



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2025 – 10:27 PM EST

PDB ID : 4JI4
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : Demirci, H.; Wang, L.; Murphy IV, F.; Murphy, E.; Carr, J.; Blanchard, S.;
Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on : 2013-03-05
Resolution : 3.69 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

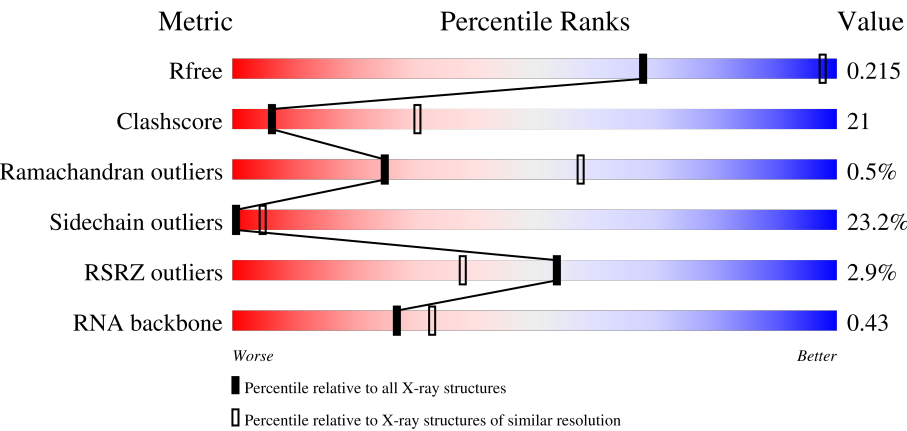
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.69 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.




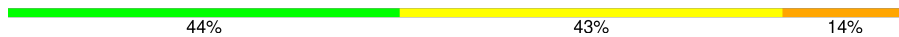
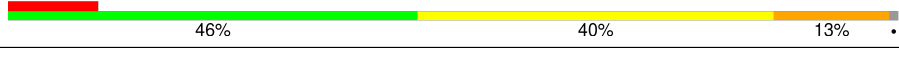
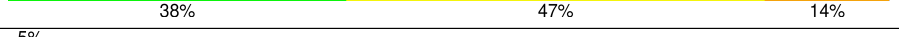
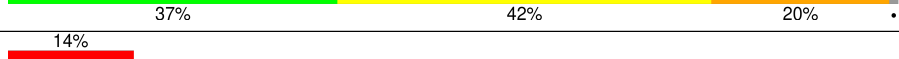
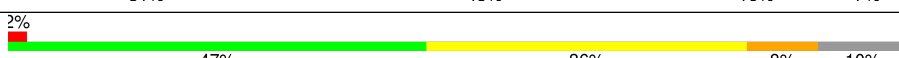

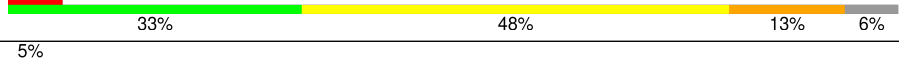
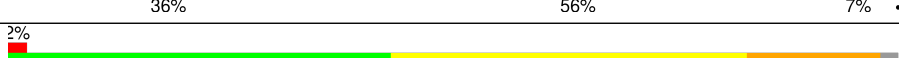
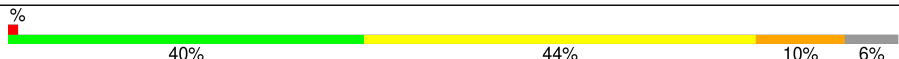
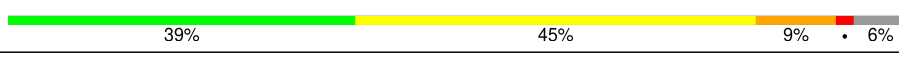
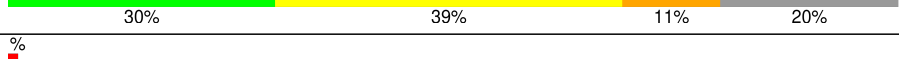
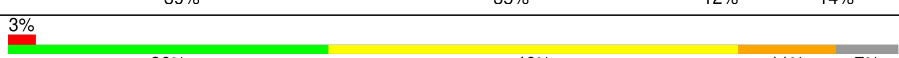



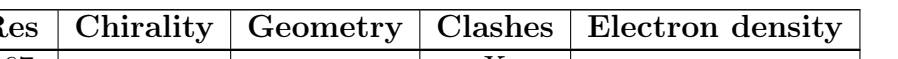
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	164625	1017 (3.80-3.60)
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)
RNA backbone	3690	1122 (4.40-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div><div>2%</div><div><div></div><div>19%</div><div>43%</div><div>31%</div><div>7%</div></div><div></div></div>
2	B	256	<div><div>%</div><div><div></div><div>39%</div><div>40%</div><div>12%</div><div>9%</div></div><div></div></div>
3	C	239	<div><div>5%</div><div><div></div><div>36%</div><div>40%</div><div>10%</div><div>14%</div></div><div></div></div>
4	D	209	<div><div>4%</div><div><div></div><div>45%</div><div>45%</div><div>9%</div></div><div></div></div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	5MC	A	967	-	-	X	-
12	0TD	L	92	-	-	X	-
22	MG	A	1632	-	-	-	X
22	MG	A	1822	-	-	-	X
22	MG	A	1855	-	-	-	X
22	MG	A	1861	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52281 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	6	0
			32644	14540	6038	10548	1518			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1490	U	C	conflict	GB M26923.1
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			973	613	195	163	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	LEU	PRO	conflict	UNP F6DEQ7

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	262	Total	Mg	0	0
			262	262		
22	B	1	Total	Mg	0	0
			1	1		
22	C	1	Total	Mg	0	0
			1	1		
22	D	3	Total	Mg	0	0
			3	3		
22	E	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		
22	H	1	Total	Mg	0	0
			1	1		
22	I	1	Total	Mg	0	0
			1	1		
22	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	1	Total 1	Mg 1	0	0
22	Q	1	Total 1	Mg 1	0	0

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

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

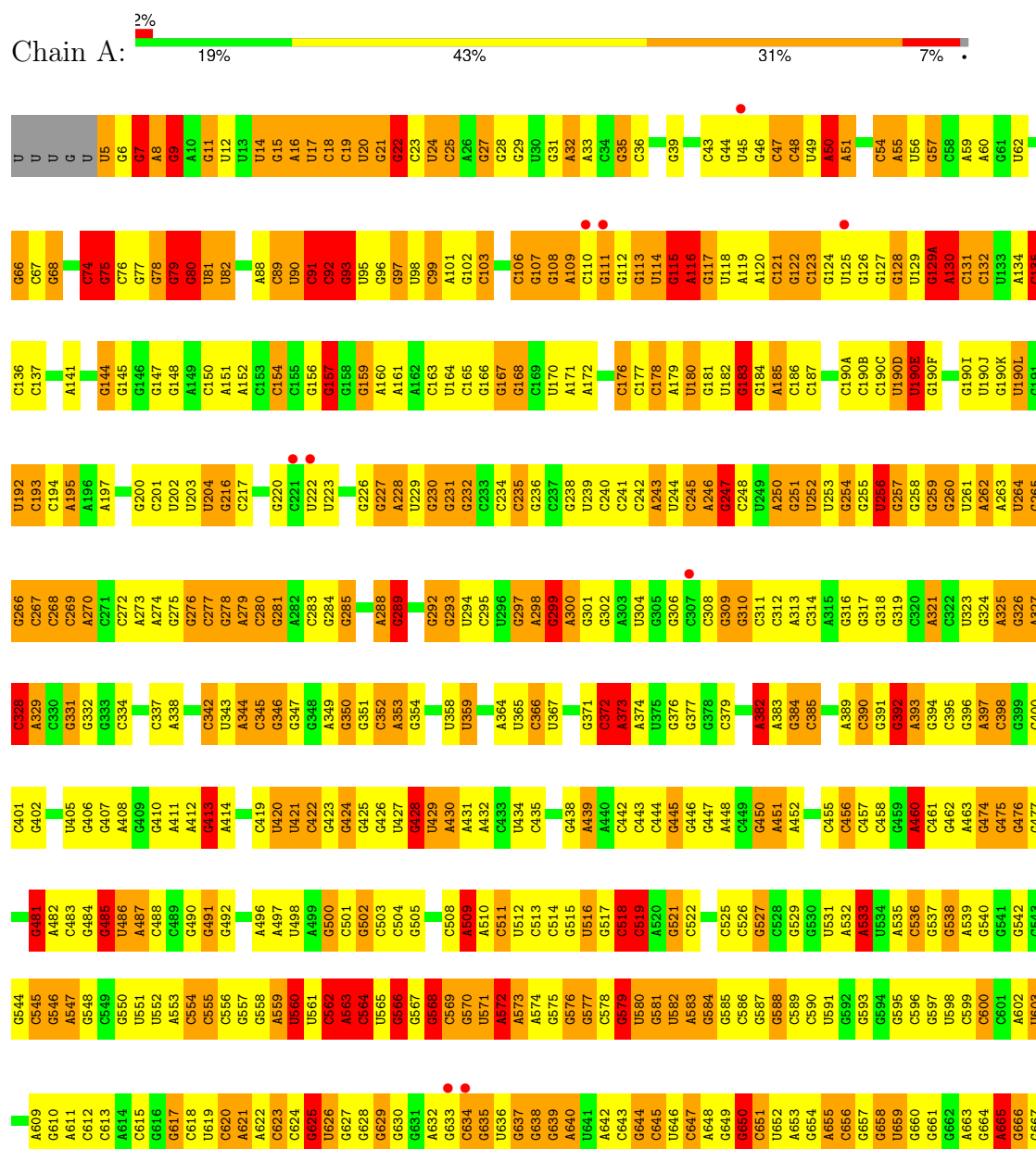
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	261	Total 261	O 261	0	0
24	C	1	Total 1	O 1	0	0
24	D	1	Total 1	O 1	0	0
24	E	6	Total 6	O 6	0	0
24	Q	2	Total 2	O 2	0	0
24	T	1	Total 1	O 1	0	0

3 Residue-property plots

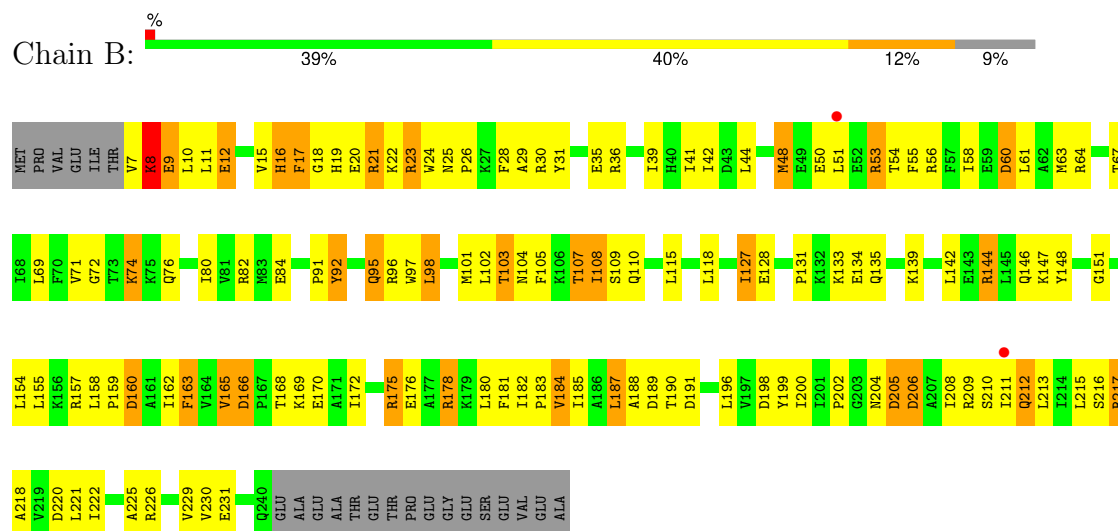
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

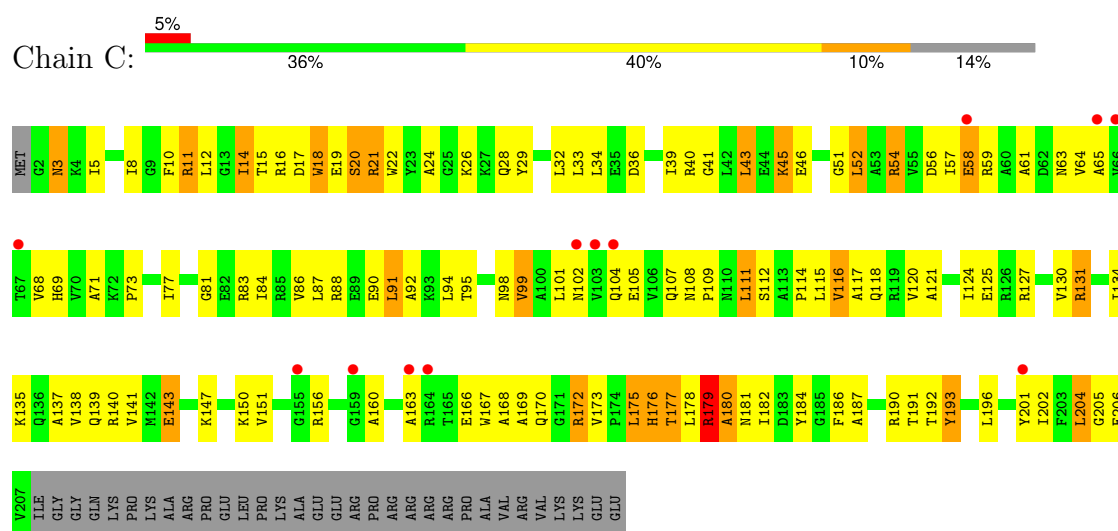


U1490	G1423	A1363	U1302	A1239	G1178	G1108	G1048	A983	G922	A860	U793	G731	G668
G1491	C1424	C1364	C1303	U1240	A1179	C1109	U1049	C994	A923	G861	U793	G731	G668
G1492	U1425	G1365	G1424	A1180	A1180	C1109	G1050	C985	A924	G862	C795	A732	U669
G1493	C1426	C1366	G1305	C1242	G1181	A1111	C1051	A986	G925	U863	C796	A733	G670
G1494	U1427	A1306	G1306	C1243	G1182	C1112	U1062	G926	G925	A864	C797	G734	G671
G1495	A1428	G1368	U1307	C1244	A1183	C1113	G1063	G927	G927	A865	C798	C735	U672
U1496	C1429	C1369	U1308	A1245	G1184	C1114	C1054	U992	G928	C866	C799	C736	G673
G1497	C1430	G1370	G1309	C1246	G1185	G1117	U1055	U993	G929	G867	C738	A737	G674
U1498	G1431	G1371	G1310	C1245	G1186	G1117	U1056	A994	G929	C868	C739	U740	A676
A1499	G1432	U1372	G1311	C1249	G1189	G1117	G1057	A994	G930	C869	U740	G741	U677
A1500	G1433	G1373	A1350	A1250	G1190	G1124	G1068	U1000	G932	U870	U804	G741	G678
A1501	A1434	A1374	C1314	A1251	G1190	U1125	C1069	A1001	G933	U871	C805	G741	C679
A1502	G1435	A1375	U1315	A1252	A1191	U1126	C1068	G1002	C934	A872	C806	C744	C680
U1503	U1436	G1376	G1316	G1253	C1192	G1127	U1062	G1003	A935	A873	C807	C745	C681
G1504	A1377	C1377	C1317	G1254	C1193	C1128	U1062	G1003A	C936	G874	C808	A746	G682
G1505	G1438	C1378	U1318	G1255	U1194	C1129	C1063	A1004	C937	C875	C809	C747	G683
U1506	G1379	A1319	A1319	A1256	C1195	A1130	G1064	A1005	A938	G876	C810	A684	A684
U1507	G1380	C1320	U1320	U1257	U1196	C1131	U1065	C1006	G939	C877	C811	C749	G685
G1441	U1381	G1382	C1321	C1258	G1197	C1132	C1066	G1007	C940	G878	C812	G750	U686
G1442	U1382	C1382	G1322	C1259	G1198	C1133	A1067	C1008	A941	C879	U813	U751	A687
C1509	G1443	C1383	G1323	G1260	U1199	G1068	U1068	G1009	G942	C880	A814	G752	G688
U1510	A1446	C1384	A1261	G1261	C1200	U1135	C1069	G1010	U943	G881	A815	A753	C689
G1511	G1447	A1385	C1262	G1263	G1201	C1136	U1070	G1011	G944	C882	A816	C754	G690
U1512	G1448	G1386	C1263	G1263	G1202	C1137	C1071	U1012	G945	C883	C817	G755	G691
A1513	C1449	C1386	C1327	C1264	C1203	G1138	G1072	G1072	A946	U884	C818	C756	U692
C1514	U1450	G1387	C1328	G1265	U1204	C1139	U1073	A1015	G947	G885	C819	U757	U693
C1515	A1451	C1388	A1329	G1266	U1205	C1140	G1074	A1016	C948	G886	U820	G758	G694
G1516	C1452	C1389	U1330	G1267	C1206	C1141	C1075	G1017	A949	G887	G821	A759	A695
G1517	G1453	U1390	G1331	C1267	G1207	C1142	C1076	C1018	U950	G888	C822	G760	A696
A1518	U1391	C1392	A1332	A1268	C1208	G1143	G1077	C1019	G951	A889	C823	G761	U697
U1519	G1455	G1392	A1333	A1269	G1208	C1143	U1077	U1020	U952	G890	C824	C762	U698
G1520	C1459	U1393	G1334	C1270	C1209	C1144	U1078	G1021	G953	U891	C826	G763	C701
G1521	A1460	C1335	C1335	C1271	C1210	C1145	U1078	G1021	G954	A892	C826	C764	A702
U1522	G1461	C1396	C1336	G1272	U1211	A1146	C1081	G1022	U955	C893	U827	G765	G703
G1523	G1462	C1395	G1337	C1273	U1212	C1147	G1081	G1023	C893	C834	A828	A766	A704
C1524	C1463	C1397	G1338	A1274	C1213	U1148	G1082	G1024	G894	G895	C829	A767	G704
G1525	G1464	A1398	A1339	C1277	C1214	C1149	U1083	U1025	A858	C895	G830	A768	U705
G1526	C1465	C1399	A1340	U1278	G1215	U1150	G1084	G1026	A959	C896	C832	G769	C706
C1527	C1466	G1400	U1341	A1279	G1216	A1151	U1085	C1027	U960	C897	C832	C770	C707
U1528	G1401	C1342	C1342	A1280	C1217	A1152	U1086	C1028	U961	G898	U833	G771	C708
G1469	C1343	A1402	G1343	U1281	C1218	C1153	G1087	G10308	G962	C899	C834	U772	G709
G1530	G1470	C1403	C1344	C1282	U1219	C1154	G1088	C10308	G963	A900	C835	C773	
A1531	G1471	C1404	U1345	G1283	G1220	C1154	G1089	G1030C	A964	A901	U835	G773	
U1532	U1472	G1405	A1346	C1284	G1221	A1157	U1090	A1030C	A965	G902	G836	G774	G713
C	A1473	U1406	G1347	A1285	C1222	C1158	U1091	G1031	G966	G902	G837	G775	G714
A	G1475	C1407	U1348	A1286	G1223	C1159	A1092	G1032	C967	G906	G838	G776	A715
C	A1408	A1408	A1287	A1287	C1224	G1160	A1093	G1033	A968	A907	U839	A777	A716
C	G1476	C1409	A1350	A1288	A1225	G1094	G1034	G1034	A969	C970	C840	C778	C717
U	C1477	U1410	U1351	A1289	C1226	C1163	U1095	A1035	C970	A908	U841	C779	C718
C	C1478	C1411	C1352	G1290	A1227	G1164	C1096	G1036	G971	A909	C848	U780	C719
C1479	C1412	G1353	C1291	G1291	C1228	C1167	C1097	C1037	C972	C912	A781	G775	C720
U1539	G1479	G1353	U1292	C1292	A1229	A1167	C1098	C1038	C973	C912	U850	A782	G721
U1540	G1480	A1413	G1354	U1292	C1293	A1168	G1099	C1039	A974	A913	C851	C783	A722
U1541	U1481	U1414	G1355	G1293	C1230	A1169	C1100	U1040	A975	A914	C852	C784	U723
U1542	G1482	G1415	G1356	G1294	G1231	A1169	C1100	U1041	A976	A915	C853	C785	G724
C1543	A1483	C1357	A1357	G1295	U1232	G1171	A1101	A1041	G976	A915	G854	G786	G725
U1544	C1484	A1416	G1417	C1296	G1233	G1172	C1102	G1042	A977	G916	C855	U787	G726
	U1485	C1418	C1359	C1297	C1234	G1173	C1103	C1043	A978	G917	G856	U788	G727
	G1486	C1419	A1360	U1298	U1235	G1174	A1044	A1044	C979	A918	U787	U788	G728
	G1487	C1420	G1361	A1299	A1236	G1175	A1105	C1045	C980	A919	C857	U788	A728
	G1488	C1421	C1361A	G1300	C1237	A1176	A1106	A1045	U981	U920	G791	C792	C729
	C1489	C1422	C1362	U1301	C1238	C1177	C1107	A1046	U982	U921	C858	U792	C730

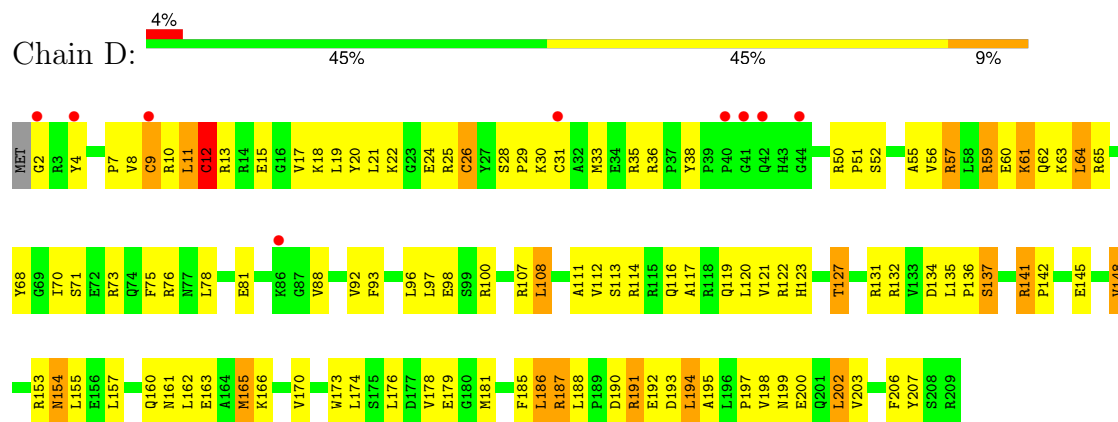
- Molecule 2: RIBOSOMAL PROTEIN S2



- Molecule 3: RIBOSOMAL PROTEIN S3

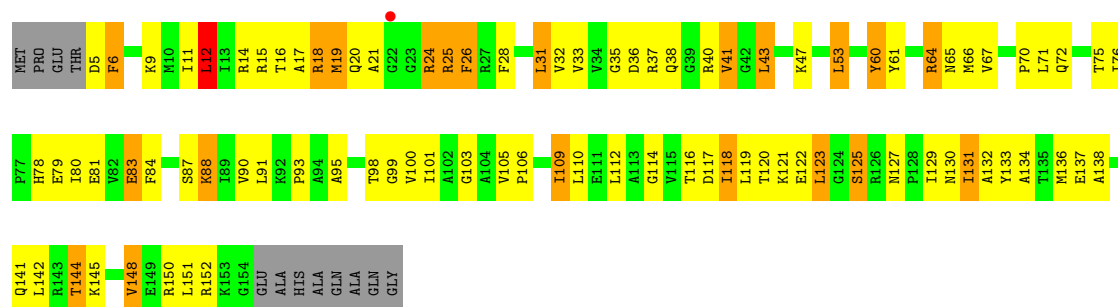


- Molecule 4: RIBOSOMAL PROTEIN S4



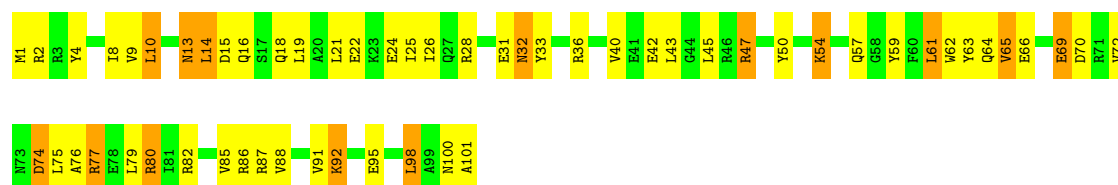
- Molecule 5: RIBOSOMAL PROTEIN S5





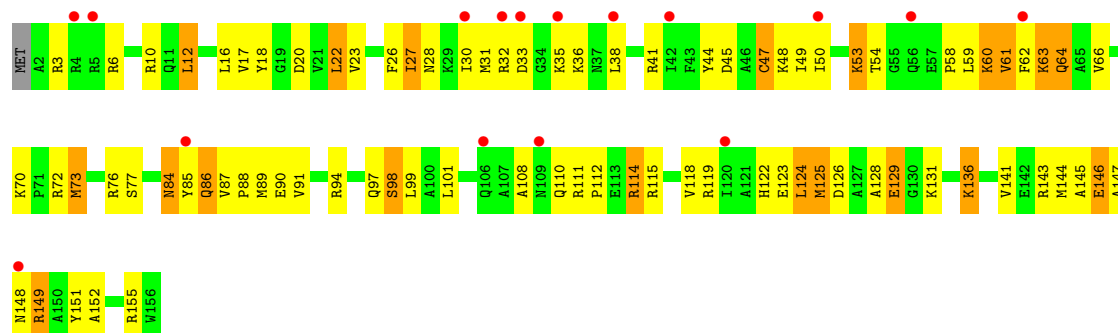
• Molecule 6: RIBOSOMAL PROTEIN S6

Chain F: 44% 43% 14%



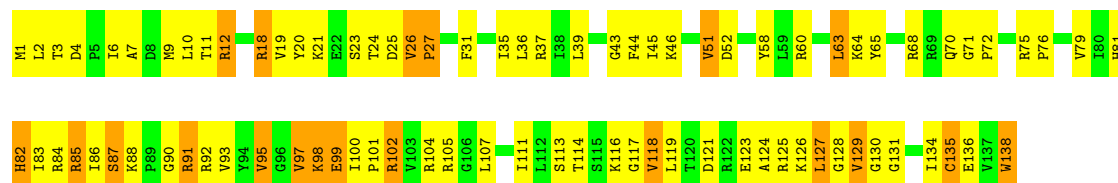
• Molecule 7: RIBOSOMAL PROTEIN S7

Chain G: 10% 46% 40% 13%



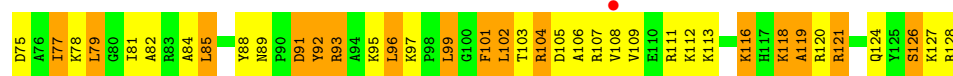
• Molecule 8: RIBOSOMAL PROTEIN S8

Chain H: 38% 47% 14%

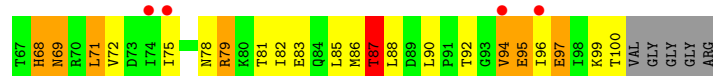
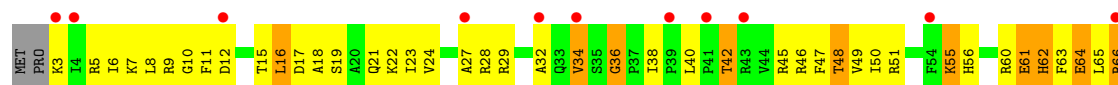


• Molecule 9: RIBOSOMAL PROTEIN S9

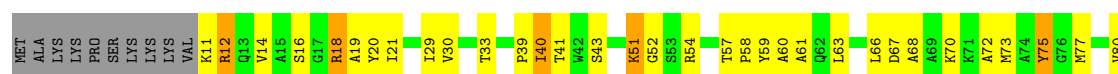
Chain I: 5% 37% 42% 20%



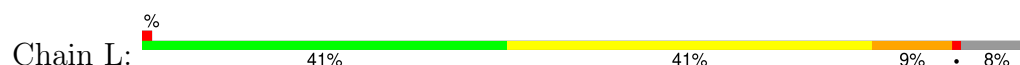
• Molecule 10: RIBOSOMAL PROTEIN S10



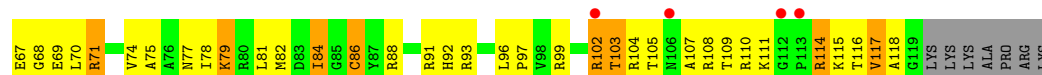
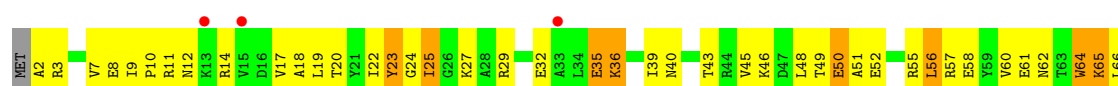
• Molecule 11: RIBOSOMAL PROTEIN S11



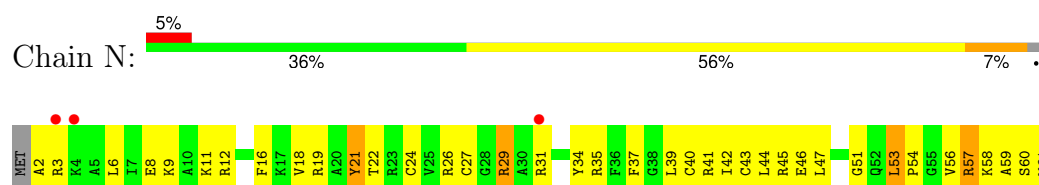
• Molecule 12: RIBOSOMAL PROTEIN S12



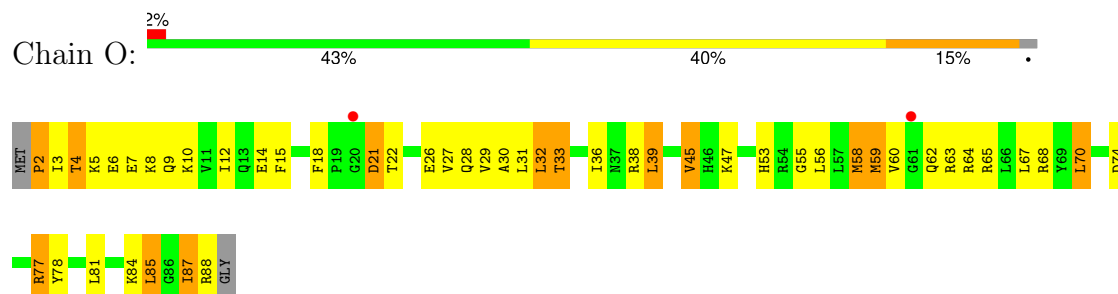
• Molecule 13: RIBOSOMAL PROTEIN S13



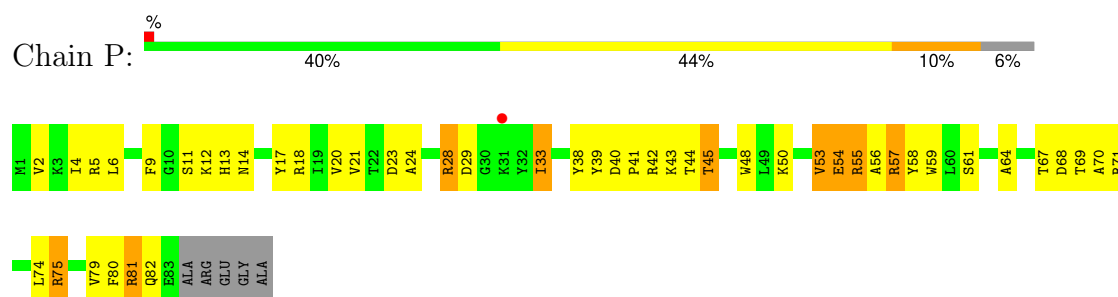
• Molecule 14: RIBOSOMAL PROTEIN S14



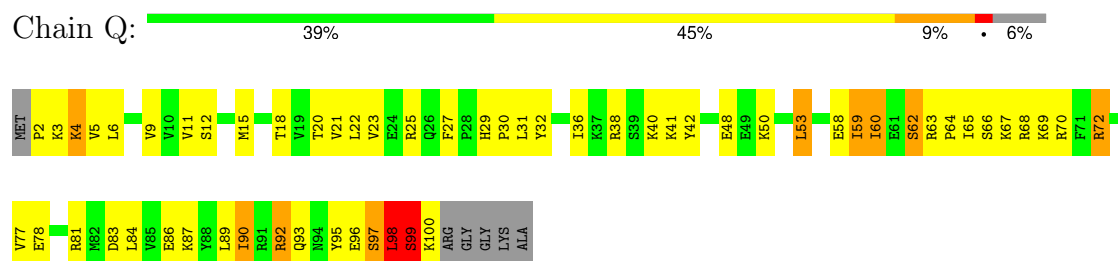
• Molecule 15: RIBOSOMAL PROTEIN S15



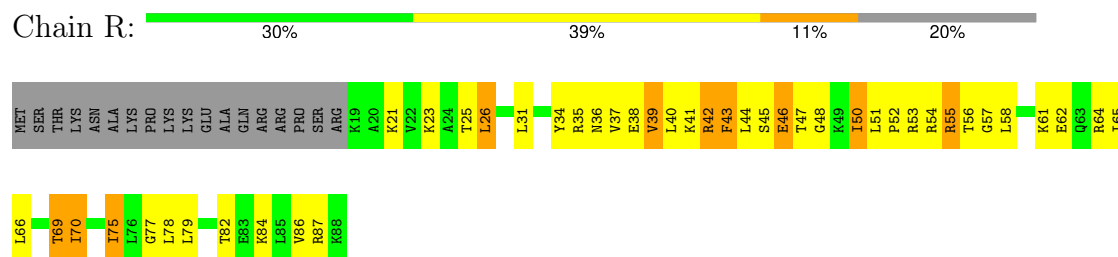
• Molecule 16: RIBOSOMAL PROTEIN S16



• Molecule 17: RIBOSOMAL PROTEIN S17

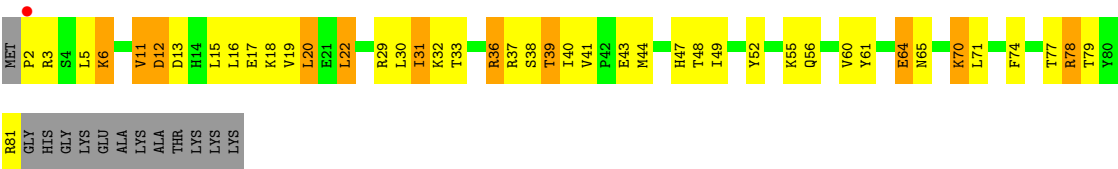


• Molecule 18: RIBOSOMAL PROTEIN S18



• Molecule 19: RIBOSOMAL PROTEIN S19

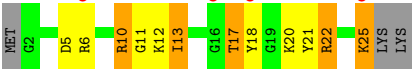




• Molecule 20: RIBOSOMAL PROTEIN S20



• Molecule 21: RIBOSOMAL PROTEIN THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.08Å 402.08Å 174.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 3.69 48.30 – 3.69	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.30-3.69) 98.4 (48.30-3.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.67Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.156 , 0.214 0.159 , 0.215	Depositor DCC
R_{free} test set	7540 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	140.3	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 189.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52281	wwPDB-VP
Average B, all atoms (Å ²)	183.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.17	188/36139 (0.5%)	1.92	1603/56396 (2.8%)
2	B	0.72	0/1935	0.88	2/2609 (0.1%)
3	C	0.54	0/1636	0.76	2/2205 (0.1%)
4	D	0.71	1/1733 (0.1%)	0.88	1/2318 (0.0%)
5	E	0.92	0/1162	1.07	1/1564 (0.1%)
6	F	0.63	0/856	0.77	0/1154
7	G	0.57	0/1276	0.77	1/1709 (0.1%)
8	H	1.05	1/1136 (0.1%)	1.11	2/1527 (0.1%)
9	I	0.53	0/1029	0.77	0/1379
10	J	0.55	0/805	0.78	0/1082
11	K	0.71	0/879	0.88	0/1187
12	L	0.72	0/977	0.99	2/1305 (0.2%)
13	M	0.60	0/947	0.81	0/1270
14	N	0.48	0/501	0.75	0/664
15	O	0.77	0/740	0.92	1/987 (0.1%)
16	P	0.84	0/716	0.95	0/963
17	Q	0.93	0/836	1.10	2/1117 (0.2%)
18	R	0.77	1/579 (0.2%)	0.94	1/768 (0.1%)
19	S	0.46	0/661	0.76	1/890 (0.1%)
20	T	0.67	0/765	0.94	1/1007 (0.1%)
21	U	0.57	0/212	0.79	0/277
All	All	1.03	191/55520 (0.3%)	1.66	1620/82378 (2.0%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2
7	G	0	1
8	H	0	2
10	J	0	4
12	L	0	1
15	O	0	1
20	T	0	2
All	All	0	17

All (191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	817	C	N1-C6	-13.12	1.29	1.37
1	A	279	A	N9-C4	-11.47	1.30	1.37
1	A	279	A	N3-C4	-11.02	1.28	1.34
1	A	822	C	N1-C6	-10.98	1.30	1.37
1	A	279	A	N7-C5	-9.71	1.33	1.39
1	A	566	G	N7-C5	-9.03	1.33	1.39
1	A	288	A	N9-C4	-8.77	1.32	1.37
1	A	1500	A	N3-C4	-8.75	1.29	1.34
1	A	574	A	N9-C4	-8.51	1.32	1.37
1	A	266	G	N7-C5	-8.50	1.34	1.39
1	A	1500	A	C6-N1	-8.48	1.29	1.35
1	A	858	G	N1-C2	8.37	1.44	1.37
1	A	876	G	N3-C4	-8.29	1.29	1.35
4	D	12	CYS	CB-SG	8.29	1.96	1.82
1	A	569	C	N3-C4	-8.28	1.28	1.33
1	A	573	A	N7-C5	-8.01	1.34	1.39
1	A	858	G	N7-C5	-7.97	1.34	1.39
1	A	130	A	N3-C4	-7.81	1.30	1.34
1	A	130	A	N9-C4	-7.78	1.33	1.37
1	A	876	G	C5-C4	-7.72	1.32	1.38
1	A	858	G	C5-C6	-7.61	1.34	1.42
1	A	1064	G	N9-C4	-7.59	1.31	1.38
1	A	568	G	C6-N1	-7.55	1.34	1.39
1	A	828	A	N7-C5	-7.51	1.34	1.39
1	A	300	A	N7-C5	-7.46	1.34	1.39
1	A	1502	A	C5-C6	-7.42	1.34	1.41
1	A	860	A	N9-C4	-7.29	1.33	1.37
1	A	1499	A	N9-C4	-7.23	1.33	1.37
1	A	109	A	N3-C4	-7.02	1.30	1.34
1	A	793	U	C2-N3	7.02	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	570	G	C6-N1	-7.00	1.34	1.39
1	A	872	A	N7-C5	-6.97	1.35	1.39
1	A	722	A	C5-C6	-6.96	1.34	1.41
1	A	1502	A	N9-C4	-6.95	1.33	1.37
1	A	329	A	C5-C6	-6.93	1.34	1.41
1	A	860	A	N3-C4	-6.91	1.30	1.34
1	A	880	C	N1-C6	-6.90	1.33	1.37
1	A	586	C	N1-C6	-6.88	1.33	1.37
1	A	918	A	C5-C4	-6.87	1.33	1.38
1	A	665	A	C5-C4	-6.86	1.33	1.38
1	A	858	G	C5-C4	6.85	1.43	1.38
1	A	569	C	N1-C6	-6.82	1.33	1.37
1	A	1499	A	N3-C4	-6.78	1.30	1.34
1	A	863	U	C2-N3	-6.73	1.33	1.37
1	A	298	A	N3-C4	-6.70	1.30	1.34
1	A	753	A	N3-C4	-6.67	1.30	1.34
1	A	243	A	N3-C4	-6.63	1.30	1.34
1	A	570	G	N1-C2	-6.59	1.32	1.37
1	A	828	A	N9-C4	-6.56	1.33	1.37
1	A	574	A	C5-C4	-6.55	1.34	1.38
1	A	574	A	N3-C4	-6.53	1.30	1.34
1	A	568	G	N3-C4	-6.52	1.30	1.35
1	A	298	A	N9-C4	-6.50	1.33	1.37
1	A	382	A	N7-C5	-6.49	1.35	1.39
1	A	753	A	N9-C4	-6.48	1.33	1.37
8	H	135	CYS	CB-SG	-6.43	1.71	1.82
1	A	868	C	N3-C4	-6.34	1.29	1.33
1	A	1064	G	N3-C4	-6.34	1.31	1.35
1	A	665	A	N9-C4	-6.32	1.34	1.37
1	A	124	G	N3-C4	-6.29	1.31	1.35
1	A	946	A	N3-C4	-6.25	1.31	1.34
1	A	1401	G	N3-C4	-6.21	1.31	1.35
1	A	915	A	N3-C4	-6.20	1.31	1.34
1	A	722	A	N7-C5	-6.20	1.35	1.39
1	A	779	C	N1-C6	-6.16	1.33	1.37
1	A	872	A	C5-C6	-6.16	1.35	1.41
1	A	895	G	N7-C5	-6.11	1.35	1.39
1	A	236	G	C6-N1	-6.11	1.35	1.39
1	A	576	G	N3-C4	-6.09	1.31	1.35
1	A	869	G	C6-N1	6.08	1.43	1.39
1	A	824	C	N1-C6	-6.08	1.33	1.37
1	A	922	G	C6-N1	-6.07	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	584	G	C5-C4	-6.07	1.34	1.38
1	A	1077	G	N9-C8	-6.04	1.33	1.37
1	A	1509	C	N1-C6	-6.03	1.33	1.37
1	A	582	U	C2-N3	-6.03	1.33	1.37
1	A	274	A	N9-C4	-6.00	1.34	1.37
1	A	602	A	N9-C4	-5.98	1.34	1.37
1	A	869	G	C5-C6	-5.95	1.36	1.42
1	A	1514	C	N1-C6	-5.92	1.33	1.37
1	A	828	A	N3-C4	-5.91	1.31	1.34
1	A	881	G	C6-N1	-5.90	1.35	1.39
1	A	766	A	N9-C4	-5.89	1.34	1.37
1	A	1401	G	C6-N1	-5.89	1.35	1.39
1	A	566	G	N9-C8	-5.88	1.33	1.37
1	A	931	C	N1-C6	-5.88	1.33	1.37
1	A	266	G	C2-N3	-5.87	1.37	1.32
1	A	665	A	N3-C4	-5.87	1.31	1.34
1	A	915	A	N9-C4	-5.86	1.34	1.37
1	A	1080	A	N3-C4	-5.86	1.31	1.34
1	A	325	A	N9-C4	-5.84	1.34	1.37
1	A	779	C	N3-C4	-5.82	1.29	1.33
1	A	21	G	N3-C4	-5.80	1.31	1.35
1	A	329	A	N9-C4	-5.80	1.34	1.37
1	A	946	A	N9-C4	-5.80	1.34	1.37
1	A	1504	G	C6-N1	-5.79	1.35	1.39
1	A	865	A	N7-C5	-5.77	1.35	1.39
1	A	757	U	N1-C2	-5.75	1.33	1.38
1	A	16	A	N3-C4	-5.75	1.31	1.34
1	A	715	A	N9-C4	-5.74	1.34	1.37
1	A	877	C	N1-C6	-5.72	1.33	1.37
1	A	125	U	C2-N3	-5.71	1.33	1.37
1	A	564	C	N1-C6	-5.71	1.33	1.37
1	A	918	A	N9-C8	-5.69	1.33	1.37
1	A	1401	G	C5-C4	-5.68	1.34	1.38
1	A	914	A	N9-C4	-5.67	1.34	1.37
1	A	1502	A	N3-C4	-5.65	1.31	1.34
1	A	589	C	N1-C6	-5.65	1.33	1.37
1	A	373	A	N9-C4	-5.62	1.34	1.37
1	A	1513	A	N9-C4	-5.62	1.34	1.37
1	A	666	G	N3-C4	-5.60	1.31	1.35
1	A	864	A	N3-C4	-5.59	1.31	1.34
1	A	918	A	N7-C5	-5.59	1.35	1.39
1	A	874	G	N9-C8	-5.58	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	635	G	C6-O6	5.58	1.29	1.24
1	A	1523	G	N3-C4	-5.57	1.31	1.35
1	A	109	A	N7-C5	-5.57	1.35	1.39
1	A	568	G	N1-C2	-5.56	1.33	1.37
1	A	787	A	N9-C4	-5.55	1.34	1.37
1	A	793	U	N3-C4	5.54	1.43	1.38
1	A	481	G	N9-C4	5.51	1.42	1.38
1	A	767	A	N3-C4	-5.51	1.31	1.34
1	A	559	A	N3-C4	-5.50	1.31	1.34
1	A	236	G	N7-C5	-5.50	1.35	1.39
1	A	1526	G	C5-C4	-5.50	1.34	1.38
1	A	109	A	N9-C4	-5.48	1.34	1.37
1	A	236	G	N9-C8	-5.47	1.34	1.37
1	A	263	A	N9-C4	-5.46	1.34	1.37
1	A	909	A	N9-C4	-5.45	1.34	1.37
1	A	236	G	C5-C4	-5.45	1.34	1.38
1	A	869	G	N9-C4	-5.43	1.33	1.38
1	A	572	A	C5-C4	-5.43	1.34	1.38
1	A	1377	A	N9-C4	-5.42	1.34	1.37
1	A	574	A	N9-C8	-5.41	1.33	1.37
1	A	243	A	N9-C4	-5.40	1.34	1.37
1	A	882	C	N3-C4	-5.39	1.30	1.33
1	A	917	G	N9-C4	-5.38	1.33	1.38
18	R	43	PHE	CB-CG	-5.38	1.42	1.51
1	A	295	C	N3-C4	-5.37	1.30	1.33
1	A	562	C	N1-C6	-5.37	1.33	1.37
1	A	879	C	N1-C6	-5.37	1.33	1.37
1	A	828	A	C5-C6	-5.37	1.36	1.41
1	A	917	G	N3-C4	-5.36	1.31	1.35
1	A	297	G	N7-C5	-5.35	1.36	1.39
1	A	882	C	N1-C6	-5.33	1.33	1.37
1	A	1529	G	N3-C4	-5.32	1.31	1.35
1	A	797	C	N3-C4	-5.30	1.30	1.33
1	A	836	G	C6-O6	5.29	1.28	1.24
1	A	868	C	N1-C6	-5.29	1.33	1.37
1	A	915	A	C5-C6	-5.29	1.36	1.41
1	A	1500	A	C5-C4	-5.29	1.35	1.38
1	A	1504	G	C5-C4	-5.28	1.34	1.38
1	A	755	G	N3-C4	-5.28	1.31	1.35
1	A	563	A	N3-C4	-5.27	1.31	1.34
1	A	1505	G	N7-C5	-5.25	1.36	1.39
1	A	1369	C	N3-C4	-5.23	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	862	C	C4-C5	-5.22	1.38	1.43
1	A	298	A	C5-C4	-5.21	1.35	1.38
1	A	116	A	N9-C4	-5.20	1.34	1.37
1	A	809	G	C6-N1	-5.19	1.35	1.39
1	A	1502	A	N7-C5	-5.18	1.36	1.39
1	A	572	A	C6-N6	-5.18	1.29	1.33
1	A	876	G	N1-C2	-5.18	1.33	1.37
1	A	793	U	C2-O2	5.17	1.27	1.22
1	A	695	A	N9-C4	-5.16	1.34	1.37
1	A	863	U	N3-C4	-5.16	1.33	1.38
1	A	782	A	C6-N1	-5.15	1.31	1.35
1	A	946	A	C6-N1	-5.14	1.31	1.35
1	A	574	A	N7-C5	-5.14	1.36	1.39
1	A	909	A	N7-C5	-5.13	1.36	1.39
1	A	862	C	C4-N4	-5.13	1.29	1.33
1	A	924	C	N1-C6	-5.12	1.34	1.37
1	A	673	G	N3-C4	-5.11	1.31	1.35
1	A	876	G	C2-N3	-5.09	1.28	1.32
1	A	107	G	N3-C4	-5.08	1.31	1.35
1	A	570	G	C5-C4	-5.08	1.34	1.38
1	A	1509	C	N3-C4	-5.07	1.30	1.33
1	A	68	G	C5-C4	-5.07	1.34	1.38
1	A	872	A	N9-C4	-5.06	1.34	1.37
1	A	21	G	N1-C2	-5.04	1.33	1.37
1	A	634	C	N1-C6	-5.04	1.34	1.37
1	A	809	G	C5-C6	-5.03	1.37	1.42
1	A	1074	G	N7-C5	-5.03	1.36	1.39
1	A	859	A	N9-C4	-5.03	1.34	1.37
1	A	1512	U	C4-O4	5.03	1.27	1.23
1	A	397	A	N7-C5	-5.02	1.36	1.39
1	A	898	G	N9-C4	-5.02	1.33	1.38
1	A	327	A	N9-C4	-5.01	1.34	1.37
1	A	728	A	N9-C4	-5.01	1.34	1.37
1	A	578	C	N3-C4	-5.01	1.30	1.33
1	A	946	A	N7-C5	-5.00	1.36	1.39

