



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 02:50 PM EST

PDB ID : 4DV1
Title : Crystal structure of the Thermus thermophilus 30S ribosomal subunit with a 16S rRNA mutation, U20G, bound with streptomycin
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2012-02-22
Resolution : 3.85 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
buster-report	:	1.1.7 (2018)
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

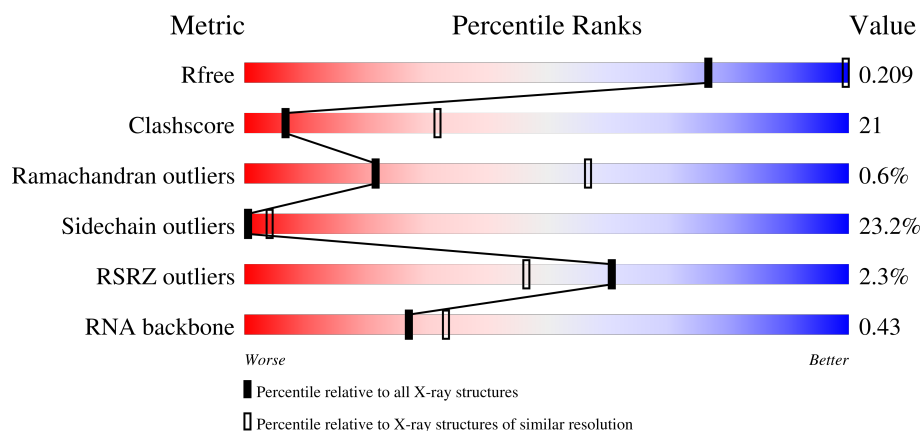
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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	1056 (4.00-3.68)
Clashscore	180529	1117 (4.00-3.68)
Ramachandran outliers	177936	1080 (4.00-3.68)
Sidechain outliers	177891	1073 (4.00-3.68)
RSRZ outliers	164620	1056 (4.00-3.68)
RNA backbone	3690	1133 (4.68-3.00)

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>21%</div> <div>42%</div> <div>29%</div> <div>8%</div> </div>
2	B	256	<div> <div>2%</div> <div>36%</div> <div>44%</div> <div>11%</div> <div>9%</div> </div>
3	C	239	<div> <div>3%</div> <div>32%</div> <div>46%</div> <div>8%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1712	-	-	-	X
23	MG	A	1730	-	-	-	X
23	MG	A	1757	-	-	-	X
23	MG	P	101	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52297 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	0	0
			32510	14478	6014	10506	1512			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	G	U	engineered mutation	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
			972	612	195	163	2			

- 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	152	141	2			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

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

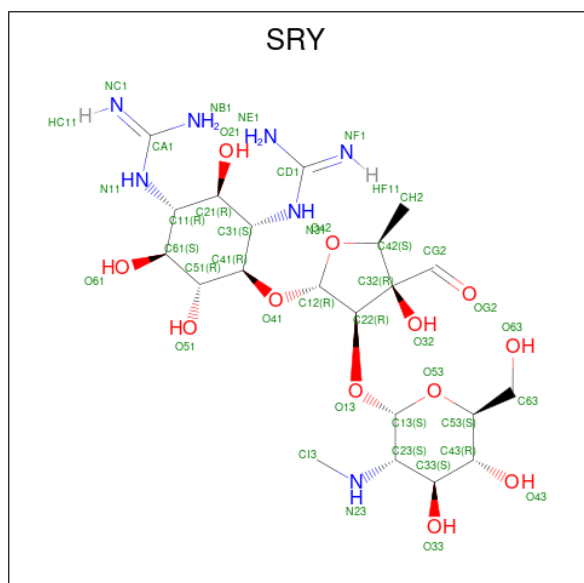
- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	230	Total 230	Mg 230	0	0
23	B	1	Total 1	Mg 1	0	0
23	D	1	Total 1	Mg 1	0	0
23	E	1	Total 1	Mg 1	0	0
23	H	2	Total 2	Mg 2	0	0
23	I	1	Total 1	Mg 1	0	0
23	J	1	Total 1	Mg 1	0	0
23	K	1	Total 1	Mg 1	0	0
23	M	2	Total 2	Mg 2	0	0
23	N	2	Total 2	Mg 2	0	0
23	P	1	Total 1	Mg 1	0	0
23	S	2	Total 2	Mg 2	0	0
23	T	2	Total 2	Mg 2	0	0

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

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	396	Total 396	O 396	0	0
25	E	6	Total 6	O 6	0	0

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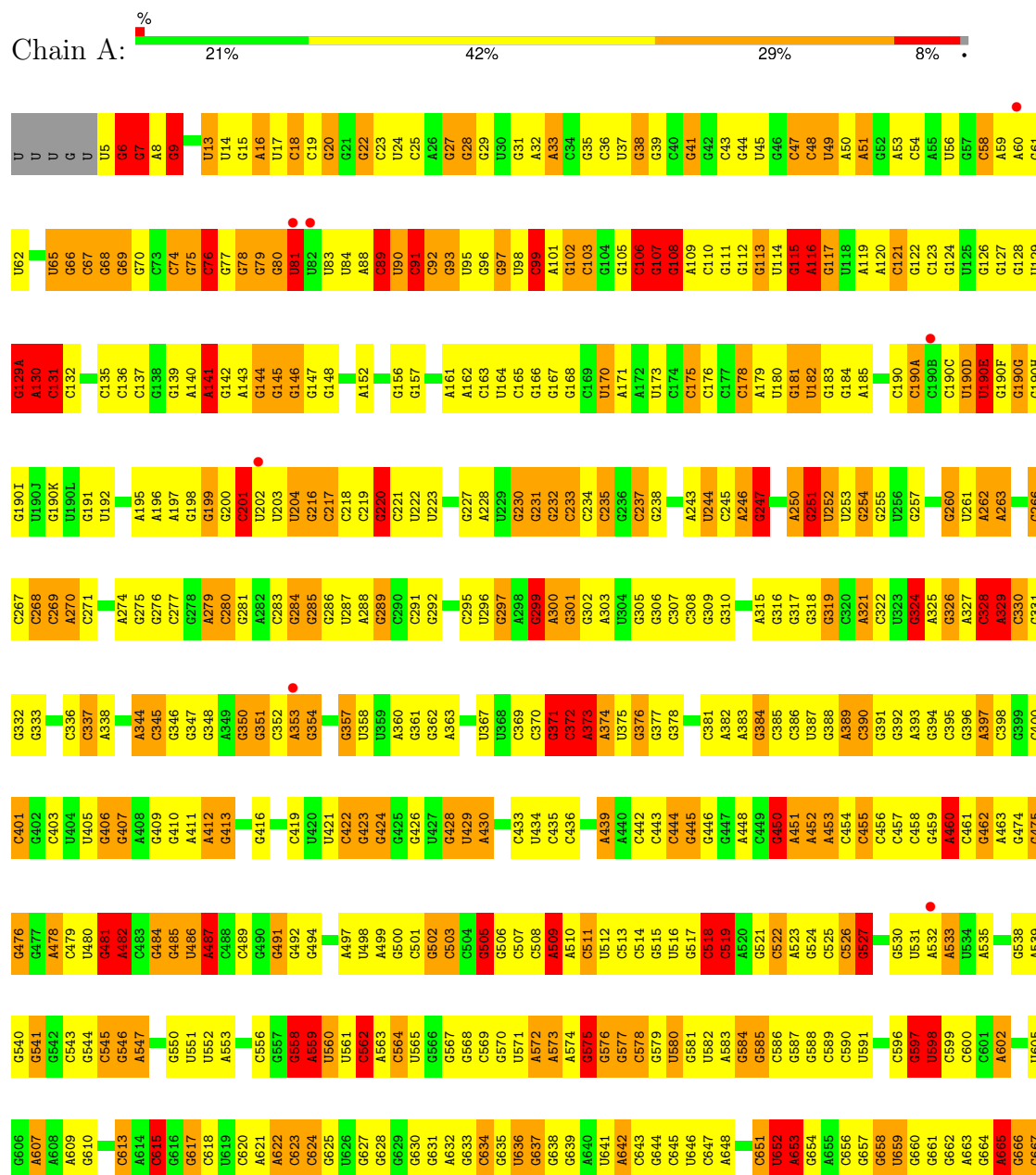
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	G	1	Total 1	O 1	0	0
25	J	1	Total 1	O 1	0	0
25	N	1	Total 1	O 1	0	0
25	Q	1	Total 1	O 1	0	0
25	T	3	Total 3	O 3	0	0
25	U	1	Total 1	O 1	0	0

3 Residue-property plots

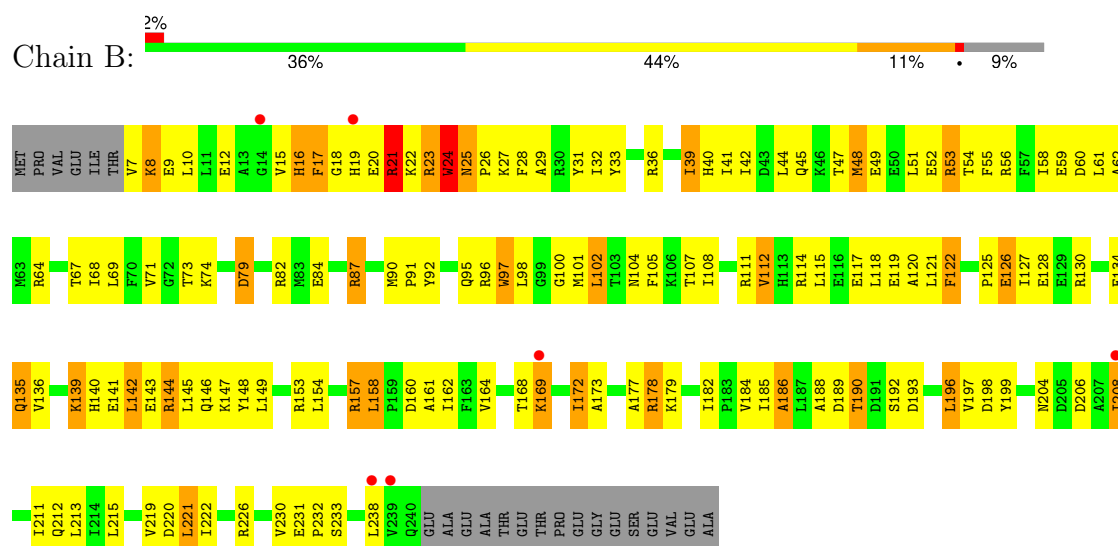
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

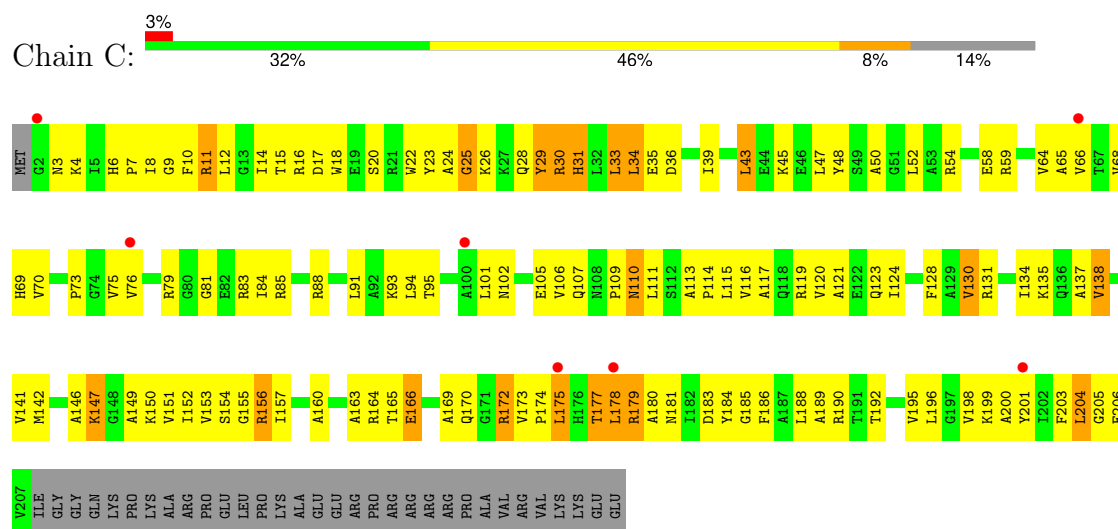


A1513	G1432	U1376	G1316	A1250	C1189	G1120	U1056	C985	G925	G861	C795	U669	G668
C1514	G1443	A1377	A1319	A1251	G1190	G1124	G1057	A956	G926	C862	C796	G670	G669
G1515	A1446	G1378	C1320	C1254	A1191	U1125	G1058	C989	G928	U863	C797	G671	G670
G1516	G1447	G1379	C1321	G1255	C1192	U1126	C1059	C990	G929	A864	G798	G672	G671
A1517	C1448	U1380	C1322	A1256	G1193	U1127	G1061	U991	C930	A865	G799	A737	A737
A1518	U1449	U1381	G1323	U1257	C1195	C1128	U1062	U992	C931	C866	G800	G674	G673
A1519	U1450	C1382	G1323	U1258	C1196	C1129	C1063	G993	C932	C867	U803	G675	G674
G1520	A1451	C1383	A1324	C1259	U1197	C1130	G1064	G998	G933	G868	A802	A765	A764
G1521	G1452	C1384	C1325	C1260	G1198	A1131	U1065	C999	C934	G869	G803	A766	A765
G1522	G1453	G1385	C1326	A1261	U1199	C1132	C1066	U1000	A935	U871	U804	U677	U676
G1523	G1454	G1385	C1327	A1261	U1199	C1132	C1066	U1000	A936	A872	C805	U678	U677
C1524	G1455	U1391	C1328	C1262	C1200	G1133	G1068	A1001	A937	A873	A807	C679	C678
G1525	G1392	C1329	A1329	C1263	A1201	G1138	C1069	G1002	A938	G874	C808	C681	C680
G1526	U1393	U1330	U1330	C1264	G1202	C1139	C1070	G1003	A939	C875	C809	G682	G681
C1527	A1394	G1331	A1331	G1265	C1203	G1140	C1071	G1003A	C940	C876	C810	U686	U685
U1528	C1395	A1332	A1332	G1266	A1204	C1141	C1072	A1004	G941	C877	C811	U687	U686
G1529	A1396	G1333	A1333	C1267	G1205	C1141	U1073	A1005	G942	C878	C812	U688	U687
G1530	C1397	G1334	G1334	A1268	G1207	C1144	G1074	C1006	U943	C879	U813	G689	G688
A1531	A1398	C1335	C1335	A1269	C1208	C1145	C1075	C1007	G944	C880	A814	C689	C688
U1532	C1399	C1336	C1336	A1270	C1209	C1146	C1075	C1008	G945	C881	A815	C690	C689
C1533	G1400	G1337	G1337	G1276	C1210	C1147	U1078	G1009	G946	C882	A816	G691	G690
C	A1473	A1338	A1338	C1277	C1211	U1148	U1079	A1014	A947	C883	C817	U692	U691
A	G1474	G1339	G1339	U1278	G1212	U1148	U1079	A1015	G948	C884	G818	U693	U692
C	G1475	A1340	U1341	U1279	A1213	C1149	A1080	U1020	A949	C885	A819	G694	G693
U	G1476	U1341	U1341	A1280	C1214	C1152	U1083	U1021	U950	C886	U820	A695	A694
C	C1477	G1342	G1342	U1281	G1215	C1153	U1084	G1022	G951	C887	G822	A696	A695
G1539	C1478	G1343	G1343	U1282	C1216	C1154	U1085	G1023	U952	C888	C823	U697	U696
U1540	C1479	C1344	C1344	C1283	C1217	G1155	G1089	G1024	G953	A889	C824	G700	G700
U1541	A1480	U1345	U1345	G1284	C1218	G1156	U1090	G1025	G954	U891	C825	A702	A701
U1542	U1481	A1346	A1346	A1285	G1219	C1157	U1091	U1026	U955	U892	C826	A703	A702
C1543	G1482	G1347	G1347	A1286	G1220	C1158	U1092	C1027	U956	A892	U827	G703	G703
U1544	A1483	U1348	U1348	A1287	C1221	C1159	A1092	C1028	U957	C893	U828	A706	A706
		A1349	A1349	A1288	G1222	U1159	C1093	C1029	A958	G894	A829	C707	C707
		C1350	C1350	A1289	C1223	G1160	A1093	G1030	A959	G895	G830	C708	C708
		U1351	U1351	G1290	C1224	C1161	U1094	C1030	U960	C896	U831	G709	G709
		G1352	G1352	G1291	A1225	C1162	C1095	G1030A	U961	C897	C832	G710	G710
		C1353	C1353	U1292	C1226	G1163	C1096	C1030B	C962	G898	C833	G711	G711
		U1354	U1354	U1293	A1227	G1164	C1097	C1032	G963	C899	U833	G712	G712
		G1355	G1355	G1294	C1228	C1165	C1098	G1033	A964	A900	C834	G713	G713
		C1356	C1356	G1295	A1229	G1174	U1099	G1034	A965	A901	U835	G714	G714
		A1357	A1357	G1296	C1230	A1168	C1100	G1034	G966	G902	G836	A715	A715
		U1358	U1358	C1297	G1231	A1169	A1101	G1038	G967	G906	G837	G719	G719
		G1359	G1359	C1297	G1232	C1171	A1102	C1039	A968	G907	U839	G720	G720
		A1360	A1360	G1300	G1233	G1172	G1103	G1042	A869	A909	C940	G721	G721
		G1361	G1361	U1301	C1234	G1173	G1104	C1043	C970	C910	U841	U722	U722
		C1361A	C1361A	U1302	U1235	G1174	A1105	C1044	C971	C911	U842	U723	U723
		C1362	C1362	U1303	A1236	G1175	G1106	C1045	A974	A914	C948	G724	G724
		A1363	A1363	C1303	C1237	G1176	C1107	C1046	A975	A915	C949	G725	G725
		U1364	U1364	G1304	G1238	G1177	G1108	C1047	A976	A916	U850	G726	G726
		G1365	G1365	G1305	A1239	G1178	C1109	C1048	A977	A917	G851	G727	G727
		C1366	C1366	U1306	U1240	G1179	A1110	C1049	A978	A918	U852	U728	U728
		G1367	G1367	U1307	G1241	A1180	A1111	C1050	A979	A919	C857	A729	A729
		C1368	C1368	U1308	C1242	G1181	C1112	C1051	A980	U920	C858	G730	G730
		A1369	A1369	G1309	C1243	G1182	C1113	C1052	A981	U921	G859	G731	G731
		G1370	G1370	U1310	C1244	A1183	C1114	C1053	A982	U922	A860	A794	A794
		A1371	A1371	G1311	A1245	G1184	C1115	C1054	A983	C924			
		G1371	G1371	G1312	C1246	G1185	C1116	U1054	A984				
		U1372	U1372	U1313	U1247	G1186	C1117	C1055	A985				
		G1373	G1373	C1314	A1248	G1187	C1118	C1056	A986				
		A1374	A1374	U1315	C1249	G1188	C1119	A1055	A987				
		U1375	U1375	U1315	C1249	G1188	C1119	A1055	A988				

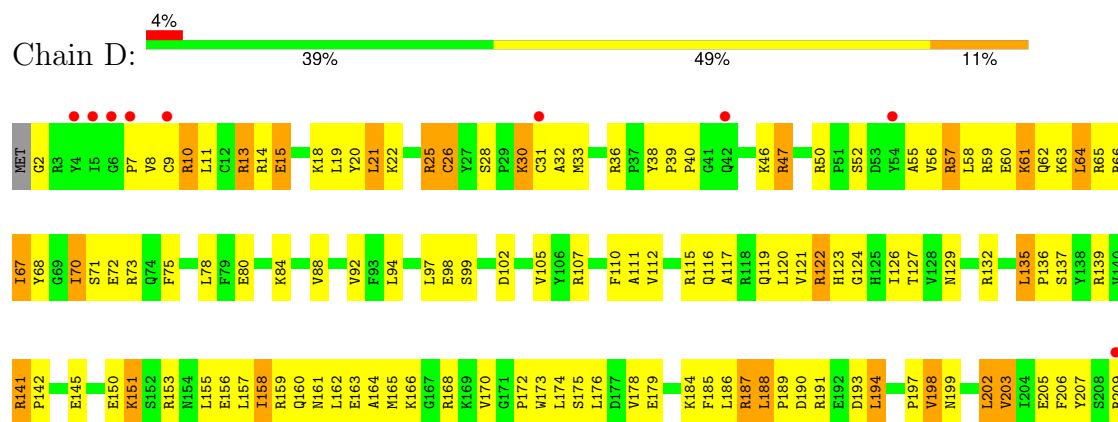
• Molecule 2: ribosomal protein S2



• Molecule 3: ribosomal protein S3

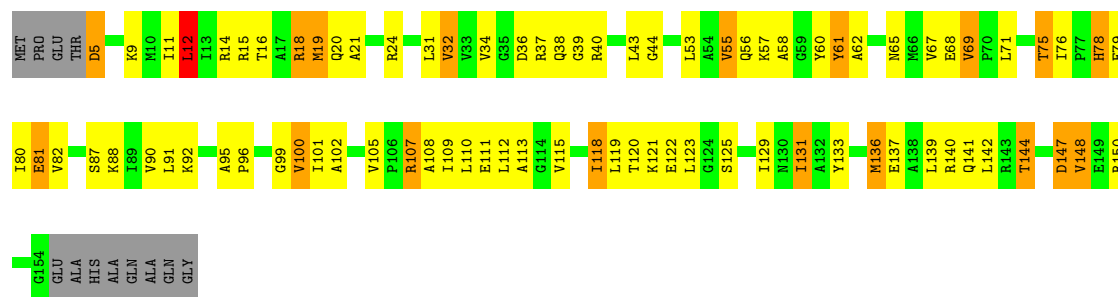


• Molecule 4: ribosomal protein S4

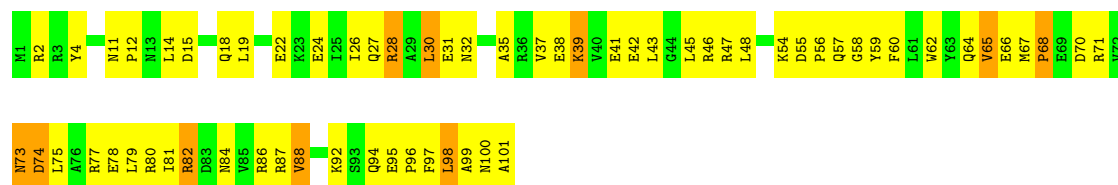


• Molecule 5: ribosomal protein S5

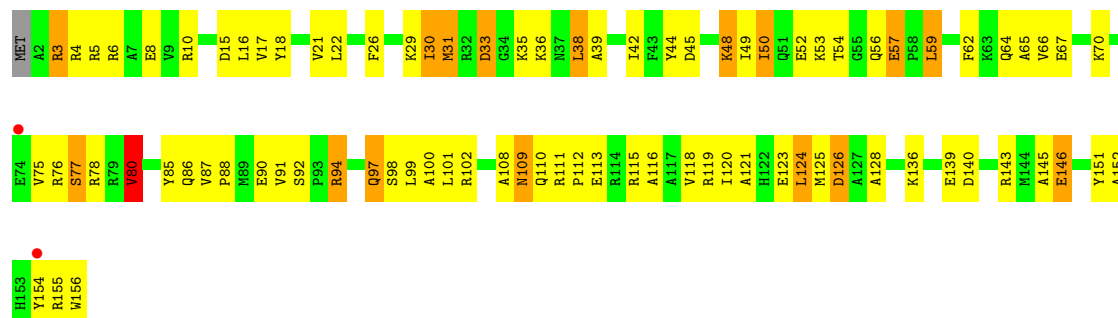
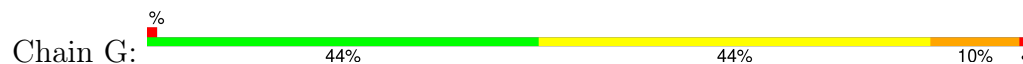




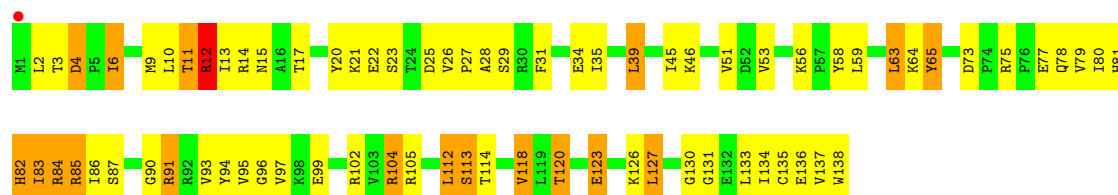
• Molecule 6: ribosomal protein S6



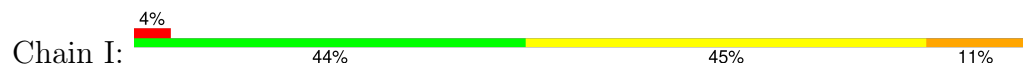
• Molecule 7: ribosomal protein S7



• Molecule 8: ribosomal protein S8

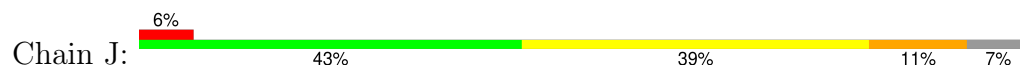


• Molecule 9: ribosomal protein S9

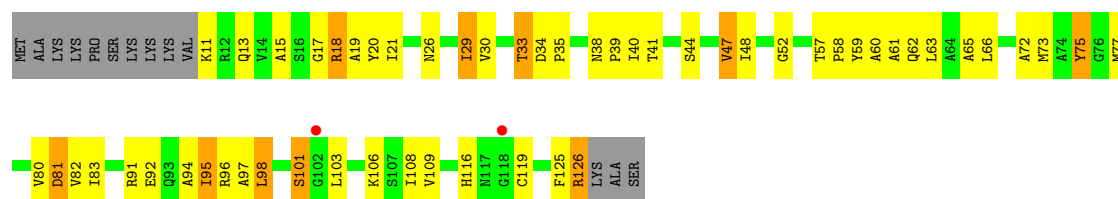




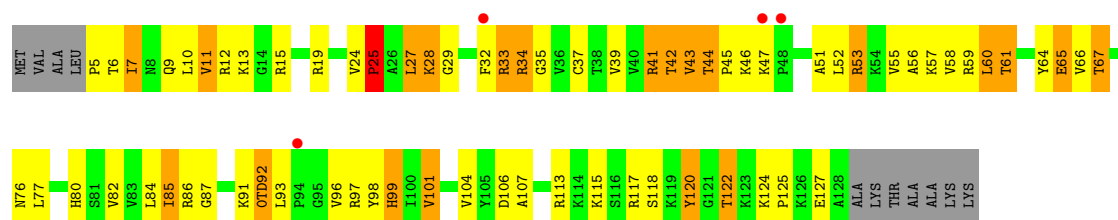
• Molecule 10: ribosomal protein S10



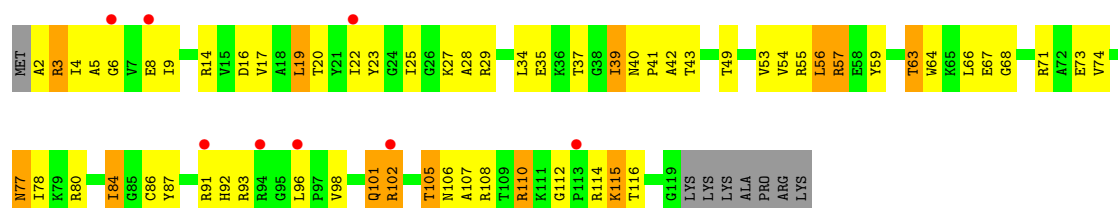
• Molecule 11: ribosomal protein S11



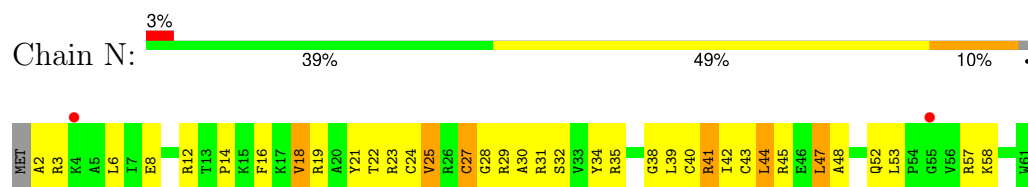
• Molecule 12: ribosomal protein S12



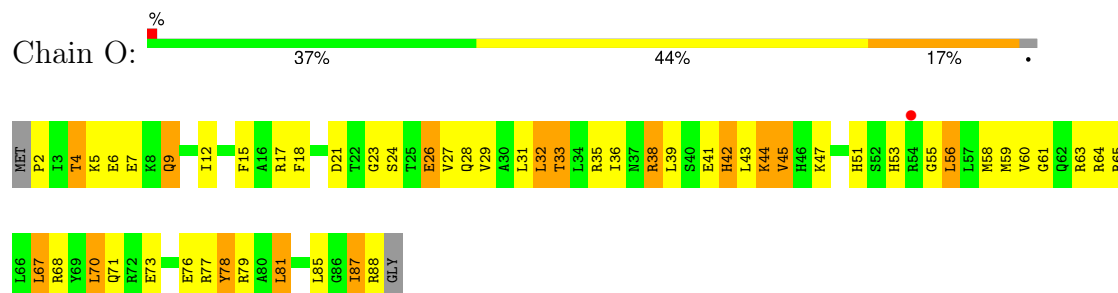
• Molecule 13: ribosomal protein S13



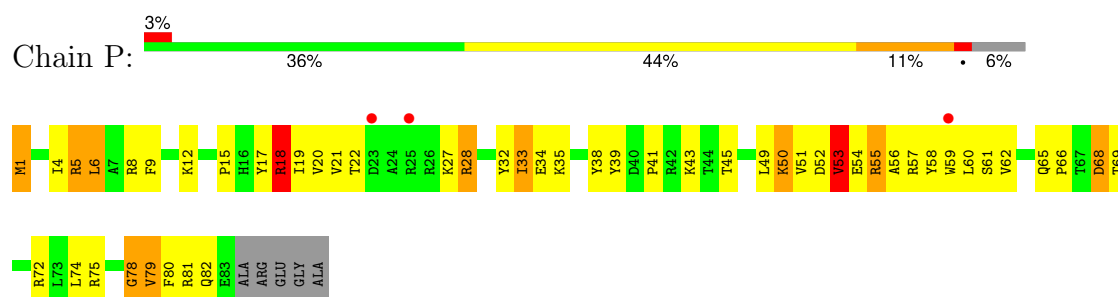
- Molecule 14: ribosomal protein S14



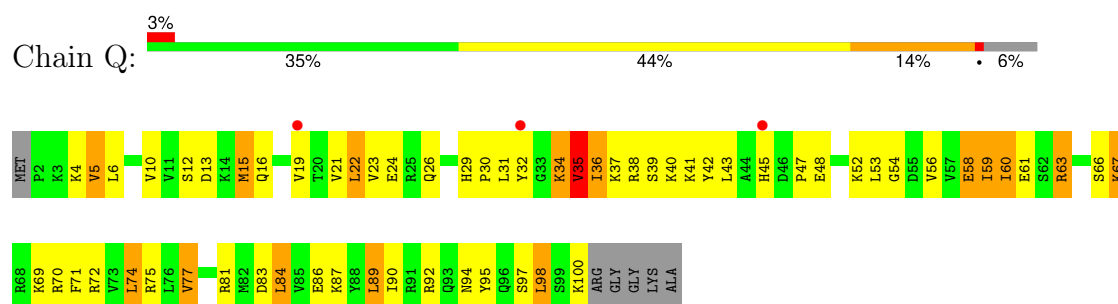
- Molecule 15: ribosomal protein S15



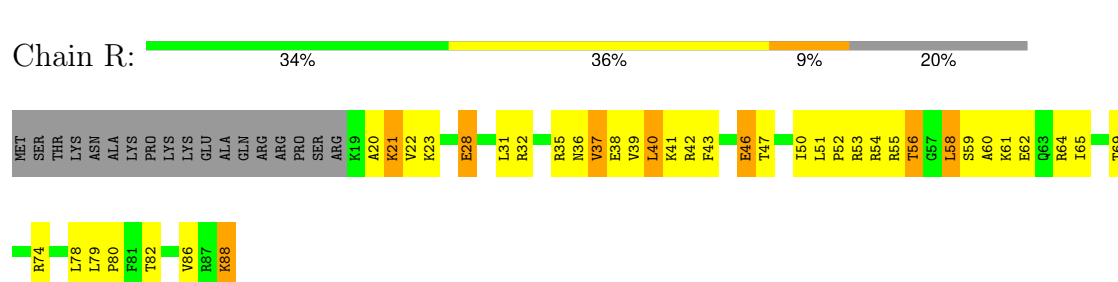
- Molecule 16: ribosomal protein S16



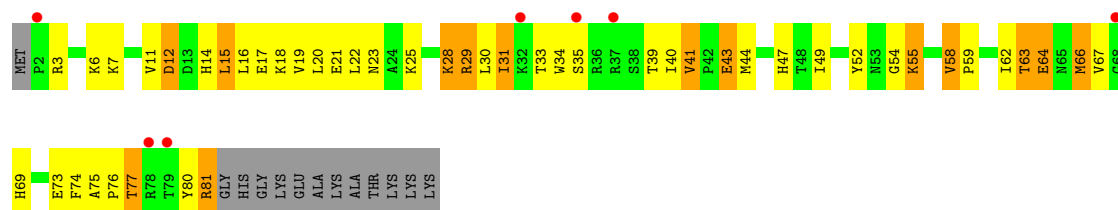
- Molecule 17: ribosomal protein S17



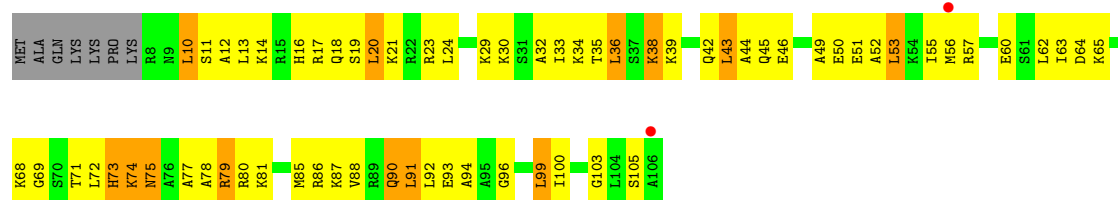
- Molecule 18: ribosomal protein S18



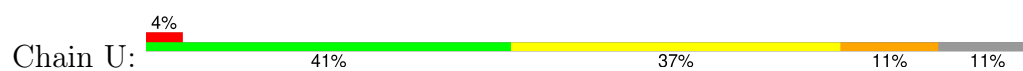
- Molecule 19: ribosomal protein S19



- 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	403.45Å 403.45Å 173.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.93 – 3.85 34.93 – 3.85	Depositor EDS
% Data completeness (in resolution range)	97.3 (34.93-3.85) 96.9 (34.93-3.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.87Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.150 , 0.212 0.150 , 0.209	Depositor DCC
R_{free} test set	6514 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	161.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 153.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52297	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: 7MG, 0TD, UR3, M2G, MG, ZN, 4OC, PSU, MA6, 2MG, 5MC, SRY

