H5'	1:A:442:C:OP2	1.88	0.74
1:A:413:G:O2'	1:A:428:G:N2	2.20	0.74
1:A:331:G:OP2	29:A:2266:HOH:O	2.06	0.74
1:A:1090:U:H2'	1:A:1091:U:H6	1.53	0.74
20:T:10:LEU:HD21	20:T:13:LEU:H	1.53	0.74
1:A:949:A:C2	1:A:1233:G:N3	2.56	0.74
4:D:52:SER:O	4:D:56:VAL:HG23	1.88	0.74
2:B:212:GLN:O	2:B:216:SER:HB3	1.88	0.73
7:G:17:VAL:HG12	7:G:18:TYR:N	2.01	0.73
2:B:75:LYS:HA	2:B:78:GLN:CG	2.16	0.73
14:N:9:LYS:HD2	14:N:9:LYS:O	1.88	0.73
13:M:87:TYR:CE1	13:M:91:ARG:HD3	2.23	0.73
1:A:289:G:OP2	29:A:2015:HOH:O	2.04	0.73
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.22	0.73
6:F:101:ALA:HA	18:R:28:GLU:HB2	1.71	0.73
6:F:25:ILE:HD12	6:F:82:ARG:HH11	1.53	0.73
1:A:1133:G:N2	1:A:1141:C:N3	2.36	0.73
10:J:63:PHE:HA	14:N:59:ALA:CB	2.18	0.73
1:A:182:U:H5	1:A:183:G:C4	2.06	0.73
17:Q:81:ARG:HE	17:Q:84:LEU:HD11	1.52	0.73
17:Q:23:VAL:HG21	17:Q:42:TYR:CD1	2.23	0.73
20:T:10:LEU:HD21	20:T:13:LEU:N	2.04	0.73
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.23	0.73
9:I:89:ASN:HB3	9:I:92:TYR:CD1	2.23	0.73
1:A:52:G:O6	29:A:2441:HOH:O	2.06	0.73
1:A:939:G:H5'	7:G:102:ARG:NH2	2.04	0.73
1:A:1286:A:H2	21:U:22:ARG:NH2	1.86	0.73
1:A:1226:C:H4'	1:A:1227:A:OP1	1.88	0.73
1:A:243:A:C2	1:A:246:A:C8	2.76	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:THR:N	2:B:176:GLU:OE1	2.20	0.73
1:A:1518[B]:MA6:N6	1:A:1519[B]:MA6:H103	2.04	0.73
1:A:1321:C:H4'	13:M:87:TYR:CE2	2.23	0.73
20:T:13:LEU:HD12	20:T:14:LYS:HA	1.71	0.73
15:O:15:PHE:CZ	15:O:85:LEU:HD21	2.24	0.72
2:B:44:LEU:H	2:B:44:LEU:HD22	1.53	0.72
1:A:1408:A:H2'	1:A:1409:C:C6	2.24	0.72
1:A:1510:U:H2'	1:A:1511:G:C8	2.23	0.72
1:A:1193:G:H2'	1:A:1194:U:H6	1.54	0.72
3:C:130:VAL:HG11	3:C:157:ILE:HG22	1.70	0.72
1:A:1407:5MC:H2'	1:A:1408:A:H5'	1.71	0.72
1:A:444:C:H42	1:A:490:G:H1	1.37	0.72
9:I:118:LYS:O	9:I:120:ARG:N	2.20	0.72
1:A:500:G:C6	1:A:501:C:N4	2.58	0.72
20:T:45:GLN:HA	20:T:91:LEU:CD2	2.19	0.72
1:A:157:G:H5'	1:A:158:G:OP2	1.90	0.72
6:F:74:ASP:N	6:F:74:ASP:OD2	2.19	0.72
6:F:82:ARG:HB2	6:F:85:VAL:HG23	1.72	0.72
1:A:421:U:OP2	1:A:422:C:N4	2.22	0.72
1:A:977:A:H2'	1:A:978:A:H5'	1.69	0.72
1:A:1403:C:O2'	1:A:1404:5MC:H5'	1.89	0.72
1:A:9:G:OP2	5:E:121:LYS:NZ	2.20	0.72
5:E:144:THR:O	5:E:148:VAL:HG23	1.89	0.72
13:M:19:LEU:O	13:M:22:ILE:HD11	1.89	0.72
1:A:427:U:OP2	1:A:428:G:O2'	2.07	0.72
1:A:345:C:OP2	1:A:345:C:H6	1.71	0.72
19:S:69:HIS:HB3	19:S:73:GLU:OE1	1.88	0.72
1:A:1537:U:H2'	1:A:1538:C:C6	2.25	0.72
1:A:1329:A:OP1	13:M:29:ARG:HG3	1.89	0.72
3:C:150:LYS:HG3	3:C:169:ALA:CB	2.18	0.72
3:C:195:VAL:C	3:C:196:LEU:HD23	2.11	0.72
1:A:928:G:O2'	1:A:1533:C:OP1	2.08	0.72
1:A:1536:C:H5	1:A:1537:U:C4	2.08	0.72
1:A:107:G:H2'	1:A:108:G:C5'	2.20	0.72
13:M:19:LEU:O	13:M:22:ILE:CD1	2.37	0.72
1:A:914:A:O5'	27:A:1928:SRV:HI33	1.88	0.72
4:D:22:LYS:CB	4:D:26:CYS:SG	2.78	0.72
18:R:47:THR:HG22	18:R:48:GLY:N	2.05	0.72
1:A:1385:G:N7	29:A:2670:HOH:O	2.23	0.72
1:A:1347:G:O2'	1:A:1348:U:OP2	2.08	0.71
1:A:1493[A]:A:O2'	1:A:1494:G:OP1	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:4OC:CM2	1:A:1403:C:H5'	2.15	0.71
16:P:22:THR:HA	16:P:33:ILE:HD12	1.71	0.71
18:R:44:LEU:HD23	18:R:44:LEU:N	2.04	0.71
10:J:16:LEU:HD21	10:J:70:ARG:CG	2.20	0.71
1:A:616:G:H1'	1:A:625:G:N2	2.05	0.71
3:C:174:PRO:O	3:C:177:THR:N	2.23	0.71
8:H:95:VAL:HG12	8:H:99:GLU:HB2	1.72	0.71
17:Q:51:TYR:CD1	17:Q:73:VAL:HG11	2.25	0.71
1:A:266:G:HO2'	1:A:267:C:P	2.12	0.71
1:A:791:G:C2'	1:A:792:A:H5'	2.20	0.71
2:B:97:TRP:CZ3	2:B:98:LEU:O	2.43	0.71
10:J:41:PRO:O	10:J:69:ASN:ND2	2.23	0.71
1:A:179:A:H2'	1:A:180:U:H6	1.55	0.71
1:A:1361(A):C:O2'	1:A:1362:C:O5'	2.05	0.71
1:A:273:A:H2'	1:A:274:A:H5'	1.71	0.71
3:C:151:VAL:C	3:C:152:ILE:HD12	2.10	0.71
1:A:532:A:N6	1:A:1207:2MG:H5'	2.06	0.71
1:A:538:G:H5''	12:L:114:LYS:CB	2.17	0.71
17:Q:81:ARG:HE	17:Q:84:LEU:CD1	2.03	0.71
1:A:1366:C:H2'	1:A:1367:C:C6	2.25	0.71
1:A:1131:G:H8	1:A:1131:G:OP2	1.72	0.71
1:A:89:C:O2'	1:A:90:U:P	2.49	0.71
1:A:447:G:H2'	1:A:485:G:N2	2.05	0.71
1:A:893:C:O2'	1:A:894:G:H5'	1.90	0.71
1:A:835:U:O4	29:A:2788:HOH:O	2.06	0.71
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:N1	2.05	0.71
1:A:382:A:O2'	1:A:383:A:H5'	1.90	0.71
1:A:1498:UR3:H4'	1:A:1519[A]:MA6:N1	2.04	0.71
7:G:46:ALA:O	7:G:50:ILE:HG12	1.91	0.71
1:A:446:G:H2'	1:A:447:G:H5'	1.72	0.71
1:A:415:A:H2'	1:A:416:G:C8	2.25	0.71
1:A:352:C:H6	1:A:352:C:H3'	1.55	0.71
11:K:40:ILE:HG23	11:K:75:TYR:CD1	2.25	0.71
1:A:951:G:OP2	13:M:102:ARG:NH2	2.24	0.71
2:B:102:LEU:HD12	2:B:102:LEU:N	2.06	0.71
3:C:10:PHE:CE1	3:C:178:LEU:HD11	2.26	0.71
10:J:81:THR:HG22	10:J:82:ILE:HG13	1.73	0.70
1:A:77:G:C4	1:A:93:G:N2	2.59	0.70
6:F:12:PRO:HG3	6:F:58:GLY:CA	2.17	0.70
1:A:537:G:H2'	1:A:538:G:H8	1.55	0.70
15:O:14:GLU:HG3	15:O:15:PHE:HD1	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:50:ILE:HG13	10:J:60:ARG:HG2	1.72	0.70
12:L:27:LEU:C	12:L:29:GLY:N	2.45	0.70
4:D:63:LYS:O	4:D:67:ILE:HD12	1.91	0.70
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.27	0.70
1:A:204:U:H4'	1:A:216:G:O5'	1.90	0.70
7:G:46:ALA:HA	7:G:49:ILE:HD12	1.74	0.70
12:L:20:LYS:CE	12:L:20:LYS:H	2.05	0.70
1:A:782:A:OP1	29:A:2280:HOH:O	2.09	0.70
14:N:22:THR:HG23	14:N:33:VAL:HG21	1.72	0.70
5:E:81:GLU:OE2	5:E:88:LYS:HD3	1.92	0.70
10:J:62:HIS:O	14:N:59:ALA:HB3	1.90	0.70
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.38	0.70
3:C:147:LYS:CE	3:C:205:GLY:H	2.04	0.70
1:A:104:G:H2'	1:A:105:G:H5''	1.72	0.70
1:A:1270:C:OP2	21:U:24:ARG:NH2	2.25	0.70
1:A:1534:C:C4	1:A:1535:A:N1	2.59	0.70
2:B:82:ARG:HA	2:B:92:TYR:CD2	2.27	0.70
17:Q:11:VAL:HG11	17:Q:88:TYR:CD2	2.26	0.70
1:A:1110:A:OP2	29:A:2142:HOH:O	2.09	0.70
8:H:118:VAL:C	8:H:119:LEU:HD23	2.12	0.70
19:S:39:THR:O	19:S:41:VAL:HG13	1.92	0.70
7:G:97:GLN:HG3	7:G:98:SER:N	2.07	0.70
1:A:689:C:C2'	1:A:690:G:H5'	2.21	0.70
5:E:11:ILE:HG22	5:E:31:LEU:HB3	1.73	0.70
2:B:238:LEU:HD23	2:B:238:LEU:O	1.91	0.70
1:A:266:G:C8	1:A:266:G:C5'	2.69	0.70
7:G:12:LEU:HD12	7:G:12:LEU:N	1.93	0.70
1:A:298:A:N6	29:A:2215:HOH:O	2.25	0.70
12:L:127:GLU:CG	12:L:128:ALA:N	2.40	0.70
1:A:918:A:H2'	1:A:919:A:C8	2.27	0.70
1:A:22:G:H2'	1:A:23:C:H6	1.57	0.70
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.21	0.70
7:G:50:ILE:CG2	7:G:58:PRO:HA	2.16	0.69
27:A:1928:SRY:O61	12:L:46:LYS:HD2	1.92	0.69
15:O:21:ASP:OD1	15:O:24:SER:HB3	1.92	0.69
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.74	0.69
8:H:73:ASP:OD2	8:H:75:ARG:HG3	1.92	0.69
2:B:25:ASN:HD21	2:B:193:ASP:HB2	1.51	0.69
1:A:1533:C:O2'	1:A:1534:C:OP1	2.09	0.69
13:M:8:GLU:OE2	13:M:22:ILE:HA	1.92	0.69
12:L:27:LEU:HG	12:L:28:LYS:N	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:G:HO2'	1:A:1301:U:P	2.14	0.69
14:N:13:THR:N	14:N:14:PRO:HD3	2.06	0.69
17:Q:51:TYR:CE1	17:Q:73:VAL:HG11	2.27	0.69
4:D:146:ILE:N	4:D:146:ILE:CD1	2.56	0.69
1:A:88:A:N7	1:A:89:C:N4	2.39	0.69
1:A:707:C:H4'	11:K:20:TYR:CE1	2.27	0.69
1:A:1130:A:OP1	1:A:1131:G:OP2	2.11	0.69
1:A:1286:A:C2	21:U:22:ARG:NH2	2.60	0.69
1:A:1213:A:H4'	1:A:1214:C:OP1	1.92	0.69
1:A:463:A:H2'	1:A:474:G:C8	2.27	0.69
1:A:21:G:H2'	1:A:22:G:C8	2.27	0.69
1:A:606:G:N1	29:A:2550:HOH:O	2.25	0.69
1:A:1454:G:N7	29:A:2825:HOH:O	2.25	0.69
1:A:1206:G:C6	1:A:1207:2MG:C5	2.81	0.69
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:C6	2.22	0.69
1:A:1527:C:O2'	1:A:1528:U:H5'	1.92	0.69
4:D:4:TYR:O	4:D:4:TYR:CD2	2.45	0.69
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.75	0.69
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.58	0.69
7:G:16:LEU:H	7:G:16:LEU:CD2	2.04	0.69
5:E:37:ARG:NH1	5:E:37:ARG:HG2	2.03	0.69
19:S:31:ILE:O	19:S:50:ALA:HB3	1.91	0.69
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.74	0.69
12:L:34:ARG:HB2	12:L:105:TYR:HE1	1.57	0.69
1:A:316:G:O2'	29:A:2463:HOH:O	2.10	0.69
3:C:62:ASP:O	3:C:97:LYS:HG2	1.92	0.69
1:A:1395:C:O2'	1:A:1396:A:H5'	1.91	0.69
1:A:924:C:O2'	1:A:1399:C:C6	2.41	0.69
3:C:58:GLU:HB2	10:J:92:THR:HG21	1.75	0.69
5:E:48:ALA:HB1	5:E:49:PRO:CD	2.22	0.69
6:F:7:ASN:ND2	18:R:34:TYR:HE1	1.91	0.69
1:A:620:C:H2'	1:A:621:A:O4'	1.93	0.69
9:I:28:VAL:O	9:I:31:GLN:N	2.25	0.69
1:A:1057:G:C4	1:A:1204:A:C2	2.81	0.69
1:A:1003:G:C2	1:A:1003(A):G:C6	2.81	0.69
15:O:70:LEU:HD22	15:O:78:TYR:HB2	1.72	0.69
14:N:15:LYS:O	14:N:16:PHE:CD2	2.46	0.69
10:J:51:ARG:HG3	10:J:59:SER:O	1.92	0.69
1:A:79:G:C2	1:A:80:G:C8	2.81	0.69
1:A:1047:G:O2'	1:A:1048:G:H5'	1.93	0.69
1:A:814:A:H2'	1:A:816:A:C5'	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:THR:HA	2:B:202:PRO:HG2	1.75	0.69
1:A:119:A:OP2	29:A:2559:HOH:O	2.11	0.69
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.27	0.68
9:I:19:LEU:HB3	9:I:59:PHE:CE2	2.28	0.68
1:A:1062:U:H2'	1:A:1063:C:C6	2.28	0.68
20:T:50:GLU:N	20:T:99:LEU:HD11	2.08	0.68
1:A:117:G:OP2	29:A:2016:HOH:O	2.11	0.68
1:A:1419:G:C6	1:A:1420:C:C4	2.81	0.68
1:A:1501:C:N4	1:A:1504:G:N3	2.42	0.68
23:W:37:A:N1	23:W:38:A:C2	2.61	0.68
18:R:59:SER:H	18:R:62:GLU:HB2	1.58	0.68
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.08	0.68
7:G:148:ASN:O	7:G:150:ALA:N	2.25	0.68
6:F:95:GLU:O	18:R:32:ARG:NH1	2.27	0.68
9:I:5:TYR:HD1	9:I:6:GLY:N	1.91	0.68
1:A:1033:G:C2'	1:A:1034:G:H5'	2.23	0.68
7:G:120:ILE:HG22	7:G:124:LEU:HD11	1.74	0.68
10:J:63:PHE:HB2	14:N:57:ARG:O	1.93	0.68
1:A:1369:C:H2'	1:A:1370:G:C8	2.28	0.68
1:A:1066:C:H2'	1:A:1067:A:H5'	1.76	0.68
1:A:392:G:H2'	1:A:393:A:C8	2.29	0.68
1:A:1279:A:H4'	1:A:1280:A:OP1	1.93	0.68
6:F:100:ASN:OD1	18:R:23:LYS:HE3	1.93	0.68
1:A:357:G:N7	29:A:2433:HOH:O	2.27	0.68
21:U:13:ILE:HG22	21:U:22:ARG:CZ	2.24	0.68
1:A:1067:A:O3'	29:A:2218:HOH:O	2.11	0.68
16:P:58:TYR:CE1	16:P:62:VAL:HG11	2.28	0.68
5:E:24:ARG:CG	5:E:24:ARG:HH11	2.07	0.68
10:J:9:ARG:CZ	10:J:9:ARG:HB3	2.23	0.68
9:I:15:ALA:HB1	9:I:77:ILE:HD12	1.76	0.68
1:A:1436:U:H2'	1:A:1437:C:H6	1.59	0.68
19:S:19:VAL:HG23	19:S:47:HIS:ND1	2.09	0.68
17:Q:29:HIS:CE1	17:Q:31:LEU:H	2.11	0.68
1:A:828:A:H4'	1:A:828:A:OP1	1.94	0.68
1:A:1311:G:N7	19:S:2:PRO:HA	2.08	0.68
9:I:55:ALA:HA	9:I:58:HIS:HB2	1.75	0.68
3:C:112:SER:O	3:C:115:LEU:HB2	1.93	0.68
3:C:85:ARG:HG2	3:C:86:VAL:N	2.09	0.68
3:C:155:GLY:HA2	3:C:164:ARG:O	1.93	0.68
14:N:24:CYS:HB2	14:N:29:ARG:HB3	1.76	0.68
1:A:865:A:C2'	1:A:866:C:H5'	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:14:GLU:CG	15:O:15:PHE:HD1	2.07	0.68
1:A:704:A:H5''	1:A:705:U:OP2	1.94	0.68
4:D:79:PHE:O	4:D:82:ALA:N	2.27	0.68
9:I:11:LYS:O	9:I:12:GLU:HB2	1.93	0.67
10:J:28:ARG:HB3	10:J:29:ARG:HD2	1.76	0.67
1:A:1003:G:N2	1:A:1039:C:C2	2.61	0.67
2:B:92:TYR:HD1	2:B:151:GLY:HA3	1.59	0.67
11:K:33:THR:HG22	11:K:39:PRO:CA	2.24	0.67
4:D:206:PHE:CD2	4:D:207:TYR:CE2	2.81	0.67
5:E:131:ILE:HG22	5:E:132:ALA:N	2.09	0.67
5:E:75:THR:HG23	5:E:76:ILE:N	2.08	0.67
17:Q:53:LEU:HD11	17:Q:85:VAL:HG11	1.76	0.67
1:A:358:U:H2'	1:A:359:U:C6	2.29	0.67
12:L:6:THR:OG1	12:L:9:GLN:HG3	1.92	0.67
1:A:1086:U:H3	1:A:1099:G:H22	1.42	0.67
1:A:1060:C:H1'	1:A:1198:G:N2	2.10	0.67
7:G:129:GLU:OE2	7:G:131:LYS:HE2	1.95	0.67
1:A:975:A:H8	1:A:975:A:H5'	1.60	0.67
1:A:1014:A:N7	1:A:1015:A:C6	2.63	0.67
7:G:69:VAL:O	7:G:69:VAL:HG12	1.93	0.67
1:A:1347:G:C2'	1:A:1348:U:OP2	2.41	0.67
1:A:1497:G:O2'	1:A:1498:UR3:H5'	1.94	0.67
13:M:87:TYR:HE1	13:M:91:ARG:HD3	1.59	0.67
8:H:57:PRO:O	8:H:57:PRO:HG2	1.95	0.67
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.29	0.67
1:A:556:C:H2'	1:A:557:G:O4'	1.95	0.67
1:A:1342:C:H2'	1:A:1343:G:C8	2.29	0.67
2:B:219:VAL:HA	2:B:222:ILE:CG1	2.24	0.67
1:A:109:A:C6	1:A:326:G:C6	2.83	0.67
15:O:4:THR:HG22	15:O:5:LYS:N	2.09	0.67
11:K:120:ARG:HG2	11:K:120:ARG:NH1	2.08	0.67
10:J:48:THR:CA	10:J:62:HIS:HB3	2.25	0.67
1:A:975:A:H8	1:A:975:A:C5'	2.07	0.67
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.77	0.67
1:A:814:A:H2'	1:A:816:A:H5'	1.77	0.67
16:P:12:LYS:O	16:P:13:HIS:HB2	1.95	0.67
1:A:785:G:C2'	1:A:786:G:H5'	2.24	0.67
2:B:61:LEU:CD1	2:B:66:GLY:HA3	2.24	0.67
1:A:1310:G:O6	19:S:2:PRO:HG3	1.94	0.67
10:J:29:ARG:H	10:J:29:ARG:HD2	1.60	0.67
1:A:995:C:O2	14:N:4:LYS:NZ	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ARG:HG3	3:C:85:ARG:HH11	1.59	0.67
1:A:606:G:O6	29:A:2549:HOH:O	2.11	0.67
1:A:804:U:H5''	1:A:805:C:OP2	1.94	0.67
1:A:170:U:O2'	1:A:171:A:H5'	1.95	0.67
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.29	0.67
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.30	0.67
1:A:509:A:H3'	1:A:509:A:C8	2.30	0.67
1:A:1443:G:C4'	1:A:1446:A:H5'	2.23	0.67
1:A:1125:U:O2'	1:A:1126:U:OP2	2.13	0.67
1:A:182:U:OP1	29:A:2183:HOH:O	2.11	0.67
20:T:55:ILE:H	20:T:55:ILE:CD1	2.08	0.67
1:A:103:C:P	20:T:17:ARG:HH12	2.17	0.67
1:A:1299:A:C6	1:A:1301:U:O2	2.48	0.67
17:Q:4:LYS:CG	17:Q:6:LEU:HD21	2.25	0.67
1:A:665:A:N3	1:A:732:C:H2'	2.10	0.67
10:J:86:MET:HG3	10:J:87:THR:N	2.05	0.66
4:D:15:GLU:CG	4:D:63:LYS:HD3	2.25	0.66
2:B:36:ARG:HG3	2:B:41:ILE:CD1	2.24	0.66
20:T:44:ALA:O	20:T:47:GLY:N	2.28	0.66
17:Q:51:TYR:CE1	17:Q:73:VAL:CG1	2.78	0.66
1:A:22:G:H2'	1:A:23:C:C6	2.30	0.66
1:A:407:G:OP1	4:D:115:ARG:NH2	2.28	0.66
16:P:10:GLY:HA3	16:P:14:ASN:O	1.94	0.66
1:A:112:G:O2'	1:A:113:G:H5'	1.96	0.66
9:I:46:ALA:HB1	9:I:77:ILE:CG2	2.25	0.66
13:M:16:ASP:O	13:M:19:LEU:N	2.28	0.66
12:L:45:PRO:HB3	12:L:93:LEU:HD23	1.77	0.66
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.75	0.66
3:C:182:ILE:HG23	3:C:202:ILE:O	1.95	0.66
20:T:29:LYS:O	20:T:32:ALA:HB3	1.95	0.66
1:A:661:G:H8	1:A:661:G:H5''	1.58	0.66
1:A:643:C:H2'	1:A:644:G:C5'	2.24	0.66
15:O:4:THR:HG22	15:O:5:LYS:H	1.60	0.66
15:O:70:LEU:HD23	15:O:70:LEU:C	2.16	0.66
21:U:18:TYR:CE1	21:U:24:ARG:HG3	2.31	0.66
1:A:1490:C:H5''	27:A:1928:SRV:NC1	2.11	0.66
12:L:93:LEU:O	12:L:96:VAL:HG23	1.95	0.66
16:P:62:VAL:O	16:P:62:VAL:HG23	1.95	0.66
3:C:58:GLU:CB	10:J:92:THR:HG21	2.24	0.66
1:A:1015:A:N6	1:A:1016:A:C6	2.63	0.66
1:A:349:A:C2'	1:A:350:G:H5'	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:U:H5''	1:A:1079:G:OP2	1.94	0.66
13:M:4:ILE:HG22	13:M:5:ALA:N	2.11	0.66
1:A:509:A:O3'	29:A:2165:HOH:O	2.14	0.66
1:A:179:A:H2'	1:A:180:U:C6	2.31	0.66
1:A:783:C:H42	1:A:799:G:H1	1.43	0.66
1:A:174:C:OP1	29:A:2211:HOH:O	2.14	0.66
1:A:458:C:OP2	29:A:2257:HOH:O	2.13	0.66
1:A:1011:G:C2'	1:A:1012:U:H5'	2.25	0.66
1:A:501:C:H2'	1:A:502:G:H8	1.61	0.66
1:A:443:C:H42	1:A:491:G:H1	1.41	0.66
1:A:273:A:C2'	1:A:274:A:H5'	2.25	0.66
2:B:162:ILE:O	2:B:185:ILE:HD12	1.94	0.66
3:C:186:PHE:CD2	3:C:187:ALA:N	2.64	0.66
1:A:946:A:H2'	1:A:947:G:C8	2.30	0.66
1:A:192:U:O4'	20:T:103:GLY:HA2	1.96	0.66
20:T:50:GLU:HA	20:T:99:LEU:HD11	1.77	0.66
18:R:87:ARG:NH2	18:R:87:ARG:HG3	1.97	0.66
5:E:13:ILE:CG2	5:E:14:ARG:N	2.59	0.66
1:A:137:C:O2'	1:A:138:G:H5''	1.96	0.66
1:A:1342:C:H2'	1:A:1343:G:H8	1.61	0.66
1:A:1054:C:C2	23:W:34:G:H5'	2.30	0.66
1:A:687:A:H4'	1:A:688:G:O5'	1.95	0.66
1:A:1026:G:C2'	1:A:1027:C:H5''	2.23	0.66
6:F:97:PHE:C	6:F:97:PHE:HD2	1.99	0.66
5:E:51:VAL:HG23	5:E:52:PRO:CD	2.26	0.66
10:J:80:LYS:HA	10:J:83:GLU:HB2	1.76	0.66
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.77	0.66
1:A:1532:U:H2'	1:A:1533:C:C5	2.31	0.66
1:A:390:C:H4'	16:P:28:ARG:HH21	1.61	0.66
4:D:135:LEU:O	4:D:135:LEU:HD12	1.96	0.66
2:B:139:LYS:O	2:B:143:GLU:HG3	1.95	0.66
1:A:944:G:OP1	29:A:2285:HOH:O	2.14	0.66
1:A:89:C:HO2'	1:A:90:U:P	2.19	0.65
10:J:63:PHE:HA	14:N:59:ALA:HB2	1.77	0.65
1:A:1480:G:H2'	1:A:1481:U:C6	2.31	0.65
1:A:76:C:C2'	1:A:77:G:H5'	2.27	0.65
18:R:39:VAL:HG13	18:R:40:LEU:N	2.11	0.65
1:A:1256:A:H8	1:A:1258:G:C2	2.15	0.65
5:E:79:GLU:HA	5:E:91:LEU:O	1.95	0.65
7:G:12:LEU:CD1	7:G:12:LEU:H	1.88	0.65
5:E:51:VAL:CG2	5:E:52:PRO:HD3	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030(A):G:H2'	1:A:1030(B):C:H5''	1.77	0.65
11:K:117:ASN:N	11:K:117:ASN:OD1	2.26	0.65
9:I:6:GLY:HA3	9:I:83:ARG:HB2	1.79	0.65
1:A:1197:G:OP1	29:A:2229:HOH:O	2.14	0.65
3:C:131:ARG:O	3:C:134:ILE:HG12	1.97	0.65
1:A:545:C:H2'	1:A:545:C:O2	1.95	0.65
14:N:21:TYR:HE2	14:N:23:ARG:HE	1.44	0.65
20:T:49:ALA:HB3	20:T:99:LEU:CD2	2.21	0.65
1:A:838:G:C3'	1:A:839:U:H5''	2.27	0.65
1:A:1480:G:H2'	1:A:1481:U:H6	1.61	0.65
6:F:26:ILE:O	6:F:30:LEU:HD12	1.96	0.65
7:G:22:LEU:HD21	7:G:66:VAL:HG21	1.77	0.65
9:I:5:TYR:CD1	9:I:6:GLY:N	2.64	0.65
1:A:1065:U:H5''	1:A:1190:G:N2	2.12	0.65
20:T:73:HIS:O	20:T:76:ALA:HB3	1.96	0.65
1:A:1407:5MC:C4	1:A:1408:A:N7	2.64	0.65
17:Q:11:VAL:HG11	17:Q:88:TYR:CE2	2.32	0.65
7:G:27:ILE:HD11	7:G:40:ALA:HA	1.77	0.65
1:A:1425:U:H2'	1:A:1426:C:H6	1.60	0.65
20:T:56:MET:CE	20:T:85:MET:HG3	2.26	0.65
9:I:108:VAL:CG1	9:I:109:VAL:H	2.05	0.65
1:A:793:U:H4'	1:A:794:A:OP2	1.97	0.65
4:D:191:ARG:HD2	4:D:200:GLU:OE2	1.97	0.65
4:D:175:SER:OG	4:D:186:LEU:HD21	1.96	0.65
1:A:474:G:H4'	16:P:81:ARG:NH2	2.11	0.65
13:M:59:TYR:O	13:M:59:TYR:HD2	1.79	0.65
2:B:161:ALA:HA	2:B:183:PRO:HD2	1.78	0.65
13:M:96:LEU:HD23	13:M:96:LEU:N	2.11	0.65
1:A:977:A:C2'	1:A:978:A:H5'	2.26	0.65
3:C:16:ARG:HG2	3:C:16:ARG:NH1	2.11	0.65
1:A:179:A:O2'	1:A:180:U:H5'	1.96	0.65
3:C:67:THR:HA	3:C:102:ASN:HB2	1.77	0.65
4:D:204:ILE:CD1	4:D:204:ILE:N	2.60	0.65
1:A:1200:C:O2	1:A:1205:U:N3	2.19	0.65
1:A:91:C:H2'	1:A:92:C:C6	2.32	0.65
1:A:913:A:O3'	27:A:1928:SRV:CI3	2.45	0.65
1:A:204:U:O2	1:A:204:U:H2'	1.97	0.65
1:A:1294:G:N7	29:A:2265:HOH:O	2.30	0.65
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.31	0.65
1:A:89:C:H2'	1:A:90:U:O5'	1.97	0.65
1:A:436:C:H2'	1:A:437:U:C6	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:G:OP2	1:A:1322:C:N4	2.30	0.65
1:A:661:G:N7	29:A:2819:HOH:O	2.30	0.65
5:E:142:LEU:C	5:E:143:ARG:HG2	2.16	0.65
2:B:87:ARG:HD2	2:B:88:ALA:N	2.12	0.65
1:A:838:G:H3'	1:A:839:U:H5''	1.79	0.65
4:D:190:ASP:HB2	4:D:193:ASP:OD2	1.97	0.65
19:S:48:THR:C	19:S:49:ILE:HD13	2.17	0.65
20:T:55:ILE:N	20:T:55:ILE:CD1	2.61	0.65
11:K:34:ASP:HB2	11:K:35:PRO:HD2	1.79	0.65
1:A:411:A:C2	1:A:413:G:H1'	2.32	0.64
7:G:50:ILE:HG21	7:G:58:PRO:CA	2.20	0.64
1:A:1047:G:H2'	1:A:1048:G:H5'	1.77	0.64
1:A:393:A:O2'	1:A:394:G:H5'	1.97	0.64
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.33	0.64
3:C:5:ILE:HD12	3:C:5:ILE:C	2.18	0.64
11:K:27:ASN:OD1	11:K:28:THR:N	2.30	0.64
7:G:71:PRO:O	7:G:96:GLN:NE2	2.24	0.64
2:B:84:GLU:OE1	2:B:216:SER:HA	1.97	0.64
1:A:1129:C:OP1	9:I:62:TYR:OH	2.15	0.64
1:A:1536:C:H5	1:A:1537:U:N3	1.94	0.64
20:T:99:LEU:HD12	20:T:100:ILE:N	2.12	0.64
4:D:180:GLY:O	4:D:182:LYS:HG2	1.98	0.64
17:Q:5:VAL:HG22	17:Q:60:ILE:HD12	1.79	0.64
5:E:11:ILE:HG22	5:E:12:LEU:N	2.10	0.64
16:P:21:VAL:O	16:P:33:ILE:HB	1.96	0.64
1:A:976:G:OP2	1:A:1358:U:O2'	2.15	0.64
15:O:14:GLU:CG	15:O:15:PHE:CD1	2.80	0.64
20:T:13:LEU:HD12	20:T:14:LYS:CA	2.27	0.64
1:A:150:C:H2'	1:A:151:A:O5'	1.97	0.64
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.78	0.64
1:A:16:A:C2'	1:A:17:U:H5'	2.27	0.64
1:A:1201:A:H4'	1:A:1202:G:O5'	1.97	0.64
6:F:97:PHE:C	6:F:97:PHE:CD2	2.70	0.64
2:B:201:ILE:O	2:B:203:GLY:N	2.31	0.64
3:C:131:ARG:NH1	5:E:50:GLU:OE1	2.31	0.64
18:R:61:LYS:O	18:R:65:ILE:HD12	1.97	0.64
4:D:189:PRO:HB2	4:D:194:LEU:CD2	2.25	0.64
1:A:514:C:O2'	1:A:515:G:H5'	1.97	0.64
1:A:1132:C:H2'	1:A:1133:G:H5'	1.79	0.64
10:J:16:LEU:CD2	10:J:70:ARG:HG3	2.28	0.64
4:D:119:GLN:HG3	4:D:123:HIS:ND1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:92:GLU:HB3	11:K:96:ARG:HH22	1.63	0.64
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.77	0.64
2:B:103:THR:HG23	2:B:176:GLU:OE1	1.98	0.64
4:D:146:ILE:N	4:D:146:ILE:HD12	2.12	0.64
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.80	0.64
4:D:131:ARG:NH1	4:D:131:ARG:HB2	2.13	0.64
16:P:8:ARG:HB2	16:P:28:ARG:NH1	2.13	0.64
20:T:55:ILE:N	20:T:55:ILE:HD12	2.13	0.64
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.79	0.64
4:D:117:ALA:O	4:D:121:VAL:HG23	1.98	0.64
1:A:689:C:O2'	1:A:690:G:H5'	1.98	0.64
4:D:32:ALA:HA	4:D:35:ARG:CB	2.22	0.64
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.28	0.64
1:A:580:U:OP2	29:A:2740:HOH:O	2.15	0.64
1:A:1330:U:OP1	13:M:23:TYR:O	2.16	0.63
6:F:8:ILE:HD13	6:F:26:ILE:HD12	1.80	0.63
2:B:157:ARG:HG3	2:B:158:LEU:N	2.13	0.63
1:A:1366:C:H2'	1:A:1367:C:H6	1.63	0.63
10:J:25:GLU:HG2	10:J:28:ARG:HD2	1.79	0.63
1:A:1303:C:H2'	1:A:1303:C:O2	1.97	0.63
3:C:62:ASP:HA	3:C:97:LYS:NZ	2.12	0.63
1:A:627:G:O2'	1:A:628:G:H5'	1.98	0.63
17:Q:29:HIS:HB2	17:Q:36:ILE:CD1	2.29	0.63
1:A:1081:G:OP1	5:E:16:THR:OG1	2.16	0.63
17:Q:74:LEU:HD22	17:Q:75:ARG:HG2	1.78	0.63
1:A:1372:U:OP1	9:I:71:SER:HB3	1.99	0.63
1:A:1493[B]:A:H2'	1:A:1494:G:N7	2.13	0.63
1:A:539:A:H2'	1:A:540:G:H8	1.63	0.63
1:A:1518[B]:MA6:C10	1:A:1519[B]:MA6:H103	2.28	0.63
8:H:97:VAL:HG12	8:H:98:LYS:N	2.13	0.63
1:A:959:A:H3'	1:A:960:U:H5''	1.81	0.63
16:P:58:TYR:C	16:P:58:TYR:CD1	2.72	0.63
1:A:1256:A:C8	1:A:1258:G:N1	2.66	0.63
1:A:15:G:H4'	5:E:24:ARG:NH2	2.12	0.63
1:A:1020:U:H2'	1:A:1021:G:H8	1.62	0.63
6:F:99:ALA:HB1	18:R:23:LYS:HZ3	1.64	0.63
1:A:943:U:C2'	1:A:944:G:H5'	2.28	0.63
2:B:119:GLU:HG3	2:B:142:LEU:HD11	1.79	0.63
9:I:17:VAL:HG13	9:I:63:ILE:CD1	2.28	0.63
1:A:790:A:C8	1:A:791:G:N7	2.67	0.63
10:J:77:PRO:HA	10:J:81:THR:OG1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:79:ARG:NH1	15:O:79:ARG:HG3	2.07	0.63
3:C:119:ARG:O	3:C:122:GLU:HB2	1.97	0.63
1:A:166:G:C2'	1:A:167:G:H5'	2.29	0.63
3:C:136:GLN:O	3:C:140:ARG:HG3	1.98	0.63
1:A:1068:G:C8	1:A:1068:G:OP2	2.48	0.63
2:B:218:ALA:O	2:B:222:ILE:HG12	1.98	0.63
1:A:1305:G:N2	1:A:1331:G:H1'	2.12	0.63
19:S:19:VAL:HG23	19:S:47:HIS:CE1	2.33	0.63
1:A:943:U:H2'	1:A:944:G:H5'	1.80	0.63
2:B:69:LEU:HD23	2:B:91:PRO:O	1.99	0.63
19:S:34:TRP:CZ2	19:S:57:HIS:HE1	2.16	0.63
1:A:1343:G:H1'	9:I:121:ARG:NH1	2.13	0.63
1:A:500:G:C6	1:A:546:G:N2	2.66	0.63
7:G:16:LEU:HD11	9:I:45:ALA:HB2	1.80	0.63
1:A:54:C:N3	1:A:352:C:C5	2.67	0.63
3:C:14:ILE:HD13	3:C:14:ILE:N	2.13	0.63
3:C:16:ARG:NH2	3:C:183:ASP:OD2	2.32	0.63
1:A:627:G:O6	29:A:2664:HOH:O	2.14	0.63
20:T:41:ILE:N	20:T:41:ILE:HD12	2.14	0.63
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.80	0.63
1:A:785:G:H2'	1:A:786:G:H5'	1.79	0.63
1:A:112:G:C2'	1:A:113:G:H5'	2.29	0.63
18:R:50:ILE:HD11	18:R:70:ILE:HG21	1.78	0.63
4:D:164:ALA:O	4:D:168:ARG:HD2	1.99	0.63
1:A:266:G:H5'	1:A:266:G:H8	1.57	0.63
10:J:30:SER:HB2	10:J:80:LYS:CB	2.21	0.63
20:T:61:SER:O	20:T:62:LEU:C	2.37	0.63
1:A:616:G:O2'	1:A:617:G:H5'	1.98	0.63
8:H:28:ALA:HA	8:H:59:LEU:HD11	1.80	0.63
20:T:13:LEU:HD12	20:T:14:LYS:N	2.14	0.63
3:C:10:PHE:O	3:C:10:PHE:HD1	1.82	0.63
2:B:179:LYS:HA	8:H:72:PRO:HD3	1.80	0.63
1:A:1291:G:H2'	1:A:1292:U:C6	2.34	0.63
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.34	0.63
1:A:1130:A:OP1	1:A:1131:G:P	2.56	0.63
1:A:1204:A:OP2	29:A:2248:HOH:O	2.15	0.63
1:A:1125:U:H3'	1:A:1126:U:H5	1.62	0.63
1:A:1125:U:O2'	1:A:1126:U:P	2.57	0.63
1:A:1281:U:C4'	1:A:1282:C:OP2	2.47	0.63
3:C:119:ARG:HH11	3:C:119:ARG:HG3	1.63	0.63
4:D:79:PHE:HD2	4:D:80:GLU:N	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:59:TYR:CD2	13:M:59:TYR:C	2.69	0.63
19:S:36:ARG:NH2	19:S:75:ALA:O	2.32	0.63
3:C:188:LEU:HD11	3:C:195:VAL:CG1	2.28	0.63
3:C:119:ARG:HH11	3:C:119:ARG:CG	2.11	0.63
1:A:235:C:N4	29:A:2113:HOH:O	2.31	0.63
9:I:121:ARG:HH11	9:I:121:ARG:CG	2.10	0.62
1:A:1003:G:N1	1:A:1003(A):G:O6	2.31	0.62
1:A:1314:C:OP2	19:S:6:LYS:CD	2.46	0.62
12:L:84:LEU:O	12:L:101:VAL:HG23	1.99	0.62
1:A:837:G:C2	1:A:850:U:O2	2.51	0.62
15:O:14:GLU:HG2	15:O:15:PHE:CE1	2.34	0.62
1:A:1001:A:H2'	1:A:1002:G:C8	2.34	0.62
3:C:191:THR:OG1	3:C:193:TYR:CE1	2.49	0.62
1:A:1126:U:OP2	1:A:1281:U:H1'	1.99	0.62
20:T:67:ALA:HA	20:T:73:HIS:H	1.65	0.62
1:A:1057:G:C5	1:A:1204:A:C2	2.87	0.62
1:A:1026:G:C8	1:A:1027:C:N3	2.68	0.62
7:G:120:ILE:HG22	7:G:124:LEU:CD1	2.29	0.62
19:S:15:LEU:HD13	19:S:16:LEU:N	2.15	0.62
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.35	0.62
23:W:37:A:N6	23:W:38:A:N1	2.47	0.62
7:G:17:VAL:CG1	7:G:18:TYR:N	2.62	0.62
1:A:1328:C:OP1	21:U:21:TYR:OH	2.13	0.62
1:A:352:C:C6	1:A:352:C:H3'	2.35	0.62
1:A:1160:G:O6	1:A:1181:G:O6	2.16	0.62
2:B:180:LEU:O	2:B:181:PHE:HB2	1.98	0.62
1:A:750:G:N3	15:O:23:GLY:HA3	2.14	0.62
8:H:127:LEU:O	8:H:127:LEU:HD23	1.99	0.62
1:A:1316:G:H2'	1:A:1317:C:H5''	1.81	0.62
1:A:1124:G:N7	1:A:1145:C:O2'	2.28	0.62
1:A:1425:U:H2'	1:A:1426:C:C6	2.34	0.62
16:P:26:ARG:HG3	16:P:27:LYS:N	2.13	0.62
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.80	0.62
2:B:87:ARG:HE	2:B:219:VAL:CG1	2.11	0.62
1:A:1519[A]:MA6:H3'	1:A:1520[A]:G:C5'	2.29	0.62
13:M:16:ASP:O	13:M:19:LEU:HB2	1.99	0.62
7:G:120:ILE:N	7:G:120:ILE:CD1	2.52	0.62
8:H:28:ALA:HA	8:H:59:LEU:CD1	2.29	0.62
20:T:13:LEU:C	20:T:13:LEU:HD12	2.20	0.62
1:A:330:C:H2'	1:A:331:G:H5'	1.81	0.62
1:A:99:C:H2'	1:A:101:A:C8	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:G:C5	1:A:507:C:C5	2.87	0.62
6:F:14:LEU:CD1	6:F:18:GLN:HB3	2.22	0.62
1:A:35:G:C6	1:A:36:C:N4	2.68	0.62
4:D:31:CYS:SG	4:D:31:CYS:O	2.57	0.62
18:R:26:LEU:N	18:R:26:LEU:HD13	2.13	0.62
16:P:74:LEU:O	16:P:79:VAL:HG23	1.99	0.62
16:P:8:ARG:HB2	16:P:28:ARG:HH11	1.64	0.62
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.82	0.62
20:T:83:ARG:O	20:T:87:LYS:HD2	2.00	0.62
17:Q:54:GLY:O	17:Q:80:GLY:HA2	1.99	0.62
1:A:544:G:C5	1:A:545:C:C5	2.88	0.62
20:T:104:LEU:N	20:T:104:LEU:HD23	2.15	0.62
4:D:150:GLU:OE1	4:D:151:LYS:HG3	2.00	0.62
1:A:975:A:H4'	1:A:976:G:H5''	1.81	0.62
15:O:14:GLU:HG2	15:O:15:PHE:CD1	2.35	0.62
8:H:113:SER:HB3	8:H:134:ILE:HD11	1.80	0.62
1:A:1052:U:H2'	1:A:1055:A:OP1	2.00	0.62
1:A:1368:G:H2'	1:A:1369:C:H5'	1.82	0.62
9:I:11:LYS:HG3	9:I:11:LYS:O	2.00	0.62
1:A:922:G:H5''	1:A:922:G:H8	1.64	0.62
1:A:592:G:O2'	1:A:593:G:H5'	2.00	0.62
1:A:551:U:H2'	1:A:552:U:C6	2.35	0.62
1:A:414:A:C2	1:A:415:A:N9	2.68	0.62
1:A:415:A:C4	1:A:416:G:C8	2.88	0.62
20:T:44:ALA:HB1	20:T:91:LEU:HB3	1.82	0.62
9:I:125:TYR:CD2	9:I:125:TYR:N	2.67	0.62
11:K:125:PHE:N	11:K:125:PHE:CD2	2.68	0.61
2:B:74:LYS:HE3	2:B:166:ASP:CB	2.28	0.61
2:B:193:ASP:C	2:B:193:ASP:OD1	2.38	0.61
1:A:501:C:H2'	1:A:502:G:C8	2.34	0.61
1:A:88:A:C5	1:A:89:C:N3	2.68	0.61
5:E:90:VAL:C	5:E:91:LEU:HD23	2.21	0.61
1:A:349:A:O2'	1:A:350:G:H5'	2.00	0.61
3:C:204:LEU:N	3:C:204:LEU:HD23	2.15	0.61
4:D:14:ARG:HD3	4:D:14:ARG:O	2.00	0.61
1:A:1406:U:C5	1:A:1407:5MC:HM52	2.35	0.61
20:T:41:ILE:H	20:T:41:ILE:HD12	1.64	0.61
1:A:986:A:C2	1:A:1220:G:C2	2.88	0.61
1:A:1338:G:H2'	1:A:1339:A:C8	2.35	0.61
3:C:156:ARG:H	3:C:163:ALA:HA	1.65	0.61
1:A:1536:C:C5	1:A:1537:U:C2	2.87	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:38:TYR:H	4:D:38:TYR:HD2	1.48	0.61
5:E:126:ARG:HG2	5:E:126:ARG:NH1	1.97	0.61
2:B:92:TYR:HE1	2:B:150:SER:HG	1.48	0.61
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	2.82	0.61
1:A:130:A:H5'	17:Q:63:ARG:HE	1.66	0.61
1:A:200:G:H2'	1:A:201:C:O4'	2.00	0.61
1:A:1385:G:C5	29:A:2670:HOH:O	2.52	0.61
7:G:135:VAL:O	7:G:139:GLU:HG3	2.00	0.61
11:K:29:ILE:HG22	11:K:43:SER:O	2.00	0.61
4:D:24:GLU:O	4:D:25:ARG:HB3	1.98	0.61
6:F:83:ASP:OD1	6:F:83:ASP:N	2.32	0.61
1:A:1194:U:O2	1:A:1194:U:H2'	2.00	0.61
1:A:544:G:C6	1:A:545:C:C5	2.89	0.61
1:A:642:A:H2'	1:A:643:C:C6	2.35	0.61
5:E:110:LEU:O	5:E:115:VAL:HB	2.01	0.61
1:A:983:A:N3	1:A:983:A:H3'	2.15	0.61
1:A:353:A:H8	1:A:353:A:C5'	2.12	0.61
11:K:16:SER:O	11:K:35:PRO:HD3	2.00	0.61
17:Q:53:LEU:HD12	17:Q:54:GLY:N	2.14	0.61
1:A:358:U:H2'	1:A:359:U:H6	1.66	0.61
2:B:178:ARG:HD2	2:B:196:LEU:O	2.00	0.61
1:A:16:A:H2'	1:A:17:U:H5'	1.81	0.61
12:L:30:ALA:HB1	12:L:31:PRO:HD2	1.82	0.61
1:A:892:A:C2	1:A:907:A:C4	2.89	0.61
1:A:188:C:C2'	1:A:189:G:H5'	2.30	0.61
1:A:831:U:H2'	1:A:832:C:H6	1.65	0.61
12:L:86:ARG:HG3	12:L:86:ARG:HH11	1.66	0.61
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.00	0.61
13:M:37:THR:CG2	13:M:39:ILE:HD13	2.31	0.61
1:A:865:A:O2'	1:A:866:C:H5'	1.99	0.61
1:A:914:A:P	27:A:1928:SRV:CI3	2.87	0.61
1:A:442:C:H2'	1:A:443:C:H5'	1.81	0.61
2:B:160:ASP:O	2:B:161:ALA:HB2	2.00	0.61
2:B:8:LYS:C	2:B:10:LEU:H	2.02	0.61
7:G:51:GLN:O	7:G:52:GLU:HG2	2.00	0.61
1:A:1348:U:H4'	9:I:120:ARG:HD2	1.81	0.61
1:A:544:G:C4	1:A:545:C:C6	2.89	0.61
1:A:923:A:O5'	1:A:923:A:H8	1.82	0.61
1:A:191:G:N3	20:T:103:GLY:O	2.34	0.61
1:A:304:U:C4	29:A:2495:HOH:O	2.48	0.61
2:B:172:ILE:H	2:B:172:ILE:HD13	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:C:H2'	1:A:138:G:C5'	2.30	0.61
1:A:414:A:H2'	1:A:414:A:N3	2.15	0.61
1:A:767:A:H2'	1:A:768:A:O4'	2.01	0.61
1:A:1482:G:N1	29:A:2362:HOH:O	2.16	0.61
7:G:21:VAL:HG23	7:G:22:LEU:H	1.65	0.61
1:A:248:C:C2'	1:A:249:U:H5'	2.31	0.61
4:D:23:GLY:HA2	4:D:112:VAL:O	2.00	0.61
20:T:22:ARG:O	20:T:23:ARG:C	2.38	0.61
1:A:829:G:O2'	1:A:830:G:H5'	2.00	0.61
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.01	0.61
1:A:778:G:H8	1:A:778:G:O5'	1.83	0.61
2:B:178:ARG:NH1	2:B:198:ASP:OD1	2.33	0.61
1:A:1103:C:H5'	2:B:98:LEU:HD12	1.82	0.61
1:A:53:A:C6	1:A:54:C:C5	2.89	0.61
1:A:448:A:C2'	1:A:449:C:H5'	2.30	0.61
17:Q:29:HIS:C	17:Q:29:HIS:ND1	2.54	0.61
14:N:15:LYS:O	14:N:16:PHE:CG	2.53	0.61
1:A:289:G:P	29:A:2015:HOH:O	2.57	0.61
23:W:32:C:O2'	23:W:33:U:O4'	2.17	0.61
2:B:88:ALA:HB2	2:B:219:VAL:CG1	2.21	0.61
1:A:1399:C:O2	1:A:1401:G:C4	2.54	0.61
1:A:109:A:H3'	1:A:110:C:H5'	1.83	0.61
1:A:114:U:H2'	1:A:115:G:H5'	1.82	0.61
4:D:159:ARG:CG	4:D:159:ARG:HH11	2.14	0.61
9:I:89:ASN:HB3	9:I:92:TYR:CE1	2.35	0.61
2:B:157:ARG:HG3	2:B:158:LEU:O	2.01	0.61
12:L:7:ILE:HG22	12:L:8:ASN:N	2.16	0.61
9:I:37:PHE:CD2	9:I:74:ILE:HD11	2.36	0.61
10:J:27:ALA:CB	10:J:74:ILE:HD12	2.31	0.61
8:H:112:LEU:N	8:H:112:LEU:CD2	2.64	0.61
1:A:1035:A:N6	1:A:1036:G:O6	2.33	0.61
1:A:182:U:C5	1:A:183:G:N9	2.69	0.61
9:I:31:GLN:NE2	9:I:36:TYR:CD1	2.66	0.60
8:H:97:VAL:O	8:H:100:ILE:HG12	2.01	0.60
17:Q:83:ASP:OD1	17:Q:84:LEU:N	2.34	0.60
4:D:131:ARG:HB2	4:D:131:ARG:HH11	1.66	0.60
2:B:15:VAL:O	2:B:42:ILE:HD12	2.01	0.60
7:G:54:THR:HG22	7:G:56:GLN:HB2	1.83	0.60
17:Q:40:LYS:CD	17:Q:42:TYR:CE1	2.83	0.60
8:H:118:VAL:O	8:H:119:LEU:HD23	2.01	0.60
1:A:1015:A:C6	1:A:1016:A:C6	2.89	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:G:O2'	1:A:260:G:H5'	2.01	0.60
4:D:170:VAL:HG22	4:D:171:GLY:N	2.16	0.60
1:A:109:A:H2'	1:A:326:G:N2	2.16	0.60
1:A:644:G:C5	1:A:645:C:C5	2.89	0.60
1:A:386:C:O2'	29:A:2002:HOH:O	2.15	0.60
3:C:91:LEU:HD23	3:C:92:ALA:N	2.16	0.60
3:C:8:ILE:HG22	3:C:9:GLY:N	2.16	0.60
1:A:633:G:H2'	1:A:634:C:C6	2.35	0.60
15:O:7:GLU:O	15:O:11:VAL:HG12	2.01	0.60
1:A:1454:G:O6	29:A:2826:HOH:O	2.16	0.60
1:A:1279:A:C4'	1:A:1280:A:OP1	2.50	0.60
1:A:783:C:O2'	1:A:784:C:H5'	2.01	0.60
7:G:37:ASN:ND2	7:G:41:ARG:HH21	1.98	0.60
9:I:46:ALA:HB1	9:I:77:ILE:HG22	1.83	0.60
1:A:1027:C:C5	1:A:1035:A:N1	2.69	0.60