All (1620) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	858	G	N1-C6-O6	25.57	135.24	119.90
1	A	858	G	C6-C5-N7	-18.08	119.55	130.40
1	A	266	G	C6-C5-N7	-17.84	119.70	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	869	G	N1-C6-O6	17.27	130.26	119.90
1	A	869	G	C4-C5-N7	16.36	117.34	110.80
1	A	858	G	C2-N3-C4	-15.93	103.93	111.90
1	A	722	A	C2-N3-C4	-15.83	102.69	110.60
1	A	869	G	C5-C6-O6	-15.77	119.14	128.60
1	A	117	G	C6-C5-N7	-15.48	121.11	130.40
1	A	117	G	N1-C6-O6	15.22	129.03	119.90
1	A	266	G	N7-C8-N9	14.78	120.49	113.10
1	A	858	G	N7-C8-N9	14.62	120.41	113.10
1	A	858	G	C5-C6-O6	-14.55	119.87	128.60
1	A	858	G	C5-N7-C8	-14.37	97.12	104.30
1	A	1370	G	C8-N9-C4	-14.14	100.74	106.40
1	A	869	G	C5-N7-C8	-13.99	97.31	104.30
1	A	1395	C	C6-N1-C2	13.50	125.70	120.30
1	A	858	G	C5-C6-N1	-13.25	104.88	111.50
1	A	858	G	C4-C5-N7	12.99	115.99	110.80
1	A	1369	C	C6-N1-C2	-12.87	115.15	120.30
1	A	766	A	O5'-P-OP2	-12.74	94.23	105.70
1	A	266	G	C4-N9-C1'	12.71	143.02	126.50
1	A	824	C	C6-N1-C2	12.58	125.33	120.30
1	A	815	A	C8-N9-C4	12.27	110.71	105.80
1	A	858	G	N3-C2-N2	-12.21	111.35	119.90
1	A	1502	A	N1-C6-N6	12.17	125.90	118.60
1	A	266	G	C5-N7-C8	-12.07	98.27	104.30
1	A	600	C	C6-N1-C2	11.94	125.07	120.30
1	A	266	G	C8-N9-C4	-11.92	101.63	106.40
1	A	281	G	N1-C6-O6	11.87	127.02	119.90
1	A	570	G	N3-C4-C5	-11.82	122.69	128.60
1	A	1532	U	C5-C6-N1	11.77	128.58	122.70
1	A	562	C	C6-N1-C2	11.76	125.00	120.30
1	A	858	G	C8-N9-C4	-11.76	101.70	106.40
1	A	722	A	N1-C6-N6	11.58	125.55	118.60
1	A	481	G	N3-C4-N9	11.55	132.93	126.00
1	A	266	G	C4-C5-N7	11.54	115.41	110.80
1	A	731	G	N1-C6-O6	11.51	126.81	119.90
1	A	570	G	N1-C6-O6	-11.49	113.01	119.90
1	A	588	G	C8-N9-C4	11.34	110.93	106.40
1	A	635	G	C5-C6-N1	-11.32	105.84	111.50
1	A	555	C	C6-N1-C2	-11.18	115.83	120.30
1	A	896	C	N3-C4-C5	11.15	126.36	121.90
1	A	119	A	O5'-P-OP2	-11.14	95.68	105.70
1	A	15	G	N1-C6-O6	11.13	126.58	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	722	A	C6-C5-N7	-11.12	124.51	132.30
1	A	658	G	N9-C4-C5	-11.07	100.97	105.40
1	A	869	G	N3-C4-C5	10.89	134.04	128.60
1	A	740	U	O5'-P-OP2	-10.88	95.91	105.70
1	A	121	C	C6-N1-C2	10.83	124.63	120.30
1	A	1502	A	C2-N3-C4	-10.73	105.24	110.60
1	A	867	G	C5-C6-O6	-10.71	122.17	128.60
1	A	647	C	C6-N1-C2	10.69	124.57	120.30
1	A	756	C	C6-N1-C2	10.65	124.56	120.30
1	A	573	A	C8-N9-C4	-10.64	101.54	105.80
1	A	1505	G	C8-N9-C4	-10.63	102.15	106.40
1	A	1200	C	C2-N1-C1'	10.59	130.44	118.80
1	A	1238	A	C8-N9-C4	-10.57	101.57	105.80
1	A	481	G	N3-C4-C5	-10.56	123.32	128.60
1	A	731	G	C5-C6-O6	-10.47	122.32	128.60
1	A	658	G	C8-N9-C4	10.47	110.59	106.40
1	A	1502	A	C5-N7-C8	-10.40	98.70	103.90
1	A	600	C	C5-C6-N1	-10.34	115.83	121.00
1	A	862	C	N3-C4-C5	10.29	126.02	121.90
1	A	1331	G	N1-C6-O6	-10.26	113.75	119.90
1	A	279	A	C2-N3-C4	-10.25	105.48	110.60
1	A	1502	A	C6-C5-N7	-10.23	125.14	132.30
1	A	872	A	N1-C6-N6	10.18	124.70	118.60
1	A	1527	C	C6-N1-C2	-10.15	116.24	120.30
1	A	266	G	C4-C5-C6	10.14	124.88	118.80
1	A	1068	G	O5'-P-OP1	-10.14	96.58	105.70
1	A	579	G	C4-C5-N7	10.12	114.85	110.80
1	A	824	C	C5-C6-N1	-10.11	115.95	121.00
1	A	835	U	C5-C4-O4	10.10	131.96	125.90
1	A	873	A	C8-N9-C4	-10.10	101.76	105.80
1	A	922	G	C8-N9-C4	-10.08	102.37	106.40
1	A	117	G	C4-C5-C6	10.04	124.83	118.80
1	A	771	G	N1-C6-O6	9.97	125.88	119.90
1	A	579	G	N1-C6-O6	9.92	125.85	119.90
1	A	852	G	C5-C6-N1	-9.89	106.55	111.50
1	A	570	G	C6-N1-C2	-9.87	119.18	125.10
1	A	793	U	N1-C2-N3	-9.79	109.02	114.90
1	A	588	G	O5'-P-OP2	-9.78	96.90	105.70
1	A	1354	C	C6-N1-C2	-9.77	116.39	120.30
1	A	948	C	C6-N1-C2	9.75	124.20	120.30
1	A	1502	A	C4-C5-N7	9.75	115.58	110.70
1	A	1181	G	C8-N9-C4	9.74	110.30	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	C	C5-C6-N1	-9.71	116.14	121.00
1	A	279	A	C4-C5-C6	9.71	121.85	117.00
1	A	572	A	C5-C6-N1	9.70	122.55	117.70
1	A	908	A	C2-N3-C4	-9.63	105.78	110.60
1	A	812	C	N3-C4-C5	-9.62	118.05	121.90
1	A	1370	G	N7-C8-N9	9.60	117.90	113.10
1	A	931	C	C5-C6-N1	-9.55	116.22	121.00
1	A	722	A	C5-C6-N1	-9.54	112.93	117.70
1	A	144	G	N1-C6-O6	9.53	125.62	119.90
1	A	382	A	C8-N9-C4	-9.50	102.00	105.80
1	A	872	A	C2-N3-C4	-9.44	105.88	110.60
1	A	570	G	C5-C6-N1	9.43	116.22	111.50
1	A	731	G	C4-C5-N7	9.42	114.57	110.80
1	A	735	C	C6-N1-C2	9.40	124.06	120.30
1	A	1420	C	C6-N1-C2	-9.40	116.54	120.30
1	A	858	G	C4-C5-C6	9.38	124.42	118.80
1	A	1238	A	N9-C4-C5	9.33	109.53	105.80
1	A	117	G	C4-N9-C1'	9.32	138.62	126.50
1	A	1197	G	O5'-P-OP1	-9.31	97.32	105.70
1	A	779	C	N1-C2-N3	9.30	125.71	119.20
1	A	117	G	C2-N3-C4	-9.27	107.27	111.90
1	A	665	A	C5-C6-N1	9.25	122.32	117.70
1	A	579	G	C5-C6-O6	-9.21	123.07	128.60
1	A	235	C	C6-N1-C2	9.20	123.98	120.30
1	A	623	C	C6-N1-C2	9.12	123.95	120.30
1	A	117	G	C5-C6-N1	-9.11	106.94	111.50
1	A	250	A	N1-C6-N6	9.11	124.07	118.60
1	A	331	G	N1-C6-O6	9.07	125.34	119.90
1	A	854	G	O5'-P-OP1	-9.06	97.55	105.70
1	A	266	G	C8-N9-C1'	-9.03	115.26	127.00
1	A	279	A	C5-C6-N1	-9.02	113.19	117.70
1	A	1527	C	N3-C2-O2	-9.02	115.59	121.90
1	A	626	U	C6-N1-C2	-9.01	115.59	121.00
1	A	562	C	C5-C6-N1	-9.00	116.50	121.00
1	A	1373	G	N3-C4-N9	9.00	131.40	126.00
1	A	771	G	C5-C6-O6	-8.99	123.20	128.60
1	A	668	G	C8-N9-C4	8.98	109.99	106.40
1	A	125	U	C5-C6-N1	-8.98	118.21	122.70
1	A	863	U	N3-C4-O4	-8.98	113.12	119.40
1	A	869	G	N7-C8-N9	8.96	117.58	113.10
1	A	588	G	N7-C8-N9	-8.94	108.63	113.10
1	A	877	C	C2-N3-C4	-8.94	115.43	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	707	C	O5'-P-OP2	-8.93	97.66	105.70
1	A	624	C	C6-N1-C2	8.90	123.86	120.30
1	A	1098	C	C6-N1-C2	8.90	123.86	120.30
1	A	658	G	C8-N9-C1'	-8.89	115.44	127.00
1	A	867	G	N1-C6-O6	8.89	125.24	119.90
1	A	970	C	N1-C2-O2	8.89	124.23	118.90
1	A	1524	C	N1-C2-O2	-8.86	113.59	118.90
1	A	1516[A]	G	C8-N9-C4	-8.85	102.86	106.40
1	A	1516[B]	G	C8-N9-C4	-8.85	102.86	106.40
1	A	117	G	C8-N9-C1'	-8.85	115.50	127.00
1	A	885	G	C2-N3-C4	-8.84	107.48	111.90
1	A	279	A	N1-C2-N3	8.80	133.70	129.30
1	A	1490	U	C5-C6-N1	8.79	127.10	122.70
1	A	650	G	C8-N9-C4	-8.79	102.89	106.40
1	A	300	A	C8-N9-C4	-8.78	102.29	105.80
1	A	232	G	N9-C4-C5	-8.77	101.89	105.40
1	A	568	G	O5'-P-OP2	-8.77	97.81	105.70
1	A	1527	C	C2-N1-C1'	8.76	128.44	118.80
1	A	279	A	O4'-C1'-N9	-8.72	101.23	108.20
1	A	835	U	N1-C2-N3	8.71	120.12	114.90
1	A	281	G	C5-C6-O6	-8.69	123.39	128.60
1	A	309	G	C4-C5-N7	8.69	114.27	110.80
1	A	25	C	C6-N1-C2	8.68	123.77	120.30
1	A	650	G	N7-C8-N9	8.68	117.44	113.10
1	A	872	A	C6-C5-N7	-8.68	126.22	132.30
17	Q	98	LEU	CA-CB-CG	8.67	135.23	115.30
1	A	1512	U	N3-C4-C5	-8.65	109.41	114.60
1	A	666	G	C2-N3-C4	-8.65	107.58	111.90
1	A	936	C	C6-N1-C2	8.65	123.76	120.30
1	A	366	C	N1-C2-O2	8.64	124.09	118.90
1	A	569	C	N3-C4-N4	-8.62	111.97	118.00
1	A	1395	C	O5'-P-OP2	-8.61	97.95	105.70
1	A	835	U	N3-C4-C5	-8.61	109.43	114.60
1	A	762	C	O5'-P-OP2	8.57	120.99	110.70
1	A	941	G	C8-N9-C4	-8.57	102.97	106.40
1	A	559	A	C6-N1-C2	-8.56	113.46	118.60
1	A	745	C	N3-C4-C5	8.56	125.33	121.90
1	A	919	A	C8-N9-C4	8.53	109.21	105.80
1	A	277	C	C6-N1-C2	8.52	123.71	120.30
1	A	635	G	N1-C6-O6	8.51	125.00	119.90
1	A	579	G	C5-N7-C8	-8.50	100.05	104.30
1	A	266	G	N1-C6-O6	8.48	124.99	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	G	C6-C5-N7	-8.43	125.34	130.40
1	A	912	C	N3-C4-N4	8.40	123.88	118.00
1	A	1442	G	N3-C4-C5	-8.40	124.40	128.60
1	A	638	G	N1-C6-O6	8.38	124.93	119.90
1	A	366	C	N3-C2-O2	-8.38	116.04	121.90
1	A	279	A	C8-N9-C4	-8.37	102.45	105.80
1	A	281	G	C4-C5-N7	8.36	114.14	110.80
1	A	922	G	N1-C6-O6	-8.35	114.89	119.90
1	A	722	A	C4-C5-N7	8.34	114.87	110.70
1	A	1531	A	N1-C6-N6	8.33	123.60	118.60
1	A	451	A	C8-N9-C4	8.32	109.13	105.80
1	A	869	G	C6-C5-N7	-8.32	125.41	130.40
1	A	877	C	C5-C6-N1	-8.32	116.84	121.00
1	A	1200	C	N1-C2-O2	8.31	123.89	118.90
1	A	257	G	N1-C6-O6	8.30	124.88	119.90
1	A	1373	G	N3-C4-C5	-8.30	124.45	128.60
1	A	281	G	N9-C4-C5	-8.29	102.08	105.40
1	A	886	G	N1-C6-O6	8.28	124.87	119.90
1	A	550	G	C2-N3-C4	-8.23	107.78	111.90
1	A	252	U	C5-C6-N1	-8.22	118.59	122.70
1	A	650	G	C6-C5-N7	-8.22	125.47	130.40
1	A	658	G	N3-C4-N9	8.21	130.93	126.00
1	A	666	G	N1-C2-N3	8.21	128.83	123.90
1	A	715	A	C2-N3-C4	-8.20	106.50	110.60
1	A	667	G	C2-N3-C4	-8.19	107.80	111.90
1	A	812	C	C4-C5-C6	8.19	121.50	117.40
1	A	326	G	C4-C5-N7	-8.18	107.53	110.80
1	A	867	G	C6-C5-N7	-8.17	125.50	130.40
1	A	867	G	C4-C5-N7	8.16	114.06	110.80
1	A	117	G	C4-C5-N7	8.15	114.06	110.80
1	A	292	G	C5-C6-O6	-8.15	123.71	128.60
1	A	1060	C	N1-C2-O2	8.14	123.78	118.90
1	A	890	G	C4-C5-N7	-8.13	107.55	110.80
1	A	292	G	N1-C6-O6	8.13	124.78	119.90
1	A	615	C	O5'-P-OP1	-8.12	98.39	105.70
1	A	859	A	N1-C6-N6	8.11	123.47	118.60
1	A	511	C	C5-C6-N1	-8.10	116.95	121.00
1	A	266	G	N3-C4-N9	8.09	130.85	126.00
1	A	626	U	N1-C2-N3	8.09	119.75	114.90
1	A	835	U	C4-C5-C6	8.08	124.55	119.70
1	A	817	C	C4-C5-C6	8.07	121.44	117.40
1	A	835	U	N3-C2-O2	-8.06	116.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	875	C	C5-C6-N1	-8.05	116.97	121.00
1	A	858	G	N3-C4-C5	8.04	132.62	128.60
1	A	815	A	N7-C8-N9	-8.04	109.78	113.80
1	A	483	C	C4-C5-C6	8.02	121.41	117.40
1	A	824	C	C2-N3-C4	-8.02	115.89	119.90
1	A	1505	G	N7-C8-N9	8.00	117.10	113.10
1	A	658	G	N1-C2-N3	8.00	128.70	123.90
1	A	1490	U	N1-C2-N3	-8.00	110.10	114.90
1	A	919	A	O5'-P-OP2	-7.99	98.51	105.70
1	A	278	G	O5'-P-OP2	-7.98	98.52	105.70
1	A	1075	C	N3-C4-C5	7.98	125.09	121.90
1	A	659	U	C2-N3-C4	-7.97	122.22	127.00
1	A	232	G	C4-C5-N7	7.96	113.98	110.80
1	A	826	C	C5-C6-N1	-7.96	117.02	121.00
1	A	1307	U	N3-C2-O2	-7.96	116.62	122.20
1	A	1226	C	N1-C2-O2	7.95	123.67	118.90
1	A	650	G	C4-N9-C1'	7.93	136.81	126.50
1	A	658	G	N1-C2-N2	-7.92	109.07	116.20
1	A	835	U	C6-N1-C2	-7.91	116.25	121.00
1	A	817	C	C6-N1-C2	7.91	123.46	120.30
1	A	822	C	C4-C5-C6	7.91	121.35	117.40
1	A	342	C	C6-N1-C2	-7.90	117.14	120.30
1	A	731	G	N9-C4-C5	-7.90	102.24	105.40
1	A	1200	C	C5-C6-N1	7.89	124.94	121.00
1	A	8	A	N9-C4-C5	7.88	108.95	105.80
1	A	251	G	C4-C5-N7	7.88	113.95	110.80
1	A	805	C	C6-N1-C2	7.86	123.44	120.30
1	A	615	C	C6-N1-C2	-7.86	117.16	120.30
1	A	863	U	C5-C4-O4	7.85	130.61	125.90
1	A	916	G	C8-N9-C4	7.84	109.53	106.40
1	A	518	C	N1-C2-O2	7.84	123.60	118.90
1	A	1282	C	C6-N1-C2	-7.83	117.17	120.30
1	A	326	G	C5-C6-O6	7.83	133.30	128.60
1	A	122	G	N1-C6-O6	7.82	124.59	119.90
1	A	941	G	N7-C8-N9	7.82	117.01	113.10
1	A	1490	U	C5-C4-O4	-7.81	121.21	125.90
1	A	1200	C	C6-N1-C2	-7.81	117.17	120.30
1	A	600	C	C2-N3-C4	-7.80	116.00	119.90
1	A	1189	C	C6-N1-C2	7.79	123.42	120.30
1	A	1108	G	C8-N9-C4	-7.77	103.29	106.40
1	A	277	C	N3-C4-C5	7.76	125.00	121.90
1	A	825	G	C8-N9-C4	7.75	109.50	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1079	G	N3-C4-C5	-7.74	124.73	128.60
1	A	757	U	C2-N1-C1'	-7.73	108.42	117.70
1	A	116	A	C2-N3-C4	-7.72	106.74	110.60
1	A	281	G	C6-C5-N7	-7.72	125.77	130.40
1	A	691	G	C8-N9-C4	-7.71	103.31	106.40
1	A	18	C	C5-C6-N1	-7.71	117.14	121.00
1	A	190(E)	U	C2-N1-C1'	-7.70	108.46	117.70
1	A	1442	G	C4-N9-C1'	7.69	136.50	126.50
1	A	970	C	N3-C2-O2	-7.69	116.52	121.90
1	A	1505	G	C6-C5-N7	-7.68	125.79	130.40
1	A	569	C	C5-C4-N4	7.67	125.57	120.20
1	A	722	A	C5-N7-C8	-7.66	100.07	103.90
1	A	1158	C	C2-N1-C1'	7.65	127.21	118.80
1	A	643	C	N3-C4-C5	7.65	124.96	121.90
1	A	854	G	C4-N9-C1'	7.64	136.43	126.50
1	A	117	G	C5-C6-O6	-7.63	124.02	128.60
1	A	755	G	N1-C6-O6	7.63	124.48	119.90
1	A	922	G	N9-C4-C5	7.62	108.45	105.40
1	A	805	C	N3-C4-C5	7.62	124.95	121.90
1	A	833	U	C5-C4-O4	7.61	130.46	125.90
1	A	931	C	C2-N3-C4	-7.61	116.10	119.90
1	A	1078	U	N1-C2-O2	7.60	128.12	122.80
1	A	722	A	N1-C2-N3	7.59	133.10	129.30
1	A	599	C	C6-N1-C2	7.59	123.34	120.30
1	A	809	G	C4-C5-N7	7.58	113.83	110.80
1	A	331	G	C5-C6-N1	-7.58	107.71	111.50
1	A	18	C	C6-N1-C2	7.57	123.33	120.30
1	A	1452	C	C6-N1-C2	7.57	123.33	120.30
1	A	944	G	C5-C6-O6	7.57	133.14	128.60
1	A	665	A	C6-N1-C2	-7.56	114.06	118.60
1	A	836	G	C5-C6-N1	-7.56	107.72	111.50
1	A	877	C	O5'-P-OP2	-7.55	98.90	105.70
1	A	928	G	C4-C5-N7	7.55	113.82	110.80
1	A	273	A	C8-N9-C4	-7.55	102.78	105.80
1	A	558	G	O5'-P-OP1	7.55	119.75	110.70
1	A	250	A	N9-C4-C5	-7.54	102.78	105.80
1	A	130	A	N1-C2-N3	7.54	133.07	129.30
1	A	1051	C	C2-N1-C1'	7.54	127.09	118.80
1	A	309	G	C5-C6-O6	-7.54	124.08	128.60
1	A	768	A	N1-C6-N6	7.53	123.12	118.60
1	A	822	C	C2-N3-C4	-7.53	116.14	119.90
1	A	771	G	C6-C5-N7	-7.52	125.89	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	C	C5-C4-N4	-7.51	114.94	120.20
1	A	7	G	O4'-C1'-N9	7.51	114.21	108.20
1	A	817	C	C5-C6-N1	-7.51	117.25	121.00
1	A	483	C	C5-C6-N1	-7.50	117.25	121.00
1	A	715	A	N3-C4-C5	7.50	132.05	126.80
1	A	299	G	N1-C6-O6	7.49	124.39	119.90
1	A	1158	C	N1-C2-O2	7.49	123.39	118.90
1	A	695	A	C2-N3-C4	-7.49	106.86	110.60
1	A	815	A	O4'-C1'-N9	-7.48	102.22	108.20
1	A	602	A	C2-N3-C4	-7.48	106.86	110.60
1	A	867	G	N9-C4-C5	-7.47	102.41	105.40
1	A	872	A	C4-C5-N7	7.46	114.43	110.70
1	A	283	C	C5-C6-N1	7.46	124.73	121.00
1	A	814	A	C8-N9-C4	7.46	108.78	105.80
1	A	1371	G	O5'-P-OP1	-7.46	98.98	105.70
1	A	941	G	C5-N7-C8	-7.45	100.58	104.30
1	A	666	G	C5-C6-N1	-7.44	107.78	111.50
1	A	318	G	N1-C6-O6	7.44	124.36	119.90
1	A	578	C	N1-C2-O2	-7.43	114.44	118.90
1	A	1060	C	N3-C2-O2	-7.43	116.70	121.90
1	A	589	C	C4-C5-C6	7.42	121.11	117.40
1	A	123	C	N3-C4-C5	-7.42	118.93	121.90
1	A	111	G	N3-C4-N9	-7.41	121.55	126.00
1	A	1064	G	N3-C4-C5	7.40	132.30	128.60
1	A	314	C	C5-C6-N1	-7.39	117.31	121.00
1	A	331	G	C6-C5-N7	-7.39	125.97	130.40
1	A	8	A	N1-C6-N6	-7.38	114.17	118.60
1	A	826	C	C6-N1-C2	7.38	123.25	120.30
1	A	1094	G	C8-N9-C4	7.38	109.35	106.40
1	A	1087	G	C4-C5-N7	7.38	113.75	110.80
1	A	168	G	C4-N9-C1'	7.37	136.07	126.50
1	A	310	G	C5-C6-O6	-7.37	124.18	128.60
1	A	29	G	N1-C6-O6	7.36	124.32	119.90
1	A	264	U	N3-C2-O2	-7.36	117.05	122.20
1	A	21	G	C8-N9-C4	7.36	109.34	106.40
1	A	880	C	C2-N3-C4	-7.35	116.22	119.90
1	A	626	U	N3-C2-O2	-7.35	117.06	122.20
1	A	51	A	C8-N9-C4	-7.34	102.86	105.80
1	A	319	G	C5-C6-O6	-7.34	124.19	128.60
1	A	127	G	N1-C6-O6	7.34	124.30	119.90
1	A	279	A	N7-C8-N9	7.33	117.47	113.80
1	A	257	G	C6-C5-N7	-7.33	126.00	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	G	C6-C5-N7	-7.33	126.00	130.40
1	A	1339	A	N1-C6-N6	-7.32	114.21	118.60
1	A	585	G	C8-N9-C4	-7.32	103.47	106.40
1	A	240	C	N3-C4-C5	7.32	124.83	121.90
1	A	746	A	C8-N9-C4	7.31	108.73	105.80
1	A	600	C	N3-C4-C5	7.31	124.82	121.90
1	A	382	A	N7-C8-N9	7.31	117.45	113.80
1	A	864	A	C5-C6-N6	7.30	129.54	123.70
1	A	266	G	N3-C4-C5	-7.30	124.95	128.60
1	A	511	C	C6-N1-C2	7.29	123.22	120.30
1	A	491	G	N1-C6-O6	7.28	124.27	119.90
1	A	771	G	N9-C4-C5	-7.28	102.49	105.40
1	A	1442	G	N3-C4-N9	7.28	130.37	126.00
1	A	1084	G	N1-C2-N3	7.28	128.26	123.90
1	A	1500	A	N9-C4-C5	7.28	108.71	105.80
1	A	1490	U	C4-C5-C6	-7.27	115.34	119.70
1	A	648	A	C5-C6-N1	7.27	121.33	117.70
1	A	880	C	C5-C4-N4	-7.26	115.12	120.20
1	A	659	U	C5-C6-N1	-7.25	119.08	122.70
1	A	1524	C	C6-N1-C2	-7.25	117.40	120.30
1	A	121	C	N3-C2-O2	7.25	126.97	121.90
1	A	949	A	C2-N3-C4	-7.24	106.98	110.60
1	A	167	G	N3-C4-N9	7.24	130.34	126.00
1	A	129(A)	G	C6-C5-N7	-7.23	126.06	130.40
1	A	533	A	N1-C6-N6	-7.23	114.26	118.60
1	A	722	A	C4-C5-C6	7.23	120.62	117.00
1	A	254	G	C2-N3-C4	-7.23	108.29	111.90
1	A	379	C	C6-N1-C2	7.23	123.19	120.30
1	A	106	C	C6-N1-C2	-7.22	117.41	120.30
1	A	1361(A)	C	C5-C6-N1	7.22	124.61	121.00
1	A	126	G	C5-C6-N1	-7.21	107.89	111.50
1	A	266	G	O4'-C1'-N9	-7.21	102.43	108.20
1	A	907	A	N1-C2-N3	7.21	132.90	129.30
1	A	763	G	C5-C6-O6	-7.20	124.28	128.60
1	A	819	A	N1-C6-N6	7.20	122.92	118.60
1	A	1512	U	N3-C4-O4	7.19	124.44	119.40
1	A	875	C	C2-N3-C4	-7.19	116.31	119.90
1	A	919	A	N7-C8-N9	-7.18	110.21	113.80
1	A	1064	G	N3-C4-N9	-7.18	121.69	126.00
1	A	519	C	C6-N1-C2	7.18	123.17	120.30
1	A	1488	G	N3-C4-C5	-7.18	125.01	128.60
1	A	21	G	N9-C4-C5	-7.18	102.53	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1235	U	N1-C2-O2	-7.17	117.78	122.80
1	A	862	C	C5-C4-N4	-7.17	115.19	120.20
1	A	117	G	N9-C4-C5	-7.16	102.53	105.40
1	A	572	A	N1-C6-N6	-7.16	114.30	118.60
1	A	793	U	C5-C6-N1	7.16	126.28	122.70
1	A	576	G	O5'-P-OP2	-7.16	99.25	105.70
1	A	579	G	C6-C5-N7	-7.15	126.11	130.40
1	A	815	A	N9-C4-C5	-7.15	102.94	105.80
1	A	1190	G	O5'-P-OP2	-7.15	99.26	105.70
1	A	581	G	C2-N3-C4	-7.14	108.33	111.90
1	A	809	G	C5-C6-O6	-7.14	124.31	128.60
4	D	12	CYS	CA-CB-SG	7.14	126.85	114.00
1	A	309	G	N9-C4-C5	-7.14	102.55	105.40
1	A	292	G	C6-C5-N7	-7.14	126.12	130.40
1	A	256	U	N1-C2-N3	-7.13	110.62	114.90
1	A	557	G	N1-C6-O6	7.13	124.18	119.90
1	A	735	C	C5-C6-N1	-7.13	117.44	121.00
1	A	1200	C	C6-N1-C1'	-7.13	112.25	120.80
1	A	1354	C	C5-C6-N1	7.13	124.56	121.00
1	A	251	G	C5-C6-O6	-7.12	124.33	128.60
1	A	736	C	N3-C2-O2	-7.12	116.92	121.90
1	A	7	G	C8-N9-C4	-7.12	103.55	106.40
1	A	397	A	C6-C5-N7	-7.12	127.32	132.30
1	A	690	G	N3-C4-C5	7.11	132.16	128.60
1	A	1246	C	N3-C4-C5	7.11	124.75	121.90
12	L	66	VAL	CB-CA-C	-7.11	97.88	111.40
1	A	1441	G	C5-C6-N1	-7.11	107.94	111.50
1	A	779	C	C2-N3-C4	-7.11	116.35	119.90
1	A	413	G	O4'-C1'-N9	7.11	113.88	108.20
1	A	771	G	C4-C5-N7	7.10	113.64	110.80
1	A	867	G	N3-C4-N9	7.09	130.26	126.00
1	A	1485	U	C5-C4-O4	7.09	130.16	125.90
1	A	568	G	OP2-P-O3'	7.08	120.79	105.20
1	A	883	C	C6-N1-C2	7.08	123.13	120.30
1	A	1490	U	N1-C2-O2	7.08	127.76	122.80
1	A	1369	C	N3-C2-O2	-7.08	116.94	121.90
1	A	650	G	C4-C5-C6	7.08	123.05	118.80
1	A	379	C	O5'-P-OP2	-7.07	99.33	105.70
1	A	722	A	N9-C4-C5	-7.07	102.97	105.80
1	A	232	G	N1-C6-O6	7.06	124.14	119.90
1	A	254	G	O5'-P-OP1	-7.06	99.34	105.70
1	A	864	A	N1-C6-N6	-7.06	114.36	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	G	N1-C2-N3	7.06	128.13	123.90
1	A	1078	U	C2-N1-C1'	7.05	126.16	117.70
1	A	385	C	C6-N1-C2	-7.05	117.48	120.30
1	A	15	G	C2-N3-C4	-7.05	108.38	111.90
1	A	655	A	C5-C6-N1	7.05	121.22	117.70
1	A	1500	A	N1-C6-N6	-7.04	114.37	118.60
1	A	1502	A	C5-C6-N1	-7.04	114.18	117.70
1	A	823	G	N1-C2-N2	-7.04	109.87	116.20
1	A	569	C	O5'-P-OP2	-7.03	99.37	105.70
1	A	719	C	N1-C2-O2	7.03	123.12	118.90
1	A	661	G	C2-N3-C4	-7.03	108.39	111.90
1	A	920	U	C5-C4-O4	7.03	130.12	125.90
1	A	150	C	C6-N1-C2	-7.02	117.49	120.30
1	A	250	A	O5'-P-OP2	-7.01	99.39	105.70
1	A	329	A	N1-C6-N6	7.01	122.80	118.60
1	A	686	U	C5-C6-N1	-7.00	119.20	122.70
1	A	597	G	C5-C6-O6	-7.00	124.40	128.60
1	A	1455	G	C8-N9-C4	-7.00	103.60	106.40
1	A	1433	A	C8-N9-C4	-6.98	103.01	105.80
1	A	242	C	C6-N1-C2	6.98	123.09	120.30
1	A	329	A	C2-N3-C4	-6.98	107.11	110.60
1	A	809	G	C5-C6-N1	6.98	114.99	111.50
1	A	894	G	C2-N3-C4	-6.98	108.41	111.90
1	A	128	G	N1-C6-O6	6.98	124.08	119.90
1	A	895	G	C8-N9-C4	-6.97	103.61	106.40
1	A	1330	U	C5-C4-O4	-6.97	121.72	125.90
1	A	1074	G	C5-C6-N1	-6.97	108.01	111.50
1	A	397	A	N1-C6-N6	6.97	122.78	118.60
1	A	481	G	C8-N9-C1'	-6.96	117.95	127.00
1	A	552	U	C5-C6-N1	-6.96	119.22	122.70
1	A	319	G	N1-C6-O6	6.95	124.07	119.90
1	A	256	U	C5-C4-O4	-6.95	121.73	125.90
1	A	7	G	N9-C4-C5	6.95	108.18	105.40
1	A	280	C	OP1-P-OP2	6.95	130.02	119.60
1	A	1078	U	N3-C2-O2	-6.95	117.34	122.20
1	A	1530	G	C2-N3-C4	-6.94	108.43	111.90
1	A	147	G	N1-C6-O6	6.93	124.06	119.90
1	A	852	G	N1-C6-O6	6.92	124.05	119.90
1	A	1077	G	N1-C2-N2	-6.91	109.98	116.20
1	A	1087	G	C5-C6-O6	-6.91	124.45	128.60
1	A	66	G	C8-N9-C4	-6.90	103.64	106.40
1	A	1307	U	N1-C2-O2	6.90	127.63	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1373	G	C8-N9-C1'	-6.90	118.03	127.00
1	A	132	C	C6-N1-C2	-6.89	117.54	120.30
1	A	770	C	C2-N3-C4	-6.89	116.45	119.90
1	A	1149	C	C6-N1-C2	-6.89	117.54	120.30
1	A	793	U	C2-N3-C4	6.89	131.13	127.00
1	A	658	G	C2-N3-C4	-6.88	108.46	111.90
1	A	698	G	C4-N9-C1'	6.88	135.45	126.50
1	A	456	C	C6-N1-C2	6.88	123.05	120.30
1	A	1365	G	C8-N9-C4	-6.87	103.65	106.40
1	A	1417	G	C8-N9-C4	-6.87	103.65	106.40
1	A	525	C	C6-N1-C2	6.86	123.05	120.30
1	A	862	C	C6-N1-C2	6.86	123.05	120.30
1	A	300	A	N7-C8-N9	6.86	117.23	113.80
1	A	232	G	C6-C5-N7	-6.86	126.28	130.40
1	A	570	G	N3-C4-N9	6.86	130.12	126.00
1	A	15	G	C5-N7-C8	-6.85	100.88	104.30
1	A	721	G	C8-N9-C1'	-6.85	118.10	127.00
1	A	1305	G	P-O3'-C3'	6.83	127.90	119.70
1	A	185	A	O5'-P-OP2	-6.83	99.56	105.70
1	A	129(A)	G	C4-N9-C1'	6.82	135.37	126.50
1	A	268	C	N1-C2-O2	6.82	122.99	118.90
1	A	578	C	N1-C2-N3	6.82	123.98	119.20
1	A	299	G	C5-C6-N1	-6.82	108.09	111.50
1	A	310	G	C8-N9-C4	6.82	109.13	106.40
1	A	310	G	N1-C6-O6	6.82	123.99	119.90
1	A	35	G	N1-C6-O6	6.82	123.99	119.90
1	A	782	A	C2-N3-C4	-6.80	107.20	110.60
1	A	279	A	C6-C5-N7	-6.80	127.54	132.30
1	A	698	G	N3-C4-C5	-6.79	125.21	128.60
1	A	770	C	O5'-P-OP2	-6.79	99.59	105.70
1	A	15	G	C5-C6-N1	-6.78	108.11	111.50
1	A	892	A	N1-C2-N3	6.78	132.69	129.30
1	A	1514	C	N1-C2-O2	-6.77	114.84	118.90
1	A	773	G	N1-C6-O6	6.77	123.96	119.90
1	A	850	U	C5-C4-O4	6.76	129.96	125.90
1	A	649	G	C5-C6-N1	6.76	114.88	111.50
1	A	226	G	N1-C2-N2	-6.75	110.12	116.20
1	A	774	G	C5-C6-O6	-6.74	124.55	128.60
1	A	634	C	C6-N1-C2	-6.74	117.60	120.30
1	A	1502	A	N7-C8-N9	6.74	117.17	113.80
1	A	1505	G	C4-C5-C6	6.74	122.84	118.80
1	A	930	C	C2-N3-C4	-6.74	116.53	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	G	N3-C2-N2	-6.74	115.19	119.90
1	A	740	U	C5-C6-N1	-6.74	119.33	122.70
1	A	865	A	C6-N1-C2	-6.72	114.56	118.60
1	A	297	G	C4-C5-C6	6.72	122.83	118.80
1	A	1074	G	C6-C5-N7	-6.72	126.37	130.40
1	A	568	G	N1-C6-O6	-6.72	115.87	119.90
1	A	1331	G	C5-C6-O6	6.72	132.63	128.60
1	A	1525	G	N1-C2-N3	6.72	127.93	123.90
1	A	251	G	C5-N7-C8	-6.71	100.94	104.30
1	A	1477	C	C6-N1-C2	-6.71	117.62	120.30
1	A	352	C	C6-N1-C2	6.71	122.98	120.30
1	A	854	G	C6-C5-N7	-6.71	126.38	130.40
1	A	1346	A	N1-C6-N6	-6.70	114.58	118.60
1	A	854	G	C8-N9-C1'	-6.70	118.29	127.00
1	A	569	C	C4-C5-C6	6.70	120.75	117.40
1	A	8	A	C8-N9-C4	-6.70	103.12	105.80
1	A	1531	A	N7-C8-N9	6.69	117.15	113.80
1	A	1460	A	N1-C6-N6	6.69	122.61	118.60
1	A	1531	A	C5-C6-N1	-6.69	114.35	117.70
1	A	450	G	C8-N9-C4	6.69	109.08	106.40
1	A	570	G	C4-N9-C1'	6.69	135.19	126.50
1	A	859	A	C2-N3-C4	-6.69	107.26	110.60
1	A	1361(A)	C	C5-C4-N4	-6.68	115.52	120.20
1	A	724	G	C5-C6-N1	6.68	114.84	111.50
1	A	302	G	C5-C6-O6	-6.67	124.59	128.60
1	A	588	G	C5-N7-C8	6.67	107.64	104.30
1	A	947	G	C6-C5-N7	-6.67	126.40	130.40
1	A	560	U	N1-C2-O2	6.67	127.47	122.80
1	A	1347	G	N3-C4-N9	6.67	130.00	126.00
1	A	1193	G	N1-C6-O6	6.66	123.90	119.90
1	A	328	C	C2-N1-C1'	6.65	126.12	118.80
1	A	1527	C	N1-C2-O2	6.65	122.89	118.90
1	A	117	G	N1-C2-N3	6.65	127.89	123.90
1	A	615	C	C5-C6-N1	6.65	124.32	121.00
1	A	190(B)	C	C5-C6-N1	6.64	124.32	121.00
1	A	944	G	C8-N9-C4	-6.64	103.74	106.40
1	A	559	A	N1-C2-N3	6.64	132.62	129.30
20	T	94	ALA	N-CA-C	-6.64	93.08	111.00
1	A	485	G	P-O3'-C3'	6.63	127.66	119.70
1	A	941	G	C4-C5-N7	6.63	113.45	110.80
1	A	659	U	N1-C2-N3	6.63	118.88	114.90
1	A	698	G	C8-N9-C4	-6.62	103.75	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1082	G	C2-N3-C4	-6.62	108.59	111.90
1	A	103	C	N3-C4-C5	-6.62	119.25	121.90
8	H	12	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	595	G	C8-N9-C1'	-6.61	118.41	127.00
1	A	67	C	C6-N1-C2	-6.61	117.66	120.30
1	A	481	G	C2-N3-C4	6.60	115.20	111.90
1	A	906	G	N1-C6-O6	6.60	123.86	119.90
1	A	167	G	C8-N9-C1'	-6.60	118.42	127.00
1	A	23	C	C4-C5-C6	6.59	120.70	117.40
1	A	1087	G	N1-C6-O6	6.58	123.85	119.90
1	A	1395	C	C5-C6-N1	-6.58	117.71	121.00
1	A	262	A	C8-N9-C4	-6.58	103.17	105.80
1	A	1380	U	C5-C4-O4	6.58	129.85	125.90
1	A	168	G	C8-N9-C1'	-6.58	118.45	127.00
1	A	1073	U	C6-N1-C2	6.58	124.95	121.00
1	A	947	G	N1-C2-N2	-6.57	110.29	116.20
1	A	1124	G	N1-C6-O6	-6.56	115.96	119.90
1	A	863	U	N3-C2-O2	-6.55	117.61	122.20
1	A	874	G	C8-N9-C1'	-6.55	118.48	127.00
1	A	1505	G	P-O3'-C3'	6.55	127.56	119.70
1	A	718	G	N1-C6-O6	6.55	123.83	119.90
1	A	1073	U	C5-C6-N1	-6.55	119.43	122.70
1	A	372	C	C6-N1-C2	6.54	122.92	120.30
1	A	16	A	N7-C8-N9	-6.54	110.53	113.80
1	A	853	G	C5-C6-N1	-6.54	108.23	111.50
1	A	190(B)	C	C6-N1-C2	-6.53	117.69	120.30
1	A	529	G	N1-C6-O6	6.53	123.82	119.90
1	A	235	C	C5-C6-N1	-6.53	117.73	121.00
1	A	451	A	N9-C4-C5	-6.53	103.19	105.80
1	A	123	C	C6-N1-C2	-6.53	117.69	120.30
1	A	326	G	C5-C6-N1	-6.53	108.24	111.50
1	A	922	G	C5-C6-O6	6.53	132.52	128.60
1	A	529	G	C6-C5-N7	-6.52	126.49	130.40
1	A	656	C	N3-C4-N4	-6.52	113.44	118.00
1	A	651	C	C6-N1-C2	6.51	122.91	120.30
1	A	944	G	N1-C6-O6	-6.51	116.00	119.90
1	A	382	A	C6-C5-N7	-6.50	127.75	132.30
1	A	283	C	C2-N3-C4	6.50	123.15	119.90
1	A	858	G	N1-C2-N3	6.50	127.80	123.90
1	A	1442	G	C8-N9-C1'	-6.50	118.55	127.00
1	A	379	C	C5-C6-N1	-6.49	117.75	121.00
1	A	573	A	C4-C5-C6	6.49	120.25	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	G	C2-N3-C4	-6.49	108.65	111.90
1	A	557	G	C6-C5-N7	-6.49	126.51	130.40
1	A	257	G	C4-C5-N7	6.49	113.39	110.80
1	A	557	G	C2-N3-C4	-6.48	108.66	111.90
1	A	732	C	C2-N3-C4	-6.47	116.66	119.90
1	A	1510	U	N1-C2-O2	6.47	127.33	122.80
1	A	658	G	C6-C5-N7	-6.47	126.52	130.40
1	A	757	U	C6-N1-C2	6.47	124.88	121.00
1	A	933	G	N1-C6-O6	6.47	123.78	119.90
1	A	798	G	C6-N1-C2	-6.46	121.22	125.10
1	A	9	G	C2-N3-C4	-6.46	108.67	111.90
1	A	329	A	C4-C5-N7	6.46	113.93	110.70
1	A	564	C	N3-C2-O2	-6.45	117.38	121.90
1	A	168	G	C4-C5-C6	6.45	122.67	118.80
1	A	25	C	N3-C2-O2	6.45	126.41	121.90
1	A	74	C	C6-N1-C2	-6.45	117.72	120.30
1	A	638	G	C6-C5-N7	-6.45	126.53	130.40
1	A	109	A	C2-N3-C4	-6.44	107.38	110.60
1	A	456	C	N1-C2-O2	6.44	122.76	118.90
1	A	1076	C	C2-N1-C1'	6.44	125.88	118.80
1	A	314	C	C2-N3-C4	-6.43	116.68	119.90
1	A	829	G	N3-C4-N9	6.43	129.86	126.00
1	A	779	C	C4-C5-C6	6.43	120.61	117.40
1	A	1074	G	N1-C6-O6	6.43	123.76	119.90
1	A	144	G	C5-C6-N1	-6.42	108.29	111.50
1	A	626	U	C2-N1-C1'	6.42	125.40	117.70
1	A	569	C	C2-N3-C4	-6.41	116.69	119.90
1	A	251	G	N1-C6-O6	6.41	123.75	119.90
1	A	321	A	O5'-P-OP2	-6.41	99.93	105.70
1	A	89	C	C2-N1-C1'	6.41	125.84	118.80
1	A	1254	C	C6-N1-C2	-6.39	117.75	120.30
1	A	812	C	N1-C2-N3	6.38	123.67	119.20
1	A	1051	C	N1-C2-O2	6.38	122.73	118.90
1	A	59	A	O5'-P-OP2	-6.38	99.96	105.70
1	A	593	G	C5-C6-O6	6.37	132.42	128.60
1	A	611	A	N1-C6-N6	-6.36	114.78	118.60
1	A	650	G	N3-C4-C5	-6.36	125.42	128.60
1	A	311	C	C2-N3-C4	-6.35	116.72	119.90
1	A	1532	U	C4-C5-C6	-6.35	115.89	119.70
1	A	1079	G	N1-C6-O6	-6.35	116.09	119.90
1	A	1453	G	C4-C5-N7	6.35	113.34	110.80
1	A	533	A	N9-C4-C5	6.34	108.34	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	C	C5-C6-N1	-6.34	117.83	121.00
1	A	876	G	C5-C6-N1	6.34	114.67	111.50
1	A	288	A	C8-N9-C4	6.34	108.34	105.80
1	A	553	A	C8-N9-C4	6.34	108.33	105.80
1	A	903	G	C4-N9-C1'	6.34	134.74	126.50
1	A	903	G	C8-N9-C1'	-6.33	118.77	127.00
1	A	1386	G	N1-C2-N3	6.33	127.70	123.90
1	A	445	G	N1-C6-O6	6.33	123.70	119.90
1	A	758	G	C2-N3-C4	-6.33	108.73	111.90
1	A	1415	G	C8-N9-C4	-6.33	103.87	106.40
1	A	1502	A	N9-C4-C5	-6.33	103.27	105.80
1	A	882	C	C2-N3-C4	-6.33	116.74	119.90
1	A	919	A	C5-C6-N1	6.33	120.86	117.70
1	A	1079	G	C4-N9-C1'	6.33	134.72	126.50
1	A	1108	G	C4-C5-C6	6.33	122.59	118.80
1	A	929	G	C2-N3-C4	-6.32	108.74	111.90
1	A	634	C	N3-C4-C5	-6.32	119.37	121.90
1	A	326	G	N1-C2-N3	6.32	127.69	123.90
1	A	548	G	N1-C6-O6	6.32	123.69	119.90
1	A	918	A	C6-N1-C2	-6.31	114.81	118.60
1	A	481	G	C5-N7-C8	6.31	107.46	104.30
1	A	1362	C	C6-N1-C2	-6.30	117.78	120.30
1	A	1531	A	C6-C5-N7	-6.30	127.89	132.30
1	A	581	G	N3-C4-N9	-6.30	122.22	126.00
1	A	949	A	C8-N9-C4	6.30	108.32	105.80
1	A	719	C	N3-C2-O2	-6.30	117.49	121.90
1	A	141	A	C8-N9-C4	6.29	108.32	105.80
1	A	873	A	C5-C6-N1	6.29	120.85	117.70
1	A	27	G	N1-C6-O6	6.29	123.67	119.90
1	A	274	A	C8-N9-C4	6.29	108.31	105.80
1	A	1393	U	C5-C4-O4	-6.29	122.13	125.90
1	A	283	C	C6-N1-C2	-6.28	117.79	120.30
1	A	526	C	C6-N1-C2	6.28	122.81	120.30
1	A	715	A	C8-N9-C4	6.28	108.31	105.80
1	A	832	C	N3-C4-C5	6.28	124.41	121.90
1	A	89	C	C5-C6-N1	6.28	124.14	121.00
1	A	129(A)	G	N3-C4-N9	6.28	129.77	126.00
1	A	580	U	N3-C4-C5	-6.28	110.83	114.60
1	A	1181	G	N7-C8-N9	-6.28	109.96	113.10
1	A	1277	C	C6-N1-C2	-6.28	117.79	120.30
1	A	854	G	N1-C2-N3	6.28	127.67	123.90
1	A	589	C	C5-C6-N1	-6.28	117.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	G	N3-C4-N9	-6.27	122.24	126.00
1	A	912	C	C5-C4-N4	-6.27	115.81	120.20
1	A	1504	G	N1-C6-O6	-6.27	116.14	119.90
1	A	297	G	OP1-P-OP2	-6.27	110.20	119.60
1	A	695	A	C5-N7-C8	-6.27	100.77	103.90
1	A	254	G	N1-C2-N3	6.26	127.66	123.90
1	A	240	C	N3-C2-O2	6.25	126.28	121.90
1	A	122	G	C6-C5-N7	-6.25	126.65	130.40
1	A	1373	G	C4-N9-C1'	6.25	134.62	126.50
1	A	1441	G	C4-C5-N7	-6.25	108.30	110.80
1	A	279	A	N9-C4-C5	6.25	108.30	105.80
1	A	779	C	C6-N1-C2	-6.25	117.80	120.30
1	A	872	A	N9-C4-C5	-6.25	103.30	105.80
1	A	1231	G	OP1-P-O3'	6.25	118.94	105.20
1	A	518	C	N3-C2-O2	-6.25	117.53	121.90
1	A	773	G	C4-C5-N7	6.24	113.30	110.80
1	A	359	U	O5'-P-OP1	-6.24	100.08	105.70
1	A	302	G	N1-C6-O6	6.23	123.64	119.90
1	A	1511	G	OP1-P-OP2	-6.23	110.26	119.60
1	A	48	C	C6-N1-C2	6.23	122.79	120.30
1	A	881	G	N1-C2-N3	6.22	127.63	123.90
1	A	130	A	C2-N3-C4	-6.21	107.49	110.60
1	A	1377	A	N1-C6-N6	-6.21	114.87	118.60
1	A	21	G	N1-C2-N2	-6.21	110.61	116.20
1	A	1228	C	N1-C2-O2	6.21	122.63	118.90
1	A	570	G	N1-C2-N2	-6.21	110.61	116.20
1	A	106	C	OP2-P-O3'	6.20	118.84	105.20
1	A	558	G	C5-N7-C8	-6.20	101.20	104.30
1	A	731	G	C6-C5-N7	-6.20	126.68	130.40
1	A	836	G	C4-C5-C6	6.20	122.52	118.80
1	A	1230	C	C5-C6-N1	6.20	124.10	121.00
1	A	872	A	C5-N7-C8	-6.19	100.80	103.90
1	A	292	G	C4-C5-N7	6.19	113.28	110.80
1	A	1084	G	N3-C4-C5	-6.19	125.50	128.60
1	A	23	C	N1-C2-N3	6.19	123.53	119.20
1	A	1282	C	C2-N1-C1'	6.18	125.60	118.80
1	A	1523	G	N3-C2-N2	-6.18	115.57	119.90
1	A	670	G	N1-C6-O6	6.18	123.61	119.90
1	A	1300	G	OP2-P-O3'	6.18	118.79	105.20
1	A	584	G	N1-C2-N2	6.17	121.75	116.20
1	A	250	A	C8-N9-C4	6.17	108.27	105.80
1	A	812	C	P-O3'-C3'	6.17	127.10	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	823	G	N1-C2-N3	6.17	127.60	123.90
1	A	780	A	C6-N1-C2	-6.17	114.90	118.60
1	A	1108	G	N3-C4-C5	-6.16	125.52	128.60
1	A	573	A	N9-C4-C5	6.16	108.26	105.80
1	A	304	U	O5'-P-OP1	-6.16	100.16	105.70
1	A	529	G	C4-C5-C6	6.16	122.49	118.80
1	A	761	G	C6-C5-N7	-6.16	126.71	130.40
1	A	836	G	C8-N9-C1'	-6.15	119.00	127.00
1	A	860	A	N1-C2-N3	6.14	132.37	129.30
1	A	573	A	N7-C8-N9	6.14	116.87	113.80
1	A	264	U	C6-N1-C2	-6.14	117.32	121.00
1	A	1498	UR3	P-O3'-C3'	6.13	127.06	119.70
1	A	266	G	C5-C6-O6	-6.13	124.92	128.60
1	A	24	U	C5-C6-N1	-6.13	119.64	122.70
1	A	747	C	C5-C6-N1	-6.13	117.94	121.00
1	A	591	U	C5-C6-N1	-6.13	119.64	122.70
1	A	676	A	C2-N3-C4	-6.13	107.54	110.60
1	A	872	A	O5'-P-OP2	-6.13	100.19	105.70
1	A	882	C	C5-C6-N1	-6.13	117.94	121.00
1	A	962	C	N1-C2-O2	6.13	122.58	118.90
1	A	903	G	C6-C5-N7	-6.12	126.73	130.40
1	A	620	C	C6-N1-C2	6.12	122.75	120.30
1	A	565	U	N1-C2-N3	-6.12	111.23	114.90
1	A	334	C	C6-N1-C2	6.11	122.74	120.30
1	A	293	G	N3-C4-C5	6.11	131.65	128.60
1	A	852	G	C2-N3-C4	-6.11	108.85	111.90
1	A	1246	C	C6-N1-C2	6.10	122.74	120.30
1	A	1301	U	O5'-P-OP2	-6.10	100.21	105.70
1	A	117	G	N3-C4-N9	6.10	129.66	126.00
1	A	558	G	C4-C5-N7	6.09	113.24	110.80
1	A	667	G	N1-C2-N3	6.09	127.56	123.90
1	A	1301	U	P-O3'-C3'	6.09	127.01	119.70
1	A	1366	C	C5-C6-N1	6.09	124.04	121.00
1	A	880	C	C4-C5-C6	6.09	120.44	117.40
1	A	851	G	C6-C5-N7	-6.08	126.75	130.40
1	A	89	C	N1-C2-O2	6.08	122.55	118.90
1	A	557	G	N1-C2-N3	6.08	127.55	123.90
1	A	661	G	N3-C4-C5	6.08	131.64	128.60
1	A	342	C	C5-C6-N1	6.08	124.04	121.00
1	A	246	A	C5-C6-N1	6.07	120.74	117.70
1	A	254	G	C5-C6-N1	-6.07	108.46	111.50
1	A	635	G	C4-C5-C6	6.07	122.44	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	923	A	N9-C4-C5	-6.07	103.37	105.80
1	A	1529	G	N1-C6-O6	6.06	123.54	119.90
1	A	1238	A	C5-C6-N6	6.06	128.55	123.70
1	A	150	C	OP2-P-O3'	6.06	118.53	105.20
1	A	67	C	N3-C4-C5	-6.05	119.48	121.90
1	A	733	A	C2-N3-C4	-6.05	107.58	110.60
1	A	1079	G	C8-N9-C4	-6.05	103.98	106.40
1	A	836	G	C4-N9-C1'	6.05	134.36	126.50
1	A	342	C	N3-C4-C5	-6.04	119.48	121.90
1	A	797	C	N3-C2-O2	-6.04	117.67	121.90
1	A	890	G	N9-C4-C5	6.04	107.82	105.40
1	A	1500	A	C8-N9-C4	-6.04	103.38	105.80
1	A	643	C	C2-N3-C4	-6.04	116.88	119.90
1	A	1158	C	N3-C2-O2	-6.04	117.67	121.90
1	A	597	G	C4-C5-N7	6.04	113.22	110.80
1	A	309	G	C6-C5-N7	-6.04	126.78	130.40
1	A	310	G	N9-C4-C5	-6.04	102.98	105.40
1	A	245	C	C2-N3-C4	-6.03	116.88	119.90
1	A	372	C	C5-C6-N1	-6.03	117.98	121.00
1	A	1512	U	C6-N1-C2	-6.03	117.38	121.00
1	A	885	G	N1-C2-N3	6.03	127.52	123.90
1	A	596	C	C6-N1-C2	6.02	122.71	120.30
1	A	364	A	C4-C5-C6	6.02	120.01	117.00
1	A	703	G	C5-C6-N1	-6.01	108.49	111.50
1	A	1074	G	C2-N3-C4	-6.01	108.89	111.90
1	A	1509	C	C5-C6-N1	-6.01	117.99	121.00
1	A	130	A	C4-C5-C6	6.01	120.01	117.00
1	A	116	A	C5-C6-N1	-6.01	114.69	117.70
1	A	180	U	C2-N1-C1'	6.01	124.91	117.70
1	A	1060	C	C2-N1-C1'	6.01	125.41	118.80
1	A	740	U	C4-C5-C6	6.00	123.30	119.70
1	A	1062	U	C5-C4-O4	6.00	129.50	125.90
1	A	819	A	C6-C5-N7	-6.00	128.10	132.30
1	A	1394	A	N1-C6-N6	6.00	122.20	118.60
1	A	27	G	C5-C6-O6	-6.00	125.00	128.60
1	A	329	A	N3-C4-C5	6.00	131.00	126.80
1	A	903	G	C4-C5-C6	5.99	122.39	118.80
1	A	190(A)	C	C6-N1-C2	-5.99	117.90	120.30
1	A	1479	C	C6-N1-C2	-5.99	117.90	120.30
1	A	167	G	C4-N9-C1'	5.99	134.28	126.50
1	A	1490	U	C2-N1-C1'	5.99	124.89	117.70
1	A	732	C	N3-C4-C5	5.99	124.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	A	N1-C2-N3	5.99	132.29	129.30
1	A	230	G	C5-C6-N1	-5.99	108.51	111.50
1	A	860	A	C2-N3-C4	-5.99	107.61	110.60
1	A	782	A	N1-C2-N3	5.98	132.29	129.30
1	A	898	G	C2-N3-C4	-5.98	108.91	111.90
1	A	1510	U	N3-C2-O2	-5.98	118.01	122.20
2	B	44	LEU	CA-CB-CG	-5.98	101.55	115.30
1	A	168	G	C5-C6-N1	-5.98	108.51	111.50
1	A	1039	C	C6-N1-C2	-5.98	117.91	120.30
1	A	92	C	C2-N1-C1'	5.98	125.37	118.80
1	A	569	C	C2-N1-C1'	-5.97	112.23	118.80
1	A	398	C	N3-C4-C5	5.97	124.29	121.90
1	A	19	C	OP1-P-OP2	5.97	128.55	119.60