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	1.12	108/36044 (0.3%)	1.81	1604/56250 (2.9%)
2	B	0.63	0/1935	0.79	0/2609
3	C	0.59	0/1636	0.78	1/2205 (0.0%)
4	D	0.69	0/1733	0.89	2/2318 (0.1%)
5	E	0.88	0/1162	1.05	3/1564 (0.2%)
6	F	0.61	0/856	0.79	1/1154 (0.1%)
7	G	0.64	0/1276	0.84	0/1709
8	H	1.01	1/1136 (0.1%)	1.12	2/1527 (0.1%)
9	I	0.61	0/1029	0.82	0/1379
10	J	0.56	0/805	0.80	0/1082
11	K	0.68	0/879	0.89	0/1187
12	L	0.77	0/977	1.01	1/1306 (0.1%)
13	M	0.66	0/947	0.85	0/1270
14	N	0.64	0/501	0.83	0/664
15	O	0.73	0/740	0.91	0/987
16	P	0.77	0/716	1.00	2/963 (0.2%)
17	Q	0.97	0/836	1.14	6/1117 (0.5%)
18	R	0.70	0/579	0.87	1/768 (0.1%)
19	S	0.55	0/661	0.75	0/890
20	T	0.74	0/765	1.00	1/1007 (0.1%)
21	U	0.64	0/212	0.78	0/277
All	All	1.00	109/55425 (0.2%)	1.58	1624/82233 (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
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1
12	L	0	1
13	M	0	1
16	P	0	2
20	T	0	1
All	All	0	9

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1509	C	N3-C4	-10.95	1.26	1.33
1	A	279	A	N9-C4	-10.62	1.31	1.37
1	A	573	A	N7-C5	-8.71	1.34	1.39
1	A	1523	G	N7-C5	-8.10	1.34	1.39
1	A	715	A	N9-C4	-8.01	1.33	1.37
1	A	266	G	N9-C4	-8.00	1.31	1.38
1	A	1513	A	N9-C4	-7.91	1.33	1.37
1	A	279	A	N3-C4	-7.87	1.30	1.34
1	A	1502	A	C5-C6	-7.79	1.34	1.41
1	A	1509	C	N1-C6	-7.73	1.32	1.37
1	A	372	C	C2-O2	7.72	1.31	1.24
1	A	1493	A	N9-C4	7.63	1.42	1.37
1	A	1504	G	N9-C8	-7.34	1.32	1.37
1	A	733	A	N9-C4	-7.22	1.33	1.37
1	A	860	A	N3-C4	-7.14	1.30	1.34
1	A	1521	G	C5-C4	-7.09	1.33	1.38
1	A	715	A	N3-C4	-7.04	1.30	1.34
1	A	569	C	N3-C4	-7.00	1.29	1.33
8	H	135	CYS	CB-SG	-6.93	1.70	1.82
1	A	572	A	N3-C4	-6.81	1.30	1.34
1	A	1523	G	C5-C6	-6.68	1.35	1.42
1	A	372	C	N3-C4	6.46	1.38	1.33
1	A	722	A	N9-C4	-6.44	1.33	1.37
1	A	1501	C	N3-C4	-6.42	1.29	1.33
1	A	1329	A	N7-C5	-6.35	1.35	1.39
1	A	792	A	N9-C4	6.34	1.41	1.37
1	A	1504	G	C6-N1	-6.30	1.35	1.39
1	A	791	G	N9-C4	6.29	1.43	1.38
1	A	1227	A	N9-C4	-6.27	1.34	1.37
1	A	1079	G	N7-C5	-6.27	1.35	1.39
1	A	88	A	N9-C4	6.14	1.41	1.37
1	A	602	A	N9-C4	-6.09	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1377	A	N3-C4	-6.04	1.31	1.34
1	A	1529	G	C6-N1	-6.03	1.35	1.39
1	A	1346	A	C3'-O3'	5.99	1.50	1.42
1	A	828	A	N9-C4	-5.92	1.34	1.37
1	A	1103	C	N3-C4	-5.92	1.29	1.33
1	A	1526	G	N7-C5	-5.89	1.35	1.39
1	A	389	A	N7-C5	-5.87	1.35	1.39
1	A	382	A	N7-C5	-5.86	1.35	1.39
1	A	482	A	N7-C5	-5.85	1.35	1.39
1	A	605	U	N3-C4	-5.82	1.33	1.38
1	A	817	C	N1-C6	-5.81	1.33	1.37
1	A	362	G	N3-C4	-5.79	1.31	1.35
1	A	274	A	N9-C4	-5.78	1.34	1.37
1	A	279	A	N7-C5	-5.76	1.35	1.39
1	A	1504	G	C5-C4	-5.75	1.34	1.38
1	A	1514	C	N3-C4	-5.74	1.29	1.33
1	A	706	A	N3-C4	-5.74	1.31	1.34
1	A	1521	G	N9-C8	-5.72	1.33	1.37
1	A	854	G	C6-N1	-5.71	1.35	1.39
1	A	190(G)	G	N7-C5	-5.69	1.35	1.39
1	A	372	C	C2-N3	5.63	1.40	1.35
1	A	584	G	N7-C5	-5.61	1.35	1.39
1	A	910	C	N3-C4	-5.61	1.30	1.33
1	A	642	A	N7-C5	-5.58	1.35	1.39
1	A	900	A	N7-C5	-5.57	1.35	1.39
1	A	1514	C	N1-C2	-5.57	1.34	1.40
1	A	1510	U	C2-N3	-5.55	1.33	1.37
1	A	291	C	N1-C6	-5.55	1.33	1.37
1	A	1377	A	N9-C4	-5.54	1.34	1.37
1	A	605	U	C2-N3	-5.53	1.33	1.37
1	A	288	A	N9-C4	-5.53	1.34	1.37
1	A	108	G	P-O5'	-5.50	1.54	1.59
1	A	782	A	N7-C5	-5.49	1.35	1.39
1	A	889	A	N9-C4	-5.49	1.34	1.37
1	A	901	A	N9-C4	-5.46	1.34	1.37
1	A	565	U	C2-O2	5.46	1.27	1.22
1	A	1520	G	N3-C4	-5.45	1.31	1.35
1	A	1526	G	C5-C6	-5.43	1.36	1.42
1	A	23	C	N1-C6	-5.43	1.33	1.37
1	A	862	C	C4-C5	-5.42	1.38	1.43
1	A	556	C	N3-C4	-5.42	1.30	1.33
1	A	771	G	N9-C4	-5.42	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	909	A	N7-C5	-5.40	1.36	1.39
1	A	1527	C	C4-C5	-5.39	1.38	1.43
1	A	481	G	N9-C4	5.37	1.42	1.38
1	A	946	A	C6-N1	-5.37	1.31	1.35
1	A	97	G	N9-C4	5.35	1.42	1.38
1	A	1180	A	N9-C4	5.33	1.41	1.37
1	A	329	A	C5-C6	-5.30	1.36	1.41
1	A	791	G	C5-C4	5.30	1.42	1.38
1	A	238	G	C2-N3	-5.29	1.28	1.32
1	A	706	A	N9-C4	-5.24	1.34	1.37
1	A	1329	A	C5-C6	-5.21	1.36	1.41
1	A	1508	G	C6-N1	-5.21	1.35	1.39
1	A	729	A	N9-C4	-5.20	1.34	1.37
1	A	568	G	C6-N1	-5.18	1.35	1.39
1	A	33	A	N3-C4	-5.17	1.31	1.34
1	A	558	G	C5-C6	-5.16	1.37	1.42
1	A	879	C	C4-C5	-5.14	1.38	1.43
1	A	574	A	N3-C4	-5.14	1.31	1.34
1	A	1505	G	N7-C5	-5.14	1.36	1.39
1	A	868	C	N1-C6	-5.13	1.34	1.37
1	A	288	A	C6-N1	-5.12	1.31	1.35
1	A	771	G	N3-C4	-5.10	1.31	1.35
1	A	635	G	C2-N3	-5.09	1.28	1.32
1	A	561	U	N1-C6	-5.08	1.33	1.38
1	A	568	G	N3-C4	-5.07	1.31	1.35
1	A	1396	A	N9-C4	-5.07	1.34	1.37
1	A	917	G	N9-C4	-5.06	1.33	1.38
1	A	574	A	C6-N1	-5.06	1.32	1.35
1	A	1500	A	N3-C4	-5.04	1.31	1.34
1	A	810	C	N1-C6	-5.04	1.34	1.37
1	A	771	G	C5-C6	-5.04	1.37	1.42
1	A	124	G	N3-C4	-5.02	1.31	1.35
1	A	453	A	N9-C4	-5.02	1.34	1.37
1	A	1504	G	N7-C5	-5.01	1.36	1.39
1	A	1401	G	N3-C4	-5.00	1.31	1.35