7:G:153:HIS:NE2	11:K:57:THR:HG22	2.16	0.60
2:B:19:HIS:O	2:B:39:ILE:HG13	2.01	0.60
1:A:1251:A:H2'	1:A:1252:A:O4'	2.02	0.60
1:A:446:G:H2'	1:A:447:G:C5'	2.32	0.60
1:A:182:U:C5	1:A:183:G:H1'	2.35	0.60
1:A:130:A:H1'	1:A:263:A:O2'	2.01	0.60
14:N:12:ARG:HH11	14:N:12:ARG:H	1.48	0.60
1:A:14:U:O2	1:A:16:A:C8	2.54	0.60
5:E:41:VAL:HG13	5:E:113:ALA:HA	1.83	0.60
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.83	0.60
1:A:1500:A:OP2	1:A:1505:G:OP1	2.19	0.60
1:A:328:C:HO2'	1:A:329:A:P	2.16	0.60
2:B:231:GLU:HB3	2:B:232:PRO:CD	2.28	0.60
9:I:9:ARG:HA	9:I:76:ALA:CB	2.31	0.60
2:B:185:ILE:H	2:B:185:ILE:HD12	1.66	0.60
1:A:972:C:OP1	10:J:57:LYS:HD2	2.02	0.60
3:C:148:GLY:HA3	3:C:172:ARG:O	2.01	0.60
1:A:875:C:O2'	8:H:14:ARG:NH1	2.35	0.60
1:A:44:G:N2	1:A:399:G:C4	2.70	0.60
14:N:29:ARG:HG2	14:N:40:CYS:CB	2.31	0.60
7:G:38:LEU:HD12	7:G:42:ILE:HD11	1.83	0.60
2:B:240:GLN:O	2:B:240:GLN:CG	2.50	0.60
1:A:1126:U:C4	1:A:1127:G:C2	2.89	0.60
1:A:740:U:O2'	1:A:741:G:H5'	2.01	0.60
4:D:79:PHE:C	4:D:79:PHE:CD2	2.75	0.60
8:H:38:ILE:O	8:H:38:ILE:HG22	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:C:C2'	1:A:1067:A:H5'	2.31	0.60
3:C:14:ILE:O	3:C:16:ARG:N	2.35	0.60
7:G:26:PHE:HD1	7:G:101:LEU:HD23	1.66	0.60
13:M:99:ARG:HB2	13:M:101:GLN:HE22	1.66	0.60
20:T:56:MET:HE3	20:T:85:MET:HG3	1.84	0.60
1:A:1518[A]:MA6:H93	1:A:1519[A]:MA6:H103	1.82	0.60
23:W:37:A:C6	23:W:38:A:C2	2.89	0.60
1:A:1004:A:N7	1:A:1037:C:N3	2.49	0.60
18:R:87:ARG:HH21	18:R:87:ARG:CB	2.13	0.60
17:Q:23:VAL:HG21	17:Q:42:TYR:HD1	1.64	0.60
2:B:100:GLY:HA2	2:B:176:GLU:OE2	2.01	0.60
10:J:63:PHE:N	10:J:63:PHE:CD1	2.68	0.60
1:A:1234:C:H1'	1:A:1364:U:O2	2.00	0.60
2:B:20:GLU:HA	2:B:39:ILE:CD1	2.31	0.60
1:A:276:G:OP1	17:Q:12:SER:OG	2.14	0.60
1:A:476:G:H2'	1:A:477:G:H8	1.66	0.60
1:A:543:C:H2'	1:A:544:G:C5'	2.30	0.60
7:G:5:ARG:NH2	7:G:8:GLU:HG2	2.17	0.60
1:A:710:G:H5'	6:F:54:LYS:CE	2.27	0.60
1:A:868:C:H2'	1:A:869:G:C5'	2.31	0.60
11:K:48:ILE:HD13	11:K:48:ILE:N	2.15	0.60
1:A:254:G:OP1	17:Q:67:LYS:O	2.20	0.60
11:K:73:MET:HG3	11:K:103:LEU:HD21	1.83	0.60
7:G:65:ALA:HB2	7:G:128:ALA:HB2	1.83	0.60
1:A:1060:C:O2	1:A:1198:G:C2	2.55	0.59
1:A:1494:G:O2'	1:A:1495:U:H5'	2.02	0.59
4:D:13:ARG:HD2	4:D:38:TYR:O	2.02	0.59
12:L:90:VAL:HG12	12:L:90:VAL:O	2.02	0.59
19:S:80:TYR:CZ	19:S:81:ARG:HG2	2.36	0.59
19:S:34:TRP:CZ2	19:S:57:HIS:CE1	2.90	0.59
15:O:60:VAL:HG12	15:O:61:GLY:N	2.17	0.59
1:A:1503:A:C4	1:A:1531:A:C2	2.90	0.59
1:A:524:G:H2'	1:A:525:C:C6	2.37	0.59
13:M:78:ILE:O	13:M:81:LEU:N	2.34	0.59
1:A:1118:C:H1'	1:A:1179:A:C4	2.37	0.59
1:A:1060:C:C2	1:A:1198:G:N1	2.70	0.59
1:A:1027:C:O4'	1:A:1027:C:O2	2.17	0.59
6:F:98:LEU:HD13	6:F:98:LEU:N	2.15	0.59
19:S:64:GLU:O	19:S:67:VAL:HG23	2.02	0.59
1:A:182:U:C5	1:A:183:G:C1'	2.85	0.59
8:H:26:VAL:HG22	8:H:27:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:73:GLU:O	13:M:77:ASN:HB2	2.02	0.59
19:S:51:VAL:CG2	19:S:58:VAL:HG23	2.33	0.59
20:T:99:LEU:HD12	20:T:100:ILE:H	1.65	0.59
1:A:89:C:O2'	1:A:90:U:O5'	2.19	0.59
18:R:58:LEU:HD12	18:R:62:GLU:HB3	1.85	0.59
7:G:74:GLU:HG2	7:G:91:VAL:CG2	2.32	0.59
17:Q:29:HIS:ND1	17:Q:30:PRO:HD2	2.17	0.59
3:C:84:ILE:HG23	3:C:88:ARG:HH12	1.67	0.59
4:D:206:PHE:CE2	4:D:207:TYR:HE2	2.20	0.59
1:A:149:A:O2'	1:A:150:C:H5'	2.03	0.59
7:G:52:GLU:N	7:G:52:GLU:OE1	2.35	0.59
1:A:667:G:H4'	15:O:51:HIS:CE1	2.38	0.59
1:A:1130:A:P	1:A:1131:G:OP2	2.60	0.59
4:D:18:LYS:HB3	4:D:33:MET:HG3	1.84	0.59
1:A:1026:G:N7	1:A:1027:C:N3	2.50	0.59
1:A:939:G:H5'	7:G:102:ARG:HH22	1.67	0.59
1:A:17:U:H2'	1:A:18:C:C6	2.37	0.59
1:A:399:G:OP1	29:A:2086:HOH:O	2.17	0.59
1:A:1399:C:O2	1:A:1401:G:C8	2.55	0.59
6:F:12:PRO:HG2	6:F:57:GLN:O	2.01	0.59
4:D:127:THR:HG23	4:D:147:ALA:O	2.03	0.59
5:E:121:LYS:HG2	5:E:123:LEU:HD21	1.84	0.59
1:A:848:C:O5'	1:A:848:C:H6	1.86	0.59
1:A:1124:G:O4'	10:J:38:ILE:HD11	2.02	0.59
5:E:80:ILE:O	5:E:80:ILE:HG23	2.03	0.59
6:F:74:ASP:O	6:F:77:ARG:HB3	2.02	0.59
1:A:380:G:N7	29:A:2680:HOH:O	2.35	0.59
5:E:36:ASP:CG	5:E:38:GLN:HB2	2.23	0.59
16:P:82:GLN:O	16:P:84:ALA:N	2.35	0.59
1:A:504:C:OP1	29:A:2163:HOH:O	2.17	0.59
13:M:70:LEU:O	13:M:74:VAL:HG22	2.03	0.59
1:A:868:C:H2'	1:A:869:G:O5'	2.02	0.59
1:A:1124:G:H2'	1:A:1145:C:H5	1.68	0.59
20:T:61:SER:HG	20:T:65:LYS:HD2	1.65	0.59
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.37	0.59
5:E:33:VAL:HG12	5:E:34:VAL:N	2.16	0.59
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.18	0.59
1:A:138:G:C8	1:A:138:G:H5'	2.34	0.59
17:Q:29:HIS:HB2	17:Q:36:ILE:HD12	1.84	0.59
11:K:47:VAL:HG12	11:K:48:ILE:HD13	1.84	0.59
3:C:6:HIS:CD2	3:C:7:PRO:HD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:GLU:O	9:I:20:ARG:HG2	2.02	0.59
1:A:747:C:H2'	1:A:748:C:O5'	2.03	0.59
1:A:960:U:H4'	1:A:961:U:C5'	2.32	0.59
19:S:22:LEU:O	19:S:26:GLY:O	2.21	0.59
6:F:5:GLU:OE1	18:R:34:TYR:OH	2.15	0.59
1:A:1527:C:C2'	1:A:1528:U:H5'	2.32	0.59
1:A:1291:G:H4'	9:I:39:GLY:CA	2.32	0.59
1:A:1190:G:H8	1:A:1190:G:C5'	2.16	0.59
1:A:500:G:C6	1:A:501:C:C4	2.91	0.59
10:J:24:VAL:HG22	10:J:28:ARG:HH12	1.68	0.59
1:A:644:G:H8	1:A:644:G:C5'	2.09	0.59
2:B:105:PHE:O	2:B:109:SER:OG	2.20	0.59
1:A:994:A:C2	1:A:995:C:C6	2.90	0.59
19:S:25:LYS:HG3	19:S:26:GLY:H	1.67	0.59
1:A:180:U:H2'	1:A:181:G:H5'	1.85	0.59
3:C:203:PHE:C	3:C:204:LEU:HD23	2.23	0.59
1:A:1499:A:H5'	1:A:1519[A]:MA6:N1	2.18	0.59
1:A:510:A:H5''	1:A:511:C:P	2.43	0.59
10:J:44:VAL:HG13	10:J:66:ARG:CD	2.29	0.59
1:A:1126:U:O4	1:A:1127:G:N2	2.35	0.59
1:A:1256:A:N6	1:A:1277:C:C6	2.71	0.59
1:A:1151:A:HO2'	1:A:1152:A:H8	1.49	0.59
8:H:87:SER:HA	8:H:93:VAL:HG23	1.84	0.59
1:A:1010:G:H22	1:A:1020:U:H1'	1.67	0.59
1:A:433:C:C2	1:A:434:U:H5	2.21	0.59
11:K:45:GLY:HA3	11:K:55:LYS:HB3	1.84	0.59
11:K:119:CYS:O	11:K:121:PRO:HD3	2.02	0.59
1:A:1493[A]:A:H2	23:W:36:A:O2'	1.83	0.58
1:A:923:A:O4'	1:A:1398:A:C2	2.56	0.58
19:S:12:ASP:O	19:S:15:LEU:CD1	2.51	0.58
17:Q:45:HIS:HE2	17:Q:47:PRO:HB3	1.67	0.58
9:I:102:LEU:HD12	9:I:102:LEU:H	1.68	0.58
5:E:15:ARG:NH1	5:E:26:PHE:CE2	2.71	0.58
11:K:125:PHE:N	11:K:125:PHE:HD2	2.02	0.58
1:A:790:A:H2'	1:A:791:G:C8	2.38	0.58
18:R:82:THR:HG23	18:R:83:GLU:N	2.17	0.58
1:A:893:C:C2'	1:A:894:G:H5'	2.32	0.58
9:I:39:GLY:O	9:I:40:LEU:HD22	2.03	0.58
1:A:1332:A:C2	1:A:1333:A:C4	2.91	0.58
1:A:529:G:C8	1:A:529:G:H3'	2.37	0.58
1:A:128:G:H4'	17:Q:3:LYS:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:14:VAL:HG23	9:I:66:ARG:O	2.03	0.58
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.85	0.58
5:E:152:ARG:HB3	8:H:43:GLY:HA3	1.83	0.58
19:S:51:VAL:O	19:S:51:VAL:HG23	2.04	0.58
1:A:364:A:H2'	1:A:365:U:O2	2.03	0.58
1:A:1018:C:O5'	1:A:1018:C:H6	1.86	0.58
9:I:55:ALA:O	9:I:56:LEU:C	2.42	0.58
12:L:113:ARG:NH1	12:L:116:SER:H	2.00	0.58
1:A:327:A:HO2'	1:A:328:C:H6	1.51	0.58
13:M:37:THR:HG23	13:M:39:ILE:CD1	2.33	0.58
1:A:864:A:H2'	1:A:865:A:C8	2.37	0.58
1:A:625:G:H4'	16:P:16:HIS:CD2	2.37	0.58
8:H:53:VAL:HG12	8:H:58:TYR:CE1	2.38	0.58
1:A:345:C:OP2	1:A:345:C:C6	2.56	0.58
3:C:186:PHE:CD2	3:C:186:PHE:C	2.76	0.58
1:A:11:G:O6	29:A:2647:HOH:O	2.16	0.58
1:A:737:A:H2'	1:A:738:C:C6	2.37	0.58
1:A:1147:C:O2	9:I:16:ARG:NH2	2.37	0.58
1:A:1371:G:C5	1:A:1372:U:C5	2.90	0.58
4:D:152:SER:O	4:D:155:LEU:HB2	2.04	0.58
1:A:1329:A:C2'	1:A:1330:U:H5'	2.34	0.58
15:O:62:GLN:O	15:O:63:ARG:C	2.39	0.58
18:R:44:LEU:HD13	18:R:48:GLY:O	2.03	0.58
4:D:100:ARG:HH12	4:D:137:SER:HA	1.68	0.58
1:A:101:A:H2'	1:A:102:G:H8	1.68	0.58
1:A:1003:G:N1	1:A:1003(A):G:C6	2.71	0.58
1:A:1035:A:C6	1:A:1036:G:O6	2.57	0.58
13:M:86:CYS:SG	13:M:87:TYR:N	2.77	0.58
1:A:820:U:H4'	1:A:821:G:OP2	2.03	0.58
1:A:1405:G:C2'	1:A:1406:U:H5'	2.33	0.58
1:A:1424:C:C4	1:A:1425:U:C5	2.91	0.58
13:M:59:TYR:HD2	13:M:59:TYR:C	2.07	0.58
8:H:103:VAL:HG21	8:H:109:ILE:C	2.24	0.58
12:L:70:ILE:CG2	12:L:75:HIS:HD2	2.02	0.58
1:A:1329:A:O2'	1:A:1330:U:H5'	2.03	0.58
19:S:44:MET:HB2	19:S:62:ILE:HD13	1.86	0.58
1:A:741:G:H5'	15:O:39:LEU:CD1	2.33	0.58
1:A:358:U:O2'	1:A:359:U:H5'	2.04	0.58
1:A:1347:G:N2	1:A:1373:G:H2'	2.18	0.58
21:U:10:ARG:NH1	21:U:10:ARG:CG	2.59	0.58
1:A:1054:C:O2'	1:A:1055:A:O5'	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ASN:ND2	2:B:193:ASP:CB	2.55	0.58
17:Q:4:LYS:HG2	17:Q:6:LEU:HD21	1.85	0.58
1:A:1124:G:O2'	1:A:1145:C:N4	2.36	0.58
1:A:162:A:H5''	1:A:163:C:OP2	2.03	0.58
11:K:11:LYS:N	11:K:75:TYR:HE2	2.01	0.58
1:A:409:G:OP1	4:D:24:GLU:O	2.21	0.58
4:D:106:TYR:O	4:D:109:GLY:N	2.29	0.58
1:A:1501:C:C4	1:A:1504:G:C4	2.92	0.58
1:A:1502:A:H2'	1:A:1504:G:N7	2.19	0.58
10:J:24:VAL:HG22	10:J:28:ARG:NH1	2.19	0.58
1:A:386:C:C2'	1:A:387:U:H5'	2.34	0.58
6:F:87:ARG:CG	6:F:87:ARG:HH11	2.14	0.58
16:P:23:ASP:OD1	16:P:25:ARG:HG3	2.02	0.58
5:E:24:ARG:HG2	5:E:24:ARG:NH1	2.18	0.58
3:C:151:VAL:O	3:C:167:TRP:O	2.20	0.58
13:M:4:ILE:HD13	13:M:57:ARG:HB2	1.85	0.58
4:D:25:ARG:NH2	4:D:30:LYS:HD3	2.19	0.58
1:A:1250:A:C2	1:A:1287:A:C2	2.91	0.58
1:A:1206:G:H2'	1:A:1207:2MG:O4'	2.04	0.58
10:J:49:VAL:HA	10:J:50:ILE:HD12	1.84	0.58
2:B:165:VAL:HG12	2:B:166:ASP:N	2.18	0.58
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.38	0.58
1:A:984:C:N4	1:A:1221:G:H1	2.01	0.58
3:C:82:GLU:HG3	3:C:83:ARG:H	1.69	0.58
1:A:1418:A:H2'	1:A:1419:G:O4'	2.04	0.58
1:A:150:C:C2'	1:A:151:A:O5'	2.51	0.58
1:A:1095:U:H2'	1:A:1096:C:O4'	2.03	0.58
2:B:97:TRP:CE2	2:B:101:MET:HG3	2.39	0.57
1:A:966:M2G:HM22	1:A:967:5MC:O2	2.04	0.57
1:A:419:C:C2'	1:A:420:U:H5'	2.34	0.57
2:B:107:THR:O	2:B:110:GLN:HB2	2.04	0.57
9:I:55:ALA:HB1	9:I:59:PHE:HB2	1.85	0.57
1:A:540:G:C6	1:A:541:G:C5	2.92	0.57
1:A:1501:C:N4	1:A:1504:G:C2	2.72	0.57
1:A:909:A:C8	1:A:910:C:C6	2.91	0.57
1:A:137:C:H2'	1:A:138:G:H5''	1.84	0.57
1:A:633:G:H2'	1:A:634:C:H6	1.68	0.57
1:A:409:G:N2	1:A:434:U:C5	2.72	0.57
10:J:50:ILE:HD12	10:J:50:ILE:N	2.19	0.57
1:A:1004:A:H2'	1:A:1005:A:H5'	1.86	0.57
7:G:16:LEU:CD1	9:I:45:ALA:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:GLN:O	3:C:122:GLU:HG3	2.04	0.57
3:C:10:PHE:C	3:C:10:PHE:HD1	2.07	0.57
5:E:116:THR:HB	5:E:117:ASP:OD2	2.04	0.57
1:A:581:G:O2'	1:A:582:U:H5'	2.04	0.57
1:A:993:G:N3	1:A:993:G:H2'	2.19	0.57
1:A:734:G:O5'	1:A:734:G:H8	1.87	0.57
1:A:1193:G:C2	1:A:1194:U:C5	2.92	0.57
1:A:691:G:H2'	1:A:692:U:C6	2.40	0.57
4:D:150:GLU:CD	4:D:150:GLU:N	2.57	0.57
1:A:53:A:N6	1:A:54:C:C4	2.73	0.57
21:U:8:THR:HG22	21:U:9:ARG:H	1.68	0.57
1:A:1063:C:H2'	1:A:1064:G:C8	2.39	0.57
1:A:1189:C:H5''	1:A:1190:G:OP2	2.04	0.57
13:M:74:VAL:HG23	13:M:75:ALA:H	1.69	0.57
1:A:134:A:N6	16:P:25:ARG:HH21	2.02	0.57
14:N:4:LYS:O	14:N:7:ILE:HG12	2.05	0.57
4:D:187:ARG:CG	4:D:188:LEU:HD12	2.35	0.57
1:A:1419:G:O6	1:A:1420:C:N4	2.38	0.57
5:E:9:LYS:NZ	5:E:111:GLU:OE1	2.38	0.57
20:T:39:LYS:O	20:T:43:LEU:HG	2.04	0.57
1:A:510:A:H5''	1:A:511:C:OP2	2.04	0.57
27:A:1928:SRV:OG2	12:L:91:LYS:NZ	2.27	0.57
12:L:92:0TD:N	12:L:92:0TD:OD1	2.36	0.57
1:A:1277:C:H1'	1:A:1282:C:H1'	1.86	0.57
17:Q:81:ARG:HG3	17:Q:84:LEU:HD12	1.87	0.57
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.02	0.57
1:A:293:G:C4	1:A:305:G:N2	2.72	0.57
9:I:26:VAL:HG12	9:I:61:ALA:HB3	1.85	0.57
9:I:31:GLN:HE22	9:I:36:TYR:HD1	1.50	0.57
1:A:1055:A:C2	1:A:1056:U:H1'	2.40	0.57
1:A:54:C:O2'	1:A:55:A:H5'	2.03	0.57
19:S:15:LEU:H	19:S:15:LEU:HD12	1.70	0.57
3:C:10:PHE:CD1	3:C:10:PHE:C	2.77	0.57
1:A:1241:G:H2'	1:A:1242:C:H6	1.70	0.57
13:M:87:TYR:HE1	13:M:91:ARG:CD	2.18	0.57
5:E:11:ILE:HD11	5:E:105:VAL:HA	1.87	0.57
18:R:43:PHE:CD2	18:R:66:LEU:HD21	2.40	0.57
1:A:54:C:N3	1:A:352:C:H5	2.02	0.57
3:C:33:LEU:O	3:C:37:GLN:HG2	2.04	0.57
17:Q:18:THR:CG2	17:Q:69:LYS:HD3	2.35	0.57
1:A:315:A:OP1	29:A:2576:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ALA:CB	2:B:219:VAL:HG13	2.22	0.57
1:A:1494:G:N3	1:A:1495:U:C6	2.73	0.57
1:A:540:G:C4	1:A:541:G:C8	2.92	0.57
1:A:1533:C:O2'	1:A:1534:C:P	2.63	0.57
13:M:40:ASN:OD1	13:M:41:PRO:HD2	2.04	0.57
13:M:87:TYR:CD1	13:M:87:TYR:C	2.77	0.57
12:L:28:LYS:HE3	12:L:33:ARG:NH2	2.19	0.57
1:A:954:G:H21	1:A:1227:A:H62	1.51	0.57
2:B:170:GLU:O	2:B:173:ALA:N	2.38	0.57
1:A:975:A:C8	1:A:975:A:C5'	2.87	0.57
4:D:79:PHE:CD2	4:D:80:GLU:N	2.73	0.57
1:A:174:C:O5'	1:A:174:C:H6	1.86	0.57
17:Q:74:LEU:C	17:Q:74:LEU:HD23	2.25	0.57
5:E:65:ASN:O	5:E:65:ASN:ND2	2.38	0.57
20:T:63:ILE:O	20:T:66:ALA:HB3	2.04	0.57
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.38	0.57
16:P:18:ARG:O	16:P:20:VAL:HG23	2.05	0.57
1:A:264:U:H2'	1:A:265:G:H5'	1.87	0.57
1:A:1279:A:H5''	1:A:1280:A:OP1	2.05	0.57
9:I:125:TYR:HD2	9:I:125:TYR:N	2.03	0.57
8:H:17:THR:O	8:H:78:GLN:NE2	2.38	0.57
11:K:80:VAL:HG13	11:K:81:ASP:N	2.20	0.57
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.86	0.56
10:J:82:ILE:HG22	10:J:82:ILE:O	2.05	0.56
13:M:87:TYR:O	13:M:90:LEU:N	2.38	0.56
16:P:23:ASP:OD1	16:P:24:ALA:N	2.39	0.56
4:D:114:ARG:HG3	4:D:114:ARG:HH11	1.70	0.56
5:E:79:GLU:HB3	5:E:92:LYS:HG2	1.87	0.56
3:C:50:ALA:O	3:C:71:ALA:HB3	2.04	0.56
13:M:4:ILE:CG2	13:M:5:ALA:N	2.68	0.56
5:E:117:ASP:OD2	5:E:117:ASP:N	2.37	0.56
9:I:105:ASP:OD2	9:I:107:ARG:HG3	2.04	0.56
1:A:1054:C:N3	23:W:34:G:C5'	2.68	0.56
1:A:1507:A:C8	1:A:1530:G:N2	2.73	0.56
1:A:502:G:H2'	1:A:503:C:O4'	2.05	0.56
8:H:114:THR:HG21	8:H:129:VAL:CG2	2.35	0.56
10:J:48:THR:HA	10:J:62:HIS:CB	2.31	0.56
1:A:994:A:C2	1:A:995:C:C5	2.92	0.56
1:A:1126:U:O4	1:A:1127:G:C2	2.58	0.56
3:C:174:PRO:O	3:C:176:HIS:N	2.38	0.56
20:T:41:ILE:O	20:T:44:ALA:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:96:PRO:HA	5:E:117:ASP:OD1	2.05	0.56
7:G:136:LYS:HD2	7:G:140:ASP:OD1	2.04	0.56
3:C:134:ILE:O	3:C:138:VAL:HG23	2.05	0.56
11:K:124:LYS:C	11:K:125:PHE:HD2	2.09	0.56
1:A:537:G:H2'	1:A:538:G:C8	2.37	0.56
1:A:1004:A:N6	1:A:1037:C:H42	2.04	0.56
17:Q:101:ARG:HD3	17:Q:101:ARG:H	1.70	0.56
13:M:87:TYR:CE1	13:M:91:ARG:CD	2.88	0.56
13:M:87:TYR:O	13:M:90:LEU:HB2	2.06	0.56
1:A:910:C:OP2	12:L:21:LYS:NZ	2.38	0.56
1:A:1126:U:H2'	1:A:1127:G:O5'	2.06	0.56
1:A:1124:G:O2'	1:A:1145:C:C5	2.58	0.56
19:S:62:ILE:HA	19:S:66:MET:CE	2.35	0.56
1:A:854:G:N2	1:A:855:G:C4	2.74	0.56
4:D:206:PHE:HD2	4:D:207:TYR:CE2	2.22	0.56
7:G:27:ILE:CD1	7:G:40:ALA:HA	2.36	0.56
1:A:667:G:H4'	15:O:51:HIS:ND1	2.19	0.56
21:U:8:THR:HG22	21:U:9:ARG:N	2.20	0.56
1:A:695:A:H2'	1:A:696:A:C8	2.41	0.56
13:M:44:ARG:HB3	13:M:46:LYS:HG3	1.86	0.56
8:H:29:SER:OG	8:H:32:LYS:HG3	2.06	0.56
21:U:18:TYR:HD1	21:U:24:ARG:CZ	2.18	0.56
1:A:1053:G:HO2'	1:A:1199:U:H5	1.54	0.56
1:A:1534:C:C2	1:A:1535:A:C2	2.93	0.56
1:A:106:C:C2'	1:A:107:G:H5'	2.34	0.56
1:A:945:G:N1	1:A:1337:G:C2	2.73	0.56
1:A:1124:G:H5'	10:J:35:SER:O	2.05	0.56
10:J:69:ASN:O	10:J:70:ARG:HD3	2.04	0.56
12:L:11:VAL:HG22	17:Q:29:HIS:CD2	2.40	0.56
2:B:36:ARG:CG	2:B:41:ILE:HD11	2.35	0.56
1:A:344:A:H5''	1:A:345:C:H5	1.70	0.56
1:A:830:G:O3'	2:B:22:LYS:HB3	2.05	0.56
1:A:1092:A:H8	1:A:1092:A:C5'	2.18	0.56
9:I:118:LYS:C	9:I:120:ARG:H	2.08	0.56
1:A:1499:A:OP1	1:A:1519[A]:MA6:N1	2.38	0.56
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.58	0.56
1:A:1125:U:H3'	1:A:1126:U:C5	2.40	0.56
19:S:41:VAL:HB	19:S:42:PRO:HD2	1.86	0.56
1:A:564:C:H5'	17:Q:32:TYR:CE2	2.41	0.56
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.41	0.56
1:A:83:U:H5	1:A:84:U:C5	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1250:A:C2	1:A:1287:A:N1	2.74	0.56
16:P:57:ARG:O	16:P:58:TYR:C	2.40	0.56
4:D:196:LEU:HD23	4:D:196:LEU:N	2.21	0.56
1:A:831:U:H2'	1:A:832:C:C6	2.41	0.56
1:A:337:C:H2'	1:A:338:A:C8	2.41	0.56
1:A:1360:A:H2'	1:A:1361:G:O5'	2.06	0.56
1:A:1065:U:O2'	1:A:1066:C:OP2	2.19	0.56
11:K:122:LYS:O	11:K:124:LYS:N	2.39	0.56
1:A:1395:C:C2'	1:A:1396:A:H5'	2.35	0.56
1:A:1400:5MC:OP1	1:A:1400:5MC:HM51	2.06	0.56
1:A:1536:C:H6	1:A:1536:C:H3'	1.69	0.56
1:A:427:U:C4	1:A:428:G:C6	2.94	0.56
3:C:8:ILE:HG12	3:C:16:ARG:HG3	1.88	0.56
4:D:173:TRP:CD1	4:D:189:PRO:HD3	2.41	0.56
1:A:827:U:O2	1:A:827:U:H2'	2.05	0.56
1:A:1014:A:N7	1:A:1015:A:N6	2.54	0.56
1:A:28:G:O2'	1:A:296:U:OP1	2.20	0.56
1:A:1128:C:O2'	1:A:1130:A:C8	2.58	0.56
8:H:102:ARG:H	8:H:102:ARG:CD	2.01	0.56
12:L:27:LEU:CG	12:L:28:LYS:H	2.05	0.56
1:A:908:A:C2	1:A:909:A:C4	2.94	0.56
16:P:21:VAL:HG12	16:P:21:VAL:O	2.05	0.56
4:D:19:LEU:HD12	4:D:67:ILE:HG13	1.86	0.56
8:H:36:LEU:HA	8:H:39:LEU:HD23	1.88	0.56
1:A:476:G:H2'	1:A:477:G:C8	2.40	0.56
3:C:105:GLU:HG2	3:C:106:VAL:N	2.21	0.56
17:Q:86:GLU:O	17:Q:90:ILE:HG12	2.05	0.56
9:I:5:TYR:HD1	9:I:6:GLY:H	1.54	0.56
10:J:55:LYS:CG	10:J:56:HIS:N	2.51	0.56
1:A:559:A:OP1	5:E:126:ARG:NH2	2.39	0.56
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.86	0.56
3:C:59:ARG:HG2	3:C:64:VAL:HG13	1.88	0.56
2:B:170:GLU:O	2:B:173:ALA:HB3	2.06	0.56
15:O:12:ILE:C	15:O:14:GLU:N	2.57	0.56
1:A:1407:5MC:C2	1:A:1408:A:C8	2.94	0.56
1:A:1082:G:C2'	1:A:1083:U:H5'	2.35	0.56
4:D:18:LYS:CE	4:D:20:TYR:HE2	2.11	0.56
12:L:127:GLU:HG3	12:L:128:ALA:O	2.05	0.56
18:R:37:VAL:O	18:R:39:VAL:N	2.39	0.56
5:E:76:ILE:HG12	5:E:118:ILE:CD1	2.36	0.56
1:A:273:A:N6	1:A:274:A:C6	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LYS:HE3	3:C:205:GLY:H	1.69	0.56
1:A:188:C:O2'	1:A:189:G:H5'	2.06	0.56
23:W:32:C:HO2'	23:W:33:U:H6	1.54	0.56
1:A:1096:C:H2'	1:A:1097:C:H6	1.71	0.56
5:E:137:GLU:HG2	5:E:140:ARG:HH11	1.71	0.56
9:I:27:THR:OG1	9:I:28:VAL:N	2.39	0.55
10:J:61:GLU:O	10:J:61:GLU:HG2	2.06	0.55
1:A:500:G:O6	1:A:501:C:N4	2.39	0.55
1:A:353:A:H5'	1:A:353:A:H8	1.70	0.55
1:A:176:C:HO2'	1:A:177:C:H5'	1.71	0.55
4:D:172:PRO:HG2	4:D:173:TRP:HE3	1.71	0.55
1:A:137:C:C2'	1:A:138:G:C5'	2.84	0.55
12:L:34:ARG:HB2	12:L:105:TYR:CE1	2.41	0.55
8:H:124:ALA:O	8:H:128:GLY:N	2.38	0.55
1:A:190(E):U:C5	17:Q:72:ARG:NH2	2.74	0.55
2:B:141:GLU:O	2:B:144:ARG:HG3	2.06	0.55
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.71	0.55
1:A:1248:A:H2'	1:A:1249:C:H5'	1.87	0.55
9:I:10:ARG:HG3	9:I:11:LYS:HG2	1.89	0.55
1:A:1399:C:O2	1:A:1401:G:N7	2.38	0.55
1:A:1436:U:C2	1:A:1437:C:C6	2.93	0.55
5:E:11:ILE:CG2	5:E:12:LEU:N	2.68	0.55
1:A:446:G:C2'	1:A:447:G:H5'	2.36	0.55
1:A:1126:U:H6	1:A:1126:U:OP1	1.89	0.55
3:C:8:ILE:CG2	3:C:9:GLY:N	2.70	0.55
19:S:13:ASP:O	19:S:16:LEU:HB3	2.06	0.55
8:H:36:LEU:O	8:H:37:ARG:C	2.44	0.55
1:A:264:U:C2'	1:A:265:G:H5'	2.37	0.55
1:A:462:G:H5'	1:A:463:A:OP2	2.07	0.55
14:N:12:ARG:HH11	14:N:12:ARG:N	2.04	0.55
1:A:939:G:H5'	7:G:102:ARG:CZ	2.36	0.55
1:A:21:G:P	29:A:2044:HOH:O	2.65	0.55
13:M:99:ARG:NH2	19:S:2:PRO:CG	2.70	0.55
7:G:66:VAL:HG12	7:G:67:GLU:N	2.21	0.55
9:I:27:THR:CG2	9:I:62:TYR:HA	2.37	0.55
1:A:1536:C:C5	1:A:1537:U:N3	2.74	0.55
1:A:89:C:C5	1:A:90:U:C4	2.84	0.55
1:A:569:C:H5''	1:A:570:G:OP1	2.07	0.55
10:J:48:THR:CB	10:J:62:HIS:HB3	2.36	0.55
1:A:414:A:C2	1:A:415:A:C4	2.93	0.55
20:T:10:LEU:CD2	20:T:13:LEU:N	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1408:A:O2'	1:A:1409:C:H5'	2.07	0.55
1:A:506:G:C2'	1:A:507:C:H5'	2.36	0.55
1:A:1360:A:C2'	1:A:1361:G:O5'	2.54	0.55
1:A:1195:C:H5''	1:A:1196:U:O5'	2.06	0.55
1:A:1027:C:O2'	1:A:1034:G:N2	2.40	0.55
1:A:1029:C:C2'	1:A:1030:C:H5'	2.37	0.55
13:M:23:TYR:CE2	13:M:70:LEU:HD13	2.42	0.55
8:H:28:ALA:HB2	8:H:58:TYR:CA	2.36	0.55
1:A:547:A:OP2	4:D:2:GLY:CA	2.55	0.55
2:B:8:LYS:C	2:B:10:LEU:N	2.58	0.55
1:A:829:G:C2'	1:A:830:G:H5'	2.35	0.55
5:E:69:VAL:HG12	5:E:70:PRO:N	2.20	0.55
9:I:128:ARG:OXT	9:I:128:ARG:HG2	2.06	0.55
12:L:83:VAL:HG12	12:L:107:ALA:HB2	1.88	0.55
7:G:75:VAL:O	7:G:75:VAL:HG22	2.06	0.55
20:T:84:LEU:O	20:T:84:LEU:HD23	2.07	0.55
1:A:255:G:O6	1:A:266:G:O6	2.25	0.55
9:I:63:ILE:HG22	9:I:63:ILE:O	2.06	0.55
1:A:922:G:N3	1:A:1398:A:H2	2.05	0.55
7:G:121:ALA:O	7:G:125:MET:HG3	2.07	0.55
1:A:1006:C:N4	1:A:1023:G:H1	2.02	0.55
1:A:1124:G:HO2'	1:A:1145:C:N4	2.03	0.55
4:D:196:LEU:HD23	4:D:196:LEU:H	1.72	0.55
5:E:76:ILE:HG12	5:E:118:ILE:HD12	1.88	0.55
1:A:1015:A:H2'	1:A:1016:A:O4'	2.05	0.55
1:A:337:C:H2'	1:A:338:A:H8	1.71	0.55
23:W:35:G:H2'	23:W:36:A:H8	1.70	0.55
8:H:57:PRO:CG	8:H:57:PRO:O	2.53	0.55
1:A:838:G:N2	1:A:849:C:C2	2.75	0.55
1:A:261:U:O2	1:A:263:A:C8	2.60	0.55
1:A:1417:G:O2'	1:A:1418:A:H5'	2.06	0.55
2:B:7:VAL:O	2:B:10:LEU:HB2	2.06	0.55
1:A:668:G:O2'	1:A:669:U:H5'	2.07	0.55
12:L:60:LEU:HB2	12:L:64:TYR:O	2.06	0.55
1:A:1448:C:H2'	1:A:1449:C:H6	1.71	0.55
1:A:933:G:OP2	7:G:3:ARG:HB3	2.07	0.55
1:A:1114:C:H1'	14:N:60:SER:OG	2.05	0.55
1:A:1139:G:N2	1:A:1143:G:N2	2.54	0.55
1:A:36:C:C2'	1:A:37:U:H5'	2.37	0.55
10:J:4:ILE:HG22	10:J:77:PRO:HD3	1.87	0.55
1:A:1028:C:N3	1:A:1034:G:C2	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:39:G:C2	23:W:40:PSU:N3	2.74	0.55
8:H:20:TYR:CZ	8:H:76:PRO:HD2	2.41	0.55
3:C:54:ARG:NH1	3:C:56:ASP:OD1	2.27	0.55
4:D:170:VAL:HG22	4:D:171:GLY:H	1.71	0.55
1:A:822:C:C2'	1:A:823:G:H5'	2.37	0.55
7:G:108:ALA:O	7:G:119:ARG:HB3	2.07	0.55
13:M:37:THR:HG23	13:M:39:ILE:HD13	1.88	0.55
13:M:27:LYS:CE	21:U:21:TYR:HE2	2.20	0.55
1:A:961:U:C2'	1:A:962:C:H5'	2.36	0.55
19:S:63:THR:OG1	19:S:66:MET:HG3	2.07	0.55
5:E:67:VAL:HG21	5:E:140:ARG:HB3	1.89	0.55
1:A:1415:G:C2'	1:A:1416:G:H5'	2.36	0.55
1:A:998:G:H2'	1:A:999:C:C6	2.41	0.55
1:A:1206:G:C6	1:A:1207:2MG:C6	2.94	0.55
1:A:545:C:O2	1:A:546:G:O4'	2.25	0.55
1:A:1005:A:C8	1:A:1026:G:N1	2.73	0.55
1:A:1027:C:C5	1:A:1035:A:C2	2.95	0.55
1:A:278:G:C6	17:Q:95:TYR:HD2	2.25	0.55
2:B:101:MET:HB2	2:B:102:LEU:HD12	1.89	0.55
3:C:59:ARG:NH1	3:C:97:LYS:HE2	2.22	0.55
8:H:4:ASP:HB3	8:H:7:ALA:HB3	1.88	0.55
3:C:5:ILE:CD1	3:C:10:PHE:HB2	2.37	0.55
2:B:56:ARG:HB2	2:B:56:ARG:NH1	2.22	0.55
1:A:107:G:C3'	1:A:108:G:H5''	2.36	0.55
1:A:597:G:N2	1:A:643:C:N3	2.40	0.55
1:A:357:G:C2	1:A:358:U:C5	2.95	0.55
1:A:1011:G:H2'	1:A:1012:U:H5'	1.87	0.55
4:D:204:ILE:HD13	4:D:204:ILE:H	1.73	0.55
1:A:1117:G:H5''	9:I:104:ARG:NH2	2.22	0.55
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.87	0.55
9:I:16:ARG:HD3	9:I:64:THR:HG22	1.89	0.54
9:I:64:THR:O	9:I:64:THR:HG22	2.07	0.54
1:A:1190:G:H5''	1:A:1190:G:C8	2.42	0.54
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.89	0.54
1:A:192:U:H1'	20:T:103:GLY:CA	2.34	0.54
12:L:76:ASN:CG	12:L:76:ASN:O	2.45	0.54
10:J:38:ILE:HG23	10:J:39:PRO:HD2	1.88	0.54
18:R:45:SER:OG	18:R:46:GLU:N	2.38	0.54
19:S:11:VAL:CG1	19:S:16:LEU:HD22	2.37	0.54
1:A:1160:G:O6	1:A:1181:G:C6	2.60	0.54
1:A:421:U:O2	1:A:421:U:O4'	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:113:GLU:HB2	7:G:119:ARG:HG2	1.89	0.54
3:C:76:VAL:HG23	3:C:77:ILE:N	2.22	0.54
3:C:130:VAL:O	3:C:134:ILE:CD1	2.56	0.54
2:B:212:GLN:HE21	2:B:235:SER:HB3	1.72	0.54
1:A:1500:A:P	1:A:1505:G:OP1	2.65	0.54
1:A:1319:A:OP1	19:S:5:LEU:HD22	2.08	0.54
1:A:132:C:O2'	1:A:133:U:H5'	2.08	0.54
6:F:98:LEU:H	6:F:98:LEU:CD1	2.17	0.54
1:A:389:A:C5	1:A:390:C:H1'	2.42	0.54
1:A:1346:A:C5	7:G:10:ARG:NH1	2.75	0.54
4:D:72:GLU:O	4:D:75:PHE:HB3	2.07	0.54
1:A:1030(A):G:C4	1:A:1030(C):G:OP2	2.60	0.54
1:A:860:A:OP2	29:A:2124:HOH:O	2.18	0.54
12:L:78:GLN:N	12:L:81:SER:OG	2.29	0.54
3:C:20:SER:HA	3:C:57:ILE:O	2.07	0.54
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.89	0.54
1:A:1381:U:C6	1:A:1382:C:C5	2.96	0.54
1:A:839:U:C5'	1:A:840:C:H5	2.18	0.54
1:A:1122:U:H2'	1:A:1123:A:H5'	1.89	0.54
1:A:676:A:O2'	1:A:677:U:H5'	2.06	0.54
1:A:178:C:C2'	1:A:179:A:H5'	2.38	0.54
1:A:529:G:C8	1:A:529:G:C3'	2.89	0.54
3:C:36:ASP:O	3:C:39:ILE:HB	2.07	0.54
1:A:568:G:N2	1:A:883:C:C2	2.75	0.54
11:K:91:ARG:O	11:K:94:ALA:N	2.35	0.54
9:I:23:ASN:OD1	9:I:25:LYS:HE3	2.07	0.54
17:Q:23:VAL:CG2	17:Q:42:TYR:HD1	2.21	0.54
2:B:172:ILE:HG12	2:B:173:ALA:N	2.22	0.54
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.90	0.54
9:I:99:LEU:N	9:I:99:LEU:HD22	2.22	0.54
6:F:53:ALA:C	6:F:54:LYS:HG2	2.28	0.54
1:A:1122:U:C2'	1:A:1123:A:H5'	2.38	0.54
19:S:42:PRO:O	19:S:45:VAL:HG23	2.06	0.54
4:D:63:LYS:NZ	4:D:197:PRO:O	2.40	0.54
1:A:448:A:H2'	1:A:449:C:H6	1.73	0.54
8:H:86:ILE:HG22	8:H:87:SER:N	2.22	0.54
1:A:22:G:C6	1:A:23:C:C4	2.96	0.54
1:A:22:G:C5	1:A:23:C:C5	2.96	0.54
7:G:51:GLN:HA	7:G:54:THR:O	2.07	0.54
1:A:998:G:H2'	1:A:999:C:H6	1.73	0.54
21:U:6:ARG:HG3	21:U:15:ARG:NH1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:G:O6	29:A:2136:HOH:O	2.16	0.54
1:A:1197:G:H2'	1:A:1198:G:H5''	1.90	0.54
2:B:74:LYS:C	2:B:76:GLN:H	2.10	0.54
1:A:1533:C:H2'	1:A:1534:C:C6	2.42	0.54
3:C:13:GLY:HA2	14:N:57:ARG:HH12	1.72	0.54
1:A:53:A:C6	1:A:54:C:C4	2.96	0.54
19:S:80:TYR:HD1	19:S:81:ARG:H	1.51	0.54
15:O:15:PHE:HE2	15:O:85:LEU:HD21	1.72	0.54
4:D:21:LEU:HD21	4:D:66:ARG:O	2.07	0.54
20:T:10:LEU:HD23	20:T:13:LEU:H	1.68	0.54
1:A:380:G:C8	29:A:2680:HOH:O	2.54	0.54
20:T:88:VAL:HG12	20:T:89:ARG:N	2.21	0.54
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:H2	2.37	0.54
1:A:39:G:H1	1:A:1532:U:H3	88.34	0.54
6:F:48:LEU:HG	6:F:57:GLN:HA	1.88	0.54
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.89	0.54
1:A:1005:A:H2'	1:A:1005:A:N3	2.23	0.54
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.43	0.54
1:A:991:U:O2'	1:A:992:U:P	2.66	0.54
1:A:1256:A:C8	1:A:1258:G:C2	2.94	0.54
19:S:19:VAL:HG23	19:S:47:HIS:HD1	1.71	0.54
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.41	0.54
8:H:4:ASP:OD1	8:H:6:ILE:N	2.40	0.54
20:T:82:SER:O	20:T:83:ARG:C	2.44	0.54
1:A:98:U:C2'	1:A:99:C:H5'	2.37	0.54
17:Q:12:SER:HB3	17:Q:20:THR:OG1	2.07	0.54
17:Q:90:ILE:O	17:Q:91:ARG:C	2.46	0.54
3:C:3:ASN:N	3:C:3:ASN:OD1	2.40	0.54
1:A:89:C:C6	1:A:90:U:N3	2.75	0.54
2:B:92:TYR:CE1	2:B:151:GLY:HA3	2.42	0.54
17:Q:81:ARG:NE	17:Q:84:LEU:CD1	2.71	0.54
17:Q:45:HIS:NE2	17:Q:47:PRO:HB3	2.22	0.54
1:A:119:A:P	29:A:2559:HOH:O	2.64	0.54
1:A:1279:A:C5'	1:A:1280:A:OP1	2.56	0.54
1:A:259:G:H2'	1:A:260:G:O5'	2.08	0.54
1:A:895:G:H2'	1:A:896:C:H6	1.73	0.54
1:A:257:G:C2	1:A:270:A:C2	2.94	0.54
5:E:107:ARG:O	5:E:108:ALA:C	2.46	0.54
12:L:59:ARG:HG3	12:L:65:GLU:OE2	2.08	0.54
1:A:1055:A:C8	1:A:1206:G:N2	2.76	0.54
3:C:156:ARG:NH1	3:C:193:TYR:HB2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:79:ARG:HD2	10:J:79:ARG:H	1.73	0.54
1:A:500:G:C6	1:A:546:G:C2	2.96	0.54
19:S:41:VAL:HG22	19:S:44:MET:HG3	1.89	0.54
3:C:6:HIS:HD2	3:C:7:PRO:HD2	1.70	0.54
14:N:9:LYS:O	14:N:11:LYS:N	2.40	0.54
7:G:54:THR:CG2	7:G:56:GLN:HB2	2.38	0.54
4:D:58:LEU:C	4:D:58:LEU:HD23	2.27	0.54
10:J:79:ARG:H	10:J:79:ARG:CD	2.21	0.54
1:A:91:C:H2'	1:A:92:C:H6	1.70	0.54
13:M:37:THR:OG1	13:M:55:ARG:HG2	2.08	0.54
5:E:11:ILE:CG2	5:E:31:LEU:HB3	2.37	0.54
1:A:1018:C:H2'	1:A:1019:C:C6	2.43	0.54
1:A:610:G:H2'	1:A:611:A:H5'	1.89	0.54
4:D:57:ARG:HG3	4:D:202:LEU:HD22	1.89	0.54
1:A:1190:G:C8	1:A:1190:G:C5'	2.91	0.53
1:A:1206:G:C4	1:A:1207:2MG:C8	2.96	0.53
1:A:1054:C:N3	23:W:34:G:H5'	2.21	0.53
1:A:1505:G:H5'	1:A:1506:U:OP1	2.08	0.53
1:A:384:G:H2'	1:A:385:C:C6	2.42	0.53
1:A:1004:A:C5'	29:A:2327:HOH:O	2.55	0.53
6:F:98:LEU:N	6:F:98:LEU:CD1	2.71	0.53
19:S:31:ILE:O	19:S:50:ALA:CB	2.56	0.53
3:C:46:GLU:HG3	3:C:83:ARG:HH21	1.71	0.53
1:A:769:G:C2'	1:A:770:C:H5'	2.38	0.53
1:A:725:G:C2'	1:A:726:C:H5'	2.38	0.53
20:T:45:GLN:HA	20:T:91:LEU:HD21	1.90	0.53
1:A:671:G:H5'	6:F:77:ARG:NH2	2.23	0.53
17:Q:48:GLU:O	17:Q:49:GLU:HB2	2.08	0.53
2:B:114:ARG:O	2:B:117:GLU:HB3	2.08	0.53
18:R:50:ILE:HG12	18:R:70:ILE:HD13	1.89	0.53
6:F:62:TRP:C	6:F:63:TYR:HD2	2.11	0.53
14:N:46:GLU:O	14:N:49:HIS:HB2	2.08	0.53
1:A:579:G:H5'	1:A:728:A:H1'	1.90	0.53
9:I:15:ALA:CB	9:I:77:ILE:HD12	2.37	0.53
1:A:689:C:H2'	1:A:690:G:H5'	1.89	0.53
1:A:691:G:H2'	1:A:692:U:H6	1.73	0.53
1:A:1502:A:N3	1:A:1502:A:C2'	2.70	0.53
1:A:1006:C:O2'	1:A:1007:C:H5'	2.08	0.53
1:A:1236:A:H4'	1:A:1304:G:H4'	1.91	0.53
1:A:865:A:H8	1:A:865:A:O5'	1.91	0.53
4:D:83:SER:CA	4:D:89:THR:HG23	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:41:VAL:HG23	19:S:43:GLU:OE2	2.07	0.53
3:C:150:LYS:HA	3:C:169:ALA:HB2	1.90	0.53
7:G:69:VAL:HA	7:G:138:LYS:HD3	1.89	0.53
17:Q:59:ILE:CG2	17:Q:71:PHE:CD1	2.90	0.53
1:A:947:G:H2'	1:A:948:C:O4'	2.08	0.53
1:A:602:A:C2	1:A:637:G:C2	2.96	0.53
1:A:890:G:O2'	1:A:906:G:O6	2.16	0.53
1:A:1278:U:O2	1:A:1278:U:H2'	2.07	0.53
12:L:55:VAL:N	12:L:70:ILE:HD12	2.23	0.53
1:A:1054:C:N4	23:W:34:G:C8	2.76	0.53
4:D:43:HIS:HA	4:D:46:LYS:HG3	1.90	0.53
1:A:34:C:H1'	12:L:32:PHE:CZ	2.43	0.53
1:A:858:G:O2'	1:A:859:A:C5'	2.44	0.53
1:A:778:G:H2'	1:A:779:C:O4'	2.08	0.53
5:E:8:GLU:CB	5:E:34:VAL:HG12	2.38	0.53
1:A:784:C:H2'	1:A:785:G:O5'	2.08	0.53
7:G:27:ILE:HG22	7:G:28:ASN:N	2.24	0.53
1:A:154:C:C2'	1:A:155:C:H5'	2.38	0.53
11:K:56:GLY:O	11:K:57:THR:C	2.45	0.53
20:T:84:LEU:HD23	20:T:84:LEU:C	2.29	0.53
1:A:256:U:O2'	1:A:257:G:H5'	2.07	0.53
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.09	0.53
21:U:18:TYR:CD1	21:U:24:ARG:HG3	2.44	0.53
1:A:688:G:H2'	1:A:689:C:C6	2.43	0.53
18:R:38:GLU:CD	18:R:38:GLU:H	2.11	0.53
12:L:19:ARG:HA	12:L:20:LYS:NZ	2.23	0.53
1:A:664:G:OP1	18:R:64:ARG:HD2	2.09	0.53
3:C:113:ALA:N	3:C:114:PRO:HD2	2.24	0.53
8:H:9:MET:SD	8:H:36:LEU:HD21	2.48	0.53
17:Q:81:ARG:HG3	17:Q:81:ARG:O	2.08	0.53
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.91	0.53
1:A:594:G:H2'	1:A:595:G:H5'	1.90	0.53
7:G:115:ARG:HG3	7:G:118:VAL:HG23	1.90	0.53
1:A:1413:A:C2	1:A:1414:U:C2	2.97	0.53
1:A:1055:A:C8	1:A:1206:G:C2	2.96	0.53
1:A:229:U:O2'	16:P:23:ASP:HB2	2.09	0.53
18:R:22:VAL:HG23	18:R:56:THR:HA	1.91	0.53
9:I:48:GLU:HB3	9:I:101:PHE:CE1	2.43	0.53
7:G:78:ARG:HD2	7:G:156:TRP:CB	2.38	0.53
2:B:30:ARG:HD2	2:B:31:TYR:CE1	2.43	0.53
7:G:59:LEU:HD23	7:G:60:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:62:PHE:CD1	7:G:62:PHE:C	2.79	0.53
5:E:51:VAL:O	5:E:54:ALA:HB3	2.09	0.53
23:W:35:G:N3	23:W:36:A:C8	2.76	0.53
10:J:29:ARG:CD	10:J:29:ARG:H	2.16	0.53
1:A:1026:G:C8	1:A:1027:C:C2	2.96	0.53
4:D:147:ALA:CB	4:D:182:LYS:HB3	2.39	0.53
1:A:1321:C:C4'	13:M:87:TYR:HE2	2.18	0.53
1:A:392:G:N3	1:A:393:A:C8	2.77	0.53
1:A:182:U:C5	1:A:183:G:C4	2.94	0.53
14:N:26:ARG:HD3	14:N:47:LEU:CD1	2.39	0.53
1:A:144:G:H1	1:A:178:C:H42	1.57	0.53
17:Q:11:VAL:HG13	17:Q:85:VAL:HG12	1.91	0.53
6:F:99:ALA:HB1	18:R:23:LYS:NZ	2.23	0.53
1:A:98:U:O2'	1:A:99:C:H5'	2.09	0.53
1:A:1472:U:H2'	1:A:1473:A:O5'	2.09	0.53
1:A:1369:C:H2'	1:A:1370:G:H8	1.73	0.53
7:G:5:ARG:CZ	7:G:8:GLU:HG2	2.37	0.53
1:A:89:C:O2'	1:A:90:U:OP1	2.23	0.53
13:M:15:VAL:O	13:M:19:LEU:HG	2.08	0.53
1:A:1212:U:C1'	1:A:1213:A:OP2	2.52	0.53
1:A:443:C:N4	1:A:491:G:H1	2.06	0.53
2:B:122:PHE:CE1	2:B:127:ILE:HD12	2.44	0.53
1:A:532:A:H61	1:A:1207:2MG:H5'	1.74	0.53
10:J:49:VAL:O	10:J:61:GLU:N	2.36	0.53
1:A:922:G:C6	1:A:923:A:C6	2.97	0.53
6:F:49:ALA:HB3	6:F:50:TYR:HD1	1.74	0.53
1:A:1026:G:C8	1:A:1027:C:O2	2.62	0.53
1:A:1303:C:N4	1:A:1304:G:C6	2.77	0.53
8:H:54:ASP:CG	8:H:55:GLY:H	2.00	0.53
2:B:100:GLY:CA	2:B:176:GLU:OE2	2.55	0.53