1	A	1508	G	C5-C6-O6	-5.96	125.02	128.60
1	A	44	G	N1-C6-O6	5.96	123.48	119.90
1	A	854	G	N1-C2-N2	-5.96	110.84	116.20
1	A	774	G	C4-C5-N7	5.96	113.18	110.80
1	A	933	G	C4-C5-N7	5.96	113.18	110.80
1	A	586	C	C5-C6-N1	-5.94	118.03	121.00
1	A	1414	U	C6-N1-C2	-5.94	117.44	121.00
1	A	5	U	P-O3'-C3'	5.93	126.82	119.70
1	A	1516[A]	G	N7-C8-N9	5.93	116.07	113.10
1	A	1516[B]	G	N7-C8-N9	5.93	116.07	113.10
1	A	168	G	N3-C4-N9	5.93	129.56	126.00
1	A	559	A	C4-C5-C6	5.93	119.97	117.00
1	A	1178	G	C8-N9-C4	-5.93	104.03	106.40
1	A	1532	U	C5-C4-O4	-5.93	122.34	125.90
1	A	752	G	C8-N9-C4	5.93	108.77	106.40
1	A	1527	C	C5-C4-N4	-5.93	116.05	120.20
1	A	691	G	C5-C6-O6	5.93	132.16	128.60
1	A	204	U	O4'-C1'-N1	-5.93	103.46	108.20
1	A	869	G	N9-C4-C5	-5.93	103.03	105.40
1	A	736	C	C5-C6-N1	-5.92	118.04	121.00
1	A	1238	A	N7-C8-N9	5.92	116.76	113.80
1	A	597	G	N3-C4-N9	5.92	129.55	126.00
1	A	755	G	C5-C6-O6	-5.92	125.05	128.60
1	A	1077	G	N3-C4-N9	5.92	129.55	126.00
1	A	869	G	C8-N9-C1'	5.92	134.70	127.00
1	A	1494	G	C8-N9-C4	-5.92	104.03	106.40
1	A	1495	U	N1-C2-N3	-5.92	111.35	114.90
1	A	19	C	N3-C4-C5	5.92	124.27	121.90
1	A	269	C	N3-C2-O2	-5.92	117.76	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	922	G	N7-C8-N9	5.92	116.06	113.10
1	A	1302	U	O4'-C1'-N1	-5.91	103.47	108.20
1	A	1361(A)	C	C4-C5-C6	-5.91	114.44	117.40
1	A	947	G	N1-C2-N3	5.91	127.45	123.90
1	A	729	A	N1-C6-N6	5.91	122.15	118.60
1	A	873	A	N9-C4-C5	5.91	108.16	105.80
1	A	80	G	N9-C4-C5	5.91	107.76	105.40
1	A	750	G	N1-C2-N3	5.91	127.44	123.90
1	A	638	G	N9-C4-C5	-5.91	103.04	105.40
1	A	721	G	C4-N9-C1'	5.90	134.17	126.50
1	A	168	G	N1-C6-O6	5.89	123.44	119.90
1	A	770	C	N3-C4-C5	5.89	124.26	121.90
1	A	251	G	C6-C5-N7	-5.89	126.87	130.40
1	A	585	G	OP1-P-OP2	5.89	128.43	119.60
1	A	1190	G	P-O3'-C3'	5.88	126.76	119.70
1	A	190(F)	G	N1-C6-O6	-5.88	116.37	119.90
1	A	522	C	N1-C2-O2	-5.88	115.37	118.90
1	A	750	G	N1-C6-O6	5.88	123.43	119.90
1	A	1346	A	N9-C4-C5	5.88	108.15	105.80
1	A	572	A	N9-C4-C5	5.88	108.15	105.80
1	A	1505	G	N3-C4-C5	-5.87	125.66	128.60
1	A	548	G	C5-C6-N1	-5.87	108.57	111.50
1	A	648	A	N7-C8-N9	-5.87	110.86	113.80
1	A	1332	A	C8-N9-C4	-5.87	103.45	105.80
1	A	635	G	N1-C2-N3	5.87	127.42	123.90
1	A	226	G	N1-C2-N3	5.86	127.42	123.90
1	A	297	G	C6-C5-N7	-5.86	126.88	130.40
1	A	1077	G	N3-C2-N2	5.86	124.00	119.90
1	A	1469	G	C5-C6-O6	-5.86	125.08	128.60
1	A	568	G	OP1-P-OP2	5.86	128.39	119.60
1	A	783	C	N3-C4-C5	5.86	124.24	121.90
1	A	1205	U	N3-C2-O2	-5.86	118.10	122.20
1	A	732	C	C5-C4-N4	-5.86	116.10	120.20
1	A	1415	G	N7-C8-N9	5.86	116.03	113.10
1	A	1431	C	N3-C4-C5	5.86	124.24	121.90
1	A	1331	G	C6-C5-N7	5.85	133.91	130.40
1	A	1143	G	N1-C6-O6	5.85	123.41	119.90
1	A	1343	G	C2-N3-C4	-5.85	108.97	111.90
1	A	729	A	C5-N7-C8	-5.84	100.98	103.90
1	A	135	C	N3-C2-O2	5.84	125.99	121.90
1	A	508	C	N3-C4-C5	5.84	124.23	121.90
7	G	124	LEU	CA-CB-CG	-5.84	101.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	689	C	N3-C4-C5	-5.84	119.56	121.90
1	A	581	G	N3-C4-C5	5.83	131.52	128.60
1	A	1542	U	C6-N1-C2	5.83	124.50	121.00
1	A	1501	C	C2-N3-C4	-5.83	116.98	119.90
1	A	552	U	C6-N1-C2	5.83	124.50	121.00
1	A	825	G	N9-C4-C5	-5.83	103.07	105.40
1	A	811	C	C6-N1-C2	5.83	122.63	120.30
1	A	902	G	C5-C6-O6	-5.83	125.11	128.60
1	A	1495	U	N1-C2-O2	5.83	126.88	122.80
1	A	864	A	N9-C4-C5	5.82	108.13	105.80
1	A	878	G	C5-C6-N1	5.82	114.41	111.50
1	A	892	A	C8-N9-C4	-5.82	103.47	105.80
1	A	21	G	C8-N9-C1'	-5.82	119.44	127.00
1	A	1281	U	N3-C4-O4	5.82	123.47	119.40
1	A	103	C	C4-C5-C6	5.82	120.31	117.40
1	A	289	G	N1-C6-O6	5.82	123.39	119.90
1	A	900	A	C8-N9-C4	-5.82	103.47	105.80
1	A	570	G	C2-N3-C4	5.81	114.81	111.90
1	A	603	U	C2-N1-C1'	-5.81	110.73	117.70
1	A	107	G	C5-N7-C8	-5.81	101.39	104.30
1	A	392	G	C6-C5-N7	-5.81	126.91	130.40
1	A	292	G	N9-C4-C5	-5.81	103.08	105.40
1	A	364	A	N1-C2-N3	5.81	132.20	129.30
1	A	502	G	C6-C5-N7	-5.81	126.92	130.40
1	A	885	G	C5-C6-N1	-5.81	108.60	111.50
3	C	5	ILE	CB-CA-C	-5.81	99.98	111.60
1	A	107	G	C4-C5-N7	5.80	113.12	110.80
1	A	814	A	N7-C8-N9	-5.80	110.90	113.80
1	A	1224	G	C4-C5-N7	-5.80	108.48	110.80
1	A	1380	U	N3-C4-O4	-5.80	115.34	119.40
1	A	1395	C	N3-C4-C5	5.80	124.22	121.90
1	A	80	G	N3-C2-N2	-5.80	115.84	119.90
1	A	311	C	N3-C4-C5	5.80	124.22	121.90
1	A	746	A	N1-C2-N3	5.80	132.20	129.30
1	A	128	G	C2-N3-C4	-5.80	109.00	111.90
1	A	600	C	N3-C4-N4	-5.80	113.94	118.00
1	A	1390	U	N3-C4-C5	-5.79	111.12	114.60
1	A	686	U	C5-C4-O4	5.79	129.38	125.90
1	A	908	A	N3-C4-C5	5.79	130.85	126.80
1	A	1058	G	C4-C5-N7	-5.79	108.48	110.80
1	A	1393	U	C6-N1-C2	5.79	124.47	121.00
1	A	485	G	OP2-P-O3'	5.79	117.94	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	779	C	N3-C2-O2	-5.79	117.85	121.90
1	A	1394	A	C8-N9-C4	5.79	108.12	105.80
1	A	1082	G	N1-C2-N3	5.79	127.37	123.90
1	A	176	C	C6-N1-C2	5.79	122.61	120.30
1	A	889	A	N1-C2-N3	5.78	132.19	129.30
1	A	931	C	C4-C5-C6	5.78	120.29	117.40
1	A	276	G	C8-N9-C4	5.78	108.71	106.40
1	A	804	U	N3-C2-O2	-5.78	118.15	122.20
1	A	1124	G	C6-C5-N7	5.78	133.87	130.40
1	A	651	C	N3-C4-C5	5.78	124.21	121.90
1	A	686	U	C4-C5-C6	5.78	123.17	119.70
1	A	638	G	C5-C6-N1	-5.78	108.61	111.50
1	A	1010	G	C8-N9-C4	-5.77	104.09	106.40
1	A	364	A	C2-N3-C4	-5.77	107.72	110.60
1	A	402	G	C8-N9-C4	-5.77	104.09	106.40
1	A	745	C	C2-N3-C4	-5.77	117.02	119.90
1	A	928	G	C5-N7-C8	-5.77	101.42	104.30
1	A	1310	G	C8-N9-C1'	-5.77	119.50	127.00
1	A	288	A	C2-N3-C4	-5.77	107.72	110.60
1	A	78	G	N1-C6-O6	5.76	123.36	119.90
1	A	1181	G	N9-C4-C5	-5.76	103.09	105.40
1	A	115	G	N3-C4-N9	5.76	129.46	126.00
1	A	698	G	C4-C5-C6	5.76	122.26	118.80
1	A	972	C	N3-C4-C5	-5.76	119.60	121.90
1	A	755	G	N3-C2-N2	-5.76	115.87	119.90
1	A	947	G	N3-C4-N9	5.76	129.46	126.00
1	A	739	C	C2-N3-C4	-5.76	117.02	119.90
1	A	1475	G	C8-N9-C4	-5.76	104.10	106.40
1	A	500	G	N1-C6-O6	5.75	123.35	119.90
1	A	1380	U	P-O3'-C3'	5.75	126.61	119.70
1	A	264	U	O5'-P-OP2	-5.75	100.52	105.70
1	A	932	C	N3-C2-O2	-5.75	117.87	121.90
1	A	1091	U	N3-C4-C5	-5.75	111.15	114.60
1	A	665	A	N1-C6-N6	-5.75	115.15	118.60
1	A	757	U	N3-C2-O2	5.75	126.22	122.20
1	A	928	G	C5-C6-O6	-5.75	125.15	128.60
1	A	103	C	C6-N1-C2	-5.75	118.00	120.30
1	A	827	U	N3-C4-C5	5.75	118.05	114.60
1	A	870	U	N1-C2-N3	-5.75	111.45	114.90
1	A	1090	U	C6-N1-C2	-5.75	117.55	121.00
1	A	667	G	N1-C6-O6	5.75	123.35	119.90
1	A	228	A	C2-N3-C4	-5.74	107.73	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1521	G	N3-C4-C5	-5.74	125.73	128.60
1	A	25	C	N1-C2-O2	-5.74	115.46	118.90
1	A	713	G	N9-C4-C5	5.73	107.69	105.40
1	A	730	G	C4-C5-N7	-5.73	108.51	110.80
1	A	730	G	N7-C8-N9	-5.73	110.23	113.10
1	A	1347	G	C6-C5-N7	-5.73	126.96	130.40
1	A	15	G	N7-C8-N9	5.73	115.97	113.10
1	A	240	C	C5-C4-N4	-5.73	116.19	120.20
1	A	289	G	C2-N3-C4	-5.73	109.04	111.90
1	A	822	C	N3-C4-N4	5.73	122.01	118.00
1	A	482	A	C8-N9-C4	-5.73	103.51	105.80
1	A	578	C	C2-N3-C4	-5.73	117.04	119.90
1	A	57	G	N1-C6-O6	-5.72	116.47	119.90
1	A	776	G	N3-C4-N9	-5.72	122.57	126.00
1	A	1051	C	C6-N1-C1'	-5.72	113.93	120.80
1	A	1179	A	C8-N9-C4	-5.72	103.51	105.80
1	A	1228	C	N3-C2-O2	-5.72	117.89	121.90
1	A	504	C	C6-N1-C2	-5.72	118.01	120.30
1	A	1434	A	C5-C6-N6	-5.72	119.12	123.70
1	A	948	C	N3-C2-O2	5.72	125.90	121.90
1	A	16	A	C8-N9-C4	5.71	108.09	105.80
1	A	144	G	C6-C5-N7	-5.71	126.97	130.40
1	A	1228	C	C2-N1-C1'	5.71	125.08	118.80
1	A	44	G	C6-C5-N7	-5.71	126.97	130.40
1	A	829	G	C4-N9-C1'	5.71	133.92	126.50
1	A	624	C	N3-C4-C5	5.71	124.18	121.90
1	A	90	U	C5-C6-N1	5.70	125.55	122.70
1	A	190(E)	U	N1-C2-O2	-5.70	118.81	122.80
1	A	965	A	C8-N9-C4	5.70	108.08	105.80
1	A	1532	U	C6-N1-C2	-5.70	117.58	121.00
1	A	1478	C	C6-N1-C2	-5.70	118.02	120.30
1	A	145	G	N1-C6-O6	5.70	123.32	119.90
1	A	609	A	N1-C2-N3	5.70	132.15	129.30
1	A	597	G	C6-C5-N7	-5.70	126.98	130.40
1	A	274	A	N7-C8-N9	-5.69	110.95	113.80
1	A	658	G	C4-N9-C1'	5.69	133.90	126.50
1	A	805	C	C2-N3-C4	-5.69	117.06	119.90
1	A	724	G	OP1-P-OP2	-5.68	111.07	119.60
1	A	66	G	N3-C2-N2	-5.68	115.92	119.90
1	A	942	G	N1-C6-O6	5.68	123.31	119.90
1	A	595	G	O4'-C1'-N9	-5.68	103.66	108.20
1	A	593	G	N1-C6-O6	-5.68	116.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	C	C5-C6-N1	-5.68	118.16	121.00
1	A	190(F)	G	C6-C5-N7	5.67	133.81	130.40
1	A	519	C	N1-C2-O2	5.67	122.30	118.90
1	A	1200	C	N3-C2-O2	-5.67	117.93	121.90
1	A	1370	G	N9-C4-C5	5.67	107.67	105.40
1	A	1078	U	O5'-P-OP2	-5.67	100.60	105.70
1	A	144	G	C5-N7-C8	-5.66	101.47	104.30
1	A	157	G	N1-C6-O6	5.66	123.30	119.90
1	A	392	G	N3-C4-N9	5.66	129.40	126.00
1	A	731	G	C5-N7-C8	-5.66	101.47	104.30
1	A	1392	G	N1-C2-N3	5.66	127.30	123.90
1	A	697	U	N3-C4-O4	-5.66	115.44	119.40
1	A	923	A	C4-C5-N7	5.66	113.53	110.70
1	A	1288	A	C8-N9-C4	-5.66	103.54	105.80
1	A	482	A	N7-C8-N9	5.66	116.63	113.80
5	E	12	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	686	U	N1-C2-N3	5.65	118.29	114.90
1	A	773	G	C5-C6-O6	-5.65	125.21	128.60
1	A	867	G	C8-N9-C1'	-5.64	119.66	127.00
1	A	120	A	C2-N3-C4	-5.64	107.78	110.60
1	A	251	G	N7-C8-N9	5.64	115.92	113.10
1	A	113	G	C6-C5-N7	-5.64	127.02	130.40
1	A	400	C	N3-C4-N4	-5.64	114.05	118.00
1	A	687	A	P-O3'-C3'	5.64	126.47	119.70
1	A	642	A	C8-N9-C4	-5.64	103.55	105.80
1	A	859	A	C4-C5-C6	5.63	119.81	117.00
1	A	1307	U	C5-C4-O4	5.63	129.28	125.90
1	A	596	C	C5-C6-N1	-5.63	118.19	121.00
1	A	858	G	N3-C4-N9	-5.62	122.62	126.00
1	A	9	G	N1-C2-N3	5.62	127.27	123.90
1	A	20	U	OP1-P-OP2	5.62	128.03	119.60
1	A	776	G	N3-C4-C5	5.62	131.41	128.60
1	A	154	C	C5-C4-N4	-5.62	116.27	120.20
1	A	589	C	N3-C4-C5	-5.62	119.65	121.90
1	A	23	C	C2-N3-C4	-5.62	117.09	119.90
1	A	836	G	N1-C2-N3	5.62	127.27	123.90
1	A	617	G	C8-N9-C4	5.62	108.65	106.40
1	A	815	A	N1-C6-N6	5.62	121.97	118.60
1	A	590	C	N1-C2-O2	-5.61	115.53	118.90
1	A	885	G	N3-C4-C5	5.61	131.41	128.60
1	A	62	U	N3-C4-C5	-5.61	111.23	114.60
1	A	880	C	N3-C4-N4	5.61	121.93	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1064	G	C2-N3-C4	-5.61	109.10	111.90
1	A	122	G	C2-N3-C4	-5.60	109.10	111.90
1	A	279	A	C5-N7-C8	-5.60	101.10	103.90
1	A	1434	A	C4-C5-N7	5.60	113.50	110.70
1	A	80	G	C8-N9-C4	-5.60	104.16	106.40
1	A	595	G	N3-C4-N9	5.60	129.36	126.00
1	A	822	C	C2-N1-C1'	5.60	124.96	118.80
1	A	881	G	C6-N1-C2	-5.60	121.74	125.10
1	A	1530	G	N1-C6-O6	5.60	123.26	119.90
1	A	912	C	N1-C2-O2	-5.59	115.54	118.90
1	A	830	G	C4-C5-N7	-5.59	108.56	110.80
1	A	1469	G	N1-C6-O6	5.59	123.25	119.90
1	A	655	A	C6-N1-C2	-5.59	115.25	118.60
1	A	864	A	C4-C5-N7	-5.59	107.91	110.70
1	A	491	G	C5-C6-N1	-5.59	108.71	111.50
1	A	874	G	C8-N9-C4	5.59	108.64	106.40
1	A	9	G	N1-C6-O6	5.58	123.25	119.90
1	A	718	G	N3-C4-C5	5.58	131.39	128.60
1	A	1441	G	C5-C6-O6	5.58	131.95	128.60
1	A	243	A	N1-C2-N3	5.58	132.09	129.30
1	A	597	G	C6-N1-C2	-5.58	121.75	125.10
1	A	945	G	C5-C6-N1	5.58	114.29	111.50
1	A	691	G	N9-C4-C5	5.58	107.63	105.40
1	A	689	C	C6-N1-C2	-5.58	118.07	120.30
1	A	760	G	C5-C6-O6	5.58	131.94	128.60
1	A	941	G	C6-C5-N7	-5.58	127.05	130.40
1	A	293	G	N3-C4-N9	-5.57	122.66	126.00
1	A	572	A	C6-N1-C2	-5.57	115.26	118.60
1	A	635	G	N3-C2-N2	-5.57	116.00	119.90
1	A	876	G	C6-N1-C2	-5.57	121.76	125.10
12	L	26	ALA	N-CA-C	-5.57	95.96	111.00
1	A	190(E)	U	C6-N1-C2	5.57	124.34	121.00
1	A	238	G	C8-N9-C4	-5.57	104.17	106.40
1	A	723	U	C5-C6-N1	5.56	125.48	122.70
1	A	933	G	C6-C5-N7	-5.56	127.06	130.40
1	A	832	C	C2-N3-C4	-5.56	117.12	119.90
1	A	268	C	N3-C2-O2	-5.56	118.01	121.90
1	A	555	C	N1-C2-N3	5.56	123.09	119.20
1	A	568	G	N1-C2-N3	5.56	127.23	123.90
1	A	750	G	O5'-P-OP2	5.56	117.37	110.70
1	A	126	G	C2-N3-C4	-5.56	109.12	111.90
1	A	658	G	C5-C6-O6	-5.55	125.27	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1068	G	OP1-P-OP2	5.55	127.93	119.60
1	A	1370	G	OP1-P-O3'	5.55	117.42	105.20
1	A	721	G	C4-C5-C6	5.55	122.13	118.80
1	A	812	C	N1-C2-O2	-5.55	115.57	118.90
1	A	251	G	O4'-C1'-N9	-5.55	103.76	108.20
1	A	770	C	C5-C6-N1	-5.55	118.22	121.00
1	A	1300	G	C4-N9-C1'	-5.55	119.29	126.50
1	A	1281	U	C5-C6-N1	5.55	125.47	122.70
1	A	1485	U	N3-C2-O2	-5.55	118.32	122.20
1	A	125	U	C2-N3-C4	-5.55	123.67	127.00
1	A	777	A	C5'-C4'-O4'	5.55	115.76	109.10
1	A	885	G	N3-C4-N9	-5.55	122.67	126.00
1	A	27	G	C8-N9-C4	-5.54	104.18	106.40
1	A	365	U	C6-N1-C1'	-5.54	113.44	121.20
1	A	873	A	N1-C6-N6	-5.54	115.28	118.60
1	A	1414	U	N3-C2-O2	-5.54	118.32	122.20
1	A	509	A	N9-C1'-C2'	-5.54	105.91	112.00
1	A	329	A	N9-C4-C5	-5.54	103.58	105.80
1	A	823	G	C6-N1-C2	-5.54	121.78	125.10
1	A	167	G	N1-C2-N2	-5.53	111.22	116.20
1	A	1091	U	C6-N1-C2	-5.53	117.68	121.00
1	A	771	G	C8-N9-C4	5.53	108.61	106.40
1	A	640	A	OP2-P-O3'	5.53	117.36	105.20
1	A	921	U	N1-C2-O2	-5.53	118.93	122.80
1	A	309	G	C2-N3-C4	-5.52	109.14	111.90
1	A	553	A	C5-C6-N6	-5.52	119.28	123.70
1	A	919	A	C4-C5-C6	-5.52	114.24	117.00
1	A	1382	C	N1-C2-O2	5.52	122.21	118.90
1	A	256	U	N3-C2-O2	5.52	126.06	122.20
1	A	1394	A	N9-C4-C5	-5.52	103.59	105.80
1	A	635	G	C2-N3-C4	-5.51	109.14	111.90
1	A	666	G	O5'-P-OP1	-5.51	100.74	105.70
1	A	690	G	N3-C4-N9	-5.51	122.69	126.00
1	A	15	G	C4-C5-N7	5.51	113.00	110.80
1	A	1490	U	C6-N1-C1'	-5.51	113.48	121.20
1	A	22	G	C6-C5-N7	-5.51	127.09	130.40
1	A	610	G	N1-C6-O6	-5.51	116.59	119.90
1	A	813	U	C2-N1-C1'	5.51	124.31	117.70
1	A	882	C	N1-C2-N3	5.51	123.06	119.20
8	H	12	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	A	1310	G	C6-C5-N7	-5.51	127.09	130.40
1	A	753	A	C2-N3-C4	-5.51	107.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	947	G	C8-N9-C1'	-5.51	119.84	127.00
1	A	1395	C	OP2-P-O3'	5.51	117.31	105.20
1	A	32	A	C6-N1-C2	-5.50	115.30	118.60
1	A	752	G	C5-C6-O6	5.50	131.90	128.60
18	R	78	LEU	CA-CB-CG	-5.50	102.64	115.30
1	A	793	U	O5'-P-OP2	-5.50	100.75	105.70
1	A	15	G	C5-C6-O6	-5.50	125.30	128.60
1	A	115	G	N3-C4-C5	-5.50	125.85	128.60
1	A	839	U	N1-C2-O2	5.50	126.65	122.80
1	A	750	G	C4-C5-C6	5.49	122.10	118.80
1	A	584	G	N1-C2-N3	-5.49	120.61	123.90
1	A	1477	C	C5-C6-N1	5.49	123.75	121.00
1	A	948	C	C2-N1-C1'	-5.49	112.76	118.80
1	A	1235	U	N1-C2-N3	5.49	118.19	114.90
1	A	1366	C	C6-N1-C2	-5.49	118.10	120.30
1	A	1075	C	C6-N1-C2	5.49	122.50	120.30
1	A	1099	G	N3-C4-N9	-5.49	122.71	126.00
1	A	1414	U	N3-C4-C5	-5.49	111.31	114.60
1	A	451	A	O4'-C1'-N9	-5.49	103.81	108.20
1	A	591	U	C2-N3-C4	-5.48	123.71	127.00
1	A	753	A	N1-C2-N3	5.48	132.04	129.30
1	A	392	G	C4-N9-C1'	5.48	133.63	126.50
1	A	879	C	C2-N3-C4	-5.48	117.16	119.90
1	A	22	G	OP2-P-O3'	5.48	117.25	105.20
1	A	487	A	C8-N9-C4	5.48	107.99	105.80
1	A	1283	G	C8-N9-C4	-5.48	104.21	106.40
1	A	111	G	N3-C4-C5	5.47	131.34	128.60
1	A	1060	C	N3-C4-C5	5.47	124.09	121.90
1	A	818	G	O5'-P-OP2	5.47	117.27	110.70
1	A	248	C	N3-C4-C5	5.47	124.09	121.90
1	A	621	A	N1-C6-N6	5.47	121.88	118.60
1	A	264	U	N1-C2-N3	5.47	118.18	114.90
1	A	761	G	C2-N3-C4	-5.47	109.17	111.90
1	A	109	A	C8-N9-C4	-5.47	103.61	105.80
1	A	623	C	N3-C4-C5	5.46	124.09	121.90
1	A	558	G	C8-N9-C4	-5.46	104.22	106.40
1	A	898	G	C8-N9-C4	5.46	108.58	106.40
1	A	933	G	C5-C6-O6	-5.46	125.32	128.60
1	A	1230	C	C6-N1-C2	-5.46	118.11	120.30
1	A	74	C	C5-C6-N1	5.46	123.73	121.00
1	A	1525	G	OP2-P-O3'	5.46	117.21	105.20
1	A	697	U	C6-N1-C2	5.46	124.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	G	N3-C4-N9	5.46	129.27	126.00
1	A	1183	A	C8-N9-C4	5.46	107.98	105.80
1	A	319	G	C4-C5-N7	5.46	112.98	110.80
1	A	17	U	C5-C6-N1	-5.45	119.97	122.70
1	A	1515[A]	C	N3-C2-O2	-5.45	118.08	121.90
1	A	1515[B]	C	N3-C2-O2	-5.45	118.08	121.90
1	A	869	G	N1-C2-N2	5.45	121.11	116.20
1	A	1526	G	O5'-P-OP2	-5.45	100.80	105.70
1	A	147	G	C5-C6-O6	-5.45	125.33	128.60
1	A	500	G	C5-C6-O6	-5.44	125.33	128.60
1	A	565	U	C5-C4-O4	-5.44	122.64	125.90
1	A	1344	C	N3-C4-N4	-5.44	114.19	118.00
1	A	1370	G	N1-C6-O6	-5.44	116.64	119.90
1	A	1393	U	N3-C2-O2	5.44	126.01	122.20
1	A	300	A	C5-N7-C8	-5.44	101.18	103.90
1	A	485	G	O4'-C1'-N9	5.44	112.55	108.20
1	A	570	G	C8-N9-C4	-5.44	104.22	106.40
1	A	836	G	N1-C6-O6	5.44	123.16	119.90
1	A	839	U	N3-C2-O2	-5.44	118.39	122.20
1	A	947	G	C4-N9-C1'	5.44	133.57	126.50
1	A	91	C	C5-C6-N1	5.44	123.72	121.00
1	A	828	A	C6-C5-N7	-5.43	128.50	132.30
1	A	668	G	N9-C4-C5	-5.43	103.23	105.40
1	A	11	G	N1-C2-N3	5.43	127.16	123.90
1	A	250	A	N3-C4-C5	5.43	130.60	126.80
1	A	129(A)	G	N3-C4-C5	-5.43	125.89	128.60
1	A	1529	G	C5-C6-O6	-5.43	125.34	128.60
1	A	106	C	O5'-P-OP1	-5.42	100.82	105.70
1	A	869	G	C2-N3-C4	-5.42	109.19	111.90
1	A	266	G	N1-C2-N2	-5.42	111.32	116.20
1	A	579	G	N7-C8-N9	5.42	115.81	113.10
1	A	25	C	C5-C6-N1	-5.42	118.29	121.00
1	A	648	A	C8-N9-C4	5.42	107.97	105.80
1	A	625	G	N3-C4-C5	-5.41	125.89	128.60
1	A	260	G	C5-C6-N1	-5.41	108.80	111.50
1	A	267	C	N3-C4-C5	5.41	124.06	121.90
1	A	47	C	C6-N1-C2	5.41	122.46	120.30
1	A	247	G	O5'-P-OP1	-5.41	100.83	105.70
1	A	890	G	O4'-C1'-N9	5.41	112.53	108.20
1	A	938	A	N1-C6-N6	-5.41	115.36	118.60
1	A	757	U	C5-C6-N1	-5.40	120.00	122.70
1	A	1434	A	N1-C6-N6	5.40	121.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	A	C4-C5-N7	-5.40	108.00	110.70
1	A	563	A	C8-N9-C4	-5.40	103.64	105.80
1	A	1380	U	C5-C6-N1	-5.40	120.00	122.70
1	A	761	G	N1-C6-O6	5.40	123.14	119.90
1	A	1354	C	N1-C2-O2	5.39	122.14	118.90
1	A	658	G	N1-C6-O6	5.39	123.14	119.90
1	A	808	C	N3-C4-C5	5.39	124.06	121.90
1	A	901	A	C2-N3-C4	-5.39	107.91	110.60
1	A	866	C	C2-N3-C4	-5.39	117.21	119.90
1	A	918	A	C5-C6-N1	5.39	120.39	117.70
1	A	923	A	C8-N9-C4	5.39	107.95	105.80
1	A	522	C	O5'-P-OP2	-5.39	100.85	105.70
1	A	1322	C	C2-N1-C1'	5.39	124.73	118.80
1	A	309	G	N1-C6-O6	5.38	123.13	119.90
1	A	886	G	C6-C5-N7	-5.38	127.17	130.40
1	A	1338	G	N1-C6-O6	-5.38	116.67	119.90
1	A	50	A	C8-N9-C4	5.38	107.95	105.80
1	A	590	C	C6-N1-C2	5.38	122.45	120.30
1	A	309	G	C5-N7-C8	-5.38	101.61	104.30
1	A	554	C	N1-C2-O2	-5.38	115.67	118.90
1	A	586	C	C4-C5-C6	5.38	120.09	117.40
1	A	1373	G	C4-C5-C6	5.38	122.03	118.80
1	A	1399	C	C6-N1-C2	-5.38	118.15	120.30
1	A	1426	C	C6-N1-C2	5.38	122.45	120.30
1	A	79	G	C2-N3-C4	5.38	114.59	111.90
1	A	502	G	N3-C4-N9	5.38	129.23	126.00
1	A	663	A	N1-C6-N6	-5.38	115.37	118.60
1	A	929	G	N3-C4-C5	5.38	131.29	128.60
1	A	485	G	C4-N9-C1'	-5.37	119.51	126.50
1	A	570	G	N1-C2-N3	5.37	127.12	123.90
1	A	621	A	C5-N7-C8	-5.37	101.22	103.90
1	A	752	G	N7-C8-N9	-5.37	110.41	113.10
1	A	667	G	C8-N9-C4	5.37	108.55	106.40
1	A	726	C	C4-C5-C6	5.37	120.08	117.40
1	A	851	G	C4-N9-C1'	5.37	133.48	126.50
1	A	317	G	C4-C5-N7	5.37	112.95	110.80
1	A	385	C	N3-C4-C5	5.37	124.05	121.90
1	A	267	C	C5-C6-N1	-5.36	118.32	121.00
1	A	1246	C	C2-N1-C1'	-5.36	112.90	118.80
17	Q	99	SER	N-CA-C	5.36	125.48	111.00
1	A	1186	G	N3-C4-C5	5.36	131.28	128.60
1	A	28	G	C6-N1-C2	-5.36	121.89	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	G	OP1-P-OP2	5.36	127.64	119.60
1	A	875	C	C6-N1-C2	5.36	122.44	120.30
1	A	1199	U	N3-C2-O2	-5.36	118.45	122.20
1	A	1368	G	C5-C6-N1	5.36	114.18	111.50
1	A	1487	G	N3-C4-C5	-5.36	125.92	128.60
1	A	14	U	N1-C2-N3	5.35	118.11	114.90
1	A	250	A	C4-C5-N7	5.35	113.38	110.70
1	A	267	C	C2-N3-C4	-5.35	117.22	119.90
1	A	825	G	C5-C6-O6	-5.35	125.39	128.60
1	A	1328	C	N3-C4-C5	5.35	124.04	121.90
1	A	565	U	C6-N1-C2	5.35	124.21	121.00
1	A	851	G	N1-C6-O6	5.35	123.11	119.90
1	A	747	C	C2-N3-C4	-5.35	117.23	119.90
1	A	1230	C	C5-C4-N4	-5.35	116.45	120.20
1	A	1509	C	C2-N3-C4	-5.35	117.22	119.90
1	A	1352	C	C6-N1-C2	-5.35	118.16	120.30
1	A	129(A)	G	C4-C5-N7	5.34	112.94	110.80
1	A	1521	G	N3-C4-N9	5.34	129.21	126.00
19	S	29	ARG	N-CA-C	5.34	125.43	111.00
1	A	125	U	N3-C2-O2	-5.34	118.46	122.20
1	A	1452	C	N1-C2-N3	-5.34	115.46	119.20
1	A	301	G	N1-C2-N3	5.34	127.10	123.90
1	A	553	A	N9-C4-C5	-5.34	103.67	105.80
1	A	722	A	N7-C8-N9	5.34	116.47	113.80
1	A	1186	G	N1-C6-O6	5.34	123.10	119.90
1	A	553	A	N1-C6-N6	5.33	121.80	118.60
1	A	873	A	N7-C8-N9	5.33	116.47	113.80
1	A	1108	G	C4-N9-C1'	5.33	133.43	126.50
1	A	243	A	C2-N3-C4	-5.33	107.93	110.60
1	A	1090	U	N3-C4-C5	-5.33	111.40	114.60
1	A	721	G	C6-C5-N7	-5.33	127.20	130.40
1	A	595	G	C4-N9-C1'	5.33	133.43	126.50
1	A	709	G	N1-C6-O6	5.32	123.09	119.90
1	A	876	G	N3-C4-N9	-5.32	122.81	126.00
1	A	1529	G	C6-C5-N7	-5.32	127.21	130.40
1	A	250	A	C6-N1-C2	5.32	121.79	118.60
1	A	306	G	C5-C6-N1	-5.32	108.84	111.50
1	A	768	A	OP2-P-O3'	5.32	116.90	105.20
1	A	1080	A	N9-C4-C5	5.32	107.93	105.80
1	A	1336	C	C6-N1-C2	5.32	122.43	120.30
1	A	931	C	N1-C2-N3	5.32	122.92	119.20
1	A	750	G	N3-C4-C5	-5.31	125.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	C	N1-C2-O2	-5.31	115.71	118.90
1	A	561	U	C5-C4-O4	-5.31	122.71	125.90
1	A	829	G	N3-C4-C5	-5.31	125.94	128.60
1	A	562	C	N1-C2-O2	5.31	122.09	118.90
1	A	829	G	C6-C5-N7	-5.31	127.21	130.40
1	A	115	G	P-O3'-C3'	5.31	126.07	119.70
1	A	366	C	C2-N1-C1'	5.31	124.64	118.80
1	A	598	U	C5-C6-N1	-5.31	120.05	122.70
1	A	28	G	C6-C5-N7	-5.30	127.22	130.40
1	A	397	A	C4-C5-N7	5.30	113.35	110.70
1	A	1506	U	N3-C2-O2	5.30	125.91	122.20
1	A	1344	C	C5-C6-N1	-5.30	118.35	121.00
1	A	428	G	P-O3'-C3'	5.30	126.06	119.70
1	A	620	C	N3-C4-C5	5.30	124.02	121.90
1	A	190(E)	U	C5-C6-N1	-5.30	120.05	122.70
1	A	756	C	N3-C4-C5	5.30	124.02	121.90
1	A	1253	G	N1-C6-O6	5.30	123.08	119.90
1	A	599	C	C5-C4-N4	-5.29	116.49	120.20
1	A	701	C	P-O3'-C3'	5.29	126.05	119.70
1	A	1103	C	N3-C2-O2	-5.29	118.19	121.90
1	A	402	G	N9-C4-C5	5.29	107.52	105.40
1	A	1158	C	C6-N1-C2	-5.29	118.18	120.30
1	A	1231	G	N1-C6-O6	5.29	123.08	119.90
1	A	740	U	N1-C2-N3	5.29	118.07	114.90
1	A	718	G	C2-N3-C4	-5.29	109.26	111.90
1	A	860	A	C5-N7-C8	-5.29	101.26	103.90
1	A	1310	G	C4-N9-C1'	5.28	133.37	126.50
1	A	227	G	N1-C6-O6	5.28	123.07	119.90
1	A	129(A)	G	C8-N9-C1'	-5.28	120.14	127.00
1	A	625	G	C5-C6-O6	-5.28	125.43	128.60
1	A	736	C	N1-C2-O2	5.27	122.06	118.90
1	A	1237	C	N3-C2-O2	-5.27	118.21	121.90
1	A	872	A	OP2-P-O3'	5.27	116.80	105.20
1	A	1106	G	C2-N3-C4	-5.27	109.26	111.90
1	A	726	C	O5'-P-OP1	-5.27	100.96	105.70
1	A	832	C	C5-C4-N4	-5.27	116.51	120.20
1	A	946	A	C8-N9-C4	-5.27	103.69	105.80
1	A	130	A	C6-C5-N7	-5.27	128.61	132.30
1	A	585	G	N7-C8-N9	5.27	115.73	113.10
1	A	1236	A	OP2-P-O3'	5.27	116.79	105.20
1	A	460	A	C2-N3-C4	5.27	113.23	110.60
1	A	802	A	C5-C6-N6	-5.27	119.49	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	829	G	N1-C2-N2	-5.27	111.46	116.20
1	A	1478	C	C5-C6-N1	5.27	123.63	121.00
1	A	1503	A	OP1-P-O3'	5.27	116.79	105.20
1	A	1530	G	C4-C5-N7	5.27	112.91	110.80
1	A	548	G	C2-N3-C4	-5.27	109.27	111.90
1	A	519	C	N1-C2-N3	-5.26	115.52	119.20
1	A	558	G	C6-C5-N7	-5.26	127.24	130.40
1	A	593	G	N1-C2-N2	-5.26	111.46	116.20
1	A	725	G	C8-N9-C4	5.26	108.51	106.40
1	A	774	G	N1-C6-O6	5.26	123.06	119.90
1	A	866	C	N1-C2-O2	-5.26	115.74	118.90
1	A	154	C	N3-C4-C5	5.26	124.00	121.90
1	A	767	A	N9-C4-C5	5.26	107.90	105.80
1	A	116	A	OP2-P-O3'	5.25	116.76	105.20
1	A	299	G	C6-C5-N7	-5.25	127.25	130.40
1	A	382	A	C5-N7-C8	-5.25	101.27	103.90
1	A	588	G	N9-C4-C5	-5.25	103.30	105.40
1	A	114	U	OP1-P-O3'	5.25	116.75	105.20
1	A	756	C	O5'-P-OP2	-5.25	100.98	105.70
1	A	809	G	C6-N1-C2	-5.25	121.95	125.10
1	A	474	G	N3-C4-C5	-5.25	125.98	128.60
1	A	51	A	C5-C6-N1	5.24	120.32	117.70
1	A	559	A	N3-C4-C5	-5.24	123.13	126.80
1	A	688	G	O5'-P-OP1	-5.24	100.98	105.70
1	A	475	G	C5-C6-N1	-5.24	108.88	111.50
1	A	668	G	N7-C8-N9	-5.24	110.48	113.10
1	A	865	A	C5-C6-N1	5.24	120.32	117.70
1	A	27	G	N7-C8-N9	5.24	115.72	113.10
1	A	257	G	N9-C4-C5	-5.24	103.31	105.40
1	A	382	A	C4-C5-C6	5.24	119.62	117.00
1	A	377	G	C5-C6-N1	-5.23	108.88	111.50
1	A	898	G	N7-C8-N9	-5.23	110.48	113.10
1	A	308	C	N1-C2-O2	5.23	122.04	118.90
1	A	1065	U	OP2-P-O3'	5.23	116.71	105.20
1	A	1406	U	N3-C4-O4	5.23	123.06	119.40
1	A	297	G	C4-N9-C1'	5.23	133.29	126.50
1	A	632	A	N1-C6-N6	5.23	121.74	118.60
1	A	1285	A	P-O3'-C3'	5.22	125.97	119.70
1	A	1393	U	C5-C6-N1	-5.22	120.09	122.70
1	A	288	A	N3-C4-C5	5.22	130.46	126.80
1	A	331	G	C4-C5-C6	5.22	121.93	118.80
1	A	1238	A	N1-C6-N6	-5.22	115.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1370	G	C5-N7-C8	-5.22	101.69	104.30
1	A	788	U	N3-C4-C5	-5.22	111.47	114.60
1	A	1344	C	N3-C4-C5	5.22	123.99	121.90
1	A	935	A	N1-C6-N6	-5.22	115.47	118.60
1	A	1528	U	O5'-P-OP2	-5.22	101.00	105.70
1	A	193	C	C6-N1-C2	5.22	122.39	120.30
1	A	392	G	C4-C5-C6	5.22	121.93	118.80
1	A	1117	G	N3-C4-C5	5.22	131.21	128.60
1	A	851	G	C8-N9-C4	-5.21	104.31	106.40
1	A	122	G	C5-C6-N1	-5.21	108.89	111.50
1	A	776	G	C2-N3-C4	-5.21	109.29	111.90
1	A	875	C	N3-C4-C5	5.21	123.98	121.90
1	A	109	A	N1-C2-N3	5.21	131.91	129.30
1	A	1087	G	C5-N7-C8	-5.21	101.69	104.30
1	A	397	A	N7-C8-N9	5.21	116.41	113.80
1	A	144	G	C4-C5-N7	5.21	112.88	110.80
1	A	932	C	C2-N1-C1'	5.21	124.53	118.80
1	A	1078	U	C5-C4-O4	-5.21	122.78	125.90
1	A	563	A	O4'-C1'-N9	5.21	112.36	108.20
1	A	328	C	O4'-C1'-N1	5.21	112.36	108.20
1	A	550	G	N1-C6-O6	5.21	123.02	119.90
1	A	727	G	C8-N9-C4	-5.20	104.32	106.40
1	A	1345	U	C5-C6-N1	-5.20	120.10	122.70
1	A	728	A	C2-N3-C4	-5.20	108.00	110.60
1	A	807	A	C8-N9-C4	5.20	107.88	105.80
1	A	54	C	N3-C4-C5	5.20	123.98	121.90
1	A	570	G	C8-N9-C1'	-5.20	120.24	127.00
1	A	568	G	C4-N9-C1'	5.20	133.25	126.50
1	A	1059	C	N3-C4-C5	-5.20	119.82	121.90
1	A	117	G	N7-C8-N9	5.19	115.70	113.10
1	A	235	C	N3-C4-C5	5.19	123.98	121.90
1	A	761	G	C5-N7-C8	-5.19	101.70	104.30
1	A	1109	C	N1-C2-O2	5.19	122.02	118.90
1	A	637	G	N1-C2-N3	5.19	127.01	123.90
1	A	1087	G	C6-C5-N7	-5.19	127.29	130.40
1	A	1420	C	C5-C6-N1	5.19	123.59	121.00
1	A	760	G	C2-N3-C4	-5.19	109.31	111.90
1	A	23	C	C5-C6-N1	-5.19	118.41	121.00
1	A	232	G	N3-C2-N2	5.18	123.53	119.90
1	A	129(A)	G	C5-C6-O6	-5.18	125.49	128.60
1	A	245	C	N3-C4-N4	5.18	121.63	118.00
1	A	854	G	C4-C5-C6	5.18	121.91	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	784	C	C2-N3-C4	-5.18	117.31	119.90
1	A	1403	C	C5-C6-N1	5.18	123.59	121.00
1	A	250	A	C5-C6-N1	-5.18	115.11	117.70
1	A	392	G	C8-N9-C1'	-5.18	120.27	127.00
1	A	259	G	C6-C5-N7	-5.18	127.29	130.40
1	A	373	A	N1-C2-N3	5.18	131.89	129.30
1	A	803	G	N9-C4-C5	5.18	107.47	105.40
1	A	824	C	N3-C4-C5	5.18	123.97	121.90
1	A	1158	C	C6-N1-C1'	-5.17	114.59	120.80
1	A	645	C	C6-N1-C2	5.17	122.37	120.30
1	A	167	G	C6-C5-N7	-5.17	127.30	130.40
1	A	192	U	C5-C6-N1	-5.17	120.11	122.70
1	A	713	G	C8-N9-C4	-5.17	104.33	106.40
1	A	82	U	C6-N1-C2	-5.17	117.90	121.00
1	A	317	G	N1-C6-O6	5.17	123.00	119.90
1	A	763	G	N3-C2-N2	-5.17	116.28	119.90
1	A	481	G	C4-N9-C1'	5.17	133.22	126.50
1	A	650	G	C8-N9-C1'	-5.17	120.28	127.00
1	A	816	A	O4'-C1'-N9	-5.17	104.07	108.20
1	A	877	C	N1-C2-N3	5.17	122.82	119.20
1	A	858	G	N1-C2-N2	5.16	120.85	116.20
1	A	115	G	C5-C6-O6	-5.16	125.50	128.60
1	A	377	G	C2-N3-C4	-5.16	109.32	111.90
1	A	717	C	N1-C2-O2	-5.16	115.80	118.90
1	A	245	C	N1-C2-O2	-5.16	115.81	118.90
1	A	405	U	C5-C6-N1	-5.16	120.12	122.70
1	A	703	G	C8-N9-C4	-5.16	104.34	106.40
1	A	1076	C	N3-C2-O2	-5.16	118.29	121.90
1	A	1453	G	C5-N7-C8	-5.16	101.72	104.30
1	A	1062	U	C6-N1-C2	-5.15	117.91	121.00
1	A	637	G	C8-N9-C4	5.15	108.46	106.40
1	A	878	G	C4-C5-N7	5.15	112.86	110.80
1	A	1228	C	OP2-P-O3'	5.15	116.53	105.20
1	A	1250	A	C8-N9-C4	-5.15	103.74	105.80
1	A	583	A	O5'-P-OP2	5.15	116.88	110.70
1	A	595	G	N1-C2-N2	-5.15	111.56	116.20
1	A	558	G	N7-C8-N9	5.15	115.67	113.10
1	A	560	U	C2-N1-C1'	5.15	123.88	117.70
1	A	822	C	N1-C2-N3	5.15	122.80	119.20
1	A	365	U	C2-N1-C1'	5.15	123.88	117.70
1	A	563	A	C4-C5-C6	5.15	119.57	117.00
1	A	597	G	C5-C6-N1	5.15	114.07	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	615	C	C5-C4-N4	-5.15	116.60	120.20
2	B	103	THR	CB-CA-C	-5.15	97.71	111.60
1	A	648	A	C6-N1-C2	-5.14	115.51	118.60
1	A	817	C	C6-N1-C1'	-5.14	114.63	120.80
1	A	247	G	OP1-P-OP2	5.14	127.31	119.60
1	A	392	G	N3-C4-C5	-5.14	126.03	128.60
1	A	865	A	C5-C6-N6	-5.14	119.59	123.70
1	A	872	A	C5-C6-N6	-5.14	119.59	123.70
1	A	1414	U	N1-C2-O2	5.14	126.40	122.80
1	A	661	G	N3-C4-N9	-5.14	122.92	126.00
1	A	1087	G	N9-C4-C5	-5.14	103.34	105.40
1	A	617	G	N9-C4-C5	-5.13	103.35	105.40
1	A	876	G	C6-C5-N7	5.13	133.48	130.40
1	A	947	G	C4-C5-C6	5.13	121.88	118.80
1	A	879	C	N1-C2-N3	5.13	122.79	119.20
1	A	275	G	C6-C5-N7	-5.13	127.32	130.40
1	A	919	A	C2-N3-C4	5.13	113.17	110.60
1	A	300	A	C6-C5-N7	-5.13	128.71	132.30
1	A	753	A	N9-C4-C5	5.13	107.85	105.80
1	A	877	C	C4-C5-C6	5.13	119.97	117.40
1	A	1078	U	C5-C6-N1	5.13	125.27	122.70
1	A	833	U	N3-C2-O2	-5.13	118.61	122.20
1	A	869	G	N3-C4-N9	-5.13	122.92	126.00
1	A	16	A	C4-C5-N7	-5.12	108.14	110.70
1	A	590	C	C5-C6-N1	-5.12	118.44	121.00
1	A	613	C	N3-C4-C5	5.12	123.95	121.90
1	A	144	G	N7-C8-N9	5.12	115.66	113.10
1	A	930	C	N1-C2-N3	5.12	122.78	119.20
1	A	1064	G	N3-C2-N2	-5.12	116.31	119.90
1	A	428	G	N1-C6-O6	-5.12	116.83	119.90
1	A	625	G	C5-C6-N1	5.12	114.06	111.50
1	A	739	C	N3-C4-C5	5.12	123.95	121.90
1	A	859	A	C6-C5-N7	-5.12	128.72	132.30
1	A	8	A	C5-C6-N6	5.12	127.79	123.70
1	A	28	G	N1-C2-N3	5.12	126.97	123.90
1	A	483	C	N1-C2-N3	5.12	122.78	119.20
1	A	615	C	N1-C2-O2	-5.12	115.83	118.90
1	A	125	U	N1-C2-N3	5.11	117.97	114.90
1	A	178	C	N1-C2-O2	5.11	121.97	118.90
1	A	945	G	C5-C6-O6	-5.11	125.53	128.60
1	A	1449	C	N3-C4-C5	5.11	123.95	121.90
1	A	93	G	OP1-P-OP2	-5.11	111.94	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	896	C	C4-C5-C6	-5.11	114.85	117.40
1	A	397	A	C5-N7-C8	-5.11	101.35	103.90
1	A	656	C	N3-C4-C5	5.10	123.94	121.90
1	A	559	A	C8-N9-C4	-5.10	103.76	105.80
1	A	634	C	N1-C2-N3	5.10	122.77	119.20
1	A	895	G	C6-C5-N7	-5.10	127.34	130.40
1	A	1433	A	N7-C8-N9	5.10	116.35	113.80
1	A	1390	U	C4-C5-C6	5.10	122.76	119.70
1	A	445	G	C5-C6-N1	-5.10	108.95	111.50
1	A	828	A	N1-C6-N6	5.10	121.66	118.60
1	A	43	C	C6-N1-C2	5.10	122.34	120.30
1	A	671	G	N1-C6-O6	5.10	122.96	119.90
1	A	829	G	C8-N9-C1'	-5.10	120.37	127.00
1	A	853	G	C4-C5-C6	5.10	121.86	118.80
1	A	266	G	N3-C2-N2	5.09	123.46	119.90
1	A	279	A	C4-N9-C1'	5.09	135.47	126.30
1	A	285	G	N3-C2-N2	-5.09	116.34	119.90
1	A	759	A	OP2-P-O3'	5.09	116.40	105.20
1	A	881	G	OP2-P-O3'	5.09	116.40	105.20
1	A	944	G	N9-C4-C5	5.09	107.44	105.40
1	A	1332	A	N1-C6-N6	-5.09	115.55	118.60
1	A	1368	G	N3-C4-C5	-5.09	126.06	128.60
1	A	16	A	C5-N7-C8	5.09	106.44	103.90
1	A	934	C	N3-C4-C5	5.09	123.93	121.90
1	A	240	C	C4-C5-C6	-5.08	114.86	117.40
1	A	577	G	OP1-P-O3'	5.08	116.37	105.20
1	A	1543	C	N1-C2-O2	5.08	121.95	118.90
1	A	460	A	C5-C6-N1	5.08	120.24	117.70
1	A	762	C	C5-C4-N4	-5.08	116.65	120.20
1	A	1329	A	N1-C6-N6	5.08	121.64	118.60
1	A	239	U	OP1-P-OP2	5.07	127.21	119.60
1	A	572	A	C2-N3-C4	5.07	113.14	110.60
1	A	75	G	C8-N9-C1'	-5.07	120.41	127.00
1	A	366	C	OP2-P-O3'	5.07	116.36	105.20
1	A	791	G	O5'-P-OP2	-5.07	101.14	105.70
1	A	863	U	O5'-P-OP1	-5.07	101.14	105.70
1	A	880	C	N1-C2-O2	-5.07	115.86	118.90
1	A	183	G	C4-C5-N7	5.07	112.83	110.80
1	A	502	G	C4-C5-N7	5.07	112.83	110.80
1	A	1465	C	N3-C4-C5	5.07	123.93	121.90
1	A	488	C	N3-C4-C5	5.07	123.93	121.90
1	A	649	G	C6-N1-C2	-5.07	122.06	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	750	G	C6-C5-N7	-5.06	127.36	130.40
1	A	721	G	N3-C4-N9	5.06	129.04	126.00
1	A	730	G	C6-N1-C2	-5.06	122.06	125.10
1	A	127	G	C2-N3-C4	-5.06	109.37	111.90
1	A	761	G	C4-C5-N7	5.06	112.82	110.80
1	A	293	G	N1-C6-O6	5.06	122.94	119.90
1	A	372	C	C4-C5-C6	5.05	119.93	117.40
1	A	1094	G	N7-C8-N9	-5.05	110.57	113.10
1	A	1499	A	C6-N1-C2	-5.05	115.57	118.60
1	A	1526	G	C5-C6-O6	-5.05	125.57	128.60
3	C	179	ARG	N-CA-C	-5.05	97.36	111.00
1	A	242	C	N3-C4-C5	5.05	123.92	121.90
1	A	568	G	C6-N1-C2	-5.05	122.07	125.10
1	A	766	A	OP1-P-OP2	5.05	127.18	119.60
1	A	962	C	N1-C2-N3	-5.05	115.66	119.20
1	A	1369	C	N1-C2-N3	5.05	122.74	119.20
1	A	306	G	N1-C6-O6	5.05	122.93	119.90
1	A	555	C	C2-N1-C1'	5.05	124.35	118.80
1	A	21	G	N1-C6-O6	5.05	122.93	119.90
1	A	227	G	C5-N7-C8	-5.05	101.78	104.30
1	A	725	G	C5-C6-N1	5.05	114.02	111.50
1	A	819	A	N7-C8-N9	5.05	116.32	113.80
1	A	827	U	C2-N3-C4	-5.05	123.97	127.00
1	A	1058	G	C5-C6-O6	5.05	131.63	128.60
1	A	1399	C	N1-C2-O2	-5.05	115.87	118.90
1	A	47	C	C6-N1-C1'	-5.04	114.75	120.80
1	A	392	G	O5'-P-OP2	-5.04	101.16	105.70
1	A	746	A	C6-N1-C2	-5.04	115.58	118.60
1	A	1336	C	O4'-C1'-N1	-5.04	104.17	108.20
1	A	819	A	C5-N7-C8	-5.04	101.38	103.90
1	A	1079	G	N1-C2-N2	-5.04	111.67	116.20
1	A	1497	G	N3-C4-C5	-5.04	126.08	128.60
15	O	85	LEU	CA-CB-CG	-5.04	103.71	115.30
1	A	609	A	C2-N3-C4	-5.04	108.08	110.60
1	A	1167	A	C8-N9-C4	-5.04	103.79	105.80
1	A	18	C	C4-C5-C6	5.03	119.92	117.40
1	A	639	G	N1-C2-N3	5.03	126.92	123.90
1	A	365	U	O4'-C1'-N1	5.03	112.22	108.20
1	A	393	A	C2-N3-C4	-5.03	108.09	110.60
1	A	1310	G	N3-C4-N9	5.03	129.02	126.00
1	A	558	G	N1-C6-O6	5.03	122.92	119.90
1	A	1338	G	C5-C6-O6	5.03	131.62	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	G	C5-C6-N1	-5.02	108.99	111.50
1	A	1331	G	C4-C5-N7	-5.02	108.79	110.80
1	A	722	A	N3-C4-C5	5.02	130.31	126.80
1	A	1512	U	N1-C2-O2	-5.02	119.29	122.80
1	A	11	G	C2-N3-C4	-5.02	109.39	111.90
1	A	267	C	N3-C4-N4	-5.02	114.49	118.00
1	A	1081	G	C5-N7-C8	-5.02	101.79	104.30
1	A	297	G	N1-C2-N3	5.01	126.91	123.90
1	A	873	A	C5-N7-C8	-5.01	101.39	103.90
1	A	1500	A	N1-C2-N3	5.01	131.81	129.30
1	A	331	G	N9-C4-C5	-5.01	103.40	105.40
1	A	822	C	C5-C4-N4	-5.01	116.69	120.20
1	A	826	C	C2-N3-C4	-5.01	117.39	119.90
1	A	584	G	C5-C6-O6	-5.01	125.59	128.60
1	A	697	U	C5-C6-N1	-5.01	120.19	122.70
1	A	256	U	C4-C5-C6	-5.01	116.69	119.70
1	A	270	A	N1-C6-N6	5.01	121.61	118.60
1	A	1239	A	O5'-P-OP2	-5.01	101.19	105.70
1	A	915	A	C2-N3-C4	-5.01	108.10	110.60
1	A	331	G	C8-N9-C1'	-5.00	120.50	127.00
1	A	747	C	C6-N1-C2	5.00	122.30	120.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	71	VAL	Peptide
2	B	8	LYS	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
4	D	195	ALA	Peptide
4	D	29	PRO	Peptide
7	G	10	ARG	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
10	J	36	GLY	Peptide
10	J	87	THR	Peptide
10	J	88	LEU	Peptide
10	J	90	LEU	Peptide
12	L	27	LEU	Peptide
15	O	2	PRO	Peptide
20	T	11	SER	Peptide