All (1624) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	573	A	C8-N9-C4	-18.34	98.46	105.80
1	A	1505	G	C8-N9-C4	-15.18	100.33	106.40
1	A	372	C	C6-N1-C2	13.96	125.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	A	C5-N7-C8	-13.43	97.18	103.90
1	A	481	G	N3-C4-N9	13.26	133.96	126.00
1	A	573	A	N7-C8-N9	13.08	120.34	113.80
1	A	873	A	C8-N9-C4	-12.91	100.64	105.80
1	A	295	C	C6-N1-C2	12.75	125.40	120.30
1	A	1496	C	C6-N1-C2	-12.70	115.22	120.30
1	A	1282	C	C6-N1-C2	-12.62	115.25	120.30
1	A	106	C	C6-N1-C2	-12.58	115.27	120.30
1	A	1370	G	C8-N9-C4	-12.57	101.37	106.40
1	A	1377	A	N1-C6-N6	-12.56	111.06	118.60
1	A	948	C	C6-N1-C2	12.39	125.26	120.30
1	A	310	G	N1-C6-O6	12.37	127.32	119.90
1	A	190(G)	G	N1-C6-O6	12.29	127.27	119.90
1	A	1505	G	N7-C8-N9	12.28	119.24	113.10
1	A	635	G	N1-C6-O6	12.25	127.25	119.90
1	A	326	G	C4-C5-N7	-12.18	105.93	110.80
1	A	279	A	N7-C8-N9	12.15	119.88	113.80
1	A	1181	G	C8-N9-C4	12.02	111.21	106.40
1	A	103	C	C6-N1-C2	-11.98	115.51	120.30
1	A	117	G	C5-C6-N1	-11.89	105.55	111.50
1	A	572	A	N9-C4-C5	11.79	110.52	105.80
1	A	1502	A	C4-C5-N7	11.63	116.52	110.70
1	A	1367	C	C6-N1-C2	-11.52	115.69	120.30
1	A	117	G	N1-C6-O6	11.47	126.78	119.90
1	A	326	G	C5-C6-O6	11.16	135.30	128.60
1	A	190(G)	G	C6-C5-N7	-11.13	123.72	130.40
1	A	331	G	N1-C6-O6	11.11	126.57	119.90
1	A	1370	G	N7-C8-N9	11.10	118.65	113.10
1	A	572	A	N1-C6-N6	-11.01	111.99	118.60
1	A	326	G	N9-C4-C5	10.93	109.77	105.40
1	A	232	G	N9-C4-C5	-10.79	101.08	105.40
1	A	1238	A	N9-C4-C5	10.76	110.11	105.80
1	A	305	G	C8-N9-C4	-10.70	102.12	106.40
1	A	372	C	N1-C2-N3	-10.67	111.73	119.20
1	A	735	C	C6-N1-C2	10.67	124.57	120.30
1	A	928	G	N1-C6-O6	10.62	126.27	119.90
1	A	232	G	C6-C5-N7	-10.51	124.09	130.40
1	A	1403	C	C6-N1-C2	10.48	124.49	120.30
1	A	725	G	C5-C6-O6	-10.44	122.33	128.60
1	A	1238	A	N1-C6-N6	-10.32	112.41	118.60
1	A	232	G	C4-C5-N7	10.30	114.92	110.80
1	A	725	G	C4-C5-N7	10.28	114.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1502	A	N1-C6-N6	10.23	124.74	118.60
1	A	1502	A	C5-N7-C8	-10.18	98.81	103.90
1	A	969	A	N1-C6-N6	10.13	124.68	118.60
1	A	565	U	N1-C2-N3	-10.06	108.86	114.90
1	A	815	A	C8-N9-C4	10.05	109.82	105.80
1	A	232	G	N1-C6-O6	10.03	125.92	119.90
1	A	1517	G	C8-N9-C4	-9.98	102.41	106.40
1	A	310	G	C5-C6-O6	-9.87	122.68	128.60
1	A	753	A	C6-N1-C2	-9.86	112.68	118.60
1	A	481	G	C8-N9-C4	9.84	110.34	106.40
1	A	1455	G	N1-C6-O6	9.81	125.78	119.90
1	A	745	C	C6-N1-C2	9.79	124.22	120.30
1	A	238	G	C5-C6-N1	-9.79	106.61	111.50
1	A	299	G	C6-C5-N7	-9.78	124.53	130.40
1	A	1523	G	C8-N9-C4	-9.76	102.50	106.40
1	A	1504	G	N3-C4-C5	-9.74	123.73	128.60
1	A	43	C	C5-C6-N1	-9.73	116.13	121.00
1	A	299	G	N1-C6-O6	9.72	125.73	119.90
1	A	946	A	N1-C6-N6	-9.71	112.77	118.60
1	A	573	A	N9-C4-C5	9.70	109.68	105.80
1	A	238	G	N1-C6-O6	9.65	125.69	119.90
1	A	1329	A	N1-C6-N6	9.65	124.39	118.60
1	A	284	G	N1-C6-O6	9.64	125.69	119.90
1	A	28	G	N1-C6-O6	9.61	125.67	119.90
1	A	715	A	C2-N3-C4	-9.58	105.81	110.60
1	A	1502	A	C6-C5-N7	-9.58	125.59	132.30
1	A	328	C	N3-C2-O2	-9.57	115.20	121.90
1	A	117	G	C8-N9-C1'	-9.57	114.56	127.00
1	A	482	A	N7-C8-N9	9.53	118.56	113.80
1	A	1513	A	C2-N3-C4	-9.52	105.84	110.60
1	A	1249	C	C6-N1-C2	-9.49	116.50	120.30
1	A	190(F)	G	N3-C4-N9	-9.46	120.33	126.00
1	A	830	G	N1-C6-O6	9.45	125.57	119.90
1	A	103	C	N3-C4-C5	-9.41	118.13	121.90
1	A	945	G	C4-C5-C6	-9.37	113.18	118.80
1	A	325	A	N1-C6-N6	-9.37	112.98	118.60
1	A	279	A	C8-N9-C4	-9.35	102.06	105.80
1	A	481	G	N9-C4-C5	-9.34	101.67	105.40
1	A	861	G	C5-C6-N1	9.32	116.16	111.50
1	A	950	U	N3-C4-C5	-9.32	109.01	114.60
1	A	1543	C	N1-C2-O2	9.32	124.49	118.90
17	Q	35	VAL	CB-CA-C	-9.31	93.70	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1339	A	N1-C6-N6	-9.30	113.02	118.60
1	A	1084	G	N3-C4-C5	-9.28	123.96	128.60
1	A	266	G	N3-C4-C5	9.26	133.23	128.60
1	A	1523	G	C5-C6-O6	-9.24	123.06	128.60
1	A	121	C	C6-N1-C2	9.20	123.98	120.30
1	A	944	G	C8-N9-C4	-9.12	102.75	106.40
1	A	1524	C	N3-C4-C5	-9.12	118.25	121.90
1	A	791	G	C8-N9-C4	-9.12	102.75	106.40
1	A	722	A	C2-N3-C4	-9.12	106.04	110.60
1	A	963	G	C8-N9-C4	-9.11	102.76	106.40
1	A	854	G	N1-C2-N3	9.05	129.33	123.90
1	A	88	A	C8-N9-C4	-9.05	102.18	105.80
1	A	117	G	C4-C5-C6	9.05	124.23	118.80
1	A	1347	G	C5-C6-O6	-9.04	123.17	128.60
1	A	635	G	C5-C6-N1	-9.01	107.00	111.50
1	A	790	A	C8-N9-C4	-9.01	102.20	105.80
1	A	283	C	C6-N1-C2	-8.99	116.70	120.30
1	A	1524	C	C6-N1-C2	-8.97	116.71	120.30
1	A	117	G	C6-C5-N7	-8.96	125.02	130.40
1	A	99	C	C6-N1-C2	-8.93	116.73	120.30
1	A	292	G	N1-C6-O6	8.89	125.23	119.90
1	A	305	G	N9-C4-C5	8.87	108.95	105.40
1	A	572	A	C8-N9-C4	-8.87	102.25	105.80
1	A	382	A	C8-N9-C4	-8.86	102.25	105.80
1	A	1079	G	N3-C4-C5	-8.86	124.17	128.60
1	A	326	G	C8-N9-C4	-8.86	102.86	106.40
1	A	16	A	C8-N9-C4	8.83	109.33	105.80
1	A	190(G)	G	C5-C6-N1	-8.81	107.09	111.50
1	A	852	G	C5-C6-N1	-8.79	107.11	111.50
1	A	106	C	N3-C2-O2	-8.78	115.75	121.90
1	A	1237	C	C6-N1-C2	-8.77	116.79	120.30
1	A	289	G	C8-N9-C4	-8.73	102.91	106.40
1	A	1231	G	N1-C6-O6	8.73	125.14	119.90
1	A	137	C	N3-C4-C5	8.69	125.38	121.90
1	A	260	G	C8-N9-C4	-8.68	102.93	106.40
1	A	288	A	C2-N3-C4	-8.67	106.26	110.60
1	A	635	G	N3-C2-N2	-8.65	113.84	119.90
1	A	27	G	N1-C6-O6	8.65	125.09	119.90
1	A	129(A)	G	C4-C5-N7	8.61	114.25	110.80
1	A	852	G	N1-C6-O6	8.61	125.06	119.90
1	A	575	G	C2-N3-C4	-8.60	107.60	111.90
1	A	108	G	N7-C8-N9	8.58	117.39	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	585	G	C8-N9-C4	8.57	109.83	106.40
1	A	946	A	N9-C4-C5	8.56	109.22	105.80
1	A	651	C	C6-N1-C2	8.56	123.72	120.30
1	A	1365	G	C8-N9-C4	-8.55	102.98	106.40
1	A	1526	G	N1-C6-O6	8.55	125.03	119.90
1	A	232	G	C5-C6-O6	-8.53	123.48	128.60
1	A	1403	C	N3-C2-O2	8.53	127.87	121.90
1	A	666	G	C5-C6-N1	-8.50	107.25	111.50
1	A	482	A	N1-C6-N6	8.49	123.69	118.60
1	A	500	G	C8-N9-C4	-8.48	103.01	106.40
1	A	328	C	N1-C2-O2	8.48	123.99	118.90
1	A	481	G	N3-C4-C5	-8.44	124.38	128.60
1	A	730	G	N1-C2-N2	-8.44	108.61	116.20
1	A	600	C	C6-N1-C2	8.44	123.67	120.30
1	A	856	C	N3-C4-C5	-8.41	118.53	121.90
1	A	285	G	N1-C6-O6	8.41	124.94	119.90
1	A	915	A	N1-C6-N6	-8.40	113.56	118.60
1	A	872	A	N1-C6-N6	8.40	123.64	118.60
1	A	569	C	N3-C4-C5	8.38	125.25	121.90
1	A	1332	A	N1-C6-N6	-8.37	113.58	118.60
1	A	326	G	N3-C4-C5	-8.33	124.43	128.60
1	A	131	C	C5-C6-N1	-8.33	116.83	121.00
1	A	1333	A	C8-N9-C4	-8.33	102.47	105.80
1	A	244	U	N1-C2-N3	-8.31	109.91	114.90
1	A	1238	A	C8-N9-C4	-8.30	102.48	105.80
1	A	190(A)	C	C6-N1-C2	-8.29	116.98	120.30
1	A	789	U	C5-C6-N1	8.28	126.84	122.70
1	A	180	U	C2-N1-C1'	8.28	127.64	117.70
1	A	279	A	C6-C5-N7	-8.25	126.53	132.30
1	A	1055	A	N1-C6-N6	-8.23	113.66	118.60
1	A	851	G	C8-N9-C4	-8.21	103.11	106.40
1	A	1354	C	C6-N1-C2	-8.20	117.02	120.30
1	A	1502	A	N9-C4-C5	-8.19	102.52	105.80
1	A	1523	G	N1-C6-O6	8.19	124.81	119.90
1	A	1200	C	C2-N1-C1'	8.19	127.81	118.80
1	A	773	G	C6-C5-N7	-8.18	125.50	130.40
1	A	624	C	C6-N1-C2	8.17	123.57	120.30
1	A	266	G	C2-N3-C4	-8.16	107.82	111.90
1	A	873	A	N9-C4-C5	8.16	109.06	105.80
1	A	482	A	C8-N9-C4	-8.16	102.54	105.80
1	A	1181	G	N7-C8-N9	-8.16	109.02	113.10
1	A	1441	G	C4-C5-N7	-8.13	107.55	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	708	C	C6-N1-C2	8.12	123.55	120.30
1	A	928	G	C6-C5-N7	-8.12	125.53	130.40
1	A	283	C	C2-N1-C1'	8.09	127.70	118.80
1	A	589	C	C5-C6-N1	-8.09	116.96	121.00
1	A	108	G	C8-N9-C4	-8.07	103.17	106.40
1	A	79	G	C8-N9-C4	-8.05	103.18	106.40
1	A	235	C	C6-N1-C2	8.05	123.52	120.30
1	A	700	G	N3-C4-N9	8.04	130.83	126.00
1	A	27	G	C5-C6-O6	-8.03	123.78	128.60
1	A	1529	G	C4-N9-C1'	8.03	136.94	126.50
1	A	331	G	C2-N3-C4	-8.01	107.90	111.90
1	A	1347	G	N9-C4-C5	-8.00	102.20	105.40
1	A	75	G	N3-C4-N9	7.99	130.79	126.00
1	A	1513	A	N1-C2-N3	7.98	133.29	129.30
1	A	950	U	C5-C4-O4	7.98	130.69	125.90
1	A	93	G	C8-N9-C4	7.98	109.59	106.40
1	A	945	G	N1-C2-N3	-7.97	119.12	123.90
1	A	856	C	N1-C2-O2	-7.97	114.12	118.90
1	A	126	G	C8-N9-C4	7.96	109.59	106.40
1	A	372	C	C5-C4-N4	-7.96	114.63	120.20
1	A	292	G	C6-C5-N7	-7.94	125.64	130.40
1	A	931	C	C5-C6-N1	-7.94	117.03	121.00
1	A	279	A	N1-C6-N6	7.93	123.36	118.60
1	A	295	C	N3-C4-C5	7.93	125.07	121.90
1	A	1526	G	C6-C5-N7	-7.93	125.64	130.40
1	A	507	C	C6-N1-C2	-7.89	117.14	120.30
1	A	27	G	C6-C5-N7	-7.89	125.67	130.40
1	A	481	G	C8-N9-C1'	-7.88	116.76	127.00
1	A	1193	G	N1-C6-O6	7.87	124.62	119.90
1	A	1527	C	C5-C4-N4	-7.87	114.69	120.20
1	A	731	G	N1-C6-O6	7.86	124.61	119.90
1	A	251	G	C6-C5-N7	-7.85	125.69	130.40
1	A	795	C	C2-N3-C4	7.84	123.82	119.90
1	A	1530	G	C8-N9-C4	7.84	109.54	106.40
1	A	78	G	N9-C4-C5	-7.84	102.26	105.40
1	A	706	A	C2-N3-C4	-7.84	106.68	110.60
1	A	815	A	N7-C8-N9	-7.84	109.88	113.80
1	A	299	G	C5-C6-O6	-7.81	123.91	128.60
1	A	1329	A	C4-C5-N7	7.81	114.61	110.70
1	A	773	G	C4-C5-N7	7.81	113.92	110.80
1	A	251	G	N1-C6-O6	7.81	124.59	119.90
1	A	1455	G	C6-C5-N7	-7.80	125.72	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	725	G	C5-N7-C8	-7.79	100.40	104.30
1	A	117	G	C4-N9-C1'	7.79	136.63	126.50
1	A	397	A	C8-N9-C4	-7.79	102.69	105.80
1	A	693	G	C4-C5-N7	7.77	113.91	110.80
1	A	854	G	C6-N1-C2	-7.76	120.44	125.10
1	A	1441	G	C5-C6-O6	7.75	133.25	128.60
1	A	936	C	C6-N1-C2	7.75	123.40	120.30
1	A	833	U	N3-C2-O2	-7.74	116.78	122.20
8	H	12	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	A	234	C	C6-N1-C2	7.74	123.40	120.30
1	A	331	G	C5-C6-N1	-7.74	107.63	111.50
1	A	728	A	C2-N3-C4	-7.73	106.73	110.60
1	A	578	C	C4-C5-C6	7.72	121.26	117.40
1	A	525	C	C6-N1-C2	7.71	123.39	120.30
1	A	18	C	C6-N1-C2	7.71	123.39	120.30
1	A	562	C	N3-C2-O2	-7.71	116.51	121.90
1	A	1187	G	N1-C6-O6	7.70	124.52	119.90
1	A	244	U	C6-N1-C2	7.70	125.62	121.00
1	A	1370	G	C5-N7-C8	-7.70	100.45	104.30
1	A	928	G	C5-C6-O6	-7.69	123.98	128.60
1	A	693	G	C5-C6-O6	-7.68	123.99	128.60
1	A	1523	G	N3-C2-N2	-7.68	114.52	119.90
1	A	811	C	N3-C4-N4	7.67	123.37	118.00
1	A	115	G	C8-N9-C4	7.67	109.47	106.40
1	A	753	A	N1-C2-N3	7.67	133.13	129.30
1	A	201	C	C6-N1-C2	-7.66	117.24	120.30
1	A	605	U	N3-C2-O2	-7.66	116.84	122.20
1	A	15	G	C8-N9-C1'	-7.66	117.05	127.00
1	A	292	G	C5-C6-O6	-7.66	124.01	128.60
1	A	969	A	C2-N3-C4	-7.66	106.77	110.60
1	A	1497	G	C8-N9-C4	-7.65	103.34	106.40
1	A	305	G	N3-C4-N9	-7.65	121.41	126.00
1	A	830	G	C5-C6-N1	-7.65	107.68	111.50
1	A	795	C	N3-C4-C5	-7.64	118.84	121.90
1	A	1531	A	N1-C6-N6	7.64	123.18	118.60
1	A	731	G	C5-C6-O6	-7.63	124.02	128.60
1	A	1209	C	C6-N1-C2	-7.62	117.25	120.30
1	A	735	C	C5-C6-N1	-7.61	117.19	121.00
1	A	190(A)	C	C5-C6-N1	7.61	124.81	121.00
1	A	658	G	C8-N9-C1'	-7.61	117.11	127.00
1	A	1442	G	C4-N9-C1'	7.60	136.38	126.50
1	A	522	C	C5-C6-N1	-7.59	117.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1438	G	C5-C6-O6	-7.59	124.05	128.60
1	A	1509	C	C4-C5-C6	7.58	121.19	117.40
1	A	1347	G	C8-N9-C4	7.57	109.43	106.40
1	A	18	C	C5-C6-N1	-7.57	117.22	121.00
1	A	795	C	N3-C4-N4	7.57	123.30	118.00
1	A	1132	C	C6-N1-C2	-7.56	117.28	120.30
1	A	578	C	N3-C4-C5	-7.56	118.88	121.90
1	A	331	G	C6-C5-N7	-7.55	125.87	130.40
1	A	482	A	C6-C5-N7	-7.55	127.02	132.30
1	A	1200	C	N1-C2-O2	7.54	123.42	118.90
1	A	190(F)	G	N3-C4-C5	7.54	132.37	128.60
1	A	253	U	N3-C2-O2	7.53	127.47	122.20
1	A	602	A	C2-N3-C4	-7.53	106.84	110.60
1	A	146	G	N1-C6-O6	7.52	124.41	119.90
1	A	326	G	N1-C6-O6	-7.51	115.39	119.90
1	A	1249	C	C5-C6-N1	7.51	124.75	121.00
1	A	1103	C	C2-N3-C4	-7.50	116.15	119.90
1	A	906	G	N1-C6-O6	7.47	124.38	119.90
1	A	1200	C	C6-N1-C1'	-7.47	111.83	120.80
1	A	279	A	C4-C5-N7	7.46	114.43	110.70
1	A	666	G	N1-C6-O6	7.46	124.38	119.90
1	A	316	G	N3-C4-N9	7.46	130.47	126.00
1	A	1161	C	C6-N1-C2	-7.45	117.32	120.30
1	A	117	G	C2-N3-C4	-7.45	108.17	111.90
1	A	23	C	C5-C6-N1	-7.45	117.27	121.00
1	A	238	G	N3-C2-N2	-7.45	114.68	119.90
1	A	598	U	C5-C6-N1	-7.45	118.97	122.70
1	A	328	C	C2-N1-C1'	7.45	126.99	118.80
1	A	820	U	N1-C2-N3	7.45	119.37	114.90
1	A	28	G	C6-C5-N7	-7.45	125.93	130.40
1	A	890	G	C4-C5-N7	-7.45	107.82	110.80
1	A	1395	C	C6-N1-C2	7.43	123.27	120.30
1	A	1249	C	C2-N1-C1'	7.43	126.97	118.80
1	A	1377	A	N7-C8-N9	-7.43	110.08	113.80
1	A	78	G	C4-C5-N7	7.42	113.77	110.80
1	A	106	C	N1-C2-N3	7.42	124.39	119.20
1	A	1517	G	N7-C8-N9	7.42	116.81	113.10
1	A	1329	A	C5-C6-N6	-7.42	117.77	123.70
1	A	190(G)	G	C4-C5-C6	7.41	123.25	118.80
1	A	875	C	C5-C6-N1	-7.41	117.30	121.00
1	A	482	A	C5-N7-C8	-7.40	100.20	103.90
1	A	950	U	C4-C5-C6	7.40	124.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	G	C8-N9-C4	-7.40	103.44	106.40
1	A	122	G	N1-C6-O6	7.40	124.34	119.90
1	A	1230	C	C6-N1-C2	-7.40	117.34	120.30
1	A	818	G	N9-C4-C5	7.40	108.36	105.40
1	A	1377	A	C6-C5-N7	7.40	137.48	132.30
1	A	873	A	N7-C8-N9	7.40	117.50	113.80
1	A	283	C	N3-C4-C5	-7.39	118.94	121.90
1	A	944	G	N7-C8-N9	7.38	116.79	113.10
1	A	1158	C	N1-C2-O2	7.38	123.33	118.90
1	A	1074	G	N1-C6-O6	7.38	124.33	119.90
1	A	97	G	C8-N9-C4	-7.37	103.45	106.40
1	A	642	A	C8-N9-C4	-7.36	102.86	105.80
1	A	1443	G	C8-N9-C4	7.36	109.34	106.40
1	A	266	G	C5-N7-C8	-7.36	100.62	104.30
1	A	945	G	C8-N9-C1'	7.36	136.57	127.00
1	A	888	G	C4-C5-C6	7.36	123.22	118.80
1	A	639	G	N1-C2-N3	7.35	128.31	123.90
1	A	669	U	N3-C2-O2	7.35	127.34	122.20
1	A	573	A	C4-C5-C6	7.34	120.67	117.00
1	A	819	A	C8-N9-C4	-7.34	102.86	105.80
1	A	766	A	N1-C6-N6	7.34	123.01	118.60
1	A	804	U	N3-C2-O2	-7.34	117.06	122.20
1	A	642	A	N7-C8-N9	7.33	117.46	113.80
1	A	310	G	C2-N3-C4	-7.33	108.24	111.90
1	A	944	G	N1-C6-O6	-7.32	115.51	119.90
1	A	1442	G	C8-N9-C1'	-7.32	117.49	127.00
1	A	299	G	C4-C5-N7	7.32	113.73	110.80
1	A	1103	C	N3-C4-N4	-7.31	112.88	118.00
1	A	14	U	C6-N1-C2	-7.31	116.61	121.00
1	A	1443	G	N3-C4-C5	7.31	132.26	128.60
1	A	693	G	N9-C4-C5	-7.31	102.48	105.40
1	A	227	G	C4-C5-N7	7.30	113.72	110.80
1	A	1504	G	N1-C6-O6	-7.30	115.52	119.90
1	A	28	G	C4-C5-C6	7.30	123.18	118.80
1	A	296	U	N3-C4-C5	-7.29	110.22	114.60
1	A	1482	G	N3-C4-C5	-7.29	124.95	128.60
1	A	1083	U	N3-C4-C5	-7.29	110.23	114.60
1	A	773	G	N7-C8-N9	7.29	116.74	113.10
1	A	1510	U	N3-C2-O2	-7.29	117.10	122.20
1	A	1501	C	C6-N1-C2	-7.27	117.39	120.30
1	A	730	G	N1-C2-N3	7.26	128.26	123.90
1	A	788	U	C5-C6-N1	7.26	126.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	C	N3-C4-C5	7.26	124.80	121.90
1	A	1411	C	C6-N1-C2	-7.25	117.40	120.30
1	A	1403	C	N1-C2-N3	-7.25	114.13	119.20
1	A	948	C	N3-C4-C5	7.24	124.80	121.90
1	A	654	G	N3-C4-N9	-7.23	121.66	126.00
1	A	383	A	C8-N9-C4	-7.23	102.91	105.80
1	A	666	G	C2-N3-C4	-7.22	108.29	111.90
1	A	778	G	C5-C6-N1	-7.22	107.89	111.50
1	A	1422	G	N3-C2-N2	-7.22	114.84	119.90
1	A	9	G	C5-C6-O6	-7.22	124.27	128.60
1	A	309	G	N1-C6-O6	7.22	124.23	119.90
1	A	890	G	N9-C4-C5	7.21	108.29	105.40
1	A	1329	A	C6-C5-N7	-7.21	127.25	132.30
1	A	945	G	C6-C5-N7	7.21	134.73	130.40
1	A	232	G	N3-C4-N9	7.21	130.33	126.00
1	A	1526	G	C5-C6-O6	-7.21	124.27	128.60
1	A	310	G	C4-C5-N7	7.20	113.68	110.80
1	A	310	G	N3-C4-C5	7.19	132.20	128.60
1	A	1354	C	N1-C2-O2	7.19	123.22	118.90
1	A	1442	G	N3-C4-C5	-7.19	125.00	128.60
1	A	589	C	C2-N3-C4	-7.19	116.31	119.90
1	A	90	U	C6-N1-C2	-7.18	116.69	121.00
1	A	569	C	C2-N3-C4	-7.18	116.31	119.90
1	A	1483	A	N1-C6-N6	-7.18	114.29	118.60
1	A	1329	A	C5-N7-C8	-7.17	100.31	103.90
1	A	1338	G	N3-C4-C5	-7.17	125.02	128.60
1	A	814	A	C8-N9-C4	7.16	108.66	105.80
1	A	296	U	C4-C5-C6	7.16	123.99	119.70
1	A	873	A	N1-C6-N6	-7.16	114.31	118.60
1	A	800	G	C4-N9-C1'	7.15	135.80	126.50
1	A	1455	G	C2-N3-C4	-7.15	108.33	111.90
1	A	1523	G	C6-C5-N7	-7.14	126.11	130.40
1	A	1377	A	C4-C5-N7	-7.14	107.13	110.70
1	A	1412	C	N3-C2-O2	-7.14	116.90	121.90
1	A	1523	G	N7-C8-N9	7.14	116.67	113.10
1	A	1496	C	N3-C4-C5	-7.13	119.05	121.90
1	A	129(A)	G	C5-N7-C8	-7.13	100.73	104.30
1	A	838	G	C8-N9-C4	7.13	109.25	106.40
1	A	929	G	C2-N3-C4	-7.12	108.34	111.90
1	A	950	U	C6-N1-C2	-7.12	116.73	121.00
1	A	671	G	N1-C6-O6	7.11	124.17	119.90
1	A	1084	G	C8-N9-C4	-7.10	103.56	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1333	A	N9-C4-C5	7.09	108.64	105.80
1	A	564	C	C2-N3-C4	7.09	123.44	119.90
1	A	814	A	N1-C6-N6	7.08	122.85	118.60
1	A	99	C	C5-C6-N1	7.08	124.54	121.00
1	A	1442	G	N3-C4-N9	7.08	130.25	126.00
1	A	266	G	N3-C4-N9	-7.07	121.76	126.00
1	A	1441	G	C5-C6-N1	-7.07	107.97	111.50
1	A	190(E)	U	C5-C6-N1	-7.06	119.17	122.70
1	A	576	G	C4-C5-C6	7.06	123.03	118.80
1	A	336	C	N3-C4-C5	7.06	124.72	121.90
1	A	1504	G	C6-N1-C2	-7.06	120.87	125.10
1	A	400	C	C6-N1-C2	7.04	123.12	120.30
1	A	863	U	N1-C2-N3	7.04	119.12	114.90
1	A	1108	G	N3-C4-C5	-7.02	125.09	128.60
1	A	881	G	C5-C6-O6	-7.02	124.39	128.60
1	A	1103	C	N3-C4-C5	7.02	124.71	121.90
1	A	357	G	N1-C6-O6	7.01	124.11	119.90
1	A	373	A	C5-N7-C8	-7.01	100.39	103.90
1	A	753	A	C4-C5-N7	-7.01	107.20	110.70
1	A	830	G	C4-C5-C6	7.00	123.00	118.80
1	A	899	C	C2-N1-C1'	6.99	126.49	118.80
1	A	589	C	C6-N1-C2	6.99	123.10	120.30
1	A	1049	U	C6-N1-C2	-6.99	116.81	121.00
1	A	723	U	C2-N1-C1'	6.98	126.07	117.70
1	A	56	U	C5-C4-O4	-6.97	121.72	125.90
1	A	729	A	N1-C6-N6	6.97	122.78	118.60
1	A	623	C	C6-N1-C2	6.97	123.09	120.30
1	A	615	C	C5-C6-N1	6.97	124.48	121.00
1	A	15	G	N9-C4-C5	-6.97	102.61	105.40
1	A	773	G	C5-N7-C8	-6.97	100.82	104.30
1	A	1346	A	C5-C6-N1	6.97	121.18	117.70
1	A	607	A	N9-C4-C5	-6.96	103.02	105.80
1	A	283	C	N3-C4-N4	6.96	122.87	118.00
1	A	318	G	N1-C6-O6	6.95	124.07	119.90
20	T	94	ALA	N-CA-C	-6.95	92.24	111.00
16	P	18	ARG	NE-CZ-NH1	-6.95	116.83	120.30
1	A	481	G	C5-C6-O6	-6.94	124.44	128.60
1	A	923	A	C2-N3-C4	-6.94	107.13	110.60
1	A	872	A	N9-C4-C5	-6.94	103.03	105.80
1	A	481	G	N7-C8-N9	-6.93	109.63	113.10
1	A	1165	C	C6-N1-C2	-6.93	117.53	120.30
1	A	190(C)	C	C6-N1-C2	-6.93	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1347	G	N1-C6-O6	6.93	124.06	119.90
1	A	1258	G	N3-C4-C5	-6.93	125.14	128.60
1	A	1502	A	C2-N3-C4	-6.92	107.14	110.60
1	A	890	G	C5-C6-O6	6.92	132.75	128.60
1	A	667	G	N1-C6-O6	6.92	124.05	119.90
1	A	818	G	C8-N9-C4	-6.91	103.64	106.40
1	A	1438	G	N1-C6-O6	6.91	124.05	119.90
1	A	1350	A	C8-N9-C4	-6.91	103.04	105.80
1	A	819	A	N7-C8-N9	6.90	117.25	113.80
1	A	889	A	C2-N3-C4	-6.90	107.15	110.60
1	A	928	G	C4-C5-N7	6.90	113.56	110.80
1	A	900	A	C2-N3-C4	-6.90	107.15	110.60
1	A	296	U	N1-C2-N3	6.89	119.04	114.90
1	A	253	U	C6-N1-C2	6.88	125.13	121.00
1	A	309	G	C5-C6-O6	-6.88	124.47	128.60
1	A	372	C	C6-N1-C1'	-6.88	112.54	120.80
1	A	950	U	N1-C2-N3	6.88	119.03	114.90
1	A	945	G	C2-N3-C4	6.88	115.34	111.90
1	A	723	U	C5-C6-N1	6.87	126.13	122.70
1	A	860	A	N1-C2-N3	6.87	132.73	129.30
1	A	765	G	C4-C5-N7	6.86	113.55	110.80
1	A	522	C	C2-N1-C1'	-6.85	111.26	118.80
1	A	868	C	N3-C4-C5	6.85	124.64	121.90
1	A	289	G	N7-C8-N9	6.85	116.52	113.10
1	A	1079	G	C4-C5-C6	6.84	122.90	118.80
1	A	450	G	C8-N9-C4	6.83	109.13	106.40
1	A	708	C	N3-C4-C5	6.83	124.63	121.90
1	A	818	G	N3-C4-N9	-6.83	121.90	126.00
1	A	733	A	C2-N3-C4	-6.83	107.19	110.60
1	A	635	G	C2-N3-C4	-6.83	108.49	111.90
1	A	746	A	C8-N9-C4	6.82	108.53	105.80
1	A	852	G	C2-N3-C4	-6.82	108.49	111.90
1	A	1235	U	N1-C2-O2	-6.82	118.03	122.80
1	A	945	G	C5-C6-N1	6.81	114.91	111.50
1	A	771	G	C2-N3-C4	-6.81	108.50	111.90
1	A	93	G	N9-C4-C5	-6.80	102.68	105.40
1	A	773	G	C5-C6-O6	-6.80	124.52	128.60
1	A	1455	G	C4-C5-N7	6.80	113.52	110.80
1	A	53	A	C8-N9-C4	-6.79	103.08	105.80
1	A	718	G	N3-C4-C5	-6.79	125.21	128.60
1	A	1525	G	N9-C4-C5	6.79	108.11	105.40
1	A	950	U	N3-C2-O2	-6.78	117.45	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1392	G	C4-C5-N7	6.78	113.51	110.80
1	A	789	U	C6-N1-C2	-6.78	116.93	121.00
1	A	451	A	C4-C5-C6	-6.78	113.61	117.00
1	A	22	G	C6-C5-N7	-6.77	126.34	130.40
1	A	107	G	N1-C6-O6	6.77	123.96	119.90
1	A	305	G	C8-N9-C1'	6.77	135.80	127.00
1	A	636	U	N3-C4-O4	6.76	124.13	119.40
1	A	577	G	C8-N9-C4	6.75	109.10	106.40
1	A	360	A	C5-N7-C8	-6.74	100.53	103.90
1	A	969	A	C6-C5-N7	-6.74	127.58	132.30
1	A	514	C	C6-N1-C2	-6.74	117.61	120.30
1	A	1345	U	N3-C2-O2	6.74	126.92	122.20
1	A	800	G	C8-N9-C1'	-6.74	118.24	127.00
1	A	851	G	C4-N9-C1'	6.74	135.25	126.50
1	A	1539	C	N3-C4-C5	6.72	124.59	121.90
1	A	963	G	N7-C8-N9	6.72	116.46	113.10
1	A	636	U	N3-C4-C5	-6.72	110.57	114.60
1	A	575	G	C4-C5-N7	6.72	113.49	110.80
1	A	1496	C	C2-N1-C1'	6.72	126.19	118.80
1	A	745	C	N3-C4-C5	6.71	124.58	121.90
1	A	791	G	N3-C4-C5	-6.71	125.24	128.60
1	A	199	G	N1-C6-O6	6.71	123.92	119.90
1	A	401	C	N3-C4-C5	6.71	124.58	121.90
1	A	252	U	C5-C6-N1	-6.71	119.35	122.70
1	A	1116	C	N3-C4-C5	6.71	124.58	121.90
1	A	931	C	C2-N3-C4	-6.70	116.55	119.90
1	A	821	G	C8-N9-C4	6.69	109.08	106.40
1	A	1079	G	C6-C5-N7	-6.69	126.39	130.40
1	A	1079	G	C8-N9-C4	-6.69	103.72	106.40
1	A	1378	C	C6-N1-C2	-6.69	117.62	120.30
1	A	687	A	C8-N9-C4	-6.69	103.13	105.80
1	A	1070	U	N1-C2-N3	6.68	118.91	114.90
1	A	190(F)	G	C4-N9-C1'	-6.68	117.81	126.50
1	A	280	C	C6-N1-C2	6.68	122.97	120.30
1	A	376	G	N7-C8-N9	-6.67	109.76	113.10
1	A	700	G	N3-C2-N2	6.67	124.57	119.90
1	A	1103	C	C5-C6-N1	-6.67	117.67	121.00
1	A	108	G	N1-C6-O6	6.67	123.90	119.90
1	A	1530	G	N3-C4-C5	6.67	131.93	128.60
1	A	1375	A	C5-N7-C8	6.67	107.23	103.90
1	A	129(A)	G	C5-C6-O6	-6.66	124.60	128.60
1	A	29	G	C2-N3-C4	-6.66	108.57	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	A	C5-C6-N1	6.66	121.03	117.70
1	A	676	A	C8-N9-C4	6.66	108.46	105.80
1	A	835	U	C5-C4-O4	6.66	129.89	125.90
1	A	530	G	C4-N9-C1'	6.65	135.15	126.50
1	A	1300	G	N1-C6-O6	-6.65	115.91	119.90
1	A	918	A	C6-N1-C2	-6.65	114.61	118.60
1	A	795	C	C5-C6-N1	6.64	124.32	121.00
1	A	43	C	C4-C5-C6	6.64	120.72	117.40
1	A	1531	A	N7-C8-N9	6.64	117.12	113.80
1	A	361	G	C8-N9-C4	6.64	109.06	106.40
1	A	1300	G	C4-C5-N7	-6.64	108.14	110.80
1	A	43	C	C6-N1-C2	6.63	122.95	120.30
1	A	15	G	N1-C6-O6	6.63	123.88	119.90
1	A	326	G	C5-N7-C8	6.63	107.61	104.30
1	A	279	A	C2-N3-C4	-6.62	107.29	110.60
1	A	771	G	N3-C4-C5	6.62	131.91	128.60
1	A	725	G	N1-C6-O6	6.62	123.87	119.90
1	A	373	A	N7-C8-N9	6.62	117.11	113.80
1	A	607	A	C4-C5-N7	6.61	114.00	110.70
1	A	871	U	N1-C2-O2	6.61	127.42	122.80
1	A	176	C	C6-N1-C2	6.59	122.94	120.30