20:T:74:LYS:HB2	20:T:76:ALA:H	1.74	0.53
11:K:48:ILE:HG22	11:K:49:GLY:N	2.22	0.53
1:A:1407:5MC:N3	1:A:1408:A:C8	2.77	0.53
12:L:50:SER:O	12:L:51:ALA:HB2	2.09	0.53
1:A:560:U:H5'	1:A:566:G:N2	2.24	0.53
12:L:79:GLU:HG2	12:L:80:HIS:NE2	2.23	0.53
1:A:1131:G:C8	1:A:1131:G:OP2	2.59	0.53
1:A:1090:U:H2'	1:A:1091:U:C6	2.38	0.53
10:J:47:PHE:HD2	14:N:34:TYR:CD2	2.27	0.53
1:A:1035:A:C4	1:A:1036:G:N7	2.76	0.53
4:D:150:GLU:O	4:D:153:ARG:N	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:65:LEU:HD12	10:J:66:ARG:N	2.24	0.53
1:A:984:C:N3	1:A:1221:G:N2	2.47	0.53
8:H:28:ALA:HB2	8:H:58:TYR:HA	1.90	0.53
9:I:53:VAL:HG21	9:I:85:LEU:CD1	2.35	0.53
16:P:15:PRO:HB2	16:P:41:PRO:HG2	1.91	0.53
7:G:37:ASN:HD22	7:G:41:ARG:HH21	1.57	0.53
1:A:1077:G:N2	1:A:1081:G:C4	2.77	0.53
1:A:456:C:H2'	1:A:457:C:C6	2.43	0.53
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.74	0.53
1:A:1349:A:OP1	9:I:118:LYS:HG3	2.08	0.53
1:A:1130:A:H5''	9:I:62:TYR:CE2	2.43	0.53
10:J:61:GLU:CG	10:J:61:GLU:O	2.57	0.53
11:K:14:VAL:O	11:K:15:ALA:HB3	2.08	0.53
1:A:1314:C:O2'	1:A:1315:U:H5'	2.08	0.53
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.30	0.53
17:Q:40:LYS:HG2	17:Q:41:LYS:H	1.73	0.53
2:B:239:VAL:HG12	2:B:239:VAL:O	2.09	0.53
15:O:14:GLU:HG3	15:O:15:PHE:CD1	2.38	0.53
7:G:139:GLU:HB3	7:G:143:ARG:HH22	1.73	0.53
1:A:781:A:C5	1:A:802:A:C2	2.97	0.53
11:K:92:GLU:HB3	11:K:96:ARG:NH2	2.24	0.53
6:F:67:MET:HB2	6:F:68:PRO:CD	2.38	0.53
18:R:50:ILE:HD11	18:R:70:ILE:CG2	2.38	0.53
20:T:105:SER:O	20:T:106:ALA:OXT	2.27	0.53
1:A:1058:G:H2'	1:A:1059:C:C6	2.43	0.52
1:A:437:U:OP2	29:A:2795:HOH:O	2.19	0.52
5:E:11:ILE:HG21	5:E:31:LEU:HD13	1.90	0.52
14:N:26:ARG:CD	14:N:47:LEU:HD11	2.36	0.52
1:A:178:C:H2'	1:A:179:A:H5'	1.92	0.52
11:K:40:ILE:CG2	11:K:75:TYR:CD1	2.92	0.52
1:A:783:C:C2'	1:A:784:C:H5'	2.39	0.52
1:A:375:U:C4	1:A:376:G:N7	2.77	0.52
8:H:19:VAL:O	8:H:19:VAL:HG23	2.09	0.52
1:A:1130:A:H5''	9:I:62:TYR:HE2	1.74	0.52
1:A:1054:C:N4	23:W:34:G:OP1	2.41	0.52
1:A:1057:G:H5''	3:C:154:SER:OG	2.08	0.52
2:B:212:GLN:NE2	2:B:235:SER:HB2	2.23	0.52
1:A:1003(A):G:N1	1:A:1038:C:N3	2.46	0.52
1:A:1320:C:C2'	1:A:1321:C:H5'	2.40	0.52
11:K:120:ARG:CG	11:K:120:ARG:NH1	2.72	0.52
18:R:47:THR:HA	18:R:83:GLU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:U:H2'	1:A:57:G:C8	2.43	0.52
5:E:152:ARG:O	8:H:64:LYS:NZ	2.42	0.52
6:F:10:LEU:HD12	6:F:10:LEU:H	1.73	0.52
1:A:514:C:H2'	1:A:515:G:H8	1.73	0.52
19:S:38:SER:HB3	19:S:71:LEU:HD12	1.91	0.52
1:A:164:U:H2'	1:A:165:C:C6	2.43	0.52
2:B:26:PRO:O	2:B:29:ALA:HB2	2.09	0.52
6:F:78:GLU:O	6:F:81:ILE:HG12	2.10	0.52
12:L:75:HIS:HB3	12:L:102:ARG:NH1	2.24	0.52
12:L:54:LYS:HD3	12:L:54:LYS:N	2.25	0.52
1:A:1054:C:C4	23:W:34:G:OP1	2.63	0.52
1:A:1517[B]:G:O6	1:A:1518[B]:MA6:H103	2.09	0.52
1:A:35:G:C5	1:A:36:C:C5	2.97	0.52
1:A:509:A:H3'	1:A:509:A:H8	1.70	0.52
7:G:46:ALA:HB1	7:G:121:ALA:HB2	1.90	0.52
1:A:1005:A:OP2	1:A:1006:C:C5	2.62	0.52
4:D:155:LEU:CD2	4:D:156:GLU:H	2.22	0.52
13:M:23:TYR:CD2	13:M:70:LEU:HD13	2.44	0.52
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.13	0.52
1:A:661:G:C8	1:A:661:G:H5''	2.42	0.52
1:A:520:A:H61	1:A:529:G:H1'	1.74	0.52
1:A:1350:A:C5	1:A:1351:U:C5	2.97	0.52
1:A:1056:U:H5'	3:C:163:ALA:CB	2.34	0.52
1:A:1391:U:H2'	1:A:1392:G:H8	1.74	0.52
1:A:1519[A]:MA6:H2'	1:A:1520[A]:G:H5'	1.90	0.52
1:A:1537:U:O5'	1:A:1537:U:H6	1.93	0.52
1:A:93:G:C2'	1:A:95:U:H5'	2.40	0.52
10:J:44:VAL:CG1	10:J:66:ARG:HD3	2.32	0.52
2:B:92:TYR:O	2:B:92:TYR:HD1	1.92	0.52
16:P:67:THR:CG2	16:P:68:ASP:N	2.63	0.52
19:S:11:VAL:HG11	19:S:16:LEU:HD22	1.91	0.52
17:Q:50:LYS:HE3	17:Q:51:TYR:CE2	2.44	0.52
4:D:2:GLY:O	4:D:3:ARG:HB3	2.08	0.52
1:A:1186:G:N2	1:A:1187:G:H1'	2.25	0.52
2:B:204:ASN:OD1	2:B:204:ASN:C	2.47	0.52
9:I:27:THR:OG1	9:I:31:GLN:O	2.19	0.52
2:B:212:GLN:NE2	2:B:235:SER:CB	2.72	0.52
6:F:48:LEU:HD11	6:F:52:ILE:HG13	1.87	0.52
1:A:746:A:O2'	1:A:747:C:H5'	2.09	0.52
1:A:1439:C:OP1	20:T:38:LYS:HE2	2.10	0.52
1:A:995:C:H1'	14:N:4:LYS:HE2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:G:N2	1:A:850:U:O2	2.42	0.52
11:K:33:THR:HG21	11:K:37:GLY:O	2.10	0.52
5:E:92:LYS:O	5:E:118:ILE:HG13	2.09	0.52
19:S:49:ILE:N	19:S:49:ILE:HD13	2.24	0.52
1:A:461:C:H4'	1:A:462:G:OP2	2.09	0.52
1:A:442:C:C2'	1:A:443:C:H5'	2.39	0.52
2:B:184:VAL:HG12	2:B:197:VAL:HG13	1.90	0.52
1:A:259:G:C2'	1:A:260:G:O5'	2.58	0.52
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.90	0.52
3:C:77:ILE:HG13	3:C:103:VAL:HG21	1.92	0.52
1:A:1085:U:C6	1:A:1094:G:N1	2.78	0.52
1:A:1069:C:O2'	1:A:1192:C:H1'	2.10	0.52
1:A:735:C:H1'	18:R:75:ILE:HD11	1.92	0.52
21:U:18:TYR:HD2	21:U:22:ARG:HD3	1.73	0.52
1:A:1392:G:N2	1:A:1502:A:H8	2.08	0.52
1:A:191:G:O2'	20:T:101:GLY:O	2.28	0.52
13:M:71:ARG:HA	13:M:74:VAL:CG2	2.40	0.52
3:C:62:ASP:HA	3:C:97:LYS:HZ1	1.74	0.52
16:P:9:PHE:HB2	16:P:16:HIS:O	2.10	0.52
1:A:182:U:H5	1:A:183:G:N9	2.05	0.52
1:A:969:A:H2'	1:A:970:C:H5'	1.90	0.52
2:B:47:THR:HG23	2:B:202:PRO:O	2.09	0.52
1:A:171:A:P	29:A:2844:HOH:O	2.68	0.52
1:A:506:G:H2'	1:A:507:C:H5'	1.92	0.52
19:S:51:VAL:HG23	19:S:58:VAL:HG23	1.91	0.52
9:I:118:LYS:HG3	9:I:118:LYS:O	2.09	0.52
1:A:1054:C:H2'	1:A:1055:A:H5''	1.92	0.52
1:A:1190:G:O2'	1:A:1191:A:O5'	2.27	0.52
1:A:532:A:N1	1:A:1207:2MG:H4'	2.25	0.52
18:R:87:ARG:HB2	18:R:87:ARG:NH2	2.25	0.52
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.92	0.52
1:A:1241:G:H2'	1:A:1242:C:C6	2.45	0.52
1:A:740:U:H4'	15:O:42:HIS:CD2	2.45	0.52
4:D:111:ALA:HB1	4:D:116:GLN:HG2	1.91	0.52
7:G:89:MET:SD	7:G:156:TRP:CZ3	3.03	0.52
1:A:1067:A:O2'	1:A:1093:A:O2'	2.07	0.52
1:A:1494:G:C2	1:A:1495:U:C6	2.98	0.52
1:A:1396:A:H4'	1:A:1397:C:H5''	1.90	0.52
1:A:35:G:C4	1:A:36:C:C5	2.98	0.52
4:D:32:ALA:C	4:D:35:ARG:H	2.13	0.52
19:S:15:LEU:HD12	19:S:15:LEU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:LEU:HD11	8:H:135:CYS:HB3	1.90	0.52
1:A:1147:C:H4'	9:I:5:TYR:CE2	2.38	0.52
1:A:1288:A:N6	1:A:1289:A:N6	2.57	0.52
6:F:14:LEU:HD12	6:F:19:LEU:HA	1.91	0.52
1:A:512:U:O2	1:A:540:G:C2	2.62	0.52
1:A:92:C:H2'	1:A:93:G:C8	2.44	0.52
1:A:909:A:C8	1:A:910:C:C5	2.98	0.52
4:D:173:TRP:C	4:D:174:LEU:HD23	2.30	0.52
1:A:414:A:C2	1:A:415:A:C8	2.98	0.52
12:L:79:GLU:HG2	12:L:80:HIS:CE1	2.45	0.52
9:I:17:VAL:HG22	9:I:63:ILE:HD11	1.92	0.52
1:A:504:C:C2	1:A:542:G:N2	2.78	0.52
1:A:132:C:C2'	1:A:133:U:H5'	2.40	0.52
10:J:48:THR:HG23	10:J:62:HIS:HB3	1.91	0.52
1:A:1124:G:C8	1:A:1145:C:C6	2.98	0.52
18:R:22:VAL:CG2	18:R:56:THR:HA	2.39	0.52
1:A:1110:A:H8	1:A:1110:A:O5'	1.92	0.52
1:A:568:G:H5''	1:A:568:G:H8	1.75	0.52
10:J:6:ILE:CD1	10:J:98:ILE:HG23	2.40	0.52
9:I:27:THR:HG22	9:I:62:TYR:HA	1.92	0.51
1:A:1003:G:H2'	1:A:1003(A):G:C8	2.45	0.51
13:M:22:ILE:HG13	13:M:25:ILE:HD12	1.91	0.51
1:A:630:G:H8	1:A:630:G:OP2	1.92	0.51
1:A:1009:G:N2	1:A:1010:G:C4	2.78	0.51
10:J:7:LYS:HE2	10:J:9:ARG:HH21	1.73	0.51
7:G:22:LEU:CD2	7:G:66:VAL:HG21	2.38	0.51
12:L:10:LEU:HD11	12:L:15:ARG:HE	1.75	0.51
5:E:55:VAL:O	5:E:56:GLN:C	2.47	0.51
3:C:34:LEU:HD12	3:C:34:LEU:O	2.10	0.51
12:L:75:HIS:HB3	12:L:102:ARG:HH12	1.75	0.51
1:A:1206:G:C5	1:A:1207:2MG:N7	2.78	0.51
10:J:32:ALA:HB2	10:J:76:ASN:OD1	2.10	0.51
1:A:428:G:H1'	1:A:429:U:OP2	2.10	0.51
1:A:1031:G:N2	1:A:1032:G:C4	2.78	0.51
1:A:1103:C:OP1	2:B:96:ARG:NH1	2.43	0.51
16:P:67:THR:CG2	16:P:68:ASP:H	2.15	0.51
3:C:78:GLY:HA3	3:C:83:ARG:HB3	1.92	0.51
13:M:99:ARG:NH2	19:S:2:PRO:HG2	2.24	0.51
7:G:54:THR:HG22	7:G:56:GLN:CB	2.40	0.51
1:A:924:C:H5'	1:A:1399:C:OP2	2.09	0.51
1:A:36:C:H2'	1:A:37:U:H5'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:47:PHE:CD2	14:N:34:TYR:CD2	2.99	0.51
1:A:328:C:C2'	1:A:329:A:OP2	2.58	0.51
13:M:22:ILE:HD13	13:M:22:ILE:N	2.25	0.51
1:A:747:C:C2'	1:A:748:C:O5'	2.58	0.51
1:A:1103:C:C5'	2:B:98:LEU:HD12	2.40	0.51
3:C:13:GLY:HA2	14:N:57:ARG:NH1	2.25	0.51
16:P:58:TYR:O	16:P:62:VAL:HG13	2.11	0.51
1:A:840:C:H5'	1:A:848:C:O2	2.11	0.51
1:A:975:A:C8	1:A:975:A:H5'	2.43	0.51
1:A:770:C:O2'	1:A:771:G:H5'	2.10	0.51
1:A:1009:G:H2'	1:A:1009:G:N3	2.25	0.51
1:A:988:G:C2	1:A:1218:C:O2	2.64	0.51
13:M:36:LYS:HB2	13:M:59:TYR:HE1	1.75	0.51
1:A:1061:G:C6	1:A:1062:U:N3	2.78	0.51
1:A:688:G:H2'	1:A:689:C:H6	1.75	0.51
11:K:122:LYS:O	11:K:123:LYS:C	2.47	0.51
6:F:14:LEU:HD21	6:F:84:ASN:OD1	2.10	0.51
2:B:219:VAL:CA	2:B:222:ILE:HG12	2.39	0.51
1:A:1519[B]:MA6:H93	1:A:1520[B]:G:H21	1.75	0.51
1:A:509:A:HO2'	1:A:510:A:P	2.25	0.51
18:R:39:VAL:HG13	18:R:40:LEU:H	1.75	0.51
13:M:23:TYR:CE2	13:M:71:ARG:HG3	2.45	0.51
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.46	0.51
1:A:1407:5MC:N3	1:A:1408:A:N7	2.58	0.51
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.92	0.51
4:D:82:ALA:HB2	4:D:96:LEU:HD22	1.92	0.51
7:G:21:VAL:HG23	7:G:22:LEU:N	2.26	0.51
1:A:1441:G:H5''	1:A:1442:G:O5'	2.10	0.51
3:C:84:ILE:HG12	3:C:88:ARG:HH22	1.75	0.51
1:A:1482:G:O5'	1:A:1482:G:H8	1.94	0.51
1:A:1168:A:H2'	1:A:1169:A:C8	2.45	0.51
1:A:1162:C:O2'	1:A:1163:C:H5'	2.10	0.51
1:A:1368:G:C2'	1:A:1369:C:H5'	2.41	0.51
23:W:35:G:C4	23:W:36:A:N7	2.79	0.51
1:A:1267:C:O2'	21:U:20:LYS:HG3	2.11	0.51
15:O:39:LEU:O	15:O:39:LEU:HD23	2.11	0.51
1:A:1152:A:OP1	10:J:68:HIS:CE1	2.63	0.51
1:A:1408:A:C4	1:A:1409:C:C5	2.99	0.51
4:D:145:GLU:C	4:D:146:ILE:HD12	2.31	0.51
7:G:111:ARG:HD3	7:G:113:GLU:HG3	1.93	0.51
1:A:658:G:C2	1:A:749:C:N3	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.44	0.51
1:A:1203:C:H2'	1:A:1204:A:O4'	2.11	0.51
1:A:509:A:C8	1:A:509:A:C3'	2.92	0.51
13:M:48:LEU:HB3	13:M:53:VAL:HG23	1.91	0.51
1:A:865:A:H2'	1:A:866:C:C6	2.45	0.51
1:A:849:C:H2'	1:A:850:U:H5'	1.92	0.51
15:O:11:VAL:HG22	15:O:12:ILE:HD13	1.92	0.51
1:A:1148:U:C4	1:A:1149:C:C2	2.99	0.51
1:A:1351:U:H5'	7:G:33:ASP:OD1	2.10	0.51
1:A:1055:A:N7	1:A:1206:G:C2	2.79	0.51
1:A:429:U:O2	1:A:430:A:C8	2.64	0.51
4:D:18:LYS:CB	4:D:33:MET:HG3	2.40	0.51
7:G:38:LEU:O	7:G:42:ILE:CG1	2.52	0.51
8:H:83:ILE:HB	8:H:137:VAL:HG22	1.93	0.51
1:A:1163:C:C2	1:A:1174:G:N2	2.79	0.51
5:E:150:ARG:HG2	5:E:151:LEU:HD23	1.92	0.51
10:J:50:ILE:HA	10:J:60:ARG:HA	1.92	0.51
1:A:1518[A]:MA6:C9	1:A:1519[A]:MA6:H103	2.41	0.51
1:A:1534:C:C4	1:A:1535:A:C2	2.99	0.51
14:N:22:THR:O	14:N:23:ARG:HG3	2.10	0.51
1:A:191:G:N2	20:T:103:GLY:O	2.43	0.51
23:W:39:G:C2	23:W:40:PSU:O4	2.64	0.51
1:A:983:A:H2	1:A:984:C:C6	2.29	0.51
1:A:1126:U:O4	1:A:1127:G:N1	2.44	0.51
1:A:676:A:H8	1:A:676:A:O5'	1.94	0.51
1:A:1020:U:H2'	1:A:1021:G:C8	2.42	0.51
2:B:83:MET:SD	2:B:234:PRO:O	2.69	0.51
1:A:22:G:C4	1:A:23:C:C5	2.99	0.51
1:A:814:A:H2'	1:A:816:A:H5''	1.93	0.51
1:A:1098:C:H2'	1:A:1099:G:O4'	2.10	0.51
1:A:433:C:H2'	1:A:434:U:H6	1.75	0.51
2:B:8:LYS:O	2:B:11:LEU:HD13	2.11	0.51
1:A:31:G:N2	1:A:48:C:OP1	2.34	0.51
1:A:266:G:H5''	1:A:268:C:H41	1.76	0.51
9:I:121:ARG:NH1	9:I:121:ARG:CG	2.69	0.51
1:A:1494:G:C2'	1:A:1495:U:H5'	2.41	0.51
1:A:922:G:C2	1:A:1396:A:C6	2.98	0.51
10:J:21:GLN:HA	10:J:24:VAL:HG12	1.93	0.51
1:A:1328:C:H2'	1:A:1329:A:H8	1.76	0.51
12:L:90:VAL:CG1	12:L:93:LEU:HG	2.41	0.51
1:A:134:A:N6	16:P:25:ARG:NH2	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:63:PHE:HB3	14:N:58:LYS:HA	1.93	0.51
1:A:1048:G:C6	1:A:1210:C:N4	2.79	0.51
1:A:352:C:C3'	1:A:352:C:C6	2.94	0.51
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.93	0.51
4:D:61:LYS:CD	4:D:61:LYS:C	2.79	0.51
1:A:1243:C:H5''	21:U:8:THR:HG23	1.91	0.51
1:A:1173:G:H2'	1:A:1174:G:C8	2.45	0.51
1:A:1088:G:C2'	1:A:1089:G:H5'	2.41	0.51
3:C:29:TYR:OH	14:N:54:PRO:O	2.29	0.51
1:A:1499:A:H5'	1:A:1519[A]:MA6:C2	2.42	0.50
1:A:981:U:H5'	14:N:21:TYR:CZ	2.45	0.50
10:J:47:PHE:CZ	14:N:37:PHE:CE1	2.88	0.50
19:S:47:HIS:O	19:S:62:ILE:HG22	2.10	0.50
1:A:475:G:O6	29:A:2600:HOH:O	2.20	0.50
1:A:297:G:N2	1:A:300:A:OP2	2.37	0.50
1:A:162:A:H3'	1:A:163:C:O4'	2.11	0.50
1:A:1081:G:P	5:E:16:THR:HG1	2.34	0.50
1:A:581:G:O3'	15:O:64:ARG:NH2	2.39	0.50
1:A:1172:C:O2'	1:A:1173:G:H5'	2.11	0.50
1:A:658:G:H2'	1:A:659:U:C6	2.46	0.50
1:A:797:C:O2'	1:A:798:G:H5'	2.10	0.50
4:D:92:VAL:O	4:D:93:PHE:C	2.47	0.50
1:A:928:G:C2	1:A:1390:U:O2	2.65	0.50
20:T:50:GLU:HA	20:T:99:LEU:CD1	2.39	0.50
17:Q:40:LYS:CD	17:Q:42:TYR:CZ	2.94	0.50
2:B:100:GLY:O	2:B:101:MET:C	2.49	0.50
1:A:1375:A:C5	1:A:1376:U:C5	2.99	0.50
1:A:1470:G:O2'	1:A:1471:G:H5'	2.11	0.50
9:I:95:LYS:HD2	9:I:95:LYS:H	1.76	0.50
1:A:973:G:H2'	1:A:974:A:OP1	2.11	0.50
1:A:1305:G:OP1	21:U:2:GLY:HA3	2.11	0.50
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.32	0.50
10:J:63:PHE:HA	14:N:59:ALA:H	1.76	0.50
1:A:976:G:C8	1:A:1358:U:C2	2.99	0.50
1:A:1110:A:N7	29:A:2140:HOH:O	2.35	0.50
1:A:1349:A:C2	1:A:1374:A:C4	3.00	0.50
21:U:13:ILE:HA	21:U:22:ARG:NH1	2.26	0.50
1:A:1052:U:C2'	1:A:1055:A:OP1	2.59	0.50
2:B:80:ILE:HD12	2:B:208:ILE:HD12	1.94	0.50
1:A:1493[B]:A:H2'	1:A:1494:G:C8	2.46	0.50
10:J:24:VAL:HG23	10:J:34:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:90:VAL:HG11	12:L:93:LEU:HD12	1.93	0.50
1:A:849:C:C2'	1:A:850:U:H5'	2.41	0.50
3:C:58:GLU:O	3:C:65:ALA:HB2	2.11	0.50
3:C:33:LEU:HD21	14:N:53:LEU:CD2	2.41	0.50
14:N:15:LYS:HG2	14:N:15:LYS:O	2.11	0.50
7:G:143:ARG:NH2	7:G:143:ARG:HB2	2.27	0.50
13:M:4:ILE:HG22	13:M:5:ALA:HB2	1.93	0.50
1:A:1179:A:H2'	1:A:1180:A:O4'	2.11	0.50
5:E:147:ASP:O	5:E:150:ARG:HB3	2.12	0.50
8:H:18:ARG:NH2	8:H:81:HIS:O	2.45	0.50
2:B:57:PHE:CG	2:B:199:TYR:CE1	2.99	0.50
12:L:55:VAL:CG1	12:L:67:THR:OG1	2.59	0.50
1:A:1517[A]:G:C6	1:A:1518[A]:MA6:C5	2.95	0.50
1:A:411:A:H3'	1:A:411:A:H8	1.77	0.50
18:R:37:VAL:O	18:R:38:GLU:C	2.49	0.50
1:A:1438:G:C6	1:A:1439:C:C4	2.99	0.50
5:E:10:MET:HA	5:E:32:VAL:HG23	1.93	0.50
9:I:48:GLU:HB3	9:I:101:PHE:HZ	1.74	0.50
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.94	0.50
12:L:39:VAL:HG12	12:L:40:VAL:N	2.27	0.50
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.12	0.50
9:I:19:LEU:HB3	9:I:59:PHE:CD2	2.47	0.50
10:J:78:ASN:CG	10:J:79:ARG:HH11	2.14	0.50
2:B:213:LEU:HB3	2:B:214:ILE:HD12	1.94	0.50
1:A:1515[A]:C:H42	1:A:1520[A]:G:H1	1.59	0.50
2:B:102:LEU:O	2:B:105:PHE:HB2	2.11	0.50
1:A:228:A:H2'	1:A:229:U:C6	2.46	0.50
1:A:1123:A:C2	10:J:39:PRO:HG3	2.47	0.50
1:A:193:C:O3'	20:T:61:SER:HB2	2.11	0.50
1:A:768:A:C5	1:A:769:G:C8	2.99	0.50
1:A:725:G:O2'	1:A:726:C:H5'	2.12	0.50
1:A:324:G:OP1	20:T:22:ARG:HD3	2.11	0.50
1:A:736:C:H2'	1:A:737:A:C8	2.47	0.50
1:A:738:C:OP1	6:F:92:LYS:HD3	2.11	0.50
1:A:83:U:C5	1:A:84:U:C6	3.00	0.50
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.94	0.50
3:C:39:ILE:HG21	3:C:57:ILE:HD11	1.94	0.50
15:O:88:ARG:NE	15:O:88:ARG:CA	2.57	0.50
2:B:211:ILE:O	2:B:215:LEU:HB2	2.11	0.50
23:W:35:G:C4	23:W:36:A:C8	2.99	0.50
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:A:OP2	29:A:2222:HOH:O	2.19	0.50
8:H:59:LEU:HD12	8:H:59:LEU:N	2.26	0.50
3:C:178:LEU:C	3:C:180:ALA:H	2.14	0.50
1:A:201:C:N4	1:A:216:G:H1	2.04	0.50
1:A:491:G:C4	1:A:492:G:C8	3.00	0.50
14:N:13:THR:N	14:N:14:PRO:CD	2.75	0.50
1:A:939:G:H2'	1:A:940:C:C6	2.46	0.50
1:A:802:A:C2'	1:A:803:G:H5'	2.42	0.50
1:A:1248:A:C2'	1:A:1249:C:H5'	2.42	0.50
1:A:690:G:H2'	1:A:691:G:O4'	2.12	0.50
1:A:1492[B]:A:H2'	1:A:1492[B]:A:N3	2.27	0.50
11:K:20:TYR:CD2	11:K:83:ILE:HB	2.47	0.50
5:E:77:PRO:O	5:E:78:HIS:HB3	2.11	0.50
1:A:740:U:H4'	15:O:42:HIS:HD2	1.77	0.50
1:A:834:C:O2'	1:A:835:U:H5'	2.12	0.50
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.46	0.50
13:M:63:THR:HG23	13:M:64:TRP:N	2.27	0.50
2:B:158:LEU:HB3	2:B:159:PRO:HD2	1.94	0.50
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.12	0.50
21:U:23:PRO:C	21:U:25:LYS:H	2.15	0.50
1:A:478:A:O2'	1:A:479:C:H5'	2.12	0.50
9:I:36:TYR:HE2	9:I:73:GLN:OE1	1.93	0.50
3:C:157:ILE:C	3:C:159:GLY:H	2.15	0.50
2:B:101:MET:C	2:B:102:LEU:HD12	2.31	0.50
1:A:264:U:H2'	1:A:265:G:C5'	2.42	0.50
17:Q:53:LEU:CD1	17:Q:54:GLY:N	2.74	0.50
13:M:4:ILE:O	13:M:6:GLY:O	2.30	0.50
20:T:56:MET:HE1	20:T:85:MET:HG3	1.92	0.50
7:G:48:LYS:O	7:G:52:GLU:OE2	2.30	0.50
1:A:1115:C:H6	1:A:1115:C:O5'	1.95	0.50
1:A:1352:C:H2'	1:A:1353:G:O4'	2.12	0.49
1:A:1368:G:OP2	9:I:114:TYR:N	2.45	0.49
1:A:1057:G:C5'	3:C:154:SER:OG	2.60	0.49
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.94	0.49
4:D:127:THR:HA	4:D:132:ARG:HA	1.94	0.49
4:D:180:GLY:O	4:D:182:LYS:CG	2.60	0.49
1:A:1434:A:H2'	1:A:1435:G:O4'	2.11	0.49
1:A:1072:G:H2'	1:A:1073:U:C6	2.46	0.49
1:A:1126:U:C2'	1:A:1127:G:O5'	2.59	0.49
1:A:1123:A:H2	10:J:39:PRO:HG3	1.77	0.49
1:A:664:G:H22	1:A:741:G:H1	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:O	15:O:42:HIS:HB3	2.12	0.49
7:G:101:LEU:O	7:G:105:VAL:HG23	2.11	0.49
1:A:172:A:O2'	1:A:173:U:H5'	2.12	0.49
2:B:195:ASP:O	8:H:68:ARG:NH2	2.45	0.49
1:A:586:C:C2'	1:A:587:G:H5'	2.41	0.49
11:K:12:ARG:O	11:K:12:ARG:HG2	2.10	0.49
1:A:540:G:C5	1:A:541:G:N7	2.80	0.49
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:N6	2.27	0.49
1:A:1031:G:C2	1:A:1032:G:C5	3.00	0.49
13:M:33:ALA:O	13:M:37:THR:HG22	2.12	0.49
1:A:866:C:H2'	1:A:867:G:O4'	2.13	0.49
1:A:130:A:H1'	1:A:263:A:HO2'	1.76	0.49
1:A:440:A:C5'	1:A:442:C:OP2	2.58	0.49
17:Q:58:GLU:C	17:Q:59:ILE:HD13	2.33	0.49
1:A:990:C:H42	1:A:1215:G:H1	1.61	0.49
23:W:30:G:N3	23:W:30:G:H2'	2.27	0.49
1:A:1090:U:C2	1:A:1091:U:C6	3.00	0.49
3:C:130:VAL:O	3:C:134:ILE:HD11	2.12	0.49
1:A:37:U:H2'	1:A:38:G:O4'	2.12	0.49
1:A:426:G:O2'	1:A:427:U:H5'	2.12	0.49
1:A:91:C:H2'	1:A:92:C:C5	2.47	0.49
4:D:19:LEU:CD2	4:D:19:LEU:H	2.21	0.49
4:D:64:LEU:HA	4:D:67:ILE:HD12	1.92	0.49
1:A:250:A:H1'	1:A:251:G:OP2	2.12	0.49
8:H:85:ARG:HD2	8:H:87:SER:O	2.12	0.49
1:A:676:A:H5''	11:K:113:PRO:HB3	1.93	0.49
1:A:357:G:O2'	1:A:358:U:H5'	2.12	0.49
11:K:43:SER:OG	11:K:44:SER:N	2.45	0.49
3:C:76:VAL:HG21	3:C:103:VAL:HG13	1.94	0.49
1:A:1326:C:OP2	21:U:6:ARG:HD3	2.12	0.49
12:L:82:VAL:HG23	12:L:106:ASP:OD1	2.13	0.49
15:O:36:ILE:HG22	15:O:37:ASN:N	2.26	0.49
7:G:72:ARG:NH1	7:G:142:GLU:OE2	2.46	0.49
1:A:922:G:O2'	1:A:1398:A:N1	2.37	0.49
1:A:106:C:H2'	1:A:107:G:H5'	1.93	0.49
1:A:1441:G:O2'	1:A:1442:G:N2	2.45	0.49
1:A:1026:G:C2'	1:A:1027:C:OP1	2.60	0.49
12:L:42:THR:HA	12:L:53:ARG:O	2.13	0.49
1:A:1300:G:C6	1:A:1335:C:C5	3.01	0.49
17:Q:6:LEU:HB3	17:Q:23:VAL:HG11	1.94	0.49
1:A:854:G:N1	1:A:855:G:C5	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:55:ILE:HD13	20:T:55:ILE:H	1.77	0.49
20:T:44:ALA:HB3	20:T:91:LEU:HD13	1.95	0.49
1:A:491:G:N3	1:A:492:G:C8	2.80	0.49
1:A:1425:U:C2	1:A:1426:C:C5	3.00	0.49
1:A:166:G:H2'	1:A:167:G:H5'	1.94	0.49
1:A:45:U:H2'	1:A:46:G:C8	2.47	0.49
1:A:19:C:O2'	1:A:20:U:H5'	2.12	0.49
16:P:40:ASP:HB3	16:P:48:TRP:CB	2.42	0.49
1:A:1305:G:P	21:U:2:GLY:HA3	2.52	0.49
1:A:1321:C:C5'	13:M:87:TYR:HE2	2.25	0.49
1:A:116:A:H3'	29:A:2018:HOH:O	2.12	0.49
20:T:10:LEU:HG	20:T:11:SER:N	2.27	0.49
1:A:1112:C:O2	3:C:179:ARG:HG3	2.12	0.49
17:Q:82:MET:O	17:Q:85:VAL:HG23	2.12	0.49
17:Q:62:SER:CB	17:Q:72:ARG:HD3	2.42	0.49
19:S:35:SER:OG	19:S:38:SER:HB2	2.13	0.49
1:A:811:C:O2'	1:A:901:A:N1	2.45	0.49
15:O:56:LEU:CD1	15:O:56:LEU:C	2.80	0.49
2:B:28:PHE:CD2	2:B:28:PHE:O	2.66	0.49
1:A:1193:G:N3	1:A:1194:U:C6	2.80	0.49
1:A:1197:G:C2'	1:A:1198:G:H5''	2.42	0.49
1:A:1501:C:C5	1:A:1504:G:C4	3.00	0.49
1:A:1532:U:C6	1:A:1533:C:H5	2.30	0.49
1:A:544:G:C2	1:A:545:C:C6	3.00	0.49
13:M:22:ILE:HG13	13:M:25:ILE:CD1	2.43	0.49
1:A:653:A:OP1	8:H:56:LYS:HE2	2.13	0.49
3:C:22:TRP:CG	3:C:59:ARG:HD2	2.48	0.49
3:C:92:ALA:O	3:C:95:THR:O	2.30	0.49
5:E:42:GLY:HA2	5:E:136:MET:CE	2.43	0.49
1:A:1166:G:C2	1:A:1171:G:C6	3.01	0.49
1:A:836:G:C6	1:A:851:G:C5	3.00	0.49
9:I:113:LYS:H	9:I:119:ALA:HA	1.77	0.49
1:A:1090:U:C2	1:A:1091:U:C5	3.00	0.49
4:D:43:HIS:ND1	4:D:46:LYS:HE2	2.28	0.49
1:A:1507:A:C5	1:A:1530:G:C2	3.00	0.49
1:A:89:C:O2'	1:A:90:U:C5'	2.61	0.49
5:E:10:MET:SD	5:E:13:ILE:HG13	2.53	0.49
4:D:194:LEU:HB3	4:D:196:LEU:HD21	1.94	0.49
1:A:741:G:H2'	1:A:742:G:O4'	2.13	0.49
1:A:741:G:H5''	15:O:39:LEU:HD12	1.95	0.49
8:H:86:ILE:HG21	8:H:133:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:LEU:N	3:C:47:LEU:HD12	2.26	0.49
17:Q:53:LEU:CD1	17:Q:85:VAL:HG11	2.43	0.49
1:A:47:C:C6	1:A:365:U:H2'	2.48	0.49
1:A:1067:A:H1'	1:A:1068:G:OP2	2.13	0.49
1:A:1057:G:C4	1:A:1204:A:H2	2.28	0.49
1:A:110:C:H2'	1:A:111:G:O4'	2.13	0.49
1:A:1047:G:C5	29:A:2425:HOH:O	2.63	0.49
16:P:2:VAL:O	16:P:64:ALA:HA	2.13	0.49
1:A:355:C:H5'	1:A:389:A:OP2	2.13	0.49
19:S:62:ILE:HA	19:S:66:MET:SD	2.52	0.49
1:A:137:C:H2'	1:A:138:G:H5'	1.94	0.49
1:A:630:G:H5'	1:A:631:G:OP2	2.13	0.49
20:T:10:LEU:HD23	20:T:13:LEU:HB3	1.95	0.49
1:A:443:C:C4	1:A:444:C:C5	3.01	0.49
1:A:490:G:C6	1:A:491:G:N7	2.81	0.49
1:A:949:A:C2	1:A:1233:G:C4	3.01	0.49
1:A:1233:G:N2	1:A:1234:C:C2	2.81	0.49
1:A:1361(A):C:C2'	1:A:1362:C:O5'	2.60	0.49
1:A:1419:G:C6	1:A:1420:C:N4	2.81	0.49
1:A:1082:G:H2'	1:A:1083:U:H5'	1.93	0.49
2:B:144:ARG:NH1	2:B:148:TYR:HE1	2.10	0.49
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.10	0.49
1:A:1128:C:H5'	9:I:16:ARG:NH2	2.28	0.49
7:G:123:GLU:O	7:G:126:ASP:N	2.46	0.49
1:A:278:G:OP2	17:Q:41:LYS:NZ	2.44	0.49
3:C:88:ARG:HB2	3:C:101:LEU:HD22	1.95	0.49
20:T:44:ALA:O	20:T:45:GLN:C	2.50	0.49
6:F:25:ILE:HD12	6:F:82:ARG:NH1	2.26	0.49
2:B:238:LEU:CD2	2:B:238:LEU:O	2.60	0.49
13:M:65:LYS:C	13:M:66:LEU:HD23	2.33	0.49
7:G:20:ASP:OD2	7:G:63:LYS:NZ	2.46	0.49
4:D:39:PRO:O	4:D:44:GLY:HA3	2.12	0.49
1:A:1352:C:H2'	1:A:1353:G:C8	2.48	0.49
1:A:1055:A:O2'	3:C:156:ARG:NH2	2.46	0.49
1:A:1202:G:H2'	1:A:1203:C:H5'	1.94	0.49
1:A:945:G:N3	1:A:945:G:H2'	2.28	0.49
5:E:32:VAL:HG12	5:E:58:ALA:HB1	1.93	0.49
4:D:187:ARG:HG2	4:D:188:LEU:N	2.27	0.49
20:T:13:LEU:C	20:T:13:LEU:CD1	2.80	0.49
13:M:11:ARG:HG3	13:M:12:ASN:H	1.74	0.49
15:O:70:LEU:HD23	15:O:78:TYR:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:A:H2'	1:A:350:G:H5'	1.95	0.49
1:A:507:C:OP2	1:A:508:C:O2'	2.25	0.49
5:E:95:ALA:O	5:E:98:THR:OG1	2.17	0.49
17:Q:65:ILE:CG2	17:Q:69:LYS:HE3	2.43	0.49
1:A:19:C:P	5:E:127:ASN:HD22	2.35	0.49
5:E:84:PHE:HB3	5:E:134:ALA:HB2	1.95	0.49
7:G:47:CYS:HA	7:G:50:ILE:HG12	1.95	0.48
1:A:77:G:O2'	1:A:78:G:H5'	2.13	0.48
1:A:79:G:N3	1:A:80:G:C8	2.81	0.48
1:A:1330:U:H2'	1:A:1331:G:H5'	1.93	0.48
2:B:220:ASP:O	2:B:223:ILE:HG13	2.13	0.48
1:A:1071:C:O2'	1:A:1072:G:H5'	2.12	0.48
17:Q:60:ILE:O	17:Q:60:ILE:HG23	2.12	0.48
1:A:954:G:N2	1:A:1227:A:H62	2.11	0.48
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.94	0.48
1:A:1357:A:H5''	1:A:1358:U:OP2	2.13	0.48
4:D:61:LYS:NZ	4:D:72:GLU:OE2	2.44	0.48
5:E:34:VAL:HG22	5:E:62:ALA:HB1	1.95	0.48
1:A:1385:G:H2'	1:A:1386:G:O4'	2.12	0.48
4:D:206:PHE:CE2	4:D:207:TYR:CE2	3.01	0.48
1:A:154:C:O2'	1:A:155:C:H5'	2.13	0.48
1:A:610:G:C2'	1:A:611:A:H5'	2.43	0.48
1:A:1248:A:C6	1:A:1249:C:C4	3.01	0.48
1:A:1350:A:OP1	9:I:121:ARG:HD2	2.12	0.48
1:A:1520[A]:G:H2'	1:A:1521:G:H8	1.78	0.48
8:H:97:VAL:HG23	8:H:129:VAL:C	2.33	0.48
1:A:570:G:C6	1:A:873:A:C2	3.01	0.48
15:O:4:THR:CG2	15:O:5:LYS:H	2.26	0.48
3:C:64:VAL:CG2	3:C:99:VAL:HB	2.43	0.48
1:A:1124:G:H2'	1:A:1145:C:C5	2.46	0.48
1:A:56:U:H2'	1:A:57:G:H8	1.78	0.48
2:B:16:HIS:HD2	2:B:17:PHE:N	2.11	0.48
14:N:11:LYS:HE3	14:N:13:THR:OG1	2.12	0.48
1:A:834:C:N4	29:A:2788:HOH:O	2.45	0.48
6:F:62:TRP:CE2	18:R:35:ARG:NH2	2.81	0.48
21:U:5:ASP:O	21:U:11:GLY:HA3	2.12	0.48
1:A:83:U:C5	1:A:84:U:C5	3.01	0.48
3:C:35:GLU:O	3:C:36:ASP:C	2.51	0.48
2:B:224:GLN:HG3	2:B:229:VAL:HG22	1.94	0.48
1:A:807:A:H2'	1:A:808:C:C6	2.49	0.48
2:B:168:THR:O	2:B:169:LYS:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:LYS:HE3	3:C:45:LYS:HA	1.95	0.48
9:I:36:TYR:HD2	9:I:37:PHE:CE1	2.31	0.48
1:A:429:U:H1'	1:A:430:A:H5''	1.95	0.48
14:N:23:ARG:HG2	14:N:29:ARG:O	2.13	0.48
7:G:43:PHE:O	7:G:46:ALA:HB3	2.13	0.48
1:A:994:A:H2'	1:A:994:A:N3	2.28	0.48
1:A:777:A:H2'	1:A:777:A:N3	2.28	0.48
8:H:82:HIS:HD1	8:H:138:TRP:HE1	1.57	0.48
3:C:82:GLU:HG3	3:C:83:ARG:N	2.28	0.48
1:A:254:G:C2	1:A:273:A:C2	3.01	0.48
5:E:142:LEU:O	5:E:143:ARG:HG2	2.13	0.48
12:L:75:HIS:CB	12:L:102:ARG:HH12	2.26	0.48
1:A:1347:G:H1'	1:A:1348:U:H5	1.78	0.48
1:A:1060:C:O2'	1:A:1061:G:H5'	2.13	0.48
2:B:212:GLN:O	2:B:213:LEU:C	2.51	0.48
1:A:1399:C:C2	1:A:1401:G:C4	3.02	0.48
1:A:923:A:C1'	1:A:1398:A:C2	2.96	0.48
17:Q:21:VAL:HG12	17:Q:22:LEU:N	2.28	0.48
16:P:8:ARG:CB	16:P:28:ARG:NH1	2.75	0.48
3:C:86:VAL:O	3:C:89:GLU:CB	2.57	0.48
3:C:50:ALA:HA	3:C:72:LYS:HG3	1.94	0.48
3:C:152:ILE:HD12	3:C:152:ILE:N	2.27	0.48
3:C:175:LEU:HD21	3:C:201:TYR:CE2	2.49	0.48
1:A:421:U:H4'	1:A:422:C:OP2	2.14	0.48
17:Q:48:GLU:OE1	17:Q:50:LYS:HG3	2.13	0.48
17:Q:9:VAL:O	17:Q:11:VAL:HG23	2.14	0.48
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.95	0.48
8:H:38:ILE:HD13	8:H:41:ARG:NH2	2.27	0.48
1:A:418:C:H2'	1:A:419:C:C6	2.48	0.48
20:T:43:LEU:N	20:T:43:LEU:HD23	2.27	0.48
20:T:18:GLN:O	20:T:19:SER:C	2.52	0.48
16:P:65:GLN:HA	16:P:65:GLN:OE1	2.13	0.48
1:A:1229:A:C2	1:A:1230:C:C4	3.02	0.48
1:A:1248:A:N6	1:A:1249:C:N4	2.62	0.48
1:A:1392:G:H21	1:A:1502:A:H8	1.61	0.48
1:A:1397:C:H4'	1:A:1398:A:OP2	2.14	0.48
1:A:39:G:C2'	1:A:39:G:N3	3.30	0.48
12:L:117:ARG:O	12:L:118:SER:C	2.52	0.48
1:A:426:G:OP1	4:D:38:TYR:OH	2.29	0.48
7:G:16:LEU:HD22	7:G:16:LEU:N	2.13	0.48
16:P:9:PHE:N	16:P:16:HIS:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:U:C2'	1:A:181:G:H5'	2.44	0.48
1:A:802:A:H2'	1:A:803:G:H5'	1.96	0.48
1:A:547:A:OP2	4:D:2:GLY:HA3	2.12	0.48
7:G:31:MET:HG3	7:G:32:ARG:N	2.28	0.48
15:O:31:LEU:N	15:O:31:LEU:HD13	2.28	0.48
2:B:212:GLN:HE22	2:B:235:SER:HB2	1.79	0.48
1:A:926:G:C6	1:A:1505:G:C6	3.01	0.48
18:R:86:VAL:O	18:R:87:ARG:NH2	2.46	0.48
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.96	0.48
1:A:1330:U:OP1	13:M:25:ILE:O	2.31	0.48
2:B:102:LEU:CD1	2:B:102:LEU:N	2.75	0.48
16:P:74:LEU:HB3	16:P:79:VAL:CG2	2.35	0.48
3:C:126:ARG:NE	3:C:128:PHE:HD1	2.11	0.48
4:D:172:PRO:HD2	4:D:173:TRP:HZ3	1.78	0.48
7:G:26:PHE:CD1	7:G:101:LEU:HD23	2.48	0.48
2:B:83:MET:SD	2:B:238:LEU:HD12	2.53	0.48
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.48	0.48
1:A:1238:A:H5'	1:A:1336:C:H41	1.78	0.48
10:J:76:ASN:C	10:J:78:ASN:N	2.59	0.48
10:J:28:ARG:HB3	10:J:29:ARG:NH1	2.25	0.48
27:A:1928:SRY:H12	27:A:1928:SRY:O53	2.13	0.48
1:A:228:A:H2'	1:A:229:U:H6	1.78	0.48
19:S:31:ILE:HG23	19:S:32:LYS:N	2.29	0.48
15:O:15:PHE:HZ	15:O:85:LEU:HD21	1.77	0.48
1:A:967:5MC:O2	1:A:967:5MC:H2'	2.13	0.48
2:B:122:PHE:HE2	2:B:139:LYS:HD2	1.78	0.48
20:T:56:MET:HE1	20:T:85:MET:CG	2.43	0.48
1:A:154:C:H6	1:A:154:C:O5'	1.97	0.48
1:A:1290:G:H2'	1:A:1291:G:C8	2.48	0.48
1:A:668:G:H1	1:A:738:C:H42	1.62	0.48
20:T:60:GLU:HA	20:T:63:ILE:HD12	1.96	0.48
1:A:1143:G:H2'	1:A:1144:G:C8	2.47	0.48
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.49	0.48
6:F:76:ALA:HA	6:F:79:LEU:HD12	1.95	0.48
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.95	0.48
1:A:1392:G:O2'	1:A:1393:U:H5'	2.14	0.48
1:A:109:A:C4	1:A:327:A:C2	3.01	0.48
1:A:945:G:O6	1:A:1236:A:N1	2.47	0.48
5:E:105:VAL:HB	5:E:106:PRO:CD	2.43	0.48
1:A:840:C:H3'	1:A:840:C:OP2	2.13	0.48
1:A:1228:C:OP1	13:M:115:LYS:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:40:ILE:HG22	19:S:67:VAL:HG13	1.96	0.48
4:D:98:GLU:CD	4:D:103:ASN:HD21	2.17	0.48
15:O:12:ILE:C	15:O:14:GLU:H	2.17	0.48
15:O:8:LYS:O	15:O:12:ILE:HG12	2.14	0.48
15:O:78:TYR:CE1	15:O:82:ILE:HD12	2.49	0.48
2:B:118:LEU:HB2	2:B:142:LEU:CD1	2.44	0.48
8:H:14:ARG:CZ	8:H:14:ARG:CB	2.91	0.48
13:M:81:LEU:HD11	13:M:88:ARG:HH22	1.77	0.48
7:G:116:ALA:O	7:G:119:ARG:N	2.47	0.48
1:A:333:G:O2'	1:A:334:C:H5'	2.13	0.48
9:I:127:LYS:HG3	9:I:127:LYS:O	2.14	0.48
12:L:57:LYS:HA	12:L:67:THR:HA	1.96	0.48
1:A:1133:G:N2	1:A:1141:C:C2	2.77	0.48
9:I:17:VAL:CG2	9:I:80:GLY:HA3	2.44	0.48
9:I:46:ALA:HB1	9:I:77:ILE:HG21	1.96	0.48
10:J:79:ARG:HD2	10:J:79:ARG:N	2.29	0.48
1:A:1391:U:H2'	1:A:1392:G:C8	2.48	0.48
13:M:99:ARG:NH2	19:S:2:PRO:CD	2.77	0.48
8:H:40:ALA:O	8:H:41:ARG:C	2.52	0.48
1:A:754:C:P	15:O:72:ARG:HH12	2.37	0.48
1:A:1371:G:C6	1:A:1372:U:C4	3.01	0.48
1:A:1054:C:N3	23:W:34:G:O4'	2.47	0.48
1:A:1441:G:H4'	1:A:1442:G:C2	2.48	0.48
1:A:1004:A:H5''	29:A:2327:HOH:O	2.13	0.48
1:A:961:U:O2'	1:A:962:C:H5'	2.13	0.48
4:D:187:ARG:HG3	4:D:188:LEU:HD12	1.94	0.48
1:A:1084:G:H5'	1:A:1102:A:OP2	2.14	0.48
1:A:782:A:P	29:A:2280:HOH:O	2.71	0.48
8:H:11:THR:O	8:H:12:ARG:C	2.53	0.48
5:E:97:GLY:N	5:E:117:ASP:OD1	2.47	0.48
7:G:111:ARG:CB	7:G:112:PRO:HD2	2.43	0.48
12:L:75:HIS:C	12:L:75:HIS:ND1	2.67	0.47
1:A:794:A:C8	1:A:794:A:H3'	2.48	0.47
1:A:1006:C:N3	1:A:1023:G:N2	2.56	0.47
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.96	0.47
17:Q:4:LYS:HG3	17:Q:6:LEU:CD2	2.44	0.47
6:F:7:ASN:OD1	6:F:7:ASN:N	2.47	0.47
15:O:70:LEU:HD22	15:O:78:TYR:CB	2.41	0.47
13:M:4:ILE:HG22	13:M:5:ALA:CB	2.44	0.47
2:B:162:ILE:HD13	2:B:177:ALA:HB2	1.95	0.47
8:H:19:VAL:CG2	8:H:21:LYS:HD3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:THR:HG23	2:B:95:GLN:O	2.14	0.47
6:F:39:LYS:HB2	6:F:39:LYS:HE3	1.66	0.47
1:A:1263:C:N4	1:A:1264:C:N4	2.62	0.47
15:O:18:PHE:HD1	15:O:19:PRO:O	1.97	0.47
1:A:1204:A:N7	1:A:1205:U:C5	2.82	0.47
1:A:500:G:N7	1:A:546:G:N2	2.60	0.47
1:A:924:C:C4'	1:A:1399:C:OP2	2.62	0.47
10:J:47:PHE:HB3	14:N:34:TYR:CE2	2.44	0.47
18:R:87:ARG:CG	18:R:87:ARG:NH2	2.53	0.47
1:A:277:C:C2'	1:A:278:G:H5'	2.44	0.47
1:A:1048:G:O6	1:A:1210:C:N4	2.47	0.47
1:A:390:C:O3'	16:P:28:ARG:NH2	2.47	0.47
8:H:27:PRO:CA	8:H:58:TYR:CD2	2.96	0.47
1:A:877:C:O2'	1:A:878:G:H5'	2.13	0.47
15:O:70:LEU:HD22	15:O:78:TYR:CA	2.44	0.47
1:A:1015:A:N6	1:A:1016:A:N6	2.61	0.47
13:M:35:GLU:HG2	13:M:36:LYS:N	2.29	0.47
5:E:38:GLN:OE1	5:E:38:GLN:HA	2.14	0.47
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.31	0.47
3:C:76:VAL:HG21	3:C:103:VAL:CG1	2.44	0.47
1:A:257:G:O5'	1:A:257:G:H8	1.97	0.47
14:N:36:PHE:CD1	14:N:36:PHE:C	2.87	0.47
5:E:5:ASP:CG	5:E:6:PHE:H	2.16	0.47
12:L:110:VAL:O	12:L:122:THR:HG21	2.13	0.47
1:A:373:A:H2'	1:A:374:A:H8	1.79	0.47
10:J:54:PHE:C	10:J:54:PHE:CD2	2.87	0.47
14:N:24:CYS:HB2	14:N:29:ARG:CB	2.43	0.47
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.97	0.47
8:H:137:VAL:O	8:H:138:TRP:HB3	2.14	0.47
1:A:1162:C:N3	1:A:1175:G:C2	2.83	0.47
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.48	0.47
2:B:121:LEU:HD23	2:B:121:LEU:C	2.35	0.47
13:M:20:THR:CG2	13:M:20:THR:O	2.62	0.47
9:I:66:ARG:HE	9:I:66:ARG:HB3	1.38	0.47
1:A:1202:G:C2'	1:A:1203:C:H5'	2.44	0.47
1:A:35:G:O2'	12:L:118:SER:O	2.20	0.47
10:J:25:GLU:HG2	10:J:28:ARG:CD	2.43	0.47
8:H:101:PRO:HA	8:H:102:ARG:HH11	1.78	0.47
1:A:60:A:H4'	1:A:61:G:O5'	2.14	0.47
1:A:1329:A:P	13:M:29:ARG:HG3	2.55	0.47