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Mol	Chain	Res	Type	Group
20	T	93	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32644	0	16503	885	0
2	B	1900	0	1951	115	0
3	C	1612	0	1677	94	0
4	D	1703	0	1763	88	0
5	E	1146	0	1207	65	0
6	F	843	0	857	43	0
7	G	1257	0	1296	67	0
8	H	1116	0	1177	73	0
9	I	1010	0	1037	81	0
10	J	792	0	835	54	0
11	K	864	0	881	34	0
12	L	973	0	1062	62	0
13	M	937	0	995	62	0
14	N	492	0	529	40	0
15	O	729	0	768	38	0
16	P	700	0	720	38	0
17	Q	823	0	891	54	0
18	R	574	0	644	44	0
19	S	647	0	673	42	0
20	T	763	0	861	44	0
21	U	208	0	221	11	0
22	A	262	0	0	0	0
22	B	1	0	0	0	0
22	C	1	0	0	0	0
22	D	3	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	H	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	P	1	0	0	0	0
22	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	261	0	0	11	0
24	C	1	0	0	1	0
24	D	1	0	0	0	0
24	E	6	0	0	0	0
24	Q	2	0	0	0	0
24	T	1	0	0	1	0
All	All	52281	0	36548	1858	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (1858) 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)
16:P:9:PHE:HD1	16:P:18:ARG:HG3	1.23	0.99
4:D:63:LYS:NZ	4:D:197:PRO:O	1.97	0.95
1:A:671:G:H4'	6:F:77:ARG:HE	1.32	0.95
1:A:1195:C:H3'	1:A:1196:U:H5''	1.49	0.94
8:H:95:VAL:HG12	8:H:99:GLU:HB2	1.51	0.93
1:A:1490:U:H2'	1:A:1491:G:H8	1.32	0.92
2:B:30:ARG:HD2	2:B:31:TYR:HE2	1.35	0.90
3:C:150:LYS:HA	3:C:169:ALA:HB3	1.54	0.90
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.53	0.90
1:A:953:G:N7	13:M:104:ARG:NH2	2.20	0.89
12:L:25:PRO:HB3	12:L:27:LEU:HD22	1.52	0.89
1:A:419:C:H42	1:A:424:G:H1	1.12	0.89
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.52	0.88
1:A:443:C:H42	1:A:491:G:H1	1.21	0.88
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.56	0.87
1:A:144:G:H1	1:A:178:C:H42	1.20	0.86
13:M:49:THR:HB	13:M:52:GLU:H	1.39	0.85
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.11	0.85
1:A:600:C:H42	1:A:638:G:H1	1.21	0.85
21:U:10:ARG:HH11	21:U:10:ARG:HB2	1.42	0.85
1:A:262:A:H5'	20:T:74:LYS:HD3	1.57	0.84
19:S:41:VAL:HG22	19:S:44:MET:HG3	1.57	0.83
1:A:1034:G:H2'	1:A:1035:A:H8	1.44	0.83
1:A:103:C:OP1	20:T:17:ARG:NH1	2.11	0.82
1:A:1051:C:N4	1:A:1207:2MG:O6	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:G:O3'	15:O:64:ARG:NH2	2.13	0.81
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.61	0.81
3:C:139:GLN:O	3:C:143:GLU:N	2.13	0.81
1:A:1300:G:OP2	1:A:1335:C:N4	2.14	0.81
1:A:1164:G:H1	1:A:1172:C:H42	1.28	0.81
1:A:1168:A:H2'	1:A:1169:A:C8	2.16	0.80
1:A:101:A:H2'	1:A:102:G:H8	1.45	0.80
18:R:51:LEU:HD22	18:R:55:ARG:HH12	1.45	0.80
20:T:54:LYS:HA	20:T:57:ARG:HD3	1.61	0.80
17:Q:48:GLU:HG3	17:Q:50:LYS:HB2	1.62	0.80
17:Q:81:ARG:HE	17:Q:84:LEU:HD11	1.47	0.79
1:A:1412:C:N4	1:A:1488:G:O6	2.13	0.79
5:E:15:ARG:HG2	5:E:28:PHE:HE2	1.47	0.79
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.15	0.79
5:E:95:ALA:O	5:E:98:THR:OG1	2.00	0.79
1:A:1064:G:N2	1:A:1190:G:H2'	1.97	0.79
1:A:1176:A:N6	1:A:1181:G:O6	2.16	0.78
2:B:60:ASP:OD2	2:B:64:ARG:NH1	2.14	0.78
10:J:48:THR:HA	10:J:62:HIS:HB3	1.63	0.78
18:R:37:VAL:O	18:R:40:LEU:N	2.17	0.78
1:A:35:G:O2'	12:L:118:SER:O	2.01	0.78
1:A:89:C:H2'	1:A:90:U:C6	2.18	0.78
1:A:278:G:OP2	17:Q:41:LYS:NZ	2.15	0.78
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.49	0.78
1:A:673:G:H5''	6:F:87:ARG:HD3	1.63	0.78
1:A:1263:C:N4	1:A:1272:G:O6	2.17	0.77
1:A:298:A:N6	24:A:2049:HOH:O	2.06	0.77
1:A:413:G:H8	1:A:428:G:H21	1.32	0.77
10:J:48:THR:OG1	10:J:62:HIS:ND1	2.17	0.77
1:A:419:C:N3	1:A:424:G:N2	2.29	0.77
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.13	0.77
3:C:108:ASN:HB3	3:C:111:LEU:HB2	1.67	0.77
8:H:116:LYS:HD2	8:H:129:VAL:HG11	1.65	0.77
12:L:102:ARG:NH2	12:L:108:ALA:O	2.17	0.77
2:B:10:LEU:HB2	2:B:11:LEU:HD12	1.68	0.76
4:D:154:ASN:OD1	4:D:154:ASN:N	2.18	0.76
10:J:50:ILE:HG13	10:J:60:ARG:HB3	1.68	0.76
1:A:1160:G:O6	1:A:1181:G:N1	2.14	0.76
14:N:8:GLU:HA	14:N:11:LYS:HB2	1.66	0.76
1:A:958:A:O2'	1:A:985:C:O2'	1.99	0.76
1:A:1309:G:OP2	13:M:99:ARG:NH1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:G:N2	1:A:1172:C:N3	2.30	0.76
12:L:27:LEU:C	12:L:29:GLY:H	1.86	0.76
1:A:869:G:N7	24:A:2098:HOH:O	2.18	0.75
3:C:176:HIS:ND1	24:C:401:HOH:O	2.19	0.75
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.67	0.75
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.67	0.75
1:A:1410:G:N2	1:A:1411:C:O2	2.19	0.75
1:A:1045:C:H2'	1:A:1046:A:H8	1.52	0.75
4:D:163:GLU:HG3	4:D:166:LYS:HE3	1.68	0.75
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.21	0.75
8:H:85:ARG:NE	8:H:87:SER:O	2.20	0.75
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.69	0.74
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.20	0.74
2:B:22:LYS:O	2:B:23:ARG:NH1	2.21	0.74
1:A:755:G:OP2	15:O:65:ARG:HD2	1.88	0.74
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.20	0.74
1:A:984:C:O2	1:A:1221:G:N2	2.18	0.73
17:Q:40:LYS:HD2	17:Q:42:TYR:CE1	2.23	0.73
1:A:132:C:O2	1:A:230:G:N2	2.20	0.73
1:A:184:G:H2'	1:A:185:A:H8	1.53	0.73
3:C:172:ARG:HB2	3:C:172:ARG:HH11	1.51	0.73
20:T:75:ASN:N	20:T:75:ASN:OD1	2.21	0.73
10:J:19:SER:HB2	10:J:94:VAL:HG21	1.70	0.73
18:R:21:LYS:HD3	18:R:57:GLY:HA2	1.70	0.73
1:A:79:G:N1	1:A:80:G:N7	2.37	0.73
1:A:241:C:H4'	12:L:19:ARG:HH22	1.53	0.73
1:A:130:A:H5'	17:Q:63:ARG:HE	1.54	0.73
1:A:1061:G:H1	1:A:1195:C:H42	1.36	0.73
1:A:1226:C:OP2	13:M:91:ARG:NH1	2.22	0.73
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.21	0.73
1:A:1055:A:N7	1:A:1200:C:N4	2.37	0.72
13:M:84:ILE:HG13	13:M:86:CYS:H	1.52	0.72
1:A:103:C:P	20:T:17:ARG:HH12	2.12	0.72
1:A:1065:U:H5''	1:A:1190:G:N2	2.05	0.72
2:B:127:ILE:HG22	2:B:135:GLN:HG2	1.72	0.72
1:A:1316:G:N1	1:A:1319:A:OP2	2.23	0.72
2:B:158:LEU:H	2:B:158:LEU:HD12	1.54	0.72
1:A:1392:G:H21	1:A:1502:A:H8	1.34	0.72
1:A:1372:U:OP2	9:I:11:LYS:NZ	2.22	0.72
3:C:86:VAL:HG12	3:C:87:LEU:HD23	1.72	0.72
1:A:951:G:OP2	13:M:102:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:G:OP1	4:D:38:TYR:OH	2.09	0.71
2:B:23:ARG:NH1	2:B:23:ARG:HA	2.06	0.71
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.22	0.71
1:A:258:G:H2'	1:A:259:G:H8	1.56	0.71
7:G:70:LYS:O	7:G:72:ARG:NH1	2.23	0.71
6:F:80:ARG:HD2	6:F:88:VAL:HB	1.72	0.71
1:A:992:U:H3	1:A:1044:A:H62	1.39	0.71
1:A:343:U:O2'	1:A:346:G:O6	2.08	0.71
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.26	0.71
5:E:15:ARG:HG2	5:E:28:PHE:CE2	2.24	0.70
13:M:3:ARG:HE	13:M:7:VAL:HA	1.55	0.70
17:Q:62:SER:HB3	17:Q:72:ARG:HD3	1.72	0.70
2:B:30:ARG:HD2	2:B:31:TYR:CE2	2.25	0.70
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.15	0.70
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.57	0.70
1:A:902:G:H2'	1:A:903:G:H8	1.57	0.70
1:A:600:C:N3	1:A:638:G:N2	2.33	0.70
10:J:11:PHE:O	10:J:68:HIS:NE2	2.24	0.70
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.55	0.70
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.74	0.69
13:M:117:VAL:HG12	13:M:118:ALA:H	1.56	0.69
1:A:1309:G:O3'	13:M:77:ASN:ND2	2.24	0.69
1:A:1070:U:H2'	1:A:1071:C:H6	1.56	0.69
1:A:1244:C:H42	1:A:1293:G:H1	1.38	0.69
3:C:84:ILE:O	3:C:88:ARG:NH1	2.26	0.69
1:A:269:C:H2'	1:A:270:A:C8	2.27	0.69
12:L:52:LEU:O	12:L:54:LYS:NZ	2.24	0.69
1:A:384:G:H2'	1:A:385:C:C6	2.27	0.69
2:B:95:GLN:HG2	2:B:148:TYR:HD2	1.58	0.69
20:T:57:ARG:HE	20:T:102:GLY:HA3	1.58	0.68
4:D:119:GLN:HE21	4:D:123:HIS:HE1	1.41	0.68
15:O:6:GLU:OE1	15:O:6:GLU:N	2.21	0.68
1:A:18:C:H5''	5:E:127:ASN:HD21	1.58	0.68
1:A:1150:U:O4	1:A:1151:A:N6	2.27	0.68
9:I:4:TYR:HB2	9:I:88:TYR:HD1	1.59	0.68
14:N:40:CYS:O	14:N:44:LEU:N	2.24	0.68
1:A:1255:G:H22	1:A:1283:G:H1'	1.57	0.68
2:B:23:ARG:HA	2:B:23:ARG:HH11	1.59	0.68
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.76	0.68
1:A:656:C:H42	1:A:750:G:H1	1.41	0.68
1:A:1418:A:H2'	1:A:1419:G:O4'	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:ILE:H	2:B:172:ILE:HD12	1.59	0.68
12:L:113:ARG:HH11	12:L:116:SER:H	1.42	0.68
1:A:235:C:N4	24:A:1980:HOH:O	2.27	0.67
1:A:1266:G:N2	1:A:1269:A:OP2	2.23	0.67
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.27	0.67
6:F:74:ASP:OD2	6:F:74:ASP:N	2.23	0.67
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.76	0.67
1:A:1262:C:H42	1:A:1273:G:H1	1.42	0.67
2:B:21:ARG:HA	2:B:39:ILE:HG23	1.76	0.67
4:D:24:GLU:HG3	4:D:112:VAL:HG11	1.76	0.67
5:E:5:ASP:OD2	5:E:6:PHE:N	2.25	0.67
1:A:1417:G:O2'	1:A:1483:A:N6	2.26	0.67
2:B:160:ASP:OD2	2:B:160:ASP:N	2.27	0.67
7:G:18:TYR:HD2	7:G:59:LEU:HD13	1.59	0.67
3:C:14:ILE:HG12	3:C:15:THR:HG23	1.74	0.67
6:F:42:GLU:HG3	6:F:61:LEU:HB3	1.75	0.67
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.27	0.67
9:I:2:GLU:HG3	9:I:3:GLN:HG2	1.75	0.67
1:A:1141:C:H2'	1:A:1142:G:H8	1.57	0.67
1:A:858:G:N7	24:A:2098:HOH:O	2.27	0.67
1:A:569:C:H42	1:A:881:G:H1	1.41	0.67
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.77	0.67
1:A:1100:C:OP2	2:B:96:ARG:NH1	2.27	0.67
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.27	0.67
2:B:9:GLU:OE2	2:B:12:GLU:N	2.28	0.67
2:B:91:PRO:HG3	2:B:155:LEU:HD21	1.77	0.67
6:F:47:ARG:H	6:F:47:ARG:HD2	1.59	0.67
9:I:104:ARG:NH1	9:I:105:ASP:O	2.26	0.67
2:B:208:ILE:H	2:B:208:ILE:HD12	1.60	0.67
11:K:40:ILE:HG23	11:K:75:TYR:HD1	1.59	0.67
14:N:53:LEU:HD12	14:N:56:VAL:HG21	1.75	0.67
18:R:46:GLU:H	18:R:46:GLU:CD	1.99	0.66
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.25	0.66
13:M:23:TYR:CE2	13:M:70:LEU:HD12	2.29	0.66
1:A:921:U:O2'	5:E:19:MET:O	2.11	0.66
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.76	0.66
7:G:114:ARG:O	7:G:119:ARG:NH1	2.28	0.66
12:L:27:LEU:C	12:L:29:GLY:N	2.48	0.66
4:D:13:ARG:NH1	4:D:38:TYR:O	2.29	0.66
16:P:38:TYR:HE2	16:P:50:LYS:HE2	1.60	0.66
10:J:86:MET:SD	10:J:87:THR:N	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.78	0.66
1:A:243:A:H4'	1:A:244:U:H5''	1.77	0.66
1:A:1033:G:H2'	1:A:1034:G:C8	2.30	0.66
1:A:1249:C:H1'	9:I:70:LYS:HE2	1.78	0.66
18:R:55:ARG:NH1	18:R:55:ARG:HB3	2.11	0.66
12:L:66:VAL:HG11	12:L:98:TYR:CE1	2.31	0.66
1:A:384:G:H2'	1:A:385:C:H6	1.60	0.65
9:I:19:LEU:HD21	9:I:59:PHE:CG	2.32	0.65
14:N:16:PHE:HB2	14:N:19:ARG:HD2	1.77	0.65
20:T:87:LYS:O	20:T:91:LEU:HB2	1.96	0.65
1:A:166:G:H2'	1:A:167:G:C8	2.32	0.65
13:M:24:GLY:O	13:M:29:ARG:HD2	1.97	0.65
1:A:130:A:OP2	1:A:190(E):U:O2'	2.09	0.65
1:A:1435:G:H2'	1:A:1436:U:C6	2.32	0.65
20:T:30:LYS:HG2	20:T:34:LYS:HE2	1.78	0.65
1:A:985:C:H42	1:A:1220:G:H1	1.42	0.65
7:G:73:MET:HA	7:G:91:VAL:HG23	1.77	0.65
1:A:1151:A:H5''	10:J:42:THR:HG22	1.78	0.65
7:G:90:GLU:HG2	7:G:91:VAL:H	1.62	0.65
7:G:88:PRO:HG2	7:G:155:ARG:HH22	1.59	0.65
11:K:57:THR:HG23	11:K:60:ALA:H	1.62	0.64
19:S:64:GLU:OE2	19:S:65:ASN:ND2	2.30	0.64
1:A:184:G:H2'	1:A:185:A:C8	2.31	0.64
1:A:547:A:OP2	4:D:2:GLY:N	2.29	0.64
4:D:155:LEU:HD13	4:D:157:LEU:H	1.61	0.64
14:N:29:ARG:NH1	14:N:40:CYS:SG	2.70	0.64
19:S:77:THR:HG23	19:S:78:ARG:HG3	1.79	0.64
1:A:1257:U:H4'	1:A:1258:G:O5'	1.96	0.64
9:I:82:ALA:HB1	9:I:96:LEU:HD21	1.79	0.64
9:I:118:LYS:HG2	9:I:121:ARG:HB3	1.80	0.64
1:A:413:G:O6	4:D:36:ARG:NH1	2.31	0.64
1:A:633:G:H2'	1:A:634:C:C6	2.33	0.64
2:B:60:ASP:O	2:B:64:ARG:HG3	1.98	0.64
1:A:1338:G:H2'	1:A:1339:A:C8	2.31	0.64
4:D:50:ARG:NH1	4:D:51:PRO:O	2.30	0.64
9:I:89:ASN:O	9:I:92:TYR:HB2	1.97	0.64
1:A:1179:A:H2'	1:A:1180:A:O4'	1.98	0.64
6:F:1:MET:HB3	6:F:66:GLU:HG2	1.80	0.64
1:A:1004:A:H5''	1:A:1025:U:C2	2.33	0.63
1:A:1195:C:H3'	1:A:1196:U:C5'	2.26	0.63
10:J:79:ARG:O	10:J:82:ILE:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:U:OP1	1:A:1108:G:N2	2.27	0.63
3:C:127:ARG:HG2	3:C:193:TYR:OH	1.98	0.63
1:A:783:C:H42	1:A:799:G:H1	1.46	0.63
1:A:1320:C:H42	19:S:36:ARG:HD3	1.62	0.63
1:A:1502:A:H2	1:A:1505:G:H1	1.47	0.63
9:I:47:LEU:HA	9:I:50:LEU:HD12	1.81	0.63
9:I:118:LYS:O	9:I:120:ARG:N	2.28	0.63
16:P:67:THR:HG22	16:P:68:ASP:H	1.64	0.63
4:D:59:ARG:HA	4:D:62:GLN:HB2	1.81	0.63
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.80	0.63
1:A:1402:4OC:H2'	1:A:1403:C:O4'	1.98	0.63
10:J:7:LYS:HD3	10:J:9:ARG:NE	2.14	0.63
12:L:92:0TD:OD1	12:L:92:0TD:N	2.30	0.63
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.38	0.63
16:P:21:VAL:HG12	16:P:33:ILE:HG13	1.79	0.63
1:A:79:G:C2	1:A:80:G:C8	2.86	0.62
1:A:9:G:OP2	5:E:121:LYS:NZ	2.28	0.62
1:A:986:A:N3	19:S:52:TYR:OH	2.24	0.62
1:A:1168:A:H2'	1:A:1169:A:H8	1.65	0.62
2:B:50:GLU:O	2:B:53:ARG:HG3	1.99	0.62
7:G:53:LYS:HB3	7:G:125:MET:HE1	1.81	0.62
9:I:43:ALA:HA	9:I:74:ILE:HD12	1.81	0.62
1:A:973:G:H3'	1:A:974:A:H5''	1.80	0.62
1:A:1301:U:O2'	1:A:1302:U:H3'	1.99	0.62
1:A:1336:C:H6	1:A:1336:C:H5''	1.64	0.62
2:B:74:LYS:HE3	2:B:206:ASP:HA	1.82	0.62
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.32	0.62
1:A:186:C:O2'	20:T:85:MET:SD	2.52	0.62
1:A:967:5MC:O3'	9:I:128:ARG:NH2	2.32	0.62
2:B:16:HIS:CB	2:B:210:SER:HB3	2.29	0.62
1:A:633:G:H2'	1:A:634:C:H6	1.65	0.62
1:A:1412:C:N3	1:A:1488:G:N1	2.40	0.62
1:A:1009:G:N2	1:A:1010:G:N3	2.46	0.62
1:A:101:A:H2'	1:A:102:G:C8	2.31	0.62
1:A:241:C:H4'	12:L:19:ARG:NH2	2.15	0.62
8:H:4:ASP:OD1	8:H:6:ILE:N	2.32	0.62
1:A:1112:C:O2'	3:C:179:ARG:NH1	2.32	0.62
3:C:88:ARG:HG3	3:C:91:LEU:HD22	1.82	0.62
1:A:1045:C:H2'	1:A:1046:A:C8	2.35	0.62
1:A:1197:G:H5''	24:A:2057:HOH:O	2.00	0.62
2:B:16:HIS:O	2:B:17:PHE:HD1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:106:ALA:O	9:I:108:VAL:HG23	1.99	0.62
1:A:80:G:H2'	1:A:81:U:H5'	1.82	0.61
1:A:1034:G:H2'	1:A:1035:A:C8	2.31	0.61
1:A:1347:G:N2	1:A:1373:G:H2'	2.15	0.61
1:A:1415:G:H2'	1:A:1416:G:H8	1.65	0.61
6:F:2:ARG:O	6:F:66:GLU:HA	2.00	0.61
1:A:937:A:H5''	1:A:938:A:OP2	2.00	0.61
2:B:82:ARG:HA	2:B:92:TYR:CE1	2.35	0.61
3:C:124:ILE:HG12	3:C:130:VAL:HG12	1.82	0.61
4:D:88:VAL:O	4:D:92:VAL:HG23	2.00	0.61
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.82	0.61
1:A:542:G:OP1	4:D:10:ARG:NH2	2.33	0.61
5:E:75:THR:OG1	5:E:76:ILE:N	2.24	0.61
1:A:1058:G:H2'	1:A:1059:C:O4'	2.00	0.61
12:L:59:ARG:HA	12:L:65:GLU:HG3	1.82	0.61
17:Q:97:SER:O	17:Q:98:LEU:HD12	2.01	0.61
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.64	0.61
13:M:40:ASN:HD22	13:M:43:THR:HG23	1.65	0.61
1:A:618:C:N3	1:A:622:A:N6	2.47	0.61
1:A:949:A:C2	1:A:1233:G:N3	2.69	0.61
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.01	0.61
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.82	0.61
12:L:126:LYS:H	12:L:126:LYS:HD2	1.65	0.61
1:A:337:C:H2'	1:A:338:A:C8	2.36	0.61
1:A:353:A:H5'	1:A:353:A:H8	1.66	0.61
1:A:691:G:H2'	1:A:692:U:C6	2.36	0.61
5:E:65:ASN:ND2	5:E:65:ASN:O	2.33	0.61
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.83	0.60
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.83	0.60
4:D:157:LEU:O	4:D:160:GLN:HB3	2.00	0.60
7:G:90:GLU:HG2	7:G:91:VAL:N	2.16	0.60
20:T:44:ALA:HB1	20:T:91:LEU:HB3	1.82	0.60
1:A:978:A:O2'	1:A:1322:C:N3	2.35	0.60
1:A:1046:A:H3'	1:A:1047:G:H8	1.67	0.60
20:T:49:ALA:HB3	20:T:99:LEU:HD12	1.84	0.60
1:A:1234:C:H1'	1:A:1364:U:O2	2.01	0.60
7:G:16:LEU:HD12	9:I:44:VAL:HG12	1.83	0.60
1:A:358:U:H2'	1:A:359:U:H6	1.66	0.60
3:C:156:ARG:HG2	3:C:160:ALA:O	2.01	0.60
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.84	0.60
12:L:89:ARG:HG2	12:L:97:ARG:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:C:H2'	1:A:680:C:C6	2.37	0.60
3:C:11:ARG:HB3	3:C:16:ARG:HB2	1.83	0.60
17:Q:97:SER:OG	17:Q:98:LEU:N	2.34	0.60
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.83	0.60
1:A:299:G:H2'	1:A:300:A:C8	2.37	0.60
1:A:625:G:H2'	1:A:626:U:C6	2.37	0.60
1:A:1074:G:O3'	2:B:103:THR:HG21	2.02	0.60
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.02	0.60
1:A:1356:G:H2'	1:A:1357:A:C8	2.37	0.60
5:E:20:GLN:NE2	5:E:25:ARG:HH21	2.00	0.60
1:A:463:A:OP1	16:P:75:ARG:NH2	2.34	0.60
1:A:912:C:OP1	12:L:46:LYS:NZ	2.33	0.60
2:B:191:ASP:N	2:B:191:ASP:OD1	2.28	0.60
4:D:4:TYR:OH	4:D:7:PRO:O	2.17	0.60
1:A:1487:G:H2'	1:A:1488:G:O4'	2.02	0.59
1:A:1520[A]:G:H2'	1:A:1521:G:H8	1.66	0.59
3:C:21:ARG:HH21	3:C:58:GLU:HG3	1.67	0.59
11:K:66:LEU:HG	11:K:97:ALA:HB1	1.84	0.59
1:A:872:A:O2'	1:A:873:A:H5''	2.02	0.59
13:M:75:ALA:O	13:M:79:LYS:NZ	2.35	0.59
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.37	0.59
8:H:39:LEU:HB3	8:H:45:ILE:HG12	1.83	0.59
21:U:10:ARG:O	21:U:13:ILE:HG12	2.03	0.59
1:A:828:A:H5''	1:A:859:A:C2	2.38	0.59
16:P:74:LEU:HB3	16:P:79:VAL:HG21	1.84	0.59
1:A:1093:A:N3	1:A:1109:C:O2'	2.34	0.59
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.03	0.59
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.17	0.59
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.83	0.59
1:A:900:A:H2'	1:A:901:A:O4'	2.03	0.59
1:A:1510:U:H2'	1:A:1511:G:C8	2.37	0.59
4:D:75:PHE:O	4:D:78:LEU:HB3	2.02	0.59
15:O:14:GLU:HG3	15:O:15:PHE:HD1	1.67	0.59
1:A:485:G:O2'	1:A:486:U:OP2	2.14	0.59
5:E:127:ASN:HB3	5:E:130:ASN:HB2	1.84	0.59
10:J:10:GLY:HA3	10:J:16:LEU:HD21	1.85	0.59
10:J:17:ASP:O	10:J:21:GLN:HB2	2.01	0.59
1:A:268:C:H2'	1:A:269:C:H6	1.67	0.59
1:A:1181:G:N2	1:A:1182:G:H22	2.01	0.59
7:G:129:GLU:HB3	7:G:131:LYS:HG2	1.85	0.59
15:O:87:ILE:HG22	15:O:88:ARG:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:G:O3'	17:Q:68:ARG:NH1	2.35	0.59
2:B:9:GLU:HB3	2:B:12:GLU:HG2	1.83	0.59
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.84	0.59
1:A:1437:C:H2'	1:A:1438:G:C8	2.39	0.58
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.36	0.58
7:G:88:PRO:HG2	7:G:155:ARG:HH12	1.67	0.58
13:M:25:ILE:HD11	13:M:66:LEU:HD11	1.85	0.58
1:A:967:5MC:H5''	1:A:968:A:H2'	1.85	0.58
1:A:1427:U:H2'	1:A:1428:A:C8	2.38	0.58
1:A:79:G:N1	1:A:80:G:C5	2.72	0.58
1:A:539:A:H2'	1:A:540:G:C8	2.37	0.58
1:A:793:U:H5'	24:A:2157:HOH:O	2.03	0.58
1:A:858:G:C6	1:A:869:G:C8	2.91	0.58
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.36	0.58
5:E:18:ARG:HG2	5:E:19:MET:N	2.16	0.58
6:F:4:TYR:HB2	6:F:65:VAL:HG22	1.84	0.58
1:A:628:G:H2'	1:A:629:G:C8	2.38	0.58
1:A:414:A:OP2	1:A:428:G:N2	2.30	0.58
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.86	0.58
17:Q:65:ILE:HB	17:Q:69:LYS:HG2	1.84	0.58
17:Q:66:SER:OG	17:Q:69:LYS:HB3	2.03	0.58
8:H:97:VAL:HG12	8:H:98:LYS:HG3	1.86	0.58
16:P:41:PRO:O	16:P:43:LYS:HE3	2.03	0.58
1:A:216:G:C2	1:A:217:C:C4	2.91	0.58
1:A:1049:U:H4'	1:A:1050:G:O5'	2.03	0.58
1:A:1111:A:N1	3:C:177:THR:HB	2.19	0.58
3:C:39:ILE:HD12	3:C:57:ILE:HD13	1.84	0.58
3:C:134:ILE:O	3:C:138:VAL:HG23	2.03	0.58
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.68	0.58
1:A:190(L):U:H3	20:T:105:SER:CB	2.17	0.58
1:A:864:A:H2'	1:A:865:A:C8	2.39	0.58
20:T:51:GLU:O	20:T:55:ILE:HG12	2.04	0.58
1:A:77:G:C6	1:A:93:G:N1	2.72	0.58
2:B:91:PRO:HB3	2:B:154:LEU:HB2	1.85	0.58
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.85	0.58
1:A:1424:C:H2'	1:A:1425:U:C6	2.39	0.58
3:C:11:ARG:HH12	3:C:178:LEU:HA	1.68	0.58
3:C:12:LEU:HD21	14:N:51:GLY:HA2	1.85	0.57
4:D:111:ALA:HB1	4:D:116:GLN:HG2	1.85	0.57
16:P:67:THR:HG22	16:P:68:ASP:N	2.19	0.57
2:B:9:GLU:O	2:B:10:LEU:HD23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:67:THR:HB	16:P:70:ALA:H	1.69	0.57
1:A:401:C:O2'	1:A:621:A:N3	2.28	0.57
3:C:88:ARG:HH21	3:C:101:LEU:HB2	1.69	0.57
12:L:111:LYS:NZ	12:L:111:LYS:H	2.01	0.57
1:A:1517[A]:G:H2'	1:A:1518[A]:MA6:H8	1.86	0.57
1:A:1530:G:H2'	1:A:1531:A:C8	2.39	0.57
2:B:175:ARG:HH11	2:B:175:ARG:HG3	1.68	0.57
18:R:34:TYR:CE1	18:R:35:ARG:HG3	2.40	0.57
18:R:47:THR:HG22	18:R:48:GLY:H	1.69	0.57
1:A:617:G:H1	1:A:623:C:H42	1.52	0.57
1:A:1291:G:H5''	7:G:41:ARG:HH21	1.69	0.57
1:A:1401:G:N2	1:A:1402:4OC:H1'	2.19	0.57
1:A:1437:C:H2'	1:A:1438:G:H8	1.70	0.57
1:A:1520[B]:G:H2'	1:A:1521:G:H8	1.69	0.57
6:F:13:ASN:OD1	6:F:13:ASN:N	2.30	0.57
9:I:32:ASP:OD2	9:I:33:PHE:N	2.38	0.57
19:S:11:VAL:HB	19:S:16:LEU:HD12	1.87	0.57
7:G:45:ASP:O	7:G:49:ILE:HG12	2.05	0.57
17:Q:3:LYS:HB3	17:Q:60:ILE:HD11	1.84	0.57
17:Q:5:VAL:O	17:Q:6:LEU:HD23	2.04	0.57
1:A:691:G:H2'	1:A:692:U:H6	1.68	0.57
6:F:50:TYR:OH	6:F:87:ARG:NH2	2.37	0.57
19:S:18:LYS:NZ	19:S:32:LYS:HG2	2.20	0.57
5:E:84:PHE:HB3	5:E:134:ALA:HB2	1.84	0.57
16:P:23:ASP:OD1	16:P:24:ALA:N	2.37	0.57
1:A:258:G:H2'	1:A:259:G:C8	2.38	0.57
1:A:442:C:H2'	1:A:443:C:H6	1.70	0.57
1:A:629:G:H2'	1:A:630:G:C8	2.39	0.57
1:A:673:G:H2'	1:A:674:G:C8	2.39	0.57
12:L:39:VAL:HG22	12:L:57:LYS:HB2	1.87	0.57
1:A:372:C:H4'	1:A:373:A:O5'	2.05	0.56
1:A:991:U:H3	1:A:1215:G:N2	2.03	0.56
3:C:179:ARG:NE	3:C:206:GLU:OE1	2.38	0.56
7:G:18:TYR:CD2	7:G:59:LEU:HD22	2.40	0.56
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.20	0.56
8:H:111:ILE:HG22	8:H:134:ILE:HD13	1.87	0.56
1:A:444:C:H42	1:A:490:G:H1	1.52	0.56
1:A:1114:C:O2'	14:N:60:SER:O	2.09	0.56
1:A:1397:C:O2'	1:A:1398:A:OP1	2.19	0.56
1:A:1415:G:H2'	1:A:1416:G:C8	2.40	0.56
13:M:48:LEU:HD12	13:M:52:GLU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:C:H2'	1:A:391:G:C8	2.41	0.56
1:A:517:G:H5'	1:A:519:C:C2	2.39	0.56
1:A:1026:G:O6	1:A:1036:G:N2	2.38	0.56
3:C:184:TYR:HE2	3:C:186:PHE:HB2	1.70	0.56
6:F:10:LEU:HB3	6:F:85:VAL:HA	1.87	0.56
6:F:82:ARG:HB3	6:F:85:VAL:HG23	1.87	0.56
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.41	0.56
1:A:264:U:H2'	1:A:265:G:O4'	2.05	0.56
12:L:25:PRO:HG3	12:L:27:LEU:HD13	1.87	0.56
13:M:17:VAL:O	13:M:20:THR:HG22	2.05	0.56
18:R:25:THR:OG1	18:R:25:THR:O	2.23	0.56
18:R:56:THR:OG1	18:R:57:GLY:N	2.38	0.56
1:A:99:C:H2'	1:A:101:A:C8	2.41	0.56
1:A:176:C:O2'	1:A:177:C:H5'	2.05	0.56
1:A:411:A:OP1	4:D:30:LYS:NZ	2.38	0.56
1:A:1425:U:H2'	1:A:1426:C:C6	2.40	0.56
2:B:118:LEU:HB3	2:B:142:LEU:HD23	1.87	0.56
4:D:190:ASP:H	4:D:193:ASP:HB2	1.70	0.56
18:R:66:LEU:HD12	18:R:66:LEU:O	2.05	0.56
1:A:1004:A:O2'	1:A:1038:C:O2	2.22	0.56
4:D:174:LEU:O	4:D:186:LEU:HD11	2.06	0.56
9:I:16:ARG:HB2	9:I:64:THR:HG23	1.87	0.56
10:J:45:ARG:HB3	10:J:65:LEU:HB3	1.88	0.56
12:L:57:LYS:HE3	12:L:65:GLU:HB3	1.88	0.56
18:R:61:LYS:HG2	18:R:65:ILE:HD11	1.87	0.56
1:A:411:A:N9	1:A:413:G:H1'	2.21	0.56
1:A:664:G:H22	1:A:741:G:H1	1.54	0.56
1:A:1004:A:H5''	1:A:1025:U:N3	2.20	0.56
13:M:3:ARG:HA	13:M:8:GLU:O	2.06	0.56
13:M:96:LEU:O	13:M:110:ARG:NH1	2.38	0.56
5:E:60:TYR:HD2	5:E:61:TYR:HD1	1.54	0.56
7:G:94:ARG:O	7:G:97:GLN:HB3	2.06	0.56
18:R:45:SER:OG	18:R:47:THR:O	2.18	0.56
1:A:95:U:H2'	1:A:96:G:H8	1.71	0.56
1:A:1009:G:H1	1:A:1020:U:H3	1.52	0.56
1:A:1201:A:H4'	1:A:1202:G:C5'	2.36	0.56
1:A:1290:G:H2'	1:A:1291:G:C8	2.41	0.56
1:A:939:G:H2'	1:A:940:C:C6	2.41	0.56
1:A:1004:A:N6	1:A:1036:G:O6	2.39	0.56
1:A:1285:A:H4'	1:A:1286:A:O5'	2.06	0.56
3:C:21:ARG:HA	14:N:54:PRO:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:187:ARG:NE	4:D:188:LEU:H	2.03	0.56
1:A:1309:G:H2'	1:A:1310:G:C8	2.40	0.55
1:A:1442:G:C5	1:A:1446:A:C6	2.93	0.55
1:A:337:C:H2'	1:A:338:A:H8	1.71	0.55
1:A:1003:G:H1	1:A:1038:C:H42	1.53	0.55
1:A:1128:C:O2'	1:A:1130:A:N7	2.39	0.55
1:A:166:G:H2'	1:A:167:G:H8	1.71	0.55
1:A:536:C:H2'	1:A:537:G:C8	2.41	0.55
1:A:1413:A:H2'	1:A:1414:U:H6	1.71	0.55
1:A:277:C:P	17:Q:68:ARG:HH12	2.28	0.55
1:A:918:A:H2'	1:A:919:A:C8	2.41	0.55
1:A:1376:U:OP1	7:G:98:SER:OG	2.12	0.55
2:B:133:LYS:NZ	2:B:133:LYS:H	2.04	0.55
11:K:109:VAL:HG11	18:R:84:LYS:HE2	1.88	0.55
11:K:120:ARG:HH22	11:K:126:ARG:HH12	1.54	0.55
12:L:66:VAL:HG11	12:L:98:TYR:HE1	1.68	0.55
18:R:44:LEU:HD13	18:R:48:GLY:O	2.06	0.55
1:A:1366:C:H2'	1:A:1367:C:H6	1.71	0.55
3:C:150:LYS:HB2	3:C:201:TYR:HB2	1.89	0.55
1:A:186:C:H2'	1:A:187:C:C6	2.41	0.55
1:A:955:U:O2'	1:A:1227:A:N6	2.40	0.55
1:A:1258:G:H2'	1:A:1259:C:C6	2.42	0.55
1:A:1488:G:H2'	1:A:1489:G:C8	2.42	0.55
9:I:104:ARG:HD3	9:I:105:ASP:H	1.72	0.55
1:A:79:G:C2	1:A:80:G:N7	2.75	0.55
1:A:443:C:N4	1:A:491:G:H1	1.98	0.55
1:A:474:G:H4'	16:P:81:ARG:NH2	2.21	0.55
1:A:620:C:H2'	1:A:621:A:O4'	2.06	0.55
2:B:103:THR:HA	2:B:180:LEU:HD11	1.87	0.55
1:A:835:U:OP1	18:R:64:ARG:NH2	2.39	0.55
2:B:166:ASP:OD2	2:B:169:LYS:N	2.30	0.55
8:H:82:HIS:C	8:H:82:HIS:ND1	2.60	0.55
1:A:560:U:H5'	1:A:566:G:C2	2.42	0.55
1:A:1232:U:H5''	9:I:124:GLN:O	2.07	0.55
1:A:1504:G:H4'	1:A:1505:G:H5'	1.89	0.55
3:C:22:TRP:CH2	3:C:32:LEU:HB3	2.42	0.55
2:B:80:ILE:HG22	2:B:215:LEU:HD12	1.89	0.55
3:C:64:VAL:HG12	3:C:65:ALA:H	1.71	0.55
4:D:60:GLU:OE2	4:D:199:ASN:N	2.32	0.55
13:M:8:GLU:OE2	13:M:22:ILE:HA	2.07	0.55
1:A:103:C:OP2	20:T:14:LYS:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1309:G:OP1	13:M:92:HIS:NE2	2.33	0.54
12:L:113:ARG:NH1	12:L:116:SER:H	2.04	0.54
13:M:67:GLU:O	13:M:71:ARG:HG2	2.07	0.54
17:Q:29:HIS:CE1	17:Q:31:LEU:H	2.24	0.54
1:A:204:U:H4'	1:A:216:G:O5'	2.08	0.54
1:A:344:A:H5'	1:A:345:C:C5	2.42	0.54
2:B:28:PHE:CD2	2:B:190:THR:HA	2.41	0.54
9:I:46:ALA:HB1	9:I:77:ILE:HG21	1.89	0.54
14:N:3:ARG:HB2	14:N:6:LEU:HB2	1.89	0.54
1:A:690:G:H2'	1:A:691:G:O4'	2.08	0.54
4:D:8:VAL:O	4:D:11:LEU:N	2.39	0.54
11:K:120:ARG:NH2	11:K:126:ARG:HH12	2.05	0.54
1:A:580:U:H2'	1:A:581:G:O4'	2.07	0.54
7:G:60:LYS:HZ3	7:G:64:GLN:HB2	1.72	0.54
8:H:123:GLU:O	8:H:127:LEU:HB2	2.08	0.54
9:I:51:ARG:HG2	9:I:56:LEU:HD11	1.89	0.54
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.42	0.54
19:S:18:LYS:HD3	19:S:31:ILE:HG13	1.90	0.54
1:A:116:A:H2'	1:A:117:G:H8	1.73	0.54
4:D:200:GLU:OE1	4:D:200:GLU:N	2.33	0.54
7:G:111:ARG:HG2	7:G:112:PRO:HD2	1.89	0.54
9:I:19:LEU:HD12	9:I:61:ALA:HB2	1.88	0.54
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.90	0.54
17:Q:11:VAL:O	17:Q:53:LEU:HD21	2.07	0.54
17:Q:83:ASP:OD1	17:Q:84:LEU:N	2.39	0.54
1:A:309:G:H2'	1:A:310:G:H8	1.72	0.54
1:A:758:G:C8	24:A:1967:HOH:O	2.60	0.54
1:A:1000:U:C4	1:A:1042:G:C6	2.96	0.54
1:A:1047:G:C2'	1:A:1048:G:H5'	2.37	0.54
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.88	0.54
7:G:18:TYR:HB3	7:G:59:LEU:HD22	1.90	0.54
8:H:87:SER:HG	8:H:93:VAL:H	1.52	0.54
1:A:413:G:H8	1:A:428:G:N2	2.04	0.54
1:A:715:A:H2'	1:A:716:A:C8	2.43	0.54
1:A:866:C:H2'	1:A:867:G:O4'	2.08	0.54
1:A:1028:C:H41	1:A:1033:G:H21	1.55	0.54
1:A:1520[A]:G:H2'	1:A:1521:G:C8	2.42	0.54
1:A:612:C:H42	1:A:628:G:H1	1.56	0.54
1:A:1143:G:H2'	1:A:1144:G:C8	2.43	0.54
5:E:80:ILE:HG22	8:H:104:ARG:NH2	2.22	0.54
10:J:19:SER:HA	10:J:22:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:79:ARG:O	10:J:83:GLU:N	2.39	0.54
17:Q:60:ILE:O	17:Q:62:SER:OG	2.26	0.54
1:A:179:A:H2'	1:A:180:U:C6	2.42	0.54
15:O:62:GLN:O	15:O:65:ARG:N	2.40	0.54
20:T:10:LEU:O	20:T:13:LEU:HB2	2.08	0.54
20:T:73:HIS:HB3	20:T:74:LYS:HG3	1.90	0.54
1:A:443:C:N3	1:A:491:G:N2	2.51	0.54
1:A:966:M2G:C5	1:A:967:5MC:HM52	2.43	0.54
15:O:4:THR:OG1	15:O:7:GLU:OE2	2.25	0.54
1:A:325:A:H2'	1:A:326:G:O4'	2.09	0.53
1:A:628:G:H2'	1:A:629:G:H8	1.71	0.53
1:A:923:A:OP1	5:E:21:ALA:HB2	2.08	0.53
1:A:1143:G:H2'	1:A:1144:G:H8	1.73	0.53
4:D:20:TYR:HB3	4:D:26:CYS:HB3	1.89	0.53
18:R:65:ILE:O	18:R:69:THR:OG1	2.25	0.53
21:U:25:LYS:HA	21:U:25:LYS:HE3	1.90	0.53
1:A:60:A:P	1:A:331:G:H22	2.31	0.53
1:A:731:G:OP1	1:A:766:A:H1'	2.07	0.53
2:B:208:ILE:HA	2:B:211:ILE:HD12	1.89	0.53
4:D:108:LEU:HD12	4:D:176:LEU:HD13	1.89	0.53
9:I:64:THR:OG1	9:I:66:ARG:NH2	2.41	0.53
10:J:49:VAL:HG12	14:N:41:ARG:HG3	1.91	0.53
12:L:97:ARG:HB2	12:L:98:TYR:CE1	2.42	0.53
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.43	0.53
1:A:170:U:O2'	1:A:171:A:H5'	2.08	0.53
1:A:444:C:N4	1:A:490:G:H1	2.06	0.53
1:A:456:C:H2'	1:A:457:C:C6	2.44	0.53
1:A:1053:G:H4'	1:A:1054:C:H5'	1.90	0.53
1:A:1461:G:H2'	1:A:1462:G:H8	1.73	0.53
2:B:91:PRO:HG3	2:B:155:LEU:CD2	2.38	0.53
18:R:25:THR:O	18:R:26:LEU:HD13	2.08	0.53
1:A:195:A:H4'	20:T:68:LYS:NZ	2.23	0.53
1:A:1422:G:H2'	1:A:1423:G:H8	1.72	0.53
6:F:91:VAL:HG12	6:F:92:LYS:O	2.08	0.53
12:L:46:LYS:HE2	12:L:47:LYS:HE3	1.91	0.53
19:S:22:LEU:HD13	19:S:47:HIS:CE1	2.44	0.53
1:A:232:G:H1'	1:A:262:A:N1	2.23	0.53
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.90	0.53
1:A:1366:C:H2'	1:A:1367:C:C6	2.44	0.53
1:A:1392:G:N2	1:A:1502:A:H8	2.03	0.53
16:P:13:HIS:O	16:P:42:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:21:VAL:O	16:P:33:ILE:HG12	2.09	0.53
1:A:279:A:H5''	1:A:281:G:O4'	2.09	0.53
1:A:407:G:C6	1:A:408:A:C6	2.96	0.53
1:A:569:C:H5''	1:A:570:G:OP1	2.08	0.53
1:A:1070:U:H2'	1:A:1071:C:C6	2.41	0.53
9:I:55:ALA:HA	9:I:58:HIS:HB2	1.90	0.53
1:A:567:G:H2'	1:A:568:G:O4'	2.08	0.53
1:A:579:G:H2'	1:A:580:U:C6	2.43	0.53
1:A:908:A:C2	1:A:909:A:C4	2.96	0.53
1:A:1255:G:O2'	1:A:1258:G:H1'	2.09	0.53
1:A:1417:G:O3'	1:A:1418:A:H8	1.91	0.53
7:G:59:LEU:HD12	7:G:62:PHE:HD1	1.71	0.53
1:A:56:U:H2'	1:A:57:G:H8	1.73	0.53
1:A:758:G:N7	24:A:1967:HOH:O	2.34	0.53
1:A:1265:G:C6	1:A:1266:G:C6	2.97	0.53
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.42	0.53
2:B:178:ARG:O	8:H:71:GLY:HA2	2.08	0.53
1:A:268:C:H2'	1:A:269:C:C6	2.44	0.53
1:A:748:C:H4'	1:A:749:C:O5'	2.09	0.53
1:A:859:A:H2'	1:A:860:A:O4'	2.09	0.53
11:K:18:ARG:HB3	11:K:20:TYR:HE1	1.74	0.53
1:A:358:U:H2'	1:A:359:U:C6	2.44	0.53
1:A:627:G:H2'	1:A:628:G:H8	1.74	0.53
2:B:189:ASP:CG	2:B:205:ASP:HB3	2.29	0.53
18:R:39:VAL:O	18:R:42:ARG:HB2	2.09	0.53
1:A:448:A:P	1:A:485:G:H22	2.31	0.52
1:A:554:C:H2'	1:A:555:C:C6	2.44	0.52
1:A:1441:G:H4'	1:A:1442:G:C5	2.43	0.52
12:L:79:GLU:OE2	12:L:80:HIS:N	2.42	0.52
1:A:969:A:OP1	10:J:55:LYS:NZ	2.40	0.52
14:N:26:ARG:HD2	14:N:47:LEU:HD21	1.91	0.52
19:S:15:LEU:HD12	19:S:16:LEU:N	2.24	0.52
1:A:600:C:N4	1:A:638:G:H1	1.97	0.52
8:H:114:THR:HG22	8:H:130:GLY:O	2.10	0.52
13:M:49:THR:HG22	13:M:51:ALA:H	1.74	0.52
15:O:14:GLU:HG3	15:O:15:PHE:CD1	2.44	0.52
17:Q:92:ARG:HB3	17:Q:92:ARG:HH11	1.75	0.52
1:A:299:G:C6	1:A:300:A:C6	2.97	0.52
1:A:536:C:H2'	1:A:537:G:H8	1.75	0.52
1:A:757:U:H2'	1:A:758:G:O4'	2.08	0.52
1:A:1047:G:H2'	1:A:1048:G:H5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.91	0.52
5:E:41:VAL:HG23	5:E:67:VAL:CG1	2.39	0.52
13:M:39:ILE:HG22	13:M:40:ASN:N	2.24	0.52
15:O:4:THR:H	15:O:7:GLU:CD	2.13	0.52
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.44	0.52
1:A:793:U:H5''	1:A:794:A:H5''	1.91	0.52
1:A:858:G:C6	1:A:869:G:N7	2.77	0.52
1:A:1327:C:P	21:U:12:LYS:HZ1	2.32	0.52
5:E:76:ILE:HB	5:E:93:PRO:HB3	1.91	0.52
5:E:145:LYS:HG3	8:H:107:LEU:HD21	1.92	0.52
8:H:81:HIS:N	8:H:138:TRP:O	2.40	0.52
1:A:277:C:H5'	17:Q:68:ARG:NH1	2.25	0.52
1:A:841:U:H3'	1:A:848:C:O4'	2.10	0.52
3:C:95:THR:HG21	3:C:99:VAL:HG13	1.92	0.52
3:C:135:LYS:O	3:C:138:VAL:HB	2.09	0.52
4:D:28:SER:O	4:D:30:LYS:N	2.37	0.52
8:H:1:MET:HG2	8:H:2:LEU:O	2.09	0.52
1:A:342:C:H2'	1:A:343:U:O4'	2.10	0.52
1:A:953:G:H2'	1:A:954:G:O4'	2.09	0.52
2:B:7:VAL:N	2:B:8:LYS:HZ2	2.08	0.52
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.24	0.52
1:A:922:G:C2	1:A:1396:A:C6	2.98	0.52
1:A:1465:C:H2'	1:A:1466:C:O4'	2.09	0.52
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.24	0.52
6:F:62:TRP:CD1	18:R:35:ARG:CZ	2.93	0.52
8:H:87:SER:HA	8:H:93:VAL:HG13	1.92	0.52
14:N:40:CYS:SG	14:N:43:CYS:N	2.67	0.52
17:Q:4:LYS:HG3	17:Q:5:VAL:N	2.24	0.52
1:A:159:G:H21	1:A:161:A:H8	1.57	0.52
1:A:284:G:H2'	1:A:285:G:H8	1.74	0.52
1:A:344:A:H4'	1:A:345:C:OP2	2.09	0.52
1:A:421:U:O4	3:C:127:ARG:NH2	2.43	0.52
1:A:502:G:H2'	1:A:503:C:O4'	2.09	0.52
1:A:986:A:O2'	19:S:55:LYS:O	2.27	0.52
1:A:1181:G:O2'	1:A:1182:G:O5'	2.21	0.52
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.91	0.52
2:B:133:LYS:H	2:B:133:LYS:HZ3	1.56	0.52
3:C:19:GLU:N	14:N:51:GLY:O	2.43	0.52
4:D:31:CYS:C	4:D:33:MET:H	2.11	0.52
4:D:121:VAL:O	4:D:134:ASP:HA	2.10	0.52
1:A:1112:C:H42	3:C:178:LEU:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:A:H4'	1:A:1202:G:H5''	1.92	0.52
1:A:1342:C:H2'	1:A:1343:G:C8	2.44	0.52
1:A:1399:C:C2	1:A:1401:G:C5	2.98	0.52
2:B:15:VAL:HG11	2:B:213:LEU:HD22	1.92	0.52
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.92	0.52
4:D:190:ASP:HB3	4:D:193:ASP:HB2	1.91	0.52
8:H:46:LYS:HG2	8:H:64:LYS:HG3	1.92	0.52
12:L:86:ARG:HH11	12:L:86:ARG:HG2	1.74	0.52
20:T:39:LYS:HG2	20:T:55:ILE:HG21	1.92	0.52
1:A:79:G:C6	1:A:80:G:N7	2.78	0.51
1:A:183:G:H21	1:A:223:U:HO2'	1.57	0.51
1:A:1053:G:HO2'	1:A:1199:U:H5	1.58	0.51
1:A:1078:U:H5''	1:A:1079:G:OP2	2.10	0.51
1:A:1141:C:H2'	1:A:1142:G:C8	2.43	0.51
1:A:1424:C:H2'	1:A:1425:U:H6	1.74	0.51
3:C:11:ARG:NH1	3:C:178:LEU:HA	2.24	0.51
3:C:24:ALA:HB3	3:C:29:TYR:CD1	2.45	0.51
13:M:19:LEU:HD11	13:M:56:LEU:HD11	1.91	0.51
19:S:30:LEU:HD22	19:S:48:THR:HB	1.92	0.51
20:T:81:LYS:O	20:T:85:MET:HG3	2.10	0.51
1:A:438:G:H4'	4:D:123:HIS:CD2	2.46	0.51
1:A:689:C:O2'	1:A:705:U:O2'	2.24	0.51
1:A:1484:C:H2'	1:A:1485:U:C6	2.45	0.51
2:B:31:TYR:N	2:B:31:TYR:HD2	2.08	0.51
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.91	0.51
6:F:28:ARG:O	6:F:32:ASN:HB2	2.10	0.51
6:F:98:LEU:HB2	6:F:101:ALA:HB2	1.92	0.51
1:A:677:U:H2'	1:A:678:U:H6	1.76	0.51
1:A:853:G:O2'	1:A:854:G:H5'	2.10	0.51
1:A:1382:C:H2'	1:A:1383:C:C6	2.45	0.51
5:E:110:LEU:HD13	5:E:118:ILE:HD13	1.92	0.51
12:L:111:LYS:H	12:L:111:LYS:HZ2	1.56	0.51
1:A:1255:G:C6	1:A:1279:A:N7	2.78	0.51
1:A:1415:G:H1	1:A:1485:U:H3	1.58	0.51
4:D:148:VAL:HG12	4:D:153:ARG:NH1	2.24	0.51
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.44	0.51
9:I:10:ARG:HE	9:I:11:LYS:HG3	1.76	0.51
12:L:25:PRO:C	12:L:27:LEU:HB2	2.30	0.51
21:U:5:ASP:O	21:U:11:GLY:HA3	2.09	0.51
1:A:935:A:H2'	1:A:936:C:O4'	2.10	0.51
1:A:1065:U:H5''	1:A:1190:G:H22	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:C:H2'	1:A:1343:G:H8	1.74	0.51
1:A:1490:U:O2'	1:A:1491:G:H5'	2.10	0.51
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.93	0.51
4:D:8:VAL:HG11	4:D:21:LEU:HB3	1.91	0.51
15:O:55:GLY:O	15:O:59:MET:HG2	2.10	0.51
1:A:1181:G:N3	1:A:1182:G:N1	2.59	0.51
19:S:64:GLU:HG3	19:S:65:ASN:H	1.76	0.51
1:A:183:G:N2	1:A:223:U:O2'	2.31	0.51
1:A:1411:C:H2'	1:A:1412:C:C6	2.46	0.51
12:L:46:LYS:HG3	12:L:92:OTD:O	2.10	0.51
18:R:21:LYS:HE3	18:R:54:ARG:O	2.11	0.51
1:A:924:C:O2'	1:A:1502:A:N6	2.43	0.51
1:A:1181:G:C2	1:A:1182:G:N1	2.79	0.51
1:A:1265:G:H1	1:A:1270:C:H42	1.57	0.51
1:A:539:A:H2'	1:A:540:G:H8	1.75	0.51
1:A:736:C:H2'	1:A:737:A:C8	2.46	0.51
1:A:858:G:O6	1:A:869:G:C8	2.63	0.51
1:A:1242:C:H42	1:A:1295:G:H1	1.59	0.51
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	2.11	0.51
8:H:43:GLY:O	8:H:64:LYS:NZ	2.41	0.51
1:A:98:U:H2'	1:A:99:C:C6	2.46	0.51
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.46	0.51
19:S:74:PHE:CD1	19:S:74:PHE:N	2.79	0.51
1:A:1096:C:H2'	1:A:1097:C:H6	1.76	0.50
1:A:1101:A:H4'	1:A:1102:A:O5'	2.10	0.50
1:A:1157:A:N7	1:A:1180:A:N6	2.59	0.50
2:B:157:ARG:HG3	2:B:158:LEU:O	2.11	0.50
3:C:3:ASN:N	3:C:3:ASN:OD1	2.42	0.50
3:C:180:ALA:HB3	3:C:182:ILE:HG13	1.92	0.50
1:A:113:G:H2'	1:A:114:U:C6	2.47	0.50
1:A:660:G:C2	1:A:746:A:C2	3.00	0.50
1:A:1152:A:H2'	1:A:1153:C:O4'	2.11	0.50
1:A:1171:G:H2'	1:A:1172:C:C6	2.46	0.50
2:B:21:ARG:HA	2:B:39:ILE:HA	1.94	0.50
3:C:46:GLU:OE1	3:C:87:LEU:HD22	2.11	0.50
10:J:92:THR:C	10:J:94:VAL:H	2.14	0.50
15:O:18:PHE:CE1	15:O:21:ASP:HB2	2.46	0.50
15:O:56:LEU:C	15:O:56:LEU:HD13	2.32	0.50
20:T:45:GLN:HG2	20:T:91:LEU:HD11	1.93	0.50
1:A:131:C:H2'	1:A:132:C:C6	2.46	0.50
1:A:1328:C:OP1	21:U:21:TYR:OH	2.17	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.93	0.50
7:G:50:ILE:HG21	7:G:58:PRO:HA	1.93	0.50
1:A:264:U:H4'	17:Q:63:ARG:HD3	1.94	0.50
1:A:448:A:C4	1:A:487:A:C2	3.00	0.50
1:A:566:G:H4'	1:A:567:G:OP1	2.11	0.50
1:A:744:C:H4'	1:A:852:G:O2'	2.11	0.50
1:A:927:G:H1	1:A:1390:U:H3	1.59	0.50
1:A:1404:5MC:HN41	1:A:1497:G:H1	1.60	0.50
9:I:113:LYS:H	9:I:119:ALA:HA	1.77	0.50
10:J:40:LEU:HB2	10:J:69:ASN:O	2.11	0.50
1:A:243:A:C2	1:A:246:A:C8	2.99	0.50
1:A:926:G:N2	1:A:1542:U:OP1	2.45	0.50
1:A:1241:G:H2'	1:A:1242:C:H6	1.76	0.50
1:A:1330:U:H2'	1:A:1331:G:H5'	1.94	0.50
1:A:1525:G:H2'	1:A:1526:G:O4'	2.11	0.50
4:D:57:ARG:HA	4:D:202:LEU:HD12	1.93	0.50
4:D:206:PHE:HD2	4:D:207:TYR:CE2	2.30	0.50
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.47	0.50
1:A:448:A:OP2	1:A:485:G:N2	2.42	0.50
1:A:895:G:H2'	1:A:896:C:H6	1.76	0.50
1:A:1240:U:C2	7:G:32:ARG:HD2	2.46	0.50
1:A:1296:C:H3'	1:A:1297:C:H6	1.76	0.50
1:A:1391:U:H2'	1:A:1392:G:C8	2.47	0.50
2:B:19:HIS:CE1	2:B:205:ASP:H	2.29	0.50
8:H:134:ILE:HD12	8:H:134:ILE:H	1.77	0.50
20:T:53:LEU:HD12	20:T:102:GLY:H	1.76	0.50
20:T:71:THR:O	20:T:72:LEU:HD23	2.12	0.50
1:A:190(C):C:H2'	1:A:190(D):U:O4'	2.12	0.50
1:A:190(L):U:H3	20:T:105:SER:HB3	1.77	0.50
1:A:619:U:N3	4:D:134:ASP:OD2	2.38	0.50
1:A:981:U:H3'	1:A:982:U:H6	1.77	0.50
3:C:91:LEU:O	3:C:95:THR:HG22	2.11	0.50
4:D:22:LYS:HB2	4:D:26:CYS:HB2	1.94	0.50
9:I:48:GLU:N	9:I:49:PRO:HD2	2.27	0.50
12:L:59:ARG:NH2	12:L:65:GLU:HG2	2.26	0.50
15:O:74:ASP:HB3	15:O:77:ARG:HG3	1.94	0.50
1:A:627:G:H2'	1:A:628:G:C8	2.47	0.50
1:A:784:C:H2'	1:A:785:G:O4'	2.11	0.50
1:A:794:A:C5	1:A:795:C:C4	2.99	0.50
1:A:1201:A:H4'	1:A:1202:G:O5'	2.11	0.50
1:A:1232:U:OP1	9:I:126:SER:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:HIS:HB2	2:B:210:SER:HB3	1.93	0.50
3:C:83:ARG:O	3:C:87:LEU:HG	2.12	0.50
5:E:122:GLU:OE1	5:E:131:ILE:HG13	2.12	0.50
10:J:42:THR:HB	10:J:68:HIS:HB3	1.94	0.50
11:K:59:TYR:CE2	11:K:63:LEU:HD11	2.47	0.50
18:R:50:ILE:HG12	18:R:70:ILE:HD13	1.93	0.50
19:S:49:ILE:HB	19:S:60:VAL:HG23	1.93	0.50
1:A:279:A:OP1	1:A:280:C:O2'	2.23	0.50
1:A:665:A:C2	1:A:732:C:C2	3.00	0.50
1:A:812:C:OP1	1:A:903:G:H1'	2.12	0.50
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.93	0.50
10:J:62:HIS:O	14:N:59:ALA:HB3	2.12	0.50
1:A:130:A:O2'	1:A:131:C:H5''	2.12	0.49
1:A:376:G:H5''	16:P:5:ARG:HD2	1.93	0.49
1:A:945:G:C2	1:A:1337:G:C2	3.00	0.49
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.77	0.49
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.76	0.49
13:M:82:MET:CE	13:M:93:ARG:HH22	2.25	0.49
13:M:107:ALA:HB3	13:M:111:LYS:HE3	1.95	0.49
1:A:1064:G:H1'	1:A:1190:G:N2	2.27	0.49
1:A:1355:G:H2'	1:A:1356:G:H8	1.76	0.49
4:D:107:ARG:HD2	4:D:173:TRP:HZ2	1.76	0.49
6:F:33:TYR:CG	6:F:75:LEU:HD23	2.47	0.49
11:K:98:LEU:O	11:K:101:SER:OG	2.17	0.49
17:Q:81:ARG:HE	17:Q:84:LEU:CD1	2.22	0.49
20:T:84:LEU:HA	20:T:87:LYS:HE2	1.94	0.49
1:A:393:A:H2'	1:A:394:G:H8	1.78	0.49
1:A:672:U:O2'	1:A:673:G:H5'	2.12	0.49
7:G:28:ASN:O	7:G:31:MET:HB3	2.12	0.49
10:J:7:LYS:HA	10:J:71:LEU:HD11	1.95	0.49
13:M:23:TYR:HE2	13:M:70:LEU:HD12	1.73	0.49
13:M:97:PRO:HA	13:M:110:ARG:HH11	1.77	0.49
17:Q:22:LEU:HD12	17:Q:40:LYS:O	2.13	0.49
1:A:1490:U:H2'	1:A:1491:G:C8	2.24	0.49
2:B:189:ASP:N	2:B:189:ASP:OD1	2.45	0.49
8:H:104:ARG:HD2	8:H:138:TRP:CG	2.48	0.49
8:H:118:VAL:O	8:H:119:LEU:HD23	2.12	0.49
12:L:90:VAL:HG21	12:L:93:LEU:HD12	1.93	0.49
1:A:410:G:N1	1:A:431:A:OP2	2.40	0.49
1:A:714:G:H2'	1:A:715:A:C8	2.48	0.49
1:A:1003:G:H2'	1:A:1003(A):G:H5''	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:C:H2'	1:A:1164:G:C8	2.47	0.49
2:B:16:HIS:HB3	2:B:210:SER:HB3	1.94	0.49
9:I:103:THR:HG22	9:I:104:ARG:O	2.13	0.49
16:P:74:LEU:O	16:P:79:VAL:HG23	2.13	0.49
17:Q:92:ARG:HB3	17:Q:92:ARG:NH1	2.28	0.49
1:A:517:G:N1	1:A:533:A:OP2	2.34	0.49
1:A:767:A:H2'	1:A:768:A:O4'	2.13	0.49
1:A:793:U:H4'	1:A:794:A:OP2	2.12	0.49
1:A:1202:G:H1'	14:N:42:ILE:HD12	1.93	0.49
1:A:1443:G:H5'	1:A:1446:A:H5''	1.93	0.49
2:B:131:PRO:HB2	2:B:134:GLU:HG3	1.95	0.49
3:C:91:LEU:HD23	3:C:92:ALA:N	2.28	0.49
7:G:146:GLU:HA	7:G:149:ARG:HB2	1.95	0.49
9:I:48:GLU:HB3	9:I:101:PHE:CZ	2.47	0.49
16:P:28:ARG:HB3	16:P:29:ASP:OD2	2.12	0.49
16:P:53:VAL:O	16:P:55:ARG:N	2.46	0.49
1:A:187:C:OP1	20:T:82:SER:OG	2.26	0.49
1:A:256:U:H2'	1:A:257:G:C8	2.48	0.49
1:A:564:C:O2'	8:H:91:ARG:NH2	2.42	0.49
1:A:1228:C:H5'	13:M:115:LYS:O	2.13	0.49
1:A:1309:G:O2'	13:M:74:VAL:HG23	2.12	0.49
9:I:118:LYS:C	9:I:120:ARG:H	2.15	0.49
10:J:24:VAL:HG23	10:J:34:VAL:HG11	1.93	0.49
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.94	0.49
1:A:420:U:H3'	1:A:422:C:N4	2.27	0.49
1:A:781:A:C5	1:A:802:A:C2	3.00	0.49
1:A:1124:G:H2'	1:A:1145:C:H41	1.77	0.49
1:A:1136:U:H5''	1:A:1137:C:C4	2.48	0.49
1:A:1279:A:OP1	10:J:7:LYS:NZ	2.40	0.49
3:C:19:GLU:OE1	3:C:54:ARG:NH2	2.45	0.49
5:E:145:LYS:O	5:E:148:VAL:HG23	2.13	0.49
8:H:36:LEU:O	8:H:37:ARG:C	2.51	0.49
9:I:19:LEU:HD11	9:I:59:PHE:HB3	1.95	0.49
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.94	0.49
17:Q:67:LYS:O	17:Q:69:LYS:N	2.46	0.49
1:A:192:U:O4'	20:T:103:GLY:HA2	2.13	0.49
1:A:229:U:O2'	1:A:230:G:H5'	2.13	0.49
1:A:803:G:C6	1:A:804:U:C4	3.00	0.49
1:A:815:A:N3	1:A:1527:C:O2'	2.42	0.49
1:A:1027:C:H2'	1:A:1034:G:H22	1.76	0.49
1:A:1425:U:H3	1:A:1475:G:H1	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.93	0.49
4:D:179:GLU:OE2	4:D:179:GLU:N	2.34	0.49
5:E:80:ILE:HD11	5:E:138:ALA:HB1	1.95	0.49
9:I:49:PRO:HD3	9:I:101:PHE:CE2	2.48	0.49
15:O:78:TYR:O	15:O:81:LEU:N	2.46	0.49
1:A:45:U:H2'	1:A:46:G:C8	2.47	0.49
1:A:113:G:H2'	1:A:114:U:H6	1.78	0.49
1:A:538:G:H5''	12:L:115:LYS:HG3	1.94	0.49
1:A:927:G:H4'	1:A:1503:A:C8	2.48	0.49
1:A:967:5MC:O2'	9:I:128:ARG:NH1	2.46	0.49
1:A:1486:G:C2	1:A:1487:G:C4	3.01	0.49
2:B:175:ARG:HG3	2:B:175:ARG:NH1	2.27	0.49
10:J:5:ARG:HB3	10:J:99:LYS:O	2.13	0.49
10:J:12:ASP:O	10:J:15:THR:HB	2.13	0.49
11:K:40:ILE:HG22	11:K:41:THR:HG22	1.94	0.49
11:K:117:ASN:OD1	11:K:117:ASN:N	2.43	0.49
16:P:53:VAL:O	16:P:56:ALA:N	2.46	0.49
1:A:243:A:H2	1:A:245:C:H2'	1.78	0.48
1:A:279:A:H5'	1:A:279:A:C8	2.48	0.48
1:A:518:C:H1'	12:L:50:SER:HB3	1.95	0.48
1:A:1149:C:O2'	1:A:1280:A:N1	2.42	0.48
8:H:9:MET:HE1	8:H:35:ILE:HG21	1.94	0.48
9:I:11:LYS:HZ2	9:I:11:LYS:HB3	1.77	0.48
12:L:41:ARG:NH2	12:L:43:VAL:HG12	2.28	0.48
12:L:76:ASN:ND2	12:L:77:LEU:HD23	2.28	0.48
21:U:12:LYS:HG3	21:U:17:THR:OG1	2.12	0.48
1:A:75:G:C6	1:A:76:C:C4	3.01	0.48
1:A:950:U:H2'	1:A:951:G:C8	2.48	0.48
1:A:97:G:H2'	1:A:98:U:O4'	2.14	0.48
1:A:429:U:P	4:D:36:ARG:HH12	2.36	0.48
1:A:603:U:H3	1:A:635:G:H1	1.61	0.48