1	A	583	A	N1-C6-N6	6.59	122.56	118.60
1	A	597	G	C6-C5-N7	-6.59	126.44	130.40
1	A	135	C	C5-C6-N1	6.59	124.30	121.00
1	A	316	G	C6-C5-N7	-6.59	126.44	130.40
1	A	577	G	N1-C6-O6	6.59	123.86	119.90
1	A	826	C	C2-N1-C1'	6.59	126.05	118.80
1	A	1487	G	N3-C4-C5	-6.58	125.31	128.60
1	A	108	G	C5-N7-C8	-6.58	101.01	104.30
1	A	572	A	C5-C6-N1	6.57	120.99	117.70
1	A	1332	A	N9-C4-C5	6.57	108.43	105.80
1	A	773	G	N1-C6-O6	6.57	123.84	119.90
1	A	235	C	N3-C4-C5	6.57	124.53	121.90
1	A	287	U	C6-N1-C2	-6.57	117.06	121.00
1	A	299	G	N9-C4-C5	-6.57	102.77	105.40
1	A	1051	C	N3-C4-C5	-6.57	119.27	121.90
1	A	180	U	N3-C4-O4	6.56	123.99	119.40
1	A	1079	G	C4-N9-C1'	6.56	135.03	126.50
1	A	1277	C	C6-N1-C2	-6.56	117.67	120.30
1	A	322	C	C6-N1-C2	6.56	122.92	120.30
1	A	945	G	N1-C6-O6	-6.56	115.96	119.90
1	A	855	G	C5-C6-O6	-6.56	124.66	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1099	G	N1-C6-O6	6.56	123.83	119.90
1	A	1529	G	C8-N9-C1'	-6.56	118.47	127.00
1	A	825	G	C8-N9-C1'	-6.55	118.48	127.00
1	A	1438	G	C4-C5-N7	6.55	113.42	110.80
1	A	1354	C	N3-C2-O2	-6.55	117.32	121.90
1	A	74	C	C2-N1-C1'	6.55	126.00	118.80
1	A	543	C	C6-N1-C2	-6.54	117.68	120.30
1	A	284	G	C5-C6-O6	-6.53	124.68	128.60
1	A	870	U	C5-C6-N1	-6.53	119.43	122.70
1	A	1280	A	N9-C4-C5	6.53	108.41	105.80
1	A	875	C	C6-N1-C2	6.53	122.91	120.30
1	A	373	A	C6-C5-N7	-6.53	127.73	132.30
1	A	245	C	C4-C5-C6	-6.53	114.14	117.40
1	A	372	C	N3-C4-N4	6.52	122.57	118.00
1	A	624	C	N3-C4-C5	6.52	124.51	121.90
1	A	774	G	C6-C5-N7	-6.52	126.49	130.40
1	A	1238	A	C5-C6-N6	6.52	128.91	123.70
1	A	108	G	C4-N9-C1'	6.51	134.97	126.50
1	A	909	A	C8-N9-C4	-6.51	103.19	105.80
1	A	875	C	N3-C4-C5	6.51	124.50	121.90
1	A	1108	G	C4-N9-C1'	6.51	134.97	126.50
1	A	328	C	N3-C4-N4	-6.51	113.45	118.00
1	A	1251	A	C8-N9-C4	-6.50	103.20	105.80
1	A	731	G	C4-C5-N7	6.50	113.40	110.80
1	A	687	A	N3-C4-C5	-6.50	122.25	126.80
1	A	245	C	C5-C6-N1	6.49	124.25	121.00
1	A	1506	U	N1-C2-O2	6.49	127.34	122.80
1	A	285	G	C2-N3-C4	-6.49	108.66	111.90
1	A	1280	A	N1-C6-N6	-6.49	114.71	118.60
1	A	576	G	N1-C2-N3	6.48	127.79	123.90
1	A	1416	G	C4-C5-N7	6.48	113.39	110.80
1	A	54	C	N3-C2-O2	-6.48	117.36	121.90
1	A	873	A	C2-N3-C4	6.47	113.84	110.60
1	A	667	G	C2-N3-C4	-6.47	108.67	111.90
1	A	730	G	N3-C4-C5	-6.47	125.36	128.60
1	A	1504	G	N3-C4-N9	6.47	129.88	126.00
1	A	809	G	N1-C6-O6	6.46	123.78	119.90
1	A	1491	G	C8-N9-C4	-6.46	103.82	106.40
1	A	28	G	C5-C6-N1	-6.46	108.27	111.50
1	A	168	G	C6-C5-N7	-6.46	126.53	130.40
1	A	773	G	C8-N9-C4	-6.45	103.82	106.40
1	A	851	G	N7-C8-N9	6.45	116.33	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1529	G	N3-C4-C5	-6.45	125.37	128.60
1	A	569	C	N1-C2-O2	-6.45	115.03	118.90
1	A	16	A	N7-C8-N9	-6.44	110.58	113.80
1	A	190(F)	G	C8-N9-C1'	6.43	135.36	127.00
1	A	1346	A	P-O3'-C3'	6.43	127.42	119.70
1	A	263	A	C5-C6-N1	6.43	120.92	117.70
1	A	515	G	N1-C6-O6	6.43	123.76	119.90
1	A	227	G	C5-C6-O6	-6.42	124.75	128.60
1	A	975	A	N1-C6-N6	6.42	122.45	118.60
1	A	765	G	C5-N7-C8	-6.42	101.09	104.30
1	A	1187	G	C5-C6-O6	-6.42	124.75	128.60
1	A	253	U	C2-N1-C1'	-6.42	110.00	117.70
1	A	1158	C	C2-N1-C1'	6.42	125.86	118.80
1	A	237	C	C6-N1-C2	-6.42	117.73	120.30
1	A	325	A	N9-C4-C5	6.41	108.36	105.80
1	A	251	G	N3-C4-N9	6.41	129.85	126.00
1	A	1429	C	C6-N1-C2	-6.41	117.74	120.30
1	A	1079	G	N1-C2-N2	-6.40	110.44	116.20
1	A	13	U	N3-C2-O2	-6.40	117.72	122.20
1	A	859	A	N1-C6-N6	6.40	122.44	118.60
1	A	885	G	C6-C5-N7	-6.40	126.56	130.40
1	A	881	G	N1-C6-O6	6.40	123.74	119.90
1	A	1524	C	C2-N1-C1'	6.39	125.83	118.80
1	A	325	A	C5-C6-N6	6.39	128.81	123.70
1	A	1149	C	C6-N1-C2	-6.39	117.74	120.30
1	A	944	G	N3-C4-C5	-6.39	125.41	128.60
1	A	397	A	N7-C8-N9	6.38	116.99	113.80
1	A	503	C	C6-N1-C2	-6.38	117.75	120.30
1	A	948	C	C5-C6-N1	-6.38	117.81	121.00
1	A	238	G	C2-N3-C4	-6.38	108.71	111.90
1	A	814	A	C2-N3-C4	-6.38	107.41	110.60
1	A	1527	C	C6-N1-C2	-6.38	117.75	120.30
1	A	289	G	N1-C2-N3	6.38	127.72	123.90
1	A	1156	G	C8-N9-C4	-6.37	103.85	106.40
1	A	108	G	C6-C5-N7	-6.37	126.58	130.40
1	A	1461	G	C4-C5-N7	6.37	113.35	110.80
1	A	237	C	N3-C2-O2	-6.37	117.44	121.90
1	A	766	A	C8-N9-C4	6.37	108.35	105.80
1	A	875	C	C2-N3-C4	-6.37	116.72	119.90
1	A	735	C	C2-N1-C1'	-6.37	111.80	118.80
1	A	871	U	N1-C2-N3	-6.37	111.08	114.90
1	A	1395	C	C2-N1-C1'	-6.37	111.80	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	825	G	C8-N9-C4	6.36	108.95	106.40
1	A	309	G	C6-C5-N7	-6.36	126.58	130.40
1	A	888	G	C4-N9-C1'	6.36	134.76	126.50
1	A	1517	G	C5-C6-N1	-6.36	108.32	111.50
1	A	297	G	C8-N9-C4	-6.35	103.86	106.40
1	A	753	A	N9-C4-C5	6.35	108.34	105.80
1	A	526	C	N3-C4-C5	6.35	124.44	121.90
1	A	1377	A	N9-C4-C5	6.34	108.34	105.80
1	A	835	U	N1-C2-N3	6.34	118.70	114.90
1	A	852	G	N3-C4-C5	6.34	131.77	128.60
1	A	522	C	N3-C4-N4	-6.34	113.56	118.00
1	A	276	G	C8-N9-C4	6.33	108.93	106.40
1	A	1487	G	C4-N9-C1'	6.33	134.73	126.50
1	A	244	U	N3-C2-O2	6.33	126.63	122.20
1	A	274	A	C8-N9-C4	6.33	108.33	105.80
1	A	308	C	N3-C4-N4	6.33	122.43	118.00
1	A	778	G	C2-N3-C4	-6.32	108.74	111.90
1	A	1344	C	N3-C4-N4	-6.32	113.58	118.00
1	A	131	C	C6-N1-C2	6.32	122.83	120.30
1	A	376	G	C8-N9-C4	6.32	108.93	106.40
1	A	744	C	C6-N1-C2	6.31	122.83	120.30
1	A	190(G)	G	C2-N3-C4	-6.31	108.74	111.90
1	A	79	G	N7-C8-N9	6.31	116.25	113.10
1	A	81	U	C6-N1-C2	-6.31	117.22	121.00
1	A	128	G	N1-C6-O6	6.30	123.68	119.90
1	A	228	A	N1-C6-N6	6.30	122.38	118.60
1	A	730	G	C4-N9-C1'	6.30	134.69	126.50
1	A	880	C	C5-C4-N4	-6.29	115.79	120.20
1	A	916	G	C4-N9-C1'	6.29	134.68	126.50
1	A	652	U	C5-C4-O4	-6.29	122.12	125.90
1	A	260	G	N7-C8-N9	6.29	116.24	113.10
1	A	110	C	N1-C2-O2	6.29	122.67	118.90
1	A	324	G	N3-C4-N9	-6.28	122.23	126.00
1	A	718	G	C4-N9-C1'	6.28	134.67	126.50
1	A	573	A	N3-C4-C5	-6.28	122.40	126.80
1	A	1300	G	C6-C5-N7	6.28	134.17	130.40
1	A	693	G	C6-C5-N7	-6.28	126.63	130.40
1	A	1359	C	C6-N1-C2	-6.27	117.79	120.30
1	A	530	G	C8-N9-C4	-6.27	103.89	106.40
1	A	830	G	C6-C5-N7	-6.27	126.64	130.40
1	A	882	C	C5-C6-N1	-6.27	117.86	121.00
1	A	6	G	C5-C6-N1	-6.27	108.37	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	G	N1-C2-N3	6.27	127.66	123.90
1	A	835	U	N3-C2-O2	-6.26	117.81	122.20
1	A	148	G	C8-N9-C4	6.26	108.91	106.40
1	A	117	G	N9-C4-C5	-6.26	102.90	105.40
1	A	295	C	C5-C6-N1	-6.25	117.87	121.00
1	A	730	G	C8-N9-C1'	-6.25	118.87	127.00
1	A	641	U	N3-C2-O2	6.25	126.58	122.20
1	A	1235	U	C6-N1-C2	-6.25	117.25	121.00
1	A	376	G	C5-N7-C8	6.24	107.42	104.30
1	A	1432	G	C5-C6-O6	6.24	132.35	128.60
1	A	91	C	C2-N1-C1'	6.24	125.67	118.80
1	A	122	G	C6-C5-N7	-6.24	126.66	130.40
1	A	1398	A	N1-C2-N3	6.24	132.42	129.30
1	A	945	G	N1-C2-N2	6.24	121.82	116.20
1	A	1043	C	C6-N1-C2	-6.24	117.80	120.30
1	A	220	G	C4-N9-C1'	6.24	134.61	126.50
1	A	1305	G	N1-C6-O6	6.24	123.64	119.90
1	A	888	G	N3-C4-C5	-6.24	125.48	128.60
1	A	828	A	N1-C6-N6	6.23	122.34	118.60
1	A	888	G	C8-N9-C4	-6.23	103.91	106.40
1	A	1332	A	C5-C6-N6	6.23	128.68	123.70
1	A	167	G	N3-C4-C5	-6.23	125.49	128.60
1	A	545	C	N3-C4-C5	-6.23	119.41	121.90
1	A	575	G	N3-C4-C5	6.22	131.71	128.60
1	A	1126	U	C5-C6-N1	6.21	125.81	122.70
1	A	1526	G	C4-C5-N7	6.21	113.29	110.80
1	A	522	C	C6-N1-C2	6.21	122.78	120.30
1	A	577	G	N9-C4-C5	-6.21	102.92	105.40
1	A	199	G	C6-C5-N7	-6.21	126.67	130.40
1	A	1061	G	N1-C6-O6	6.20	123.62	119.90
1	A	41	G	N7-C8-N9	6.20	116.20	113.10
1	A	587	G	C4-C5-N7	-6.20	108.32	110.80
1	A	918	A	C5-C6-N1	6.20	120.80	117.70
1	A	1533	C	C2-N1-C1'	6.20	125.62	118.80
1	A	820	U	N1-C2-O2	-6.20	118.46	122.80
1	A	481	G	C5-N7-C8	6.19	107.40	104.30
1	A	769	G	C8-N9-C4	-6.19	103.92	106.40
1	A	1333	A	C5-C6-N6	6.19	128.65	123.70
1	A	1461	G	N9-C4-C5	-6.19	102.92	105.40
1	A	564	C	N1-C2-N3	-6.19	114.87	119.20
1	A	81	U	C5-C6-N1	6.18	125.79	122.70
1	A	182	U	C5-C6-N1	6.18	125.79	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1281	U	C6-N1-C2	-6.18	117.29	121.00
1	A	585	G	N7-C8-N9	-6.18	110.01	113.10
1	A	1505	G	C5-N7-C8	-6.18	101.21	104.30
1	A	780	A	C6-N1-C2	-6.18	114.89	118.60
1	A	1438	G	C6-C5-N7	-6.18	126.69	130.40
1	A	400	C	N3-C4-C5	6.17	124.37	121.90
1	A	1158	C	N3-C2-O2	-6.17	117.58	121.90
1	A	946	A	C8-N9-C4	-6.17	103.33	105.80
1	A	137	C	C6-N1-C2	6.17	122.77	120.30
1	A	305	G	N3-C2-N2	-6.17	115.58	119.90
1	A	766	A	N9-C4-C5	-6.17	103.33	105.80
1	A	919	A	C2-N3-C4	6.17	113.68	110.60
1	A	97	G	N3-C4-C5	-6.16	125.52	128.60
1	A	570	G	C4-N9-C1'	6.16	134.51	126.50
1	A	1078	U	C5-C6-N1	6.16	125.78	122.70
1	A	693	G	N1-C6-O6	6.16	123.60	119.90
1	A	506	G	N1-C6-O6	-6.16	116.21	119.90
1	A	93	G	N3-C4-N9	6.16	129.69	126.00
1	A	1075	C	C2-N1-C1'	6.16	125.57	118.80
1	A	1100	C	C6-N1-C2	-6.16	117.84	120.30
1	A	119	A	N9-C4-C5	6.15	108.26	105.80
1	A	1332	A	C8-N9-C4	-6.15	103.34	105.80
1	A	333	G	N1-C6-O6	6.15	123.59	119.90
1	A	820	U	C5-C6-N1	-6.15	119.62	122.70
1	A	1282	C	C5-C6-N1	6.15	124.08	121.00
1	A	1505	G	C6-C5-N7	-6.15	126.71	130.40
1	A	247	G	N3-C2-N2	-6.15	115.60	119.90
1	A	1335	C	N3-C2-O2	-6.14	117.60	121.90
1	A	642	A	C5-N7-C8	-6.14	100.83	103.90
1	A	522	C	C5-C4-N4	6.14	124.50	120.20
1	A	1505	G	N9-C4-C5	6.13	107.85	105.40
1	A	1093	A	N1-C6-N6	6.13	122.28	118.60
1	A	562	C	N1-C2-O2	6.13	122.58	118.90
1	A	825	G	N1-C6-O6	6.13	123.58	119.90
1	A	111	G	N3-C4-N9	-6.12	122.33	126.00
1	A	812	C	C5-C4-N4	6.12	124.49	120.20
1	A	180	U	C5-C6-N1	6.12	125.76	122.70
1	A	1354	C	C5-C6-N1	6.12	124.06	121.00
1	A	98	U	C5-C6-N1	6.12	125.76	122.70
1	A	597	G	C4-N9-C1'	6.12	134.45	126.50
1	A	867	G	C2-N3-C4	-6.12	108.84	111.90
1	A	1361(A)	C	C5-C6-N1	6.12	124.06	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	872	A	C2-N3-C4	-6.11	107.54	110.60
1	A	167	G	C8-N9-C4	-6.11	103.95	106.40
1	A	736	C	N3-C4-C5	6.11	124.34	121.90
1	A	901	A	C2-N3-C4	-6.11	107.54	110.60
1	A	654	G	C2-N3-C4	-6.11	108.84	111.90
1	A	896	C	C6-N1-C2	-6.11	117.86	120.30
1	A	711	G	N1-C6-O6	6.11	123.56	119.90
1	A	1467	G	N3-C4-C5	6.11	131.66	128.60
1	A	1347	G	C4-C5-N7	6.10	113.24	110.80
1	A	1476	G	C8-N9-C4	-6.10	103.96	106.40
1	A	1342	C	N3-C4-N4	6.10	122.27	118.00
1	A	570	G	C8-N9-C1'	-6.10	119.07	127.00
1	A	1544	U	N3-C4-O4	6.09	123.67	119.40
1	A	541	G	N1-C6-O6	6.09	123.56	119.90
1	A	303	A	N1-C6-N6	6.09	122.25	118.60
1	A	220	G	C6-C5-N7	-6.09	126.75	130.40
1	A	576	G	C4-N9-C1'	6.09	134.41	126.50
1	A	747	C	C6-N1-C2	6.09	122.73	120.30
1	A	753	A	N3-C4-C5	-6.08	122.54	126.80
1	A	859	A	N7-C8-N9	6.08	116.84	113.80
1	A	659	U	C5-C6-N1	-6.08	119.66	122.70
1	A	651	C	N3-C4-C5	6.08	124.33	121.90
1	A	658	G	N9-C4-C5	-6.08	102.97	105.40
1	A	1415	G	N1-C6-O6	6.08	123.55	119.90
1	A	476	G	C8-N9-C4	-6.07	103.97	106.40
1	A	820	U	C2-N3-C4	-6.07	123.36	127.00
1	A	107	G	C4-C5-N7	6.07	113.23	110.80
1	A	382	A	C6-C5-N7	-6.07	128.05	132.30
1	A	1181	G	C4-N9-C1'	-6.07	118.61	126.50
1	A	1281	U	C5-C6-N1	6.07	125.73	122.70
1	A	79	G	N1-C6-O6	6.07	123.54	119.90
1	A	129(A)	G	N1-C6-O6	6.07	123.54	119.90
1	A	228	A	C2-N3-C4	-6.07	107.57	110.60
1	A	800	G	N1-C2-N3	6.07	127.54	123.90
1	A	283	C	C5-C6-N1	6.07	124.03	121.00
1	A	110	C	N3-C2-O2	-6.06	117.66	121.90
1	A	113	G	C6-C5-N7	-6.06	126.76	130.40
1	A	289	G	C6-C5-N7	-6.06	126.76	130.40
1	A	382	A	N7-C8-N9	6.06	116.83	113.80
1	A	577	G	C4-C5-N7	6.06	113.22	110.80
1	A	773	G	C4-N9-C1'	6.06	134.38	126.50
1	A	190(G)	G	C4-N9-C1'	6.05	134.37	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	A	C4-C5-C6	6.05	120.03	117.00
1	A	1379	G	N3-C4-C5	-6.05	125.57	128.60
1	A	1509	C	C5-C6-N1	-6.05	117.97	121.00
1	A	753	A	N1-C6-N6	-6.05	114.97	118.60
1	A	285	G	C6-C5-N7	-6.05	126.77	130.40
1	A	1530	G	N1-C6-O6	6.05	123.53	119.90
1	A	945	G	C4-N9-C1'	-6.04	118.64	126.50
1	A	1374	A	C4-C5-C6	6.04	120.02	117.00
1	A	1377	A	C5-C6-N6	6.04	128.53	123.70
1	A	74	C	C6-N1-C1'	-6.04	113.56	120.80
1	A	928	G	N9-C4-C5	-6.04	102.98	105.40
1	A	899	C	C6-N1-C2	-6.04	117.89	120.30
1	A	916	G	N3-C4-C5	-6.04	125.58	128.60
1	A	926	G	N3-C4-C5	-6.04	125.58	128.60
1	A	726	C	C2-N3-C4	-6.03	116.88	119.90
1	A	654	G	N3-C2-N2	-6.03	115.68	119.90
1	A	558	G	C4-C5-N7	6.03	113.21	110.80
1	A	968	A	N1-C6-N6	6.02	122.21	118.60
1	A	859	A	C5-C6-N6	-6.02	118.88	123.70
1	A	1104	G	N3-C4-N9	6.02	129.61	126.00
1	A	115	G	N7-C8-N9	-6.02	110.09	113.10
1	A	825	G	N9-C4-C5	-6.02	102.99	105.40
1	A	167	G	N1-C6-O6	-6.01	116.29	119.90
1	A	970	C	N1-C2-O2	6.01	122.50	118.90
1	A	597	G	N1-C2-N3	6.00	127.50	123.90
1	A	1056	U	N1-C2-N3	-6.00	111.30	114.90
1	A	9	G	N9-C4-C5	-6.00	103.00	105.40
1	A	450	G	N7-C8-N9	-6.00	110.10	113.10
1	A	658	G	C8-N9-C4	6.00	108.80	106.40
1	A	1523	G	C5-N7-C8	-5.99	101.30	104.30
1	A	777	A	C8-N9-C4	-5.99	103.40	105.80
1	A	731	G	N9-C4-C5	-5.99	103.00	105.40
1	A	969	A	C4-C5-N7	5.99	113.69	110.70
1	A	78	G	C5-C6-O6	-5.99	125.01	128.60
1	A	572	A	C2-N3-C4	5.99	113.59	110.60
1	A	204	U	C2-N1-C1'	5.98	124.88	117.70
1	A	1353	G	C5-C6-N1	5.98	114.49	111.50
1	A	299	G	N3-C4-N9	5.98	129.59	126.00
1	A	1377	A	C6-N1-C2	-5.97	115.02	118.60
1	A	1422	G	C5-C6-N1	-5.97	108.51	111.50
1	A	692	U	N3-C2-O2	-5.97	118.02	122.20
1	A	725	G	C6-C5-N7	-5.97	126.82	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	755	G	C5-C6-N1	5.97	114.49	111.50
1	A	1523	G	C4-C5-N7	5.97	113.19	110.80
1	A	613	C	C6-N1-C2	5.97	122.69	120.30
1	A	1374	A	N1-C2-N3	5.97	132.28	129.30
1	A	1511	G	C4-C5-N7	5.97	113.19	110.80
1	A	521	G	C5-C6-N1	5.96	114.48	111.50
1	A	576	G	N3-C4-C5	-5.96	125.62	128.60
1	A	895	G	C8-N9-C4	-5.96	104.02	106.40
1	A	981	U	N3-C2-O2	5.96	126.37	122.20
1	A	1083	U	C6-N1-C2	-5.95	117.43	121.00
1	A	1237	C	C4-C5-C6	5.95	120.37	117.40
1	A	1446	A	C8-N9-C4	5.94	108.18	105.80
1	A	868	C	C2-N3-C4	-5.94	116.93	119.90
1	A	942	G	N1-C6-O6	5.94	123.47	119.90
1	A	1306	A	C4-C5-C6	5.94	119.97	117.00
1	A	1533	C	C5-C6-N1	5.94	123.97	121.00
1	A	98	U	C6-N1-C2	-5.94	117.44	121.00
1	A	906	G	C6-C5-N7	-5.94	126.84	130.40
1	A	605	U	N1-C2-O2	5.94	126.95	122.80
1	A	1079	G	N3-C4-N9	5.93	129.56	126.00
1	A	751	U	N3-C2-O2	5.93	126.35	122.20
1	A	269	C	C6-N1-C2	-5.92	117.93	120.30
1	A	576	G	C8-N9-C1'	-5.92	119.30	127.00
1	A	1108	G	N3-C4-N9	5.92	129.56	126.00
1	A	1346	A	C6-N1-C2	-5.92	115.05	118.60
1	A	863	U	C4-C5-C6	5.92	123.25	119.70
1	A	1502	A	C5-C6-N6	-5.92	118.97	123.70
1	A	970	C	N3-C2-O2	-5.92	117.76	121.90
1	A	1344	C	C5-C6-N1	-5.92	118.04	121.00
1	A	233	C	N1-C2-O2	5.91	122.45	118.90
1	A	277	C	C6-N1-C2	5.91	122.66	120.30
1	A	1432	G	C5-C6-N1	-5.91	108.55	111.50
1	A	936	C	N1-C2-O2	5.91	122.44	118.90
1	A	372	C	N3-C2-O2	5.91	126.03	121.90
1	A	793	U	C5-C6-N1	5.91	125.65	122.70
1	A	487	A	C8-N9-C4	5.90	108.16	105.80
1	A	23	C	C2-N3-C4	-5.90	116.95	119.90
1	A	670	G	C8-N9-C1'	-5.90	119.33	127.00
1	A	605	U	N3-C4-O4	-5.90	115.27	119.40
1	A	20	G	C2-N3-C4	-5.89	108.95	111.90
1	A	15	G	C4-N9-C1'	5.89	134.16	126.50
1	A	573	A	C6-N1-C2	-5.89	115.07	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1069	C	C6-N1-C2	5.89	122.66	120.30
1	A	1308	U	N3-C2-O2	5.89	126.32	122.20
1	A	1496	C	N3-C2-O2	-5.89	117.78	121.90
1	A	971	G	C4-C5-N7	-5.89	108.44	110.80
1	A	279	A	N1-C2-N3	5.89	132.24	129.30
1	A	697	U	C2-N1-C1'	-5.89	110.64	117.70
1	A	764	C	C6-N1-C2	-5.89	117.94	120.30
1	A	1061	G	C5-C6-N1	-5.89	108.56	111.50
1	A	897	C	N3-C4-N4	5.88	122.12	118.00
1	A	251	G	N9-C4-C5	-5.88	103.05	105.40
1	A	587	G	N1-C6-O6	-5.88	116.37	119.90
1	A	9	G	C8-N9-C1'	-5.88	119.36	127.00
1	A	565	U	C4-C5-C6	-5.88	116.17	119.70
1	A	722	A	C5-N7-C8	-5.88	100.96	103.90
1	A	833	U	N1-C2-O2	5.87	126.91	122.80
1	A	1449	C	C6-N1-C2	5.87	122.65	120.30
1	A	590	C	C6-N1-C2	5.87	122.65	120.30
1	A	779	C	C4-C5-C6	5.87	120.34	117.40
1	A	1467	G	N3-C4-N9	-5.87	122.48	126.00
1	A	454	C	C6-N1-C2	-5.87	117.95	120.30
1	A	116	A	N1-C6-N6	5.87	122.12	118.60
1	A	371	G	C5-C6-N1	5.87	114.43	111.50
1	A	872	A	C6-C5-N7	-5.87	128.19	132.30
1	A	1527	C	C2-N1-C1'	5.87	125.25	118.80
1	A	1441	G	C4-C5-C6	5.86	122.32	118.80
1	A	1195	C	C5-C6-N1	5.86	123.93	121.00
1	A	201	C	C6-N1-C1'	5.86	127.83	120.80
1	A	127	G	N1-C6-O6	5.86	123.42	119.90
1	A	796	C	C6-N1-C2	-5.86	117.96	120.30
17	Q	22	LEU	CA-CB-CG	-5.85	101.84	115.30
1	A	23	C	C4-C5-C6	5.85	120.33	117.40
1	A	530	G	N7-C8-N9	5.85	116.03	113.10
1	A	864	A	N9-C4-C5	5.85	108.14	105.80
1	A	1455	G	C5-C6-N1	-5.85	108.57	111.50
1	A	113	G	N3-C4-N9	5.85	129.51	126.00
1	A	637	G	C8-N9-C1'	-5.85	119.39	127.00
1	A	1093	A	C5-C6-N6	-5.85	119.02	123.70
1	A	1202	G	N1-C6-O6	-5.85	116.39	119.90
1	A	838	G	N7-C8-N9	-5.85	110.18	113.10
1	A	919	A	C8-N9-C4	5.85	108.14	105.80
1	A	1179	A	N1-C6-N6	-5.84	115.09	118.60
1	A	580	U	C4-C5-C6	5.84	123.21	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	G	N1-C6-O6	-5.84	116.39	119.90
1	A	654	G	N3-C4-C5	5.84	131.52	128.60
1	A	599	C	N3-C2-O2	5.84	125.99	121.90
1	A	637	G	N3-C4-N9	5.84	129.50	126.00
1	A	766	A	C5-C6-N6	-5.84	119.03	123.70
1	A	220	G	N3-C4-N9	5.84	129.50	126.00
1	A	310	G	C6-C5-N7	-5.83	126.90	130.40
1	A	75	G	N3-C4-C5	-5.83	125.68	128.60
1	A	639	G	N1-C2-N2	-5.83	110.95	116.20
1	A	634	C	N3-C2-O2	-5.83	117.82	121.90
1	A	785	G	N1-C6-O6	5.82	123.39	119.90
1	A	830	G	N3-C2-N2	-5.82	115.82	119.90
1	A	856	C	C4-C5-C6	5.82	120.31	117.40
1	A	1181	G	N3-C4-C5	5.82	131.51	128.60
1	A	636	U	C4-C5-C6	5.82	123.19	119.70
1	A	730	G	C4-C5-C6	5.82	122.29	118.80
17	Q	35	VAL	CG1-CB-CG2	5.82	120.21	110.90
1	A	909	A	C6-N1-C2	-5.81	115.11	118.60
1	A	658	G	C4-N9-C1'	5.80	134.04	126.50
1	A	1416	G	N1-C6-O6	5.80	123.38	119.90
1	A	260	G	N3-C2-N2	-5.80	115.84	119.90
1	A	707	C	C6-N1-C2	5.79	122.62	120.30
1	A	556	C	C5-C6-N1	-5.79	118.11	121.00
1	A	1408	A	N1-C6-N6	5.79	122.07	118.60
1	A	733	A	C8-N9-C4	5.79	108.11	105.80
1	A	305	G	N7-C8-N9	5.79	115.99	113.10
1	A	1063	C	C4-C5-C6	5.79	120.29	117.40
1	A	266	G	C4-C5-N7	5.78	113.11	110.80
1	A	396	G	C6-C5-N7	-5.78	126.93	130.40
1	A	1483	A	N9-C4-C5	5.78	108.11	105.80
1	A	1084	G	N1-C6-O6	-5.77	116.44	119.90
1	A	1107	C	C6-N1-C2	-5.77	117.99	120.30
1	A	119	A	C8-N9-C4	-5.77	103.49	105.80
1	A	794	A	C4-C5-N7	-5.77	107.81	110.70
1	A	1517	G	C4-C5-C6	5.77	122.26	118.80
1	A	719	C	N1-C2-O2	5.77	122.36	118.90
1	A	886	G	C2-N3-C4	-5.77	109.02	111.90
1	A	782	A	C6-N1-C2	-5.77	115.14	118.60
1	A	1503	A	C8-N9-C4	5.77	108.11	105.80
1	A	1446	A	N7-C8-N9	-5.76	110.92	113.80
1	A	331	G	N9-C4-C5	-5.76	103.09	105.40
1	A	1497	G	N7-C8-N9	5.76	115.98	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	G	N1-C2-N3	5.76	127.36	123.90
1	A	508	C	N1-C2-O2	5.76	122.36	118.90
1	A	47	C	N3-C2-O2	-5.75	117.87	121.90
1	A	275	G	C8-N9-C4	5.75	108.70	106.40
1	A	1287	A	C8-N9-C4	-5.75	103.50	105.80
1	A	1300	G	C5-C6-O6	5.75	132.05	128.60
1	A	1091	U	N1-C2-O2	5.75	126.83	122.80
1	A	374	A	N1-C6-N6	-5.75	115.15	118.60
1	A	715	A	C5-C6-N1	-5.75	114.83	117.70
1	A	307	C	N1-C2-O2	5.75	122.35	118.90
1	A	637	G	N3-C4-C5	-5.75	125.73	128.60
1	A	509	A	C8-N9-C4	-5.74	103.50	105.80
1	A	1187	G	C4-C5-N7	5.74	113.10	110.80
1	A	220	G	C8-N9-C1'	-5.74	119.54	127.00
1	A	881	G	C6-C5-N7	-5.74	126.96	130.40
1	A	121	C	C5-C6-N1	-5.74	118.13	121.00
1	A	803	G	N1-C2-N2	-5.74	111.04	116.20
1	A	144	G	N1-C6-O6	5.73	123.34	119.90
1	A	1079	G	N1-C2-N3	5.73	127.34	123.90
1	A	103	C	C5-C6-N1	5.73	123.87	121.00
1	A	862	C	C5-C4-N4	-5.73	116.19	120.20
1	A	78	G	C8-N9-C4	5.73	108.69	106.40
1	A	117	G	C8-N9-C4	5.72	108.69	106.40
1	A	578	C	N1-C2-N3	5.72	123.21	119.20
1	A	791	G	N7-C8-N9	5.72	115.96	113.10
1	A	653	A	N1-C6-N6	-5.72	115.17	118.60
1	A	1496	C	C5-C6-N1	5.72	123.86	121.00
1	A	1523	G	N1-C2-N2	5.72	121.34	116.20
1	A	382	A	C4-C5-C6	5.71	119.86	117.00
1	A	308	C	C5-C4-N4	-5.71	116.20	120.20
1	A	15	G	N3-C4-N9	5.71	129.42	126.00
1	A	190(E)	U	C2-N3-C4	-5.71	123.58	127.00
1	A	44	G	C6-C5-N7	-5.70	126.98	130.40
1	A	824	C	N1-C2-O2	-5.70	115.48	118.90
1	A	862	C	C5-C6-N1	5.70	123.85	121.00
1	A	1348	U	C2-N1-C1'	5.70	124.54	117.70
1	A	204	U	C5-C6-N1	5.70	125.55	122.70
1	A	328	C	N3-C4-C5	5.70	124.18	121.90
1	A	190(F)	G	C6-C5-N7	5.69	133.82	130.40
1	A	948	C	C2-N1-C1'	-5.69	112.54	118.80
1	A	657	G	C5-C6-N1	-5.69	108.65	111.50
1	A	1371	G	N3-C4-N9	5.69	129.42	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	742	G	N3-C4-N9	-5.69	122.59	126.00
1	A	519	C	N3-C4-C5	-5.68	119.63	121.90
1	A	6	G	C4-N9-C1'	5.68	133.89	126.50
1	A	1524	C	N3-C4-N4	5.68	121.98	118.00
1	A	397	A	C4-C5-C6	5.68	119.84	117.00
1	A	1337	G	C8-N9-C4	-5.68	104.13	106.40
1	A	27	G	C4-C5-N7	5.68	113.07	110.80
1	A	115	G	P-O3'-C3'	5.68	126.51	119.70
1	A	179	A	N1-C6-N6	5.68	122.01	118.60
1	A	765	G	N1-C6-O6	5.67	123.31	119.90
1	A	1195	C	C6-N1-C2	-5.67	118.03	120.30
1	A	1401	G	C6-C5-N7	-5.67	127.00	130.40
1	A	545	C	C6-N1-C2	-5.67	118.03	120.30
1	A	1238	A	C4-C5-N7	-5.67	107.86	110.70
1	A	1083	U	C4-C5-C6	5.67	123.10	119.70
1	A	1530	G	C4-N9-C1'	-5.67	119.13	126.50
1	A	558	G	C6-C5-N7	-5.67	127.00	130.40
1	A	653	A	N9-C4-C5	5.67	108.07	105.80
1	A	1394	A	N1-C6-N6	-5.67	115.20	118.60
1	A	93	G	N3-C2-N2	5.67	123.87	119.90
1	A	728	A	N1-C2-N3	5.66	132.13	129.30
5	E	12	LEU	CA-CB-CG	5.66	128.31	115.30
6	F	37	VAL	CB-CA-C	-5.66	100.65	111.40
1	A	268	C	N1-C2-O2	5.66	122.29	118.90
1	A	511	C	C5-C6-N1	-5.66	118.17	121.00
1	A	6	G	C6-C5-N7	-5.65	127.01	130.40
1	A	7	G	C6-N1-C2	-5.65	121.71	125.10
1	A	715	A	N1-C2-N3	5.65	132.13	129.30
1	A	9	G	N1-C6-O6	5.65	123.29	119.90
1	A	1264	C	C6-N1-C2	-5.65	118.04	120.30
1	A	29	G	N1-C2-N3	5.65	127.29	123.90
1	A	316	G	C5-C6-O6	-5.65	125.21	128.60
1	A	591	U	C2-N3-C4	-5.65	123.61	127.00
1	A	916	G	C8-N9-C1'	-5.65	119.66	127.00
1	A	577	G	C2-N3-C4	-5.65	109.08	111.90
1	A	122	G	C5-C6-N1	-5.64	108.68	111.50
1	A	1527	C	N3-C4-N4	5.64	121.95	118.00
8	H	4	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	48	C	C6-N1-C2	5.64	122.56	120.30
1	A	1187	G	C6-C5-N7	-5.64	127.01	130.40
1	A	126	G	N7-C8-N9	-5.64	110.28	113.10
1	A	638	G	C6-C5-N7	-5.64	127.02	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	G	C8-N9-C4	5.64	108.66	106.40
1	A	936	C	C5-C6-N1	-5.64	118.18	121.00
1	A	700	G	N9-C4-C5	-5.64	103.14	105.40
1	A	1487	G	C4-C5-C6	5.64	122.18	118.80
1	A	1247	U	C6-N1-C2	-5.64	117.62	121.00
1	A	1353	G	N3-C4-C5	-5.64	125.78	128.60