1:A:116:A:H61	1:A:313:A:H1'	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:66:LEU:O	18:R:66:LEU:HD12	2.13	0.47
16:P:8:ARG:C	16:P:9:PHE:HD2	2.17	0.47
19:S:40:ILE:HG23	19:S:62:ILE:CD1	2.44	0.47
3:C:112:SER:O	3:C:116:VAL:HG23	2.15	0.47
17:Q:29:HIS:ND1	17:Q:30:PRO:CD	2.76	0.47
17:Q:11:VAL:CG1	17:Q:88:TYR:CD2	2.94	0.47
5:E:69:VAL:CG1	5:E:71:LEU:HD23	2.44	0.47
1:A:609:A:N6	29:A:2320:HOH:O	2.39	0.47
3:C:52:LEU:HA	3:C:70:VAL:HA	1.97	0.47
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.41	0.47
1:A:1402:4OC:HM22	1:A:1402:4OC:O3'	2.15	0.47
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:C2	2.78	0.47
12:L:113:ARG:HH11	12:L:116:SER:H	1.62	0.47
7:G:50:ILE:HB	7:G:58:PRO:HB3	1.97	0.47
1:A:645:C:C2	1:A:646:U:C6	3.02	0.47
13:M:95:GLY:C	13:M:96:LEU:HD23	2.34	0.47
1:A:1381:U:C6	1:A:1382:C:C6	3.02	0.47
1:A:838:G:H3'	1:A:839:U:C5'	2.42	0.47
1:A:956:U:O2'	1:A:957:U:H5'	2.14	0.47
1:A:969:A:C2'	1:A:970:C:H5'	2.45	0.47
1:A:147:G:C2	1:A:148:G:C8	3.03	0.47
1:A:892:A:C2	1:A:907:A:C5	3.02	0.47
3:C:130:VAL:O	3:C:134:ILE:HG12	2.15	0.47
1:A:1520[A]:G:H2'	1:A:1521:G:C8	2.49	0.47
20:T:102:GLY:O	20:T:104:LEU:N	2.47	0.47
1:A:437:U:H5'	4:D:155:LEU:HD21	1.96	0.47
2:B:101:MET:HA	2:B:108:ILE:HD12	1.96	0.47
3:C:22:TRP:CD1	3:C:59:ARG:HD2	2.50	0.47
10:J:63:PHE:HA	14:N:59:ALA:HB3	1.95	0.47
3:C:173:VAL:N	3:C:174:PRO:HD3	2.29	0.47
20:T:41:ILE:CD1	20:T:41:ILE:H	2.27	0.47
17:Q:47:PRO:HD2	17:Q:48:GLU:H	1.79	0.47
13:M:99:ARG:C	13:M:101:GLN:HE22	2.17	0.47
1:A:70:G:C2	1:A:99:C:O2	2.67	0.47
1:A:506:G:C6	1:A:507:C:C4	3.02	0.47
7:G:78:ARG:HD2	7:G:156:TRP:HB3	1.95	0.47
16:P:40:ASP:OD1	16:P:44:THR:OG1	2.31	0.47
1:A:836:G:C6	1:A:851:G:C6	3.03	0.47
1:A:1148:U:C5	1:A:1149:C:C4	3.03	0.47
1:A:1286:A:H3'	1:A:1287:A:H5''	1.96	0.47
1:A:1351:U:O2'	1:A:1352:C:H5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:45:ARG:HH11	14:N:45:ARG:CG	2.28	0.47
1:A:1060:C:C2	1:A:1198:G:C2	3.03	0.47
10:J:21:GLN:O	10:J:24:VAL:HG12	2.15	0.47
10:J:85:LEU:O	10:J:86:MET:HB3	2.15	0.47
1:A:78:G:C6	1:A:79:G:N7	2.83	0.47
1:A:77:G:C6	1:A:93:G:N1	2.83	0.47
1:A:1027:C:O2	1:A:1027:C:H5''	2.13	0.47
18:R:36:ASN:CG	18:R:39:VAL:HG11	2.35	0.47
4:D:177:ASP:OD1	4:D:179:GLU:N	2.47	0.47
13:M:27:LYS:HD2	13:M:28:ALA:N	2.30	0.47
13:M:54:VAL:HG13	13:M:55:ARG:N	2.30	0.47
13:M:90:LEU:HD23	13:M:90:LEU:HA	1.81	0.47
1:A:1435:G:C4	1:A:1436:U:C5	3.03	0.47
16:P:8:ARG:O	16:P:9:PHE:CD2	2.68	0.47
1:A:284:G:N3	1:A:285:G:C8	2.82	0.47
19:S:41:VAL:O	19:S:42:PRO:C	2.52	0.47
4:D:12:CYS:HA	4:D:19:LEU:CD2	2.44	0.47
15:O:46:HIS:C	15:O:48:LYS:H	2.17	0.47
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.30	0.47
1:A:976:G:H5'	1:A:1358:U:O2'	2.15	0.47
1:A:232:G:H1'	1:A:262:A:N1	2.29	0.47
20:T:54:LYS:HG2	20:T:55:ILE:N	2.28	0.47
9:I:48:GLU:N	9:I:49:PRO:CD	2.78	0.47
1:A:514:C:H2'	1:A:515:G:C8	2.48	0.47
1:A:1503:A:C5	1:A:1531:A:C2	3.02	0.47
17:Q:66:SER:OG	17:Q:69:LYS:HG3	2.14	0.47
1:A:1092:A:H8	1:A:1092:A:O5'	1.98	0.47
9:I:95:LYS:HD2	9:I:95:LYS:N	2.29	0.47
1:A:19:C:H2'	1:A:20:U:H6	1.80	0.47
1:A:811:C:H4'	1:A:900:A:N6	2.30	0.47
3:C:117:ALA:HB2	3:C:200:ALA:HB2	1.96	0.47
3:C:26:LYS:NZ	3:C:26:LYS:HB2	2.29	0.47
4:D:31:CYS:O	4:D:32:ALA:HB3	2.14	0.47
1:A:644:G:C6	1:A:645:C:C5	3.01	0.47
15:O:17:ARG:HA	15:O:17:ARG:HD2	1.78	0.47
1:A:1035:A:C6	1:A:1036:G:C6	3.02	0.47
13:M:39:ILE:N	13:M:39:ILE:HD12	2.30	0.47
1:A:868:C:H2'	1:A:869:G:H5'	1.97	0.47
1:A:1073:U:O2	2:B:104:ASN:ND2	2.45	0.47
1:A:1228:C:H4'	13:M:116:THR:HA	1.96	0.47
4:D:188:LEU:H	4:D:188:LEU:CD1	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:75:ASN:O	20:T:76:ALA:C	2.53	0.47
1:A:1405:G:H2'	1:A:1406:U:H5'	1.95	0.47
7:G:103:TRP:NE1	7:G:137:LYS:HE2	2.30	0.47
7:G:153:HIS:CE1	7:G:154:TYR:CE2	3.03	0.47
11:K:57:THR:HG22	11:K:58:PRO:HD2	1.95	0.47
1:A:1163:C:C6	1:A:1163:C:H3'	2.49	0.47
1:A:1131:G:H2'	1:A:1132:C:C6	2.50	0.47
1:A:1288:A:H2'	1:A:1289:A:C8	2.50	0.47
1:A:1061:G:C2	1:A:1062:U:O2	2.67	0.47
1:A:1533:C:HO2'	1:A:1534:C:P	2.30	0.47
7:G:123:GLU:O	7:G:124:LEU:C	2.53	0.47
12:L:19:ARG:HH12	12:L:21:LYS:HB3	1.79	0.47
18:R:45:SER:HB3	18:R:47:THR:O	2.15	0.47
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.95	0.47
15:O:11:VAL:O	15:O:14:GLU:HB3	2.15	0.47
1:A:262:A:C6	1:A:263:A:C6	3.03	0.47
3:C:175:LEU:HD12	3:C:175:LEU:H	1.80	0.47
1:A:826:C:C2	1:A:827:U:C5	3.02	0.47
1:A:802:A:O2'	29:A:2374:HOH:O	2.20	0.47
1:A:129(A):G:N3	1:A:190(E):U:H5''	2.29	0.47
1:A:875:C:H1'	8:H:15:ASN:HD21	1.80	0.47
1:A:1360:A:HO2'	1:A:1361:G:P	2.38	0.47
1:A:1360:A:O2'	1:A:1361:G:H5'	2.15	0.47
1:A:1286:A:C8	1:A:1286:A:H3'	2.50	0.47
1:A:1206:G:O6	1:A:1207:2MG:C6	2.68	0.47
1:A:1054:C:N3	23:W:34:G:OP1	2.48	0.47
7:G:47:CYS:HA	7:G:50:ILE:CG1	2.45	0.47
10:J:86:MET:CG	10:J:87:THR:H	2.09	0.47
8:H:100:ILE:HG12	8:H:100:ILE:H	1.52	0.47
1:A:913:A:O3'	27:A:1928:SRY:HI33	2.10	0.47
9:I:8:GLY:HA2	9:I:79:LEU:CD1	2.38	0.47
3:C:121:ALA:HB1	3:C:189:ALA:HB2	1.95	0.47
1:A:1182:G:H4'	1:A:1183:A:O5'	2.14	0.47
17:Q:17:LYS:HG2	17:Q:47:PRO:HA	1.97	0.47
4:D:145:GLU:O	4:D:145:GLU:HG3	2.13	0.47
7:G:69:VAL:HG22	7:G:135:VAL:HG22	1.96	0.47
1:A:248:C:H2'	1:A:249:U:H5'	1.95	0.47
10:J:99:LYS:HD2	10:J:99:LYS:N	2.30	0.47
1:A:401:C:H1'	1:A:622:A:H1'	1.97	0.47
9:I:64:THR:HG23	9:I:66:ARG:NH2	2.30	0.46
21:U:10:ARG:NH1	21:U:10:ARG:HG3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:14:LEU:HD13	6:F:18:GLN:CB	2.24	0.46
2:B:208:ILE:HD13	2:B:211:ILE:HD12	1.96	0.46
1:A:925:G:H1'	1:A:1502:A:N9	2.30	0.46
1:A:77:G:N2	1:A:92:C:O2	2.48	0.46
1:A:385:C:H2'	1:A:386:C:H6	1.81	0.46
13:M:17:VAL:HG12	13:M:18:ALA:N	2.30	0.46
2:B:97:TRP:HH2	2:B:176:GLU:OE2	1.98	0.46
11:K:120:ARG:CZ	11:K:126:ARG:HE	2.28	0.46
1:A:353:A:C8	1:A:353:A:C5'	2.96	0.46
1:A:819:A:H4'	1:A:820:U:OP2	2.15	0.46
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.52	0.46
4:D:107:ARG:HH11	4:D:114:ARG:NH2	2.13	0.46
1:A:1181:G:C2	1:A:1182:G:N2	2.83	0.46
15:O:70:LEU:HD23	15:O:70:LEU:O	2.14	0.46
1:A:22:G:C6	1:A:23:C:N4	2.83	0.46
15:O:55:GLY:O	15:O:59:MET:HG3	2.16	0.46
15:O:56:LEU:HD12	15:O:56:LEU:C	2.35	0.46
1:A:339:C:H2'	1:A:340:U:C6	2.51	0.46
3:C:157:ILE:CD1	3:C:166:GLU:HG2	2.45	0.46
10:J:4:ILE:HG23	10:J:74:ILE:O	2.15	0.46
12:L:90:VAL:O	12:L:91:LYS:C	2.53	0.46
7:G:126:ASP:OD2	7:G:131:LYS:HE3	2.15	0.46
1:A:983:A:H5'	1:A:984:C:OP2	2.16	0.46
1:A:983:A:OP1	14:N:3:ARG:NH2	2.41	0.46
1:A:1258:G:O2'	1:A:1259:C:H5'	2.15	0.46
1:A:264:U:O2'	17:Q:63:ARG:HD3	2.15	0.46
1:A:822:C:H2'	1:A:823:G:H5'	1.97	0.46
16:P:48:TRP:CD1	16:P:48:TRP:N	2.81	0.46
2:B:132:LYS:O	2:B:136:VAL:HG23	2.15	0.46
3:C:15:THR:HB	3:C:181:ASN:HA	1.97	0.46
1:A:743:U:H2'	1:A:744:C:H6	1.81	0.46
12:L:54:LYS:HB2	12:L:70:ILE:HB	1.97	0.46
1:A:1367:C:N3	1:A:1368:G:C8	2.84	0.46
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.97	0.46
1:A:1054:C:C3'	1:A:1054:C:C2	2.98	0.46
1:A:1064:G:H1'	1:A:1190:G:H21	1.81	0.46
6:F:15:ASP:OD2	6:F:18:GLN:HB2	2.15	0.46
10:J:28:ARG:CB	10:J:29:ARG:HH11	2.25	0.46
1:A:570:G:H2'	1:A:571:U:C6	2.50	0.46
1:A:918:A:OP2	29:A:2624:HOH:O	2.21	0.46
12:L:90:VAL:HG11	12:L:93:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:20:TYR:O	11:K:30:VAL:HA	2.16	0.46
1:A:653:A:OP1	8:H:56:LYS:NZ	2.45	0.46
3:C:64:VAL:HG23	3:C:99:VAL:HB	1.95	0.46
1:A:116:A:H5''	29:A:2018:HOH:O	2.15	0.46
1:A:853:G:C2	1:A:854:G:C8	3.02	0.46
8:H:4:ASP:HB3	8:H:7:ALA:CB	2.45	0.46
1:A:162:A:H1'	1:A:348:G:O2'	2.16	0.46
1:A:1290:G:H2'	1:A:1291:G:H8	1.81	0.46
1:A:44:G:C2	1:A:399:G:C4	3.04	0.46
1:A:669:U:H2'	1:A:670:G:C8	2.51	0.46
1:A:419:C:O2'	1:A:420:U:H5'	2.16	0.46
3:C:20:SER:HB3	3:C:57:ILE:HB	1.97	0.46
1:A:861:G:H8	1:A:861:G:O5'	1.98	0.46
1:A:81:U:C6	1:A:81:U:H3'	2.49	0.46
1:A:1519[B]:MA6:C9	1:A:1520[B]:G:H21	2.29	0.46
1:A:1519[A]:MA6:H3'	1:A:1520[A]:G:H5'	1.98	0.46
1:A:544:G:H2'	1:A:545:C:O5'	2.14	0.46
4:D:8:VAL:C	4:D:10:ARG:N	2.69	0.46
13:M:25:ILE:HG23	13:M:29:ARG:HB2	1.97	0.46
1:A:553:A:O2'	12:L:29:GLY:O	2.31	0.46
1:A:285:G:C2	1:A:286:G:C8	3.03	0.46
1:A:391:G:C6	1:A:392:G:C5	3.04	0.46
1:A:575:G:C8	1:A:881:G:N2	2.83	0.46
3:C:119:ARG:NH1	3:C:119:ARG:CG	2.76	0.46
14:N:9:LYS:C	14:N:9:LYS:HD2	2.36	0.46
8:H:96:GLY:H	8:H:99:GLU:CD	2.18	0.46
1:A:382:A:H2'	1:A:383:A:C8	2.50	0.46
1:A:547:A:OP2	4:D:2:GLY:HA2	2.15	0.46
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.62	0.46
1:A:433:C:H2'	1:A:434:U:C6	2.50	0.46
12:L:30:ALA:CB	12:L:31:PRO:HD2	2.43	0.46
1:A:11:G:H2'	1:A:12:U:O4'	2.15	0.46
9:I:126:SER:C	9:I:128:ARG:H	2.18	0.46
16:P:19:ILE:HG22	16:P:36:ILE:CG1	2.45	0.46
2:B:121:LEU:HD23	2:B:121:LEU:O	2.15	0.46
1:A:1148:U:C5	1:A:1149:C:C5	3.03	0.46
1:A:1393:U:C3'	1:A:1393:U:C6	2.99	0.46
1:A:92:C:H2'	1:A:93:G:H8	1.81	0.46
13:M:2:ALA:O	13:M:10:PRO:HD2	2.15	0.46
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.81	0.46
7:G:74:GLU:HA	7:G:141:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:G:O6	29:A:2233:HOH:O	2.17	0.46
1:A:1109:C:OP2	3:C:176:HIS:ND1	2.48	0.46
2:B:16:HIS:NE2	2:B:17:PHE:HD2	2.12	0.46
1:A:491:G:C2	1:A:492:G:C4	3.04	0.46
1:A:1233:G:H2'	1:A:1234:C:C6	2.51	0.46
1:A:966:M2G:N7	1:A:967:5MC:HM52	2.30	0.46
2:B:107:THR:HG23	2:B:110:GLN:OE1	2.16	0.46
8:H:105:ARG:HD3	8:H:105:ARG:HA	1.73	0.46
10:J:12:ASP:O	10:J:12:ASP:OD2	2.33	0.46
1:A:1300:G:O2'	1:A:1301:U:OP2	2.34	0.46
8:H:54:ASP:CG	8:H:55:GLY:N	2.61	0.46
2:B:97:TRP:HZ2	2:B:102:LEU:CD1	2.18	0.46
7:G:150:ALA:HA	11:K:59:TYR:CD2	2.51	0.46
10:J:9:ARG:HB3	10:J:9:ARG:NH1	2.31	0.46
2:B:185:ILE:N	2:B:185:ILE:HD12	2.29	0.46
1:A:610:G:H5'	29:A:2771:HOH:O	2.14	0.46
4:D:122:ARG:HA	4:D:134:ASP:O	2.15	0.46
1:A:652:U:O4	1:A:752:G:O2'	2.29	0.46
3:C:142:MET:O	3:C:142:MET:HE3	2.16	0.46
1:A:1148:U:C6	1:A:1149:C:C6	3.04	0.46
1:A:1370:G:C2	1:A:1371:G:C8	3.04	0.46
1:A:643:C:C2'	1:A:644:G:C5'	2.87	0.46
1:A:89:C:C6	1:A:90:U:C2	3.03	0.46
18:R:39:VAL:CG1	18:R:40:LEU:N	2.79	0.46
1:A:1314:C:OP2	19:S:6:LYS:HG2	2.15	0.46
1:A:961:U:H2'	1:A:962:C:C5'	2.45	0.46
7:G:64:GLN:HA	7:G:64:GLN:OE1	2.15	0.46
1:A:1407:5MC:H2'	1:A:1408:A:C5'	2.43	0.46
1:A:666:G:H5'	1:A:726:C:H1'	1.98	0.46
11:K:11:LYS:N	11:K:75:TYR:CE2	2.82	0.46
13:M:59:TYR:CE2	13:M:63:THR:HG21	2.50	0.46
1:A:668:G:C2'	1:A:669:U:H5'	2.46	0.46
7:G:111:ARG:HD3	7:G:113:GLU:CG	2.45	0.46
1:A:164:U:H2'	1:A:165:C:H6	1.81	0.46
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.97	0.46
1:A:538:G:C2	1:A:539:A:C4	3.04	0.46
1:A:1502:A:C2	1:A:1504:G:C2	3.04	0.46
1:A:1519[B]:MA6:C9	1:A:1520[B]:G:N2	2.79	0.46
1:A:499:A:C4'	1:A:500:G:OP1	2.49	0.46
1:A:923:A:H1'	1:A:1398:A:N3	2.30	0.46
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.51	0.46
4:D:107:ARG:NH1	4:D:114:ARG:NH2	2.64	0.46
1:A:460:A:C6	1:A:462:G:C6	3.04	0.46
1:A:344:A:C5'	1:A:345:C:H5	2.27	0.46
6:F:45:LEU:HB3	6:F:59:TYR:HD1	1.81	0.46
5:E:84:PHE:CE1	5:E:133:TYR:HB3	2.50	0.46
5:E:84:PHE:CB	5:E:134:ALA:HB2	2.46	0.46
2:B:115:LEU:HD21	2:B:153:ARG:NH1	2.31	0.46
1:A:1413:A:H2'	1:A:1414:U:O4'	2.15	0.46
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.98	0.46
1:A:923:A:C2'	1:A:924:C:H5'	2.45	0.46
1:A:411:A:C8	1:A:411:A:H3'	2.51	0.46
4:D:127:THR:HG22	4:D:149:ALA:HB2	1.97	0.46
1:A:630:G:C5'	1:A:631:G:OP2	2.64	0.46
1:A:1511:G:H2'	1:A:1512:U:O4'	2.16	0.46
1:A:1015:A:C5	1:A:1016:A:C5	3.04	0.46
1:A:920:U:H2'	1:A:921:U:C6	2.51	0.46
19:S:51:VAL:O	19:S:51:VAL:CG2	2.64	0.46
9:I:103:THR:HG22	9:I:104:ARG:O	2.15	0.46
5:E:45:PHE:CE2	5:E:47:LYS:HE3	2.51	0.46
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.51	0.46
1:A:66:G:C2	1:A:67:C:C6	3.03	0.46
10:J:46:ARG:HH11	10:J:46:ARG:HG3	1.80	0.46
9:I:17:VAL:CG1	9:I:63:ILE:HD11	2.40	0.46
9:I:77:ILE:O	9:I:78:LYS:C	2.54	0.46
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.98	0.46
1:A:510:A:P	29:A:2165:HOH:O	2.74	0.46
1:A:511:C:O2'	1:A:534:U:H1'	2.16	0.46
18:R:36:ASN:OD1	18:R:39:VAL:CG1	2.64	0.46
12:L:27:LEU:CG	12:L:28:LYS:N	2.75	0.46
1:A:978:A:O2'	1:A:1322:C:O2	2.27	0.46
3:C:113:ALA:O	3:C:116:VAL:N	2.50	0.46
3:C:178:LEU:HA	3:C:178:LEU:HD13	1.78	0.46
4:D:52:SER:O	4:D:55:ALA:HB3	2.16	0.46
1:A:1454:G:C5	29:A:2825:HOH:O	2.65	0.46
1:A:803:G:C6	1:A:804:U:C4	3.04	0.46
1:A:407:G:C5'	4:D:3:ARG:HH12	2.29	0.46
11:K:116:HIS:N	11:K:116:HIS:ND1	2.62	0.46
1:A:166:G:O2'	1:A:167:G:H5'	2.15	0.46
3:C:39:ILE:HG22	3:C:40:ARG:N	2.31	0.46
13:M:65:LYS:HE3	13:M:65:LYS:HB2	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:C:N4	29:A:2573:HOH:O	2.49	0.46
1:A:342:C:H2'	1:A:343:U:H5'	1.98	0.46
9:I:15:ALA:HA	9:I:65:VAL:HG13	1.98	0.45
20:T:57:ARG:HD3	20:T:102:GLY:CA	2.45	0.45
1:A:642:A:C4	8:H:114:THR:O	2.70	0.45
1:A:76:C:H2'	1:A:77:G:H8	1.82	0.45
1:A:1032:G:H2'	1:A:1033:G:H8	1.82	0.45
1:A:1304:G:C6	1:A:1305:G:N1	2.83	0.45
13:M:40:ASN:HD22	13:M:43:THR:HG23	1.81	0.45
12:L:44:THR:HA	12:L:45:PRO:HD3	1.76	0.45
1:A:1125:U:C3'	1:A:1126:U:H5	2.28	0.45
4:D:172:PRO:HG2	4:D:173:TRP:CE3	2.51	0.45
4:D:196:LEU:CD2	4:D:196:LEU:H	2.29	0.45
4:D:120:LEU:HD23	4:D:125:HIS:HB2	1.98	0.45
1:A:182:U:P	29:A:2183:HOH:O	2.73	0.45
8:H:9:MET:O	8:H:10:LEU:C	2.54	0.45
3:C:5:ILE:HD11	3:C:10:PHE:CD2	2.51	0.45
1:A:515:G:C6	1:A:516:PSU:C2	3.04	0.45
16:P:34:GLU:OE2	16:P:55:ARG:HD2	2.15	0.45
1:A:1379:G:C6	1:A:1380:U:C5	3.04	0.45
1:A:1368:G:H2'	1:A:1369:C:C5'	2.46	0.45
1:A:1068:G:O4'	1:A:1068:G:OP2	2.33	0.45
1:A:1190:G:HO2'	1:A:1191:A:P	2.39	0.45
1:A:792:A:C4'	1:A:793:U:OP1	2.48	0.45
4:D:31:CYS:C	4:D:33:MET:H	2.19	0.45
1:A:109:A:C3'	1:A:110:C:H5'	2.46	0.45
1:A:642:A:H2'	1:A:643:C:H6	1.76	0.45
1:A:89:C:C5	1:A:90:U:C2	3.03	0.45
1:A:386:C:H2'	1:A:387:U:H5'	1.97	0.45
4:D:155:LEU:HD22	4:D:156:GLU:H	1.80	0.45
1:A:1315:U:H2'	1:A:1316:G:O4'	2.16	0.45
12:L:46:LYS:C	12:L:48:PRO:HD2	2.36	0.45
15:O:5:LYS:HA	15:O:5:LYS:HZ3	1.72	0.45
15:O:46:HIS:C	15:O:48:LYS:N	2.70	0.45
1:A:1151:A:O2'	1:A:1152:A:H8	1.99	0.45
8:H:4:ASP:CG	8:H:7:ALA:H	2.20	0.45
4:D:159:ARG:CG	4:D:159:ARG:NH1	2.77	0.45
1:A:179:A:C2'	1:A:180:U:H5'	2.46	0.45
1:A:1425:U:H3	1:A:1475:G:H1	1.64	0.45
1:A:1290:G:C6	1:A:1291:G:C6	3.04	0.45
1:A:1178:G:N2	1:A:1180:A:H3'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:A:C2	1:A:482:A:C6	3.04	0.45
1:A:1502:A:H2'	1:A:1504:G:C8	2.51	0.45
10:J:47:PHE:HD2	14:N:34:TYR:CE2	2.34	0.45
1:A:437:U:C5'	4:D:155:LEU:HD21	2.46	0.45
15:O:4:THR:CG2	15:O:5:LYS:N	2.76	0.45
1:A:575:G:H4'	1:A:576:G:OP1	2.16	0.45
4:D:188:LEU:H	4:D:188:LEU:HD12	1.81	0.45
1:A:631:G:H2'	1:A:632:A:C8	2.51	0.45
1:A:853:G:O2'	1:A:854:G:H5'	2.17	0.45
12:L:11:VAL:HG12	12:L:12:ARG:N	2.31	0.45
4:D:61:LYS:CD	4:D:62:GLN:N	2.75	0.45
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.98	0.45
15:O:78:TYR:CZ	15:O:82:ILE:HD12	2.51	0.45
7:G:148:ASN:C	7:G:150:ALA:N	2.66	0.45
17:Q:59:ILE:HA	17:Q:59:ILE:HD12	1.59	0.45
8:H:20:TYR:HE1	8:H:76:PRO:HG2	1.81	0.45
2:B:200:ILE:HG23	2:B:201:ILE:N	2.29	0.45
11:K:58:PRO:O	11:K:61:ALA:HB3	2.16	0.45
15:O:61:GLY:O	15:O:65:ARG:HD2	2.17	0.45
1:A:1503:A:C4	1:A:1531:A:N3	2.85	0.45
17:Q:18:THR:HG23	17:Q:69:LYS:HD3	1.99	0.45
1:A:566:G:H4'	1:A:567:G:OP1	2.16	0.45
13:M:66:LEU:O	13:M:69:GLU:HG2	2.16	0.45
18:R:53:ARG:HG3	18:R:63:GLN:NE2	2.31	0.45
3:C:27:LYS:HA	3:C:30:ARG:HH12	1.81	0.45
9:I:37:PHE:HB3	9:I:43:ALA:HB2	1.99	0.45
1:A:1400:5MC:O5'	1:A:1400:5MC:H6	2.00	0.45
1:A:1518[A]:MA6:H2'	1:A:1519[A]:MA6:H8	1.98	0.45
1:A:1519[A]:MA6:C3'	1:A:1520[A]:G:H5'	2.47	0.45
1:A:411:A:N3	1:A:413:G:H1'	2.32	0.45
4:D:38:TYR:N	4:D:38:TYR:CD2	2.84	0.45
14:N:27:CYS:SG	14:N:29:ARG:CB	2.86	0.45
4:D:149:ALA:O	4:D:152:SER:HB2	2.15	0.45
13:M:74:VAL:HG23	13:M:75:ALA:N	2.31	0.45
1:A:1319:A:H4'	1:A:1320:C:OP1	2.16	0.45
16:P:67:THR:HB	16:P:70:ALA:H	1.80	0.45
19:S:10:PHE:CD2	19:S:10:PHE:C	2.89	0.45
5:E:144:THR:HB	5:E:146:ALA:HB3	1.98	0.45
1:A:626:U:H2'	1:A:627:G:C8	2.51	0.45
1:A:1084:G:N2	29:A:2128:HOH:O	2.50	0.45
3:C:199:LYS:HB3	3:C:201:TYR:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:81:ARG:CG	17:Q:81:ARG:O	2.65	0.45
1:A:557:G:H5'	1:A:558:G:OP2	2.16	0.45
1:A:101:A:N3	1:A:102:G:C8	2.85	0.45
12:L:7:ILE:O	12:L:8:ASN:C	2.55	0.45
1:A:933:G:OP1	7:G:4:ARG:HG3	2.17	0.45
1:A:1415:G:C6	1:A:1486:G:C6	3.04	0.45
2:B:77:ALA:O	2:B:81:VAL:HG23	2.16	0.45
1:A:1286:A:H3'	1:A:1286:A:H8	1.81	0.45
1:A:1288:A:C6	1:A:1289:A:C6	3.04	0.45
15:O:17:ARG:HD3	15:O:26:GLU:OE2	2.16	0.45
1:A:77:G:C2	1:A:93:G:C2	3.05	0.45
1:A:1003(A):G:N1	1:A:1004:A:H1'	2.32	0.45
1:A:1005:A:C8	1:A:1026:G:O6	2.70	0.45
4:D:177:ASP:OD1	4:D:177:ASP:C	2.54	0.45
13:M:91:ARG:HH21	13:M:96:LEU:CB	2.30	0.45
2:B:223:ILE:HD13	2:B:230:VAL:HG23	1.99	0.45
6:F:97:PHE:HD2	6:F:98:LEU:N	2.14	0.45
18:R:56:THR:HB	18:R:58:LEU:HD23	1.97	0.45
4:D:70:ILE:CG2	4:D:71:SER:O	2.59	0.45
9:I:32:ASP:CG	9:I:33:PHE:N	2.69	0.45
20:T:73:HIS:HB3	20:T:74:LYS:HG2	1.99	0.45
1:A:1112:C:C2	3:C:178:LEU:HB2	2.51	0.45
4:D:119:GLN:HG3	4:D:123:HIS:CE1	2.51	0.45
1:A:1233:G:C2	1:A:1234:C:C4	3.05	0.45
14:N:12:ARG:NH1	14:N:12:ARG:H	2.13	0.45
14:N:14:PRO:O	14:N:15:LYS:CB	2.64	0.45
7:G:148:ASN:O	7:G:149:ARG:C	2.55	0.45
7:G:150:ALA:HA	11:K:59:TYR:HD2	1.82	0.45
20:T:31:SER:O	20:T:32:ALA:C	2.55	0.45
11:K:116:HIS:C	11:K:117:ASN:OD1	2.54	0.45
13:M:77:ASN:O	13:M:80:ARG:HB3	2.16	0.45
1:A:590:C:O2'	1:A:591:U:H5'	2.16	0.45
1:A:1250:A:C6	1:A:1251:A:N1	2.84	0.45
14:N:41:ARG:HG3	14:N:42:ILE:N	2.32	0.45
1:A:1494:G:C2	1:A:1495:U:C5	3.05	0.45
1:A:1393:U:H3'	1:A:1393:U:C6	2.52	0.45
14:N:27:CYS:HB3	14:N:43:CYS:SG	2.57	0.45
1:A:646:U:H2'	1:A:647:C:C6	2.51	0.45
1:A:90:U:O2'	1:A:91:C:O5'	2.33	0.45
1:A:1003(A):G:C6	1:A:1004:A:H1'	2.51	0.45
18:R:25:THR:OG1	18:R:26:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:112:LEU:C	5:E:114:GLY:N	2.70	0.45
1:A:769:G:H2'	1:A:770:C:H5'	1.98	0.45
1:A:770:C:C2'	1:A:771:G:H5'	2.47	0.45
17:Q:47:PRO:CD	17:Q:48:GLU:H	2.30	0.45
1:A:147:G:O2'	1:A:148:G:H5'	2.17	0.45
1:A:434:U:H2'	1:A:434:U:O2	2.14	0.45
4:D:92:VAL:O	4:D:95:GLY:N	2.49	0.45
4:D:102:ASP:OD1	4:D:102:ASP:N	2.48	0.45
1:A:1514:C:N4	1:A:1515[B]:C:H41	2.15	0.45
2:B:231:GLU:CB	2:B:232:PRO:HD2	2.30	0.45
11:K:20:TYR:HD2	11:K:83:ILE:HB	1.80	0.45
10:J:63:PHE:HD1	10:J:63:PHE:H	1.60	0.45
1:A:1112:C:H1'	3:C:179:ARG:HH11	1.82	0.45
20:T:79:ARG:HD2	20:T:83:ARG:HH12	1.82	0.45
13:M:97:PRO:HB3	13:M:101:GLN:OE1	2.16	0.45
6:F:61:LEU:HB3	6:F:63:TYR:HE2	1.81	0.45
1:A:507:C:H3'	1:A:508:C:H2'	1.98	0.45
1:A:129:U:O3'	1:A:129(A):G:H3'	2.16	0.45
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.27	0.45
1:A:651:C:O2'	1:A:652:U:H5'	2.17	0.45
20:T:8:ARG:HG3	20:T:9:ASN:HB3	1.99	0.45
1:A:1054:C:O2'	1:A:1056:U:OP2	2.32	0.45
1:A:1194:U:H5''	1:A:1195:C:OP2	2.17	0.45
11:K:124:LYS:HE3	11:K:125:PHE:HE2	1.82	0.45
7:G:8:GLU:HG3	7:G:8:GLU:O	2.17	0.45
1:A:1277:C:C1'	1:A:1282:C:H1'	2.46	0.45
1:A:1157:A:C4	1:A:1181:G:C2	3.05	0.45
9:I:89:ASN:O	9:I:92:TYR:HB2	2.16	0.45
13:M:7:VAL:O	13:M:9:ILE:CD1	2.65	0.45
1:A:946:A:H2'	1:A:947:G:H8	1.79	0.45
19:S:52:TYR:CE2	19:S:54:GLY:CA	3.00	0.45
1:A:1162:C:C2	1:A:1175:G:C2	3.05	0.45
1:A:1166:G:N2	1:A:1171:G:C6	2.85	0.45
1:A:1345:U:P	29:A:2503:HOH:O	2.74	0.45
1:A:613:C:O2'	1:A:614:A:H5'	2.15	0.45
12:L:68:ALA:HB1	12:L:100:ILE:HD12	1.99	0.45
2:B:226:ARG:H	2:B:226:ARG:HG2	1.43	0.45
1:A:1451:A:H8	1:A:1451:A:O5'	2.00	0.45
5:E:83:GLU:O	5:E:83:GLU:CG	2.65	0.45
1:A:1059:C:N3	1:A:1198:G:O6	2.50	0.45
1:A:1090:U:N3	1:A:1091:U:C5	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:G:N1	1:A:1446:A:N6	2.63	0.45
11:K:14:VAL:HG12	11:K:15:ALA:N	2.32	0.45
7:G:120:ILE:H	7:G:120:ILE:CD1	2.16	0.45
18:R:56:THR:HB	18:R:58:LEU:CD2	2.47	0.45
1:A:283:C:C2	1:A:284:G:C8	3.04	0.45
17:Q:10:VAL:CG2	17:Q:19:VAL:HB	2.47	0.45
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.52	0.45
3:C:84:ILE:CG2	3:C:85:ARG:N	2.80	0.45
3:C:46:GLU:HB3	3:C:47:LEU:CD1	2.42	0.45
1:A:438:G:N2	1:A:496:A:C8	2.85	0.45
1:A:186:C:H5'	20:T:78:ALA:HB1	1.98	0.45
1:A:1420:C:H2'	1:A:1421:G:H8	1.81	0.45
7:G:69:VAL:O	7:G:69:VAL:CG1	2.63	0.45
4:D:204:ILE:HD12	4:D:204:ILE:N	2.32	0.45
2:B:197:VAL:HG11	2:B:200:ILE:HG13	1.99	0.45
1:A:582:U:H5''	15:O:64:ARG:HH21	1.82	0.45
2:B:53:ARG:HA	2:B:56:ARG:HH12	1.80	0.45
1:A:533:A:OP1	29:A:2170:HOH:O	2.21	0.45
3:C:90:GLU:H	3:C:90:GLU:HG3	1.57	0.45
1:A:1248:A:C6	1:A:1249:C:N4	2.85	0.45
1:A:503:C:OP2	12:L:116:SER:CB	2.63	0.45
1:A:1029:C:H2'	1:A:1030:C:H5'	1.98	0.45
11:K:72:ALA:HB1	11:K:77:MET:HE2	1.98	0.45
4:D:63:LYS:O	4:D:67:ILE:CD1	2.63	0.45
1:A:741:G:H5''	15:O:39:LEU:HD11	1.98	0.45
1:A:677:U:C2'	1:A:678:U:H5'	2.47	0.45
1:A:713:G:N2	1:A:714:G:C2	2.85	0.45
11:K:34:ASP:HB2	11:K:35:PRO:CD	2.45	0.45
1:A:1110:A:C8	29:A:2140:HOH:O	2.69	0.45
1:A:1015:A:N3	1:A:1218:C:O2'	2.50	0.45
2:B:196:LEU:H	2:B:196:LEU:HG	1.28	0.45
1:A:895:G:C5	1:A:896:C:C5	3.05	0.45
16:P:53:VAL:O	16:P:54:GLU:C	2.53	0.45
11:K:114:VAL:HG22	11:K:115:PRO:O	2.17	0.45
2:B:68:ILE:O	2:B:90:MET:HB3	2.16	0.45
1:A:1130:A:OP2	1:A:1130:A:H3'	2.17	0.44
1:A:1201:A:H4'	1:A:1202:G:C5'	2.46	0.44
1:A:1003(A):G:N1	1:A:1038:C:C2	2.77	0.44
4:D:177:ASP:CG	4:D:180:GLY:H	2.18	0.44
1:A:1303:C:C2'	1:A:1303:C:O2	2.56	0.44
13:M:10:PRO:HB3	13:M:18:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1314:C:OP2	19:S:6:LYS:CG	2.65	0.44
8:H:56:LYS:HB3	8:H:57:PRO:HD2	2.00	0.44
5:E:37:ARG:HA	5:E:114:GLY:CA	2.47	0.44
1:A:355:C:C5'	1:A:389:A:OP2	2.65	0.44
17:Q:10:VAL:O	17:Q:10:VAL:CG1	2.65	0.44
3:C:5:ILE:C	3:C:5:ILE:CD1	2.85	0.44
7:G:103:TRP:HE1	7:G:137:LYS:HE2	1.82	0.44
1:A:44:G:H2'	1:A:45:U:O4'	2.17	0.44
2:B:57:PHE:CD1	2:B:199:TYR:CE1	3.05	0.44
2:B:224:GLN:OE1	2:B:229:VAL:HG22	2.16	0.44
1:A:306:G:H2'	1:A:307:C:H6	1.82	0.44
1:A:1313:U:H5	19:S:4:SER:HB2	1.81	0.44
9:I:28:VAL:HA	9:I:63:ILE:HG22	1.99	0.44
1:A:1052:U:O4	1:A:1200:C:C2	2.70	0.44
1:A:1053:G:C4'	1:A:1054:C:H5'	2.47	0.44
3:C:131:ARG:C	3:C:134:ILE:HG12	2.36	0.44
1:A:1054:C:N3	23:W:34:G:P	2.91	0.44
23:W:36:A:N3	23:W:36:A:H2'	2.33	0.44
1:A:1507:A:C4	1:A:1530:G:C2	3.05	0.44
13:M:22:ILE:H	13:M:22:ILE:HD13	1.82	0.44
13:M:52:GLU:O	13:M:53:VAL:C	2.54	0.44
23:W:39:G:N2	23:W:40:PSU:C4	2.86	0.44
16:P:20:VAL:HG13	16:P:32:TYR:HD2	1.82	0.44
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.99	0.44
1:A:55:A:C2	1:A:56:U:H1'	2.51	0.44
19:S:41:VAL:CG2	19:S:43:GLU:OE2	2.65	0.44
8:H:104:ARG:HD2	8:H:138:TRP:CD2	2.53	0.44
1:A:784:C:C2'	1:A:785:G:O5'	2.65	0.44
5:E:98:THR:HB	5:E:117:ASP:HB3	1.98	0.44
1:A:400:C:N4	1:A:401:C:N4	2.65	0.44
1:A:42:G:C2	1:A:43:C:C2	3.05	0.44
11:K:86:GLY:H	11:K:112:THR:HG23	1.81	0.44
1:A:1055:A:N1	1:A:1056:U:H1'	2.32	0.44
14:N:24:CYS:SG	14:N:40:CYS:N	2.83	0.44
13:M:19:LEU:HA	13:M:19:LEU:HD23	1.48	0.44
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.90	0.44
13:M:115:LYS:HB2	13:M:115:LYS:HE2	1.72	0.44
7:G:40:ALA:O	7:G:41:ARG:C	2.53	0.44
1:A:1291:G:O5'	1:A:1291:G:H8	2.00	0.44
7:G:113:GLU:O	7:G:119:ARG:HD3	2.17	0.44
7:G:59:LEU:O	7:G:62:PHE:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:56:VAL:O	17:Q:76:LEU:HD12	2.17	0.44
20:T:42:GLN:OE1	20:T:42:GLN:HA	2.17	0.44
1:A:1347:G:H2'	1:A:1348:U:OP2	2.15	0.44
2:B:76:GLN:O	2:B:208:ILE:HD11	2.16	0.44
1:A:1403:C:O2'	1:A:1404:5MC:C5'	2.61	0.44
1:A:925:G:C1'	1:A:1502:A:C8	3.01	0.44
1:A:229:U:H2'	1:A:230:G:C5'	2.41	0.44
16:P:57:ARG:HD3	16:P:79:VAL:O	2.18	0.44
18:R:47:THR:CG2	18:R:48:GLY:N	2.76	0.44
1:A:616:G:C2'	1:A:617:G:H5'	2.47	0.44
5:E:148:VAL:O	5:E:152:ARG:HG3	2.18	0.44
1:A:629:G:H2'	1:A:630:G:O4'	2.17	0.44
8:H:4:ASP:OD2	8:H:85:ARG:CZ	2.64	0.44
1:A:1014:A:C5	1:A:1015:A:C6	3.06	0.44
2:B:139:LYS:HA	2:B:139:LYS:HD2	1.72	0.44
1:A:514:C:C2'	1:A:515:G:H5'	2.47	0.44
11:K:54:ARG:O	11:K:57:THR:OG1	2.35	0.44
11:K:88:GLY:O	11:K:89:ALA:C	2.56	0.44
1:A:256:U:C2'	1:A:257:G:H5'	2.48	0.44
16:P:6:LEU:HD23	16:P:17:TYR:CB	2.47	0.44
3:C:69:HIS:HA	3:C:104:GLN:O	2.17	0.44
1:A:681:C:C2	1:A:682:G:C8	3.06	0.44
10:J:19:SER:HA	10:J:22:LYS:HB3	1.99	0.44
1:A:1297:C:HO2'	1:A:1298:C:P	2.39	0.44
1:A:1488:G:H2'	1:A:1489:G:H8	1.83	0.44
1:A:1347:G:C6	9:I:107:ARG:NH1	2.85	0.44
9:I:64:THR:HG23	9:I:66:ARG:CZ	2.47	0.44
1:A:1394:A:C6	1:A:1501:C:H4'	2.53	0.44
1:A:1518[A]:MA6:N6	1:A:1519[A]:MA6:H103	2.33	0.44
1:A:1519[B]:MA6:H93	1:A:1520[B]:G:N2	2.32	0.44
10:J:33:GLN:C	10:J:34:VAL:HG23	2.38	0.44
13:M:67:GLU:HB3	13:M:68:GLY:H	1.20	0.44
1:A:868:C:C2'	1:A:869:G:O5'	2.63	0.44
1:A:1126:U:H3	1:A:1127:G:N2	2.15	0.44
1:A:1126:U:H6	1:A:1126:U:P	2.40	0.44
1:A:176:C:C2'	1:A:177:C:H5'	2.46	0.44
1:A:1227:A:H2'	1:A:1228:C:O5'	2.18	0.44
4:D:190:ASP:O	4:D:194:LEU:HD23	2.17	0.44
1:A:448:A:C4	1:A:449:C:C5	3.05	0.44
1:A:778:G:H2'	1:A:779:C:C5'	2.48	0.44
8:H:10:LEU:HA	8:H:10:LEU:HD22	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:A:C8	1:A:442:C:C6	3.05	0.44
1:A:444:C:N4	1:A:490:G:H1	2.12	0.44
1:A:815:A:O2'	1:A:1527:C:H1'	2.18	0.44
1:A:942:G:H2'	1:A:942:G:N3	2.31	0.44
9:I:97:LYS:HD2	9:I:97:LYS:O	2.18	0.44
5:E:36:ASP:OD2	5:E:38:GLN:HB2	2.18	0.44
1:A:862:C:H5''	29:A:2609:HOH:O	2.16	0.44
1:A:1350:A:C4	1:A:1351:U:C6	3.06	0.44
1:A:532:A:H61	1:A:1207:2MG:C5'	2.30	0.44
10:J:50:ILE:CD1	10:J:50:ILE:N	2.80	0.44
1:A:540:G:H2'	1:A:541:G:O4'	2.18	0.44
1:A:108:G:N3	1:A:108:G:H5'	2.33	0.44
10:J:85:LEU:HB3	10:J:86:MET:H	1.61	0.44
8:H:102:ARG:CD	8:H:102:ARG:N	2.64	0.44
1:A:1027:C:H5	1:A:1035:A:C2	2.36	0.44
1:A:1437:C:O2	1:A:1437:C:H2'	2.17	0.44
1:A:630:G:H3'	1:A:631:G:H5''	1.99	0.44
1:A:1346:A:N3	7:G:10:ARG:NH1	2.66	0.44
1:A:1245:A:C2	1:A:1293:G:N3	2.86	0.44
3:C:7:PRO:CB	3:C:11:ARG:HH21	2.30	0.44
1:A:73:C:N4	1:A:74:C:H41	2.15	0.44
1:A:155:C:C2	1:A:167:G:C2	3.06	0.44
9:I:40:LEU:HD13	9:I:40:LEU:HA	1.56	0.44
6:F:91:VAL:HG12	6:F:92:LYS:O	2.17	0.44
1:A:1088:G:H2'	1:A:1089:G:H5'	2.00	0.44
5:E:135:THR:O	5:E:136:MET:C	2.52	0.44
18:R:76:LEU:HA	18:R:76:LEU:HD23	1.38	0.44
4:D:158:ILE:HA	4:D:158:ILE:HD13	1.88	0.44
1:A:1347:G:O2'	1:A:1348:U:O5'	2.36	0.44
1:A:428:G:C1'	1:A:429:U:OP2	2.65	0.44
1:A:77:G:H2'	1:A:78:G:O5'	2.18	0.44
1:A:54:C:C2	1:A:352:C:H5	2.36	0.44
4:D:114:ARG:HG3	4:D:114:ARG:NH1	2.33	0.44
5:E:90:VAL:O	5:E:120:THR:HA	2.17	0.44
4:D:62:GLN:HB3	4:D:66:ARG:NH1	2.32	0.44
8:H:87:SER:C	8:H:88:LYS:HG3	2.38	0.44
9:I:49:PRO:HG3	9:I:101:PHE:HD1	1.82	0.44
2:B:178:ARG:O	8:H:71:GLY:HA2	2.18	0.44
1:A:154:C:H2'	1:A:155:C:H5'	1.99	0.44
1:A:433:C:C2	1:A:434:U:C5	3.02	0.44
1:A:595:G:C2	1:A:641:U:C2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:84:PHE:C	5:E:84:PHE:CD2	2.90	0.44
1:A:521:G:O2'	1:A:522:C:H5'	2.17	0.44
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.35	0.44
15:O:53:HIS:O	15:O:54:ARG:C	2.54	0.44
1:A:1113:C:H6	1:A:1113:C:O5'	2.01	0.44
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.17	0.44
1:A:510:A:H1'	1:A:543:C:O4'	2.18	0.44
1:A:710:G:N7	29:A:2472:HOH:O	2.36	0.44
1:A:653:A:OP1	8:H:56:LYS:CE	2.66	0.44
1:A:277:C:O2'	1:A:278:G:H5'	2.18	0.44
1:A:960:U:H1'	1:A:1223:C:H5'	1.99	0.44
13:M:108:ARG:HH21	13:M:114:ARG:HA	1.81	0.44
1:A:1112:C:N3	3:C:178:LEU:HB2	2.32	0.44
1:A:21:G:H2'	1:A:22:G:H8	1.78	0.44
1:A:1527:C:H2'	1:A:1528:U:H5'	1.98	0.44
2:B:30:ARG:HD2	2:B:31:TYR:CZ	2.53	0.44
4:D:101:LEU:O	4:D:101:LEU:HG	2.17	0.44
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.34	0.44
5:E:51:VAL:CB	5:E:52:PRO:HD3	2.48	0.44
8:H:116:LYS:HD2	8:H:129:VAL:HG11	2.00	0.44
1:A:89:C:O2'	1:A:90:U:H5'	2.17	0.44
1:A:1003(A):G:C2	1:A:1004:A:H1'	2.53	0.44
13:M:68:GLY:C	13:M:70:LEU:N	2.70	0.44
2:B:231:GLU:O	2:B:232:PRO:C	2.55	0.44
9:I:9:ARG:HA	9:I:76:ALA:HB1	2.00	0.44
2:B:92:TYR:CE1	2:B:151:GLY:CA	3.00	0.44
16:P:4:ILE:HB	16:P:66:PRO:HA	1.99	0.44
16:P:1:MET:O	16:P:2:VAL:C	2.56	0.44
18:R:61:LYS:O	18:R:62:GLU:C	2.54	0.44
1:A:1271:G:H2'	1:A:1272:G:H8	1.83	0.44
20:T:92:LEU:HD23	20:T:92:LEU:N	2.33	0.44
14:N:5:ALA:O	14:N:8:GLU:HG3	2.18	0.44
19:S:52:TYR:CE1	19:S:55:LYS:C	2.91	0.44
5:E:43:LEU:HD12	5:E:43:LEU:O	2.18	0.44
3:C:73:PRO:HD3	3:C:105:GLU:HB2	1.99	0.44
1:A:594:G:C2'	1:A:595:G:H5'	2.47	0.44
5:E:42:GLY:HA2	5:E:136:MET:HE1	2.00	0.44
2:B:168:THR:HG22	2:B:169:LYS:N	2.33	0.44
1:A:236:G:H2'	1:A:237:C:O4'	2.18	0.44
1:A:886:G:H1	1:A:911:U:H3	1.66	0.44
1:A:1250:A:H4'	9:I:68:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1401:G:C5	1:A:1402:4OC:C5	3.01	0.43
10:J:47:PHE:CD2	14:N:34:TYR:HD2	2.36	0.43
18:R:36:ASN:O	18:R:40:LEU:HG	2.18	0.43
13:M:27:LYS:C	13:M:27:LYS:HD2	2.38	0.43
21:U:21:TYR:N	21:U:21:TYR:CD1	2.86	0.43
1:A:1436:U:H2'	1:A:1437:C:C6	2.47	0.43
1:A:1124:G:C2'	1:A:1145:C:C5	3.01	0.43
1:A:285:G:O6	29:A:2039:HOH:O	2.20	0.43
1:A:956:U:C2	1:A:1225:A:C2	3.06	0.43
4:D:70:ILE:HD13	4:D:70:ILE:HA	1.79	0.43
8:H:36:LEU:HG	8:H:36:LEU:H	1.65	0.43
5:E:33:VAL:CG1	5:E:34:VAL:N	2.80	0.43
1:A:102:G:O2'	1:A:151:A:N3	2.39	0.43
3:C:34:LEU:HD13	14:N:25:VAL:CG2	2.48	0.43
10:J:99:LYS:H	10:J:99:LYS:HD2	1.83	0.43
12:L:39:VAL:HG23	12:L:57:LYS:HB3	1.99	0.43
9:I:37:PHE:CE2	9:I:74:ILE:HD11	2.52	0.43
1:A:1537:U:H2'	1:A:1538:C:N1	2.33	0.43
14:N:29:ARG:HG2	14:N:40:CYS:HB3	2.00	0.43
1:A:1004:A:N6	1:A:1037:C:N4	2.66	0.43
18:R:38:GLU:CD	18:R:38:GLU:N	2.71	0.43
1:A:1071:C:H42	1:A:1104:G:H1	1.66	0.43
16:P:4:ILE:O	16:P:66:PRO:HA	2.18	0.43
1:A:1255:G:C2	1:A:1283:G:C2	3.06	0.43
5:E:89:ILE:HD12	5:E:90:VAL:H	1.82	0.43
3:C:114:PRO:O	3:C:118:GLN:HG3	2.18	0.43
20:T:10:LEU:O	20:T:10:LEU:HD23	2.18	0.43
8:H:20:TYR:CE1	8:H:76:PRO:CD	3.00	0.43
2:B:114:ARG:NE	2:B:118:LEU:HD21	2.33	0.43
1:A:81:U:C5'	1:A:82:U:OP2	2.66	0.43
1:A:1465:C:C5	1:A:1466:C:C5	3.06	0.43
8:H:63:LEU:HA	8:H:63:LEU:HD13	1.53	0.43
1:A:1342:C:O2'	1:A:1343:G:H5'	2.18	0.43
1:A:1502:A:H2	1:A:1505:G:H1	1.66	0.43
1:A:1242:C:H4'	1:A:1304:G:OP1	2.17	0.43
2:B:98:LEU:HB2	2:B:101:MET:SD	2.59	0.43
1:A:134:A:H2'	1:A:135:C:O4'	2.18	0.43
3:C:62:ASP:HA	3:C:97:LYS:HZ2	1.82	0.43
19:S:44:MET:HB2	19:S:62:ILE:CD1	2.48	0.43
13:M:99:ARG:CB	13:M:101:GLN:HE22	2.31	0.43
6:F:90:VAL:HG12	6:F:91:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.19	0.43
1:A:537:G:C2	1:A:538:G:C5	3.06	0.43
10:J:4:ILE:HD12	10:J:5:ARG:N	2.32	0.43
1:A:644:G:C8	1:A:644:G:C4'	3.02	0.43
12:L:33:ARG:C	12:L:84:LEU:HD12	2.38	0.43
1:A:707:C:H4'	11:K:20:TYR:HD1	1.74	0.43
18:R:43:PHE:HE2	18:R:58:LEU:HD21	1.83	0.43
1:A:1225:A:C5'	1:A:1226:C:OP2	2.58	0.43
8:H:45:ILE:HG13	8:H:47:GLY:N	2.34	0.43
4:D:61:LYS:HD2	4:D:61:LYS:C	2.38	0.43
3:C:37:GLN:OE1	14:N:47:LEU:CD2	2.66	0.43
1:A:1407:5MC:O2'	1:A:1408:A:H5'	2.18	0.43
15:O:82:ILE:HG22	15:O:83:GLU:N	2.34	0.43
20:T:44:ALA:O	20:T:46:GLU:N	2.51	0.43
1:A:949:A:N1	1:A:1233:G:C4	2.86	0.43
13:M:99:ARG:HB2	13:M:101:GLN:NE2	2.32	0.43
13:M:63:THR:HG23	13:M:64:TRP:H	1.84	0.43