1:A:794:A:H2'	1:A:795:C:C6	2.48	0.48
1:A:824:C:H2'	1:A:825:G:C8	2.48	0.48
1:A:1227:A:N7	19:S:81:ARG:NH2	2.57	0.48
1:A:1358:U:O3'	14:N:35:ARG:HD2	2.13	0.48
2:B:135:GLN:O	2:B:139:LYS:HB2	2.13	0.48
3:C:81:GLY:O	3:C:84:ILE:HG22	2.13	0.48
5:E:103:GLY:HA3	5:E:106:PRO:HD2	1.95	0.48
10:J:42:THR:HB	10:J:68:HIS:HA	1.95	0.48
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.56	0.48
18:R:55:ARG:HB3	18:R:55:ARG:HH11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:G:C6	1:A:812:C:C2	3.01	0.48
1:A:860:A:N6	1:A:861:G:C2	2.82	0.48
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.95	0.48
11:K:33:THR:HA	11:K:39:PRO:HA	1.96	0.48
12:L:48:PRO:HD2	12:L:92:0TD:CSB	2.43	0.48
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.96	0.48
1:A:77:G:H2'	1:A:78:G:C8	2.48	0.48
1:A:109:A:C6	1:A:326:G:C6	3.01	0.48
1:A:247:G:OP2	17:Q:99:SER:HB2	2.13	0.48
1:A:463:A:H2'	1:A:474:G:O4'	2.14	0.48
1:A:950:U:H2'	1:A:951:G:H8	1.78	0.48
1:A:1148:U:H4'	9:I:14:VAL:HG11	1.95	0.48
2:B:31:TYR:N	2:B:31:TYR:CD2	2.80	0.48
3:C:39:ILE:O	3:C:43:LEU:HB2	2.13	0.48
6:F:4:TYR:CE2	6:F:72:VAL:HG21	2.48	0.48
11:K:98:LEU:HD23	11:K:98:LEU:HA	1.56	0.48
1:A:11:G:C5	1:A:12:U:C5	3.02	0.48
1:A:90:U:O2'	1:A:91:C:O5'	2.24	0.48
1:A:255:G:C2	1:A:272:C:C2	3.02	0.48
1:A:984:C:H2'	1:A:985:C:C6	2.49	0.48
1:A:1010:G:H1	1:A:1019:C:H42	1.61	0.48
1:A:1026:G:H3'	1:A:1027:C:C6	2.48	0.48
1:A:1310:G:N2	1:A:1328:C:N3	2.61	0.48
4:D:111:ALA:HB3	4:D:117:ALA:HB2	1.96	0.48
5:E:83:GLU:HG3	5:E:88:LYS:HB2	1.94	0.48
13:M:56:LEU:O	13:M:60:VAL:HG23	2.12	0.48
1:A:1086:U:H3	1:A:1099:G:H22	1.61	0.48
1:A:1310:G:P	13:M:77:ASN:HD21	2.36	0.48
1:A:1416:G:C2'	1:A:1417:G:H5'	2.43	0.48
1:A:1493:A:O3'	1:A:1494:G:H8	1.97	0.48
3:C:88:ARG:O	3:C:91:LEU:HB3	2.14	0.48
1:A:255:G:P	17:Q:69:LYS:HZ1	2.37	0.48
1:A:571:U:H5''	1:A:572:A:OP2	2.14	0.48
7:G:84:ASN:O	7:G:85:TYR:HD2	1.97	0.48
9:I:97:LYS:HD2	9:I:102:LEU:HD11	1.95	0.48
12:L:113:ARG:NH2	12:L:120:TYR:HE1	2.12	0.48
18:R:38:GLU:HA	18:R:41:LYS:HE3	1.96	0.48
1:A:176:C:H2'	1:A:177:C:H6	1.79	0.48
1:A:671:G:H5'	6:F:77:ARG:HH21	1.78	0.48
1:A:828:A:C8	1:A:828:A:H3'	2.49	0.48
1:A:985:C:N4	1:A:1220:G:H1	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:G:OP2	14:N:3:ARG:NH1	2.47	0.48
1:A:1373:G:H5''	7:G:36:LYS:HE2	1.95	0.48
2:B:80:ILE:CD1	2:B:212:GLN:HG2	2.43	0.48
3:C:116:VAL:O	3:C:120:VAL:HG23	2.13	0.48
8:H:6:ILE:HG13	8:H:31:PHE:CE2	2.49	0.48
9:I:104:ARG:CD	9:I:105:ASP:H	2.27	0.48
11:K:73:MET:CG	11:K:103:LEU:HD21	2.44	0.48
1:A:17:U:H2'	1:A:18:C:C6	2.48	0.48
1:A:501:C:H2'	1:A:502:G:C8	2.49	0.48
1:A:1228:C:H4'	13:M:116:THR:HA	1.95	0.48
9:I:51:ARG:HD3	9:I:56:LEU:HD21	1.95	0.48
16:P:18:ARG:O	16:P:20:VAL:HG13	2.13	0.48
1:A:164:U:H2'	1:A:165:C:C6	2.49	0.47
1:A:190(D):U:H6	1:A:190(D):U:O5'	1.97	0.47
1:A:1226:C:OP2	13:M:103:THR:HG21	2.13	0.47
1:A:1438:G:H1	1:A:1463:C:H42	1.62	0.47
3:C:125:GLU:O	3:C:127:ARG:HG3	2.14	0.47
8:H:25:ASP:OD1	8:H:25:ASP:N	2.47	0.47
10:J:6:ILE:HB	10:J:72:VAL:HB	1.96	0.47
12:L:48:PRO:HD2	12:L:92:OTD:H8	1.94	0.47
1:A:77:G:C4	1:A:93:G:N2	2.83	0.47
1:A:95:U:O2'	1:A:96:G:H5'	2.15	0.47
1:A:902:G:H2'	1:A:903:G:C8	2.44	0.47
1:A:983:A:O2'	1:A:1050:G:OP2	2.32	0.47
1:A:1267:C:O2	21:U:20:LYS:HD2	2.14	0.47
2:B:180:LEU:HB2	2:B:182:ILE:HG13	1.96	0.47
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.95	0.47
17:Q:15:MET:HB3	17:Q:18:THR:HB	1.95	0.47
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.49	0.47
1:A:349:A:H2'	1:A:350:G:H5''	1.97	0.47
1:A:809:G:C6	1:A:810:C:C5	3.03	0.47
1:A:1006:C:OP1	1:A:1037:C:O2'	2.32	0.47
1:A:1372:U:H5''	9:I:71:SER:HB3	1.96	0.47
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.50	0.47
5:E:18:ARG:HE	5:E:18:ARG:HB3	1.40	0.47
5:E:144:THR:O	5:E:148:VAL:HG22	2.14	0.47
6:F:76:ALA:O	6:F:80:ARG:HD3	2.13	0.47
13:M:55:ARG:O	13:M:58:GLU:HB2	2.14	0.47
1:A:562:C:N3	12:L:16:GLU:HG2	2.29	0.47
1:A:779:C:H2'	1:A:780:A:O4'	2.13	0.47
1:A:1311:G:C2	1:A:1327:C:N3	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1389:C:H2'	1:A:1390:U:O4'	2.14	0.47
1:A:1454:G:O2'	1:A:1455:G:H5'	2.14	0.47
3:C:130:VAL:O	3:C:134:ILE:HG13	2.13	0.47
5:E:43:LEU:HD23	5:E:43:LEU:HA	1.64	0.47
7:G:16:LEU:HD11	9:I:42:ARG:HG3	1.96	0.47
7:G:115:ARG:HB3	7:G:118:VAL:HG23	1.96	0.47
13:M:35:GLU:HG3	13:M:36:LYS:N	2.28	0.47
1:A:35:G:H21	12:L:118:SER:HB3	1.80	0.47
1:A:216:G:H2'	1:A:217:C:C6	2.49	0.47
1:A:451:A:N7	1:A:481:G:N1	2.62	0.47
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.49	0.47
1:A:1532:U:H2'	1:A:1533:C:H5''	1.96	0.47
7:G:76:ARG:HB2	7:G:89:MET:SD	2.55	0.47
11:K:124:LYS:HG3	11:K:125:PHE:N	2.29	0.47
1:A:109:A:C4	1:A:327:A:C2	3.02	0.47
1:A:345:C:OP2	1:A:345:C:H6	1.97	0.47
1:A:509:A:H5'	4:D:55:ALA:HB2	1.96	0.47
1:A:665:A:N3	1:A:732:C:H2'	2.29	0.47
1:A:974:A:C8	14:N:31:ARG:HD2	2.49	0.47
1:A:1309:G:H5'	13:M:78:ILE:HD11	1.97	0.47
2:B:105:PHE:O	2:B:108:ILE:N	2.47	0.47
2:B:131:PRO:HD2	2:B:134:GLU:OE2	2.15	0.47
7:G:108:ALA:O	7:G:119:ARG:HB3	2.15	0.47
16:P:40:ASP:HB3	16:P:48:TRP:HB2	1.96	0.47
17:Q:21:VAL:HG23	17:Q:42:TYR:HB2	1.95	0.47
1:A:74:C:C4	1:A:75:G:N7	2.82	0.47
1:A:116:A:H2'	1:A:117:G:C8	2.49	0.47
1:A:434:U:H2'	1:A:435:C:C6	2.49	0.47
1:A:491:G:H2'	1:A:492:G:H8	1.78	0.47
1:A:1245:A:H61	1:A:1292:U:H3	1.63	0.47
1:A:1410:G:H1'	1:A:1491:G:H22	1.79	0.47
1:A:1416:G:H2'	1:A:1417:G:H5'	1.96	0.47
4:D:194:LEU:HA	4:D:194:LEU:HD13	1.66	0.47
8:H:82:HIS:CE1	8:H:138:TRP:CZ2	3.03	0.47
8:H:124:ALA:O	8:H:128:GLY:N	2.27	0.47
9:I:46:ALA:HB1	9:I:77:ILE:CG2	2.45	0.47
9:I:89:ASN:HB2	9:I:92:TYR:CD1	2.50	0.47
11:K:19:ALA:HB2	11:K:80:VAL:HG11	1.96	0.47
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.80	0.47
17:Q:38:ARG:HD3	17:Q:38:ARG:HA	1.46	0.47
20:T:83:ARG:NH2	24:T:201:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:C:H2'	1:A:177:C:C6	2.49	0.47
1:A:1461:G:H2'	1:A:1462:G:C8	2.50	0.47
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.97	0.47
2:B:72:GLY:HA3	2:B:165:VAL:HB	1.97	0.47
5:E:90:VAL:O	5:E:120:THR:HA	2.15	0.47
11:K:115:PRO:C	11:K:117:ASN:H	2.18	0.47
12:L:47:LYS:HD2	12:L:48:PRO:HD3	1.96	0.47
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.96	0.47
1:A:19:C:P	5:E:127:ASN:HD22	2.38	0.47
1:A:92:C:O2	1:A:93:G:C8	2.68	0.47
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.47
1:A:1059:C:H2'	1:A:1060:C:C6	2.49	0.47
1:A:1107:C:OP1	3:C:172:ARG:NH1	2.47	0.47
2:B:9:GLU:OE2	2:B:11:LEU:N	2.47	0.47
10:J:99:LYS:HD3	10:J:100:THR:H	1.79	0.47
13:M:11:ARG:HD2	13:M:12:ASN:H	1.79	0.47
14:N:37:PHE:C	14:N:39:LEU:H	2.17	0.47
16:P:45:THR:O	16:P:48:TRP:HD1	1.98	0.47
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.97	0.47
1:A:227:G:H2'	1:A:228:A:O4'	2.15	0.47
1:A:897:C:H42	1:A:902:G:H1	1.63	0.47
1:A:1450:U:O2'	1:A:1451:A:H2'	2.14	0.47
4:D:119:GLN:HG3	4:D:123:HIS:CE1	2.50	0.47
4:D:174:LEU:C	4:D:186:LEU:HD21	2.35	0.47
7:G:143:ARG:O	7:G:147:ALA:HB2	2.14	0.47
1:A:259:G:C2	1:A:260:G:C4	3.03	0.46
1:A:457:C:H2'	1:A:458:C:H6	1.80	0.46
1:A:926:G:H2'	1:A:1505:G:N3	2.29	0.46
1:A:1505:G:C8	1:A:1505:G:H3'	2.49	0.46
2:B:180:LEU:O	2:B:181:PHE:HB2	2.15	0.46
12:L:25:PRO:HA	12:L:27:LEU:HD13	1.98	0.46
16:P:17:TYR:HB2	16:P:39:TYR:HB3	1.96	0.46
1:A:7:G:H5'	1:A:298:A:O4'	2.14	0.46
1:A:95:U:H2'	1:A:96:G:C8	2.49	0.46
1:A:892:A:H2'	1:A:893:C:C6	2.50	0.46
2:B:74:LYS:HZ1	2:B:76:GLN:HG2	1.80	0.46
3:C:83:ARG:HG2	3:C:87:LEU:HD21	1.98	0.46
8:H:104:ARG:NH1	8:H:138:TRP:CE2	2.83	0.46
9:I:5:TYR:O	9:I:84:ALA:HA	2.16	0.46
9:I:53:VAL:HG21	9:I:85:LEU:HG	1.98	0.46
1:A:230:G:H2'	1:A:231:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:C:H2'	1:A:652:U:C6	2.49	0.46
1:A:1022:G:N2	1:A:1023:G:N7	2.55	0.46
1:A:1057:G:H2'	1:A:1058:G:O4'	2.16	0.46
1:A:1144:G:N2	1:A:1145:C:O2	2.48	0.46
1:A:1480:G:C2	1:A:1481:U:C2	3.03	0.46
3:C:175:LEU:HD11	3:C:201:TYR:CE2	2.50	0.46
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.50	0.46
9:I:2:GLU:HG3	9:I:3:GLN:N	2.31	0.46
10:J:36:GLY:O	10:J:38:ILE:HG13	2.15	0.46
16:P:6:LEU:HD12	16:P:6:LEU:N	2.30	0.46
20:T:10:LEU:HD22	20:T:10:LEU:HA	1.47	0.46
1:A:35:G:C6	1:A:36:C:N4	2.83	0.46
1:A:827:U:H5''	1:A:828:A:OP2	2.14	0.46
1:A:1223:C:P	19:S:78:ARG:HH21	2.38	0.46
1:A:1398:A:H5''	1:A:1401:G:H4'	1.97	0.46
2:B:80:ILE:HG21	2:B:211:ILE:HG22	1.96	0.46
2:B:131:PRO:O	2:B:134:GLU:HB2	2.15	0.46
6:F:14:LEU:HD22	6:F:14:LEU:HA	1.73	0.46
7:G:53:LYS:HE3	7:G:125:MET:HE2	1.96	0.46
9:I:75:ASP:O	9:I:78:LYS:HG2	2.15	0.46
11:K:58:PRO:O	11:K:61:ALA:HB3	2.15	0.46
12:L:58:VAL:HG12	12:L:59:ARG:O	2.15	0.46
15:O:2:PRO:O	15:O:3:ILE:HG13	2.15	0.46
1:A:103:C:O2'	1:A:172:A:N1	2.45	0.46
1:A:446:G:H3'	1:A:447:G:H8	1.80	0.46
1:A:1008:C:H42	1:A:1021:G:H1	1.64	0.46
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:H2	2.45	0.46
3:C:167:TRP:CG	3:C:168:ALA:N	2.84	0.46
4:D:78:LEU:HD11	4:D:96:LEU:HB3	1.98	0.46
5:E:90:VAL:C	5:E:91:LEU:HD23	2.35	0.46
8:H:71:GLY:HA3	8:H:72:PRO:HD2	1.67	0.46
13:M:91:ARG:HH22	13:M:103:THR:HG21	1.81	0.46
19:S:31:ILE:HG21	19:S:49:ILE:HG23	1.97	0.46
1:A:54:C:O2'	1:A:55:A:H5''	2.16	0.46
1:A:284:G:H2'	1:A:285:G:C8	2.50	0.46
1:A:474:G:H2'	1:A:475:G:O4'	2.15	0.46
1:A:819:A:H4'	1:A:820:U:OP2	2.15	0.46
1:A:1304:G:C6	1:A:1305:G:N1	2.83	0.46
6:F:54:LYS:N	6:F:54:LYS:HD2	2.30	0.46
8:H:114:THR:N	8:H:117:GLY:O	2.42	0.46
19:S:11:VAL:HG12	19:S:15:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:G:H2'	1:A:217:C:H6	1.80	0.46
1:A:424:G:C2	1:A:425:G:C5	3.03	0.46
1:A:977:A:H2'	1:A:978:A:H5'	1.97	0.46
1:A:1297:C:O2'	1:A:1298:C:OP2	2.30	0.46
1:A:1502:A:H2'	1:A:1504:G:C8	2.50	0.46
8:H:26:VAL:HG23	8:H:27:PRO:HD2	1.97	0.46
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.61	0.46
11:K:21:ILE:HD12	11:K:95:ILE:HG12	1.98	0.46
1:A:15:G:H4'	5:E:24:ARG:NH2	2.30	0.46
1:A:276:G:O2'	17:Q:68:ARG:NH1	2.49	0.46
1:A:491:G:H2'	1:A:492:G:C8	2.50	0.46
1:A:636:U:H2'	1:A:637:G:C8	2.50	0.46
1:A:650:G:C5'	1:A:650:G:H8	2.29	0.46
1:A:792:A:H1'	1:A:793:U:OP2	2.16	0.46
1:A:921:U:H2'	1:A:922:G:O4'	2.16	0.46
1:A:948:C:H42	1:A:1233:G:H1	1.64	0.46
1:A:1172:C:H2'	1:A:1173:G:H8	1.80	0.46
1:A:1245:A:N1	1:A:1293:G:C2	2.84	0.46
1:A:1481:U:H2'	1:A:1482:G:O4'	2.15	0.46
4:D:21:LEU:HD12	4:D:21:LEU:HA	1.70	0.46
5:E:98:THR:O	5:E:101:ILE:HD11	2.15	0.46
5:E:121:LYS:HG2	5:E:123:LEU:HD23	1.97	0.46
7:G:49:ILE:O	7:G:53:LYS:HB2	2.16	0.46
9:I:99:LEU:HD22	9:I:99:LEU:H	1.81	0.46
10:J:99:LYS:CD	10:J:100:THR:H	2.29	0.46
20:T:91:LEU:HD22	20:T:91:LEU:HA	1.74	0.46
1:A:14:U:O2	1:A:16:A:C8	2.69	0.46
1:A:243:A:C2	1:A:245:C:H2'	2.51	0.46
1:A:509:A:C8	1:A:509:A:H3'	2.51	0.46
1:A:583:A:H2'	1:A:584:G:O4'	2.16	0.46
1:A:1321:C:O2'	19:S:78:ARG:NH1	2.49	0.46
1:A:1392:G:O2'	1:A:1393:U:H5'	2.16	0.46
2:B:144:ARG:NH1	2:B:148:TYR:OH	2.49	0.46
8:H:104:ARG:HD2	8:H:138:TRP:CD1	2.50	0.46
13:M:2:ALA:N	13:M:9:ILE:HG23	2.31	0.46
1:A:134:A:C6	1:A:135:C:N3	2.84	0.46
1:A:945:G:H2'	1:A:945:G:N3	2.31	0.46
1:A:1416:G:N2	1:A:1485:U:H1'	2.31	0.46
7:G:108:ALA:HB2	7:G:123:GLU:HG2	1.98	0.46
8:H:102:ARG:HG3	8:H:102:ARG:O	2.16	0.46
11:K:72:ALA:HB1	11:K:77:MET:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:G:H4'	16:P:81:ARG:CZ	2.46	0.45
1:A:1020:U:H2'	1:A:1021:G:H8	1.82	0.45
1:A:1418:A:H3'	1:A:1418:A:OP2	2.15	0.45
7:G:22:LEU:HD23	7:G:62:PHE:CZ	2.52	0.45
14:N:24:CYS:CB	14:N:40:CYS:HB3	2.45	0.45
19:S:19:VAL:HA	19:S:22:LEU:HB2	1.98	0.45
1:A:293:G:C6	1:A:294:U:C4	3.03	0.45
1:A:644:G:C5	1:A:645:C:C5	3.04	0.45
2:B:24:TRP:CG	2:B:25:ASN:N	2.84	0.45
3:C:10:PHE:CZ	3:C:178:LEU:HD12	2.51	0.45
3:C:40:ARG:HE	3:C:57:ILE:HD12	1.81	0.45
3:C:156:ARG:H	3:C:163:ALA:HA	1.81	0.45
4:D:111:ALA:HA	4:D:161:ASN:ND2	2.30	0.45
5:E:40:ARG:HG2	5:E:40:ARG:HH11	1.81	0.45
7:G:26:PHE:HD1	7:G:101:LEU:HD23	1.81	0.45
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	1.97	0.45
1:A:136:C:H2'	1:A:137:C:H6	1.82	0.45
1:A:666:G:H5'	1:A:726:C:H1'	1.97	0.45
1:A:836:G:C6	1:A:851:G:C6	3.04	0.45
2:B:74:LYS:HZ2	2:B:76:GLN:H	1.64	0.45
2:B:187:LEU:HD22	2:B:187:LEU:HA	1.40	0.45
3:C:51:GLY:O	3:C:71:ALA:N	2.39	0.45
4:D:113:SER:OG	4:D:114:ARG:N	2.49	0.45
8:H:102:ARG:HH11	8:H:105:ARG:HD3	1.82	0.45
10:J:18:ALA:O	10:J:22:LYS:HG3	2.16	0.45
15:O:4:THR:H	15:O:4:THR:HG1	1.46	0.45
16:P:53:VAL:O	16:P:54:GLU:C	2.53	0.45
16:P:58:TYR:O	16:P:61:SER:HB3	2.16	0.45
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.15	0.45
1:A:11:G:H2'	1:A:12:U:H6	1.80	0.45
1:A:27:G:H1	1:A:556:C:N4	2.15	0.45
1:A:882:C:O2'	1:A:883:C:H5'	2.17	0.45
1:A:1074:G:C4'	2:B:104:ASN:HB2	2.47	0.45
1:A:1148:U:H2'	1:A:1149:C:O4'	2.17	0.45
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.50	0.45
7:G:18:TYR:CD2	7:G:59:LEU:HD13	2.46	0.45
7:G:28:ASN:HA	7:G:31:MET:HE2	1.97	0.45
8:H:100:ILE:HA	8:H:101:PRO:HD3	1.50	0.45
9:I:105:ASP:OD1	9:I:107:ARG:HG3	2.17	0.45
14:N:8:GLU:O	14:N:12:ARG:N	2.50	0.45
20:T:41:ILE:HD12	20:T:41:ILE:HA	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:A:H2'	1:A:229:U:C6	2.51	0.45
1:A:376:G:N3	1:A:389:A:C2	2.85	0.45
1:A:447:G:H2'	1:A:485:G:N2	2.31	0.45
1:A:485:G:O2'	1:A:486:U:P	2.75	0.45
1:A:1001:A:N6	1:A:1041:A:H61	2.14	0.45
1:A:1088:G:C6	1:A:1089:G:C5	3.05	0.45
1:A:1096:C:H2'	1:A:1097:C:C6	2.51	0.45
1:A:1130:A:H4'	9:I:20:ARG:HH21	1.81	0.45
1:A:1368:G:OP2	9:I:112:LYS:NZ	2.33	0.45
2:B:74:LYS:NZ	2:B:76:GLN:H	2.15	0.45
12:L:120:TYR:N	12:L:120:TYR:CD2	2.84	0.45
14:N:54:PRO:O	14:N:56:VAL:HG23	2.16	0.45
15:O:53:HIS:O	15:O:56:LEU:HB3	2.16	0.45
17:Q:29:HIS:CE1	17:Q:32:TYR:H	2.33	0.45
1:A:563:A:H2'	1:A:567:G:C8	2.51	0.45
1:A:1181:G:HO2'	1:A:1182:G:P	2.36	0.45
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.99	0.45
2:B:48:MET:HA	2:B:51:LEU:HB2	1.97	0.45
2:B:95:GLN:NE2	2:B:147:LYS:HE3	2.31	0.45
9:I:89:ASN:HB3	9:I:91:ASP:OD1	2.16	0.45
11:K:18:ARG:HB3	11:K:20:TYR:CE1	2.51	0.45
18:R:25:THR:OG1	18:R:42:ARG:NH1	2.49	0.45
19:S:17:GLU:HA	19:S:20:LEU:HD23	1.98	0.45
1:A:118:U:H3'	1:A:288:A:H61	1.82	0.45
1:A:391:G:C6	1:A:392:G:C5	3.05	0.45
1:A:420:U:H3'	1:A:422:C:H41	1.81	0.45
1:A:1347:G:H1'	1:A:1348:U:H5	1.81	0.45
3:C:150:LYS:HG3	3:C:173:VAL:HG21	1.98	0.45
7:G:12:LEU:H	7:G:12:LEU:HG	1.60	0.45
7:G:86:GLN:HB2	7:G:148:ASN:HD22	1.81	0.45
7:G:152:ALA:HA	7:G:155:ARG:CZ	2.46	0.45
13:M:79:LYS:NZ	13:M:79:LYS:HB2	2.32	0.45
15:O:5:LYS:HB2	15:O:5:LYS:HE2	1.76	0.45
17:Q:62:SER:OG	17:Q:72:ARG:HG2	2.16	0.45
18:R:43:PHE:C	18:R:44:LEU:HD23	2.37	0.45
1:A:521:G:P	12:L:54:LYS:HE2	2.57	0.45
1:A:739:C:OP2	6:F:2:ARG:NH2	2.49	0.45
1:A:1171:G:H2'	1:A:1172:C:H6	1.81	0.45
1:A:1184:G:H2'	1:A:1185:G:H8	1.80	0.45
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.40	0.45
3:C:121:ALA:O	3:C:124:ILE:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:109:ILE:HG22	5:E:110:LEU:N	2.31	0.45
10:J:3:LYS:NZ	10:J:3:LYS:HB2	2.32	0.45
11:K:40:ILE:HG23	11:K:75:TYR:CD1	2.44	0.45
13:M:45:VAL:O	13:M:48:LEU:HD23	2.17	0.45
15:O:56:LEU:O	15:O:60:VAL:HG12	2.17	0.45
1:A:115:G:O2'	1:A:116:A:OP2	2.26	0.45
1:A:1028:C:N4	1:A:1033:G:H21	2.14	0.45
1:A:1064:G:H22	1:A:1190:G:H2'	1.79	0.45
2:B:217:ARG:HA	2:B:217:ARG:HD3	1.52	0.45
3:C:77:ILE:HG12	3:C:84:ILE:HD12	1.99	0.45
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.33	0.45
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.70	0.45
13:M:99:ARG:NH1	19:S:2:PRO:HG3	2.32	0.45
14:N:57:ARG:NH1	14:N:57:ARG:HB2	2.32	0.45
15:O:29:VAL:O	15:O:33:THR:HB	2.17	0.45
1:A:222:U:H2'	1:A:223:U:C6	2.51	0.45
1:A:959:A:O2'	1:A:984:C:O2'	2.32	0.45
1:A:1412:C:H2'	1:A:1413:A:H8	1.82	0.45
2:B:84:GLU:OE1	2:B:216:SER:HA	2.17	0.45
4:D:119:GLN:NE2	4:D:123:HIS:HE1	2.11	0.45
10:J:71:LEU:HD12	10:J:71:LEU:HA	1.80	0.45
1:A:76:C:N4	1:A:93:G:H1	2.16	0.44
1:A:122:G:C2	1:A:123:C:C2	3.04	0.44
1:A:411:A:C8	1:A:413:G:H1'	2.52	0.44
1:A:569:C:N4	1:A:881:G:H1	2.12	0.44
1:A:1236:A:H4'	1:A:1304:G:H4'	1.99	0.44
1:A:1278:U:H5''	1:A:1279:A:H5'	1.99	0.44
5:E:19:MET:SD	5:E:24:ARG:HB3	2.57	0.44
8:H:2:LEU:HA	8:H:2:LEU:HD23	1.46	0.44
15:O:12:ILE:HG23	15:O:27:VAL:HG11	1.99	0.44
19:S:30:LEU:HD13	19:S:48:THR:O	2.16	0.44
1:A:429:U:H1'	1:A:430:A:H5''	1.99	0.44
1:A:646:U:H2'	1:A:647:C:C6	2.52	0.44
1:A:1111:A:H2'	1:A:1112:C:O4'	2.16	0.44
1:A:1198:G:H2'	1:A:1199:U:C6	2.52	0.44
1:A:1260:C:O5'	1:A:1284:C:H4'	2.17	0.44
6:F:22:GLU:OE2	6:F:82:ARG:HG2	2.17	0.44
8:H:6:ILE:HG13	8:H:31:PHE:HE2	1.82	0.44
8:H:63:LEU:HD13	8:H:63:LEU:N	2.32	0.44
8:H:95:VAL:HG23	8:H:131:GLY:O	2.17	0.44
10:J:81:THR:O	10:J:85:LEU:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:47:THR:HG22	18:R:48:GLY:N	2.32	0.44
19:S:30:LEU:HB3	19:S:31:ILE:H	1.53	0.44
1:A:112:G:O2'	1:A:113:G:H5'	2.17	0.44
1:A:382:A:H2'	1:A:383:A:C8	2.52	0.44
1:A:684:A:N3	11:K:39:PRO:HD2	2.32	0.44
1:A:858:G:O6	1:A:869:G:N7	2.50	0.44
1:A:991:U:O2	1:A:993:G:H8	2.00	0.44
1:A:1003(A):G:N2	1:A:1006:C:H41	2.16	0.44
1:A:1057:G:C4	1:A:1058:G:C8	3.05	0.44
3:C:20:SER:OG	3:C:40:ARG:NH2	2.50	0.44
3:C:52:LEU:HD23	3:C:69:HIS:O	2.18	0.44
4:D:15:GLU:OE1	4:D:62:GLN:HB3	2.17	0.44
5:E:98:THR:HB	5:E:117:ASP:HB3	1.99	0.44
7:G:145:ALA:C	7:G:147:ALA:H	2.20	0.44
8:H:127:LEU:HD22	8:H:127:LEU:HA	1.77	0.44
13:M:39:ILE:CG2	13:M:40:ASN:N	2.80	0.44
1:A:20:U:H2'	1:A:21:G:H5'	1.99	0.44
1:A:78:G:N1	1:A:92:C:N4	2.65	0.44
1:A:455:C:O5'	1:A:455:C:H6	2.01	0.44
1:A:1225:A:H5''	13:M:103:THR:HG23	1.99	0.44
1:A:1476:G:H2'	1:A:1477:C:C6	2.53	0.44
3:C:88:ARG:HA	3:C:91:LEU:HB3	1.98	0.44
8:H:97:VAL:HG12	8:H:98:LYS:HZ2	1.81	0.44
10:J:63:PHE:HD2	14:N:57:ARG:O	2.01	0.44
1:A:152:A:N6	1:A:170:U:C2	2.85	0.44
1:A:1010:G:N2	1:A:1019:C:N3	2.64	0.44
3:C:137:ALA:HA	3:C:140:ARG:HE	1.83	0.44
5:E:17:ALA:CA	5:E:26:PHE:HB3	2.35	0.44
5:E:36:ASP:OD2	5:E:38:GLN:HB2	2.18	0.44
10:J:79:ARG:NH1	10:J:82:ILE:HG13	2.32	0.44
16:P:33:ILE:HG12	16:P:33:ILE:H	1.39	0.44
18:R:40:LEU:HD23	18:R:40:LEU:HA	1.64	0.44
1:A:346:G:H2'	1:A:347:G:O4'	2.18	0.44
1:A:650:G:H8	1:A:650:G:H5''	1.83	0.44
1:A:1035:A:H2'	1:A:1036:G:C8	2.53	0.44
3:C:73:PRO:HD3	3:C:105:GLU:OE2	2.17	0.44
4:D:107:ARG:HD2	4:D:173:TRP:CZ2	2.52	0.44
4:D:120:LEU:HD23	4:D:120:LEU:HA	1.68	0.44
12:L:85:ILE:HG23	12:L:98:TYR:HB3	2.00	0.44
13:M:108:ARG:HG3	13:M:114:ARG:HH12	1.82	0.44
13:M:108:ARG:HG3	13:M:114:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:G:OP1	4:D:73:ARG:HG2	2.18	0.44
1:A:775:G:H2'	1:A:776:G:O4'	2.16	0.44
1:A:895:G:H2'	1:A:896:C:C6	2.52	0.44
1:A:1031:G:H2'	1:A:1032:G:H8	1.83	0.44
1:A:1227:A:H2	1:A:1228:C:H1'	1.83	0.44
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.99	0.44
2:B:84:GLU:HG3	2:B:215:LEU:HB3	2.00	0.44
2:B:165:VAL:HG12	2:B:166:ASP:N	2.32	0.44
3:C:43:LEU:HD11	3:C:68:VAL:HG21	2.00	0.44
7:G:48:LYS:HA	7:G:48:LYS:HD3	1.89	0.44
9:I:51:ARG:HG2	9:I:56:LEU:HD21	2.00	0.44
9:I:111:ARG:O	9:I:119:ALA:HB2	2.17	0.44
1:A:21:G:H2'	1:A:22:G:C8	2.52	0.44
1:A:88:A:H2'	1:A:89:C:O4'	2.17	0.44
1:A:130:A:H5'	17:Q:63:ARG:NE	2.29	0.44
1:A:659:U:OP1	15:O:8:LYS:HD3	2.17	0.44
1:A:1191:A:P	3:C:3:ASN:HD22	2.41	0.44
3:C:112:SER:O	3:C:115:LEU:HB2	2.18	0.44
4:D:31:CYS:O	4:D:31:CYS:SG	2.75	0.44
6:F:75:LEU:O	6:F:79:LEU:HD13	2.17	0.44
10:J:7:LYS:HD3	10:J:9:ARG:HE	1.80	0.44
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.99	0.44
15:O:39:LEU:HB3	15:O:56:LEU:HD23	1.99	0.44
1:A:476:G:C5	1:A:477:G:C8	3.06	0.44
1:A:514:C:H2'	1:A:515:G:H8	1.82	0.44
1:A:824:C:H2'	1:A:825:G:H8	1.81	0.44
1:A:1295:G:C6	1:A:1296:C:C4	3.05	0.44
1:A:1454:G:H2'	1:A:1455:G:H8	1.81	0.44
4:D:78:LEU:O	4:D:81:GLU:HB3	2.16	0.44
4:D:112:VAL:HG23	4:D:116:GLN:OE1	2.18	0.44
10:J:28:ARG:HG2	10:J:29:ARG:HG2	2.00	0.44
16:P:71:ARG:HG3	16:P:80:PHE:HE1	1.83	0.44
17:Q:29:HIS:HA	17:Q:30:PRO:HD3	1.72	0.44
20:T:50:GLU:HA	20:T:100:ILE:HG13	2.00	0.44
1:A:91:C:H5'	1:A:92:C:OP2	2.17	0.43
1:A:117:G:P	24:A:1912:HOH:O	2.75	0.43
1:A:1355:G:C6	1:A:1368:G:C6	3.06	0.43
1:A:1385:G:H2'	1:A:1386:G:O4'	2.17	0.43
2:B:92:TYR:CE2	2:B:151:GLY:HA3	2.53	0.43
2:B:220:ASP:HA	2:B:230:VAL:HG21	2.00	0.43
3:C:131:ARG:H	3:C:131:ARG:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:TYR:CE2	3:C:186:PHE:HB2	2.51	0.43
12:L:7:ILE:O	12:L:8:ASN:C	2.55	0.43
18:R:53:ARG:HD2	18:R:58:LEU:O	2.17	0.43
1:A:144:G:N2	1:A:178:C:N3	2.42	0.43
1:A:431:A:H2'	1:A:432:A:H8	1.82	0.43
1:A:456:C:N4	1:A:457:C:H41	2.16	0.43
1:A:581:G:C8	24:A:1966:HOH:O	2.71	0.43
1:A:1055:A:H1'	3:C:156:ARG:HH21	1.83	0.43
1:A:1085:U:C6	1:A:1094:G:N1	2.86	0.43
1:A:1134:G:H1	1:A:1140:C:H42	1.66	0.43
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.53	0.43
4:D:17:VAL:HG22	4:D:18:LYS:H	1.83	0.43
4:D:162:LEU:HA	4:D:165:MET:HB2	2.00	0.43
5:E:9:LYS:N	5:E:33:VAL:O	2.50	0.43
5:E:137:GLU:O	5:E:141:GLN:HG2	2.18	0.43
8:H:18:ARG:NH2	8:H:81:HIS:O	2.51	0.43
12:L:34:ARG:O	12:L:61:THR:HG23	2.18	0.43
13:M:32:GLU:HG2	13:M:64:TRP:HZ2	1.83	0.43
16:P:12:LYS:C	16:P:14:ASN:H	2.21	0.43
20:T:53:LEU:HD22	20:T:53:LEU:HA	1.71	0.43
1:A:617:G:H1	1:A:623:C:N4	2.15	0.43
1:A:687:A:H4'	1:A:688:G:O5'	2.18	0.43
1:A:1065:U:C5	1:A:1190:G:H1'	2.54	0.43
2:B:107:THR:O	2:B:110:GLN:HB2	2.18	0.43
2:B:118:LEU:HA	2:B:118:LEU:HD23	1.79	0.43
2:B:166:ASP:HB2	2:B:205:ASP:OD2	2.18	0.43
20:T:20:LEU:O	20:T:23:ARG:HB3	2.18	0.43
1:A:683:G:H2'	1:A:684:A:C8	2.52	0.43
1:A:1199:U:O5'	1:A:1199:U:H6	2.02	0.43
1:A:1242:C:N4	1:A:1295:G:H1	2.16	0.43
1:A:1412:C:H2'	1:A:1413:A:C8	2.53	0.43
1:A:1505:G:H3'	1:A:1505:G:H8	1.82	0.43
9:I:79:LEU:HD22	9:I:79:LEU:HA	1.69	0.43
13:M:65:LYS:H	13:M:65:LYS:HD3	1.84	0.43
1:A:75:G:C2	1:A:96:G:C2	3.06	0.43
1:A:505:G:C6	1:A:535:A:C2	3.06	0.43
1:A:1094:G:H5''	1:A:1095:U:H5	1.83	0.43
3:C:114:PRO:HB2	3:C:118:GLN:NE2	2.34	0.43
10:J:51:ARG:HA	14:N:45:ARG:HD2	2.00	0.43
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.53	0.43
17:Q:40:LYS:HB3	17:Q:42:TYR:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:C:H5''	5:E:127:ASN:ND2	2.28	0.43
1:A:56:U:H2'	1:A:57:G:C8	2.52	0.43
1:A:78:G:N2	1:A:92:C:C4	2.86	0.43
1:A:564:C:C6	17:Q:31:LEU:HD11	2.53	0.43
1:A:664:G:OP1	18:R:64:ARG:HD2	2.19	0.43
1:A:737:A:H2'	1:A:738:C:C6	2.54	0.43
1:A:1355:G:H2'	1:A:1356:G:C8	2.54	0.43
1:A:1441:G:O2'	1:A:1460:A:N6	2.51	0.43
2:B:51:LEU:O	2:B:55:PHE:HB2	2.18	0.43
2:B:213:LEU:HD12	2:B:213:LEU:HA	1.73	0.43
13:M:11:ARG:HD2	13:M:12:ASN:N	2.34	0.43
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.99	0.43
16:P:74:LEU:HB3	16:P:79:VAL:CG2	2.49	0.43
1:A:24:U:H2'	1:A:25:C:C6	2.54	0.43
1:A:190(I):G:H2'	1:A:190(J):U:O4'	2.19	0.43
1:A:392:G:H2'	1:A:393:A:C8	2.54	0.43
1:A:953:G:C5'	1:A:965:A:H61	2.32	0.43
1:A:1031:G:H2'	1:A:1032:G:C8	2.54	0.43
1:A:1098:C:H2'	1:A:1099:G:O4'	2.18	0.43
1:A:1228:C:O3'	13:M:116:THR:HG23	2.19	0.43
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.53	0.43
3:C:28:GLN:HG3	3:C:32:LEU:HD22	1.99	0.43
7:G:35:LYS:HD3	7:G:38:LEU:HD13	2.01	0.43
7:G:44:TYR:HD2	7:G:44:TYR:HA	1.61	0.43
8:H:97:VAL:HA	8:H:100:ILE:HD11	2.01	0.43
9:I:19:LEU:HG	9:I:60:ASP:O	2.19	0.43
13:M:71:ARG:O	13:M:74:VAL:HG12	2.19	0.43
19:S:2:PRO:HD2	19:S:3:ARG:HH21	1.84	0.43
19:S:3:ARG:NH1	19:S:3:ARG:HB3	2.33	0.43
1:A:179:A:H2'	1:A:180:U:H6	1.83	0.43
1:A:1281:U:OP2	1:A:1282:C:N4	2.43	0.43
1:A:1486:G:H2'	1:A:1487:G:O4'	2.19	0.43
2:B:17:PHE:CD1	2:B:18:GLY:N	2.87	0.43
2:B:218:ALA:O	2:B:222:ILE:HG13	2.19	0.43
3:C:54:ARG:HH12	3:C:56:ASP:HB2	1.83	0.43
5:E:152:ARG:HA	8:H:64:LYS:HZ1	1.83	0.43
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.71	0.43
9:I:33:PHE:CZ	9:I:47:LEU:HD21	2.53	0.43
13:M:57:ARG:O	13:M:61:GLU:HB2	2.18	0.43
15:O:59:MET:HG2	15:O:59:MET:H	1.56	0.43
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:A:H8	1:A:300:A:O5'	2.02	0.43
1:A:517:G:H5'	1:A:519:C:N3	2.34	0.43
1:A:728:A:H2'	1:A:729:A:O4'	2.19	0.43
1:A:976:G:OP2	1:A:1358:U:O2'	2.31	0.43
2:B:185:ILE:HA	2:B:199:TYR:O	2.19	0.43
8:H:119:LEU:HB3	8:H:123:GLU:HB3	2.00	0.43
9:I:2:GLU:HG3	9:I:3:GLN:H	1.84	0.43
10:J:19:SER:O	10:J:22:LYS:HB2	2.18	0.43
12:L:30:ALA:HB1	12:L:31:PRO:HD2	1.99	0.43
18:R:56:THR:OG1	18:R:58:LEU:HG	2.19	0.43
19:S:18:LYS:O	19:S:22:LEU:HB2	2.19	0.43
1:A:297:G:N2	1:A:300:A:OP2	2.46	0.43
1:A:328:C:H4'	1:A:329:A:H5'	2.01	0.43
1:A:923:A:O2'	1:A:1398:A:H2'	2.19	0.43
1:A:940:C:H2'	1:A:941:G:O4'	2.19	0.43
1:A:1250:A:C6	1:A:1287:A:C2	3.06	0.43
1:A:1277:C:H1'	1:A:1282:C:H1'	2.01	0.43
1:A:1323:G:H2'	1:A:1324:A:C8	2.54	0.43
3:C:180:ALA:O	3:C:181:ASN:HB3	2.18	0.43
4:D:127:THR:HA	4:D:132:ARG:HA	2.01	0.43
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.51	0.43
9:I:99:LEU:HB3	9:I:101:PHE:HD1	1.84	0.43
15:O:28:GLN:O	15:O:32:LEU:HB2	2.19	0.43
1:A:129:U:O3'	1:A:129(A):G:H3'	2.18	0.42
1:A:500:G:C6	1:A:546:G:C2	3.06	0.42
1:A:582:U:P	15:O:64:ARG:NH2	2.92	0.42
1:A:689:C:HO2'	1:A:705:U:HO2'	1.52	0.42
1:A:1256:A:H5''	1:A:1258:G:N9	2.34	0.42
1:A:1476:G:H2'	1:A:1477:C:H6	1.84	0.42
2:B:42:ILE:N	2:B:42:ILE:HD12	2.33	0.42
2:B:61:LEU:HD21	2:B:160:ASP:HB2	2.01	0.42
2:B:80:ILE:HD11	2:B:212:GLN:HG2	2.01	0.42
5:E:152:ARG:CZ	8:H:44:PHE:HE1	2.32	0.42
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.84	0.42
7:G:88:PRO:HG2	7:G:155:ARG:NH2	2.29	0.42
8:H:84:ARG:O	8:H:135:CYS:HB2	2.19	0.42
10:J:7:LYS:HD2	10:J:97:GLU:HB2	2.01	0.42
11:K:84:VAL:HG11	11:K:91:ARG:HD3	2.01	0.42
1:A:102:G:H2'	1:A:103:C:H6	1.83	0.42
1:A:707:C:H2'	1:A:708:C:H6	1.84	0.42
1:A:1018:C:H2'	1:A:1019:C:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:G:O2'	9:I:16:ARG:NH2	2.51	0.42
1:A:1199:U:H5''	1:A:1200:C:OP2	2.19	0.42
2:B:42:ILE:HD12	2:B:42:ILE:H	1.84	0.42
2:B:182:ILE:HA	2:B:183:PRO:HD3	1.92	0.42
3:C:10:PHE:O	3:C:178:LEU:HD11	2.19	0.42
3:C:21:ARG:NH2	3:C:58:GLU:HG3	2.34	0.42
5:E:53:LEU:HD22	5:E:53:LEU:HA	1.62	0.42
5:E:152:ARG:HB3	8:H:43:GLY:HA3	2.01	0.42
10:J:9:ARG:HB2	10:J:95:GLU:HB3	2.01	0.42
13:M:50:GLU:HG3	13:M:51:ALA:N	2.34	0.42
1:A:515:G:H2'	1:A:516:PSU:H6	1.84	0.42
1:A:575:G:OP1	1:A:575:G:H4'	2.20	0.42
1:A:791:G:C6	1:A:792:A:N6	2.86	0.42
1:A:865:A:O5'	1:A:865:A:H8	2.03	0.42
1:A:986:A:H1'	19:S:55:LYS:HA	2.01	0.42
1:A:1206:G:H22	1:A:1207:2MG:HM22	1.84	0.42
1:A:1250:A:H3'	1:A:1251:A:C8	2.53	0.42
1:A:1404:5MC:N4	1:A:1498:UR3:H3U2	2.34	0.42
1:A:1418:A:C8	1:A:1483:A:N6	2.88	0.42
1:A:1441:G:H4'	1:A:1442:G:C6	2.55	0.42
1:A:1489:G:H2'	1:A:1490:U:C6	2.54	0.42
3:C:114:PRO:O	3:C:117:ALA:HB3	2.20	0.42
7:G:63:LYS:HD3	7:G:63:LYS:N	2.33	0.42
9:I:81:ILE:HD13	9:I:81:ILE:HA	1.89	0.42
11:K:51:LYS:HE3	11:K:51:LYS:HA	2.00	0.42
11:K:84:VAL:HG21	11:K:95:ILE:HD11	2.02	0.42
17:Q:27:PHE:CE2	17:Q:36:ILE:HG13	2.55	0.42
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.19	0.42
19:S:33:THR:HG21	19:S:71:LEU:HD21	2.02	0.42
20:T:29:LYS:O	20:T:32:ALA:HB3	2.18	0.42
1:A:78:G:C6	1:A:79:G:C8	3.07	0.42
1:A:587:G:N2	1:A:754:C:OP2	2.48	0.42
1:A:1163:C:N3	1:A:1174:G:C2	2.87	0.42
1:A:1425:U:H2'	1:A:1426:C:H6	1.85	0.42
2:B:158:LEU:HB3	2:B:159:PRO:HD2	2.01	0.42
4:D:108:LEU:HD13	4:D:108:LEU:HA	1.93	0.42
7:G:20:ASP:HB3	7:G:23:VAL:HG23	2.00	0.42
8:H:7:ALA:HB2	8:H:85:ARG:HD2	2.01	0.42
8:H:116:LYS:HD3	8:H:127:LEU:HD11	2.00	0.42
9:I:50:LEU:HG	9:I:81:ILE:HG21	2.01	0.42
12:L:82:VAL:HG12	12:L:106:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:110:VAL:HG12	12:L:111:LYS:O	2.19	0.42
14:N:24:CYS:SG	14:N:40:CYS:HB3	2.59	0.42
17:Q:21:VAL:HG21	17:Q:59:ILE:HG13	2.02	0.42
1:A:445:G:C2	1:A:490:G:N1	2.88	0.42
1:A:625:G:H2'	1:A:626:U:H6	1.82	0.42
1:A:636:U:H5'	17:Q:2:PRO:HG3	2.00	0.42
1:A:794:A:C6	1:A:795:C:N4	2.88	0.42
1:A:1184:G:H2'	1:A:1185:G:C8	2.54	0.42
1:A:1291:G:H2'	1:A:1292:U:H6	1.84	0.42
2:B:163:PHE:HA	2:B:185:ILE:HB	2.01	0.42
4:D:70:ILE:HG22	4:D:71:SER:O	2.19	0.42
8:H:86:ILE:HG22	8:H:87:SER:N	2.32	0.42
8:H:114:THR:OG1	8:H:117:GLY:O	2.21	0.42
8:H:116:LYS:HD3	8:H:127:LEU:CD1	2.49	0.42
15:O:4:THR:HB	15:O:6:GLU:OE1	2.19	0.42
18:R:37:VAL:HG13	18:R:79:LEU:HD21	2.00	0.42
18:R:61:LYS:O	18:R:62:GLU:C	2.58	0.42
21:U:18:TYR:HD2	21:U:22:ARG:HD3	1.84	0.42
1:A:411:A:C4	1:A:413:G:H1'	2.55	0.42
1:A:639:G:O2'	1:A:640:A:H5'	2.20	0.42
1:A:657:G:H2'	1:A:658:G:H8	1.84	0.42
1:A:807:A:C6	1:A:808:C:C4	3.08	0.42
1:A:1181:G:N3	1:A:1182:G:C2	2.87	0.42
1:A:1407:5MC:H2'	1:A:1408:A:H8	1.85	0.42
7:G:151:TYR:O	7:G:155:ARG:NH2	2.53	0.42
9:I:27:THR:OG1	9:I:28:VAL:N	2.53	0.42
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.55	0.42
18:R:61:LYS:O	18:R:65:ILE:HG13	2.19	0.42
19:S:15:LEU:HD21	19:S:38:SER:OG	2.20	0.42
1:A:21:G:C2	1:A:22:G:C6	3.08	0.42
1:A:110:C:H2'	1:A:111:G:O4'	2.19	0.42
1:A:204:U:H4'	1:A:216:G:O4'	2.20	0.42
1:A:376:G:C4	1:A:389:A:C2	3.07	0.42
1:A:451:A:O5'	1:A:451:A:H8	2.01	0.42
1:A:544:G:C5	1:A:545:C:C5	3.08	0.42
1:A:570:G:O6	1:A:873:A:C2	2.72	0.42
1:A:1051:C:N4	1:A:1207:2MG:C6	2.85	0.42
1:A:1427:U:H2'	1:A:1428:A:H8	1.84	0.42
1:A:1520[B]:G:O2'	1:A:1521:G:H5'	2.19	0.42
2:B:208:ILE:H	2:B:208:ILE:CD1	2.26	0.42
3:C:137:ALA:O	3:C:141:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:ARG:O	3:C:181:ASN:N	2.53	0.42
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.83	0.42
5:E:84:PHE:CE2	5:E:133:TYR:HB2	2.55	0.42
5:E:99:GLY:H	5:E:117:ASP:CG	2.23	0.42
5:E:118:ILE:C	5:E:119:LEU:HD23	2.39	0.42
7:G:16:LEU:HG	9:I:42:ARG:HA	2.01	0.42
7:G:141:VAL:HA	7:G:144:MET:SD	2.60	0.42
9:I:127:LYS:HD2	9:I:127:LYS:HA	1.91	0.42
10:J:24:VAL:HG13	10:J:28:ARG:NH2	2.34	0.42
11:K:52:GLY:C	11:K:54:ARG:N	2.72	0.42
13:M:68:GLY:O	13:M:71:ARG:HG3	2.20	0.42
14:N:2:ALA:HB2	14:N:29:ARG:HA	2.01	0.42
14:N:9:LYS:HG3	14:N:21:TYR:O	2.20	0.42
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.20	0.42
19:S:39:THR:HG22	19:S:40:ILE:H	1.84	0.42
1:A:734:G:N2	18:R:75:ILE:HD11	2.35	0.42
1:A:946:A:H2'	1:A:947:G:C8	2.53	0.42
1:A:992:U:H4'	1:A:993:G:O5'	2.20	0.42
1:A:1015:A:H2'	1:A:1016:A:O4'	2.20	0.42
1:A:1332:A:H2'	1:A:1333:A:H8	1.84	0.42
1:A:1430:C:O2	1:A:1471:G:N2	2.53	0.42
2:B:55:PHE:HA	2:B:58:ILE:HD12	2.02	0.42
8:H:65:TYR:HA	8:H:79:VAL:HG23	2.01	0.42
14:N:61:TRP:OXT	14:N:61:TRP:CG	2.73	0.42
18:R:26:LEU:HD12	18:R:26:LEU:HA	1.87	0.42
20:T:61:SER:O	20:T:62:LEU:C	2.58	0.42
1:A:200:G:C6	1:A:201:C:C4	3.07	0.42
1:A:681:C:H2'	1:A:682:G:O4'	2.20	0.42
1:A:868:C:H2'	1:A:869:G:O4'	2.20	0.42
1:A:1163:C:N3	1:A:1174:G:N2	2.67	0.42
1:A:1255:G:N2	1:A:1283:G:H1'	2.30	0.42
2:B:162:ILE:HB	2:B:184:VAL:HG23	2.01	0.42
3:C:175:LEU:HD11	3:C:201:TYR:CD2	2.54	0.42
4:D:9:CYS:O	4:D:12:CYS:HB2	2.20	0.42
4:D:190:ASP:CG	4:D:191:ARG:N	2.73	0.42
10:J:32:ALA:O	10:J:34:VAL:HG23	2.19	0.42
11:K:12:ARG:HE	11:K:12:ARG:HA	1.85	0.42
17:Q:9:VAL:O	17:Q:9:VAL:HG13	2.20	0.42
19:S:15:LEU:HD13	19:S:44:MET:HE1	2.02	0.42
1:A:106:C:H2'	1:A:107:G:O4'	2.19	0.42
1:A:474:G:C2	1:A:475:G:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:A:H2'	1:A:768:A:C8	2.55	0.42
1:A:979:C:H3'	1:A:980:C:C6	2.55	0.42
1:A:1399:C:C2	1:A:1502:A:N6	2.88	0.42
2:B:36:ARG:O	2:B:39:ILE:HD12	2.19	0.42
4:D:200:GLU:O	4:D:203:VAL:N	2.53	0.42
5:E:129:ILE:H	5:E:129:ILE:HG12	1.60	0.42
8:H:60:ARG:HH11	8:H:60:ARG:HG3	1.83	0.42
9:I:92:TYR:O	9:I:96:LEU:HB2	2.20	0.42
10:J:66:ARG:HG3	14:N:57:ARG:HD2	2.02	0.42
15:O:67:LEU:HA	15:O:67:LEU:HD23	1.46	0.42
20:T:84:LEU:HA	20:T:84:LEU:HD23	1.80	0.42
1:A:68:G:H5'	1:A:171:A:O2'	2.20	0.41
1:A:156:G:N1	1:A:157:G:C5	2.87	0.41
1:A:413:G:H2'	1:A:428:G:N2	2.35	0.41
1:A:451:A:N6	1:A:481:G:C4	2.88	0.41
1:A:853:G:C2	1:A:854:G:C8	3.07	0.41
1:A:877:C:O2	8:H:3:THR:HG21	2.20	0.41
1:A:1008:C:N4	1:A:1021:G:H1	2.19	0.41
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.54	0.41
1:A:1218:C:H2'	1:A:1219:U:C6	2.54	0.41
2:B:188:ALA:O	2:B:202:PRO:HA	2.20	0.41
3:C:61:ALA:C	3:C:63:ASN:H	2.24	0.41
5:E:41:VAL:HG23	5:E:67:VAL:HG13	2.02	0.41
6:F:100:ASN:HB2	18:R:23:LYS:HE2	2.02	0.41
7:G:47:CYS:HB3	7:G:48:LYS:NZ	2.35	0.41
7:G:61:VAL:HG22	7:G:128:ALA:HB1	2.01	0.41
12:L:60:LEU:HD13	12:L:60:LEU:HA	1.67	0.41
13:M:49:THR:CG2	13:M:51:ALA:H	2.33	0.41
16:P:2:VAL:O	16:P:64:ALA:HA	2.19	0.41
19:S:12:ASP:OD2	19:S:37:ARG:NH1	2.34	0.41
20:T:67:ALA:HA	20:T:72:LEU:HB2	2.02	0.41
1:A:828:A:C8	1:A:828:A:C3'	3.03	0.41
1:A:977:A:O2'	1:A:980:C:N4	2.53	0.41
1:A:1249:C:HO2'	9:I:73:GLN:NE2	2.18	0.41
2:B:24:TRP:HA	2:B:190:THR:O	2.20	0.41
3:C:138:VAL:HG11	3:C:170:GLN:H	1.85	0.41
4:D:57:ARG:HG3	4:D:202:LEU:HD13	2.01	0.41
4:D:206:PHE:CD2	4:D:207:TYR:CE2	3.08	0.41
6:F:8:ILE:HB	6:F:61:LEU:HD12	2.02	0.41
7:G:136:LYS:HE3	7:G:136:LYS:HB3	1.86	0.41
8:H:70:GLN:OE1	8:H:70:GLN:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:116:LYS:HB3	9:I:121:ARG:O	2.20	0.41
11:K:33:THR:HA	11:K:40:ILE:H	1.85	0.41
1:A:261:U:OP2	20:T:79:ARG:NH2	2.53	0.41
1:A:979:C:N4	24:A:2063:HOH:O	2.54	0.41
1:A:1008:C:H1'	1:A:1023:G:H1	1.85	0.41
1:A:1181:G:C4	1:A:1182:G:C6	3.09	0.41
1:A:1349:A:C2	1:A:1374:A:C4	3.09	0.41
1:A:1414:U:H2'	1:A:1415:G:C8	2.56	0.41
1:A:1521:G:C2	1:A:1522:U:C2	3.08	0.41
3:C:147:LYS:HD3	3:C:205:GLY:H	1.86	0.41
6:F:2:ARG:HG3	6:F:69:GLU:HG2	2.02	0.41
12:L:98:TYR:CD1	12:L:98:TYR:N	2.88	0.41
16:P:57:ARG:HH11	16:P:57:ARG:HB3	1.85	0.41
18:R:55:ARG:HB3	18:R:55:ARG:CZ	2.49	0.41
1:A:78:G:H2'	1:A:79:G:C5'	2.50	0.41
1:A:312:C:H2'	1:A:313:A:O4'	2.20	0.41
1:A:721:G:C6	1:A:733:A:C2	3.08	0.41
1:A:840:C:H5''	1:A:841:U:OP1	2.20	0.41
1:A:981:U:H3'	1:A:982:U:C6	2.56	0.41
1:A:1016:A:H2'	1:A:1017:G:O4'	2.20	0.41
1:A:1094:G:H5''	1:A:1095:U:C5	2.54	0.41
1:A:1372:U:H5''	9:I:71:SER:CB	2.49	0.41
1:A:1402:4OC:H2'	1:A:1403:C:H6	1.85	0.41
6:F:9:VAL:HA	6:F:59:TYR:O	2.20	0.41
7:G:60:LYS:NZ	7:G:64:GLN:HB2	2.36	0.41
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.20	0.41
13:M:62:ASN:OD1	13:M:62:ASN:N	2.53	0.41
15:O:10:LYS:O	15:O:14:GLU:HB3	2.21	0.41
1:A:428:G:C5	1:A:430:A:C6	3.08	0.41
1:A:629:G:H2'	1:A:630:G:H8	1.83	0.41
1:A:865:A:H1'	1:A:918:A:O2'	2.21	0.41
1:A:967:5MC:H4'	9:I:128:ARG:CZ	2.50	0.41
1:A:1233:G:H2'	1:A:1234:C:C6	2.55	0.41
3:C:108:ASN:N	3:C:109:PRO:HD3	2.35	0.41
4:D:93:PHE:O	4:D:96:LEU:N	2.54	0.41
5:E:91:LEU:HD23	5:E:91:LEU:N	2.35	0.41
18:R:52:PRO:O	18:R:56:THR:HG23	2.20	0.41
19:S:12:ASP:CG	19:S:37:ARG:HH12	2.22	0.41
1:A:46:G:H2'	1:A:366:C:H5	1.85	0.41
1:A:395:C:H2'	1:A:396:G:C8	2.56	0.41
1:A:665:A:H2'	1:A:732:C:O2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:A:O3'	1:A:723:U:H6	2.03	0.41
1:A:815:A:O2'	1:A:816:A:OP1	2.30	0.41
1:A:939:G:H2'	1:A:940:C:H6	1.83	0.41
1:A:964:A:O2'	10:J:55:LYS:HD3	2.20	0.41
1:A:1222:G:P	19:S:77:THR:HG1	2.44	0.41
1:A:1262:C:N4	1:A:1273:G:H1	2.14	0.41
1:A:1422:G:C2	1:A:1423:G:N7	2.88	0.41
9:I:19:LEU:HD21	9:I:59:PHE:CD2	2.56	0.41
9:I:49:PRO:HG2	9:I:81:ILE:HG21	2.02	0.41
19:S:5:LEU:O	19:S:6:LYS:HD3	2.20	0.41
1:A:128:G:C2	1:A:234:C:C2	3.09	0.41
1:A:654:G:H2'	1:A:655:A:H8	1.84	0.41
1:A:671:G:H5'	6:F:77:ARG:NH2	2.36	0.41
1:A:1405:G:O2'	1:A:1406:U:H5'	2.20	0.41
1:A:1426:C:H2'	1:A:1427:U:H6	1.86	0.41
1:A:1486:G:C6	1:A:1487:G:C6	3.09	0.41
3:C:22:TRP:CD2	3:C:59:ARG:HD2	2.56	0.41
4:D:57:ARG:HB3	4:D:206:PHE:HD1	1.86	0.41
5:E:53:LEU:O	5:E:53:LEU:HD13	2.21	0.41
8:H:36:LEU:HD23	8:H:39:LEU:HD12	2.02	0.41
14:N:37:PHE:C	14:N:39:LEU:N	2.74	0.41
15:O:15:PHE:CE1	15:O:84:LYS:HE2	2.56	0.41
20:T:65:LYS:O	20:T:68:LYS:HB3	2.21	0.41
20:T:73:HIS:O	20:T:76:ALA:HB3	2.21	0.41
1:A:832:C:H2'	1:A:833:U:O4'	2.21	0.41
1:A:1192:C:H2'	1:A:1193:G:O4'	2.19	0.41
1:A:1227:A:C2	1:A:1228:C:H1'	2.55	0.41
3:C:130:VAL:HG23	3:C:131:ARG:N	2.36	0.41
4:D:100:ARG:NH1	4:D:137:SER:HA	2.35	0.41
7:G:22:LEU:HD12	7:G:97:GLN:HE22	1.84	0.41
8:H:51:VAL:HG23	8:H:52:ASP:N	2.35	0.41
10:J:8:LEU:HD21	10:J:72:VAL:HG23	2.02	0.41
12:L:41:ARG:CZ	12:L:43:VAL:HG12	2.51	0.41
12:L:94:LEU:HD22	12:L:94:LEU:HA	1.72	0.41
12:L:102:ARG:HE	12:L:102:ARG:HB3	1.52	0.41
13:M:65:LYS:O	13:M:66:LEU:HD23	2.20	0.41
14:N:57:ARG:HB2	14:N:57:ARG:CZ	2.50	0.41
16:P:38:TYR:CE2	16:P:50:LYS:HE2	2.49	0.41
17:Q:90:ILE:O	17:Q:90:ILE:HD13	2.21	0.41
18:R:43:PHE:O	18:R:44:LEU:HD23	2.21	0.41
1:A:49:U:O2'	1:A:50:A:H2'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:G:C6	1:A:76:C:N4	2.88	0.41
1:A:439:A:OP1	4:D:123:HIS:HD2	2.04	0.41
1:A:677:U:H2'	1:A:678:U:C6	2.55	0.41
1:A:979:C:H3'	1:A:980:C:H6	1.86	0.41
1:A:981:U:H2'	1:A:982:U:H5	1.85	0.41
1:A:1103:C:H4'	2:B:98:LEU:HD21	2.01	0.41
1:A:1157:A:N1	1:A:1181:G:N3	2.69	0.41
1:A:1164:G:H1	1:A:1172:C:N4	2.06	0.41
1:A:1278:U:H6	1:A:1278:U:H2'	1.67	0.41
1:A:1320:C:OP1	19:S:70:LYS:HG2	2.20	0.41
1:A:1328:C:H2'	1:A:1329:A:O4'	2.20	0.41
1:A:1498:UR3:H1'	1:A:1499:A:N7	2.36	0.41
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.24	0.41
3:C:41:GLY:O	3:C:45:LYS:HB2	2.21	0.41
4:D:52:SER:O	4:D:56:VAL:HG23	2.19	0.41
4:D:141:ARG:HB2	4:D:141:ARG:CZ	2.51	0.41
4:D:173:TRP:H	4:D:173:TRP:HE3	1.67	0.41
5:E:125:SER:OG	5:E:127:ASN:HB2	2.21	0.41
8:H:9:MET:HG3	8:H:26:VAL:HG21	2.03	0.41
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.56	0.41
9:I:27:THR:HG23	9:I:62:TYR:HA	2.01	0.41
10:J:21:GLN:HA	10:J:24:VAL:HG12	2.03	0.41
10:J:46:ARG:CG	10:J:64:GLU:HB3	2.51	0.41
17:Q:62:SER:CB	17:Q:72:ARG:HD3	2.46	0.41
19:S:2:PRO:HD2	19:S:3:ARG:NH2	2.36	0.41
20:T:56:MET:CE	20:T:104:LEU:HD21	2.51	0.41
1:A:193:C:H2'	1:A:194:C:H6	1.86	0.41
1:A:491:G:C2	1:A:492:G:C5	3.08	0.41
1:A:513:C:H42	1:A:538:G:H1	1.68	0.41
1:A:803:G:C5	1:A:804:U:C4	3.09	0.41
1:A:836:G:H5''	1:A:836:G:H8	1.84	0.41
1:A:1203:C:O5'	1:A:1203:C:H6	2.04	0.41
1:A:1314:C:H2'	1:A:1315:U:C6	2.56	0.41
1:A:1409:C:H2'	1:A:1410:G:H8	1.85	0.41
12:L:46:LYS:HB2	12:L:92:OTD:H8	2.03	0.41
17:Q:5:VAL:HA	17:Q:59:ILE:O	2.21	0.41
18:R:37:VAL:O	18:R:39:VAL:N	2.55	0.41
20:T:87:LYS:HE2	20:T:87:LYS:HB2	1.63	0.41
1:A:108:G:H5'	1:A:109:A:H2	1.85	0.40
1:A:254:G:OP1	17:Q:67:LYS:O	2.39	0.40
1:A:778:G:H2'	1:A:779:C:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:A:H2'	1:A:861:G:O4'	2.21	0.40
1:A:966:M2G:H2'	1:A:967:5MC:H6	1.85	0.40
1:A:1400:5MC:H3'	1:A:1401:G:C5'	2.52	0.40
1:A:1414:U:H3'	1:A:1415:G:H8	1.86	0.40
2:B:74:LYS:HB2	2:B:165:VAL:HG11	2.03	0.40
3:C:186:PHE:CG	3:C:187:ALA:N	2.88	0.40
4:D:61:LYS:HZ3	4:D:62:GLN:N	2.18	0.40
6:F:15:ASP:HB3	6:F:18:GLN:CG	2.51	0.40
8:H:113:SER:HB2	8:H:134:ILE:HD11	2.03	0.40
12:L:84:LEU:HA	12:L:84:LEU:HD12	1.69	0.40
19:S:44:MET:O	19:S:47:HIS:HD2	2.03	0.40
1:A:394:G:H2'	1:A:395:C:H6	1.85	0.40
1:A:500:G:C5	1:A:546:G:N2	2.89	0.40
1:A:673:G:O3'	6:F:87:ARG:NH1	2.54	0.40
1:A:770:C:O2'	1:A:771:G:H5'	2.20	0.40
1:A:980:C:H2'	1:A:981:U:O4'	2.21	0.40
1:A:1255:G:C2	1:A:1283:G:N3	2.89	0.40
1:A:1511:G:H2'	1:A:1512:U:O4'	2.22	0.40
2:B:196:LEU:HD23	2:B:196:LEU:HA	1.86	0.40
5:E:37:ARG:O	5:E:114:GLY:HA3	2.22	0.40
7:G:88:PRO:HG2	7:G:155:ARG:NH1	2.34	0.40
17:Q:93:GLN:HG2	17:Q:96:GLU:OE2	2.20	0.40
20:T:61:SER:O	20:T:64:ASP:N	2.54	0.40
1:A:92:C:O2	1:A:92:C:H2'	2.21	0.40
1:A:323:U:H2'	1:A:324:G:O4'	2.20	0.40
1:A:460:A:C6	1:A:462:G:C5	3.09	0.40
1:A:475:G:H2'	1:A:476:G:O4'	2.21	0.40
1:A:551:U:O2'	12:L:86:ARG:HD2	2.21	0.40
1:A:1287:A:N7	1:A:1288:A:N6	2.70	0.40
2:B:16:HIS:CG	2:B:17:PHE:N	2.89	0.40
2:B:23:ARG:HA	2:B:23:ARG:CZ	2.50	0.40
2:B:184:VAL:HG12	2:B:198:ASP:H	1.86	0.40
4:D:22:LYS:HB2	4:D:26:CYS:CB	2.50	0.40
4:D:121:VAL:HG11	4:D:136:PRO:HA	2.03	0.40
5:E:64:ARG:H	5:E:64:ARG:HG2	1.45	0.40
7:G:53:LYS:HB3	7:G:53:LYS:HE3	1.88	0.40
13:M:8:GLU:CD	13:M:22:ILE:HA	2.42	0.40
18:R:58:LEU:HB3	18:R:62:GLU:HB3	2.04	0.40
1:A:618:C:H3'	1:A:619:U:H5''	2.03	0.40
1:A:809:G:HO2'	1:A:810:C:P	2.44	0.40
1:A:1295:G:C5	1:A:1296:C:C5	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:G:C2	1:A:1319:A:OP2	2.75	0.40
1:A:1531:A:C8	1:A:1531:A:OP2	2.74	0.40
3:C:127:ARG:HB2	3:C:127:ARG:CZ	2.51	0.40
6:F:15:ASP:CG	6:F:16:GLN:H	2.25	0.40
10:J:50:ILE:N	10:J:50:ILE:HD12	2.36	0.40
11:K:16:SER:CB	11:K:106:LYS:HZ1	2.35	0.40
11:K:122:LYS:HE2	11:K:122:LYS:HB3	1.79	0.40
12:L:28:LYS:HD3	12:L:28:LYS:HA	1.93	0.40
13:M:88:ARG:NH1	19:S:3:ARG:HH22	2.20	0.40
14:N:45:ARG:HG2	14:N:45:ARG:HH11	1.85	0.40
19:S:40:ILE:HA	19:S:44:MET:SD	2.61	0.40
1:A:27:G:H1	1:A:556:C:H42	1.70	0.40
1:A:115:G:O2'	1:A:289:G:H5''	2.22	0.40
1:A:154:C:C2	1:A:168:G:N2	2.90	0.40
1:A:253:U:H2'	1:A:254:G:C8	2.56	0.40
1:A:427:U:OP1	4:D:13:ARG:NH2	2.54	0.40
1:A:451:A:N6	1:A:481:G:C5	2.90	0.40
1:A:570:G:C2	1:A:571:U:C4	3.09	0.40
1:A:735:C:O2'	1:A:736:C:H5'	2.22	0.40
1:A:945:G:N2	1:A:1337:G:N2	2.69	0.40
1:A:1243:C:OP1	21:U:10:ARG:NH1	2.55	0.40
1:A:1244:C:H5''	1:A:1245:A:OP2	2.22	0.40
2:B:21:ARG:HE	2:B:22:LYS:H	1.67	0.40
3:C:134:ILE:HG23	3:C:151:VAL:CG1	2.52	0.40
4:D:9:CYS:HA	4:D:12:CYS:HB2	2.03	0.40
5:E:80:ILE:O	5:E:80:ILE:HG13	2.21	0.40
7:G:3:ARG:HG2	7:G:3:ARG:HH11	1.84	0.40
8:H:82:HIS:C	8:H:82:HIS:HD1	2.25	0.40
8:H:124:ALA:O	8:H:125:ARG:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	206 (89%)	23 (10%)	3 (1%)	10	40
3	C	204/239 (85%)	179 (88%)	24 (12%)	1 (0%)	25	57
4	D	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	E	148/162 (91%)	139 (94%)	8 (5%)	1 (1%)	19	51
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	137 (90%)	16 (10%)	0	100	100
8	H	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	16	49
10	J	96/105 (91%)	78 (81%)	17 (18%)	1 (1%)	13	44
11	K	114/129 (88%)	101 (89%)	13 (11%)	0	100	100
12	L	121/135 (90%)	109 (90%)	11 (9%)	1 (1%)	16	49
13	M	116/126 (92%)	102 (88%)	12 (10%)	2 (2%)	7	36
14	N	58/61 (95%)	48 (83%)	10 (17%)	0	100	100
15	O	85/89 (96%)	74 (87%)	10 (12%)	1 (1%)	11	41
16	P	81/88 (92%)	72 (89%)	9 (11%)	0	100	100
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	R	68/88 (77%)	58 (85%)	10 (15%)	0	100	100
19	S	78/93 (84%)	71 (91%)	6 (8%)	1 (1%)	10	40
20	T	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
All	All	2336/2541 (92%)	2096 (90%)	228 (10%)	12 (0%)	25	57