1	A	1500	A	N1-C6-N6	-5.64	115.22	118.60
1	A	58	C	N3-C4-C5	5.63	124.15	121.90
1	A	190(I)	G	C8-N9-C4	5.63	108.65	106.40
1	A	565	U	C6-N1-C2	5.63	124.38	121.00
1	A	888	G	C4-C5-N7	-5.63	108.55	110.80
1	A	1104	G	C5-C6-O6	-5.63	125.22	128.60
1	A	9	G	N3-C4-N9	5.63	129.38	126.00
1	A	357	G	C8-N9-C4	5.63	108.65	106.40
1	A	790	A	N7-C8-N9	5.63	116.61	113.80
1	A	570	G	N1-C2-N2	-5.63	111.13	116.20
1	A	107	G	C5-C6-O6	-5.63	125.22	128.60
1	A	607	A	N1-C6-N6	5.63	121.98	118.60
1	A	706	A	N1-C2-N3	5.62	132.11	129.30
1	A	572	A	C6-N1-C2	-5.62	115.23	118.60
1	A	931	C	C6-N1-C2	5.62	122.55	120.30
1	A	654	G	N1-C2-N3	5.62	127.27	123.90
1	A	1543	C	N1-C2-N3	-5.62	115.27	119.20
1	A	90	U	C5-C6-N1	5.61	125.51	122.70
1	A	198	G	N1-C6-O6	5.61	123.27	119.90
1	A	1195	C	C2-N1-C1'	5.61	124.97	118.80
1	A	877	C	N1-C2-N3	5.61	123.13	119.20
1	A	106	C	C4-C5-C6	5.60	120.20	117.40
1	A	397	A	N1-C2-N3	5.60	132.10	129.30
1	A	74	C	N1-C2-O2	5.60	122.26	118.90
1	A	1083	U	N3-C4-O4	5.60	123.32	119.40
1	A	852	G	N3-C2-N2	-5.60	115.98	119.90
1	A	88	A	N7-C8-N9	5.60	116.60	113.80
1	A	723	U	N1-C2-O2	5.60	126.72	122.80
1	A	1342	C	C5-C6-N1	5.60	123.80	121.00
1	A	66	G	C2-N3-C4	-5.60	109.10	111.90
1	A	66	G	N1-C6-O6	5.60	123.26	119.90
1	A	310	G	N3-C2-N2	-5.59	115.98	119.90
1	A	190(G)	G	C4-C5-N7	5.59	113.04	110.80
1	A	397	A	C4-N9-C1'	5.59	136.37	126.30
1	A	558	G	N1-C6-O6	5.59	123.25	119.90
1	A	1365	G	N9-C4-C5	5.59	107.64	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1500	A	C6-N1-C2	-5.59	115.25	118.60
1	A	1103	C	N3-C2-O2	-5.59	117.99	121.90
1	A	70	G	N1-C6-O6	5.59	123.25	119.90
1	A	703	G	C4-C5-N7	-5.59	108.56	110.80
1	A	1504	G	N1-C2-N2	-5.58	111.17	116.20
1	A	43	C	C2-N1-C1'	-5.58	112.66	118.80
1	A	297	G	N7-C8-N9	5.58	115.89	113.10
1	A	981	U	C5-C4-O4	-5.58	122.55	125.90
1	A	700	G	N1-C2-N2	-5.58	111.18	116.20
1	A	815	A	N9-C4-C5	-5.58	103.57	105.80
1	A	809	G	C6-C5-N7	-5.58	127.05	130.40
1	A	227	G	N1-C6-O6	5.57	123.24	119.90
1	A	230	G	N1-C2-N2	-5.57	111.18	116.20
1	A	860	A	N9-C4-C5	5.57	108.03	105.80
1	A	1504	G	C4-C5-N7	-5.57	108.57	110.80
1	A	1250	A	N9-C4-C5	5.57	108.03	105.80
1	A	297	G	C6-C5-N7	-5.57	127.06	130.40
1	A	565	U	N3-C4-C5	5.57	117.94	114.60
1	A	658	G	N3-C4-N9	5.57	129.34	126.00
1	A	818	G	N3-C2-N2	-5.57	116.00	119.90
1	A	597	G	N7-C8-N9	5.57	115.88	113.10
1	A	1517	G	C4-N9-C1'	5.57	133.74	126.50
1	A	577	G	C5-C6-O6	-5.56	125.26	128.60
1	A	1237	C	N1-C2-N3	5.56	123.09	119.20
1	A	372	C	N1-C2-O2	5.56	122.24	118.90
1	A	1056	U	N3-C2-O2	5.56	126.09	122.20
1	A	1377	A	C5-N7-C8	5.56	106.68	103.90
1	A	1521	G	C5-C6-N1	5.56	114.28	111.50
1	A	1543	C	C6-N1-C1'	-5.56	114.13	120.80
1	A	632	A	N1-C6-N6	5.55	121.93	118.60
1	A	628	G	N3-C4-C5	-5.55	125.82	128.60
1	A	331	G	C4-C5-C6	5.55	122.13	118.80
1	A	1203	C	C5-C6-N1	5.55	123.78	121.00
1	A	816	A	C2-N3-C4	-5.55	107.83	110.60
1	A	523	A	C2-N3-C4	-5.55	107.83	110.60
1	A	819	A	C4-C5-C6	5.55	119.77	117.00
1	A	292	G	C4-C5-N7	5.54	113.02	110.80
1	A	1345	U	N1-C2-O2	-5.54	118.92	122.80
1	A	923	A	N1-C6-N6	5.54	121.92	118.60
1	A	123	C	N3-C4-C5	-5.54	119.69	121.90
1	A	676	A	N7-C8-N9	-5.54	111.03	113.80
1	A	1231	G	C4-C5-N7	5.54	113.02	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1514	C	C2-N1-C1'	-5.53	112.72	118.80
1	A	43	C	C2-N3-C4	-5.53	117.14	119.90
1	A	171	A	C6-N1-C2	-5.53	115.28	118.60
1	A	1378	C	C5-C6-N1	5.53	123.77	121.00
1	A	885	G	C5-C6-N1	-5.53	108.74	111.50
1	A	894	G	N1-C6-O6	5.53	123.22	119.90
1	A	1338	G	N1-C2-N2	-5.53	111.23	116.20
1	A	13	U	N1-C2-N3	5.52	118.21	114.90
1	A	130	A	C8-N9-C4	5.52	108.01	105.80
1	A	190(G)	G	N7-C8-N9	5.52	115.86	113.10
1	A	790	A	N9-C4-C5	5.52	108.01	105.80
1	A	6	G	N1-C2-N3	5.52	127.21	123.90
1	A	166	G	C8-N9-C4	5.52	108.61	106.40
1	A	337	C	N3-C4-C5	5.52	124.11	121.90
1	A	1441	G	N9-C4-C5	5.52	107.61	105.40
1	A	780	A	N1-C6-N6	-5.52	115.29	118.60
1	A	874	G	C5-C6-O6	-5.52	125.29	128.60
1	A	969	A	C5-N7-C8	-5.52	101.14	103.90
1	A	867	G	N1-C2-N3	5.51	127.21	123.90
1	A	935	A	C5-C6-N1	5.51	120.46	117.70
1	A	505	G	N9-C4-C5	-5.51	103.19	105.40
1	A	407	G	N3-C4-N9	-5.51	122.69	126.00
1	A	785	G	C6-C5-N7	-5.51	127.09	130.40
1	A	1078	U	C6-N1-C2	-5.51	117.69	121.00
1	A	297	G	C4-N9-C1'	5.51	133.66	126.50
1	A	1483	A	C6-N1-C2	-5.51	115.30	118.60
1	A	1487	G	C8-N9-C1'	-5.50	119.84	127.00
1	A	53	A	C6-N1-C2	-5.50	115.30	118.60
1	A	482	A	C5-C6-N6	-5.50	119.30	123.70
1	A	1303	C	C6-N1-C2	5.50	122.50	120.30
1	A	828	A	C2-N3-C4	-5.49	107.85	110.60
1	A	1335	C	C5-C4-N4	5.49	124.04	120.20
1	A	1370	G	C4-C5-N7	5.49	113.00	110.80
1	A	729	A	C5-C6-N6	-5.49	119.31	123.70
1	A	1333	A	N1-C6-N6	-5.49	115.31	118.60
1	A	284	G	C6-C5-N7	-5.49	127.11	130.40
1	A	1189	C	C6-N1-C2	5.49	122.50	120.30
1	A	787	A	C4-C5-C6	5.49	119.74	117.00
1	A	499	A	C8-N9-C4	-5.48	103.61	105.80
1	A	9	G	C6-C5-N7	-5.48	127.11	130.40
1	A	886	G	N1-C2-N3	5.48	127.19	123.90
1	A	946	A	C4-C5-N7	-5.48	107.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1392	G	C6-C5-N7	-5.48	127.11	130.40
1	A	589	C	N3-C4-C5	5.48	124.09	121.90
1	A	1230	C	C5-C6-N1	5.48	123.74	121.00
1	A	1454	G	C5-C6-O6	-5.48	125.31	128.60
1	A	303	A	C5-N7-C8	-5.48	101.16	103.90
1	A	825	G	N3-C4-N9	5.48	129.29	126.00
1	A	47	C	C2-N1-C1'	5.47	124.82	118.80
1	A	610	G	C8-N9-C4	-5.47	104.21	106.40
1	A	653	A	C8-N9-C4	-5.47	103.61	105.80
1	A	1067	A	P-O3'-C3'	5.47	126.27	119.70
1	A	1203	C	C6-N1-C2	-5.47	118.11	120.30
1	A	723	U	C6-N1-C2	-5.47	117.72	121.00
1	A	761	G	N1-C2-N2	-5.47	111.28	116.20
1	A	765	G	N3-C4-C5	5.47	131.34	128.60
1	A	58	C	C6-N1-C2	-5.47	118.11	120.30
1	A	289	G	C4-C5-C6	5.47	122.08	118.80
1	A	400	C	C5-C6-N1	-5.47	118.27	121.00
1	A	958	A	N1-C6-N6	-5.47	115.32	118.60
1	A	271	C	C6-N1-C2	-5.46	118.11	120.30
1	A	1531	A	C6-C5-N7	-5.46	128.48	132.30
1	A	309	G	C4-C5-N7	5.46	112.98	110.80
1	A	482	A	C4-C5-N7	5.46	113.43	110.70
1	A	1015	A	N1-C6-N6	-5.46	115.33	118.60
1	A	1502	A	N7-C8-N9	5.46	116.53	113.80
1	A	27	G	C4-N9-C1'	5.46	133.59	126.50
1	A	665	A	C5-C6-N1	5.46	120.43	117.70
1	A	865	A	C8-N9-C4	-5.46	103.62	105.80
1	A	897	C	C5-C4-N4	-5.46	116.38	120.20
1	A	1375	A	N7-C8-N9	-5.46	111.07	113.80
1	A	1331	G	N1-C6-O6	-5.45	116.63	119.90
1	A	732	C	C2-N1-C1'	5.45	124.80	118.80
1	A	1392	G	N9-C4-C5	-5.45	103.22	105.40
1	A	861	G	N1-C6-O6	-5.45	116.63	119.90
1	A	22	G	N1-C6-O6	5.44	123.17	119.90
1	A	585	G	N3-C4-C5	5.44	131.32	128.60
1	A	670	G	N3-C4-N9	5.44	129.26	126.00
1	A	809	G	C5-C6-O6	-5.44	125.33	128.60
1	A	102	G	C8-N9-C4	-5.43	104.23	106.40
1	A	747	C	N3-C4-C5	5.43	124.07	121.90
1	A	1509	C	N3-C2-O2	-5.43	118.10	121.90
1	A	276	G	N1-C6-O6	5.42	123.16	119.90
1	A	80	G	C8-N9-C4	-5.42	104.23	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	G	C4-N9-C1'	5.42	133.55	126.50
1	A	823	G	N1-C2-N3	5.42	127.15	123.90
1	A	831	U	C6-N1-C2	-5.42	117.75	121.00
1	A	981	U	N3-C4-O4	5.42	123.19	119.40
5	E	115	VAL	CB-CA-C	-5.42	101.11	111.40
1	A	316	G	N1-C6-O6	5.42	123.15	119.90
1	A	238	G	N3-C4-N9	-5.41	122.75	126.00
1	A	750	G	N1-C6-O6	5.41	123.15	119.90
1	A	568	G	C4-N9-C1'	5.41	133.53	126.50
1	A	797	C	C6-N1-C2	5.41	122.46	120.30
1	A	722	A	N3-C4-C5	5.41	130.58	126.80
1	A	1104	G	N9-C4-C5	-5.41	103.24	105.40
1	A	1231	G	C5-N7-C8	-5.41	101.60	104.30
1	A	1403	C	C2-N3-C4	5.41	122.60	119.90
1	A	139	G	N1-C6-O6	5.40	123.14	119.90
1	A	288	A	C5-C6-N6	5.40	128.02	123.70
1	A	297	G	C4-C5-C6	5.40	122.04	118.80
1	A	502	G	C5-N7-C8	-5.40	101.60	104.30
1	A	199	G	C5-C6-O6	-5.40	125.36	128.60
1	A	1543	C	C2-N1-C1'	5.40	124.74	118.80
1	A	1079	G	C6-N1-C2	-5.39	121.86	125.10
1	A	864	A	N1-C6-N6	-5.39	115.37	118.60
1	A	15	G	C8-N9-C4	5.39	108.56	106.40
1	A	251	G	C8-N9-C1'	-5.39	120.00	127.00
1	A	190(C)	C	N3-C4-C5	-5.38	119.75	121.90
1	A	722	A	C4-C5-N7	5.38	113.39	110.70
1	A	1398	A	N1-C6-N6	-5.38	115.37	118.60
1	A	1514	C	N3-C4-N4	-5.38	114.23	118.00
1	A	671	G	C2-N3-C4	-5.38	109.21	111.90
1	A	7	G	N3-C4-C5	-5.38	125.91	128.60
1	A	331	G	C8-N9-C4	5.38	108.55	106.40
1	A	373	A	N1-C6-N6	5.38	121.83	118.60
1	A	662	G	C5-C6-N1	-5.38	108.81	111.50
1	A	599	C	N1-C2-O2	-5.38	115.67	118.90
1	A	1108	G	C4-C5-C6	5.38	122.03	118.80
4	D	56	VAL	CB-CA-C	-5.38	101.18	111.40
1	A	1504	G	C5-N7-C8	5.37	106.99	104.30
1	A	1524	C	C4-C5-C6	5.37	120.09	117.40
16	P	28	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	1224	G	C8-N9-C4	5.37	108.55	106.40
1	A	879	C	C5-C4-N4	-5.37	116.44	120.20
1	A	999	C	C6-N1-C2	-5.37	118.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1380	U	C6-N1-C2	-5.37	117.78	121.00
1	A	899	C	C5-C6-N1	5.37	123.68	121.00
1	A	6	G	C2-N3-C4	-5.37	109.22	111.90
1	A	91	C	C6-N1-C1'	-5.36	114.37	120.80
1	A	296	U	N3-C2-O2	-5.36	118.45	122.20
1	A	308	C	C5-C6-N1	5.36	123.68	121.00
1	A	373	A	C8-N9-C4	-5.36	103.66	105.80
1	A	481	G	C2-N3-C4	5.36	114.58	111.90
1	A	451	A	N3-C4-C5	5.36	130.55	126.80
1	A	452	A	N7-C8-N9	-5.36	111.12	113.80
1	A	635	G	C6-C5-N7	-5.36	127.18	130.40
1	A	793	U	C6-N1-C2	-5.36	117.78	121.00
1	A	888	G	C5-C6-N1	-5.36	108.82	111.50
1	A	47	C	C6-N1-C2	-5.36	118.16	120.30
1	A	108	G	C4-C5-N7	5.36	112.94	110.80
1	A	803	G	C5-C6-O6	5.36	131.81	128.60
1	A	666	G	C6-C5-N7	-5.35	127.19	130.40
1	A	190(E)	U	N3-C4-O4	-5.35	115.65	119.40
17	Q	67	LYS	N-CA-C	-5.35	96.55	111.00
1	A	288	A	N3-C4-C5	5.35	130.54	126.80
1	A	1297	C	N3-C4-C5	5.35	124.04	121.90
1	A	1329	A	N7-C8-N9	5.35	116.47	113.80
1	A	730	G	N3-C4-N9	5.34	129.21	126.00
1	A	1508	G	N3-C2-N2	-5.34	116.16	119.90
1	A	882	C	C2-N3-C4	-5.34	117.23	119.90
1	A	1055	A	C4-C5-N7	-5.34	108.03	110.70
1	A	65	U	N3-C4-C5	-5.34	111.40	114.60
1	A	396	G	C4-N9-C1'	5.34	133.44	126.50
1	A	832	C	C2-N3-C4	-5.34	117.23	119.90
1	A	1182	G	N3-C4-N9	5.34	129.20	126.00
1	A	780	A	N9-C4-C5	5.34	107.94	105.80
1	A	171	A	N1-C2-N3	5.33	131.97	129.30
1	A	328	C	C6-N1-C2	-5.33	118.17	120.30
1	A	855	G	C4-C5-N7	5.33	112.93	110.80
1	A	1377	A	C5-C6-N1	5.33	120.37	117.70
1	A	1055	A	C2-N3-C4	5.33	113.27	110.60
1	A	383	A	N7-C8-N9	5.33	116.46	113.80
1	A	190(H)	G	C5-C6-N1	-5.33	108.84	111.50
1	A	733	A	N1-C2-N3	5.33	131.96	129.30
1	A	201	C	N3-C4-C5	-5.32	119.77	121.90
1	A	361	G	N7-C8-N9	-5.32	110.44	113.10
1	A	759	A	C4-C5-C6	5.32	119.66	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1306	A	C5-C6-N1	-5.32	115.04	117.70
1	A	1148	U	C5-C6-N1	5.32	125.36	122.70
1	A	1353	G	C2-N3-C4	5.32	114.56	111.90
1	A	271	C	C5-C6-N1	5.32	123.66	121.00
1	A	378	G	C8-N9-C4	5.32	108.53	106.40
1	A	580	U	C5-C4-O4	5.31	129.09	125.90
1	A	933	G	C6-C5-N7	-5.31	127.22	130.40
1	A	1178	G	N9-C4-C5	5.31	107.52	105.40
1	A	1480	G	C5-C6-O6	5.31	131.78	128.60
1	A	89	C	C5-C6-N1	5.31	123.65	121.00
1	A	324	G	N3-C2-N2	-5.31	116.19	119.90
1	A	882	C	N3-C4-N4	-5.31	114.29	118.00
1	A	119	A	N1-C6-N6	-5.30	115.42	118.60
1	A	667	G	C8-N9-C4	5.30	108.52	106.40
1	A	1334	G	N3-C4-C5	5.30	131.25	128.60
1	A	260	G	N1-C6-O6	5.30	123.08	119.90
1	A	297	G	C5-C6-N1	-5.30	108.85	111.50
1	A	761	G	C6-C5-N7	-5.29	127.22	130.40
1	A	1380	U	N1-C2-N3	5.29	118.08	114.90
1	A	777	A	N7-C8-N9	5.29	116.45	113.80
1	A	851	G	N3-C4-C5	-5.29	125.95	128.60
1	A	811	C	C5-C4-N4	-5.29	116.50	120.20
1	A	79	G	C6-C5-N7	-5.29	127.23	130.40
1	A	573	A	C5-N7-C8	-5.29	101.25	103.90
1	A	700	G	C6-C5-N7	-5.29	127.23	130.40
1	A	1355	G	N1-C6-O6	5.28	123.07	119.90
3	C	25	GLY	N-CA-C	5.28	126.30	113.10
1	A	983	A	C2-N3-C4	5.28	113.24	110.60
1	A	1480	G	N3-C4-C5	-5.28	125.96	128.60
1	A	270	A	C8-N9-C4	-5.28	103.69	105.80
1	A	1509	C	N1-C2-N3	5.28	122.89	119.20
1	A	316	G	N3-C4-C5	-5.28	125.96	128.60
1	A	1333	A	N7-C8-N9	5.27	116.44	113.80
1	A	1416	G	C5-N7-C8	-5.27	101.66	104.30
1	A	360	A	C4-C5-N7	5.27	113.34	110.70
18	R	50	ILE	CB-CA-C	-5.27	101.06	111.60
1	A	946	A	C5-C6-N6	5.27	127.92	123.70
1	A	1504	G	C4-C5-C6	5.27	121.96	118.80
1	A	396	G	N7-C8-N9	5.27	115.73	113.10
1	A	481	G	N3-C2-N2	5.27	123.59	119.90
1	A	577	G	N3-C4-C5	5.27	131.23	128.60
1	A	1517	G	C6-C5-N7	-5.27	127.24	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1126	U	C2-N1-C1'	5.26	124.02	117.70
1	A	180	U	C6-N1-C2	-5.26	117.84	121.00
1	A	559	A	C6-N1-C2	-5.26	115.44	118.60
1	A	181	G	N3-C4-C5	-5.26	125.97	128.60
1	A	1488	G	N9-C4-C5	5.26	107.50	105.40
1	A	97	G	N7-C8-N9	5.26	115.73	113.10
1	A	303	A	C4-C5-N7	5.26	113.33	110.70
1	A	881	G	N9-C4-C5	-5.26	103.30	105.40
1	A	170	U	C2-N1-C1'	-5.25	111.39	117.70
1	A	1229	A	C8-N9-C4	5.25	107.90	105.80
1	A	505	G	C4-C5-N7	5.25	112.90	110.80
1	A	526	C	C2-N3-C4	-5.25	117.27	119.90
1	A	867	G	N1-C6-O6	5.25	123.05	119.90
1	A	105	G	N1-C6-O6	-5.25	116.75	119.90
1	A	926	G	C5-N7-C8	5.25	106.93	104.30
1	A	38	G	C8-N9-C4	5.25	108.50	106.40
1	A	232	G	C8-N9-C1'	-5.25	120.18	127.00
1	A	736	C	N3-C4-N4	-5.24	114.33	118.00
1	A	1107	C	N3-C4-C5	-5.24	119.80	121.90
1	A	1139	G	C8-N9-C4	-5.24	104.30	106.40
1	A	1510	U	C2-N3-C4	-5.24	123.86	127.00
1	A	331	G	C8-N9-C1'	-5.24	120.19	127.00
1	A	362	G	C5-C6-N1	-5.24	108.88	111.50
1	A	1353	G	N1-C6-O6	-5.24	116.76	119.90
1	A	821	G	N7-C8-N9	-5.23	110.48	113.10
1	A	1055	A	C5-N7-C8	5.23	106.52	103.90
1	A	1108	G	C8-N9-C1'	-5.23	120.20	127.00
1	A	1505	G	C4-C5-C6	5.23	121.94	118.80
1	A	826	C	C6-N1-C2	-5.23	118.21	120.30
1	A	518	C	N1-C2-O2	5.22	122.03	118.90
1	A	199	G	C4-C5-N7	5.22	112.89	110.80
1	A	730	G	C5-C6-O6	5.22	131.73	128.60
1	A	288	A	N1-C6-N6	-5.22	115.47	118.60
1	A	935	A	C4-C5-C6	-5.21	114.39	117.00
1	A	872	A	C5-C6-N6	-5.21	119.53	123.70
1	A	1461	G	C5-C6-O6	-5.21	125.47	128.60
1	A	564	C	C6-N1-C1'	-5.21	114.55	120.80
1	A	665	A	C6-N1-C2	-5.21	115.47	118.60
1	A	929	G	C5-C6-N1	-5.21	108.89	111.50
1	A	122	G	C4-C5-N7	5.21	112.88	110.80
1	A	253	U	N1-C2-O2	-5.21	119.15	122.80
1	A	1188	A	C4-C5-C6	5.21	119.61	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	C	C4-C5-C6	5.21	120.00	117.40
1	A	103	C	N3-C4-N4	5.21	121.64	118.00
1	A	141	A	C5-N7-C8	-5.21	101.30	103.90
1	A	729	A	C5-N7-C8	-5.21	101.30	103.90
17	Q	98	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	491	G	C8-N9-C1'	-5.21	120.23	127.00
1	A	751	U	C6-N1-C2	5.21	124.12	121.00
1	A	559	A	C5-C6-N1	5.20	120.30	117.70
1	A	1301	U	P-O3'-C3'	5.20	125.94	119.70
1	A	852	G	N3-C4-N9	-5.20	122.88	126.00
1	A	1224	G	N3-C4-C5	5.20	131.20	128.60
1	A	324	G	N1-C2-N2	5.20	120.88	116.20
1	A	887	G	C6-N1-C2	-5.20	121.98	125.10
1	A	1104	G	C4-C5-N7	5.20	112.88	110.80
1	A	1374	A	C5-C6-N1	-5.20	115.10	117.70
1	A	877	C	C5-C6-N1	-5.20	118.40	121.00
1	A	1231	G	C6-C5-N7	-5.19	127.28	130.40
1	A	1533	C	N1-C2-O2	5.19	122.02	118.90
1	A	777	A	C5-N7-C8	-5.19	101.31	103.90
1	A	888	G	N9-C4-C5	5.18	107.47	105.40
1	A	166	G	C5-C6-O6	-5.18	125.49	128.60
1	A	915	A	N9-C4-C5	5.18	107.87	105.80
1	A	508	C	N3-C2-O2	-5.18	118.27	121.90
1	A	881	G	C2-N3-C4	-5.18	109.31	111.90
1	A	1379	G	C2-N3-C4	5.18	114.49	111.90
1	A	190(K)	G	C8-N9-C1'	5.17	133.73	127.00
1	A	1268	A	C2-N3-C4	5.17	113.19	110.60
1	A	691	G	C8-N9-C4	-5.17	104.33	106.40
1	A	1055	A	C5-C6-N1	5.17	120.29	117.70
1	A	1441	G	C8-N9-C4	-5.17	104.33	106.40
1	A	306	G	C8-N9-C4	5.17	108.47	106.40
1	A	444	C	C6-N1-C2	-5.17	118.23	120.30
1	A	970	C	N3-C4-C5	5.17	123.97	121.90
1	A	300	A	C8-N9-C4	-5.17	103.73	105.80
1	A	460	A	C8-N9-C4	-5.16	103.73	105.80
1	A	788	U	N3-C2-O2	5.16	125.81	122.20
1	A	1409	C	C6-N1-C2	-5.16	118.23	120.30
1	A	703	G	C5-C6-O6	5.16	131.70	128.60
1	A	1197	G	N3-C4-N9	5.16	129.10	126.00
1	A	1338	G	N1-C6-O6	-5.16	116.80	119.90
1	A	863	U	C5-C4-O4	5.16	129.00	125.90
1	A	732	C	C6-N1-C1'	-5.16	114.61	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	814	A	N9-C4-C5	-5.16	103.74	105.80
1	A	922	G	C8-N9-C4	-5.16	104.34	106.40
1	A	1454	G	C4-C5-N7	5.16	112.86	110.80
1	A	251	G	C4-C5-N7	5.16	112.86	110.80
1	A	597	G	C4-C5-C6	5.16	121.89	118.80
1	A	867	G	N9-C4-C5	-5.16	103.34	105.40
1	A	318	G	C5-C6-O6	-5.16	125.51	128.60
1	A	700	G	N3-C4-C5	-5.16	126.02	128.60
1	A	822	C	C6-N1-C2	-5.16	118.24	120.30
1	A	1116	C	N1-C2-O2	5.16	121.99	118.90
1	A	1231	G	N7-C8-N9	5.16	115.68	113.10
1	A	565	U	N3-C2-O2	5.15	125.81	122.20
1	A	818	G	C5-C6-N1	-5.15	108.92	111.50
1	A	1231	G	C5-C6-O6	-5.15	125.51	128.60
1	A	804	U	N1-C2-O2	5.15	126.41	122.80
1	A	877	C	C4-C5-C6	5.15	119.97	117.40
1	A	1291	G	C8-N9-C4	-5.15	104.34	106.40
1	A	1311	G	N3-C2-N2	-5.15	116.30	119.90
12	L	85	ILE	CB-CA-C	-5.15	101.31	111.60
1	A	301	G	C8-N9-C4	-5.15	104.34	106.40
17	Q	5	VAL	CB-CA-C	-5.15	101.62	111.40
1	A	156	G	N1-C6-O6	5.14	122.99	119.90
1	A	237	C	N1-C2-N3	5.14	122.80	119.20
1	A	232	G	N3-C2-N2	5.14	123.50	119.90
1	A	869	G	C5-C6-O6	5.14	131.69	128.60
1	A	1099	G	C6-C5-N7	-5.14	127.31	130.40
1	A	1533	C	C6-N1-C1'	-5.14	114.63	120.80
1	A	269	C	N3-C2-O2	-5.14	118.30	121.90
1	A	375	U	C6-N1-C2	-5.14	117.92	121.00
1	A	782	A	N1-C2-N3	5.14	131.87	129.30
1	A	820	U	C4-C5-C6	5.14	122.78	119.70
1	A	1149	C	C5-C6-N1	5.14	123.57	121.00
1	A	1413	A	C6-N1-C2	-5.14	115.52	118.60
1	A	1528	U	C6-N1-C2	5.14	124.08	121.00
1	A	362	G	C5-C6-O6	5.14	131.68	128.60
1	A	769	G	N3-C4-C5	-5.14	126.03	128.60
1	A	511	C	C2-N3-C4	-5.13	117.33	119.90
1	A	596	C	C6-N1-C2	5.13	122.35	120.30
1	A	1461	G	N1-C6-O6	5.13	122.98	119.90
1	A	445	G	N1-C6-O6	5.13	122.98	119.90
1	A	891	U	C6-N1-C2	5.13	124.08	121.00
1	A	462	G	N3-C4-C5	-5.13	126.03	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	G	C8-N9-C4	-5.13	104.35	106.40
1	A	993	G	C8-N9-C4	-5.13	104.35	106.40
1	A	1300	G	C5-N7-C8	5.13	106.86	104.30
1	A	1544	U	C5-C4-O4	-5.13	122.82	125.90
1	A	326	G	C4-C5-C6	5.13	121.88	118.80
1	A	668	G	C8-N9-C4	5.13	108.45	106.40
1	A	824	C	C5-C6-N1	-5.13	118.44	121.00
1	A	1531	A	C8-N9-C4	-5.12	103.75	105.80
1	A	51	A	C8-N9-C4	5.12	107.85	105.80
1	A	262	A	N1-C6-N6	-5.12	115.53	118.60
1	A	1331	G	C4-C5-N7	-5.12	108.75	110.80
1	A	1363	A	C8-N9-C4	5.12	107.85	105.80
1	A	665	A	N7-C8-N9	-5.12	111.24	113.80
1	A	668	G	N7-C8-N9	-5.12	110.54	113.10
1	A	780	A	C5-C6-N1	5.12	120.26	117.70
1	A	860	A	C8-N9-C4	-5.12	103.75	105.80
1	A	319	G	C6-C5-N7	-5.12	127.33	130.40
1	A	617	G	C8-N9-C4	5.12	108.45	106.40
1	A	66	G	N3-C2-N2	-5.12	116.32	119.90
1	A	131	C	C4-C5-C6	5.12	119.96	117.40
1	A	587	G	N9-C4-C5	5.12	107.45	105.40
1	A	374	A	C2-N3-C4	5.12	113.16	110.60
1	A	1148	U	N1-C2-O2	5.12	126.38	122.80
1	A	1337	G	N9-C4-C5	5.12	107.45	105.40
1	A	1367	C	C5-C6-N1	5.12	123.56	121.00
1	A	1395	C	C5-C6-N1	-5.12	118.44	121.00
1	A	285	G	C5-C6-N1	-5.11	108.94	111.50
1	A	693	G	N3-C4-N9	5.11	129.07	126.00
1	A	899	C	N3-C4-N4	5.11	121.58	118.00
1	A	1487	G	N3-C4-N9	5.11	129.07	126.00
1	A	482	A	C4-C5-C6	5.11	119.56	117.00
1	A	916	G	N3-C4-N9	5.11	129.06	126.00
1	A	1490	C	C4-C5-C6	-5.11	114.84	117.40
1	A	190(D)	U	C5-C6-N1	-5.11	120.15	122.70
1	A	660	G	C5-C6-O6	-5.11	125.54	128.60
1	A	861	G	C4-C5-C6	-5.11	115.73	118.80
1	A	1543	C	C5-C6-N1	5.11	123.55	121.00
1	A	276	G	C2-N3-C4	-5.10	109.35	111.90
1	A	715	A	N1-C6-N6	5.10	121.66	118.60
1	A	1113	C	C5-C6-N1	5.10	123.55	121.00
1	A	509	A	C3'-C2'-C1'	-5.10	97.42	101.50
1	A	660	G	N1-C6-O6	5.10	122.96	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1181	G	N9-C4-C5	-5.10	103.36	105.40
1	A	317	G	N1-C6-O6	5.10	122.96	119.90
1	A	570	G	N3-C4-N9	5.10	129.06	126.00
1	A	1258	G	N3-C4-N9	5.10	129.06	126.00
1	A	1282	C	N3-C4-C5	-5.10	119.86	121.90
1	A	29	G	C8-N9-C4	5.10	108.44	106.40
1	A	324	G	N1-C6-O6	5.10	122.96	119.90
1	A	7	G	N1-C2-N3	5.10	126.96	123.90
1	A	13	U	C6-N1-C2	-5.10	117.94	121.00
1	A	302	G	C8-N9-C1'	-5.10	120.38	127.00
1	A	1339	A	N9-C4-C5	5.10	107.84	105.80
1	A	1434	A	N1-C6-N6	5.10	121.66	118.60
1	A	546	G	N1-C6-O6	-5.09	116.84	119.90
1	A	141	A	C4-C5-N7	5.09	113.25	110.70
1	A	853	G	C6-C5-N7	-5.09	127.34	130.40
1	A	677	U	N3-C4-C5	-5.09	111.55	114.60
1	A	1203	C	C2-N1-C1'	5.09	124.40	118.80
1	A	416	G	N7-C8-N9	5.08	115.64	113.10
1	A	862	C	C4-C5-C6	-5.08	114.86	117.40
1	A	1333	A	N1-C2-N3	5.08	131.84	129.30
1	A	300	A	C6-N1-C2	-5.08	115.55	118.60
1	A	357	G	C5-C6-N1	-5.08	108.96	111.50
1	A	782	A	C4-C5-C6	5.08	119.54	117.00
1	A	1483	A	C5-C6-N1	5.08	120.24	117.70
1	A	570	G	N1-C2-N3	5.08	126.95	123.90
1	A	708	C	C5-C6-N1	-5.08	118.46	121.00
1	A	899	C	N1-C2-O2	5.08	121.95	118.90
1	A	1305	G	N3-C4-C5	5.08	131.14	128.60
1	A	1308	U	N1-C2-O2	-5.08	119.24	122.80
1	A	227	G	C5-N7-C8	-5.08	101.76	104.30
1	A	1186	G	C5-C6-N1	-5.08	108.96	111.50
1	A	67	C	N3-C4-N4	-5.08	114.45	118.00
1	A	1055	A	N9-C4-C5	5.08	107.83	105.80
1	A	651	C	C5-C6-N1	-5.07	118.46	121.00
1	A	301	G	C4-N9-C1'	5.07	133.09	126.50
1	A	567	G	C4-C5-N7	-5.07	108.77	110.80
1	A	587	G	C5-C6-O6	5.07	131.64	128.60
1	A	788	U	N3-C4-O4	5.07	122.95	119.40
1	A	8	A	N9-C4-C5	5.07	107.83	105.80
1	A	1180	A	C2-N3-C4	5.07	113.13	110.60
1	A	863	U	N1-C2-O2	-5.07	119.25	122.80
1	A	788	U	C2-N3-C4	5.07	130.04	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	812	C	P-O3'-C3'	5.07	125.78	119.70
1	A	1197	G	C4-N9-C1'	5.07	133.09	126.50
1	A	1093	A	C4-C5-N7	5.06	113.23	110.70
1	A	1342	C	C6-N1-C2	-5.06	118.28	120.30
1	A	1430	C	N3-C2-O2	5.06	125.44	121.90
1	A	310	G	N9-C4-C5	-5.06	103.38	105.40
1	A	360	A	C2-N3-C4	-5.06	108.07	110.60
1	A	877	C	C2-N3-C4	-5.06	117.37	119.90
1	A	1191	A	N1-C6-N6	-5.06	115.57	118.60
1	A	324	G	C5-C6-N1	-5.06	108.97	111.50
1	A	794	A	C6-C5-N7	5.06	135.84	132.30
1	A	1359	C	N3-C4-C5	-5.06	119.88	121.90
1	A	116	A	N9-C4-C5	-5.05	103.78	105.80
1	A	660	G	C4-C5-N7	5.05	112.82	110.80
1	A	971	G	N7-C8-N9	-5.05	110.58	113.10
1	A	1338	G	C8-N9-C4	-5.05	104.38	106.40
1	A	799	G	C5-C6-O6	-5.05	125.57	128.60
1	A	858	G	C2-N3-C4	-5.05	109.38	111.90
1	A	326	G	C2-N3-C4	5.04	114.42	111.90
1	A	893	C	N1-C2-N3	-5.04	115.67	119.20
1	A	328	C	C6-N1-C1'	-5.04	114.75	120.80
1	A	1131	G	N3-C4-N9	5.04	129.02	126.00
1	A	120	A	N1-C2-N3	5.04	131.82	129.30
1	A	1116	C	N3-C4-N4	-5.04	114.47	118.00
1	A	1506	U	C2-N1-C1'	5.04	123.75	117.70
1	A	285	G	C4-C5-N7	5.04	112.81	110.80
1	A	764	C	C5-C6-N1	5.04	123.52	121.00
1	A	1347	G	N3-C4-N9	5.04	129.02	126.00
1	A	1100	C	N3-C2-O2	-5.03	118.38	121.90
1	A	923	A	C4-C5-N7	5.03	113.22	110.70
1	A	53	A	N1-C2-N3	5.03	131.81	129.30
1	A	75	G	C8-N9-C1'	-5.03	120.46	127.00
1	A	190(G)	G	C8-N9-C1'	-5.03	120.46	127.00