1:A:986:A:O2'	19:S:55:LYS:O	2.35	0.43
8:H:127:LEU:CD2	8:H:127:LEU:O	2.65	0.43
7:G:51:GLN:HB2	7:G:52:GLU:OE1	2.18	0.43
13:M:78:ILE:O	13:M:81:LEU:HB2	2.19	0.43
1:A:1332:A:C2	1:A:1333:A:N9	2.86	0.43
1:A:1163:C:C6	1:A:1163:C:C3'	3.02	0.43
5:E:84:PHE:C	5:E:84:PHE:HD2	2.22	0.43
11:K:19:ALA:HA	11:K:32:ILE:HD13	2.00	0.43
11:K:110:ASP:N	18:R:85:LEU:O	2.39	0.43
1:A:1515[B]:C:C4	1:A:1520[B]:G:O6	2.69	0.43
7:G:127:ALA:C	7:G:129:GLU:N	2.71	0.43
17:Q:4:LYS:HG3	17:Q:6:LEU:HD21	1.98	0.43
1:A:1221:G:C4	1:A:1222:G:C8	3.06	0.43
1:A:353:A:H5'	1:A:353:A:C8	2.50	0.43
9:I:47:LEU:HD23	9:I:47:LEU:HA	1.59	0.43
1:A:778:G:C6	1:A:779:C:N3	2.87	0.43
8:H:9:MET:HG3	8:H:26:VAL:HG21	2.01	0.43
1:A:231:G:C2	1:A:232:G:C8	3.06	0.43
3:C:78:GLY:HA3	3:C:83:ARG:CB	2.48	0.43
2:B:44:LEU:H	2:B:44:LEU:CD2	2.25	0.43
20:T:44:ALA:HA	20:T:92:LEU:CD2	2.43	0.43
1:A:1526:G:C2'	1:A:1527:C:H5'	2.48	0.43
6:F:35:ALA:CB	6:F:67:MET:HB3	2.49	0.43
1:A:1082:G:H2'	1:A:1083:U:C5'	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:58:LEU:C	4:D:58:LEU:CD2	2.86	0.43
1:A:1168:A:C6	1:A:1169:A:C6	3.07	0.43
15:O:36:ILE:HA	15:O:59:MET:CE	2.49	0.43
1:A:1166:G:N2	1:A:1171:G:C5	2.86	0.43
10:J:97:GLU:HG2	10:J:99:LYS:HE2	2.01	0.43
3:C:111:LEU:N	3:C:111:LEU:HD23	2.33	0.43
1:A:1132:C:H3'	1:A:1132:C:C6	2.52	0.43
1:A:1351:U:C2'	1:A:1352:C:H5'	2.48	0.43
1:A:1054:C:OP1	1:A:1197:G:P	2.76	0.43
3:C:135:LYS:NZ	5:E:50:GLU:HG2	2.34	0.43
1:A:925:G:C2	1:A:927:G:C8	3.07	0.43
20:T:99:LEU:CD1	20:T:100:ILE:H	2.32	0.43
1:A:90:U:C2'	1:A:91:C:O5'	2.66	0.43
1:A:1039:C:N3	1:A:1040:U:C4	2.86	0.43
1:A:132:C:H2'	1:A:133:U:H5'	2.01	0.43
5:E:13:ILE:HA	5:E:29:GLY:O	2.19	0.43
1:A:484:G:C2'	1:A:485:G:OP2	2.66	0.43
10:J:40:LEU:CB	10:J:69:ASN:HB2	2.39	0.43
4:D:173:TRP:H	4:D:173:TRP:HE3	1.64	0.43
1:A:448:A:C2	1:A:449:C:C5	3.06	0.43
20:T:41:ILE:CD1	20:T:41:ILE:N	2.82	0.43
2:B:155:LEU:HD22	2:B:157:ARG:O	2.19	0.43
7:G:54:THR:HG22	7:G:56:GLN:H	1.84	0.43
11:K:89:ALA:O	11:K:90:GLY:C	2.56	0.43
9:I:126:SER:O	9:I:128:ARG:N	2.52	0.43
1:A:360:A:C6	1:A:361:G:C6	3.06	0.43
2:B:145:LEU:HD23	2:B:145:LEU:HA	1.85	0.43
1:A:1501:C:C4	1:A:1504:G:C2	3.07	0.43
1:A:1517[B]:G:H2'	1:A:1518[B]:MA6:H8	2.00	0.43
1:A:1521:G:C2	1:A:1522:U:C2	3.07	0.43
1:A:77:G:N2	1:A:78:G:C4	2.86	0.43
5:E:121:LYS:CG	5:E:123:LEU:CD2	2.96	0.43
2:B:223:ILE:HD13	2:B:230:VAL:CG2	2.49	0.43
1:A:909:A:H2'	1:A:910:C:O4'	2.18	0.43
5:E:76:ILE:HA	5:E:77:PRO:HD3	1.89	0.43
1:A:443:C:N3	1:A:491:G:N2	2.58	0.43
4:D:78:LEU:HD23	4:D:78:LEU:HA	1.81	0.43
4:D:24:GLU:O	4:D:25:ARG:CB	2.67	0.43
1:A:236:G:C6	1:A:237:C:C2	3.06	0.43
1:A:397:A:C6	1:A:548:G:C8	3.07	0.43
5:E:139:LEU:HD23	5:E:139:LEU:HA	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:G:O3'	1:A:1054:C:H4'	2.18	0.43
1:A:1056:U:H2'	1:A:1057:G:H8	1.84	0.43
3:C:156:ARG:NE	3:C:160:ALA:O	2.51	0.43
4:D:7:PRO:HG2	4:D:10:ARG:HD2	2.00	0.43
1:A:78:G:C6	1:A:79:G:C8	3.06	0.43
1:A:1032:G:C4	1:A:1033:G:C8	3.06	0.43
12:L:90:VAL:HG11	12:L:93:LEU:HG	1.99	0.43
1:A:1048:G:H5''	14:N:3:ARG:HG3	2.01	0.43
1:A:848:C:H3'	1:A:848:C:C6	2.53	0.43
1:A:1126:U:C4	1:A:1127:G:N2	2.87	0.43
1:A:1480:G:C4	1:A:1481:U:C5	3.07	0.43
1:A:234:C:H2'	1:A:235:C:H6	1.83	0.43
4:D:28:SER:O	4:D:30:LYS:N	2.41	0.43
7:G:65:ALA:HB2	7:G:128:ALA:CA	2.49	0.43
2:B:56:ARG:HB2	2:B:56:ARG:HH11	1.82	0.43
10:J:45:ARG:HH11	14:N:36:PHE:HE2	1.65	0.43
1:A:702:A:OP2	29:A:2798:HOH:O	2.21	0.43
6:F:46:ARG:HB3	6:F:46:ARG:HE	1.59	0.43
1:A:1287:A:C6	1:A:1288:A:C6	3.07	0.43
1:A:1519[A]:MA6:C2'	1:A:1520[A]:G:H5'	2.49	0.43
1:A:93:G:O2'	1:A:95:U:H5'	2.19	0.43
3:C:33:LEU:HD11	14:N:53:LEU:HA	2.01	0.43
14:N:11:LYS:HG3	14:N:13:THR:OG1	2.19	0.43
14:N:12:ARG:C	14:N:14:PRO:HD3	2.39	0.43
12:L:104:VAL:O	12:L:105:TYR:HB2	2.19	0.43
1:A:988:G:N2	1:A:1218:C:O2	2.51	0.43
8:H:20:TYR:CE1	8:H:76:PRO:CG	3.02	0.43
1:A:46:G:C2	1:A:396:G:C2	3.06	0.43
1:A:680:C:H2'	1:A:681:C:H6	1.82	0.43
1:A:1298:C:OP2	7:G:114:ARG:NH2	2.51	0.43
1:A:1478:C:H2'	1:A:1479:C:H6	1.84	0.43
2:B:43:ASP:OD2	2:B:46:LYS:HB2	2.19	0.43
1:A:266:G:C4'	1:A:266:G:C8	3.01	0.43
9:I:16:ARG:CD	9:I:64:THR:HG22	2.49	0.43
2:B:74:LYS:C	2:B:76:GLN:N	2.72	0.43
1:A:110:C:N4	1:A:111:G:C6	2.87	0.43
15:O:26:GLU:OE1	15:O:77:ARG:HB2	2.18	0.43
1:A:77:G:C2'	1:A:78:G:O5'	2.67	0.43
12:L:93:LEU:O	12:L:94:PRO:C	2.56	0.43
1:A:1135:U:N3	1:A:1137:C:O2	2.52	0.43
6:F:97:PHE:HE1	18:R:61:LYS:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:G:C2	1:A:58:C:C2	3.07	0.43
1:A:284:G:C4	1:A:285:G:C8	3.07	0.43
19:S:15:LEU:HD13	19:S:16:LEU:H	1.82	0.43
8:H:36:LEU:HA	8:H:39:LEU:CD2	2.49	0.43
3:C:6:HIS:HE1	14:N:50:LYS:HE2	1.83	0.43
15:O:78:TYR:CZ	15:O:82:ILE:CD1	3.01	0.43
18:R:78:LEU:HD23	18:R:78:LEU:N	2.34	0.43
18:R:78:LEU:CD2	18:R:78:LEU:N	2.79	0.43
2:B:11:LEU:H	2:B:11:LEU:CD1	2.31	0.43
5:E:69:VAL:HG21	5:E:113:ALA:HB1	2.01	0.43
11:K:53:SER:O	11:K:55:LYS:N	2.51	0.43
20:T:60:GLU:O	20:T:63:ILE:HB	2.18	0.43
1:A:1326:C:P	21:U:6:ARG:HD3	2.59	0.43
1:A:1472:U:C2'	1:A:1473:A:O5'	2.67	0.43
5:E:135:THR:O	5:E:138:ALA:HB3	2.18	0.43
1:A:702:A:H3'	1:A:703:G:C5'	2.49	0.43
13:M:94:ARG:H	13:M:94:ARG:HG2	1.54	0.43
3:C:21:ARG:O	3:C:21:ARG:HG2	2.18	0.43
3:C:156:ARG:HB3	3:C:196:LEU:HD21	2.01	0.42
11:K:124:LYS:HG2	11:K:125:PHE:CE2	2.55	0.42
1:A:1501:C:C4	1:A:1504:G:N3	2.87	0.42
1:A:327:A:HO2'	1:A:328:C:C1'	2.31	0.42
4:D:150:GLU:C	4:D:152:SER:N	2.72	0.42
13:M:37:THR:HG23	13:M:39:ILE:HD12	2.01	0.42
1:A:995:C:C2'	1:A:996:A:H5'	2.49	0.42
1:A:1126:U:C6	1:A:1126:U:OP1	2.71	0.42
1:A:54:C:C5	1:A:352:C:H5	2.35	0.42
2:B:61:LEU:HD13	2:B:66:GLY:CA	2.41	0.42
5:E:148:VAL:HG23	5:E:148:VAL:H	1.31	0.42
1:A:976:G:N7	1:A:1358:U:N3	2.67	0.42
3:C:84:ILE:HG12	3:C:88:ARG:NH2	2.32	0.42
4:D:62:GLN:HA	4:D:62:GLN:OE1	2.19	0.42
1:A:497:A:H4'	1:A:498:U:OP2	2.19	0.42
1:A:942:G:C2	1:A:943:U:C6	3.07	0.42
1:A:248:C:O2'	1:A:249:U:H5'	2.19	0.42
11:K:57:THR:O	11:K:60:ALA:HB3	2.18	0.42
7:G:113:GLU:HG2	7:G:113:GLU:H	1.32	0.42
2:B:27:LYS:C	2:B:29:ALA:H	2.23	0.42
10:J:6:ILE:O	10:J:72:VAL:HG23	2.19	0.42
1:A:81:U:C6	1:A:81:U:C3'	3.02	0.42
10:J:90:LEU:HD22	10:J:90:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:G:C3'	1:A:1054:C:H5'	2.48	0.42
1:A:1190:G:O3'	3:C:3:ASN:HB2	2.19	0.42
6:F:14:LEU:HD22	6:F:14:LEU:HA	1.70	0.42
23:W:37:A:C6	23:W:38:A:N1	2.87	0.42
1:A:106:C:O2'	1:A:107:G:H5'	2.19	0.42
8:H:100:ILE:HA	8:H:101:PRO:HD2	1.57	0.42
1:A:134:A:H62	16:P:25:ARG:HH21	1.67	0.42
1:A:1126:U:N3	1:A:1127:G:C2	2.87	0.42
3:C:109:PRO:HA	3:C:115:LEU:HD12	2.01	0.42
1:A:826:C:H2'	1:A:827:U:H6	1.84	0.42
11:K:58:PRO:HB2	11:K:93:GLN:HG3	2.01	0.42
5:E:43:LEU:O	5:E:65:ASN:ND2	2.52	0.42
20:T:8:ARG:CG	20:T:9:ASN:HB3	2.50	0.42
12:L:100:ILE:HD12	12:L:100:ILE:N	2.34	0.42
1:A:397:A:H5'	1:A:398:C:OP1	2.19	0.42
1:A:1508:G:C5	1:A:1509:C:C5	3.07	0.42
1:A:1341:U:O2'	1:A:1342:C:H5'	2.19	0.42
1:A:1052:U:O2'	1:A:1055:A:OP1	2.38	0.42
1:A:1193:G:C4	1:A:1194:U:C5	3.08	0.42
1:A:792:A:C6	1:A:794:A:C2	3.07	0.42
1:A:1321:C:C5'	13:M:87:TYR:CE2	3.02	0.42
1:A:1437:C:C2	1:A:1438:G:C8	3.07	0.42
23:W:39:G:C2	23:W:40:PSU:C4	3.07	0.42
1:A:245:C:C6	1:A:284:G:N2	2.87	0.42
3:C:16:ARG:CG	3:C:16:ARG:NH1	2.78	0.42
2:B:172:ILE:H	2:B:172:ILE:CD1	2.32	0.42
17:Q:31:LEU:HA	17:Q:31:LEU:HD12	1.44	0.42
15:O:15:PHE:CD1	15:O:15:PHE:N	2.86	0.42
8:H:27:PRO:HB3	8:H:58:TYR:CE2	2.54	0.42
20:T:75:ASN:OD1	20:T:75:ASN:N	2.52	0.42
8:H:133:LEU:CD2	8:H:133:LEU:C	2.85	0.42
2:B:6:THR:N	2:B:48:MET:HE1	2.35	0.42
1:A:731:G:O2'	1:A:732:C:H5'	2.19	0.42
1:A:1480:G:C5	1:A:1481:U:C5	3.07	0.42
7:G:51:GLN:C	7:G:53:LYS:H	2.23	0.42
1:A:1092:A:C4'	1:A:1092:A:C8	3.02	0.42
16:P:39:TYR:CG	16:P:73:LEU:HD11	2.54	0.42
1:A:1297:C:O2'	1:A:1298:C:OP2	2.29	0.42
12:L:52:LEU:O	12:L:54:LYS:NZ	2.41	0.42
1:A:1367:C:C2	1:A:1368:G:C8	3.08	0.42
1:A:925:G:O4'	1:A:1502:A:C5	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:G:HO2'	1:A:1027:C:P	2.23	0.42
1:A:1104:G:P	2:B:111:ARG:HD2	2.60	0.42
1:A:1221:G:C6	1:A:1222:G:N7	2.87	0.42
1:A:961:U:H2'	1:A:962:C:H5'	2.01	0.42
4:D:192:GLU:CA	4:D:192:GLU:OE2	2.68	0.42
4:D:173:TRP:O	4:D:186:LEU:HG	2.19	0.42
3:C:88:ARG:HB2	3:C:101:LEU:CD2	2.49	0.42
2:B:36:ARG:CB	2:B:41:ILE:HD11	2.48	0.42
14:N:8:GLU:OE2	14:N:11:LYS:HD3	2.20	0.42
1:A:833:U:H2'	1:A:834:C:C6	2.53	0.42
17:Q:11:VAL:CG1	17:Q:88:TYR:CE2	3.01	0.42
7:G:65:ALA:HB2	7:G:128:ALA:N	2.33	0.42
1:A:1503:A:H5'	1:A:1531:A:H1'	2.01	0.42
1:A:518:C:O3'	12:L:50:SER:HB3	2.19	0.42
15:O:56:LEU:HA	15:O:56:LEU:HD13	1.83	0.42
1:A:1263:C:N4	1:A:1264:C:H41	2.17	0.42
1:A:903:G:H2'	1:A:904:C:H6	1.85	0.42
21:U:10:ARG:HG3	21:U:10:ARG:HH11	1.79	0.42
3:C:157:ILE:HD12	3:C:164:ARG:NH1	2.34	0.42
1:A:1518[B]:MA6:C9	1:A:1519[B]:MA6:H103	2.49	0.42
20:T:99:LEU:O	20:T:101:GLY:N	2.52	0.42
1:A:596:C:C2	1:A:644:G:N2	2.88	0.42
8:H:114:THR:OG1	8:H:117:GLY:O	2.34	0.42
1:A:1241:G:C4	1:A:1242:C:C5	3.07	0.42
1:A:914:A:OP1	27:A:1928:SRV:HI33	2.19	0.42
1:A:320:C:O2'	1:A:1435:G:H1'	2.20	0.42
1:A:1072:G:C5	1:A:1073:U:C4	3.07	0.42
2:B:97:TRP:CZ2	2:B:101:MET:HG3	2.55	0.42
2:B:100:GLY:N	2:B:176:GLU:OE2	2.52	0.42
15:O:79:ARG:CG	15:O:79:ARG:NH1	2.76	0.42
18:R:58:LEU:CD2	18:R:58:LEU:N	2.82	0.42
1:A:1225:A:H1'	19:S:78:ARG:HH11	1.83	0.42
1:A:366:C:H1'	1:A:394:G:H22	1.84	0.42
1:A:1358:U:H5''	14:N:35:ARG:HG3	2.01	0.42
15:O:8:LYS:O	15:O:9:GLN:C	2.55	0.42
6:F:82:ARG:CB	6:F:85:VAL:HG23	2.46	0.42
1:A:157:G:H2'	1:A:157:G:N3	2.35	0.42
8:H:121:ASP:O	8:H:124:ALA:N	2.49	0.42
4:D:76:ARG:O	4:D:80:GLU:HG2	2.19	0.42
1:A:1077:G:N2	1:A:1081:G:C5	2.88	0.42
17:Q:90:ILE:HA	17:Q:93:GLN:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:60:SER:O	14:N:61:TRP:HB3	2.19	0.42
14:N:61:TRP:CD1	14:N:61:TRP:O	2.73	0.42
1:A:1115:C:C4	1:A:1116:C:C5	3.08	0.42
15:O:31:LEU:HA	15:O:31:LEU:HD12	1.56	0.42
1:A:1379:G:OP2	7:G:6:ARG:HG2	2.20	0.42
15:O:2:PRO:O	15:O:3:ILE:HG13	2.20	0.42
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.83	0.42
1:A:1401:G:C5	1:A:1402:4OC:C6	3.03	0.42
1:A:922:G:C5'	1:A:922:G:H8	2.32	0.42
4:D:147:ALA:HB2	4:D:182:LYS:HB3	2.00	0.42
4:D:191:ARG:HB3	4:D:192:GLU:OE2	2.20	0.42
19:S:44:MET:O	19:S:62:ILE:HG21	2.19	0.42
4:D:64:LEU:CA	4:D:67:ILE:HD12	2.50	0.42
1:A:448:A:N3	1:A:449:C:C6	2.87	0.42
4:D:100:ARG:NH2	4:D:136:PRO:HB2	2.35	0.42
1:A:665:A:H3'	1:A:725:G:H21	1.84	0.42
1:A:891:U:C2'	1:A:892:A:H5'	2.49	0.42
1:A:376:G:H5''	16:P:5:ARG:HD2	2.01	0.42
8:H:19:VAL:HG21	8:H:21:LYS:HD3	2.02	0.42
16:P:17:TYR:HB2	16:P:39:TYR:HB3	2.02	0.42
1:A:1493[B]:A:O2'	1:A:1494:G:C8	2.66	0.42
1:A:1505:G:C5'	1:A:1506:U:OP1	2.67	0.42
1:A:429:U:H4'	1:A:430:A:O5'	2.19	0.42
1:A:1004:A:O2'	1:A:1005:A:OP1	2.27	0.42
13:M:37:THR:HG21	13:M:39:ILE:HD13	2.00	0.42
1:A:114:U:C2'	1:A:115:G:C5'	2.92	0.42
1:A:1255:G:O2'	1:A:1258:G:H1'	2.19	0.42
1:A:53:A:C5	1:A:54:C:C5	3.08	0.42
4:D:17:VAL:O	4:D:17:VAL:HG13	2.19	0.42
3:C:112:SER:HB3	3:C:115:LEU:HD12	2.01	0.42
1:A:415:A:C5	1:A:416:G:C5	3.08	0.42
8:H:39:LEU:HB3	8:H:45:ILE:HG23	2.01	0.42
4:D:21:LEU:HD12	4:D:21:LEU:N	2.34	0.42
3:C:82:GLU:CG	3:C:83:ARG:H	2.31	0.42
12:L:105:TYR:CD2	12:L:105:TYR:N	2.83	0.42
2:B:115:LEU:HD21	2:B:153:ARG:HH12	1.85	0.42
10:J:19:SER:O	10:J:22:LYS:HB3	2.20	0.42
1:A:885:G:O2'	1:A:886:G:H5'	2.20	0.42
1:A:934:C:H5''	29:A:2502:HOH:O	2.20	0.42
2:B:154:LEU:HA	2:B:154:LEU:HD23	1.74	0.42
6:F:1:MET:HE2	6:F:1:MET:H1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:A:C2	1:A:1146:A:H1'	2.54	0.42
1:A:1053:G:H4'	1:A:1054:C:H5'	2.02	0.42
4:D:8:VAL:O	4:D:10:ARG:N	2.53	0.42
1:A:425:G:C2'	1:A:426:G:H5'	2.48	0.42
5:E:126:ARG:CG	5:E:126:ARG:NH1	2.65	0.42
13:M:16:ASP:O	13:M:17:VAL:C	2.58	0.42
13:M:54:VAL:CG1	13:M:55:ARG:N	2.83	0.42
4:D:188:LEU:HA	4:D:189:PRO:HD2	1.79	0.42
15:O:15:PHE:HD1	15:O:15:PHE:N	2.17	0.42
3:C:173:VAL:O	3:C:175:LEU:HD12	2.19	0.42
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.52	0.42
1:A:49:U:O2'	1:A:50:A:H2'	2.20	0.42
9:I:22:GLY:O	9:I:57:GLY:O	2.38	0.42
19:S:72:GLY:O	19:S:74:PHE:N	2.53	0.42
13:M:21:TYR:N	13:M:21:TYR:CD1	2.87	0.42
12:L:71:PRO:HG2	12:L:102:ARG:HG3	2.01	0.42
1:A:1250:A:N1	1:A:1287:A:C2	2.88	0.42
1:A:1368:G:H5'	9:I:112:LYS:O	2.19	0.42
1:A:1051:C:H2'	1:A:1052:U:O5'	2.19	0.42
1:A:1199:U:H4'	10:J:54:PHE:CD1	2.55	0.42
1:A:1493[B]:A:C2'	1:A:1494:G:C8	3.03	0.42
1:A:1040:U:O2'	1:A:1041:A:H5'	2.20	0.42
13:M:22:ILE:H	13:M:22:ILE:CD1	2.33	0.42
2:B:101:MET:HB2	2:B:102:LEU:CD1	2.49	0.42
1:A:605:U:H3'	1:A:605:U:C6	2.55	0.42
3:C:8:ILE:HG22	3:C:9:GLY:H	1.84	0.42
3:C:115:LEU:HA	3:C:115:LEU:HD23	1.59	0.42
1:A:877:C:OP1	8:H:88:LYS:HE3	2.19	0.42
1:A:1182:G:H2'	1:A:1182:G:H8	1.78	0.42
1:A:496:A:H4'	1:A:497:A:OP1	2.18	0.42
1:A:442:C:H42	1:A:492:G:H1	1.68	0.42
1:A:1086:U:O5'	1:A:1086:U:H6	2.02	0.42
1:A:407:G:H5'	4:D:3:ARG:NH1	2.35	0.42
7:G:70:LYS:HB3	7:G:96:GLN:HG2	2.02	0.42
19:S:34:TRP:CD1	19:S:52:TYR:HB3	2.54	0.42
9:I:99:LEU:HD22	9:I:99:LEU:H	1.85	0.42
5:E:5:ASP:OD1	5:E:6:PHE:N	2.49	0.42
21:U:12:LYS:HD3	21:U:17:THR:OG1	2.20	0.42
1:A:1379:G:C6	1:A:1380:U:C4	3.07	0.42
1:A:397:A:C6	1:A:548:G:N7	2.88	0.42
1:A:505:G:C5	1:A:535:A:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:U:OP1	12:L:23:LYS:HE2	2.20	0.42
1:A:309:G:O2'	1:A:310:G:H5'	2.20	0.42
1:A:1204:A:C5	1:A:1205:U:C6	3.08	0.42
1:A:924:C:C3'	1:A:924:C:C6	3.03	0.42
7:G:5:ARG:NH1	7:G:8:GLU:HG2	2.34	0.42
8:H:52:ASP:HA	8:H:57:PRO:HA	2.02	0.42
1:A:1381:U:C5	1:A:1382:C:C6	3.08	0.42
1:A:415:A:C5	1:A:416:G:N7	2.88	0.42
5:E:80:ILE:HA	8:H:104:ARG:NH2	2.35	0.42
1:A:491:G:H2'	1:A:492:G:H8	1.85	0.42
17:Q:54:GLY:HA3	17:Q:82:MET:HG2	2.02	0.42
6:F:10:LEU:HD12	6:F:10:LEU:N	2.35	0.42
6:F:35:ALA:HA	6:F:67:MET:HB3	2.02	0.42
1:A:154:C:C3'	1:A:154:C:C6	3.03	0.42
2:B:10:LEU:CD1	2:B:15:VAL:HG21	2.50	0.42
17:Q:20:THR:HA	17:Q:43:LEU:CD2	2.50	0.42
17:Q:18:THR:HG21	17:Q:69:LYS:HD3	2.01	0.42
1:A:1172:C:O5'	1:A:1172:C:H6	2.03	0.42
15:O:52:SER:O	15:O:53:HIS:C	2.58	0.42
1:A:1190:G:H5'	3:C:4:LYS:H	1.85	0.41
1:A:1536:C:C6	1:A:1536:C:C3'	3.03	0.41
8:H:129:VAL:HG23	8:H:130:GLY:N	2.35	0.41
1:A:1032:G:H2'	1:A:1033:G:O4'	2.20	0.41
13:M:49:THR:C	13:M:51:ALA:N	2.73	0.41
4:D:83:SER:HA	4:D:89:THR:CG2	2.37	0.41
16:P:66:PRO:HG2	16:P:71:ARG:NH1	2.35	0.41
1:A:1222:G:N2	1:A:1223:C:C2	2.88	0.41
14:N:7:ILE:N	14:N:7:ILE:HD13	2.35	0.41
1:A:114:U:H1'	1:A:353:A:H1'	2.01	0.41
19:S:40:ILE:HG23	19:S:62:ILE:HD12	2.02	0.41
3:C:120:VAL:HG12	3:C:124:ILE:HD11	2.02	0.41
1:A:1111:A:O2'	1:A:1112:C:H5'	2.20	0.41
6:F:45:LEU:HA	6:F:59:TYR:HA	2.02	0.41
1:A:316:G:C5	29:A:2572:HOH:O	2.72	0.41
2:B:47:THR:HA	2:B:202:PRO:CG	2.46	0.41
1:A:1310:G:H2'	1:A:1311:G:O4'	2.20	0.41
2:B:135:GLN:O	2:B:139:LYS:HB2	2.20	0.41
13:M:63:THR:CG2	13:M:64:TRP:H	2.32	0.41
18:R:78:LEU:HD22	18:R:78:LEU:HA	1.73	0.41
12:L:60:LEU:HA	12:L:60:LEU:HD13	1.33	0.41
1:A:560:U:H4'	1:A:561:U:H5''	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1410:G:C4	1:A:1411:C:C5	3.08	0.41
16:P:38:TYR:O	16:P:49:LEU:HD12	2.19	0.41
1:A:1288:A:H2'	1:A:1289:A:H8	1.85	0.41
1:A:1190:G:C8	1:A:1190:G:C4'	3.02	0.41
1:A:973:G:C2'	1:A:974:A:OP1	2.68	0.41
1:A:1502:A:C2	1:A:1504:G:N3	2.88	0.41
1:A:1536:C:C6	1:A:1536:C:H3'	2.52	0.41
8:H:100:ILE:HG21	8:H:112:LEU:HD11	2.02	0.41
1:A:78:G:C2	1:A:79:G:C8	3.08	0.41
1:A:79:G:N3	1:A:91:C:O2	2.54	0.41
1:A:1241:G:OP1	7:G:35:LYS:NZ	2.53	0.41
13:M:70:LEU:HD23	13:M:70:LEU:HA	1.75	0.41
9:I:9:ARG:HA	9:I:76:ALA:HB2	2.00	0.41
16:P:4:ILE:HG22	16:P:4:ILE:O	2.18	0.41
1:A:1137:C:H4'	1:A:1138:G:O5'	2.19	0.41
6:F:97:PHE:CE1	18:R:61:LYS:HE2	2.55	0.41
1:A:574:A:H5''	1:A:575:G:OP2	2.20	0.41
4:D:19:LEU:CD1	4:D:67:ILE:HG13	2.50	0.41
9:I:33:PHE:HD1	9:I:33:PHE:HA	1.66	0.41
1:A:1376:U:OP1	7:G:98:SER:OG	2.25	0.41
3:C:78:GLY:CA	3:C:83:ARG:HB3	2.50	0.41
1:A:665:A:H3'	1:A:725:G:N2	2.36	0.41
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.53	0.41
5:E:69:VAL:HA	5:E:70:PRO:HD3	1.82	0.41
19:S:51:VAL:HG11	19:S:71:LEU:HD22	2.01	0.41
21:U:23:PRO:C	21:U:25:LYS:N	2.74	0.41
7:G:79:ARG:CB	7:G:83:ALA:O	2.68	0.41
4:D:162:LEU:O	4:D:165:MET:HB2	2.20	0.41
1:A:268:C:H2'	1:A:269:C:H6	1.85	0.41
1:A:1128:C:O2'	1:A:1130:A:H8	2.02	0.41
1:A:1052:U:O2	1:A:1207:2MG:N2	2.54	0.41
1:A:922:G:N3	1:A:1398:A:C2	2.86	0.41
22:V:1:U:N3	23:W:37:A:C2	2.88	0.41
15:O:5:LYS:O	15:O:6:GLU:C	2.57	0.41
1:A:243:A:C2	1:A:246:A:N7	2.88	0.41
5:E:105:VAL:O	5:E:106:PRO:C	2.56	0.41
4:D:19:LEU:HD23	4:D:19:LEU:N	2.22	0.41
1:A:140:A:O2'	1:A:141:A:H5'	2.20	0.41
17:Q:32:TYR:HA	17:Q:32:TYR:HD2	1.62	0.41
3:C:174:PRO:HB2	3:C:177:THR:HB	2.02	0.41
1:A:101:A:C2	1:A:102:G:C8	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:63:TYR:N	6:F:63:TYR:CD2	2.89	0.41
20:T:105:SER:O	20:T:106:ALA:C	2.58	0.41
1:A:937:A:N6	1:A:1345:U:O4	2.53	0.41
17:Q:76:LEU:HD12	17:Q:77:VAL:N	2.35	0.41
9:I:50:LEU:HD23	9:I:55:ALA:HB3	2.01	0.41
1:A:1091:U:O2	1:A:1093:A:C8	2.74	0.41
2:B:208:ILE:HD13	2:B:208:ILE:HA	1.85	0.41
1:A:504:C:C2	1:A:542:G:C2	3.09	0.41
1:A:89:C:H5	1:A:90:U:O4	2.02	0.41
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.50	0.41
1:A:1329:A:C5'	13:M:29:ARG:HD2	2.50	0.41
2:B:230:VAL:HG12	2:B:231:GLU:N	2.35	0.41
17:Q:95:TYR:O	17:Q:97:SER:N	2.53	0.41
5:E:105:VAL:CB	5:E:106:PRO:HD3	2.49	0.41
15:O:21:ASP:OD1	15:O:24:SER:CB	2.66	0.41
1:A:850:U:H6	1:A:850:U:H3'	1.86	0.41
1:A:684:A:N3	11:K:39:PRO:HD2	2.36	0.41
4:D:17:VAL:HG11	4:D:63:LYS:HD2	2.02	0.41
17:Q:27:PHE:CE2	17:Q:36:ILE:HD11	2.55	0.41
15:O:12:ILE:O	15:O:14:GLU:N	2.53	0.41
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.20	0.41
2:B:158:LEU:HB3	2:B:159:PRO:CD	2.50	0.41
1:A:986:A:H1'	19:S:52:TYR:OH	2.19	0.41
1:A:892:A:C6	1:A:907:A:C8	3.09	0.41
5:E:95:ALA:HB1	5:E:96:PRO:HD2	2.03	0.41
13:M:20:THR:O	13:M:20:THR:HG22	2.19	0.41
1:A:505:G:C6	1:A:535:A:C2	3.07	0.41
1:A:370:C:C2	1:A:371:G:C8	3.09	0.41
9:I:17:VAL:HG11	9:I:81:ILE:HA	2.01	0.41
1:A:1195:C:H5''	1:A:1196:U:P	2.61	0.41
1:A:1492[B]:A:C6	1:A:1493[B]:A:H1'	2.56	0.41
1:A:794:A:N6	1:A:795:C:N4	2.68	0.41
1:A:88:A:N7	1:A:89:C:N3	2.68	0.41
1:A:247:G:OP2	17:Q:99:SER:HB2	2.20	0.41
13:M:27:LYS:HE2	21:U:21:TYR:HE2	1.84	0.41
27:A:1928:SRY:C61	12:L:46:LYS:HD2	2.51	0.41
17:Q:22:LEU:HD12	17:Q:23:VAL:N	2.36	0.41
4:D:22:LYS:HB3	4:D:26:CYS:SG	2.59	0.41
16:P:20:VAL:CG1	16:P:21:VAL:N	2.78	0.41
1:A:313:A:H2'	1:A:314:C:O4'	2.21	0.41
18:R:59:SER:OG	18:R:62:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:C:N4	1:A:740:U:C4	2.89	0.41
1:A:777:A:N6	1:A:778:G:C2	2.89	0.41
2:B:16:HIS:HB3	2:B:44:LEU:HD11	2.02	0.41
1:A:188:C:H2'	1:A:189:G:H5'	2.02	0.41
3:C:26:LYS:HZ2	3:C:26:LYS:HB2	1.86	0.41
10:J:8:LEU:HD21	10:J:96:ILE:HG23	2.02	0.41
1:A:62:U:H2'	1:A:63:C:C6	2.56	0.41
4:D:141:ARG:HB2	4:D:141:ARG:HE	1.48	0.41
21:U:13:ILE:HG13	21:U:14:TRP:N	2.35	0.41
1:A:1068:G:OP1	29:A:2218:HOH:O	2.20	0.41
2:B:215:LEU:O	2:B:219:VAL:HG23	2.21	0.41
1:A:544:G:N3	1:A:545:C:C6	2.88	0.41
1:A:924:C:H3'	1:A:924:C:C6	2.55	0.41
1:A:328:C:OP1	1:A:328:C:H4'	2.19	0.41
1:A:1022:G:C2	1:A:1023:G:C8	3.08	0.41
1:A:1029:C:C4	1:A:1030:C:H5	2.39	0.41
17:Q:101:ARG:HD3	17:Q:101:ARG:N	2.34	0.41
5:E:31:LEU:HD23	5:E:44:GLY:O	2.21	0.41
19:S:15:LEU:N	19:S:15:LEU:CD1	2.83	0.41
1:A:21:G:C2	1:A:22:G:C6	3.09	0.41
1:A:22:G:C5	1:A:23:C:C4	3.09	0.41
1:A:584:G:C2'	1:A:585:G:H5'	2.50	0.41
16:P:19:ILE:CG2	16:P:36:ILE:HG13	2.51	0.41
7:G:23:VAL:HA	7:G:62:PHE:HE2	1.85	0.41
1:A:536:C:OP2	29:A:2174:HOH:O	2.22	0.41
16:P:78:GLY:C	16:P:80:PHE:N	2.69	0.41
1:A:1350:A:OP2	9:I:118:LYS:HD2	2.21	0.41
9:I:108:VAL:CG1	9:I:109:VAL:N	2.68	0.41
21:U:10:ARG:HA	21:U:13:ILE:HG12	2.02	0.41
1:A:1497:G:O2'	1:A:1518[A]:MA6:N1	2.53	0.41
1:A:922:G:N3	1:A:1396:A:C2	2.89	0.41
1:A:106:C:H2'	1:A:107:G:C5'	2.50	0.41
4:D:150:GLU:O	4:D:152:SER:N	2.54	0.41
1:A:552:U:H2'	1:A:553:A:C8	2.56	0.41
12:L:25:PRO:C	12:L:27:LEU:N	2.73	0.41
2:B:102:LEU:HB2	2:B:176:GLU:OE1	2.20	0.41
16:P:32:TYR:CD1	16:P:32:TYR:N	2.88	0.41
1:A:1121:U:O2'	1:A:1122:U:H5'	2.21	0.41
1:A:1124:G:C4'	10:J:38:ILE:HD11	2.50	0.41
18:R:22:VAL:HG21	18:R:56:THR:HG22	2.02	0.41
15:O:15:PHE:CE2	15:O:30:ALA:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:G:C2	1:A:492:G:C8	3.08	0.41
1:A:357:G:C2	1:A:358:U:C6	3.09	0.41
2:B:20:GLU:HG2	2:B:39:ILE:HD11	2.02	0.41
17:Q:89:LEU:O	17:Q:93:GLN:HB3	2.20	0.41
7:G:78:ARG:HD2	7:G:156:TRP:HB2	2.02	0.41
6:F:39:LYS:HG2	6:F:40:VAL:N	2.36	0.41
1:A:1377:A:O2'	7:G:2:ALA:HB3	2.21	0.41
1:A:756:C:H2'	1:A:757:U:O4'	2.20	0.41
6:F:11:ASN:HD22	6:F:86:ARG:NH1	2.19	0.41
5:E:101:ILE:HD13	5:E:101:ILE:N	2.36	0.41
1:A:1042:G:C6	1:A:1043:C:C4	3.08	0.41
1:A:1202:G:H1'	14:N:42:ILE:HD12	2.02	0.41
2:B:86:GLU:O	2:B:88:ALA:O	2.38	0.41
14:N:29:ARG:HG2	14:N:40:CYS:HB2	2.02	0.41
7:G:50:ILE:CB	7:G:58:PRO:HB3	2.50	0.41
6:F:52:ILE:O	6:F:53:ALA:HB3	2.21	0.41
1:A:1006:C:H2'	1:A:1007:C:H6	1.85	0.41
18:R:87:ARG:NH2	18:R:87:ARG:CB	2.79	0.41
1:A:133:U:O5'	1:A:133:U:H6	2.03	0.41
18:R:47:THR:CG2	18:R:48:GLY:H	2.27	0.41
5:E:76:ILE:HA	5:E:76:ILE:HD12	1.46	0.41
1:A:740:U:C4'	15:O:42:HIS:CD2	3.03	0.41
3:C:112:SER:OG	3:C:115:LEU:HB2	2.20	0.41
3:C:175:LEU:CD2	3:C:201:TYR:HE2	2.34	0.41
2:B:16:HIS:NE2	2:B:17:PHE:CD2	2.89	0.41
1:A:1010:G:C2	1:A:1020:U:O2	2.74	0.41
9:I:49:PRO:HD3	9:I:101:PHE:HE1	1.85	0.41
14:N:9:LYS:O	14:N:11:LYS:HB2	2.20	0.41
1:A:112:G:H2'	1:A:113:G:H5'	2.02	0.41
4:D:204:ILE:HD13	4:D:204:ILE:N	2.31	0.41
1:A:148:G:N2	1:A:149:A:C4	2.89	0.41
11:K:58:PRO:O	11:K:61:ALA:N	2.54	0.41
8:H:11:THR:OG1	8:H:14:ARG:NH2	2.50	0.41
2:B:24:TRP:CZ2	2:B:26:PRO:HB3	2.56	0.41
3:C:107:GLN:HG3	3:C:108:ASN:N	2.34	0.41
13:M:82:MET:HE2	13:M:82:MET:HB2	1.80	0.41
5:E:119:LEU:HD23	5:E:119:LEU:HA	1.56	0.41
1:A:1343:G:H2'	1:A:1344:C:C6	2.56	0.41
9:I:5:TYR:O	9:I:84:ALA:HA	2.21	0.41
1:A:1063:C:H2'	1:A:1064:G:H8	1.83	0.41
2:B:216:SER:OG	2:B:217:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:G:N2	1:A:1518[A]:MA6:C9	2.84	0.41
12:L:117:ARG:C	12:L:119:LYS:N	2.70	0.41
1:A:500:G:C5	1:A:501:C:C4	3.09	0.41
15:O:26:GLU:HG3	15:O:81:LEU:HG	2.03	0.41
1:A:674:G:H5'	6:F:50:TYR:CE2	2.56	0.41
6:F:50:TYR:CD1	6:F:50:TYR:N	2.88	0.41
1:A:1038:C:O2'	1:A:1039:C:H5'	2.21	0.41
13:M:49:THR:HB	13:M:52:GLU:CG	2.35	0.41
3:C:125:GLU:C	3:C:127:ARG:H	2.24	0.41
16:P:66:PRO:C	16:P:67:THR:O	2.59	0.41
1:A:392:G:C2	1:A:393:A:C8	3.09	0.41
1:A:575:G:C6	1:A:821:G:N7	2.89	0.41
4:D:64:LEU:HA	4:D:67:ILE:CD1	2.50	0.41
4:D:107:ARG:HH11	4:D:114:ARG:HH21	1.68	0.41
4:D:100:ARG:HH12	4:D:137:SER:CA	2.34	0.41
1:A:262:A:H5'	20:T:74:LYS:HD3	2.03	0.41
8:H:35:ILE:O	8:H:39:LEU:HD22	2.21	0.41
3:C:85:ARG:CG	3:C:85:ARG:HH11	2.29	0.41
3:C:85:ARG:O	3:C:86:VAL:C	2.60	0.41
3:C:178:LEU:C	3:C:180:ALA:N	2.73	0.41
3:C:6:HIS:CD2	3:C:6:HIS:C	2.94	0.41
1:A:1406:U:C6	1:A:1407:5MC:HM52	2.56	0.41
6:F:101:ALA:HA	18:R:28:GLU:CB	2.46	0.41
17:Q:81:ARG:NE	17:Q:84:LEU:HD12	2.34	0.41
3:C:56:ASP:HB3	3:C:67:THR:HB	2.03	0.41
19:S:52:TYR:CE2	19:S:54:GLY:HA2	2.56	0.41
23:W:33:U:O2	23:W:33:U:H2'	2.21	0.41
2:B:20:GLU:HA	2:B:39:ILE:HD11	2.01	0.41
5:E:41:VAL:HG13	5:E:113:ALA:CA	2.49	0.41
12:L:10:LEU:HD11	12:L:15:ARG:NE	2.35	0.41
14:N:36:PHE:CD1	14:N:36:PHE:O	2.73	0.41
1:A:652:U:O2'	1:A:752:G:N1	2.54	0.41
5:E:28:PHE:O	5:E:47:LYS:HA	2.21	0.41
12:L:68:ALA:HB3	12:L:100:ILE:HD11	2.03	0.41
11:K:69:ALA:O	11:K:70:LYS:C	2.58	0.41
4:D:108:LEU:HD23	4:D:108:LEU:HA	1.73	0.41
1:A:1190:G:O2'	1:A:1191:A:P	2.79	0.41
1:A:1022:G:N3	1:A:1022:G:H2'	2.35	0.41
1:A:1038:C:C2	1:A:1039:C:C6	3.09	0.41
1:A:1330:U:C2'	1:A:1331:G:H5'	2.50	0.41
1:A:1104:G:H4'	2:B:111:ARG:NE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:120:ARG:NH2	11:K:126:ARG:NE	2.69	0.41
16:P:67:THR:N	16:P:70:ALA:HB3	2.35	0.41
1:A:447:G:H2'	1:A:485:G:C2	2.54	0.41
1:A:1318:A:H5'	19:S:10:PHE:CD1	2.56	0.41
8:H:86:ILE:N	8:H:134:ILE:O	2.54	0.41
3:C:182:ILE:HA	3:C:202:ILE:O	2.20	0.41
1:A:474:G:C2	1:A:475:G:C8	3.09	0.41
1:A:442:C:N4	1:A:492:G:H1	2.19	0.41
1:A:179:A:C4	1:A:180:U:C5	3.09	0.41
17:Q:53:LEU:HD13	17:Q:53:LEU:HA	1.79	0.41
8:H:73:ASP:HA	8:H:74:PRO:HD2	1.73	0.41
1:A:16:A:C2	1:A:920:U:O2	2.74	0.41
17:Q:86:GLU:O	17:Q:87:LYS:C	2.60	0.41
1:A:143:A:C2	1:A:221:C:O2	2.74	0.41
9:I:118:LYS:HE2	9:I:118:LYS:HB3	1.90	0.40
1:A:1404:5MC:C2	1:A:1499:A:N1	2.89	0.40
12:L:113:ARG:NH2	12:L:120:TYR:CE1	2.89	0.40
1:A:411:A:C3'	1:A:411:A:C8	3.05	0.40
1:A:1005:A:C8	1:A:1026:G:C6	3.10	0.40
5:E:121:LYS:HG3	5:E:123:LEU:CD2	2.50	0.40
1:A:865:A:H1'	1:A:918:A:O2'	2.21	0.40
12:L:19:ARG:HA	12:L:20:LYS:HZ3	1.86	0.40
2:B:239:VAL:O	2:B:240:GLN:HB3	2.21	0.40
4:D:19:LEU:CD2	4:D:19:LEU:N	2.83	0.40
1:A:1102:A:O2'	2:B:99:GLY:N	2.54	0.40
14:N:11:LYS:C	14:N:13:THR:H	2.22	0.40
6:F:25:ILE:HD12	6:F:82:ARG:HD3	2.02	0.40
1:A:1418:A:H61	1:A:1482:G:H1'	1.86	0.40
10:J:7:LYS:HE2	10:J:9:ARG:NH2	2.35	0.40
2:B:183:PRO:HA	2:B:198:ASP:OD2	2.21	0.40
2:B:157:ARG:CG	2:B:158:LEU:N	2.83	0.40
1:A:891:U:O2'	1:A:892:A:H5'	2.21	0.40
7:G:51:GLN:CB	7:G:52:GLU:OE1	2.69	0.40
7:G:75:VAL:CG2	7:G:86:GLN:HB3	2.51	0.40
1:A:1415:G:H2'	1:A:1416:G:H5'	2.02	0.40
2:B:60:ASP:O	2:B:64:ARG:HB2	2.20	0.40
13:M:106:ASN:HB3	13:M:107:ALA:H	1.50	0.40
1:A:1390:U:H2'	1:A:1391:U:C6	2.57	0.40
1:A:1517[A]:G:H2'	1:A:1518[A]:MA6:H8	2.04	0.40
1:A:1518[A]:MA6:C2	1:A:1519[A]:MA6:C5	2.99	0.40
1:A:427:U:O4	1:A:428:G:C6	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:G:H2'	1:A:109:A:OP1	2.21	0.40
1:A:1305:G:P	21:U:2:GLY:N	2.94	0.40
1:A:919:A:O5'	1:A:919:A:H8	2.04	0.40
1:A:1124:G:N2	1:A:1127:G:H21	2.19	0.40
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.85	0.40
19:S:31:ILE:HG21	19:S:49:ILE:HD12	2.02	0.40
17:Q:63:ARG:HA	17:Q:64:PRO:HD3	1.90	0.40
3:C:88:ARG:NH2	3:C:101:LEU:HD23	2.36	0.40
17:Q:9:VAL:HG23	17:Q:9:VAL:H	1.70	0.40
13:M:6:GLY:O	13:M:7:VAL:C	2.59	0.40
1:A:149:A:H2'	1:A:150:C:C6	2.56	0.40
2:B:15:VAL:O	2:B:15:VAL:HG12	2.21	0.40
1:A:972:C:OP1	10:J:57:LYS:NZ	2.50	0.40
11:K:73:MET:HE3	11:K:73:MET:HB2	1.97	0.40
7:G:65:ALA:HA	7:G:128:ALA:HA	2.03	0.40
7:G:65:ALA:HB2	7:G:128:ALA:CB	2.50	0.40
1:A:47:C:H6	1:A:365:U:H2'	1.86	0.40
1:A:367:U:O2	1:A:369:C:C6	2.73	0.40
19:S:3:ARG:HD3	19:S:3:ARG:HA	1.76	0.40
3:C:131:ARG:HH21	3:C:166:GLU:CD	2.25	0.40
2:B:214:ILE:N	2:B:214:ILE:HD12	2.36	0.40
1:A:643:C:C3'	1:A:644:G:H5''	2.52	0.40
1:A:79:G:N1	1:A:80:G:C5	2.89	0.40
1:A:1440:C:H2'	1:A:1441:G:O4'	2.22	0.40
1:A:1027:C:C6	1:A:1035:A:C2	3.10	0.40
1:A:1236:A:OP1	21:U:3:LYS:HG3	2.21	0.40
1:A:660:G:C2	1:A:746:A:C2	3.10	0.40
1:A:246:A:C4	1:A:279:A:N6	2.90	0.40
5:E:112:LEU:C	5:E:114:GLY:H	2.25	0.40
1:A:838:G:C2	1:A:849:C:C2	3.10	0.40
1:A:848:C:C6	1:A:848:C:C3'	3.05	0.40
1:A:393:A:N3	1:A:394:G:C8	2.89	0.40
17:Q:27:PHE:HA	17:Q:28:PRO:HD3	1.84	0.40
1:A:777:A:N3	1:A:777:A:C2'	2.85	0.40
2:B:16:HIS:CD2	2:B:17:PHE:CD2	2.96	0.40
8:H:120:THR:O	8:H:121:ASP:C	2.59	0.40
1:A:166:G:C6	1:A:167:G:N7	2.89	0.40
12:L:86:ARG:HG3	12:L:86:ARG:NH1	2.33	0.40
23:W:32:C:O2'	23:W:33:U:H6	2.03	0.40
7:G:111:ARG:HG2	7:G:112:PRO:HD2	2.03	0.40
1:A:1133:G:H1	1:A:1141:C:N4	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:18:TYR:CD2	21:U:22:ARG:HD3	2.56	0.40
1:A:36:C:C2	1:A:37:U:C6	3.10	0.40
1:A:543:C:C2'	1:A:544:G:C5'	2.79	0.40
7:G:5:ARG:HE	7:G:7:ALA:HA	1.86	0.40
1:A:1032:G:H2'	1:A:1033:G:C8	2.57	0.40
1:A:1027:C:H5	1:A:1035:A:N1	2.16	0.40
13:M:23:TYR:CZ	13:M:71:ARG:HG3	2.57	0.40
1:A:747:C:C6	1:A:747:C:C3'	3.04	0.40
13:M:91:ARG:HH21	13:M:96:LEU:HB2	1.86	0.40
12:L:45:PRO:HB3	12:L:93:LEU:CD2	2.49	0.40
2:B:109:SER:O	2:B:112:VAL:HB	2.21	0.40
5:E:12:LEU:HG	5:E:13:ILE:N	2.36	0.40
15:O:16:ALA:CB	15:O:21:ASP:HB3	2.38	0.40
1:A:977:A:C2'	1:A:978:A:C5'	2.98	0.40
1:A:115:G:O2'	1:A:116:A:OP2	2.22	0.40
1:A:392:G:C4	1:A:393:A:C8	3.09	0.40
3:C:126:ARG:HE	3:C:128:PHE:HD1	1.68	0.40
19:S:62:ILE:HG13	19:S:66:MET:HE2	2.03	0.40
2:B:130:ARG:HA	2:B:131:PRO:HD2	1.88	0.40
1:A:632:A:H5''	1:A:633:G:OP2	2.21	0.40
1:A:1158:C:C5	1:A:1160:G:C8	3.09	0.40
15:O:70:LEU:HD22	15:O:78:TYR:HA	2.02	0.40
20:T:78:ALA:O	20:T:79:ARG:C	2.59	0.40
1:A:1425:U:O2	1:A:1426:C:C6	2.75	0.40
1:A:1244:C:C2	1:A:1294:G:N2	2.90	0.40
2:B:180:LEU:HB2	2:B:182:ILE:HG13	2.04	0.40
7:G:51:GLN:O	7:G:52:GLU:CG	2.69	0.40
1:A:735:C:H1'	18:R:75:ILE:CD1	2.52	0.40
1:A:1372:U:H2'	1:A:1373:G:O4'	2.22	0.40
9:I:70:LYS:O	9:I:74:ILE:HG12	2.21	0.40
10:J:79:ARG:HB3	10:J:80:LYS:HE2	2.03	0.40
1:A:1502:A:H2	1:A:1505:G:N1	2.20	0.40
1:A:35:G:H2'	1:A:36:C:H6	1.87	0.40
1:A:503:C:H2'	1:A:504:C:C6	2.55	0.40
12:L:113:ARG:CZ	12:L:120:TYR:HD1	2.35	0.40
1:A:328:C:O2'	1:A:329:A:P	2.74	0.40
2:B:75:LYS:HG2	2:B:78:GLN:HG3	2.04	0.40
1:A:961:U:H2'	1:A:962:C:O4'	2.22	0.40
2:B:172:ILE:HD13	2:B:172:ILE:N	2.33	0.40
15:O:42:HIS:HE1	15:O:46:HIS:CD2	2.39	0.40
3:C:47:LEU:O	3:C:50:ALA:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:C:C3'	1:A:443:C:H5'	2.51	0.40
1:A:490:G:C4	1:A:491:G:C8	3.10	0.40
1:A:1234:C:C2'	1:A:1235:U:H5'	2.52	0.40
6:F:73:ASN:O	6:F:74:ASP:C	2.59	0.40
10:J:9:ARG:CB	10:J:9:ARG:NH1	2.85	0.40
13:M:63:THR:CG2	13:M:64:TRP:N	2.84	0.40
8:H:14:ARG:CZ	8:H:14:ARG:HB2	2.50	0.40
3:C:31:HIS:HA	3:C:34:LEU:HB3	2.04	0.40
1:A:1378:C:O2	7:G:76:ARG:NH1	2.55	0.40
1:A:765:G:C6	1:A:812:C:C2	3.09	0.40
10:J:11:PHE:HD2	10:J:11:PHE:HA	1.63	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:U:O2	1:A:1400:5MC:N4[3_545]	2.15	0.05
5:E:73:ASN:N	5:E:149:GLU:OE1[7_555]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/256 (91%)	197 (84%)	34 (14%)	3 (1%)	15	61
3	C	205/239 (86%)	169 (82%)	35 (17%)	1 (0%)	34	77
4	D	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	34	77
5	E	149/162 (92%)	137 (92%)	11 (7%)	1 (1%)	26	72
6	F	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	G	153/156 (98%)	132 (86%)	21 (14%)	0	100	100
8	H	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	26	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	24	70
10	J	97/105 (92%)	77 (79%)	17 (18%)	3 (3%)	5	45
11	K	115/129 (89%)	98 (85%)	17 (15%)	0	100	100
12	L	122/135 (90%)	110 (90%)	8 (7%)	4 (3%)	5	44
13	M	116/126 (92%)	99 (85%)	16 (14%)	1 (1%)	21	68
14	N	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
15	O	86/89 (97%)	72 (84%)	14 (16%)	0	100	100
16	P	82/88 (93%)	74 (90%)	7 (8%)	1 (1%)	16	63
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	R	69/88 (78%)	60 (87%)	9 (13%)	0	100	100
19	S	79/93 (85%)	68 (86%)	9 (11%)	2 (2%)	7	49
20	T	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	19	66
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2349/2541 (92%)	2046 (87%)	283 (12%)	20 (1%)	21	68