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
12	L	28	LYS
19	S	31	ILE
2	B	95	GLN
9	I	119	ALA
3	C	180	ALA
13	M	23	TYR
5	E	70	PRO
2	B	229	VAL
10	J	34	VAL
13	M	84	ILE

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Mol	Chain	Res	Type
15	O	45	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	157 (78%)	45 (22%)	1	5
3	C	160/188 (85%)	121 (76%)	39 (24%)	0	4
4	D	180/181 (99%)	146 (81%)	34 (19%)	1	8
5	E	115/123 (94%)	77 (67%)	38 (33%)	0	1
6	F	90/90 (100%)	64 (71%)	26 (29%)	0	2
7	G	126/127 (99%)	99 (79%)	27 (21%)	1	6
8	H	119/119 (100%)	90 (76%)	29 (24%)	0	4
9	I	98/99 (99%)	68 (69%)	30 (31%)	0	1
10	J	87/92 (95%)	67 (77%)	20 (23%)	0	5
11	K	88/99 (89%)	67 (76%)	21 (24%)	0	4
12	L	103/110 (94%)	84 (82%)	19 (18%)	1	8
13	M	94/101 (93%)	73 (78%)	21 (22%)	1	5
14	N	49/50 (98%)	42 (86%)	7 (14%)	2	16
15	O	79/80 (99%)	62 (78%)	17 (22%)	1	6
16	P	72/74 (97%)	59 (82%)	13 (18%)	1	9
17	Q	94/97 (97%)	74 (79%)	20 (21%)	1	6
18	R	61/77 (79%)	48 (79%)	13 (21%)	1	6
19	S	71/80 (89%)	56 (79%)	15 (21%)	1	6
20	T	76/82 (93%)	55 (72%)	21 (28%)	0	2
21	U	19/22 (86%)	13 (68%)	6 (32%)	0	1
All	All	1983/2111 (94%)	1522 (77%)	461 (23%)	0	5