1	A	615	C	C4-C5-C6	-5.03	114.88	117.40
1	A	1295	G	C8-N9-C4	-5.03	104.39	106.40
1	A	868	C	C5-C4-N4	-5.03	116.68	120.20
1	A	891	U	C5-C6-N1	-5.03	120.19	122.70
1	A	1101	A	N1-C6-N6	5.03	121.62	118.60
1	A	1488	G	C6-N1-C2	-5.03	122.08	125.10
1	A	170	U	N1-C2-O2	-5.03	119.28	122.80
1	A	622	A	C8-N9-C4	5.03	107.81	105.80
1	A	1104	G	C6-C5-N7	-5.02	127.39	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1026	G	C8-N9-C4	5.02	108.41	106.40
1	A	1095	U	C5-C4-O4	-5.02	122.89	125.90
1	A	1412	C	C2-N3-C4	-5.02	117.39	119.90
1	A	288	A	C8-N9-C4	5.02	107.81	105.80
1	A	778	G	N1-C2-N3	5.02	126.91	123.90
1	A	582	U	N3-C2-O2	-5.02	118.69	122.20
1	A	863	U	C6-N1-C1'	5.02	128.23	121.20
1	A	1231	G	C8-N9-C4	-5.02	104.39	106.40
1	A	1543	C	C4-C5-C6	-5.02	114.89	117.40
1	A	232	G	C5-N7-C8	-5.02	101.79	104.30
1	A	325	A	C4-C5-N7	-5.02	108.19	110.70
1	A	687	A	C4-C5-C6	5.02	119.51	117.00
1	A	285	G	N9-C4-C5	-5.02	103.39	105.40
1	A	580	U	C5-C6-N1	-5.02	120.19	122.70
1	A	221	C	N3-C4-C5	5.01	123.91	121.90
1	A	920	U	C5-C4-O4	5.01	128.91	125.90
1	A	1489	G	N1-C2-N3	5.01	126.91	123.90
1	A	1525	G	N3-C2-N2	-5.01	116.39	119.90
1	A	247	G	N1-C6-O6	5.01	122.90	119.90
1	A	1512	U	N1-C2-O2	-5.01	119.30	122.80
1	A	66	G	C6-C5-N7	-5.00	127.40	130.40
1	A	266	G	C5-C6-N1	-5.00	109.00	111.50
1	A	876	G	N1-C2-N3	5.00	126.90	123.90
4	D	30	LYS	N-CA-C	5.00	124.50	111.00
5	E	148	VAL	CB-CA-C	-5.00	101.90	111.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	186	ALA	Peptide
2	B	8	LYS	Peptide
8	H	90	GLY	Peptide
10	J	87	THR	Peptide
12	L	25	PRO	Peptide
13	M	105	THR	Peptide
16	P	19	ILE	Peptide
16	P	78	GLY	Peptide
20	T	93	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32510	0	16434	862	0
2	B	1900	0	1951	98	0
3	C	1612	0	1677	122	0
4	D	1703	0	1763	105	0
5	E	1146	0	1207	59	0
6	F	843	0	857	47	0
7	G	1257	0	1296	69	0
8	H	1116	0	1177	60	0
9	I	1010	0	1037	75	0
10	J	792	0	835	49	0
11	K	864	0	881	37	0
12	L	972	0	1058	67	0
13	M	937	0	995	51	0
14	N	492	0	529	49	0
15	O	729	0	768	37	0
16	P	700	0	720	49	0
17	Q	823	0	893	52	0
18	R	574	0	644	41	0
19	S	647	0	673	34	0
20	T	763	0	861	49	0
21	U	208	0	221	15	0
22	A	40	0	37	7	0
23	A	230	0	0	0	0
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	2	0	0	0	0
23	I	1	0	0	0	0
23	J	1	0	0	0	0
23	K	1	0	0	0	0
23	M	2	0	0	0	0
23	N	2	0	0	0	0
23	P	1	0	0	0	0
23	S	2	0	0	0	0
23	T	2	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	396	0	0	4	0
25	E	6	0	0	0	0
25	G	1	0	0	1	0
25	J	1	0	0	0	0
25	N	1	0	0	0	0
25	Q	1	0	0	0	0
25	T	3	0	0	1	0
25	U	1	0	0	0	0
All	All	52297	0	36514	1832	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 (1832) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:G:H5''	1:A:1446:A:H5'	1.37	1.01
1:A:103:C:OP1	20:T:17:ARG:NH1	1.98	0.95
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.50	0.91
1:A:279:A:OP2	17:Q:95:TYR:OH	1.89	0.90
4:D:68:TYR:OH	4:D:98:GLU:OE1	1.91	0.89
1:A:1358:U:H5''	14:N:35:ARG:HG3	1.53	0.89
1:A:1255:G:H2'	1:A:1279:A:H61	1.37	0.88
1:A:1498:UR3:O2'	1:A:1499:A:OP2	1.92	0.88
6:F:100:ASN:HD22	18:R:28:GLU:HG3	1.38	0.87
19:S:33:THR:HG22	19:S:35:SER:H	1.40	0.87
1:A:1316:G:N2	1:A:1319:A:OP2	2.08	0.86
12:L:57:LYS:HD2	12:L:67:THR:HG23	1.57	0.86
7:G:111:ARG:HD3	7:G:112:PRO:HD2	1.58	0.85
1:A:1128:C:OP1	9:I:66:ARG:NH2	2.09	0.85
1:A:235:C:N4	25:A:1969:HOH:O	2.09	0.85
1:A:147:G:H1	1:A:175:C:H42	1.20	0.85
1:A:1412:C:H2'	1:A:1413:A:C8	2.10	0.85
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.42	0.85
6:F:101:ALA:HA	18:R:28:GLU:HB3	1.60	0.84
10:J:31:GLY:HA2	10:J:78:ASN:HB2	1.57	0.84
1:A:419:C:N3	1:A:424:G:N2	2.26	0.84
2:B:17:PHE:HA	2:B:44:LEU:HD11	1.60	0.84
3:C:6:HIS:HD2	3:C:9:GLY:H	1.25	0.83
1:A:1008:C:H42	1:A:1021:G:H22	1.23	0.83
1:A:1125:U:OP2	1:A:1145:C:N4	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:GLU:HG3	6:F:96:PRO:HD2	1.61	0.83
1:A:1376:U:O4	7:G:10:ARG:NH1	2.13	0.82
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.60	0.82
1:A:998:G:N2	1:A:1043:C:N3	2.28	0.81
8:H:83:ILE:HB	8:H:137:VAL:HG22	1.62	0.81
1:A:1055:A:N6	1:A:1205:U:O2	2.14	0.81
1:A:1124:G:N2	1:A:1126:U:O4	2.13	0.80
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.17	0.80
1:A:113:G:H1'	1:A:354:G:H5'	1.63	0.79
3:C:156:ARG:H	3:C:163:ALA:HA	1.45	0.79
4:D:155:LEU:HB2	4:D:158:ILE:HD11	1.63	0.79
2:B:60:ASP:OD2	2:B:64:ARG:NH2	2.15	0.79
1:A:106:C:H2'	1:A:107:G:H5'	1.65	0.79
10:J:3:LYS:HG2	10:J:75:ILE:HD12	1.65	0.79
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.48	0.79
2:B:82:ARG:NH1	2:B:92:TYR:OH	2.15	0.79
17:Q:29:HIS:HB2	17:Q:36:ILE:HD13	1.65	0.78
1:A:1007:C:H1'	1:A:1023:G:H1	1.48	0.78
1:A:563:A:N6	25:A:1931:HOH:O	2.13	0.77
5:E:100:VAL:O	5:E:107:ARG:NH2	2.17	0.77
15:O:35:ARG:NH1	15:O:59:MET:SD	2.57	0.77
20:T:44:ALA:HB1	20:T:91:LEU:HB3	1.66	0.77
1:A:936:C:O2	1:A:1382:C:N4	2.16	0.77
1:A:1124:G:N2	1:A:1149:C:N3	2.32	0.77
1:A:613:C:H42	1:A:627:G:H1	1.32	0.76
2:B:157:ARG:HG2	2:B:158:LEU:HD12	1.68	0.76
1:A:1510:U:H2'	1:A:1511:G:C8	2.20	0.76
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.17	0.76
4:D:13:ARG:NH1	4:D:38:TYR:O	2.18	0.76
1:A:1195:C:H3'	1:A:1196:U:H5''	1.67	0.76
3:C:75:VAL:O	3:C:83:ARG:NH1	2.18	0.76
1:A:1426:C:H42	1:A:1474:G:H1	1.32	0.76
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.13	0.76
4:D:190:ASP:H	4:D:193:ASP:HB2	1.51	0.75
1:A:1053:G:H4'	1:A:1054:C:H5'	1.69	0.75
1:A:1266:G:N2	1:A:1269:A:OP2	2.20	0.75
1:A:1130:A:H4'	9:I:20:ARG:HH22	1.52	0.75
6:F:22:GLU:OE2	6:F:82:ARG:NH1	2.19	0.75
1:A:501:C:H2'	1:A:502:G:H8	1.51	0.75
1:A:1112:C:O2	3:C:179:ARG:NH1	2.20	0.75
1:A:1255:G:N2	1:A:1259:C:O2	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1303:C:H2'	1:A:1304:G:H5'	1.69	0.74
13:M:5:ALA:HB2	13:M:22:ILE:HD13	1.68	0.74
18:R:46:GLU:N	18:R:46:GLU:OE1	2.20	0.74
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.21	0.74
1:A:1255:G:O2'	1:A:1258:G:H1'	1.87	0.74
1:A:409:G:H1	1:A:433:C:H42	1.36	0.74
15:O:6:GLU:OE1	15:O:6:GLU:N	2.17	0.74
21:U:12:LYS:O	21:U:22:ARG:NH1	2.20	0.74
1:A:836:G:OP1	18:R:61:LYS:NZ	2.19	0.73
1:A:1119:C:N3	1:A:1154:G:N2	2.31	0.73
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.71	0.73
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.70	0.73
1:A:250:A:H4'	1:A:251:G:O5'	1.88	0.73
1:A:1505:G:C8	1:A:1505:G:H3'	2.24	0.73
12:L:46:LYS:HG2	12:L:47:LYS:H	1.52	0.73
1:A:948:C:H42	1:A:1233:G:H1	1.35	0.73
1:A:953:G:H5'	1:A:965:A:H61	1.54	0.73
4:D:173:TRP:CE2	4:D:189:PRO:HG3	2.24	0.72
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.71	0.72
1:A:1357:A:H2'	1:A:1358:U:C6	2.24	0.72
1:A:1258:G:H1	1:A:1277:C:H42	1.37	0.72
1:A:938:A:H5'	7:G:76:ARG:HH22	1.54	0.72
19:S:11:VAL:HG22	19:S:39:THR:HB	1.72	0.72
21:U:10:ARG:HD3	21:U:13:ILE:HG21	1.70	0.72
9:I:50:LEU:HD11	9:I:81:ILE:HD12	1.71	0.72
1:A:1120:G:N1	1:A:1154:G:N3	2.38	0.72
20:T:12:ALA:HA	25:T:303:HOH:O	1.88	0.72
3:C:25:GLY:H	3:C:28:GLN:HB2	1.53	0.71
19:S:47:HIS:HB2	19:S:49:ILE:HD11	1.72	0.71
1:A:1195:C:H3'	1:A:1196:U:C5'	2.20	0.71
1:A:1328:C:H2'	1:A:1329:A:H8	1.55	0.71
5:E:32:VAL:HG22	5:E:58:ALA:HB1	1.72	0.71
15:O:39:LEU:HD22	15:O:56:LEU:HB2	1.72	0.71
1:A:759:A:H2'	1:A:760:G:H5'	1.71	0.71
7:G:38:LEU:O	7:G:42:ILE:HG13	1.90	0.71
3:C:156:ARG:NH1	3:C:160:ALA:O	2.24	0.71
1:A:106:C:C2'	1:A:107:G:H5'	2.20	0.70
1:A:419:C:H42	1:A:424:G:H1	1.38	0.70
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.26	0.70
1:A:1240:U:OP2	7:G:116:ALA:N	2.23	0.70
1:A:103:C:P	20:T:17:ARG:HH12	2.14	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:G:H2'	1:A:1436:U:C6	2.27	0.70
3:C:6:HIS:CD2	3:C:9:GLY:H	2.08	0.70
1:A:80:G:H1	1:A:89:C:H42	1.40	0.69
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.75	0.69
12:L:53:ARG:NH1	12:L:92:OTD:OD2	2.25	0.69
1:A:442:C:H42	1:A:492:G:H1	1.41	0.69
1:A:13:U:O2	1:A:914:A:H3'	1.92	0.69
10:J:30:SER:O	10:J:78:ASN:ND2	2.24	0.69
16:P:15:PRO:HG2	16:P:41:PRO:HG3	1.72	0.69
1:A:129(A):G:N3	1:A:190(E):U:H5''	2.07	0.69
1:A:390:C:O3'	16:P:28:ARG:NH2	2.25	0.69
5:E:118:ILE:O	5:E:119:LEU:HD23	1.93	0.69
8:H:120:THR:N	8:H:123:GLU:OE1	2.26	0.69
1:A:517:G:N1	1:A:533:A:OP2	2.24	0.69
1:A:147:G:H1	1:A:175:C:N4	1.91	0.69
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.74	0.68
7:G:16:LEU:HD21	9:I:42:ARG:HG2	1.75	0.68
1:A:1103:C:H5'	2:B:98:LEU:HD12	1.76	0.68
1:A:1158:C:N3	1:A:1181:G:N2	2.41	0.68
14:N:6:LEU:HB3	14:N:23:ARG:NH2	2.09	0.68
9:I:45:ALA:HA	9:I:48:GLU:HB3	1.74	0.68
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.76	0.68
18:R:32:ARG:HA	18:R:69:THR:HG21	1.76	0.68
8:H:64:LYS:HG3	8:H:79:VAL:HG21	1.74	0.68
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.76	0.68
1:A:677:U:H3	1:A:713:G:H22	1.39	0.68
1:A:978:A:H62	1:A:1360:A:N6	1.92	0.68
1:A:1063:C:H2'	1:A:1064:G:C8	2.29	0.68
4:D:150:GLU:HA	4:D:153:ARG:HE	1.59	0.68
1:A:1412:C:H2'	1:A:1413:A:H8	1.55	0.67
3:C:84:ILE:HG23	3:C:88:ARG:HH21	1.59	0.67
1:A:1048:G:H2'	1:A:1050:G:C8	2.28	0.67
1:A:501:C:H2'	1:A:502:G:C8	2.29	0.67
1:A:615:C:H42	1:A:625:G:H1	1.39	0.67
1:A:1368:G:OP2	9:I:112:LYS:NZ	2.24	0.67
3:C:11:ARG:NH1	3:C:177:THR:O	2.20	0.67
3:C:150:LYS:HE3	3:C:173:VAL:HB	1.76	0.67
4:D:57:ARG:HA	4:D:202:LEU:HD12	1.77	0.67
1:A:789:U:O2'	1:A:791:G:N7	2.27	0.67
1:A:1505:G:H3'	1:A:1505:G:H8	1.58	0.67
1:A:192:U:H4'	20:T:57:ARG:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:TYR:CE2	4:D:97:LEU:HB3	2.30	0.67
1:A:107:G:C2	1:A:108:G:H1'	2.30	0.67
1:A:501:C:OP1	12:L:117:ARG:NH2	2.28	0.67
1:A:409:G:N2	1:A:433:C:N3	2.36	0.67
1:A:485:G:O2'	1:A:486:U:O5'	2.13	0.67
3:C:142:MET:HA	3:C:146:ALA:HB3	1.77	0.66
1:A:664:G:H22	1:A:741:G:H1	1.43	0.66
3:C:111:LEU:HD13	3:C:204:LEU:HD13	1.78	0.66
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.76	0.66
1:A:411:A:C5	1:A:413:G:H1'	2.31	0.66
1:A:481:G:HO2'	1:A:482:A:H8	1.41	0.66
3:C:106:VAL:HG12	3:C:109:PRO:HA	1.77	0.66
16:P:53:VAL:O	16:P:56:ALA:N	2.28	0.66
17:Q:87:LYS:HA	17:Q:90:ILE:HD12	1.77	0.66
1:A:1236:A:H4'	1:A:1304:G:H4'	1.77	0.66
22:A:1601:SRV:O61	12:L:46:LYS:HD3	1.95	0.66
9:I:108:VAL:HG12	9:I:109:VAL:H	1.61	0.66
1:A:617:G:H1	1:A:623:C:H42	1.44	0.66
1:A:1245:A:H61	1:A:1292:U:H3	1.43	0.66
14:N:24:CYS:SG	14:N:28:GLY:N	2.68	0.66
1:A:946:A:O2'	1:A:1333:A:N3	2.24	0.66
1:A:968:A:C8	1:A:1062:U:H4'	2.31	0.66
17:Q:34:LYS:HG3	17:Q:35:VAL:N	2.11	0.66
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.36	0.66
13:M:37:THR:O	13:M:55:ARG:NH1	2.27	0.66
5:E:75:THR:OG1	5:E:76:ILE:N	2.29	0.65
3:C:138:VAL:HG13	3:C:151:VAL:HG23	1.77	0.65
11:K:57:THR:HG23	11:K:60:ALA:H	1.62	0.65
13:M:68:GLY:HA2	13:M:71:ARG:HD2	1.76	0.65
1:A:95:U:H2'	1:A:96:G:H8	1.60	0.65
1:A:518:C:H5''	1:A:519:C:C6	2.32	0.65
1:A:837:G:H1	1:A:849:C:H42	1.44	0.65
1:A:1065:U:H5''	1:A:1190:G:N2	2.12	0.65
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.78	0.65
13:M:14:ARG:HE	13:M:42:ALA:HA	1.61	0.65
17:Q:81:ARG:HB3	17:Q:84:LEU:HD11	1.76	0.65
2:B:185:ILE:HG23	2:B:199:TYR:HB2	1.78	0.65
19:S:22:LEU:HD13	19:S:28:LYS:HD2	1.78	0.65
1:A:1183:A:O2'	1:A:1184:G:OP1	2.14	0.65
4:D:18:LYS:HG2	4:D:33:MET:HG2	1.77	0.65
1:A:527:7MG:H5''	1:A:527:7MG:H81	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:70:LEU:HB3	15:O:78:TYR:HB2	1.79	0.65
1:A:714:G:H2'	1:A:715:A:C8	2.31	0.65
1:A:1290:G:H2'	1:A:1291:G:H8	1.61	0.65
1:A:76:C:O2'	1:A:77:G:H5'	1.97	0.64
1:A:1008:C:H42	1:A:1021:G:N2	1.94	0.64
1:A:547:A:OP2	4:D:2:GLY:N	2.31	0.64
3:C:150:LYS:HG2	3:C:169:ALA:HB2	1.80	0.64
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.79	0.64
18:R:51:LEU:HD13	18:R:52:PRO:HD2	1.79	0.64
1:A:115:G:O2'	1:A:116:A:OP2	2.12	0.64
1:A:1347:G:N2	1:A:1374:A:OP2	2.19	0.64
3:C:142:MET:HE3	3:C:149:ALA:HB3	1.80	0.64
18:R:59:SER:OG	18:R:60:ALA:N	2.30	0.64
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.16	0.64
3:C:23:TYR:HD2	10:J:95:GLU:HG3	1.63	0.64
12:L:85:ILE:CG2	12:L:98:TYR:HB3	2.28	0.64
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.78	0.64
1:A:539:A:H2'	1:A:540:G:H8	1.62	0.64
1:A:539:A:H2'	1:A:540:G:C8	2.31	0.64
1:A:1347:G:H3'	9:I:108:VAL:O	1.97	0.64
1:A:1465:C:H2'	1:A:1466:C:O4'	1.98	0.64
3:C:130:VAL:O	3:C:134:ILE:HG12	1.98	0.64
5:E:18:ARG:HG2	5:E:19:MET:N	2.12	0.64
6:F:100:ASN:ND2	18:R:28:GLU:HG3	2.12	0.63
1:A:1111:A:N1	3:C:177:THR:OG1	2.32	0.63
1:A:1257:U:H4'	1:A:1258:G:O5'	1.97	0.63
4:D:57:ARG:NH2	5:E:107:ARG:HD3	2.13	0.63
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.81	0.63
2:B:79:ASP:OD1	2:B:79:ASP:N	2.31	0.63
12:L:27:LEU:C	12:L:29:GLY:H	2.01	0.63
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.33	0.63
9:I:93:ARG:HD2	9:I:97:LYS:NZ	2.14	0.63
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.80	0.63
1:A:1255:G:H2'	1:A:1279:A:N6	2.12	0.63
8:H:46:LYS:HG3	8:H:64:LYS:HB3	1.81	0.63
18:R:59:SER:N	18:R:62:GLU:OE1	2.32	0.63
1:A:1202:G:O4'	14:N:29:ARG:NH1	2.32	0.62
1:A:1174:G:H2'	1:A:1175:G:H8	1.64	0.62
4:D:191:ARG:HH12	4:D:198:VAL:HG12	1.64	0.62
9:I:53:VAL:HG21	9:I:85:LEU:HD23	1.80	0.62
21:U:10:ARG:HA	21:U:13:ILE:HB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:LEU:HG	3:C:76:VAL:HG11	1.80	0.62
8:H:21:LYS:O	8:H:65:TYR:OH	2.16	0.62
16:P:57:ARG:HH21	16:P:79:VAL:HA	1.63	0.62
20:T:10:LEU:HD13	20:T:12:ALA:H	1.64	0.62
1:A:1242:C:H42	1:A:1295:G:H1	1.46	0.62
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.32	0.62
6:F:14:LEU:HD21	6:F:84:ASN:ND2	2.14	0.62
12:L:117:ARG:HB3	12:L:122:THR:HG23	1.82	0.62
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.81	0.62
15:O:41:GLU:OE2	15:O:44:LYS:NZ	2.33	0.62
1:A:1405:G:H1	1:A:1496:C:H5	1.48	0.62
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.80	0.62
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.81	0.62
1:A:737:A:O2'	6:F:73:ASN:ND2	2.32	0.62
1:A:973:G:H3'	1:A:974:A:H5''	1.82	0.62
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.64	0.62
12:L:85:ILE:HG21	12:L:98:TYR:HB3	1.80	0.62
1:A:384:G:H2'	1:A:385:C:C6	2.35	0.62
1:A:958:A:O2'	1:A:985:C:O2'	2.17	0.62
6:F:74:ASP:OD1	6:F:74:ASP:N	2.31	0.62
13:M:29:ARG:HD3	13:M:64:TRP:CE2	2.35	0.62
19:S:22:LEU:HD22	19:S:28:LYS:HG3	1.82	0.62
20:T:60:GLU:HG3	20:T:81:LYS:HE3	1.82	0.62
1:A:838:G:O6	1:A:848:C:N4	2.33	0.61
1:A:1028:C:N3	1:A:1034:G:N2	2.47	0.61
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.82	0.61
1:A:731:G:OP1	1:A:766:A:H1'	2.00	0.61
20:T:77:ALA:O	20:T:80:ARG:N	2.34	0.61
1:A:1239:A:H4'	1:A:1240:U:H5''	1.81	0.61
1:A:1300:G:OP2	1:A:1335:C:N4	2.32	0.61
16:P:32:TYR:HE2	16:P:35:LYS:HB2	1.63	0.61
1:A:1030:C:H5	1:A:1030(A):G:C6	2.18	0.61
1:A:1496:C:O2'	1:A:1497:G:O4'	2.17	0.61
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.82	0.61
5:E:147:ASP:O	5:E:150:ARG:HB3	2.01	0.61
1:A:74:C:H42	1:A:96:G:H1	1.48	0.61
20:T:10:LEU:HD22	20:T:11:SER:H	1.66	0.61
1:A:1359:C:O2'	1:A:1361(A):C:N4	2.33	0.61
1:A:1397:C:O2'	1:A:1398:A:OP1	2.19	0.61
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.81	0.61
1:A:1432:G:O2'	1:A:1468:A:N6	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1504:G:OP1	1:A:1507:A:H4'	2.01	0.61
7:G:48:LYS:HG2	7:G:49:ILE:HD12	1.82	0.61
7:G:78:ARG:HD2	7:G:156:TRP:CE3	2.36	0.61
7:G:88:PRO:HG2	7:G:155:ARG:NH1	2.16	0.61
1:A:1243:C:OP2	21:U:10:ARG:NH2	2.32	0.61
1:A:1375:A:H4'	7:G:29:LYS:HE3	1.82	0.61
5:E:65:ASN:ND2	5:E:65:ASN:O	2.34	0.61
6:F:12:PRO:HG3	6:F:57:GLN:HG3	1.83	0.61
17:Q:47:PRO:HG2	17:Q:48:GLU:HG2	1.83	0.61
16:P:8:ARG:NH1	16:P:15:PRO:HB3	2.16	0.60
1:A:935:A:H61	7:G:3:ARG:HG3	1.66	0.60
1:A:953:G:H2'	1:A:954:G:O4'	2.02	0.60
3:C:26:LYS:HG2	10:J:45:ARG:HH12	1.65	0.60
7:G:30:ILE:HG22	7:G:39:ALA:HB1	1.83	0.60
7:G:70:LYS:HG3	7:G:100:ALA:HB2	1.83	0.60
13:M:16:ASP:OD1	13:M:16:ASP:N	2.26	0.60
1:A:143:A:H2	1:A:220:G:H22	1.47	0.60
3:C:101:LEU:HG	3:C:102:ASN:H	1.66	0.60
6:F:4:TYR:HB2	6:F:65:VAL:HG22	1.82	0.60
14:N:39:LEU:HD13	14:N:43:CYS:HB3	1.82	0.60
1:A:1234:C:H1'	1:A:1364:U:O2	2.01	0.60
4:D:47:ARG:NE	4:D:47:ARG:O	2.33	0.60
10:J:84:GLN:HG3	10:J:85:LEU:HD12	1.83	0.60
1:A:392:G:H2'	1:A:393:A:H8	1.67	0.60
1:A:1346:A:H5''	9:I:120:ARG:HH12	1.66	0.60
4:D:65:ARG:HB2	4:D:75:PHE:CE1	2.36	0.60
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.83	0.60
1:A:35:G:H2'	1:A:36:C:C6	2.37	0.60
1:A:393:A:OP2	16:P:12:LYS:NZ	2.23	0.60
1:A:1338:G:H2'	1:A:1339:A:C8	2.36	0.60
12:L:6:THR:HG1	12:L:9:GLN:H	1.48	0.60
3:C:150:LYS:HB2	3:C:201:TYR:HB2	1.83	0.60
7:G:108:ALA:HB2	7:G:123:GLU:HG2	1.83	0.60
14:N:8:GLU:O	14:N:12:ARG:N	2.32	0.60
1:A:620:C:H2'	1:A:621:A:O4'	2.02	0.60
1:A:144:G:H1	1:A:178:C:H42	1.49	0.60
2:B:164:VAL:HG23	2:B:186:ALA:HA	1.83	0.60
1:A:102:G:H2'	1:A:103:C:H6	1.65	0.59
1:A:285:G:H2'	1:A:286:G:H8	1.67	0.59
1:A:636:U:H2'	1:A:637:G:C8	2.36	0.59
1:A:826:C:O2	8:H:15:ASN:ND2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.31	0.59
1:A:1222:G:OP1	19:S:77:THR:HG21	2.02	0.59
1:A:79:G:C6	1:A:80:G:C6	2.90	0.59
2:B:73:THR:HG23	2:B:95:GLN:O	2.01	0.59
3:C:14:ILE:HD11	14:N:57:ARG:HH22	1.67	0.59
9:I:91:ASP:OD1	9:I:91:ASP:N	2.31	0.59
13:M:101:GLN:OE1	13:M:101:GLN:N	2.34	0.59
14:N:52:GLN:O	14:N:53:LEU:HD23	2.03	0.59
20:T:92:LEU:O	20:T:96:GLY:HA2	2.02	0.59
1:A:571:U:O4	1:A:864:A:N6	2.35	0.59
5:E:144:THR:O	5:E:148:VAL:HG23	2.03	0.59
6:F:35:ALA:HA	6:F:67:MET:HB3	1.83	0.59
15:O:15:PHE:CE2	15:O:85:LEU:HD21	2.38	0.59
1:A:439:A:OP2	1:A:494:G:N1	2.36	0.59
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.85	0.59
3:C:6:HIS:HD2	3:C:9:GLY:N	1.98	0.59
1:A:913:A:OP2	12:L:91:LYS:NZ	2.36	0.59
1:A:1518:MA6:H102	1:A:1519:MA6:H103	1.84	0.59
8:H:73:ASP:OD1	8:H:75:ARG:HB2	2.03	0.59
1:A:512:U:OP1	4:D:46:LYS:NZ	2.34	0.59
1:A:1267:C:N3	1:A:1327:C:O2'	2.36	0.59
1:A:1376:U:H2'	1:A:1377:A:C8	2.38	0.59
20:T:35:THR:HA	20:T:38:LYS:HE2	1.84	0.59
20:T:50:GLU:HG3	20:T:51:GLU:HG2	1.83	0.59
1:A:578:C:O2'	1:A:728:A:N3	2.35	0.59
1:A:918:A:H2'	1:A:919:A:C8	2.37	0.59
1:A:1201:A:H4'	1:A:1202:G:O5'	2.03	0.59
1:A:1255:G:C6	1:A:1279:A:N7	2.71	0.59
3:C:25:GLY:HA2	3:C:29:TYR:N	2.17	0.59
3:C:188:LEU:HD22	3:C:195:VAL:HG22	1.84	0.59
1:A:109:A:H62	1:A:324:G:H21	1.48	0.58
1:A:394:G:H2'	1:A:395:C:H6	1.68	0.58
1:A:1238:A:H5'	1:A:1336:C:H41	1.66	0.58
3:C:155:GLY:HA2	3:C:164:ARG:O	2.03	0.58
3:C:155:GLY:HA2	3:C:164:ARG:H	1.68	0.58
8:H:123:GLU:HA	8:H:126:LYS:HB3	1.84	0.58
1:A:452:A:O2'	16:P:72:ARG:HD2	2.03	0.58
2:B:162:ILE:O	2:B:185:ILE:HD12	2.03	0.58
20:T:71:THR:O	20:T:72:LEU:HD23	2.03	0.58
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.38	0.58
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:VAL:H	3:C:166:GLU:HB3	1.67	0.58
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.21	0.58
12:L:33:ARG:O	12:L:85:ILE:HD12	2.02	0.58
18:R:58:LEU:HD23	18:R:58:LEU:H	1.68	0.58
1:A:376:G:O3'	16:P:5:ARG:NH1	2.36	0.58
9:I:19:LEU:HD11	9:I:81:ILE:HA	1.83	0.58
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.85	0.58
1:A:90:U:H2'	1:A:91:C:O4'	2.03	0.58
1:A:200:G:H1	1:A:217:C:H42	1.51	0.58
1:A:407:G:OP1	4:D:115:ARG:NH2	2.31	0.58
3:C:123:GLN:O	3:C:128:PHE:HB2	2.03	0.58
13:M:63:THR:HG23	13:M:64:TRP:H	1.68	0.58
16:P:75:ARG:HB2	16:P:80:PHE:HD1	1.69	0.58
20:T:69:GLY:O	20:T:73:HIS:ND1	2.37	0.58
1:A:95:U:H2'	1:A:96:G:C8	2.37	0.58
1:A:1255:G:C4	1:A:1279:A:N6	2.71	0.58
1:A:1007:C:H2'	1:A:1008:C:C5	2.39	0.58
2:B:184:VAL:HG12	2:B:197:VAL:HG13	1.84	0.58
9:I:103:THR:HG22	9:I:104:ARG:O	2.04	0.58
13:M:14:ARG:HB2	13:M:17:VAL:HG23	1.86	0.58
1:A:943:U:C2'	1:A:944:G:H5'	2.34	0.58
1:A:1360:A:H2	14:N:18:VAL:HB	1.68	0.58
14:N:40:CYS:C	14:N:44:LEU:HD22	2.24	0.58
1:A:112:G:O2'	1:A:113:G:H5'	2.04	0.58
1:A:192:U:O4'	20:T:103:GLY:HA2	2.04	0.58
5:E:105:VAL:HG11	5:E:131:ILE:HG22	1.85	0.58
5:E:118:ILE:HG12	5:E:119:LEU:H	1.69	0.58
10:J:57:LYS:NZ	10:J:60:ARG:HH22	2.02	0.58
1:A:642:A:N3	8:H:113:SER:OG	2.37	0.57
6:F:80:ARG:HH12	6:F:88:VAL:H	1.51	0.57
17:Q:24:GLU:HA	17:Q:39:SER:HB3	1.86	0.57
1:A:707:C:H2'	1:A:708:C:C6	2.39	0.57
1:A:972:C:OP2	10:J:57:LYS:HE3	2.04	0.57
1:A:1030(A):G:H2'	1:A:1030(B):C:H5''	1.86	0.57
9:I:15:ALA:HA	9:I:65:VAL:HG12	1.87	0.57
1:A:327:A:O2'	1:A:328:C:O4'	2.22	0.57
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.87	0.57
5:E:102:ALA:HA	5:E:120:THR:HB	1.86	0.57
1:A:1479:C:H2'	1:A:1480:G:H8	1.68	0.57
9:I:16:ARG:HB2	9:I:16:ARG:HH11	1.68	0.57
1:A:598:U:H4'	8:H:94:TYR:CD1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:G:C6	1:A:851:G:C6	2.93	0.57
1:A:1202:G:O2'	14:N:27:CYS:SG	2.62	0.57
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.37	0.57
3:C:180:ALA:HB1	3:C:205:GLY:O	2.05	0.57
6:F:80:ARG:NH1	6:F:88:VAL:H	2.02	0.57
14:N:24:CYS:SG	14:N:29:ARG:N	2.71	0.57
1:A:184:G:H2'	1:A:185:A:H8	1.70	0.57
1:A:353:A:H5'	1:A:353:A:H8	1.70	0.57
1:A:451:A:H2	1:A:480:U:C5	2.22	0.57
1:A:452:A:O2'	1:A:453:A:O5'	2.22	0.57
1:A:646:U:H2'	1:A:647:C:C6	2.39	0.57
1:A:1520:G:H2'	1:A:1521:G:H8	1.68	0.57
5:E:99:GLY:O	5:E:101:ILE:HD12	2.03	0.57
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.86	0.57
16:P:5:ARG:HE	16:P:22:THR:HG21	1.69	0.57
1:A:1379:G:OP2	7:G:6:ARG:NH2	2.38	0.57
2:B:114:ARG:NH1	2:B:117:GLU:OE2	2.33	0.57
17:Q:40:LYS:HE3	17:Q:42:TYR:OH	2.04	0.57
1:A:687:A:H4'	1:A:688:G:O5'	2.04	0.57
1:A:825:G:H1	1:A:875:C:H42	1.52	0.57
3:C:150:LYS:HZ3	3:C:175:LEU:HD11	1.69	0.57
9:I:20:ARG:O	9:I:60:ASP:N	2.38	0.57
1:A:992:U:O2'	1:A:993:G:OP2	2.20	0.57
1:A:1328:C:H2'	1:A:1329:A:C8	2.37	0.57
2:B:19:HIS:CG	2:B:20:GLU:H	2.23	0.57
3:C:10:PHE:CE1	3:C:178:LEU:HD21	2.40	0.57
9:I:93:ARG:HD2	9:I:97:LYS:HZ2	1.68	0.57
16:P:78:GLY:C	16:P:80:PHE:H	2.07	0.57
1:A:1163:C:H2'	1:A:1164:G:C8	2.40	0.57
2:B:118:LEU:HB2	2:B:142:LEU:HD23	1.86	0.57
7:G:26:PHE:HA	7:G:101:LEU:HD23	1.87	0.57
7:G:42:ILE:HG22	7:G:120:ILE:HD12	1.87	0.57
7:G:90:GLU:N	7:G:90:GLU:OE2	2.38	0.57
1:A:129:U:O3'	1:A:129(A):G:H3'	2.04	0.56
1:A:1168:A:H2'	1:A:1169:A:C8	2.40	0.56
3:C:88:ARG:HA	3:C:91:LEU:HB3	1.86	0.56
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.87	0.56
4:D:60:GLU:OE1	4:D:60:GLU:HA	2.05	0.56
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.87	0.56
1:A:411:A:N7	1:A:413:G:H1'	2.20	0.56
1:A:545:C:OP2	4:D:62:GLN:NE2	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:A:OP1	22:A:1601:SRV:HI33	2.04	0.56