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	15	THR
9	I	119	ALA
12	L	28	LYS
16	P	83	GLU
19	S	31	ILE
10	J	81	THR
10	J	86	MET
19	S	6	LYS
12	L	115	LYS
20	T	73	HIS
2	B	21	ARG
2	B	95	GLN
2	B	229	VAL
5	E	153	LYS
8	H	121	ASP
12	L	27	LEU
10	J	34	VAL
12	L	71	PRO
13	M	7	VAL
4	D	67	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	201/220 (91%)	151 (75%)	50 (25%)	1	6
3	C	160/188 (85%)	119 (74%)	41 (26%)	0	6
4	D	180/181 (99%)	134 (74%)	46 (26%)	0	6
5	E	115/123 (94%)	75 (65%)	40 (35%)	0	2
6	F	90/90 (100%)	60 (67%)	30 (33%)	0	2
7	G	126/127 (99%)	92 (73%)	34 (27%)	0	5
8	H	119/119 (100%)	83 (70%)	36 (30%)	0	4
9	I	98/99 (99%)	75 (76%)	23 (24%)	1	7
10	J	87/92 (95%)	70 (80%)	17 (20%)	2	13
11	K	89/99 (90%)	72 (81%)	17 (19%)	2	13
12	L	103/110 (94%)	80 (78%)	23 (22%)	1	9
13	M	94/101 (93%)	64 (68%)	30 (32%)	0	3
14	N	49/50 (98%)	35 (71%)	14 (29%)	0	4
15	O	79/80 (99%)	60 (76%)	19 (24%)	1	7
16	P	72/74 (97%)	54 (75%)	18 (25%)	1	6
17	Q	95/97 (98%)	74 (78%)	21 (22%)	1	9
18	R	62/77 (80%)	48 (77%)	14 (23%)	1	8
19	S	71/80 (89%)	55 (78%)	16 (22%)	1	9
20	T	76/82 (93%)	51 (67%)	25 (33%)	0	3
21	U	19/22 (86%)	16 (84%)	3 (16%)	3	23
All	All	1985/2111 (94%)	1468 (74%)	517 (26%)	0	5