All (461) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	12	GLU
2	B	16	HIS
2	B	17	PHE
2	B	20	GLU
2	B	23	ARG
2	B	35	GLU
2	B	48	MET
2	B	53	ARG
2	B	56	ARG
2	B	60	ASP
2	B	67	THR
2	B	69	LEU
2	B	74	LYS
2	B	92	TYR
2	B	98	LEU
2	B	107	THR
2	B	108	ILE
2	B	109	SER
2	B	115	LEU
2	B	127	ILE
2	B	128	GLU
2	B	144	ARG
2	B	146	GLN
2	B	160	ASP
2	B	163	PHE
2	B	165	VAL
2	B	166	ASP
2	B	168	THR
2	B	170	GLU
2	B	175	ARG
2	B	178	ARG
2	B	184	VAL
2	B	187	LEU
2	B	200	ILE
2	B	204	ASN
2	B	205	ASP
2	B	206	ASP
2	B	209	ARG
2	B	212	GLN
2	B	217	ARG
2	B	221	LEU

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Mol	Chain	Res	Type
2	B	226	ARG
2	B	231	GLU
3	C	3	ASN
3	C	8	ILE
3	C	11	ARG
3	C	14	ILE
3	C	17	ASP
3	C	18	TRP
3	C	20	SER
3	C	21	ARG
3	C	26	LYS
3	C	33	LEU
3	C	34	LEU
3	C	36	ASP
3	C	43	LEU
3	C	45	LYS
3	C	52	LEU
3	C	54	ARG
3	C	58	GLU
3	C	90	GLU
3	C	91	LEU
3	C	94	LEU
3	C	98	ASN
3	C	99	VAL
3	C	102	ASN
3	C	104	GLN
3	C	107	GLN
3	C	111	LEU
3	C	116	VAL
3	C	131	ARG
3	C	143	GLU
3	C	172	ARG
3	C	175	LEU
3	C	176	HIS
3	C	177	THR
3	C	190	ARG
3	C	191	THR
3	C	192	THR
3	C	193	TYR
3	C	196	LEU
3	C	204	LEU
4	D	9	CYS

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Mol	Chain	Res	Type
4	D	11	LEU
4	D	12	CYS
4	D	19	LEU
4	D	25	ARG
4	D	26	CYS
4	D	35	ARG
4	D	57	ARG
4	D	59	ARG
4	D	61	LYS
4	D	64	LEU
4	D	65	ARG
4	D	76	ARG
4	D	97	LEU
4	D	108	LEU
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	135	LEU
4	D	137	SER
4	D	141	ARG
4	D	145	GLU
4	D	148	VAL
4	D	154	ASN
4	D	165	MET
4	D	170	VAL
4	D	178	VAL
4	D	181	MET
4	D	186	LEU
4	D	187	ARG
4	D	191	ARG
4	D	192	GLU
4	D	194	LEU
4	D	202	LEU
5	E	6	PHE
5	E	12	LEU
5	E	14	ARG
5	E	16	THR
5	E	18	ARG
5	E	19	MET
5	E	24	ARG
5	E	25	ARG
5	E	26	PHE

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Mol	Chain	Res	Type
5	E	31	LEU
5	E	32	VAL
5	E	41	VAL
5	E	43	LEU
5	E	47	LYS
5	E	53	LEU
5	E	60	TYR
5	E	64	ARG
5	E	66	MET
5	E	71	LEU
5	E	72	GLN
5	E	78	HIS
5	E	79	GLU
5	E	83	GLU
5	E	87	SER
5	E	88	LYS
5	E	100	VAL
5	E	105	VAL
5	E	109	ILE
5	E	116	THR
5	E	118	ILE
5	E	123	LEU
5	E	125	SER
5	E	131	ILE
5	E	136	MET
5	E	144	THR
5	E	148	VAL
5	E	150	ARG
5	E	151	LEU
6	F	10	LEU
6	F	13	ASN
6	F	14	LEU
6	F	19	LEU
6	F	21	LEU
6	F	24	GLU
6	F	25	ILE
6	F	31	GLU
6	F	32	ASN
6	F	36	ARG
6	F	40	VAL
6	F	43	LEU
6	F	45	LEU

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Mol	Chain	Res	Type
6	F	47	ARG
6	F	54	LYS
6	F	61	LEU
6	F	65	VAL
6	F	69	GLU
6	F	70	ASP
6	F	74	ASP
6	F	77	ARG
6	F	80	ARG
6	F	86	ARG
6	F	92	LYS
6	F	95	GLU
6	F	98	LEU
7	G	6	ARG
7	G	12	LEU
7	G	22	LEU
7	G	27	ILE
7	G	47	CYS
7	G	53	LYS
7	G	54	THR
7	G	60	LYS
7	G	61	VAL
7	G	63	LYS
7	G	64	GLN
7	G	66	VAL
7	G	73	MET
7	G	77	SER
7	G	84	ASN
7	G	86	GLN
7	G	87	VAL
7	G	98	SER
7	G	110	GLN
7	G	114	ARG
7	G	122	HIS
7	G	125	MET
7	G	126	ASP
7	G	129	GLU
7	G	136	LYS
7	G	146	GLU
7	G	149	ARG
8	H	11	THR
8	H	12	ARG

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Mol	Chain	Res	Type
8	H	18	ARG
8	H	19	VAL
8	H	21	LYS
8	H	23	SER
8	H	24	THR
8	H	26	VAL
8	H	51	VAL
8	H	63	LEU
8	H	68	ARG
8	H	82	HIS
8	H	85	ARG
8	H	87	SER
8	H	88	LYS
8	H	91	ARG
8	H	92	ARG
8	H	95	VAL
8	H	97	VAL
8	H	98	LYS
8	H	99	GLU
8	H	102	ARG
8	H	118	VAL
8	H	121	ASP
8	H	126	LYS
8	H	127	LEU
8	H	129	VAL
8	H	136	GLU
8	H	138	TRP
9	I	12	GLU
9	I	16	ARG
9	I	26	VAL
9	I	27	THR
9	I	29	ASN
9	I	44	VAL
9	I	47	LEU
9	I	48	GLU
9	I	56	LEU
9	I	58	HIS
9	I	64	THR
9	I	66	ARG
9	I	70	LYS
9	I	77	ILE
9	I	79	LEU

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Mol	Chain	Res	Type
9	I	85	LEU
9	I	91	ASP
9	I	92	TYR
9	I	93	ARG
9	I	95	LYS
9	I	96	LEU
9	I	99	LEU
9	I	101	PHE
9	I	102	LEU
9	I	104	ARG
9	I	109	VAL
9	I	116	LYS
9	I	118	LYS
9	I	121	ARG
9	I	126	SER
10	J	16	LEU
10	J	23	ILE
10	J	42	THR
10	J	48	THR
10	J	55	LYS
10	J	61	GLU
10	J	62	HIS
10	J	64	GLU
10	J	66	ARG
10	J	68	HIS
10	J	69	ASN
10	J	71	LEU
10	J	75	ILE
10	J	78	ASN
10	J	79	ARG
10	J	87	THR
10	J	94	VAL
10	J	95	GLU
10	J	96	ILE
10	J	97	GLU
11	K	11	LYS
11	K	12	ARG
11	K	14	VAL
11	K	18	ARG
11	K	29	ILE
11	K	30	VAL
11	K	40	ILE

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Mol	Chain	Res	Type
11	K	51	LYS
11	K	67	ASP
11	K	70	LYS
11	K	75	TYR
11	K	81	ASP
11	K	91	ARG
11	K	92	GLU
11	K	105	VAL
11	K	108	ILE
11	K	114	VAL
11	K	123	LYS
11	K	124	LYS
11	K	125	PHE
11	K	126	ARG
12	L	6	THR
12	L	10	LEU
12	L	20	LYS
12	L	33	ARG
12	L	37	CYS
12	L	39	VAL
12	L	47	LYS
12	L	55	VAL
12	L	59	ARG
12	L	60	LEU
12	L	62	SER
12	L	64	TYR
12	L	66	VAL
12	L	79	GLU
12	L	96	VAL
12	L	97	ARG
12	L	111	LYS
12	L	113	ARG
12	L	120	TYR
13	M	14	ARG
13	M	25	ILE
13	M	27	LYS
13	M	35	GLU
13	M	36	LYS
13	M	46	LYS
13	M	50	GLU
13	M	56	LEU
13	M	64	TRP