1:A:975:A:H5'	1:A:975:A:H8	1.70	0.56
1:A:1095:U:OP1	1:A:1108:G:N2	2.32	0.56
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.39	0.56
1:A:1399:C:O2	1:A:1401:G:C5	2.58	0.56
4:D:98:GLU:HG2	4:D:189:PRO:HG2	1.87	0.56
7:G:50:ILE:O	7:G:54:THR:OG1	2.17	0.56
8:H:2:LEU:HD23	8:H:3:THR:N	2.19	0.56
9:I:32:ASP:OD2	9:I:33:PHE:N	2.38	0.56
2:B:87:ARG:HH21	2:B:233:SRR:HB2	1.68	0.56
8:H:91:ARG:NH1	17:Q:32:TYR:O	2.38	0.56
10:J:19:SRR:HB2	10:J:91:PRO:HG3	1.87	0.56
14:N:39:LEU:HD22	14:N:43:CYS:CB	2.35	0.56
16:P:49:LEU:HD12	16:P:50:LYS:H	1.71	0.56
1:A:1281:U:H4'	1:A:1282:C:OP2	2.05	0.56
3:C:35:GLU:O	3:C:39:ILE:HG13	2.06	0.56
5:E:95:ALA:HB1	5:E:96:PRO:HD2	1.87	0.56
9:I:10:ARG:HH21	9:I:11:LYS:HE3	1.71	0.56
1:A:1227:A:O3'	13:M:115:LYS:HG2	2.06	0.56
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.41	0.56
1:A:83:U:O2'	1:A:84:U:H5'	2.05	0.56
1:A:613:C:N4	1:A:627:G:H1	2.02	0.56
1:A:1477:C:H2'	1:A:1478:C:H6	1.70	0.56
1:A:1198:G:H2'	1:A:1199:U:C6	2.41	0.56
8:H:80:ILE:H	8:H:80:ILE:HD12	1.71	0.56
19:S:64:GLU:O	19:S:67:VAL:HG23	2.06	0.56
1:A:463:A:H2'	1:A:474:G:H8	1.71	0.56
1:A:981:U:H2'	1:A:982:U:C5	2.41	0.56
1:A:1130:A:H4'	9:I:20:ARG:NH2	2.18	0.56
1:A:1250:A:H2'	1:A:1251:A:C8	2.41	0.56
1:A:1414:U:H2'	1:A:1415:G:H8	1.70	0.56
20:T:36:LEU:O	20:T:39:LYS:HB3	2.06	0.56
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.88	0.56
1:A:451:A:N7	1:A:481:G:C2	2.74	0.56
4:D:99:SRR:HB2	4:D:139:ARG:HD3	1.87	0.56
12:L:86:ARG:HH11	12:L:86:ARG:HG3	1.71	0.56
1:A:142:G:O2'	1:A:196:A:N1	2.31	0.55
1:A:254:G:OP1	17:Q:67:LYS:O	2.24	0.55
1:A:76:C:H2'	1:A:77:G:C8	2.40	0.55
1:A:651:C:H2'	1:A:652:U:C6	2.41	0.55
1:A:1103:C:H5'	2:B:98:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:O2'	1:A:1348:U:P	2.64	0.55
6:F:80:ARG:NH2	6:F:88:VAL:O	2.40	0.55
1:A:9:G:OP2	5:E:121:LYS:NZ	2.28	0.55
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.88	0.55
1:A:562:C:H1'	12:L:15:ARG:HD2	1.88	0.55
1:A:973:G:O3'	14:N:41:ARG:NH2	2.35	0.55
2:B:178:ARG:HD3	2:B:196:LEU:HD22	1.88	0.55
8:H:63:LEU:HD22	8:H:63:LEU:H	1.71	0.55
8:H:65:TYR:N	8:H:65:TYR:CD1	2.75	0.55
13:M:14:ARG:NE	13:M:42:ALA:HA	2.21	0.55
1:A:1020:U:H2'	1:A:1021:G:H8	1.72	0.55
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.89	0.55
1:A:478:A:H2'	1:A:479:C:C6	2.42	0.55
1:A:481:G:O2'	1:A:482:A:H8	1.90	0.55
1:A:1071:C:H42	1:A:1104:G:H1	1.53	0.55
1:A:1205:U:H5''	3:C:190:ARG:HE	1.71	0.55
4:D:191:ARG:NH1	4:D:198:VAL:HG12	2.21	0.55
6:F:98:LEU:HD22	6:F:101:ALA:HB2	1.88	0.55
1:A:974:A:OP2	14:N:41:ARG:NH1	2.40	0.55
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.89	0.55
9:I:86:VAL:HG21	9:I:102:LEU:HD21	1.89	0.55
1:A:13:U:O4	1:A:20:G:N2	2.34	0.55
1:A:164:U:H2'	1:A:165:C:C6	2.42	0.55
1:A:1279:A:OP2	10:J:9:ARG:NH2	2.40	0.55
1:A:1405:G:N2	1:A:1497:G:C4	2.74	0.55
1:A:1442:G:C2	1:A:1446:A:N7	2.75	0.55
2:B:53:ARG:HA	2:B:56:ARG:NH1	2.21	0.55
12:L:41:ARG:HH12	12:L:43:VAL:HG13	1.72	0.55
1:A:658:G:H2'	1:A:659:U:H6	1.72	0.55
1:A:960:U:H4'	1:A:961:U:C5'	2.37	0.55
1:A:1355:G:H2'	1:A:1356:G:C8	2.41	0.55
6:F:97:PHE:CE2	6:F:99:ALA:HB2	2.42	0.55
8:H:123:GLU:O	8:H:127:LEU:HB2	2.07	0.55
1:A:509:A:C8	1:A:509:A:H3'	2.42	0.55
1:A:538:G:OP1	12:L:115:LYS:N	2.40	0.55
4:D:55:ALA:O	4:D:59:ARG:HG2	2.06	0.55
19:S:21:GLU:O	19:S:25:LYS:HD3	2.06	0.55
5:E:40:ARG:HG2	5:E:68:GLU:HA	1.89	0.55
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.42	0.55
1:A:706:A:O2'	11:K:29:ILE:HD11	2.07	0.54
1:A:1494:G:C2	1:A:1495:U:C5	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:LEU:HD13	3:C:47:LEU:HD13	1.88	0.54
15:O:38:ARG:HB3	15:O:38:ARG:HH11	1.72	0.54
1:A:384:G:H2'	1:A:385:C:H6	1.70	0.54
1:A:1007:C:O2'	1:A:1023:G:N2	2.38	0.54
1:A:1068:G:OP2	1:A:1068:G:H8	1.89	0.54
1:A:1419:G:H1	1:A:1481:U:H3	1.55	0.54
2:B:21:ARG:HA	2:B:39:ILE:HG23	1.89	0.54
3:C:117:ALA:HB2	3:C:200:ALA:HB2	1.89	0.54
3:C:186:PHE:HE1	3:C:199:LYS:HZ2	1.55	0.54
7:G:123:GLU:O	7:G:126:ASP:N	2.39	0.54
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.89	0.54
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.89	0.54
17:Q:29:HIS:CE1	17:Q:31:LEU:H	2.24	0.54
1:A:887:G:H1	1:A:910:C:H42	1.55	0.54
1:A:954:G:H21	1:A:1227:A:H62	1.55	0.54
1:A:1376:U:H2'	1:A:1377:A:H8	1.72	0.54
1:A:1413:A:H2	1:A:1487:G:H22	1.53	0.54
2:B:12:GLU:HB2	2:B:213:LEU:HD11	1.89	0.54
4:D:28:SER:O	4:D:30:LYS:N	2.37	0.54
12:L:85:ILE:HG23	12:L:99:HIS:O	2.08	0.54
19:S:18:LYS:O	19:S:22:LEU:HG	2.06	0.54
1:A:451:A:N7	1:A:481:G:N2	2.55	0.54
5:E:109:ILE:HG22	5:E:110:LEU:HD23	1.89	0.54
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.40	0.54
9:I:19:LEU:HD12	9:I:84:ALA:HB3	1.89	0.54
13:M:86:CYS:SG	13:M:87:TYR:N	2.80	0.54
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.23	0.54
15:O:61:GLY:O	15:O:65:ARG:HD3	2.06	0.54
17:Q:10:VAL:HG21	17:Q:52:LYS:O	2.08	0.54
20:T:49:ALA:HB3	20:T:99:LEU:HB2	1.90	0.54
2:B:172:ILE:HD12	2:B:173:ALA:H	1.72	0.54
14:N:18:VAL:HG22	14:N:19:ARG:HD2	1.90	0.54
1:A:474:G:H4'	16:P:81:ARG:HH21	1.72	0.54
1:A:770:C:H42	1:A:809:G:H1	1.55	0.54
1:A:788:U:H5''	1:A:789:U:OP2	2.08	0.54
1:A:1004:A:O2'	1:A:1005:A:OP1	2.24	0.54
1:A:1148:U:H2'	1:A:1149:C:O4'	2.07	0.54
1:A:1270:C:HO2'	1:A:1313:U:HO2'	1.43	0.54
11:K:66:LEU:HD21	11:K:97:ALA:HB1	1.89	0.54
1:A:35:G:H2'	1:A:36:C:H6	1.71	0.54
1:A:1097:C:H2'	1:A:1098:C:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:37:ARG:HH22	5:E:111:GLU:HG2	1.73	0.54
9:I:10:ARG:NH1	9:I:105:ASP:OD2	2.40	0.54
11:K:81:ASP:CG	11:K:106:LYS:HB2	2.27	0.54
12:L:87:GLY:H	12:L:99:HIS:H	1.55	0.54
21:U:18:TYR:CG	21:U:24:ARG:HG2	2.43	0.54
1:A:113:G:C1'	1:A:354:G:H5'	2.34	0.54
1:A:130:A:H5'	17:Q:63:ARG:NH2	2.22	0.54
8:H:17:THR:HB	8:H:78:GLN:HE22	1.73	0.54
14:N:39:LEU:HB3	14:N:44:LEU:HD13	1.88	0.54
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.40	0.54
1:A:1301:U:HO2'	1:A:1302:U:C5'	2.21	0.54
1:A:1305:G:N2	1:A:1331:G:H1'	2.23	0.54
22:A:1601:SRV:O21	22:A:1601:SRV:NE1	2.41	0.54
4:D:25:ARG:HA	4:D:28:SER:HB2	1.90	0.54
6:F:11:ASN:HB2	6:F:86:ARG:NE	2.23	0.54
1:A:75:G:H2'	1:A:76:C:C6	2.43	0.54
1:A:90:U:C4	1:A:91:C:C4	2.96	0.54
1:A:952:U:H2'	1:A:953:G:H8	1.72	0.54
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.41	0.54
1:A:1172:C:H2'	1:A:1173:G:C8	2.43	0.54
4:D:8:VAL:O	4:D:11:LEU:N	2.40	0.54
6:F:95:GLU:O	18:R:32:ARG:NH1	2.41	0.54
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.89	0.54
20:T:78:ALA:HA	20:T:81:LYS:HD3	1.90	0.54
1:A:792:A:N6	1:A:794:A:C2	2.76	0.53
13:M:39:ILE:HD12	13:M:40:ASN:H	1.74	0.53
17:Q:56:VAL:O	17:Q:77:VAL:HG23	2.08	0.53
1:A:369:C:H42	1:A:392:G:H1	1.55	0.53
1:A:757:U:H2'	1:A:758:G:O4'	2.06	0.53
1:A:1056:U:O2'	1:A:1057:G:H5'	2.08	0.53
1:A:1290:G:H2'	1:A:1291:G:C8	2.41	0.53
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.72	0.53
4:D:63:LYS:O	4:D:67:ILE:HG13	2.08	0.53
4:D:187:ARG:NH1	4:D:188:LEU:HD23	2.24	0.53
10:J:16:LEU:HD21	10:J:94:VAL:HA	1.90	0.53
1:A:1006:C:H2'	1:A:1007:C:C6	2.43	0.53
2:B:16:HIS:CD2	2:B:204:ASN:H	2.27	0.53
15:O:21:ASP:OD1	15:O:24:SER:OG	2.20	0.53
19:S:69:HIS:HB3	19:S:73:GLU:CD	2.28	0.53
1:A:1329:A:P	13:M:28:ALA:HB3	2.49	0.53
3:C:188:LEU:HD23	3:C:196:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:9:PHE:CE2	16:P:18:ARG:HD2	2.43	0.53
17:Q:81:ARG:NH2	17:Q:83:ASP:OD2	2.41	0.53
1:A:372:C:H1'	1:A:373:A:OP2	2.09	0.53
1:A:914:A:P	22:A:1601:SRV:HI33	2.49	0.53
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.08	0.53
1:A:1258:G:H1	1:A:1277:C:N4	2.03	0.53
1:A:1531:A:O5'	1:A:1531:A:H8	1.91	0.53
4:D:10:ARG:HA	4:D:13:ARG:HG2	1.89	0.53
1:A:17:U:H2'	1:A:18:C:C6	2.43	0.53
1:A:200:G:H2'	1:A:201:C:O2	2.07	0.53
1:A:1163:C:H2'	1:A:1164:G:H8	1.74	0.53
7:G:139:GLU:O	7:G:143:ARG:HB3	2.09	0.53
8:H:87:SER:HA	8:H:93:VAL:HG23	1.90	0.53
1:A:505:G:H1	1:A:526:C:H42	1.57	0.53
1:A:965:A:C2	1:A:969:A:C2	2.97	0.53
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.44	0.53
7:G:5:ARG:NH2	25:G:201:HOH:O	2.37	0.53
8:H:85:ARG:NE	8:H:87:SER:O	2.42	0.53
13:M:96:LEU:O	13:M:110:ARG:NH1	2.41	0.53
15:O:2:PRO:O	15:O:38:ARG:NH2	2.41	0.53
1:A:451:A:N6	1:A:481:G:C4	2.77	0.53
1:A:1145:C:H1'	1:A:1146:A:N7	2.24	0.53
4:D:162:LEU:HA	4:D:165:MET:HB2	1.90	0.53
1:A:775:G:C2'	1:A:776:G:H5'	2.39	0.53
3:C:81:GLY:O	3:C:84:ILE:HG22	2.08	0.53
3:C:180:ALA:CB	3:C:203:PHE:HE1	2.22	0.53
4:D:190:ASP:OD1	4:D:191:ARG:N	2.42	0.53
5:E:122:GLU:O	5:E:123:LEU:HD23	2.09	0.53
8:H:9:MET:O	8:H:13:ILE:HD12	2.09	0.53
1:A:392:G:H2'	1:A:393:A:C8	2.44	0.53
3:C:66:VAL:HG12	3:C:68:VAL:HG23	1.91	0.53
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.90	0.53
7:G:140:ASP:HA	7:G:143:ARG:HD2	1.89	0.53
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.44	0.53
16:P:68:ASP:OD1	16:P:68:ASP:N	2.42	0.53
18:R:46:GLU:H	18:R:46:GLU:CD	2.10	0.53
1:A:1014:A:H2'	1:A:1015:A:O4'	2.08	0.52
1:A:1204:A:C5	1:A:1205:U:C5	2.97	0.52
1:A:1278:U:H4'	1:A:1279:A:N3	2.24	0.52
1:A:1392:G:N2	1:A:1502:A:H8	2.07	0.52
1:A:1493:A:H2'	1:A:1494:G:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.15	0.52
12:L:6:THR:OG1	12:L:9:GLN:N	2.37	0.52
14:N:40:CYS:O	14:N:44:LEU:N	2.30	0.52
16:P:9:PHE:HE2	16:P:18:ARG:HD2	1.74	0.52
1:A:463:A:OP1	16:P:75:ARG:NH1	2.37	0.52
1:A:760:G:H2'	1:A:761:G:O4'	2.08	0.52
1:A:1057:G:H5''	3:C:154:SER:HB2	1.92	0.52
1:A:1064:G:N2	1:A:1191:A:OP2	2.36	0.52
1:A:1354:C:H2'	1:A:1355:G:H8	1.74	0.52
1:A:1392:G:H21	1:A:1502:A:H8	1.57	0.52
13:M:59:TYR:O	13:M:63:THR:HG22	2.09	0.52
1:A:403:C:O2'	4:D:122:ARG:NH1	2.43	0.52
1:A:1218:C:H2'	1:A:1219:U:C6	2.45	0.52
1:A:1355:G:H2'	1:A:1356:G:H8	1.73	0.52
13:M:22:ILE:HG22	13:M:23:TYR:N	2.25	0.52
14:N:2:ALA:HB2	14:N:28:GLY:HA3	1.91	0.52
1:A:89:C:H2'	1:A:90:U:C6	2.44	0.52
1:A:1525:G:H2'	1:A:1526:G:H8	1.74	0.52
3:C:11:ARG:NH1	3:C:178:LEU:HA	2.24	0.52
4:D:119:GLN:HG3	4:D:123:HIS:CD2	2.44	0.52
7:G:80:VAL:HG11	7:G:154:TYR:HE2	1.75	0.52
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.24	0.52
8:H:114:THR:HG22	8:H:131:GLY:HA3	1.92	0.52
4:D:10:ARG:O	4:D:13:ARG:HG2	2.08	0.52
10:J:8:LEU:HD21	10:J:96:ILE:HG23	1.90	0.52
13:M:2:ALA:O	13:M:4:ILE:HD12	2.10	0.52
14:N:24:CYS:O	14:N:28:GLY:HA2	2.10	0.52
1:A:75:G:C6	1:A:96:G:N1	2.77	0.52
1:A:767:A:H2'	1:A:768:A:O4'	2.09	0.52
22:A:1601:SRY:O21	22:A:1601:SRY:NB1	2.42	0.52
2:B:136:VAL:O	2:B:140:HIS:ND1	2.41	0.52
4:D:13:ARG:NH2	4:D:40:PRO:HA	2.25	0.52
6:F:2:ARG:O	6:F:66:GLU:HA	2.09	0.52
6:F:41:GLU:O	6:F:62:TRP:HB3	2.09	0.52
6:F:70:ASP:OD1	6:F:71:ARG:HG2	2.09	0.52
13:M:74:VAL:O	13:M:78:ILE:HG13	2.10	0.52
1:A:37:U:H2'	1:A:38:G:O4'	2.10	0.52
1:A:130:A:H5'	17:Q:63:ARG:CZ	2.40	0.52
1:A:371:G:O2'	1:A:372:C:H5'	2.10	0.52
1:A:372:C:H4'	1:A:373:A:O5'	2.10	0.52
1:A:975:A:H4'	1:A:976:G:O5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:A:H4'	1:A:1102:A:O5'	2.10	0.52
8:H:82:HIS:CE1	8:H:138:TRP:NE1	2.77	0.52
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.91	0.52
9:I:48:GLU:N	9:I:49:PRO:HD2	2.25	0.52
1:A:463:A:H1'	16:P:82:GLN:HG3	1.92	0.52
5:E:20:GLN:CD	5:E:21:ALA:H	2.13	0.52
1:A:609:A:N6	25:A:2089:HOH:O	2.42	0.52
1:A:644:G:C5	1:A:645:C:C5	2.98	0.52
1:A:1256:A:H4'	1:A:1257:U:O5'	2.10	0.52
1:A:1328:C:OP2	21:U:7:ARG:NH1	2.43	0.52
2:B:168:THR:HG22	2:B:169:LYS:HD2	1.92	0.52
5:E:69:VAL:HG21	5:E:113:ALA:HB1	1.92	0.52
12:L:86:ARG:HG3	12:L:86:ARG:NH1	2.23	0.52
17:Q:58:GLU:HB3	17:Q:74:LEU:HB3	1.92	0.52
1:A:411:A:H62	1:A:413:G:N2	2.08	0.52
1:A:721:G:C6	1:A:733:A:C2	2.98	0.52
3:C:23:TYR:CD2	10:J:95:GLU:HG3	2.44	0.52
8:H:12:ARG:NH1	8:H:27:PRO:HD3	2.24	0.52
8:H:82:HIS:CE1	8:H:138:TRP:CD1	2.98	0.52
1:A:269:C:H2'	1:A:270:A:C8	2.45	0.51
1:A:1197:G:H5''	1:A:1198:G:OP2	2.11	0.51
1:A:1404:5MC:H1'	1:A:1499:A:H2	1.73	0.51
2:B:27:LYS:HD3	2:B:193:ASP:OD1	2.10	0.51
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.92	0.51
3:C:36:ASP:O	3:C:39:ILE:HB	2.11	0.51
4:D:163:GLU:HG3	4:D:166:LYS:HE2	1.91	0.51
9:I:50:LEU:O	9:I:53:VAL:HG12	2.10	0.51
1:A:422:C:H4'	1:A:423:G:O5'	2.10	0.51
1:A:1052:U:C2	1:A:1200:C:N4	2.78	0.51
25:A:2110:HOH:O	2:B:96:ARG:HG2	2.11	0.51
11:K:72:ALA:HA	11:K:75:TYR:HB2	1.91	0.51
1:A:750:G:N3	15:O:23:GLY:HA3	2.25	0.51
1:A:757:U:H5''	1:A:822:C:O2	2.10	0.51
1:A:974:A:H8	1:A:974:A:OP1	1.94	0.51
2:B:55:PHE:HA	2:B:58:ILE:HD12	1.91	0.51
5:E:5:ASP:OD1	5:E:5:ASP:N	2.43	0.51
14:N:47:LEU:O	14:N:53:LEU:HG	2.11	0.51
1:A:633:G:H2'	1:A:634:C:C6	2.46	0.51
1:A:1357:A:H2'	1:A:1358:U:H6	1.71	0.51
2:B:68:ILE:H	2:B:90:MET:HG2	1.74	0.51
3:C:26:LYS:HG2	10:J:45:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.93	0.51
17:Q:66:SER:H	17:Q:69:LYS:HB2	1.74	0.51
8:H:82:HIS:CE1	8:H:138:TRP:HE1	2.28	0.51
1:A:230:G:H2'	1:A:231:G:O4'	2.11	0.51
1:A:1030:C:N3	1:A:1032:G:N1	2.58	0.51
1:A:1172:C:H2'	1:A:1173:G:H8	1.76	0.51
3:C:120:VAL:HG12	3:C:124:ILE:HD11	1.92	0.51
7:G:145:ALA:O	7:G:146:GLU:HG2	2.10	0.51
10:J:91:PRO:HB2	10:J:94:VAL:HG13	1.91	0.51
1:A:658:G:H1	1:A:747:C:H42	1.59	0.51
3:C:16:ARG:HG3	3:C:17:ASP:H	1.76	0.51
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.45	0.51
1:A:279:A:OP1	1:A:280:C:O2'	2.17	0.51
1:A:710:G:H5''	6:F:54:LYS:HE3	1.91	0.51
1:A:1029:C:N3	1:A:1033:G:N2	2.58	0.51
1:A:1095:U:H5''	1:A:1109:C:O2	2.11	0.51
4:D:31:CYS:C	4:D:33:MET:H	2.13	0.51
5:E:39:GLY:O	5:E:69:VAL:HG23	2.11	0.51
12:L:6:THR:HG23	12:L:9:GLN:OE1	2.10	0.51
15:O:56:LEU:O	15:O:60:VAL:HG23	2.10	0.51
1:A:575:G:OP1	1:A:575:G:H4'	2.11	0.51
1:A:1094:G:O2'	1:A:1108:G:N2	2.44	0.51
2:B:18:GLY:HA2	2:B:42:ILE:HG12	1.93	0.51
4:D:111:ALA:HA	4:D:161:ASN:ND2	2.25	0.51
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.45	0.51
20:T:43:LEU:HD12	20:T:52:ALA:HA	1.93	0.51
1:A:552:U:H2'	1:A:553:A:C8	2.46	0.51
1:A:1302:U:O4	13:M:14:ARG:NH1	2.44	0.51
1:A:1368:G:OP1	9:I:111:ARG:NH1	2.44	0.51
1:A:1505:G:C8	1:A:1505:G:C3'	2.91	0.51
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.92	0.51
9:I:118:LYS:O	9:I:120:ARG:N	2.43	0.51
11:K:95:ILE:HA	11:K:98:LEU:CD1	2.41	0.51
12:L:87:GLY:HA2	12:L:98:TYR:CA	2.32	0.51
1:A:789:U:H2'	1:A:791:G:OP2	2.11	0.50
1:A:984:C:N3	1:A:1221:G:N2	2.54	0.50
1:A:1003:G:H2'	1:A:1003(A):G:C8	2.46	0.50
1:A:1120:G:H22	1:A:1154:G:H1'	1.75	0.50
2:B:49:GLU:O	2:B:52:GLU:HB3	2.11	0.50
3:C:116:VAL:O	3:C:120:VAL:HG23	2.11	0.50
7:G:77:SER:HA	7:G:86:GLN:HA	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:53:VAL:O	16:P:55:ARG:N	2.44	0.50
17:Q:4:LYS:HG3	17:Q:5:VAL:N	2.24	0.50
1:A:738:C:OP1	6:F:92:LYS:HD3	2.11	0.50
1:A:1074:G:C6	1:A:1075:C:C4	2.99	0.50
3:C:30:ARG:HG2	3:C:31:HIS:H	1.76	0.50
3:C:121:ALA:HB1	3:C:189:ALA:HB2	1.91	0.50
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	2.95	0.50
9:I:53:VAL:HG22	9:I:92:TYR:CZ	2.46	0.50
15:O:39:LEU:CD2	15:O:56:LEU:HB2	2.41	0.50
17:Q:13:ASP:O	17:Q:15:MET:N	2.44	0.50
1:A:93:G:C2	1:A:95:U:C2	2.99	0.50
1:A:299:G:H2'	1:A:300:A:C8	2.47	0.50
10:J:37:PRO:HA	10:J:71:LEU:H	1.75	0.50
1:A:502:G:C2	1:A:503:C:C2	2.99	0.50
1:A:803:G:C6	1:A:804:U:C4	2.99	0.50
1:A:882:C:O2'	1:A:883:C:H5'	2.11	0.50
5:E:44:GLY:HA3	5:E:62:ALA:HB2	1.93	0.50
7:G:62:PHE:O	7:G:66:VAL:HG23	2.11	0.50
8:H:25:ASP:OD1	8:H:25:ASP:N	2.44	0.50
20:T:29:LYS:O	20:T:32:ALA:HB3	2.11	0.50
1:A:247:G:OP2	17:Q:100:LYS:HD3	2.11	0.50
1:A:909:A:H2'	1:A:910:C:O4'	2.11	0.50
1:A:962:C:H1'	1:A:1201:A:N1	2.26	0.50
1:A:1112:C:H1'	3:C:179:ARG:HH12	1.76	0.50
1:A:1279:A:OP1	10:J:7:LYS:NZ	2.45	0.50
1:A:1411:C:H42	1:A:1489:G:H1	1.60	0.50
3:C:142:MET:CE	3:C:170:GLN:HB2	2.42	0.50
4:D:7:PRO:HB2	4:D:10:ARG:HG2	1.92	0.50
8:H:84:ARG:HD2	8:H:85:ARG:O	2.12	0.50
9:I:61:ALA:HB1	9:I:63:ILE:HG12	1.94	0.50
12:L:117:ARG:NH2	12:L:124:LYS:HD3	2.27	0.50
19:S:34:TRP:HA	19:S:52:TYR:HB3	1.92	0.50
1:A:435:C:H2'	1:A:436:C:H6	1.77	0.50
1:A:1211:U:O2'	1:A:1212:U:OP2	2.26	0.50
4:D:173:TRP:NE1	4:D:189:PRO:HG3	2.25	0.50
5:E:81:GLU:OE2	5:E:81:GLU:N	2.38	0.50
7:G:57:GLU:OE1	7:G:59:LEU:HB3	2.11	0.50
16:P:53:VAL:O	16:P:54:GLU:C	2.50	0.50
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.94	0.50
18:R:58:LEU:HD23	18:R:58:LEU:N	2.26	0.50
1:A:299:G:C6	1:A:300:A:C6	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:G:H2'	1:A:742:G:O4'	2.12	0.50
1:A:932:C:H5'	7:G:4:ARG:HG2	1.94	0.50
1:A:1078:U:H5''	1:A:1079:G:OP2	2.11	0.50
1:A:1526:G:O2'	1:A:1527:C:H5'	2.12	0.50
6:F:97:PHE:HE2	6:F:99:ALA:HB2	1.76	0.50
11:K:92:GLU:HG3	11:K:96:ARG:NH1	2.26	0.50
1:A:559:A:O2'	1:A:560:U:OP2	2.24	0.50
4:D:170:VAL:HG11	4:D:175:SER:HA	1.92	0.50
1:A:90:U:O4	1:A:91:C:N4	2.45	0.50
1:A:232:G:H2'	1:A:233:C:H6	1.77	0.50
1:A:450:G:OP1	16:P:43:LYS:NZ	2.45	0.50
1:A:1229:A:OP1	13:M:116:THR:OG1	2.26	0.50
15:O:33:THR:HG21	15:O:85:LEU:HD13	1.94	0.50
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.12	0.50
20:T:35:THR:HA	20:T:38:LYS:NZ	2.27	0.50
20:T:50:GLU:HG3	20:T:51:GLU:H	1.77	0.50
1:A:945:G:N1	1:A:1337:G:C2	2.80	0.49
1:A:1310:G:OP1	13:M:77:ASN:ND2	2.44	0.49
1:A:1483:A:H2'	1:A:1484:C:O4'	2.12	0.49
4:D:155:LEU:HB2	4:D:158:ILE:CD1	2.37	0.49
7:G:65:ALA:HB2	7:G:128:ALA:HB2	1.94	0.49
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.94	0.49
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.92	0.49
14:N:39:LEU:HD13	14:N:43:CYS:C	2.33	0.49
15:O:6:GLU:HA	15:O:9:GLN:HB2	1.94	0.49
1:A:337:C:H2'	1:A:338:A:C8	2.46	0.49
1:A:394:G:H2'	1:A:395:C:C6	2.47	0.49
1:A:429:U:H1'	1:A:430:A:H5''	1.95	0.49
1:A:948:C:N4	1:A:1233:G:H1	2.07	0.49
1:A:954:G:C5	1:A:955:U:C4	3.00	0.49
1:A:1119:C:H42	1:A:1154:G:H1	1.60	0.49
1:A:1301:U:HO2'	1:A:1302:U:P	2.34	0.49
7:G:115:ARG:HD2	7:G:118:VAL:HG21	1.94	0.49
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.45	0.49
12:L:19:ARG:H	12:L:19:ARG:HD2	1.77	0.49
17:Q:22:LEU:HD12	17:Q:23:VAL:H	1.77	0.49
1:A:942:G:H21	9:I:124:GLN:HE22	1.59	0.49
1:A:1285:A:H4'	1:A:1286:A:O5'	2.12	0.49
1:A:922:G:C6	1:A:923:A:C6	3.01	0.49
1:A:945:G:C6	1:A:1337:G:C2	3.00	0.49
1:A:954:G:N2	1:A:1227:A:H62	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:G:H2'	1:A:1175:G:C8	2.45	0.49
1:A:1258:G:OP2	1:A:1258:G:H8	1.96	0.49
2:B:177:ALA:HB1	2:B:182:ILE:HB	1.94	0.49
5:E:43:LEU:HD22	5:E:136:MET:HG2	1.93	0.49
10:J:71:LEU:HD22	10:J:71:LEU:N	2.26	0.49
12:L:59:ARG:NH1	12:L:65:GLU:HB3	2.27	0.49
1:A:49:U:H6	1:A:49:U:H5''	1.76	0.49
1:A:533:A:O2'	1:A:535:A:OP2	2.28	0.49
1:A:983:A:OP1	14:N:3:ARG:NH2	2.44	0.49
1:A:1220:G:H2'	1:A:1221:G:O4'	2.13	0.49
3:C:25:GLY:N	3:C:28:GLN:HB2	2.26	0.49
4:D:63:LYS:NZ	4:D:197:PRO:O	2.40	0.49
5:E:43:LEU:HD11	5:E:133:TYR:HD2	1.77	0.49
11:K:17:GLY:HA2	11:K:35:PRO:HG3	1.95	0.49
1:A:232:G:H1'	1:A:262:A:N1	2.28	0.49
1:A:748:C:H4'	1:A:749:C:O5'	2.12	0.49
1:A:967:5MC:H4'	9:I:128:ARG:NE	2.26	0.49
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.95	0.49
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.46	0.49
19:S:80:TYR:CG	19:S:81:ARG:N	2.81	0.49
1:A:443:C:H2'	1:A:444:C:H6	1.78	0.49
1:A:737:A:H1'	6:F:73:ASN:HD21	1.78	0.49
1:A:942:G:C2	1:A:943:U:C2	3.00	0.49
1:A:1326:C:H5''	21:U:18:TYR:O	2.12	0.49
1:A:1403:C:H2'	1:A:1404:5MC:C6	2.48	0.49
7:G:87:VAL:HG13	7:G:151:TYR:HB3	1.93	0.49
4:D:57:ARG:NH2	4:D:205:GLU:OE2	2.46	0.49
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.48	0.49
11:K:62:GLN:O	11:K:66:LEU:HG	2.13	0.49
13:M:84:ILE:HG13	13:M:86:CYS:H	1.78	0.49
20:T:75:ASN:N	20:T:75:ASN:OD1	2.46	0.49
1:A:344:A:H4'	1:A:345:C:OP2	2.13	0.49
2:B:143:GLU:O	2:B:147:LYS:HG3	2.12	0.49
2:B:184:VAL:O	2:B:198:ASP:HB2	2.12	0.49
12:L:27:LEU:C	12:L:29:GLY:N	2.66	0.49
15:O:76:GLU:N	15:O:79:ARG:HH21	2.10	0.49
16:P:57:ARG:HH21	16:P:79:VAL:CA	2.24	0.49
19:S:63:THR:HG22	19:S:64:GLU:H	1.77	0.49
1:A:691:G:H2'	1:A:692:U:H6	1.77	0.49
1:A:881:G:OP2	12:L:12:ARG:NH2	2.46	0.49
1:A:1206:G:H2'	1:A:1207:2MG:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:88:PRO:HG2	7:G:155:ARG:HH12	1.75	0.49
15:O:36:ILE:HG13	15:O:59:MET:HE3	1.94	0.49
18:R:61:LYS:O	18:R:65:ILE:HG13	2.13	0.49
1:A:67:C:H2'	1:A:68:G:C8	2.48	0.48
1:A:485:G:O2'	1:A:486:U:P	2.71	0.48
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.28	0.48
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.94	0.48
1:A:27:G:H2'	1:A:28:G:O4'	2.14	0.48
1:A:161:A:N1	1:A:347:G:O2'	2.42	0.48
1:A:1190:G:OP1	3:C:4:LYS:HA	2.13	0.48
1:A:1203:C:OP1	14:N:2:ALA:N	2.46	0.48
4:D:141:ARG:HG2	4:D:142:PRO:HD2	1.95	0.48
13:M:5:ALA:CB	13:M:22:ILE:HD13	2.40	0.48
16:P:6:LEU:HD12	16:P:6:LEU:HA	1.60	0.48
3:C:10:PHE:CD1	3:C:178:LEU:HD21	2.48	0.48
3:C:137:ALA:O	3:C:141:VAL:HG23	2.12	0.48
5:E:82:VAL:O	5:E:88:LYS:HA	2.14	0.48
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.60	0.48
8:H:34:GLU:HB3	8:H:118:VAL:HG21	1.94	0.48
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.95	0.48
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.96	0.48
1:A:217:C:H2'	1:A:218:C:H6	1.77	0.48
1:A:455:C:H2'	1:A:456:C:H6	1.78	0.48
1:A:828:A:H4'	1:A:828:A:OP1	2.14	0.48
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.93	0.48
12:L:58:VAL:O	12:L:65:GLU:HA	2.13	0.48
1:A:452:A:O2'	1:A:453:A:O4'	2.29	0.48
1:A:484:G:H5'	1:A:486:U:H1'	1.95	0.48
1:A:517:G:H5'	1:A:519:C:C2	2.49	0.48
3:C:147:LYS:HB3	3:C:203:PHE:CE2	2.48	0.48
12:L:56:ALA:O	12:L:58:VAL:HG23	2.12	0.48
20:T:35:THR:HA	20:T:38:LYS:CE	2.43	0.48
1:A:76:C:H2'	1:A:77:G:H8	1.77	0.48
1:A:191:G:H1'	20:T:105:SER:HA	1.94	0.48
1:A:502:G:P	12:L:118:SER:HG	2.36	0.48
1:A:781:A:C4	1:A:802:A:C2	3.02	0.48
1:A:1426:C:H2'	1:A:1427:U:H6	1.78	0.48
20:T:51:GLU:O	20:T:55:ILE:HG12	2.13	0.48
1:A:695:A:C2	1:A:787:A:H1'	2.49	0.48
1:A:865:A:O5'	1:A:865:A:H8	1.97	0.48
1:A:1520:G:O2'	1:A:1521:G:H5'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:LEU:HD22	3:C:18:TRP:CD1	2.48	0.48
4:D:9:CYS:SG	4:D:31:CYS:O	2.72	0.48
4:D:156:GLU:HG3	4:D:160:GLN:HE22	1.78	0.48
9:I:50:LEU:HD23	9:I:85:LEU:HD21	1.95	0.48
13:M:108:ARG:HD3	13:M:114:ARG:NH2	2.29	0.48
1:A:35:G:C6	1:A:36:C:N4	2.81	0.48
1:A:1020:U:C2	1:A:1021:G:C8	3.02	0.48
1:A:1126:U:H3	1:A:1149:C:H1'	1.79	0.48
1:A:1363:A:H4'	1:A:1364:U:H5''	1.93	0.48
1:A:1373:G:H5''	7:G:36:LYS:HD3	1.95	0.48
1:A:1508:G:C5	1:A:1509:C:C5	3.01	0.48
12:L:84:LEU:O	12:L:101:VAL:HG23	2.14	0.48
16:P:51:VAL:HG12	16:P:53:VAL:N	2.29	0.48
1:A:79:G:N1	1:A:80:G:C6	2.82	0.48
1:A:721:G:H4'	1:A:722:A:O4'	2.13	0.48