All (517) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	11	LEU
2	B	16	HIS

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Mol	Chain	Res	Type
2	B	17	PHE
2	B	20	GLU
2	B	30	ARG
2	B	33	TYR
2	B	35	GLU
2	B	39	ILE
2	B	44	LEU
2	B	53	ARG
2	B	61	LEU
2	B	63	MET
2	B	64	ARG
2	B	67	THR
2	B	69	LEU
2	B	92	TYR
2	B	97	TRP
2	B	101	MET
2	B	107	THR
2	B	109	SER
2	B	111	ARG
2	B	114	ARG
2	B	115	LEU
2	B	122	PHE
2	B	127	ILE
2	B	128	GLU
2	B	144	ARG
2	B	150	SER
2	B	153	ARG
2	B	162	ILE
2	B	163	PHE
2	B	169	LYS
2	B	172	ILE
2	B	182	ILE
2	B	187	LEU
2	B	189	ASP
2	B	193	ASP
2	B	196	LEU
2	B	200	ILE
2	B	204	ASN
2	B	209	ARG
2	B	210	SER
2	B	212	GLN
2	B	215	LEU

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Mol	Chain	Res	Type
2	B	216	SER
2	B	221	LEU
2	B	226	ARG
2	B	236	TYR
2	B	240	GLN
3	C	3	ASN
3	C	8	ILE
3	C	10	PHE
3	C	14	ILE
3	C	16	ARG
3	C	21	ARG
3	C	22	TRP
3	C	31	HIS
3	C	33	LEU
3	C	43	LEU
3	C	45	LYS
3	C	52	LEU
3	C	58	GLU
3	C	64	VAL
3	C	70	VAL
3	C	72	LYS
3	C	75	VAL
3	C	79	ARG
3	C	85	ARG
3	C	99	VAL
3	C	101	LEU
3	C	111	LEU
3	C	119	ARG
3	C	126	ARG
3	C	127	ARG
3	C	130	VAL
3	C	134	ILE
3	C	144	SER
3	C	147	LYS
3	C	156	ARG
3	C	165	THR
3	C	167	TRP
3	C	170	GLN
3	C	175	LEU
3	C	186	PHE
3	C	188	LEU
3	C	190	ARG

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Mol	Chain	Res	Type
3	C	192	THR
3	C	193	TYR
3	C	196	LEU
3	C	204	LEU
4	D	10	ARG
4	D	19	LEU
4	D	20	TYR
4	D	26	CYS
4	D	28	SER
4	D	47	ARG
4	D	49	ARG
4	D	57	ARG
4	D	61	LYS
4	D	66	ARG
4	D	73	ARG
4	D	78	LEU
4	D	84	LYS
4	D	85	LYS
4	D	86	LYS
4	D	91	SER
4	D	92	VAL
4	D	96	LEU
4	D	107	ARG
4	D	108	LEU
4	D	114	ARG
4	D	115	ARG
4	D	119	GLN
4	D	120	LEU
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	132	ARG
4	D	145	GLU
4	D	146	ILE
4	D	150	GLU
4	D	159	ARG
4	D	163	GLU
4	D	169	LYS
4	D	177	ASP
4	D	178	VAL
4	D	179	GLU
4	D	182	LYS

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Mol	Chain	Res	Type
4	D	187	ARG
4	D	188	LEU
4	D	190	ASP
4	D	192	GLU
4	D	193	ASP
4	D	194	LEU
4	D	196	LEU
4	D	204	ILE
5	E	6	PHE
5	E	11	ILE
5	E	12	LEU
5	E	16	THR
5	E	18	ARG
5	E	24	ARG
5	E	31	LEU
5	E	32	VAL
5	E	37	ARG
5	E	38	GLN
5	E	43	LEU
5	E	47	LYS
5	E	51	VAL
5	E	53	LEU
5	E	55	VAL
5	E	60	TYR
5	E	65	ASN
5	E	66	MET
5	E	67	VAL
5	E	68	GLU
5	E	75	THR
5	E	76	ILE
5	E	78	HIS
5	E	79	GLU
5	E	80	ILE
5	E	82	VAL
5	E	83	GLU
5	E	84	PHE
5	E	100	VAL
5	E	105	VAL
5	E	110	LEU
5	E	116	THR
5	E	123	LEU
5	E	125	SER

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Mol	Chain	Res	Type
5	E	126	ARG
5	E	131	ILE
5	E	145	LYS
5	E	147	ASP
5	E	148	VAL
5	E	150	ARG
6	F	1	MET
6	F	2	ARG
6	F	7	ASN
6	F	9	VAL
6	F	10	LEU
6	F	14	LEU
6	F	16	GLN
6	F	21	LEU
6	F	24	GLU
6	F	25	ILE
6	F	28	ARG
6	F	37	VAL
6	F	39	LYS
6	F	43	LEU
6	F	54	LYS
6	F	64	GLN
6	F	65	VAL
6	F	74	ASP
6	F	75	LEU
6	F	80	ARG
6	F	83	ASP
6	F	84	ASN
6	F	86	ARG
6	F	87	ARG
6	F	89	MET
6	F	93	SER
6	F	94	GLN
6	F	97	PHE
6	F	98	LEU
6	F	100	ASN
7	G	9	VAL
7	G	10	ARG
7	G	12	LEU
7	G	15	ASP
7	G	16	LEU
7	G	17	VAL

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Mol	Chain	Res	Type
7	G	22	LEU
7	G	27	ILE
7	G	29	LYS
7	G	38	LEU
7	G	41	ARG
7	G	49	ILE
7	G	52	GLU
7	G	60	LYS
7	G	62	PHE
7	G	66	VAL
7	G	72	ARG
7	G	75	VAL
7	G	78	ARG
7	G	87	VAL
7	G	92	SER
7	G	97	GLN
7	G	101	LEU
7	G	113	GLU
7	G	114	ARG
7	G	115	ARG
7	G	120	ILE
7	G	122	HIS
7	G	124	LEU
7	G	126	ASP
7	G	129	GLU
7	G	135	VAL
7	G	146	GLU
7	G	156	TRP
8	H	1	MET
8	H	3	THR
8	H	8	ASP
8	H	10	LEU
8	H	11	THR
8	H	14	ARG
8	H	18	ARG
8	H	19	VAL
8	H	22	GLU
8	H	39	LEU
8	H	45	ILE
8	H	51	VAL
8	H	53	VAL
8	H	57	PRO

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Mol	Chain	Res	Type
8	H	59	LEU
8	H	63	LEU
8	H	81	HIS
8	H	83	ILE
8	H	85	ARG
8	H	87	SER
8	H	91	ARG
8	H	95	VAL
8	H	97	VAL
8	H	98	LYS
8	H	100	ILE
8	H	102	ARG
8	H	104	ARG
8	H	105	ARG
8	H	112	LEU
8	H	113	SER
8	H	119	LEU
8	H	121	ASP
8	H	127	LEU
8	H	133	LEU
8	H	135	CYS
8	H	136	GLU
9	I	2	GLU
9	I	5	TYR
9	I	14	VAL
9	I	16	ARG
9	I	23	ASN
9	I	29	ASN
9	I	33	PHE
9	I	34	ASN
9	I	40	LEU
9	I	48	GLU
9	I	59	PHE
9	I	62	TYR
9	I	63	ILE
9	I	64	THR
9	I	65	VAL
9	I	66	ARG
9	I	79	LEU
9	I	85	LEU
9	I	99	LEU
9	I	102	LEU

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Mol	Chain	Res	Type
9	I	109	VAL
9	I	112	LYS
9	I	125	TYR
10	J	4	ILE
10	J	9	ARG
10	J	12	ASP
10	J	19	SER
10	J	28	ARG
10	J	29	ARG
10	J	33	GLN
10	J	44	VAL
10	J	62	HIS
10	J	63	PHE
10	J	67	THR
10	J	78	ASN
10	J	89	ASP
10	J	90	LEU
10	J	94	VAL
10	J	98	ILE
10	J	99	LYS
11	K	11	LYS
11	K	29	ILE
11	K	40	ILE
11	K	57	THR
11	K	70	LYS
11	K	75	TYR
11	K	78	GLN
11	K	80	VAL
11	K	92	GLU
11	K	96	ARG
11	K	99	GLN
11	K	105	VAL
11	K	116	HIS
11	K	117	ASN
11	K	120	ARG
11	K	125	PHE
11	K	126	ARG
12	L	7	ILE
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS
12	L	32	PHE

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Mol	Chain	Res	Type
12	L	34	ARG
12	L	36	VAL
12	L	43	VAL
12	L	44	THR
12	L	50	SER
12	L	52	LEU
12	L	53	ARG
12	L	54	LYS
12	L	60	LEU
12	L	75	HIS
12	L	81	SER
12	L	82	VAL
12	L	98	TYR
12	L	101	VAL
12	L	113	ARG
12	L	116	SER
12	L	122	THR
12	L	127	GLU
13	M	7	VAL
13	M	11	ARG
13	M	14	ARG
13	M	17	VAL
13	M	22	ILE
13	M	27	LYS
13	M	32	GLU
13	M	44	ARG
13	M	46	LYS
13	M	48	LEU
13	M	50	GLU
13	M	52	GLU
13	M	55	ARG
13	M	56	LEU
13	M	57	ARG
13	M	58	GLU
13	M	59	TYR
13	M	64	TRP
13	M	67	GLU
13	M	69	GLU
13	M	70	LEU
13	M	74	VAL
13	M	81	LEU
13	M	84	ILE

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Mol	Chain	Res	Type
13	M	87	TYR
13	M	88	ARG
13	M	94	ARG
13	M	99	ARG
13	M	102	ARG
13	M	105	THR
14	N	3	ARG
14	N	6	LEU
14	N	7	ILE
14	N	9	LYS
14	N	12	ARG
14	N	17	LYS
14	N	24	CYS
14	N	27	CYS
14	N	29	ARG
14	N	33	VAL
14	N	45	ARG
14	N	46	GLU
14	N	49	HIS
14	N	58	LYS
15	O	6	GLU
15	O	11	VAL
15	O	17	ARG
15	O	24	SER
15	O	26	GLU
15	O	31	LEU
15	O	38	ARG
15	O	39	LEU
15	O	40	SER
15	O	45	VAL
15	O	47	LYS
15	O	54	ARG
15	O	56	LEU
15	O	57	LEU
15	O	67	LEU
15	O	73	GLU
15	O	81	LEU
15	O	87	ILE
15	O	88	ARG
16	P	1	MET
16	P	8	ARG
16	P	11	SER

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Mol	Chain	Res	Type
16	P	18	ARG
16	P	22	THR
16	P	25	ARG
16	P	42	ARG
16	P	45	THR
16	P	48	TRP
16	P	53	VAL
16	P	54	GLU
16	P	55	ARG
16	P	62	VAL
16	P	69	THR
16	P	72	ARG
16	P	75	ARG
16	P	79	VAL
16	P	81	ARG
17	Q	10	VAL
17	Q	13	ASP
17	Q	23	VAL
17	Q	27	PHE
17	Q	29	HIS
17	Q	36	ILE
17	Q	40	LYS
17	Q	43	LEU
17	Q	50	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	62	SER
17	Q	70	ARG
17	Q	72	ARG
17	Q	77	VAL
17	Q	85	VAL
17	Q	90	ILE
17	Q	91	ARG
17	Q	92	ARG
17	Q	93	GLN
17	Q	98	LEU
18	R	18	ARG
18	R	26	LEU
18	R	31	LEU
18	R	38	GLU
18	R	42	ARG
18	R	44	LEU

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Mol	Chain	Res	Type
18	R	46	GLU
18	R	58	LEU
18	R	70	ILE
18	R	78	LEU
18	R	82	THR
18	R	86	VAL
18	R	87	ARG
18	R	88	LYS
19	S	4	SER
19	S	7	LYS
19	S	11	VAL
19	S	14	HIS
19	S	15	LEU
19	S	16	LEU
19	S	17	GLU
19	S	27	GLU
19	S	29	ARG
19	S	31	ILE
19	S	37	ARG
19	S	39	THR
19	S	43	GLU
19	S	58	VAL
19	S	64	GLU
19	S	71	LEU
20	T	8	ARG
20	T	9	ASN
20	T	10	LEU
20	T	11	SER
20	T	13	LEU
20	T	15	ARG
20	T	17	ARG
20	T	19	SER
20	T	20	LEU
20	T	24	LEU
20	T	33	ILE
20	T	45	GLN
20	T	55	ILE
20	T	62	LEU
20	T	72	LEU
20	T	74	LYS
20	T	75	ASN
20	T	80	ARG

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Mol	Chain	Res	Type
20	T	85	MET
20	T	86	ARG
20	T	87	LYS
20	T	91	LEU
20	T	99	LEU
20	T	100	ILE
20	T	104	LEU
21	U	10	ARG
21	U	15	ARG
21	U	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	212	GLN
3	C	6	HIS
4	D	125	HIS
5	E	65	ASN
7	G	37	ASN
9	I	73	GLN
12	L	75	HIS
13	M	101	GLN
15	O	42	HIS
16	P	16	HIS
19	S	23	ASN
19	S	57	HIS
20	T	9	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1522 (98%)	377 (25%)	48 (3%)
22	V	3/4 (75%)	1 (33%)	0
23	W	10/11 (90%)	2 (20%)	0
24	a	7/8 (87%)	4 (57%)	0
25	b	2/3 (66%)	0	0
All	All	1525/1548 (98%)	384 (25%)	48 (3%)

All (384) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	16	A
1	A	31	G
1	A	32	A
1	A	33	A
1	A	34	C
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	81	U
1	A	82	U
1	A	88	A
1	A	89	C
1	A	90	U
1	A	91	C
1	A	95	U
1	A	99	C
1	A	105	G
1	A	108	G
1	A	109	A
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	138	G
1	A	144	G
1	A	151	A
1	A	157	G
1	A	159	G
1	A	162	A
1	A	163	C
1	A	170	U
1	A	173	U
1	A	181	G
1	A	182	U
1	A	183	G
1	A	190(B)	C
1	A	190(E)	U

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Mol	Chain	Res	Type
1	A	190(G)	G
1	A	195	A
1	A	197	A
1	A	199	G
1	A	201	C
1	A	202	U
1	A	216	G
1	A	222	U
1	A	225	C
1	A	230	G
1	A	246	A
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	253	U
1	A	254	G
1	A	258	G
1	A	260	G
1	A	266	G
1	A	267	C
1	A	276	G
1	A	289	G
1	A	299	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	345	C
1	A	346	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	381	C
1	A	384	G
1	A	387	U

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Mol	Chain	Res	Type
1	A	388	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	410	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	435	C
1	A	439	A
1	A	442	C
1	A	443	C
1	A	449	C
1	A	450	G
1	A	452	A
1	A	460	A
1	A	461	C
1	A	462	G
1	A	475	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	500	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	520	A
1	A	527	7MG
1	A	530	G
1	A	532	A
1	A	533	A
1	A	544	G
1	A	545	C
1	A	547	A
1	A	550	G

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Mol	Chain	Res	Type
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	566	G
1	A	568	G
1	A	569	C
1	A	571	U
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	578	C
1	A	587	G
1	A	588	G
1	A	607	A
1	A	624	C
1	A	629	G
1	A	631	G
1	A	644	G
1	A	651	C
1	A	653	A
1	A	661	G
1	A	665	A
1	A	671	G
1	A	673	G
1	A	675	A
1	A	687	A
1	A	688	G
1	A	695	A
1	A	698	G
1	A	701	C
1	A	702	A
1	A	704	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	728	A
1	A	731	G
1	A	734	G

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Mol	Chain	Res	Type
1	A	741	G
1	A	747	C
1	A	748	C
1	A	752	G
1	A	755	G
1	A	777	A
1	A	785	G
1	A	786	G
1	A	788	U
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	804	U
1	A	812	C
1	A	813	U
1	A	815	A
1	A	816	A
1	A	817	C
1	A	827	U
1	A	828	A
1	A	829	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	866	C
1	A	867	G
1	A	868	C
1	A	869	G
1	A	873	A
1	A	889	A
1	A	902	G
1	A	905	U
1	A	914	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	933	G
1	A	934	C

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Mol	Chain	Res	Type
1	A	935	A
1	A	944	G
1	A	950	U
1	A	954	G
1	A	961	U
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
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
1	A	992	U
1	A	993	G
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1021	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1030(B)	C
1	A	1030(C)	G
1	A	1045	C
1	A	1048	G
1	A	1050	G
1	A	1052	U
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U

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Mol	Chain	Res	Type
1	A	1079	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1104	G
1	A	1111	A
1	A	1122	U
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1141	C
1	A	1142	G
1	A	1143	G
1	A	1159	U
1	A	1162	C
1	A	1164	G
1	A	1171	G
1	A	1178	G
1	A	1181	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1193	G
1	A	1196	U
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

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Mol	Chain	Res	Type
1	A	1215	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1235	U
1	A	1238	A
1	A	1245	A
1	A	1249	C
1	A	1250	A
1	A	1251	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1273	G
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1312	G
1	A	1313	U
1	A	1317	C
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1328	C
1	A	1338	G
1	A	1348	U
1	A	1353	G
1	A	1356	G
1	A	1359	C

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Mol	Chain	Res	Type
1	A	1360	A
1	A	1361	G
1	A	1362	C
1	A	1363	A
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1382	C
1	A	1393	U
1	A	1394	A
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1401	G
1	A	1406	U
1	A	1407	5MC
1	A	1414	U
1	A	1418	A
1	A	1419	G
1	A	1420	C
1	A	1442	G
1	A	1443	G
1	A	1447	G
1	A	1451	A
1	A	1455	G
1	A	1478	C
1	A	1487	G
1	A	1494	G
1	A	1497	G
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1526	G
1	A	1529	G
1	A	1530	G
1	A	1534	C
1	A	1538	C
22	V	2	U
23	W	31	C

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Mol	Chain	Res	Type
23	W	33	U
24	a	35	G
24	a	37	A
24	a	39	G
24	a	40	PSU

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	89	C
1	A	115	G
1	A	129(A)	G
1	A	150	C
1	A	181	G
1	A	204	U
1	A	246	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	328	C
1	A	344	A
1	A	428	G
1	A	429	U
1	A	484	G
1	A	499	A
1	A	509	A
1	A	544	G
1	A	559	A
1	A	560	U
1	A	587	G
1	A	687	A
1	A	701	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	991	U
1	A	1026	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1137	C

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Mol	Chain	Res	Type
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1212	U
1	A	1256	A
1	A	1279	A
1	A	1281	U
1	A	1300	G
1	A	1319	A
1	A	1347	G
1	A	1360	A
1	A	1361(A)	C
1	A	1397	C
1	A	1528	U
1	A	1533	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	2MG	A	1207	1	17,26,27	2.63	6 (35%)	21,38,41	2.47	2 (9%)
1	5MC	A	1400	1	13,22,23	1.55	3 (23%)	15,32,35	0.77	0
1	4OC	A	1402	1	13,23,24	1.32	2 (15%)	18,32,35	1.16	1 (5%)
1	5MC	A	1404	1	13,22,23	1.05	1 (7%)	15,32,35	1.09	2 (13%)
1	5MC	A	1407	1	13,22,23	2.02	3 (23%)	15,32,35	1.09	1 (6%)
1	UR3	A	1498	1	12,22,23	0.86	1 (8%)	16,32,35	1.33	3 (18%)
1	MA6	A	1518[A]	1	16,26,27	1.36	3 (18%)	18,38,41	1.10	2 (11%)
1	MA6	A	1518[B]	1	16,26,27	1.19	2 (12%)	18,38,41	1.14	2 (11%)
1	MA6	A	1519[A]	1	16,26,27	1.12	2 (12%)	18,38,41	1.38	4 (22%)
1	MA6	A	1519[B]	1	16,26,27	2.06	5 (31%)	18,38,41	1.15	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	A	1540	1	13,21,22	1.15	1 (7%)	18,30,33	3.80	4 (22%)
1	PSU	A	516	1	13,21,22	1.47	2 (15%)	18,30,33	3.95	4 (22%)
1	7MG	A	527	1	19,26,27	2.87	5 (26%)	24,39,42	1.70	4 (16%)
1	M2G	A	966	1	17,27,28	1.38	3 (17%)	22,40,43	2.02	3 (13%)
1	5MC	A	967	1	13,22,23	0.89	0	15,32,35	0.96	1 (6%)
12	0TD	L	92	12	4,9,10	1.07	0	4,11,13	4.01	3 (75%)
23	PSU	W	40	23	13,21,22	1.10	2 (15%)	18,30,33	3.58	5 (27%)
24	PSU	a	40	24,1	13,21,22	1.77	2 (15%)	18,30,33	4.25	5 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	0/3/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/3/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[B]	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	0/7/37/38	0/3/3/3
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	5MC	A	967	1	-	0/3/25/26	0/2/2/2
12	0TD	L	92	12	-	0/2/12/14	0/0/0/0
23	PSU	W	40	23	-	0/7/25/26	0/2/2/2
24	PSU	a	40	24,1	-	0/7/25/26	0/2/2/2