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Mol	Chain	Res	Type
13	M	65	LYS
13	M	69	GLU
13	M	71	ARG
13	M	79	LYS
13	M	81	LEU
13	M	86	CYS
13	M	102	ARG
13	M	103	THR
13	M	105	THR
13	M	109	THR
13	M	114	ARG
13	M	117	VAL
14	N	21	TYR
14	N	22	THR
14	N	27	CYS
14	N	29	ARG
14	N	46	GLU
14	N	53	LEU
14	N	57	ARG
15	O	4	THR
15	O	9	GLN
15	O	21	ASP
15	O	22	THR
15	O	32	LEU
15	O	33	THR
15	O	36	ILE
15	O	38	ARG
15	O	39	LEU
15	O	45	VAL
15	O	47	LYS
15	O	58	MET
15	O	59	MET
15	O	68	ARG
15	O	70	LEU
15	O	77	ARG
15	O	87	ILE
16	P	11	SER
16	P	28	ARG
16	P	33	ILE
16	P	44	THR
16	P	45	THR
16	P	53	VAL

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Mol	Chain	Res	Type
16	P	54	GLU
16	P	55	ARG
16	P	57	ARG
16	P	69	THR
16	P	75	ARG
16	P	81	ARG
16	P	82	GLN
17	Q	4	LYS
17	Q	12	SER
17	Q	20	THR
17	Q	23	VAL
17	Q	25	ARG
17	Q	53	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	62	SER
17	Q	72	ARG
17	Q	77	VAL
17	Q	78	GLU
17	Q	86	GLU
17	Q	89	LEU
17	Q	90	ILE
17	Q	92	ARG
17	Q	97	SER
17	Q	98	LEU
17	Q	99	SER
17	Q	100	LYS
18	R	26	LEU
18	R	31	LEU
18	R	39	VAL
18	R	42	ARG
18	R	46	GLU
18	R	50	ILE
18	R	55	ARG
18	R	69	THR
18	R	70	ILE
18	R	75	ILE
18	R	82	THR
18	R	86	VAL
18	R	87	ARG
19	S	6	LYS
19	S	11	VAL

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Mol	Chain	Res	Type
19	S	12	ASP
19	S	13	ASP
19	S	20	LEU
19	S	22	LEU
19	S	36	ARG
19	S	39	THR
19	S	43	GLU
19	S	56	GLN
19	S	61	TYR
19	S	64	GLU
19	S	70	LYS
19	S	78	ARG
19	S	79	THR
20	T	10	LEU
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	36	LEU
20	T	41	ILE
20	T	43	LEU
20	T	53	LEU
20	T	54	LYS
20	T	57	ARG
20	T	60	GLU
20	T	71	THR
20	T	75	ASN
20	T	80	ARG
20	T	86	ARG
20	T	87	LYS
20	T	91	LEU
20	T	92	LEU
21	U	6	ARG
21	U	10	ARG
21	U	13	ILE
21	U	17	THR
21	U	22	ARG
21	U	25	LYS

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

Mol	Chain	Res	Type
4	D	42	GLN
4	D	43	HIS
4	D	123	HIS
5	E	127	ASN
6	F	7	ASN
9	I	73	GLN
13	M	77	ASN
19	S	47	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	379 (25%)	43 (2%)

All (379) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	22	G
1	A	31	G
1	A	32	A
1	A	33	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	55	A
1	A	66	G
1	A	74	C
1	A	75	G
1	A	79	G
1	A	80	G
1	A	81	U
1	A	82	U
1	A	92	C
1	A	93	G
1	A	97	G
1	A	99	C

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Mol	Chain	Res	Type
1	A	108	G
1	A	115	G
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	135	C
1	A	148	G
1	A	151	A
1	A	157	G
1	A	159	G
1	A	160	A
1	A	163	C
1	A	181	G
1	A	182	U
1	A	183	G
1	A	190(D)	U
1	A	190(E)	U
1	A	190(L)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	247	G
1	A	251	G
1	A	252	U
1	A	256	U
1	A	265	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	292	G
1	A	299	G
1	A	316	G
1	A	321	A
1	A	328	C
1	A	332	G
1	A	344	A

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Mol	Chain	Res	Type
1	A	345	C
1	A	346	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	374	A
1	A	382	A
1	A	384	G
1	A	390	C
1	A	392	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	420	U
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	450	G
1	A	452	A
1	A	460	A
1	A	461	C
1	A	476	G
1	A	481	G
1	A	485	G
1	A	486	U
1	A	496	A
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A

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Mol	Chain	Res	Type
1	A	511	C
1	A	512	U
1	A	518	C
1	A	519	C
1	A	521	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	536	C
1	A	538	G
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	566	G
1	A	568	G
1	A	571	U
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	625	G
1	A	629	G
1	A	644	G
1	A	650	G
1	A	653	A
1	A	665	A
1	A	670	G
1	A	671	G
1	A	687	A
1	A	688	G
1	A	693	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	723	U

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Mol	Chain	Res	Type
1	A	724	G
1	A	731	G
1	A	733	A
1	A	734	G
1	A	740	U
1	A	749	C
1	A	755	G
1	A	761	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	783	C
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	810	C
1	A	812	C
1	A	813	U
1	A	817	C
1	A	818	G
1	A	827	U
1	A	828	A
1	A	829	G
1	A	838	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	855	G
1	A	857	C
1	A	859	A
1	A	872	A
1	A	873	A
1	A	888	G
1	A	889	A
1	A	897	C
1	A	902	G
1	A	922	G
1	A	925	G

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Mol	Chain	Res	Type
1	A	927	G
1	A	931	C
1	A	932	C
1	A	934	C
1	A	935	A
1	A	936	C
1	A	937	A
1	A	941	G
1	A	944	G
1	A	954	G
1	A	960	U
1	A	962	C
1	A	963	G
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	982	U
1	A	983	A
1	A	984	C
1	A	985	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1011	G
1	A	1012	U
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1030(B)	C
1	A	1030(C)	G

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Mol	Chain	Res	Type
1	A	1030(D)	A
1	A	1040	U
1	A	1042	G
1	A	1045	C
1	A	1048	G
1	A	1050	G
1	A	1053	G
1	A	1055	A
1	A	1060	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1078	U
1	A	1079	G
1	A	1081	G
1	A	1085	U
1	A	1092	A
1	A	1093	A
1	A	1095	U
1	A	1101	A
1	A	1103	C
1	A	1104	G
1	A	1111	A
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	1132	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1153	C
1	A	1154	G
1	A	1157	A
1	A	1159	U
1	A	1164	G
1	A	1171	G

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Mol	Chain	Res	Type
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1207	2MG
1	A	1209	C
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1233	G
1	A	1238	A
1	A	1241	G
1	A	1243	C
1	A	1244	C
1	A	1250	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1263	C
1	A	1270	C
1	A	1273	G
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1289	A
1	A	1297	C

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Mol	Chain	Res	Type
1	A	1298	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1306	A
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1336	C
1	A	1340	A
1	A	1352	C
1	A	1353	G
1	A	1359	C
1	A	1360	A
1	A	1363	A
1	A	1364	U
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1390	U
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1411	C
1	A	1413	A
1	A	1416	G
1	A	1417	G
1	A	1418	A
1	A	1436	U
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1473	A
1	A	1475	G
1	A	1477	C
1	A	1483	A
1	A	1484	C

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Mol	Chain	Res	Type
1	A	1489	G
1	A	1490	U
1	A	1491	G
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1500	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1533	C
1	A	1540	PSU

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	91	C
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	250	A
1	A	251	G
1	A	344	A
1	A	350	G
1	A	372	C
1	A	422	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	509	A
1	A	518	C
1	A	559	A
1	A	687	A
1	A	701	C

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Mol	Chain	Res	Type
1	A	748	C
1	A	777	A
1	A	792	A
1	A	809	G
1	A	812	C
1	A	828	A
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1139	G
1	A	1145	C
1	A	1181	G
1	A	1196	U
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1358	U
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1400	1	19,22,23	1.44	5 (26%)	26,32,35	1.12	1 (3%)
1	MA6	A	1519[B]	1	19,26,27	1.64	5 (26%)	18,38,41	0.71	0
1	PSU	A	516	1	18,21,22	1.19	1 (5%)	21,30,33	1.79	4 (19%)
1	7MG	A	527	22,1	23,26,27	3.75	7 (30%)	27,39,42	2.28	10 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	M2G	A	966	1	20,27,28	1.33	2 (10%)	19,40,43	1.47	2 (10%)
1	MA6	A	1518[B]	1	19,26,27	1.31	3 (15%)	18,38,41	0.74	0
1	MA6	A	1519[A]	1	19,26,27	1.22	2 (10%)	18,38,41	0.67	0
1	PSU	A	1540	1	18,21,22	1.16	1 (5%)	21,30,33	1.86	5 (23%)
1	MA6	A	1518[A]	1	19,26,27	1.12	2 (10%)	18,38,41	0.68	0
1	PSU	A	1541	1	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
1	4OC	A	1402	1	20,23,24	1.78	5 (25%)	25,32,35	0.76	0
1	2MG	A	1207	1	18,26,27	1.72	4 (22%)	16,38,41	1.45	3 (18%)
1	5MC	A	1404	1	19,22,23	1.54	3 (15%)	26,32,35	1.52	4 (15%)
1	5MC	A	1407	1	19,22,23	1.64	4 (21%)	26,32,35	1.24	2 (7%)
1	UR3	A	1498	1	19,22,23	1.05	2 (10%)	26,32,35	1.40	4 (15%)
1	5MC	A	967	1	19,22,23	1.33	2 (10%)	26,32,35	1.02	2 (7%)
12	0TD	L	92	12	8,9,10	1.16	0	6,11,13	3.02	4 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1519[B]	1	-	5/7/29/30	0/3/3/3
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	22,1	-	2/7/37/38	0/3/3/3
1	M2G	A	966	1	-	2/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	3/7/29/30	0/3/3/3
1	MA6	A	1519[A]	1	-	3/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	2/7/29/30	0/3/3/3
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	4/9/29/30	0/2/2/2
1	2MG	A	1207	1	-	4/5/27/28	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	4/7/25/26	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-15.91	1.35	1.45
1	A	1407	5MC	C5-C4	5.48	1.48	1.44
1	A	1404	5MC	C5-C4	5.15	1.48	1.44
1	A	1207	2MG	C6-N1	4.63	1.44	1.37
1	A	967	5MC	C5-C4	-4.41	1.40	1.44
1	A	527	7MG	C5-N7	4.30	1.41	1.35
1	A	1402	4OC	CM4-N4	4.14	1.53	1.45
1	A	516	PSU	C6-C5	3.95	1.39	1.35
1	A	966	M2G	C2-N3	3.95	1.36	1.30
1	A	1540	PSU	C6-C5	3.90	1.39	1.35
1	A	1541	PSU	C6-C5	3.80	1.39	1.35
1	A	1402	4OC	C4-N4	3.78	1.43	1.36
1	A	1519[B]	MA6	C6-N1	3.76	1.37	1.32
1	A	1518[B]	MA6	C6-N1	3.75	1.37	1.32
1	A	1519[B]	MA6	C4-N3	3.37	1.40	1.35
1	A	527	7MG	C2-N2	3.37	1.42	1.34
1	A	1519[A]	MA6	C6-N1	3.37	1.37	1.32
1	A	1207	2MG	C2-N1	3.27	1.41	1.36
1	A	1518[A]	MA6	C6-C5	-3.22	1.39	1.44
1	A	1519[B]	MA6	C2-N3	3.07	1.36	1.32
1	A	1402	4OC	C2-N1	3.00	1.46	1.40
1	A	527	7MG	O6-C6	-2.99	1.17	1.23
1	A	1402	4OC	C2-N3	2.92	1.42	1.36
1	A	1400	5MC	C6-C5	2.91	1.39	1.34
1	A	1407	5MC	C2-N1	2.90	1.46	1.40
1	A	1400	5MC	C2-N3	2.89	1.42	1.36
1	A	1207	2MG	C2-N2	2.88	1.39	1.33
1	A	1519[B]	MA6	C2-N1	2.82	1.38	1.33
1	A	1498	UR3	C4-N3	-2.76	1.35	1.40
1	A	527	7MG	C4-N9	-2.76	1.34	1.37
1	A	966	M2G	C2-N2	2.75	1.40	1.35
1	A	1400	5MC	C2-N1	2.74	1.45	1.40
1	A	1404	5MC	C2-N1	2.74	1.45	1.40
1	A	527	7MG	C6-N1	-2.63	1.33	1.38
1	A	1518[A]	MA6	C6-N1	2.63	1.36	1.32
1	A	1207	2MG	C5-C6	-2.62	1.42	1.47
1	A	1498	UR3	C6-N1	-2.60	1.31	1.38
1	A	1519[A]	MA6	C6-C5	-2.53	1.41	1.44
1	A	967	5MC	C2-N3	2.52	1.41	1.36
1	A	1400	5MC	C4-N4	2.42	1.40	1.34
1	A	1407	5MC	C2-N3	2.39	1.41	1.36
1	A	527	7MG	C2-N1	-2.37	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1519[B]	MA6	C6-C5	-2.36	1.41	1.44
1	A	1518[B]	MA6	C2-N1	2.13	1.37	1.33
1	A	1400	5MC	C5-C4	2.12	1.45	1.44
1	A	1402	4OC	C5-C4	2.12	1.45	1.41
1	A	1404	5MC	C2-N3	2.06	1.40	1.36
1	A	1518[B]	MA6	C6-N6	2.03	1.42	1.37
1	A	1407	5MC	C4-N4	2.01	1.39	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	5.76	121.07	110.94
1	A	1540	PSU	C4-N3-C2	-4.86	119.68	126.37
1	A	1541	PSU	N1-C2-N3	4.86	120.29	115.17
1	A	1541	PSU	C4-N3-C2	-4.64	119.99	126.37
1	A	1540	PSU	N1-C2-N3	4.50	119.91	115.17
1	A	516	PSU	N1-C2-N3	4.43	119.84	115.17
1	A	966	M2G	O6-C6-N1	-4.42	115.37	120.62
1	A	527	7MG	C2-N3-C4	4.35	119.80	112.30
1	A	1404	5MC	N4-C4-N3	-4.27	110.78	118.51
12	L	92	0TD	CSB-SB-CB	-4.26	94.71	102.36
12	L	92	0TD	CB-CA-N	-4.22	100.55	109.10
1	A	516	PSU	C4-N3-C2	-4.20	120.59	126.37
1	A	527	7MG	C6-C5-C4	-3.96	115.44	122.40
1	A	1207	2MG	O6-C6-N1	-3.88	116.02	120.62
1	A	527	7MG	C6-C5-N7	3.74	137.73	131.93
1	A	1407	5MC	N4-C4-N3	-3.51	112.15	118.51
1	A	966	M2G	O6-C6-C5	3.44	131.14	124.32
1	A	527	7MG	C5-C4-N3	-3.44	121.68	128.13
1	A	516	PSU	C6-N1-C2	-3.36	119.57	122.69
1	A	1207	2MG	O6-C6-C5	3.32	130.90	124.32
1	A	1404	5MC	C5-C4-N3	3.22	125.06	121.75
1	A	1541	PSU	O2-C2-N1	-3.16	119.53	122.79
1	A	1404	5MC	C5-C6-N1	-3.12	119.92	123.31
12	L	92	0TD	OD1-CG-CB	-3.11	115.93	122.44
1	A	527	7MG	C2-N1-C6	-2.92	119.81	125.11
1	A	527	7MG	N9-C8-N7	2.85	107.40	103.37
1	A	516	PSU	O2-C2-N1	-2.82	119.88	122.79
1	A	1404	5MC	C4-N3-C2	-2.81	116.91	120.81
1	A	967	5MC	C5-C4-N3	2.75	124.58	121.75
1	A	1498	UR3	O3'-C3'-C2'	2.70	120.47	111.82
1	A	527	7MG	N9-C4-N3	2.58	129.24	125.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1400	5MC	N4-C4-N3	-2.51	113.96	118.51
1	A	1541	PSU	C6-N1-C2	-2.46	120.41	122.69
1	A	1498	UR3	C6-N1-C2	-2.38	119.85	121.80
1	A	1540	PSU	O2-C2-N1	-2.37	120.34	122.79
1	A	527	7MG	O6-C6-C5	-2.36	121.83	127.62
1	A	1498	UR3	O2-C2-N3	-2.33	118.11	121.33
1	A	1540	PSU	O4'-C1'-C2'	2.22	108.22	105.15
1	A	1407	5MC	C5-C4-N3	2.19	124.00	121.75
1	A	527	7MG	C5-C4-N9	2.15	109.09	106.33
1	A	1540	PSU	C6-N1-C2	-2.11	120.73	122.69
1	A	967	5MC	N4-C4-N3	-2.09	114.72	118.51
1	A	1207	2MG	N2-C2-N3	-2.09	117.85	120.51
12	L	92	0TD	O-C-CA	-2.07	119.45	124.77
1	A	1498	UR3	C2'-C3'-C4'	2.02	106.51	102.61

There are no chirality outliers.

All (39) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	O4'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
1	A	1519[A]	MA6	C5-C6-N6-C10
1	A	1519[B]	MA6	C5-C6-N6-C9
12	L	92	0TD	SB-CB-CG-OD1
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	1498	UR3	C3'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD2
1	A	967	5MC	C2'-C1'-N1-C6
1	A	967	5MC	C2'-C1'-N1-C2
1	A	1519[B]	MA6	N1-C6-N6-C10
1	A	1402	4OC	C2'-C1'-N1-C6
1	A	1519[B]	MA6	C3'-C4'-C5'-O5'
1	A	1402	4OC	C2'-C1'-N1-C2

There are no ring outliers.

12 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1400	5MC	3	0
1	A	516	PSU	1	0
1	A	966	M2G	3	0
1	A	1519[A]	MA6	2	0
1	A	1518[A]	MA6	2	0
1	A	1402	4OC	4	0
1	A	1207	2MG	3	0
1	A	1404	5MC	3	0
1	A	1407	5MC	1	0
1	A	1498	UR3	6	0
1	A	967	5MC	7	0
12	L	92	0TD	6	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 276 ligands modelled in this entry, 276 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.48	29 (1%) 66 47	62, 162, 316, 389	4 (0%)
2	B	234/256 (91%)	-0.52	2 (0%) 81 64	133, 184, 270, 282	0
3	C	206/239 (86%)	-0.01	12 (5%) 30 23	206, 252, 287, 299	0
4	D	208/209 (99%)	-0.19	9 (4%) 40 30	111, 168, 217, 268	0
5	E	150/162 (92%)	-0.50	1 (0%) 84 68	94, 134, 188, 231	0
6	F	101/101 (100%)	-0.80	0 100 100	133, 181, 218, 291	0
7	G	155/156 (99%)	0.12	16 (10%) 13 13	158, 220, 277, 309	0
8	H	138/138 (100%)	-0.66	0 100 100	95, 124, 178, 206	0
9	I	127/128 (99%)	-0.16	6 (4%) 37 28	171, 232, 283, 313	0
10	J	98/105 (93%)	0.56	15 (15%) 6 9	209, 279, 336, 389	0
11	K	116/129 (89%)	-0.50	2 (1%) 69 50	115, 162, 201, 226	0
12	L	123/135 (91%)	-0.45	1 (0%) 82 66	107, 168, 206, 263	0
13	M	118/126 (93%)	0.02	7 (5%) 29 23	154, 195, 252, 307	0
14	N	60/61 (98%)	0.22	3 (5%) 35 26	202, 244, 301, 320	0
15	O	87/89 (97%)	-0.11	2 (2%) 61 43	118, 158, 219, 250	0
16	P	83/88 (94%)	-0.26	1 (1%) 76 57	111, 173, 212, 270	0
17	Q	99/105 (94%)	-0.54	0 100 100	103, 137, 184, 194	0
18	R	70/88 (79%)	-0.71	0 100 100	118, 173, 224, 263	0
19	S	80/93 (86%)	-0.35	1 (1%) 74 55	207, 262, 310, 335	0
20	T	99/106 (93%)	-0.20	3 (3%) 52 37	127, 166, 233, 261	0
21	U	24/27 (88%)	0.77	4 (16%) 5 7	150, 219, 232, 233	0
All	All	3874/4063 (95%)	-0.35	114 (2%) 54 38	62, 177, 288, 389	4 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1516[A]	G	6.2
7	G	32	ARG	6.1
14	N	31	ARG	5.4
10	J	74	ILE	5.3
21	U	25	LYS	5.1
1	A	1517[A]	G	4.7
10	J	66	ARG	4.4
10	J	75	ILE	4.3
7	G	56	GLN	4.0
20	T	64	ASP	4.0
4	D	4	TYR	3.9
3	C	66	VAL	3.9
1	A	633	G	3.9
1	A	1148	U	3.8
1	A	110	C	3.7
3	C	67	THR	3.7
9	I	15	ALA	3.6
13	M	15	VAL	3.6
14	N	4	LYS	3.5
1	A	1240	U	3.5
4	D	40	PRO	3.5
20	T	68	LYS	3.5
10	J	43	ARG	3.5
3	C	201	TYR	3.4
21	U	18	TYR	3.3
9	I	9	ARG	3.2
1	A	871	U	3.1
7	G	148	ASN	3.1
7	G	109	ASN	3.1
3	C	163	ALA	3.0
4	D	86	LYS	3.0
5	E	22	GLY	3.0
3	C	164	ARG	3.0
13	M	113	PRO	3.0
1	A	1416	G	2.9
13	M	106	ASN	2.9
13	M	112	GLY	2.9
3	C	65	ALA	2.9
16	P	31	LYS	2.9
1	A	221	C	2.9
1	A	993	G	2.8
7	G	33	ASP	2.8
13	M	102	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
7	G	38	LEU	2.8
19	S	2	PRO	2.8
2	B	211	ILE	2.8
1	A	1149	C	2.7
9	I	14	VAL	2.7
7	G	106	GLN	2.7
1	A	1533	C	2.7
7	G	35	LYS	2.7
4	D	44	GLY	2.6
4	D	31	CYS	2.6
7	G	42	ILE	2.6
7	G	5	ARG	2.6
1	A	222	U	2.6
3	C	58	GLU	2.6
10	J	39	PRO	2.6
1	A	853	G	2.5
1	A	634	C	2.5
3	C	102	ASN	2.5
21	U	16	GLY	2.5
10	J	3	LYS	2.5
13	M	33	ALA	2.4
9	I	66	ARG	2.4
10	J	12	ASP	2.4
15	O	61	GLY	2.4
1	A	1520[A]	G	2.4
11	K	126	ARG	2.4
1	A	45	U	2.3
1	A	307	C	2.3
1	A	1280	A	2.3
7	G	4	ARG	2.3
10	J	27	ALA	2.3
10	J	96	ILE	2.3
13	M	13	LYS	2.3
1	A	111	G	2.3
1	A	1017	G	2.3
3	C	104	GLN	2.3
4	D	42	GLN	2.3
1	A	852	G	2.3
10	J	34	VAL	2.2
4	D	9	CYS	2.2
1	A	1227	A	2.2
11	K	111	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	155	GLY	2.2
10	J	94	VAL	2.2
1	A	125	U	2.2
2	B	51	LEU	2.2
1	A	758	G	2.2
7	G	120	ILE	2.2
10	J	41	PRO	2.2
7	G	62	PHE	2.2
4	D	2	GLY	2.2
7	G	85	TYR	2.2
12	L	128	ALA	2.2
7	G	50	ILE	2.2
4	D	41	GLY	2.1
7	G	30	ILE	2.1
9	I	108	VAL	2.1
1	A	1255	G	2.1
10	J	32	ALA	2.1
10	J	54	PHE	2.1
9	I	64	THR	2.1
3	C	159	GLY	2.1
15	O	20	GLY	2.1
14	N	3	ARG	2.0
21	U	6	ARG	2.0
10	J	4	ILE	2.0
3	C	103	VAL	2.0
1	A	1190	G	2.0
1	A	1387	G	2.0
1	A	1388	C	2.0
20	T	11	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1540	20/21	0.83	0.23	318,324,373,375	0
1	PSU	A	516	20/21	0.87	0.11	169,189,225,229	0
1	PSU	A	1541	20/21	0.91	0.18	303,317,323,326	0
1	2MG	A	1207	24/25	0.94	0.10	239,249,316,321	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	7MG	A	527	24/25	0.95	0.12	142,153,170,174	0
1	5MC	A	1407	21/22	0.96	0.07	180,203,212,220	0
1	UR3	A	1498	21/22	0.96	0.12	131,139,164,169	0
1	5MC	A	1400	21/22	0.97	0.08	125,139,150,167	0
1	MA6	A	1518[A]	24/25	0.97	0.15	133,147,161,163	24
1	MA6	A	1518[B]	24/25	0.97	0.15	132,148,153,153	24
1	4OC	A	1402	22/23	0.97	0.07	130,142,160,168	0
1	M2G	A	966	25/26	0.97	0.09	168,177,186,189	0
1	5MC	A	967	21/22	0.98	0.07	154,169,181,182	0
1	5MC	A	1404	21/22	0.98	0.07	132,144,188,193	0
1	MA6	A	1519[A]	24/25	0.99	0.09	118,127,134,135	24
1	MA6	A	1519[B]	24/25	0.99	0.09	123,131,165,167	24
12	0TD	L	92	10/11	0.99	0.10	161,185,287,345	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1802	1/1	0.41	0.35	180,180,180,180	0
22	MG	A	1747	1/1	0.47	0.37	132,132,132,132	0
22	MG	A	1742	1/1	0.51	0.35	152,152,152,152	0
22	MG	A	1789	1/1	0.57	0.33	157,157,157,157	0
22	MG	A	1843	1/1	0.57	0.39	132,132,132,132	0
22	MG	B	301	1/1	0.58	0.19	132,132,132,132	0
22	MG	A	1702	1/1	0.64	0.34	166,166,166,166	0
22	MG	A	1838	1/1	0.67	0.26	150,150,150,150	0
22	MG	A	1827	1/1	0.68	0.27	151,151,151,151	0
22	MG	A	1857	1/1	0.68	0.29	128,128,128,128	0
22	MG	A	1808	1/1	0.68	0.23	164,164,164,164	0
22	MG	A	1850	1/1	0.69	0.08	450,450,450,450	0
22	MG	A	1667	1/1	0.70	0.23	157,157,157,157	0
22	MG	Q	201	1/1	0.70	0.20	142,142,142,142	0
22	MG	A	1683	1/1	0.71	0.36	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1807	1/1	0.71	0.21	141,141,141,141	0
22	MG	A	1795	1/1	0.72	0.21	182,182,182,182	0
22	MG	A	1855	1/1	0.74	0.42	143,143,143,143	0
22	MG	A	1731	1/1	0.74	0.28	145,145,145,145	0
22	MG	A	1797	1/1	0.75	0.18	146,146,146,146	0
22	MG	A	1815	1/1	0.75	0.24	124,124,124,124	0
22	MG	A	1816	1/1	0.75	0.21	181,181,181,181	0
22	MG	A	1822	1/1	0.75	0.42	148,148,148,148	0
22	MG	A	1675	1/1	0.75	0.28	143,143,143,143	0
22	MG	A	1624	1/1	0.75	0.26	134,134,134,134	0
22	MG	A	1847	1/1	0.76	0.14	145,145,145,145	0
22	MG	A	1861	1/1	0.76	0.61	178,178,178,178	0
22	MG	A	1641	1/1	0.76	0.20	130,130,130,130	0
22	MG	A	1829	1/1	0.76	0.36	156,156,156,156	0
22	MG	A	1673	1/1	0.77	0.16	211,211,211,211	0
22	MG	A	1831	1/1	0.78	0.29	160,160,160,160	0
22	MG	A	1632	1/1	0.78	0.46	131,131,131,131	0
22	MG	A	1678	1/1	0.78	0.16	350,350,350,350	0
22	MG	D	304	1/1	0.78	0.35	147,147,147,147	0
22	MG	A	1856	1/1	0.78	0.25	143,143,143,143	0
22	MG	A	1796	1/1	0.79	0.24	121,121,121,121	0
22	MG	A	1704	1/1	0.79	0.13	211,211,211,211	0
22	MG	A	1849	1/1	0.80	0.15	550,550,550,550	0
22	MG	A	1746	1/1	0.80	0.34	111,111,111,111	0
22	MG	A	1605	1/1	0.80	0.36	103,103,103,103	0
22	MG	A	1743	1/1	0.81	0.21	147,147,147,147	0
22	MG	A	1791	1/1	0.81	0.05	294,294,294,294	0
22	MG	A	1834	1/1	0.81	0.15	138,138,138,138	0
22	MG	A	1771	1/1	0.82	0.15	127,127,127,127	0
22	MG	A	1689	1/1	0.82	0.78	214,214,214,214	0
22	MG	A	1739	1/1	0.82	0.15	139,139,139,139	0
22	MG	A	1729	1/1	0.82	0.15	119,119,119,119	0
22	MG	A	1785	1/1	0.83	0.10	184,184,184,184	0
22	MG	A	1759	1/1	0.83	0.11	126,126,126,126	0
22	MG	A	1769	1/1	0.83	0.23	151,151,151,151	0
22	MG	A	1662	1/1	0.83	0.32	108,108,108,108	0
22	MG	A	1811	1/1	0.83	0.34	156,156,156,156	0
22	MG	A	1781	1/1	0.83	0.23	158,158,158,158	0
22	MG	A	1854	1/1	0.84	0.37	149,149,149,149	0
22	MG	A	1833	1/1	0.84	0.15	182,182,182,182	0
22	MG	A	1688	1/1	0.84	0.12	164,164,164,164	0
22	MG	A	1826	1/1	0.84	0.19	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1770	1/1	0.84	0.24	103,103,103,103	0
22	MG	A	1682	1/1	0.84	0.12	180,180,180,180	0
22	MG	A	1734	1/1	0.84	0.23	139,139,139,139	0
22	MG	A	1832	1/1	0.84	0.33	149,149,149,149	0
22	MG	A	1858	1/1	0.85	0.32	147,147,147,147	0
22	MG	A	1859	1/1	0.85	0.11	147,147,147,147	0
22	MG	A	1844	1/1	0.85	0.19	132,132,132,132	0
22	MG	A	1862	1/1	0.85	0.23	161,161,161,161	0
22	MG	A	1836	1/1	0.85	0.58	143,143,143,143	0
22	MG	A	1776	1/1	0.85	0.21	139,139,139,139	0
22	MG	A	1735	1/1	0.85	0.23	93,93,93,93	0
22	MG	A	1800	1/1	0.86	0.19	158,158,158,158	0
22	MG	A	1818	1/1	0.86	0.33	109,109,109,109	0
22	MG	A	1812	1/1	0.86	0.08	417,417,417,417	0
22	MG	A	1798	1/1	0.86	0.08	163,163,163,163	0
22	MG	A	1813	1/1	0.87	0.18	520,520,520,520	0
22	MG	A	1686	1/1	0.87	0.08	241,241,241,241	0
22	MG	J	201	1/1	0.87	0.18	128,128,128,128	0
22	MG	A	1810	1/1	0.87	0.29	143,143,143,143	0
22	MG	A	1835	1/1	0.88	0.29	139,139,139,139	0
22	MG	A	1730	1/1	0.88	0.29	138,138,138,138	0
22	MG	A	1792	1/1	0.88	0.12	313,313,313,313	0
22	MG	A	1841	1/1	0.88	0.19	147,147,147,147	0
22	MG	A	1752	1/1	0.88	0.23	142,142,142,142	0
22	MG	A	1727	1/1	0.88	0.19	106,106,106,106	0
22	MG	A	1774	1/1	0.88	0.25	157,157,157,157	0
22	MG	A	1732	1/1	0.89	0.18	94,94,94,94	0
22	MG	A	1690	1/1	0.89	0.08	169,169,169,169	0
22	MG	A	1764	1/1	0.89	0.16	137,137,137,137	0
22	MG	A	1661	1/1	0.89	0.40	120,120,120,120	0
22	MG	A	1630	1/1	0.89	0.39	124,124,124,124	0
22	MG	A	1665	1/1	0.89	0.26	111,111,111,111	0
22	MG	A	1618	1/1	0.89	0.44	141,141,141,141	0
22	MG	A	1612	1/1	0.89	0.09	178,178,178,178	0
22	MG	A	1643	1/1	0.89	0.15	102,102,102,102	0
22	MG	A	1782	1/1	0.89	0.17	159,159,159,159	0
22	MG	A	1824	1/1	0.89	0.26	139,139,139,139	0
22	MG	A	1803	1/1	0.89	0.39	115,115,115,115	0
22	MG	A	1806	1/1	0.89	0.13	127,127,127,127	0
22	MG	A	1809	1/1	0.90	0.17	114,114,114,114	0
22	MG	A	1820	1/1	0.90	0.36	144,144,144,144	0
22	MG	A	1860	1/1	0.90	0.38	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1711	1/1	0.90	0.10	185,185,185,185	0
22	MG	A	1778	1/1	0.90	0.15	127,127,127,127	0
22	MG	A	1715	1/1	0.90	0.07	112,112,112,112	0
22	MG	A	1677	1/1	0.90	0.18	128,128,128,128	0
22	MG	H	201	1/1	0.90	0.20	167,167,167,167	0
22	MG	A	1694	1/1	0.90	0.27	105,105,105,105	0
22	MG	A	1762	1/1	0.90	0.40	124,124,124,124	0
22	MG	A	1723	1/1	0.91	0.16	120,120,120,120	0
22	MG	A	1685	1/1	0.91	0.17	159,159,159,159	0
22	MG	A	1714	1/1	0.91	0.29	162,162,162,162	0
22	MG	A	1853	1/1	0.91	0.33	150,150,150,150	0
22	MG	A	1783	1/1	0.91	0.15	119,119,119,119	0
22	MG	A	1828	1/1	0.91	0.21	114,114,114,114	0
22	MG	A	1784	1/1	0.91	0.08	175,175,175,175	0
22	MG	A	1745	1/1	0.91	0.12	169,169,169,169	0
22	MG	A	1625	1/1	0.91	0.41	101,101,101,101	0
22	MG	A	1687	1/1	0.92	0.10	234,234,234,234	0
22	MG	A	1666	1/1	0.92	0.17	141,141,141,141	0
22	MG	A	1719	1/1	0.92	0.22	514,514,514,514	0
22	MG	A	1721	1/1	0.92	0.27	149,149,149,149	0
22	MG	A	1772	1/1	0.92	0.22	120,120,120,120	0
22	MG	A	1679	1/1	0.92	0.14	124,124,124,124	0
22	MG	A	1775	1/1	0.92	0.16	146,146,146,146	0
22	MG	A	1725	1/1	0.92	0.10	156,156,156,156	0
22	MG	A	1680	1/1	0.92	0.23	175,175,175,175	0
22	MG	A	1657	1/1	0.92	0.11	146,146,146,146	0
22	MG	A	1821	1/1	0.92	0.38	138,138,138,138	0
22	MG	A	1842	1/1	0.92	0.64	152,152,152,152	0
22	MG	D	303	1/1	0.92	0.17	137,137,137,137	0
22	MG	A	1634	1/1	0.92	0.07	161,161,161,161	0
22	MG	A	1601	1/1	0.92	0.25	152,152,152,152	0
22	MG	A	1825	1/1	0.92	0.17	139,139,139,139	0
22	MG	A	1627	1/1	0.92	0.28	101,101,101,101	0
22	MG	A	1604	1/1	0.93	0.06	123,123,123,123	0
22	MG	A	1740	1/1	0.93	0.21	119,119,119,119	0
22	MG	A	1636	1/1	0.93	0.24	90,90,90,90	0
22	MG	A	1848	1/1	0.93	0.27	527,527,527,527	0
22	MG	A	1696	1/1	0.93	0.18	160,160,160,160	0
22	MG	A	1823	1/1	0.93	0.19	128,128,128,128	0
22	MG	C	301	1/1	0.93	0.06	143,143,143,143	0
22	MG	A	1660	1/1	0.93	0.11	155,155,155,155	0
22	MG	A	1613	1/1	0.93	0.20	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1684	1/1	0.93	0.13	135,135,135,135	0
22	MG	A	1726	1/1	0.93	0.10	349,349,349,349	0
22	MG	A	1753	1/1	0.93	0.17	136,136,136,136	0
22	MG	A	1851	1/1	0.94	0.10	366,366,366,366	0
22	MG	A	1852	1/1	0.94	0.26	530,530,530,530	0
22	MG	A	1830	1/1	0.94	0.08	130,130,130,130	0
22	MG	A	1637	1/1	0.94	0.31	116,116,116,116	0
22	MG	A	1755	1/1	0.94	0.07	150,150,150,150	0
22	MG	A	1756	1/1	0.94	0.12	112,112,112,112	0
22	MG	A	1817	1/1	0.94	0.16	148,148,148,148	0
22	MG	A	1758	1/1	0.94	0.26	103,103,103,103	0
22	MG	A	1638	1/1	0.94	0.16	189,189,189,189	0
22	MG	A	1761	1/1	0.94	0.13	147,147,147,147	0
22	MG	A	1804	1/1	0.94	0.06	120,120,120,120	0
22	MG	A	1610	1/1	0.94	0.12	112,112,112,112	0
22	MG	A	1611	1/1	0.94	0.09	184,184,184,184	0
22	MG	A	1765	1/1	0.94	0.07	126,126,126,126	0
22	MG	A	1846	1/1	0.94	0.22	126,126,126,126	0
22	MG	A	1645	1/1	0.94	0.29	141,141,141,141	0
22	MG	A	1748	1/1	0.94	0.06	177,177,177,177	0
22	MG	I	201	1/1	0.94	0.20	138,138,138,138	0
22	MG	A	1749	1/1	0.94	0.19	157,157,157,157	0
22	MG	P	101	1/1	0.94	0.42	106,106,106,106	0
22	MG	A	1703	1/1	0.94	0.14	291,291,291,291	0
22	MG	A	1733	1/1	0.95	0.14	147,147,147,147	0
22	MG	A	1790	1/1	0.95	0.07	217,217,217,217	0
22	MG	A	1664	1/1	0.95	0.17	121,121,121,121	0
22	MG	A	1623	1/1	0.95	0.05	129,129,129,129	0
22	MG	A	1724	1/1	0.95	0.09	169,169,169,169	0
22	MG	A	1646	1/1	0.95	0.11	236,236,236,236	0
22	MG	A	1741	1/1	0.95	0.11	128,128,128,128	0
22	MG	A	1705	1/1	0.95	0.12	319,319,319,319	0
22	MG	A	1780	1/1	0.95	0.12	143,143,143,143	0
22	MG	A	1628	1/1	0.95	0.14	141,141,141,141	0
22	MG	A	1617	1/1	0.95	0.20	175,175,175,175	0
22	MG	A	1608	1/1	0.95	0.05	169,169,169,169	0
22	MG	A	1718	1/1	0.95	0.20	134,134,134,134	0
22	MG	A	1626	1/1	0.95	0.58	105,105,105,105	0
22	MG	A	1840	1/1	0.95	0.19	143,143,143,143	0
22	MG	A	1668	1/1	0.96	0.20	134,134,134,134	0
22	MG	A	1754	1/1	0.96	0.09	137,137,137,137	0
22	MG	A	1793	1/1	0.96	0.22	444,444,444,444	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1814	1/1	0.96	0.13	70,70,70,70	0
22	MG	A	1773	1/1	0.96	0.13	156,156,156,156	0
22	MG	A	1670	1/1	0.96	0.09	199,199,199,199	0
22	MG	A	1744	1/1	0.96	0.04	127,127,127,127	0
22	MG	A	1672	1/1	0.96	0.23	146,146,146,146	0
22	MG	A	1819	1/1	0.96	0.09	137,137,137,137	0
22	MG	A	1654	1/1	0.96	0.17	156,156,156,156	0
22	MG	A	1760	1/1	0.96	0.15	140,140,140,140	0
22	MG	A	1738	1/1	0.96	0.12	113,113,113,113	0
22	MG	A	1710	1/1	0.96	0.16	94,94,94,94	0
22	MG	D	302	1/1	0.96	0.08	137,137,137,137	0
22	MG	A	1845	1/1	0.96	0.13	113,113,113,113	0
22	MG	A	1805	1/1	0.96	0.05	119,119,119,119	0
22	MG	A	1763	1/1	0.96	0.19	111,111,111,111	0
22	MG	A	1722	1/1	0.96	0.06	122,122,122,122	0
22	MG	A	1750	1/1	0.96	0.10	157,157,157,157	0
22	MG	A	1751	1/1	0.96	0.17	104,104,104,104	0
22	MG	A	1656	1/1	0.96	0.21	106,106,106,106	0
22	MG	A	1619	1/1	0.97	0.10	106,106,106,106	0
22	MG	A	1799	1/1	0.97	0.23	125,125,125,125	0
22	MG	A	1659	1/1	0.97	0.09	128,128,128,128	0
22	MG	A	1699	1/1	0.97	0.12	124,124,124,124	0
22	MG	A	1777	1/1	0.97	0.15	111,111,111,111	0
22	MG	A	1757	1/1	0.97	0.13	103,103,103,103	0
22	MG	A	1779	1/1	0.97	0.11	112,112,112,112	0
22	MG	A	1669	1/1	0.97	0.04	149,149,149,149	0
22	MG	A	1620	1/1	0.97	0.13	162,162,162,162	0
22	MG	A	1671	1/1	0.97	0.11	170,170,170,170	0
22	MG	A	1635	1/1	0.97	0.06	99,99,99,99	0
22	MG	A	1728	1/1	0.97	0.43	138,138,138,138	0
22	MG	A	1629	1/1	0.97	0.34	131,131,131,131	0
22	MG	A	1786	1/1	0.97	0.16	131,131,131,131	0
22	MG	A	1787	1/1	0.97	0.04	147,147,147,147	0
22	MG	A	1788	1/1	0.97	0.07	151,151,151,151	0
22	MG	A	1651	1/1	0.97	0.09	113,113,113,113	0
22	MG	A	1676	1/1	0.97	0.04	136,136,136,136	0
22	MG	A	1767	1/1	0.97	0.14	130,130,130,130	0
22	MG	E	201	1/1	0.97	0.07	177,177,177,177	0
22	MG	A	1602	1/1	0.97	0.11	168,168,168,168	0
22	MG	A	1631	1/1	0.97	0.09	154,154,154,154	0
22	MG	A	1691	1/1	0.97	0.06	155,155,155,155	0
22	MG	A	1720	1/1	0.97	0.27	196,196,196,196	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1737	1/1	0.97	0.12	119,119,119,119	0
23	ZN	D	301	1/1	0.97	0.19	154,154,154,154	0
22	MG	A	1701	1/1	0.98	0.06	161,161,161,161	0
22	MG	A	1606	1/1	0.98	0.05	107,107,107,107	0
22	MG	A	1609	1/1	0.98	0.05	120,120,120,120	0
22	MG	A	1607	1/1	0.98	0.08	105,105,105,105	0
22	MG	A	1647	1/1	0.98	0.07	175,175,175,175	0
22	MG	A	1801	1/1	0.98	0.12	129,129,129,129	0
22	MG	A	1706	1/1	0.98	0.09	105,105,105,105	0
22	MG	A	1707	1/1	0.98	0.07	208,208,208,208	0
22	MG	A	1709	1/1	0.98	0.18	169,169,169,169	0
22	MG	A	1649	1/1	0.98	0.05	150,150,150,150	0
22	MG	A	1650	1/1	0.98	0.07	104,104,104,104	0
22	MG	A	1736	1/1	0.98	0.07	99,99,99,99	0
22	MG	A	1713	1/1	0.98	0.05	229,229,229,229	0
22	MG	A	1616	1/1	0.98	0.11	85,85,85,85	0
22	MG	A	1621	1/1	0.98	0.05	149,149,149,149	0
22	MG	A	1692	1/1	0.98	0.05	165,165,165,165	0
22	MG	A	1837	1/1	0.98	0.08	87,87,87,87	0
22	MG	A	1633	1/1	0.98	0.06	198,198,198,198	0
22	MG	A	1839	1/1	0.98	0.24	144,144,144,144	0
22	MG	A	1695	1/1	0.98	0.06	113,113,113,113	0
22	MG	A	1642	1/1	0.98	0.13	98,98,98,98	0
22	MG	A	1697	1/1	0.98	0.05	133,133,133,133	0
22	MG	A	1768	1/1	0.98	0.05	166,166,166,166	0
22	MG	A	1698	1/1	0.98	0.04	186,186,186,186	0
22	MG	A	1658	1/1	0.98	0.05	156,156,156,156	0
22	MG	A	1794	1/1	0.98	0.13	278,278,278,278	0
22	MG	A	1700	1/1	0.98	0.03	204,204,204,204	0
23	ZN	N	101	1/1	0.98	0.07	223,223,223,223	0
22	MG	A	1716	1/1	0.99	0.06	118,118,118,118	0
22	MG	A	1717	1/1	0.99	0.08	157,157,157,157	0
22	MG	A	1652	1/1	0.99	0.03	132,132,132,132	0
22	MG	A	1674	1/1	0.99	0.05	136,136,136,136	0
22	MG	A	1663	1/1	0.99	0.04	162,162,162,162	0
22	MG	A	1653	1/1	0.99	0.07	76,76,76,76	0
22	MG	A	1639	1/1	0.99	0.05	82,82,82,82	0
22	MG	A	1655	1/1	0.99	0.14	156,156,156,156	0
22	MG	A	1640	1/1	0.99	0.13	186,186,186,186	0
22	MG	A	1693	1/1	0.99	0.05	160,160,160,160	0
22	MG	A	1614	1/1	0.99	0.04	141,141,141,141	0
22	MG	F	201	1/1	0.99	0.03	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1681	1/1	0.99	0.10	167,167,167,167	0
22	MG	A	1648	1/1	0.99	0.15	149,149,149,149	0
22	MG	A	1712	1/1	0.99	0.18	324,324,324,324	0
22	MG	A	1622	1/1	0.99	0.04	106,106,106,106	0
22	MG	A	1603	1/1	0.99	0.02	137,137,137,137	0
22	MG	A	1766	1/1	0.99	0.05	126,126,126,126	0
22	MG	A	1644	1/1	0.99	0.03	111,111,111,111	0
22	MG	A	1615	1/1	1.00	0.06	81,81,81,81	0
22	MG	A	1708	1/1	1.00	0.04	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.