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-9.11	1.32	1.45
1	A	527	7MG	CM7-N7	-2.81	1.41	1.46
1	A	527	7MG	C8-N7	-2.44	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C4-N3	-2.24	1.30	1.34
1	A	1498	UR3	C6-N1	-2.19	1.32	1.35
23	W	40	PSU	C5-C1'	-2.09	1.50	1.52
1	A	1407	5MC	C4-N4	2.01	1.39	1.34
1	A	1519[A]	MA6	C5-C4	2.02	1.45	1.40
1	A	1207	2MG	C4-N3	2.04	1.38	1.35
1	A	1404	5MC	C5-C4	2.12	1.44	1.41
1	A	966	M2G	C2-N1	2.30	1.38	1.34
1	A	966	M2G	C4-N3	2.32	1.39	1.35
1	A	1400	5MC	C6-N1	2.34	1.38	1.35
1	A	1207	2MG	C5-C4	2.38	1.45	1.40
1	A	1519[A]	MA6	C2-N1	2.39	1.38	1.33
1	A	1518[A]	MA6	C4-N3	2.43	1.39	1.35
23	W	40	PSU	C4-N3	2.61	1.37	1.33
1	A	1518[B]	MA6	C6-N1	2.61	1.37	1.34
24	a	40	PSU	C4-N3	2.67	1.38	1.33
1	A	1407	5MC	C6-N1	2.68	1.39	1.35
1	A	1518[B]	MA6	C2-N1	2.71	1.39	1.33
1	A	1519[B]	MA6	C4-N3	2.71	1.39	1.35
1	A	1402	4OC	CM4-N4	2.72	1.50	1.45
1	A	1518[A]	MA6	C2-N1	2.79	1.39	1.33
1	A	516	PSU	C5-C1'	2.92	1.54	1.52
1	A	1518[A]	MA6	C5-C4	2.92	1.47	1.40
1	A	1400	5MC	C4-N4	3.01	1.41	1.34
1	A	1400	5MC	C5-C4	3.05	1.46	1.41
1	A	1207	2MG	C2-N1	3.07	1.45	1.34
1	A	1519[B]	MA6	C5-C4	3.14	1.47	1.40
1	A	1540	PSU	C4-N3	3.22	1.39	1.33
1	A	1519[B]	MA6	C2-N3	3.34	1.38	1.32
1	A	516	PSU	C4-N3	3.37	1.39	1.33
1	A	1207	2MG	C6-C5	3.49	1.48	1.41
1	A	966	M2G	C6-N1	3.86	1.40	1.33
1	A	1519[B]	MA6	C2-N1	4.17	1.41	1.33
1	A	527	7MG	C4-N3	4.29	1.39	1.34
1	A	1519[B]	MA6	C6-N1	4.49	1.40	1.34
1	A	527	7MG	C2-N2	4.51	1.43	1.34
24	a	40	PSU	C5-C1'	5.22	1.56	1.52
1	A	1207	2MG	C2-N2	5.95	1.41	1.34
1	A	1407	5MC	C5-C4	6.05	1.50	1.41
1	A	1207	2MG	C6-N1	6.67	1.45	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	40	PSU	N1-C2-N3	-15.39	118.52	128.33
1	A	516	PSU	N1-C2-N3	-14.33	119.19	128.33
1	A	1540	PSU	N1-C2-N3	-14.07	119.36	128.33
23	W	40	PSU	N1-C2-N3	-12.77	120.19	128.33
1	A	1207	2MG	C5-C6-N1	-9.52	110.58	123.59
1	A	966	M2G	C5-C6-N1	-8.37	112.14	123.59
12	L	92	0TD	CB-CA-N	-6.15	96.33	109.66
1	A	527	7MG	C5-C4-N3	-5.65	121.31	126.82
12	L	92	0TD	CSB-SB-CB	-4.23	93.56	101.54
1	A	1402	4OC	CM4-N4-C4	-3.99	119.52	122.98
23	W	40	PSU	C5-C1'-C2'	-3.25	109.75	115.52
24	a	40	PSU	C5-C6-N1	-3.23	119.83	124.39
1	A	1407	5MC	N4-C4-N3	-3.05	112.52	116.95
23	W	40	PSU	C5-C6-N1	-2.97	120.20	124.39
1	A	966	M2G	C2-N3-C4	-2.34	112.27	115.09
12	L	92	0TD	C-CA-N	-2.31	105.00	109.83
1	A	1498	UR3	C5-C4-N3	-2.31	112.57	117.45
1	A	1519[A]	MA6	C1'-N9-C4	-2.19	123.64	126.94
1	A	966	M2G	N1-C2-N2	-2.19	114.69	117.16
1	A	1498	UR3	C3U-N3-C2	-2.06	115.08	119.51
1	A	1519[A]	MA6	C2'-C1'-N9	-2.02	111.21	114.29
1	A	1404	5MC	CM5-C5-C6	2.03	122.70	118.62
1	A	1404	5MC	C5-C4-N3	2.11	124.79	121.27
1	A	527	7MG	C6-N1-C2	2.19	118.98	115.94
1	A	527	7MG	N3-C4-N9	2.28	130.18	126.75
1	A	1518[B]	MA6	N3-C2-N1	2.32	130.67	128.89
1	A	527	7MG	C2-N3-C4	2.48	121.76	114.53
1	A	1519[B]	MA6	N3-C2-N1	2.51	130.81	128.89
1	A	1540	PSU	O4'-C1'-C2'	2.60	107.38	104.73
1	A	1519[B]	MA6	C2-N1-C6	2.66	117.08	111.43
1	A	1519[A]	MA6	C2-N1-C6	2.69	117.16	111.43
1	A	1519[A]	MA6	N3-C2-N1	2.70	130.96	128.89
1	A	1518[A]	MA6	C2-N1-C6	2.76	117.30	111.43
1	A	967	5MC	CM5-C5-C6	2.76	124.18	118.62
1	A	1518[A]	MA6	N3-C2-N1	2.80	131.04	128.89
1	A	1518[B]	MA6	C2-N1-C6	2.84	117.48	111.43
23	W	40	PSU	C6-N1-C2	3.03	120.33	115.47
1	A	1498	UR3	C6-C5-C4	3.21	123.29	117.28
1	A	516	PSU	C6-N1-C2	3.24	120.68	115.47
1	A	516	PSU	O4'-C1'-C2'	3.36	108.16	104.73
1	A	1540	PSU	C6-N1-C2	3.38	120.91	115.47
24	a	40	PSU	C5-C1'-C2'	4.59	123.66	115.52
24	a	40	PSU	C6-N1-C2	5.08	123.63	115.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C6-N1-C2	5.15	122.80	115.31
24	a	40	PSU	C4-N3-C2	5.33	119.85	115.25
1	A	1540	PSU	C4-N3-C2	5.75	120.22	115.25
23	W	40	PSU	C4-N3-C2	5.78	120.25	115.25
1	A	516	PSU	C4-N3-C2	6.45	120.82	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	11	0
1	A	1400	5MC	5	1
1	A	1402	4OC	5	0
1	A	1404	5MC	5	0
1	A	1407	5MC	10	0
1	A	1498	UR3	8	0
1	A	1518[A]	MA6	10	0
1	A	1518[B]	MA6	9	0
1	A	1519[A]	MA6	18	0
1	A	1519[B]	MA6	11	0
1	A	516	PSU	1	0
1	A	527	7MG	1	0
1	A	966	M2G	3	0
1	A	967	5MC	4	0
12	L	92	0TD	2	0
23	W	40	PSU	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 347 ligands modelled in this entry, 346 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
27	SRY	A	1928	-	33,42,42	1.48	5 (15%)	36,63,63	2.60	15 (41%)

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
27	SRY	A	1928	-	-	0/16/87/87	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1928	SRY	O53-C53	-3.48	1.35	1.44
27	A	1928	SRY	C11-N11	-3.32	1.41	1.47
27	A	1928	SRY	C23-N23	-3.04	1.42	1.47
27	A	1928	SRY	C21-C11	-2.31	1.48	1.53
27	A	1928	SRY	O51-C51	-2.00	1.38	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	1928	SRY	C43-C33-C23	-8.01	99.32	110.43
27	A	1928	SRY	C13-O13-C22	-5.30	106.79	116.30
27	A	1928	SRY	C61-C11-N11	-4.35	98.51	111.38
27	A	1928	SRY	O51-C51-C61	-3.03	103.52	110.34
27	A	1928	SRY	O53-C53-C63	-2.41	100.26	106.36
27	A	1928	SRY	O63-C63-C53	-2.15	104.24	111.33
27	A	1928	SRY	C63-C53-C43	-2.07	107.92	113.02
27	A	1928	SRY	O51-C51-C41	2.01	114.63	109.87
27	A	1928	SRY	O43-C43-C33	2.36	115.64	110.34
27	A	1928	SRY	O21-C21-C31	2.97	115.72	109.66
27	A	1928	SRY	C51-C61-C11	3.34	115.05	110.43
27	A	1928	SRY	O32-C32-C22	3.49	119.76	111.64
27	A	1928	SRY	O41-C41-C51	3.81	116.99	107.17
27	A	1928	SRY	O53-C53-C43	3.82	116.86	109.68
27	A	1928	SRY	O53-C13-C23	3.85	119.15	110.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	1928	SRY	14	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1500/1522 (98%)	-0.43	2 (0%) 95 93	80, 129, 232, 327	0
2	B	236/256 (92%)	-0.15	2 (0%) 87 77	62, 153, 220, 247	0
3	C	207/239 (86%)	-0.22	5 (2%) 62 46	94, 191, 226, 244	0
4	D	208/209 (99%)	-0.22	5 (2%) 62 46	105, 149, 198, 214	0
5	E	151/162 (93%)	-0.43	0 100 100	80, 114, 166, 193	0
6	F	101/101 (100%)	-0.46	1 (0%) 84 72	110, 150, 182, 226	0
7	G	155/156 (99%)	-0.38	3 (1%) 70 54	121, 160, 223, 238	0
8	H	138/138 (100%)	-0.42	0 100 100	75, 104, 138, 155	0
9	I	127/128 (99%)	0.10	3 (2%) 62 46	125, 184, 217, 240	0
10	J	99/105 (94%)	0.16	4 (4%) 42 28	81, 203, 272, 295	0
11	K	117/129 (90%)	-0.39	0 100 100	88, 130, 160, 167	0
12	L	124/135 (91%)	0.06	5 (4%) 42 28	97, 136, 168, 247	0
13	M	118/126 (93%)	0.08	5 (4%) 40 27	127, 158, 192, 211	0
14	N	60/61 (98%)	-0.19	1 (1%) 73 58	144, 169, 210, 246	0
15	O	88/89 (98%)	0.02	2 (2%) 64 47	94, 127, 182, 225	0
16	P	84/88 (95%)	-0.21	0 100 100	96, 126, 164, 239	0
17	Q	100/105 (95%)	-0.31	0 100 100	83, 111, 150, 189	0
18	R	71/88 (80%)	-0.30	0 100 100	95, 132, 178, 229	0
19	S	81/93 (87%)	0.19	2 (2%) 61 44	84, 184, 228, 234	0
20	T	99/106 (93%)	-0.25	0 100 100	95, 126, 167, 212	0
21	U	25/27 (92%)	0.42	2 (8%) 15 9	77, 163, 192, 220	0
22	V	4/4 (100%)	3.91	4 (100%) 0 0	263, 267, 272, 275	0
23	W	10/11 (90%)	6.93	10 (100%) 0 0	234, 291, 345, 387	5 (50%)
24	a	7/8 (87%)	0.71	1 (14%) 4 3	200, 217, 290, 330	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	b	3/3 (100%)	1.07	0 100 100	172, 172, 206, 218	0
All	All	3913/4089 (95%)	-0.25	57 (1%) 76 62	62, 140, 222, 387	5 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	W	32	C	12.9
23	W	31	C	8.5
23	W	33	U	8.1
1	A	1129	C	7.7
23	W	35	G	7.4
23	W	30	G	7.4
12	L	129	ALA	7.1
15	O	89	GLY	6.9
23	W	38	A	5.9
23	W	37	A	5.9
22	V	2	U	5.1
22	V	3	U	4.9
23	W	36	A	4.8
23	W	34	G	4.8
21	U	18	TYR	4.6
10	J	33	GLN	4.3
10	J	34	VAL	3.8
23	W	39	G	3.6
9	I	15	ALA	3.6
12	L	65	GLU	3.5
22	V	4	U	3.3
6	F	101	ALA	3.2
7	G	83	ALA	3.1
13	M	2	ALA	3.1
7	G	84	ASN	3.0
13	M	117	VAL	2.9
7	G	82	GLY	2.8
3	C	157	ILE	2.8
3	C	158	GLY	2.8
12	L	33	ARG	2.8
12	L	128	ALA	2.8
3	C	155	GLY	2.7
4	D	42	GLN	2.7
14	N	12	ARG	2.7
1	A	82	U	2.6
19	S	38	SER	2.6

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Mol	Chain	Res	Type	RSRZ
10	J	74	ILE	2.6
3	C	189	ALA	2.5
3	C	193	TYR	2.5
4	D	13	ARG	2.5
24	a	34	G	2.4
9	I	65	VAL	2.4
22	V	1	U	2.3
15	O	88	ARG	2.3
13	M	116	THR	2.3
19	S	12	ASP	2.3
13	M	15	VAL	2.3
10	J	87	THR	2.3
2	B	72	GLY	2.2
12	L	64	TYR	2.2
21	U	17	THR	2.2
13	M	5	ALA	2.1
4	D	43	HIS	2.1
9	I	66	ARG	2.1
2	B	188	ALA	2.1
4	D	45	GLN	2.0
4	D	40	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	5MC	A	967	21/22	0.97	0.12	-	117,131,145,146	0
1	5MC	A	1404	21/22	0.95	0.17	-	102,129,148,149	0
1	7MG	A	527	24/25	0.97	0.17	-	91,114,123,126	0
1	M2G	A	966	25/26	0.94	0.18	-	122,137,142,145	0
1	2MG	A	1207	24/25	0.96	0.15	-	154,167,200,202	0
1	UR3	A	1498	21/22	0.95	0.25	-	111,124,183,193	0
1	MA6	A	1518[A]	24/25	0.94	0.20	-	110,122,127,131	24
1	5MC	A	1407	21/22	0.96	0.11	-	127,152,158,162	0
12	0TD	L	92	10/11	0.99	0.22	-	113,121,127,289	0
23	PSU	W	40	20/21	0.68	0.33	-	291,301,325,326	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PSU	A	516	20/21	0.96	0.10	-	123,147,168,168	0
1	4OC	A	1402	22/23	0.92	0.21	-	104,119,127,142	0
1	PSU	A	1540	20/21	0.71	0.35	-	253,269,289,293	0
1	MA6	A	1519[A]	24/25	0.96	0.30	-	100,115,125,126	24
1	MA6	A	1518[B]	24/25	0.94	0.20	-	107,122,137,148	24
1	MA6	A	1519[B]	24/25	0.96	0.30	-	101,116,129,130	24
24	PSU	a	40	20/21	0.81	0.32	-	208,236,258,262	0
1	5MC	A	1400	21/22	0.95	0.17	-	103,130,148,159	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1870	1/1	0.94	0.48	51.50	406,406,406,406	0
26	MG	A	1834	1/1	0.83	0.93	45.54	412,412,412,412	1
26	MG	A	1759	1/1	0.78	0.86	33.73	86,86,86,86	0
26	MG	A	1804	1/1	0.89	0.50	22.88	447,447,447,447	0
26	MG	A	1670	1/1	0.86	0.47	15.78	234,234,234,234	0
26	MG	A	1904	1/1	0.64	0.65	15.63	97,97,97,97	0
26	MG	A	1728	1/1	0.82	0.86	14.98	114,114,114,114	0
26	MG	A	1761	1/1	0.98	0.59	12.51	105,105,105,105	0
26	MG	N	102	1/1	0.79	0.54	11.89	107,107,107,107	0
26	MG	A	1740	1/1	0.84	0.56	10.67	93,93,93,93	0
26	MG	A	1812	1/1	0.94	0.73	10.31	444,444,444,444	0
26	MG	E	201	1/1	0.94	0.34	7.43	95,95,95,95	0
26	MG	A	1659	1/1	0.94	0.30	6.60	90,90,90,90	0
26	MG	A	1655	1/1	0.89	0.30	6.09	125,125,125,125	0
26	MG	A	1743	1/1	0.79	0.35	6.08	105,105,105,105	0
26	MG	A	1665	1/1	0.63	0.67	5.79	117,117,117,117	0
26	MG	A	1869	1/1	0.91	0.27	5.22	431,431,431,431	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1784	1/1	0.85	0.28	5.05	122,122,122,122	0
26	MG	A	1888	1/1	0.93	0.32	4.30	89,89,89,89	0
26	MG	A	1656	1/1	0.98	0.22	4.12	236,236,236,236	0
26	MG	A	1637	1/1	0.95	0.28	3.53	228,228,228,228	0
26	MG	A	1721	1/1	0.96	0.26	3.42	92,92,92,92	0
26	MG	A	1900	1/1	0.84	0.33	3.39	93,93,93,93	0
26	MG	Q	201	1/1	0.90	0.47	3.35	145,145,145,145	0
26	MG	A	1621	1/1	0.92	0.16	3.23	131,131,131,131	0
26	MG	A	1709	1/1	0.93	0.21	3.12	245,245,245,245	0
26	MG	A	1764	1/1	0.98	0.44	2.99	78,78,78,78	0
26	MG	A	1715	1/1	0.96	0.22	2.89	229,229,229,229	0
26	MG	A	1701	1/1	0.97	0.22	2.68	108,108,108,108	0
26	MG	A	1708	1/1	0.96	0.22	2.42	152,152,152,152	0
26	MG	A	1741	1/1	0.95	0.16	2.26	105,105,105,105	0
26	MG	A	1733	1/1	0.98	0.19	2.25	70,70,70,70	0
26	MG	A	1768	1/1	0.94	0.35	2.25	107,107,107,107	0
26	MG	A	1723	1/1	0.84	0.26	2.23	117,117,117,117	0
26	MG	E	204	1/1	0.80	0.26	2.11	128,128,128,128	0
26	MG	A	1763	1/1	0.92	0.29	2.02	120,120,120,120	0
26	MG	A	1732	1/1	0.88	0.20	2.01	100,100,100,100	0
26	MG	A	1650	1/1	0.94	0.20	1.96	151,151,151,151	0
26	MG	A	1757	1/1	0.93	0.21	1.66	88,88,88,88	0
26	MG	A	1895	1/1	0.91	0.19	1.55	106,106,106,106	0
26	MG	A	1796	1/1	0.90	0.22	1.36	416,416,416,416	0
26	MG	A	1720	1/1	0.89	0.25	1.30	74,74,74,74	0
28	ZN	D	301	1/1	0.98	0.29	0.49	138,138,138,138	0
26	MG	A	1608	1/1	0.98	0.21	0.23	73,73,73,73	0
26	MG	A	1750	1/1	0.98	0.19	0.20	74,74,74,74	0
26	MG	A	1646	1/1	0.93	0.17	0.19	136,136,136,136	0
26	MG	D	303	1/1	0.96	0.21	0.17	104,104,104,104	0
26	MG	A	1847	1/1	0.98	0.18	0.02	441,441,441,441	0
26	MG	A	1617	1/1	0.89	0.22	-0.04	85,85,85,85	0
26	MG	A	1859	1/1	0.99	0.16	-0.05	427,427,427,427	0
26	MG	A	1919	1/1	0.91	0.18	-0.06	78,78,78,78	0
26	MG	A	1746	1/1	0.94	0.16	-0.08	104,104,104,104	0
26	MG	A	1736	1/1	0.98	0.15	-0.25	123,123,123,123	0
26	MG	A	1702	1/1	0.95	0.13	-0.32	279,279,279,279	0
28	ZN	N	101	1/1	0.97	0.16	-0.33	164,164,164,164	0
26	MG	A	1920	1/1	0.91	0.07	-0.39	138,138,138,138	0
26	MG	A	1776	1/1	0.96	0.17	-0.49	96,96,96,96	0
26	MG	A	1697	1/1	0.87	0.18	-0.54	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1693	1/1	0.97	0.10	-0.76	108,108,108,108	0
26	MG	A	1616	1/1	0.98	0.17	-0.77	63,63,63,63	0
27	SRV	A	1928	40/40	0.96	0.15	-0.83	70,100,124,130	0
26	MG	A	1775	1/1	0.97	0.12	-0.86	79,79,79,79	0
26	MG	A	1689	1/1	0.97	0.14	-0.92	126,126,126,126	0
26	MG	A	1786	1/1	0.91	0.09	-1.10	109,109,109,109	0
26	MG	A	1662	1/1	0.98	0.12	-1.38	123,123,123,123	0
26	MG	A	1713	1/1	0.99	0.11	-1.41	211,211,211,211	0
26	MG	A	1703	1/1	0.99	0.14	-1.45	97,97,97,97	0
26	MG	A	1672	1/1	0.98	0.10	-1.48	166,166,166,166	0
26	MG	A	1731	1/1	0.95	0.18	-1.74	68,68,68,68	0
26	MG	A	1623	1/1	0.99	0.13	-1.97	67,67,67,67	0
26	MG	A	1607	1/1	0.99	0.11	-2.19	154,154,154,154	0
26	MG	A	1638	1/1	0.99	0.13	-2.52	86,86,86,86	0
26	MG	A	1631	1/1	0.96	0.09	-2.75	158,158,158,158	0
26	MG	A	1643	1/1	0.95	0.08	-2.77	71,71,71,71	0
26	MG	A	1827	1/1	0.99	0.08	-2.79	251,251,251,251	0
26	MG	A	1906	1/1	0.96	0.13	-3.03	64,64,64,64	0
26	MG	A	1690	1/1	0.98	0.07	-3.28	114,114,114,114	0
26	MG	A	1611	1/1	1.00	0.10	-4.21	113,113,113,113	0
26	MG	A	1705	1/1	0.96	0.13	-4.40	74,74,74,74	0
26	MG	A	1835	1/1	0.95	0.13	-	309,309,309,309	0
26	MG	E	203	1/1	0.96	0.12	-	101,101,101,101	0
26	MG	A	1667	1/1	0.98	0.18	-	119,119,119,119	0
26	MG	G	201	1/1	0.61	0.83	-	117,117,117,117	0
26	MG	A	1640	1/1	0.93	0.22	-	172,172,172,172	0
26	MG	A	1907	1/1	0.91	0.27	-	120,120,120,120	0
26	MG	A	1632	1/1	0.78	0.34	-	248,248,248,248	0
26	MG	A	1606	1/1	0.97	0.41	-	87,87,87,87	0
26	MG	A	1716	1/1	0.98	0.24	-	132,132,132,132	0
26	MG	A	1781	1/1	0.73	0.35	-	104,104,104,104	0
26	MG	A	1845	1/1	0.91	0.31	-	410,410,410,410	0
26	MG	A	1829	1/1	0.90	0.28	-	489,489,489,489	0
26	MG	A	1921	1/1	0.68	0.39	-	84,84,84,84	0
26	MG	A	1657	1/1	0.89	0.34	-	220,220,220,220	0
26	MG	A	1603	1/1	0.97	0.13	-	277,277,277,277	0
26	MG	A	1896	1/1	0.96	0.13	-	114,114,114,114	0
26	MG	A	1649	1/1	0.83	0.33	-	84,84,84,84	0
26	MG	A	1725	1/1	0.90	0.26	-	92,92,92,92	0
26	MG	A	1682	1/1	0.87	0.07	-	242,242,242,242	0
26	MG	A	1604	1/1	0.94	0.25	-	91,91,91,91	0
26	MG	A	1807	1/1	0.84	0.47	-	517,517,517,517	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1860	1/1	0.93	0.22	-	460,460,460,460	0
26	MG	A	1626	1/1	0.99	0.26	-	245,245,245,245	0
26	MG	A	1668	1/1	0.97	0.25	-	173,173,173,173	0
26	MG	A	1855	1/1	0.93	0.18	-	401,401,401,401	0
26	MG	A	1612	1/1	0.95	0.45	-	281,281,281,281	0
26	MG	A	1816	1/1	0.92	0.44	-	454,454,454,454	0
26	MG	A	1853	1/1	0.92	0.25	-	502,502,502,502	0
26	MG	A	1926	1/1	0.51	0.58	-	116,116,116,116	0
26	MG	A	1858	1/1	0.99	0.23	-	355,355,355,355	0
26	MG	A	1641	1/1	0.95	0.17	-	102,102,102,102	0
26	MG	A	1633	1/1	0.98	0.18	-	118,118,118,118	0
26	MG	A	1675	1/1	0.53	1.12	-	122,122,122,122	0
26	MG	A	1873	1/1	0.98	0.12	-	361,361,361,361	0
26	MG	A	1753	1/1	0.93	0.24	-	109,109,109,109	0
26	MG	A	1622	1/1	0.62	0.51	-	81,81,81,81	0
26	MG	H	201	1/1	0.82	0.33	-	67,67,67,67	0
26	MG	A	1609	1/1	0.92	0.07	-	157,157,157,157	0
26	MG	A	1780	1/1	0.96	0.33	-	119,119,119,119	0
26	MG	A	1910	1/1	0.10	0.29	-	120,120,120,120	0
26	MG	A	1914	1/1	0.68	1.02	-	99,99,99,99	0
26	MG	A	1771	1/1	0.96	0.57	-	102,102,102,102	0
26	MG	A	1918	1/1	0.92	0.20	-	75,75,75,75	0
26	MG	A	1848	1/1	0.93	0.21	-	407,407,407,407	0
26	MG	A	1676	1/1	0.90	0.28	-	158,158,158,158	0
26	MG	A	1801	1/1	0.95	0.20	-	464,464,464,464	0
26	MG	A	1838	1/1	0.88	0.56	-	538,538,538,538	0
26	MG	A	1688	1/1	0.91	0.41	-	186,186,186,186	0
26	MG	A	1824	1/1	0.94	0.26	-	503,503,503,503	0
26	MG	A	1788	1/1	0.90	0.10	-	285,285,285,285	0
26	MG	A	1864	1/1	0.94	0.20	-	393,393,393,393	0
26	MG	A	1878	1/1	0.89	0.20	-	346,346,346,346	0
26	MG	A	1779	1/1	0.83	0.32	-	102,102,102,102	0
26	MG	A	1830	1/1	0.97	0.27	-	480,480,480,480	0
26	MG	A	1729	1/1	0.59	0.55	-	101,101,101,101	0
26	MG	A	1791	1/1	0.96	0.19	-	283,283,283,283	0
26	MG	A	1844	1/1	0.92	0.09	-	420,420,420,420	0
26	MG	A	1739	1/1	0.91	0.17	-	78,78,78,78	0
26	MG	A	1917	1/1	0.63	0.86	-	128,128,128,128	0
26	MG	A	1880	1/1	0.76	0.49	-	508,508,508,508	0
26	MG	A	1745	1/1	0.89	0.48	-	92,92,92,92	0
26	MG	A	1644	1/1	0.87	0.37	-	127,127,127,127	0
26	MG	A	1724	1/1	0.75	0.54	-	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1911	1/1	0.99	0.12	-	100,100,100,100	0
26	MG	A	1862	1/1	0.96	0.35	-	268,268,268,268	0
26	MG	A	1680	1/1	0.95	0.23	-	214,214,214,214	0
26	MG	A	1634	1/1	0.97	0.08	-	107,107,107,107	0
26	MG	A	1679	1/1	0.81	0.18	-	369,369,369,369	0
26	MG	A	1698	1/1	0.97	0.18	-	124,124,124,124	0
26	MG	A	1666	1/1	0.98	0.08	-	149,149,149,149	0
26	MG	A	1852	1/1	0.80	0.33	-	450,450,450,450	0
26	MG	A	1794	1/1	0.42	0.27	-	518,518,518,518	0
26	MG	A	1828	1/1	0.97	0.13	-	432,432,432,432	0
26	MG	A	1923	1/1	0.78	0.77	-	86,86,86,86	0
26	MG	A	1727	1/1	0.88	0.65	-	84,84,84,84	0
26	MG	A	1822	1/1	0.95	0.12	-	293,293,293,293	0
26	MG	A	1819	1/1	0.85	0.52	-	493,493,493,493	0
26	MG	A	1793	1/1	0.76	0.27	-	483,483,483,483	0
26	MG	A	1774	1/1	0.73	0.41	-	109,109,109,109	0
26	MG	A	1890	1/1	0.90	0.18	-	112,112,112,112	0
26	MG	A	1814	1/1	0.87	0.18	-	440,440,440,440	0
26	MG	A	1803	1/1	0.98	0.20	-	345,345,345,345	0
26	MG	A	1755	1/1	0.94	0.50	-	74,74,74,74	0
26	MG	A	1815	1/1	0.91	0.23	-	506,506,506,506	0
26	MG	A	1671	1/1	0.92	0.24	-	96,96,96,96	0
26	MG	A	1636	1/1	0.84	0.41	-	88,88,88,88	0
26	MG	A	1898	1/1	0.82	0.64	-	89,89,89,89	0
26	MG	A	1887	1/1	0.79	0.55	-	102,102,102,102	0
26	MG	A	1837	1/1	0.83	0.24	-	469,469,469,469	0
26	MG	A	1823	1/1	0.93	0.11	-	422,422,422,422	0
26	MG	A	1658	1/1	0.96	0.18	-	115,115,115,115	0
26	MG	A	1885	1/1	0.96	0.08	-	84,84,84,84	0
26	MG	A	1642	1/1	0.94	0.28	-	78,78,78,78	0
26	MG	S	101	1/1	0.92	0.11	-	115,115,115,115	0
26	MG	A	1800	1/1	0.96	0.32	-	415,415,415,415	1
26	MG	A	1678	1/1	0.88	0.11	-	217,217,217,217	0
26	MG	A	1851	1/1	0.97	0.27	-	328,328,328,328	0
26	MG	A	1694	1/1	0.85	0.39	-	87,87,87,87	0
26	MG	A	1866	1/1	0.91	0.20	-	434,434,434,434	0
26	MG	A	1901	1/1	0.24	0.36	-	101,101,101,101	0
26	MG	A	1661	1/1	0.91	0.28	-	244,244,244,244	0
26	MG	A	1908	1/1	0.83	0.30	-	81,81,81,81	0
26	MG	A	1899	1/1	0.77	0.33	-	68,68,68,68	0
26	MG	A	1767	1/1	0.91	0.33	-	111,111,111,111	0
26	MG	A	1783	1/1	0.95	0.13	-	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1663	1/1	0.92	0.14	-	160,160,160,160	0
26	MG	A	1686	1/1	0.98	0.38	-	184,184,184,184	0
26	MG	A	1778	1/1	0.97	0.11	-	119,119,119,119	1
26	MG	J	201	1/1	0.94	0.42	-	109,109,109,109	0
26	MG	A	1839	1/1	0.91	0.05	-	467,467,467,467	0
26	MG	A	1712	1/1	0.94	0.20	-	170,170,170,170	0
26	MG	A	1808	1/1	0.62	0.44	-	498,498,498,498	0
26	MG	A	1639	1/1	0.88	0.19	-	87,87,87,87	0
26	MG	A	1710	1/1	0.97	0.13	-	253,253,253,253	0
26	MG	A	1630	1/1	0.96	0.26	-	158,158,158,158	0
26	MG	A	1876	1/1	0.87	0.48	-	463,463,463,463	1
26	MG	A	1700	1/1	0.80	0.37	-	302,302,302,302	0
26	MG	A	1881	1/1	0.88	0.13	-	414,414,414,414	0
26	MG	A	1696	1/1	0.96	0.32	-	263,263,263,263	0
26	MG	A	1717	1/1	0.89	0.22	-	152,152,152,152	0
26	MG	F	601	1/1	0.88	0.06	-	102,102,102,102	0
26	MG	A	1785	1/1	0.90	0.21	-	108,108,108,108	0
26	MG	A	1836	1/1	0.86	0.22	-	416,416,416,416	1
26	MG	A	1893	1/1	0.82	0.44	-	114,114,114,114	0
26	MG	A	1648	1/1	0.98	0.25	-	93,93,93,93	0
26	MG	P	101	1/1	0.80	0.32	-	58,58,58,58	0
26	MG	A	1699	1/1	0.75	0.07	-	414,414,414,414	0
26	MG	A	1818	1/1	0.98	0.09	-	189,189,189,189	0
26	MG	A	1738	1/1	1.00	0.05	-	68,68,68,68	0
26	MG	A	1748	1/1	0.91	0.14	-	110,110,110,110	0
26	MG	A	1865	1/1	0.83	0.39	-	457,457,457,457	0
26	MG	A	1897	1/1	0.84	0.43	-	114,114,114,114	0
26	MG	A	1916	1/1	0.75	0.19	-	119,119,119,119	0
26	MG	A	1654	1/1	0.98	0.09	-	161,161,161,161	0
26	MG	A	1773	1/1	0.92	0.10	-	103,103,103,103	0
26	MG	A	1787	1/1	0.96	0.24	-	496,496,496,496	0
26	MG	A	1820	1/1	0.94	0.22	-	373,373,373,373	0
26	MG	A	1894	1/1	0.79	0.21	-	94,94,94,94	0
26	MG	A	1868	1/1	0.96	0.44	-	380,380,380,380	0
26	MG	A	1737	1/1	0.88	0.69	-	89,89,89,89	0
26	MG	P	103	1/1	0.74	0.47	-	96,96,96,96	0
26	MG	A	1628	1/1	0.80	0.28	-	152,152,152,152	0
26	MG	A	1806	1/1	0.93	0.19	-	505,505,505,505	0
26	MG	A	1915	1/1	0.93	0.66	-	117,117,117,117	0
26	MG	A	1863	1/1	0.82	0.22	-	409,409,409,409	0
26	MG	A	1912	1/1	0.75	0.55	-	104,104,104,104	0
26	MG	A	1770	1/1	0.61	0.63	-	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1902	1/1	0.83	0.35	-	119,119,119,119	0
26	MG	A	1742	1/1	0.91	0.35	-	97,97,97,97	0
26	MG	A	1685	1/1	0.97	0.50	-	126,126,126,126	0
26	MG	A	1627	1/1	1.00	0.11	-	141,141,141,141	0
26	MG	A	1674	1/1	0.96	0.08	-	260,260,260,260	0
26	MG	A	1817	1/1	0.92	0.18	-	419,419,419,419	0
26	MG	A	1872	1/1	0.96	0.25	-	359,359,359,359	0
26	MG	A	1811	1/1	0.97	1.57	-	468,468,468,468	0
26	MG	A	1809	1/1	0.79	0.24	-	494,494,494,494	0
26	MG	A	1846	1/1	0.54	0.32	-	449,449,449,449	0
26	MG	E	202	1/1	0.91	0.12	-	124,124,124,124	0
26	MG	A	1605	1/1	0.98	0.09	-	254,254,254,254	0
26	MG	A	1886	1/1	-0.01	1.21	-	121,121,121,121	0
26	MG	A	1647	1/1	0.87	0.30	-	104,104,104,104	0
26	MG	A	1619	1/1	0.98	0.12	-	64,64,64,64	0
26	MG	A	1602	1/1	0.97	0.47	-	66,66,66,66	1
26	MG	A	1782	1/1	0.90	0.59	-	87,87,87,87	0
26	MG	A	1762	1/1	0.89	0.43	-	82,82,82,82	0
26	MG	A	1645	1/1	0.97	0.40	-	227,227,227,227	0
26	MG	D	304	1/1	0.35	0.54	-	455,455,455,455	0
26	MG	A	1620	1/1	0.96	0.21	-	166,166,166,166	0
26	MG	A	1730	1/1	0.64	0.72	-	97,97,97,97	0
26	MG	A	1610	1/1	0.99	0.23	-	81,81,81,81	0
26	MG	A	1925	1/1	0.82	0.15	-	114,114,114,114	0
26	MG	P	102	1/1	0.69	0.35	-	101,101,101,101	0
26	MG	A	1913	1/1	0.78	0.79	-	108,108,108,108	0
26	MG	A	1695	1/1	0.92	0.06	-	176,176,176,176	0
26	MG	A	1922	1/1	0.95	0.34	-	110,110,110,110	0
26	MG	A	1927	1/1	0.92	0.21	-	112,112,112,112	0
26	MG	A	1760	1/1	0.76	0.60	-	88,88,88,88	0
26	MG	A	1726	1/1	0.85	0.17	-	98,98,98,98	0
26	MG	A	1677	1/1	0.98	0.23	-	235,235,235,235	0
26	MG	A	1722	1/1	0.87	0.89	-	95,95,95,95	0
26	MG	A	1772	1/1	0.89	0.12	-	93,93,93,93	0
26	MG	A	1826	1/1	0.87	0.08	-	395,395,395,395	0
26	MG	A	1810	1/1	0.91	0.37	-	474,474,474,474	0
26	MG	A	1879	1/1	0.89	0.28	-	438,438,438,438	0
26	MG	A	1850	1/1	0.93	0.07	-	236,236,236,236	0
26	MG	A	1861	1/1	0.94	0.11	-	443,443,443,443	0
26	MG	A	1765	1/1	0.91	0.16	-	104,104,104,104	0
26	MG	A	1789	1/1	0.96	0.16	-	378,378,378,378	0
26	MG	A	1849	1/1	0.96	0.31	-	471,471,471,471	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1875	1/1	0.93	0.20	-	460,460,460,460	0
26	MG	A	1735	1/1	0.96	0.12	-	106,106,106,106	0
26	MG	A	1795	1/1	0.90	1.11	-	359,359,359,359	0
26	MG	A	1874	1/1	0.96	0.09	-	467,467,467,467	0
26	MG	A	1909	1/1	0.71	0.34	-	93,93,93,93	0
26	MG	A	1704	1/1	0.98	0.15	-	104,104,104,104	0
26	MG	A	1882	1/1	0.99	0.34	-	315,315,315,315	0
26	MG	A	1749	1/1	0.97	0.14	-	84,84,84,84	0
26	MG	A	1871	1/1	0.80	0.25	-	392,392,392,392	0
26	MG	A	1618	1/1	0.83	0.39	-	130,130,130,130	0
26	MG	A	1758	1/1	0.70	0.32	-	101,101,101,101	0
26	MG	A	1651	1/1	0.98	0.17	-	110,110,110,110	0
26	MG	A	1798	1/1	0.91	0.07	-	464,464,464,464	0
26	MG	A	1857	1/1	0.93	0.33	-	308,308,308,308	0
26	MG	A	1805	1/1	0.91	0.09	-	331,331,331,331	0
26	MG	A	1714	1/1	0.93	0.24	-	108,108,108,108	0
26	MG	A	1840	1/1	0.93	0.17	-	467,467,467,467	1
26	MG	A	1683	1/1	0.91	0.05	-	154,154,154,154	0
26	MG	A	1883	1/1	0.93	0.27	-	443,443,443,443	0
26	MG	A	1625	1/1	0.99	0.06	-	113,113,113,113	0
26	MG	A	1614	1/1	0.86	0.17	-	285,285,285,285	0
26	MG	A	1856	1/1	0.90	0.06	-	478,478,478,478	0
26	MG	A	1867	1/1	0.98	0.55	-	413,413,413,413	1
26	MG	A	1747	1/1	0.97	0.15	-	115,115,115,115	0
26	MG	S	102	1/1	0.96	0.13	-	106,106,106,106	0
26	MG	A	1707	1/1	0.85	0.36	-	135,135,135,135	0
26	MG	A	1718	1/1	0.93	0.24	-	326,326,326,326	0
26	MG	A	1832	1/1	0.98	0.08	-	278,278,278,278	0
26	MG	A	1669	1/1	0.97	0.09	-	123,123,123,123	0
26	MG	A	1877	1/1	0.77	0.43	-	456,456,456,456	1
26	MG	A	1684	1/1	0.83	0.13	-	109,109,109,109	0
26	MG	A	1924	1/1	0.96	0.11	-	131,131,131,131	0
26	MG	A	1635	1/1	0.99	0.14	-	74,74,74,74	0
26	MG	A	1613	1/1	0.92	0.15	-	202,202,202,202	0
26	MG	A	1744	1/1	0.72	0.32	-	82,82,82,82	0
26	MG	A	1792	1/1	0.92	0.17	-	415,415,415,415	0
26	MG	D	302	1/1	0.81	0.38	-	104,104,104,104	0
26	MG	A	1664	1/1	0.96	0.19	-	154,154,154,154	0
26	MG	A	1691	1/1	0.95	0.21	-	186,186,186,186	0
26	MG	A	1711	1/1	0.77	0.99	-	133,133,133,133	0
26	MG	A	1624	1/1	0.43	1.10	-	147,147,147,147	0
26	MG	A	1802	1/1	0.94	0.11	-	355,355,355,355	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1905	1/1	0.90	0.20	-	105,105,105,105	0
26	MG	A	1734	1/1	0.75	0.52	-	124,124,124,124	0
26	MG	A	1889	1/1	0.88	0.22	-	95,95,95,95	0
26	MG	A	1615	1/1	0.97	0.09	-	147,147,147,147	0
26	MG	A	1673	1/1	0.90	0.93	-	91,91,91,91	0
26	MG	A	1777	1/1	0.91	0.15	-	94,94,94,94	0
26	MG	A	1681	1/1	0.94	0.03	-	256,256,256,256	0
26	MG	A	1903	1/1	0.93	0.21	-	78,78,78,78	0
26	MG	A	1843	1/1	0.98	0.68	-	357,357,357,357	0
26	MG	A	1751	1/1	0.91	0.46	-	76,76,76,76	0
26	MG	A	1825	1/1	0.94	0.20	-	436,436,436,436	0
26	MG	A	1653	1/1	0.99	0.25	-	96,96,96,96	0
26	MG	A	1752	1/1	0.93	0.22	-	91,91,91,91	0
26	MG	A	1841	1/1	0.93	0.26	-	496,496,496,496	0
26	MG	A	1797	1/1	0.87	0.16	-	502,502,502,502	0
26	MG	A	1754	1/1	0.97	0.16	-	85,85,85,85	0
26	MG	A	1813	1/1	0.76	0.65	-	471,471,471,471	0
26	MG	A	1692	1/1	0.99	0.20	-	182,182,182,182	0
26	MG	A	1884	1/1	0.82	1.04	-	119,119,119,119	0
26	MG	A	1756	1/1	0.91	0.16	-	126,126,126,126	0
26	MG	A	1706	1/1	0.95	0.13	-	190,190,190,190	0
26	MG	A	1719	1/1	0.96	0.08	-	262,262,262,262	0
26	MG	A	1660	1/1	0.89	0.23	-	224,224,224,224	0
26	MG	A	1766	1/1	0.83	0.52	-	105,105,105,105	0
26	MG	A	1842	1/1	0.92	0.50	-	488,488,488,488	0
26	MG	A	1821	1/1	0.96	0.29	-	428,428,428,428	0
26	MG	A	1892	1/1	0.54	0.38	-	92,92,92,92	0
26	MG	A	1854	1/1	0.95	0.51	-	418,418,418,418	0
26	MG	A	1769	1/1	0.67	0.54	-	127,127,127,127	0
26	MG	A	1891	1/1	0.75	0.16	-	127,127,127,127	0
26	MG	A	1833	1/1	0.98	0.12	-	335,335,335,335	0
26	MG	A	1652	1/1	0.97	0.09	-	72,72,72,72	0
26	MG	A	1687	1/1	0.97	0.14	-	106,106,106,106	0
26	MG	A	1831	1/1	0.95	0.18	-	395,395,395,395	0
26	MG	A	1799	1/1	0.90	0.22	-	426,426,426,426	0
26	MG	A	1790	1/1	0.91	0.14	-	444,444,444,444	0
26	MG	A	1629	1/1	0.90	0.26	-	223,223,223,223	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.