1:A:956:U:H4'	19:S:80:TYR:HE1	1.79	0.48
2:B:47:THR:HG22	2:B:51:LEU:HD12	1.96	0.48
6:F:28:ARG:O	6:F:32:ASN:HB2	2.13	0.48
10:J:5:ARG:H	10:J:5:ARG:HG3	1.44	0.48
15:O:26:GLU:OE2	15:O:77:ARG:HD2	2.13	0.48
16:P:8:ARG:CZ	16:P:15:PRO:HB3	2.44	0.48
16:P:58:TYR:CD1	16:P:58:TYR:C	2.85	0.48
18:R:43:PHE:CD2	18:R:56:THR:HG22	2.33	0.48
1:A:113:G:H2'	1:A:114:U:C6	2.49	0.48
1:A:411:A:N6	1:A:413:G:N3	2.61	0.48
1:A:785:G:C2	1:A:786:G:C8	3.02	0.48
1:A:946:A:H2'	1:A:947:G:C8	2.49	0.48
1:A:949:A:C2	1:A:1233:G:N3	2.82	0.48
1:A:1130:A:N6	1:A:1144:G:H21	2.12	0.48
1:A:1240:U:H5	7:G:109:ASN:HD21	1.59	0.48
1:A:1242:C:N4	1:A:1295:G:H1	2.09	0.48
1:A:1254:C:H2'	1:A:1255:G:C8	2.49	0.48
2:B:84:GLU:O	2:B:87:ARG:HB2	2.14	0.48
7:G:66:VAL:HG12	7:G:70:LYS:HZ3	1.78	0.48
9:I:104:ARG:HD2	9:I:105:ASP:H	1.79	0.48
14:N:39:LEU:CD2	14:N:43:CYS:HB3	2.44	0.48
1:A:478:A:H2'	1:A:479:C:H6	1.79	0.47
1:A:837:G:H1	1:A:849:C:N4	2.11	0.47
1:A:1510:U:H2'	1:A:1511:G:H8	1.75	0.47
7:G:31:MET:HB2	7:G:35:LYS:O	2.14	0.47
10:J:46:ARG:HD2	10:J:64:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:G:H2'	1:A:377:G:H8	1.79	0.47
1:A:505:G:C6	1:A:535:A:C2	3.01	0.47
1:A:679:C:H2'	1:A:680:C:C6	2.48	0.47
1:A:933:G:OP2	7:G:3:ARG:HB3	2.15	0.47
1:A:975:A:O2'	14:N:32:SER:HB2	2.15	0.47
1:A:1191:A:H2'	1:A:1192:C:C6	2.49	0.47
2:B:95:GLN:HG3	2:B:148:TYR:HA	1.95	0.47
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.39	0.47
17:Q:38:ARG:HD3	17:Q:38:ARG:HA	1.55	0.47
1:A:90:U:C4	1:A:91:C:N4	2.83	0.47
1:A:558:G:H5''	1:A:559:A:H3'	1.95	0.47
1:A:663:A:H2'	1:A:664:G:O4'	2.14	0.47
1:A:691:G:H2'	1:A:692:U:C6	2.49	0.47
1:A:943:U:H2'	1:A:944:G:H5'	1.96	0.47
1:A:976:G:OP2	1:A:1358:U:H1'	2.14	0.47
1:A:1191:A:H5''	3:C:4:LYS:NZ	2.29	0.47
1:A:1452:C:H4'	1:A:1453:G:O5'	2.14	0.47
2:B:36:ARG:CG	2:B:41:ILE:HD11	2.45	0.47
4:D:8:VAL:O	4:D:10:ARG:N	2.47	0.47
11:K:39:PRO:O	11:K:40:ILE:HD13	2.14	0.47
15:O:70:LEU:HD22	15:O:70:LEU:HA	1.38	0.47
1:A:968:A:H8	1:A:968:A:OP1	1.98	0.47
16:P:43:LYS:HB2	16:P:43:LYS:HE2	1.72	0.47
1:A:956:U:H2'	1:A:957:U:O4'	2.15	0.47
1:A:1004:A:O2'	1:A:1005:A:P	2.71	0.47
1:A:1120:G:C2	1:A:1154:G:N3	2.82	0.47
2:B:96:ARG:HH12	2:B:172:ILE:HD11	1.80	0.47
3:C:84:ILE:HG23	3:C:88:ARG:NH2	2.28	0.47
6:F:48:LEU:HG	6:F:57:GLN:HA	1.96	0.47
9:I:6:GLY:HA3	9:I:83:ARG:HB3	1.97	0.47
9:I:114:TYR:H	9:I:114:TYR:HD2	1.60	0.47
19:S:11:VAL:HG13	19:S:39:THR:O	2.15	0.47
1:A:979:C:H42	14:N:18:VAL:HG23	1.78	0.47
1:A:1263:C:H2'	1:A:1264:C:O4'	2.14	0.47
1:A:1301:U:O2'	1:A:1302:U:O5'	2.30	0.47
1:A:1442:G:C6	1:A:1446:A:N6	2.78	0.47
1:A:1493:A:H2'	1:A:1494:G:C8	2.49	0.47
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.96	0.47
3:C:22:TRP:CD1	3:C:59:ARG:HG2	2.50	0.47
3:C:110:ASN:N	3:C:110:ASN:OD1	2.47	0.47
9:I:79:LEU:HD13	9:I:83:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:29:VAL:O	15:O:33:THR:HB	2.14	0.47
20:T:87:LYS:HD3	20:T:90:GLN:HE21	1.79	0.47
1:A:75:G:C6	1:A:96:G:C6	3.02	0.47
1:A:484:G:O2'	1:A:485:G:OP2	2.22	0.47
1:A:653:A:O4'	8:H:56:LYS:HE2	2.14	0.47
1:A:877:C:O2	8:H:3:THR:HG21	2.15	0.47
1:A:1007:C:O2	1:A:1023:G:N1	2.48	0.47
1:A:1392:G:C2'	1:A:1393:U:H5'	2.45	0.47
1:A:1500:A:OP2	1:A:1505:G:OP1	2.33	0.47
2:B:17:PHE:HD1	2:B:18:GLY:N	2.13	0.47
2:B:112:VAL:HG23	2:B:149:LEU:HD13	1.96	0.47
2:B:122:PHE:CZ	2:B:139:LYS:HE2	2.50	0.47
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.97	0.47
7:G:75:VAL:HG22	7:G:88:PRO:HA	1.96	0.47
13:M:108:ARG:NH2	13:M:112:GLY:O	2.48	0.47
14:N:41:ARG:HG3	14:N:42:ILE:N	2.30	0.47
16:P:78:GLY:C	16:P:80:PHE:N	2.66	0.47
19:S:41:VAL:HG23	19:S:44:MET:HG3	1.96	0.47
1:A:60:A:H4'	1:A:61:G:O5'	2.15	0.47
1:A:837:G:C2	1:A:850:U:O2	2.68	0.47
1:A:853:G:C2	1:A:854:G:C8	3.03	0.47
1:A:952:U:H2'	1:A:953:G:C8	2.49	0.47
2:B:196:LEU:HA	2:B:196:LEU:HD23	1.66	0.47
3:C:190:ARG:HG3	3:C:195:VAL:HB	1.96	0.47
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.96	0.47
8:H:96:GLY:HA2	8:H:130:GLY:HA3	1.96	0.47
10:J:51:ARG:HG3	10:J:59:SER:HB2	1.97	0.47
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.47	0.47
19:S:34:TRP:HD1	19:S:52:TYR:CG	2.32	0.47
1:A:219:C:O2'	1:A:381:C:H5'	2.15	0.47
1:A:260:G:C4	1:A:261:U:C5	3.03	0.47
1:A:344:A:H5'	1:A:345:C:C5	2.50	0.47
1:A:690:G:C6	1:A:691:G:C6	3.03	0.47
1:A:1339:A:H5''	1:A:1340:A:OP2	2.14	0.47
7:G:57:GLU:H	7:G:57:GLU:HG3	1.48	0.47
9:I:75:ASP:O	9:I:78:LYS:HB3	2.15	0.47
11:K:65:ALA:HB1	11:K:98:LEU:HB3	1.97	0.47
13:M:105:THR:O	13:M:107:ALA:N	2.48	0.47
18:R:55:ARG:HB3	18:R:55:ARG:CZ	2.45	0.47
1:A:694:A:N1	1:A:787:A:O2'	2.46	0.47
1:A:792:A:O2'	1:A:793:U:OP2	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:A:H1'	19:S:54:GLY:O	2.15	0.47
1:A:1070:U:O2	1:A:1106:G:C2	2.69	0.47
1:A:1499:A:H1'	1:A:1520:G:OP1	2.13	0.47
3:C:36:ASP:HA	3:C:39:ILE:CD1	2.43	0.47
6:F:38:GLU:HB2	6:F:64:GLN:O	2.15	0.47
14:N:23:ARG:HH12	14:N:30:ALA:HB2	1.80	0.47
16:P:60:LEU:HA	16:P:60:LEU:HD23	1.73	0.47
17:Q:61:GLU:HA	17:Q:71:PHE:CE1	2.50	0.47
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.97	0.47
1:A:315:A:O2'	1:A:330:C:O2'	2.26	0.46
1:A:1145:C:H1'	1:A:1146:A:C8	2.49	0.46
1:A:1303:C:H2'	1:A:1304:G:C5'	2.42	0.46
1:A:1347:G:O2'	1:A:1348:U:O5'	2.33	0.46
1:A:1373:G:H5''	7:G:36:LYS:HB2	1.97	0.46
2:B:7:VAL:HG21	2:B:221:LEU:HD23	1.97	0.46
2:B:119:GLU:HG3	2:B:142:LEU:HD11	1.97	0.46
4:D:124:GLY:O	4:D:132:ARG:HG3	2.16	0.46
8:H:31:PHE:O	8:H:35:ILE:HG12	2.15	0.46
11:K:47:VAL:HG12	11:K:48:ILE:N	2.30	0.46
1:A:131:C:H2'	1:A:132:C:C6	2.50	0.46
1:A:457:C:H2'	1:A:458:C:C6	2.50	0.46
1:A:544:G:C5	1:A:545:C:C5	3.02	0.46
1:A:953:G:C5'	1:A:965:A:H61	2.23	0.46
1:A:1232:U:H5''	9:I:124:GLN:O	2.15	0.46
1:A:1325:C:H4'	21:U:17:THR:HG21	1.97	0.46
1:A:1399:C:C2	1:A:1401:G:C4	3.04	0.46
3:C:172:ARG:HB2	3:C:172:ARG:NH1	2.29	0.46
4:D:61:LYS:HE2	4:D:72:GLU:OE1	2.15	0.46
4:D:187:ARG:CZ	4:D:188:LEU:HB2	2.45	0.46
9:I:111:ARG:HH11	9:I:113:LYS:HA	1.80	0.46
12:L:11:VAL:HG22	17:Q:29:HIS:CD2	2.51	0.46
1:A:102:G:H2'	1:A:103:C:C6	2.49	0.46
1:A:1003:G:N2	1:A:1039:C:N3	2.62	0.46
1:A:1261:A:H1'	1:A:1283:G:H5''	1.96	0.46
2:B:82:ARG:NH1	2:B:82:ARG:HB2	2.30	0.46
2:B:115:LEU:HD23	2:B:153:ARG:NE	2.30	0.46
6:F:12:PRO:HD3	6:F:58:GLY:HA2	1.97	0.46
13:M:17:VAL:O	13:M:20:THR:HB	2.14	0.46
15:O:17:ARG:HB2	15:O:18:PHE:CD2	2.51	0.46
17:Q:10:VAL:HG23	17:Q:54:GLY:H	1.79	0.46
1:A:707:C:H4'	11:K:20:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:ALA:HA	3:C:116:VAL:HG23	1.96	0.46
17:Q:40:LYS:HE3	17:Q:42:TYR:CZ	2.50	0.46
19:S:29:ARG:H	19:S:29:ARG:HD2	1.80	0.46
1:A:268:C:H2'	1:A:269:C:H6	1.80	0.46
1:A:1030:C:N4	1:A:1032:G:O6	2.47	0.46
1:A:1065:U:C5	1:A:1190:G:H1'	2.50	0.46
3:C:147:LYS:HZ3	3:C:203:PHE:HE2	1.63	0.46
7:G:16:LEU:HD11	9:I:45:ALA:HB2	1.97	0.46
12:L:60:LEU:HA	12:L:60:LEU:HD13	1.60	0.46
18:R:53:ARG:NH1	18:R:58:LEU:O	2.49	0.46
19:S:15:LEU:O	19:S:19:VAL:HG12	2.16	0.46
1:A:406:G:H21	4:D:119:GLN:HE22	1.63	0.46
1:A:666:G:H5'	1:A:726:C:H1'	1.96	0.46
1:A:1003:G:H22	1:A:1039:C:H42	1.64	0.46
1:A:1124:G:H5''	1:A:1125:U:OP1	2.15	0.46
2:B:24:TRP:CE3	2:B:26:PRO:HA	2.51	0.46
7:G:50:ILE:HD11	7:G:125:MET:HB2	1.97	0.46
8:H:77:GLU:HG2	8:H:78:GLN:N	2.30	0.46
16:P:17:TYR:HD1	16:P:39:TYR:HD2	1.63	0.46
1:A:184:G:H2'	1:A:185:A:C8	2.48	0.46
1:A:691:G:H3'	11:K:26:ASN:HD21	1.79	0.46
1:A:792:A:N6	1:A:794:A:N1	2.63	0.46
1:A:935:A:N6	7:G:3:ARG:HG3	2.29	0.46
1:A:986:A:O2'	19:S:52:TYR:OH	2.26	0.46
4:D:15:GLU:CD	4:D:59:ARG:HH21	2.18	0.46
4:D:64:LEU:HD22	4:D:67:ILE:HD12	1.98	0.46
12:L:25:PRO:C	12:L:27:LEU:N	2.64	0.46
1:A:452:A:HO2'	1:A:453:A:C4'	2.29	0.46
1:A:694:A:C2	1:A:695:A:H1'	2.50	0.46
1:A:781:A:C5	1:A:802:A:C2	3.04	0.46
1:A:792:A:C6	1:A:794:A:C2	3.04	0.46
1:A:881:G:OP1	12:L:13:LYS:NZ	2.48	0.46
3:C:105:GLU:O	3:C:107:GLN:NE2	2.49	0.46
9:I:19:LEU:HD11	9:I:81:ILE:HD13	1.98	0.46
12:L:25:PRO:HB3	12:L:27:LEU:HD12	1.98	0.46
1:A:269:C:H2'	1:A:270:A:H8	1.80	0.46
1:A:370:C:N3	1:A:392:G:C2	2.84	0.46
1:A:788:U:H3'	1:A:789:U:O4'	2.16	0.46
2:B:125:PRO:HG2	2:B:126:GLU:OE1	2.16	0.46
3:C:70:VAL:O	3:C:106:VAL:HG23	2.16	0.46
3:C:142:MET:HE1	3:C:170:GLN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:30:LYS:O	4:D:32:ALA:N	2.48	0.46
4:D:107:ARG:NH1	4:D:194:LEU:HD11	2.31	0.46
5:E:110:LEU:HD12	5:E:118:ILE:HG21	1.98	0.46
12:L:44:THR:HA	12:L:45:PRO:HD3	1.54	0.46
12:L:82:VAL:O	12:L:106:ASP:HB2	2.16	0.46
1:A:78:G:N1	1:A:92:C:C4	2.84	0.46
1:A:268:C:H2'	1:A:269:C:C6	2.51	0.46
1:A:701:C:O2'	1:A:702:A:OP2	2.24	0.46
1:A:738:C:P	6:F:92:LYS:HD3	2.56	0.46
1:A:923:A:O4'	1:A:1398:A:C2	2.68	0.46
1:A:940:C:H2'	1:A:941:G:O4'	2.16	0.46
1:A:1323:G:H2'	1:A:1324:A:C8	2.51	0.46
1:A:1542:U:H2'	1:A:1543:C:C6	2.51	0.46
10:J:27:ALA:O	10:J:31:GLY:N	2.44	0.46
11:K:94:ALA:O	11:K:98:LEU:HD12	2.16	0.46
13:M:91:ARG:HB3	13:M:98:VAL:HG22	1.97	0.46
18:R:54:ARG:HE	18:R:54:ARG:HB2	1.58	0.46
1:A:350:G:O2'	1:A:351:G:H5'	2.16	0.45
1:A:389:A:C6	1:A:390:C:H1'	2.51	0.45
1:A:459:G:H1'	1:A:463:A:H61	1.81	0.45
1:A:479:C:H2'	1:A:480:U:O4'	2.16	0.45
1:A:806:C:H2'	1:A:807:A:H8	1.81	0.45
1:A:942:G:N2	1:A:943:U:C2	2.83	0.45
1:A:1060:C:C2	1:A:1198:G:C2	3.04	0.45
2:B:44:LEU:O	2:B:47:THR:HB	2.16	0.45
2:B:52:GLU:HG2	2:B:56:ARG:HH22	1.81	0.45
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.51	0.45
7:G:17:VAL:HG11	7:G:44:TYR:CE2	2.51	0.45
9:I:8:GLY:H	9:I:83:ARG:NH1	2.14	0.45
10:J:57:LYS:HG3	10:J:58:ASP:OD2	2.15	0.45
1:A:345:C:OP2	1:A:345:C:H6	1.98	0.45
1:A:485:G:HO2'	1:A:486:U:P	2.39	0.45
1:A:945:G:N1	1:A:1337:G:N2	2.63	0.45
1:A:1267:C:O2'	21:U:20:LYS:HG3	2.16	0.45
1:A:1360:A:C2	14:N:18:VAL:HB	2.49	0.45
4:D:94:LEU:O	4:D:97:LEU:HB2	2.17	0.45
10:J:8:LEU:HA	10:J:95:GLU:O	2.16	0.45
15:O:85:LEU:HD23	15:O:85:LEU:N	2.31	0.45
1:A:152:A:N6	1:A:170:U:C2	2.85	0.45
1:A:337:C:H2'	1:A:338:A:H8	1.82	0.45
1:A:452:A:HO2'	1:A:453:A:C5'	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.45
1:A:983:A:P	14:N:3:ARG:HH22	2.39	0.45
1:A:1482:G:HO2'	1:A:1483:A:H8	1.62	0.45
4:D:112:VAL:HG23	4:D:116:GLN:OE1	2.16	0.45
4:D:194:LEU:HD13	4:D:194:LEU:HA	1.63	0.45
6:F:26:ILE:O	6:F:30:LEU:HD12	2.16	0.45
17:Q:74:LEU:HD22	17:Q:74:LEU:HA	1.66	0.45
1:A:459:G:H1'	1:A:463:A:N6	2.32	0.45
1:A:550:G:C5	1:A:551:U:C5	3.04	0.45
1:A:671:G:H1	1:A:735:C:H42	1.63	0.45
1:A:825:G:H21	8:H:11:THR:HG21	1.80	0.45
1:A:1014:A:N6	1:A:1015:A:N1	2.64	0.45
1:A:1048:G:H2'	1:A:1050:G:H8	1.81	0.45
1:A:1053:G:OP1	1:A:1054:C:H5''	2.16	0.45
1:A:1094:G:OP2	1:A:1095:U:H5	2.00	0.45
2:B:74:LYS:NZ	2:B:206:ASP:OD1	2.35	0.45
5:E:55:VAL:HG12	5:E:56:GLN:N	2.32	0.45
5:E:123:LEU:HD23	5:E:123:LEU:HA	1.55	0.45
9:I:32:ASP:HB3	9:I:35:GLU:OE1	2.16	0.45
10:J:20:ALA:O	10:J:24:VAL:HG12	2.16	0.45
14:N:3:ARG:HE	14:N:6:LEU:HD23	1.82	0.45
1:A:75:G:O6	1:A:96:G:C6	2.70	0.45
1:A:951:G:OP2	13:M:102:ARG:NH2	2.47	0.45
1:A:977:A:H8	1:A:1223:C:N3	2.14	0.45
3:C:150:LYS:NZ	3:C:175:LEU:HD11	2.30	0.45
4:D:13:ARG:HB2	4:D:38:TYR:O	2.16	0.45
4:D:102:ASP:HA	4:D:121:VAL:HG21	1.99	0.45
7:G:5:ARG:HB3	7:G:6:ARG:H	1.62	0.45
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.20	0.45
9:I:118:LYS:C	9:I:120:ARG:H	2.19	0.45
18:R:56:THR:HB	18:R:58:LEU:CD2	2.46	0.45
1:A:77:G:C6	1:A:93:G:N1	2.85	0.45
1:A:89:C:H2'	1:A:90:U:O4'	2.16	0.45
1:A:718:G:O6	18:R:74:ARG:NH1	2.48	0.45
1:A:723:U:O2	1:A:723:U:H2'	2.16	0.45
1:A:880:C:OP2	12:L:6:THR:HG21	2.17	0.45
1:A:1422:G:C2	1:A:1423:G:C8	3.05	0.45
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.99	0.45
3:C:175:LEU:HD22	3:C:201:TYR:CD2	2.52	0.45
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.98	0.45
20:T:16:HIS:CE1	20:T:20:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:45:GLN:N	20:T:45:GLN:OE1	2.49	0.45
1:A:435:C:H2'	1:A:436:C:C6	2.51	0.45
1:A:661:G:H1	1:A:744:C:H42	1.63	0.45
1:A:975:A:H5'	1:A:975:A:C8	2.49	0.45
1:A:1058:G:H2'	1:A:1059:C:C6	2.51	0.45
1:A:1089:G:C6	1:A:1090:U:C4	3.05	0.45
1:A:1202:G:H2'	1:A:1203:C:O4'	2.16	0.45
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.17	0.45
3:C:30:ARG:H	3:C:30:ARG:HD3	1.80	0.45
3:C:85:ARG:HH11	3:C:88:ARG:HH12	1.63	0.45
5:E:36:ASP:C	5:E:38:GLN:H	2.19	0.45
5:E:92:LYS:O	5:E:118:ILE:HG12	2.17	0.45
9:I:86:VAL:HG23	9:I:96:LEU:HD22	1.98	0.45
12:L:42:THR:HA	12:L:53:ARG:O	2.16	0.45
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.98	0.45
14:N:16:PHE:HD1	14:N:19:ARG:NE	2.15	0.45
1:A:79:G:C2	1:A:80:G:C4	3.05	0.45
1:A:457:C:H2'	1:A:458:C:H6	1.82	0.45
1:A:977:A:H8	1:A:1223:C:C4	2.34	0.45
1:A:1267:C:O2	21:U:20:LYS:HD2	2.16	0.45
1:A:1511:G:H2'	1:A:1512:U:O4'	2.15	0.45
4:D:173:TRP:CE2	4:D:174:LEU:HD11	2.51	0.45
5:E:11:ILE:HB	5:E:31:LEU:CB	2.46	0.45
9:I:20:ARG:HB2	9:I:60:ASP:HB3	1.99	0.45
12:L:92:0TD:OD1	12:L:92:0TD:N	2.49	0.45
18:R:56:THR:HB	18:R:58:LEU:HD21	1.99	0.45
1:A:6:G:O2'	1:A:7:G:H5'	2.17	0.45
1:A:489:C:OP1	4:D:132:ARG:NH2	2.49	0.45
1:A:620:C:N1	4:D:135:LEU:HD13	2.31	0.45
1:A:922:G:C2	1:A:1396:A:C6	3.05	0.45
1:A:946:A:N1	1:A:1236:A:C2	2.85	0.45
1:A:974:A:P	14:N:41:ARG:HH22	2.39	0.45
1:A:1338:G:C6	1:A:1339:A:C6	3.05	0.45
3:C:175:LEU:H	3:C:175:LEU:HG	1.46	0.45
4:D:20:TYR:HA	4:D:26:CYS:SG	2.57	0.45
8:H:6:ILE:HG13	8:H:31:PHE:HE2	1.81	0.45
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.52	0.45
8:H:112:LEU:H	8:H:112:LEU:HD12	1.82	0.45
11:K:44:SER:H	11:K:47:VAL:HB	1.81	0.45
13:M:27:LYS:HD2	13:M:27:LYS:HA	1.36	0.45
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:102:ARG:HG3	13:M:102:ARG:O	2.17	0.45
13:M:105:THR:OG1	13:M:106:ASN:HB2	2.16	0.45
14:N:41:ARG:HG3	14:N:42:ILE:H	1.82	0.45
16:P:39:TYR:HE2	16:P:41:PRO:HB3	1.82	0.45
18:R:22:VAL:HG23	18:R:56:THR:HA	1.99	0.45
18:R:60:ALA:O	18:R:64:ARG:HG3	2.17	0.45
1:A:92:C:H2'	1:A:93:G:H8	1.81	0.45
1:A:456:C:C2	1:A:457:C:C5	3.04	0.45
1:A:1080:A:H5''	5:E:16:THR:OG1	2.17	0.45
1:A:1202:G:C4	14:N:42:ILE:HD12	2.52	0.45
4:D:31:CYS:O	4:D:31:CYS:SG	2.75	0.45
4:D:159:ARG:O	4:D:163:GLU:HB2	2.17	0.45
18:R:43:PHE:O	18:R:51:LEU:HD23	2.16	0.45
19:S:15:LEU:HD12	19:S:16:LEU:N	2.32	0.45
20:T:30:LYS:O	20:T:33:ILE:HB	2.17	0.45
1:A:1342:C:H2'	1:A:1343:G:C8	2.51	0.44
6:F:27:GLN:O	6:F:31:GLU:HG3	2.17	0.44
7:G:121:ALA:O	7:G:124:LEU:HD12	2.16	0.44
9:I:6:GLY:CA	9:I:83:ARG:HB3	2.46	0.44
11:K:125:PHE:C	11:K:126:ARG:HG3	2.37	0.44
1:A:450:G:N7	1:A:481:G:O6	2.50	0.44
1:A:517:G:H5'	1:A:519:C:O2	2.16	0.44
1:A:1265:G:C6	1:A:1266:G:C6	3.05	0.44
1:A:1329:A:OP1	13:M:28:ALA:HB3	2.17	0.44
3:C:150:LYS:HG2	3:C:169:ALA:CB	2.46	0.44
14:N:39:LEU:CD1	14:N:43:CYS:HB3	2.47	0.44
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.69	0.44
18:R:52:PRO:O	18:R:56:THR:OG1	2.29	0.44
20:T:51:GLU:HG2	20:T:51:GLU:H	1.56	0.44
1:A:92:C:O2'	1:A:93:G:H5'	2.17	0.44
1:A:328:C:O2	1:A:328:C:H2'	2.17	0.44
1:A:370:C:H2'	1:A:371:G:O4'	2.17	0.44
1:A:401:C:H1'	1:A:622:A:H1'	1.99	0.44
1:A:451:A:H2	1:A:480:U:C4	2.35	0.44
1:A:546:G:OP1	4:D:73:ARG:HG2	2.16	0.44
1:A:575:G:HO2'	1:A:821:G:H5'	1.82	0.44
1:A:665:A:H2'	1:A:732:C:O2	2.17	0.44
1:A:712:A:H2'	1:A:713:G:O4'	2.18	0.44
1:A:1196:U:H3'	1:A:1196:U:OP1	2.18	0.44
3:C:181:ASN:O	3:C:181:ASN:ND2	2.50	0.44
5:E:65:ASN:OD1	5:E:140:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:73:ASN:HD22	6:F:73:ASN:N	2.14	0.44
7:G:88:PRO:HG2	7:G:155:ARG:CZ	2.47	0.44
12:L:120:TYR:N	12:L:120:TYR:CD2	2.85	0.44
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.98	0.44
1:A:279:A:H5'	1:A:279:A:H8	1.82	0.44
1:A:411:A:H62	1:A:413:G:H21	1.65	0.44
1:A:1423:G:N2	1:A:1477:C:O2	2.40	0.44
1:A:1532:U:H2'	1:A:1533:C:H3'	2.00	0.44
10:J:57:LYS:HE2	10:J:57:LYS:HB2	1.86	0.44
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.81	0.44
13:M:3:ARG:HA	13:M:8:GLU:O	2.17	0.44
1:A:263:A:OP2	20:T:79:ARG:NH1	2.48	0.44
1:A:429:U:H4'	1:A:430:A:O5'	2.17	0.44
1:A:602:A:C2	1:A:637:G:C2	3.06	0.44
1:A:658:G:H2'	1:A:659:U:C6	2.52	0.44
1:A:803:G:H8	1:A:803:G:O5'	1.99	0.44
1:A:829:G:O2'	1:A:830:G:H5'	2.18	0.44
1:A:1235:U:O3'	21:U:3:LYS:HB2	2.18	0.44
1:A:1391:U:H2'	1:A:1392:G:C8	2.53	0.44
1:A:1400:5MC:H3'	1:A:1401:G:C5'	2.46	0.44
2:B:36:ARG:HG3	2:B:41:ILE:HD11	1.99	0.44
2:B:100:GLY:O	2:B:104:ASN:N	2.49	0.44
2:B:114:ARG:NE	2:B:141:GLU:OE2	2.46	0.44
2:B:139:LYS:HZ2	2:B:143:GLU:HG3	1.82	0.44
8:H:28:ALA:HB2	8:H:59:LEU:HG	1.99	0.44
9:I:5:TYR:CE2	9:I:18:PHE:HE2	2.35	0.44
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.53	0.44
12:L:28:LYS:HG3	12:L:33:ARG:NH1	2.32	0.44
12:L:34:ARG:O	12:L:34:ARG:HG3	2.18	0.44
1:A:222:U:H2'	1:A:223:U:C6	2.53	0.44
1:A:642:A:C5	1:A:643:C:C5	3.05	0.44
1:A:956:U:HO2'	19:S:80:TYR:HD1	1.63	0.44
1:A:1342:C:H2'	1:A:1343:G:H8	1.82	0.44
1:A:1540:PSU:HN1	1:A:1541:PSU:HN1	1.64	0.44
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.17	0.44
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.79	0.44
12:L:5:PRO:HG2	12:L:10:LEU:HD11	1.99	0.44
17:Q:95:TYR:O	17:Q:97:SER:N	2.50	0.44
1:A:410:G:OP2	4:D:25:ARG:HG3	2.17	0.44
1:A:538:G:OP2	12:L:115:LYS:HB2	2.17	0.44
1:A:695:A:OP2	11:K:52:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:TYR:CD2	2:B:31:TYR:N	2.85	0.44
2:B:48:MET:HA	2:B:51:LEU:HB2	1.99	0.44
7:G:50:ILE:HD13	7:G:50:ILE:HA	1.61	0.44
8:H:134:ILE:HA	8:H:134:ILE:HD13	1.70	0.44
1:A:69:G:H1	1:A:99:C:H42	1.66	0.44
1:A:815:A:N6	1:A:1509:C:H1'	2.33	0.44
1:A:838:G:C2	1:A:849:C:C2	3.05	0.44
1:A:1004:A:HO2'	1:A:1005:A:P	2.41	0.44
1:A:1014:A:H4'	19:S:14:HIS:CD2	2.53	0.44
1:A:1424:C:H2'	1:A:1425:U:H6	1.83	0.44
2:B:87:ARG:HB3	2:B:87:ARG:HH11	1.82	0.44
15:O:42:HIS:CD2	15:O:43:LEU:HD23	2.53	0.44
17:Q:29:HIS:HA	17:Q:30:PRO:HD3	1.57	0.44
17:Q:58:GLU:HB3	17:Q:74:LEU:CB	2.47	0.44
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.50	0.44
19:S:18:LYS:HD2	19:S:31:ILE:HD11	2.00	0.44
20:T:53:LEU:HD22	20:T:56:MET:HE2	2.00	0.44
1:A:61:G:H2'	1:A:62:U:O4'	2.18	0.44
1:A:1072:G:C6	1:A:1073:U:C4	3.06	0.44
1:A:1228:C:O3'	13:M:116:THR:HG23	2.18	0.44
1:A:1494:G:C2	1:A:1495:U:C4	3.05	0.44
1:A:1496:C:O2'	1:A:1497:G:O5'	2.35	0.44
2:B:15:VAL:HG11	2:B:213:LEU:HD12	2.00	0.44
3:C:7:PRO:HG2	3:C:184:TYR:CD1	2.53	0.44
3:C:11:ARG:HD3	3:C:181:ASN:HA	1.99	0.44
4:D:70:ILE:HA	4:D:70:ILE:HD13	1.63	0.44
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.50	0.44
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.99	0.44
6:F:78:GLU:O	6:F:81:ILE:HG22	2.18	0.44
11:K:73:MET:HG3	11:K:103:LEU:HD21	1.98	0.44
13:M:19:LEU:HD11	13:M:56:LEU:CD1	2.48	0.44
15:O:17:ARG:HD3	15:O:26:GLU:OE2	2.18	0.44
17:Q:22:LEU:HD12	17:Q:22:LEU:HA	1.52	0.44
1:A:16:A:O2'	1:A:17:U:H5'	2.18	0.43
1:A:434:U:H2'	1:A:435:C:C6	2.53	0.43
1:A:667:G:H4'	15:O:51:HIS:ND1	2.32	0.43
1:A:673:G:H2'	1:A:674:G:C8	2.53	0.43
1:A:838:G:N2	1:A:849:C:C2	2.86	0.43
1:A:1244:C:H42	1:A:1293:G:H1	1.64	0.43
1:A:1426:C:H2'	1:A:1427:U:C6	2.52	0.43
2:B:62:ALA:HB1	2:B:222:ILE:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:TRP:CH2	3:C:33:LEU:HD21	2.53	0.43
5:E:110:LEU:HD23	5:E:110:LEU:N	2.33	0.43
6:F:11:ASN:HA	6:F:12:PRO:HD2	1.73	0.43
8:H:35:ILE:HG12	8:H:35:ILE:H	1.61	0.43
10:J:5:ARG:HD3	10:J:99:LYS:HB3	1.98	0.43
12:L:51:ALA:O	12:L:52:LEU:HD23	2.18	0.43
12:L:113:ARG:HH12	12:L:115:LYS:HB3	1.83	0.43
19:S:43:GLU:OE1	19:S:43:GLU:N	2.49	0.43
20:T:65:LYS:O	20:T:68:LYS:HB3	2.18	0.43
1:A:77:G:C6	1:A:93:G:C6	3.06	0.43
1:A:1293:G:H2'	1:A:1294:G:O4'	2.18	0.43
3:C:173:VAL:HG12	3:C:175:LEU:HD23	2.00	0.43
4:D:57:ARG:HG3	4:D:202:LEU:CD1	2.48	0.43
8:H:12:ARG:HH11	8:H:26:VAL:HA	1.82	0.43
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.66	0.43
12:L:53:ARG:HG2	12:L:93:LEU:HD11	2.00	0.43
1:A:146:G:C2	1:A:147:G:C4	3.06	0.43
1:A:448:A:P	1:A:485:G:H22	2.40	0.43
1:A:679:C:H2'	1:A:680:C:H6	1.83	0.43
1:A:1133:G:N2	1:A:1141:C:N3	2.63	0.43
1:A:1178:G:P	9:I:97:LYS:HZ3	2.41	0.43
1:A:1498:UR3:O5'	1:A:1498:UR3:H6	2.18	0.43
3:C:114:PRO:N	3:C:185:GLY:HA3	2.33	0.43
5:E:90:VAL:O	5:E:91:LEU:HD23	2.19	0.43
1:A:83:U:C2'	1:A:84:U:H5'	2.48	0.43
1:A:109:A:H2'	1:A:326:G:N2	2.33	0.43
1:A:357:G:C2	1:A:358:U:C5	3.07	0.43
1:A:445:G:H2'	1:A:446:G:H8	1.83	0.43
1:A:959:A:O2'	1:A:984:C:O2'	2.34	0.43
3:C:73:PRO:HG3	3:C:105:GLU:OE1	2.19	0.43
5:E:90:VAL:C	5:E:91:LEU:HD23	2.39	0.43
7:G:124:LEU:H	7:G:124:LEU:HG	1.44	0.43
15:O:85:LEU:HB2	15:O:87:ILE:HD12	2.01	0.43
17:Q:63:ARG:CB	17:Q:63:ARG:HH11	2.32	0.43
21:U:5:ASP:O	21:U:8:THR:OG1	2.35	0.43
1:A:90:U:C4	1:A:91:C:C5	3.06	0.43
1:A:321:A:N6	1:A:329:A:OP2	2.49	0.43
1:A:946:A:C6	1:A:1236:A:C2	3.06	0.43
1:A:964:A:O2'	10:J:55:LYS:NZ	2.22	0.43
1:A:1084:G:O2'	1:A:1085:U:OP1	2.34	0.43
1:A:1226:C:H4'	1:A:1227:A:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:G:H2'	1:A:1475:G:C8	2.54	0.43
4:D:25:ARG:HA	4:D:28:SER:H	1.83	0.43
4:D:30:LYS:C	4:D:32:ALA:H	2.20	0.43
7:G:17:VAL:HG21	7:G:44:TYR:CZ	2.53	0.43
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.54	0.43
9:I:17:VAL:HG22	9:I:63:ILE:HD12	2.00	0.43
9:I:48:GLU:HA	9:I:51:ARG:HD2	2.00	0.43
13:M:16:ASP:HB3	13:M:34:LEU:HD12	1.99	0.43
1:A:279:A:H5'	1:A:279:A:C8	2.53	0.43
1:A:410:G:N1	1:A:429:U:O2	2.51	0.43
1:A:920:U:H2'	1:A:921:U:C6	2.54	0.43
1:A:1054:C:OP1	1:A:1197:G:OP1	2.37	0.43
1:A:1117:G:H5''	9:I:104:ARG:NH2	2.33	0.43
1:A:1301:U:O2'	1:A:1302:U:P	2.77	0.43
2:B:54:THR:O	2:B:58:ILE:HG13	2.19	0.43
4:D:119:GLN:HG3	4:D:123:HIS:NE2	2.33	0.43
8:H:17:THR:HG22	8:H:63:LEU:HG	2.01	0.43
12:L:59:ARG:HA	12:L:59:ARG:HH11	1.84	0.43
15:O:4:THR:O	15:O:7:GLU:HB2	2.19	0.43
17:Q:6:LEU:O	17:Q:58:GLU:HG3	2.17	0.43
20:T:33:ILE:HG12	20:T:62:LEU:CD2	2.48	0.43
20:T:50:GLU:H	20:T:50:GLU:HG2	1.34	0.43
1:A:190:C:O2'	1:A:190(A):C:H5'	2.18	0.43
1:A:284:G:H2'	1:A:285:G:C8	2.53	0.43
1:A:391:G:C6	1:A:392:G:C5	3.07	0.43
1:A:1008:C:N4	1:A:1021:G:H22	2.04	0.43
1:A:1347:G:H2'	1:A:1373:G:C6	2.53	0.43
1:A:1521:G:H2'	1:A:1522:U:C6	2.54	0.43
2:B:188:ALA:HB1	2:B:192:SER:OG	2.18	0.43
4:D:88:VAL:O	4:D:92:VAL:HG23	2.17	0.43
4:D:126:ILE:O	4:D:132:ARG:HA	2.18	0.43
10:J:8:LEU:CD2	10:J:96:ILE:HG23	2.49	0.43
12:L:35:GLY:HA3	12:L:60:LEU:HD13	2.00	0.43
17:Q:40:LYS:HG3	17:Q:41:LYS:N	2.33	0.43
18:R:37:VAL:HG13	18:R:41:LYS:HD3	2.00	0.43
18:R:88:LYS:HB3	18:R:88:LYS:NZ	2.33	0.43
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.66	0.43
1:A:1094:G:O2'	1:A:1095:U:OP1	2.37	0.43
1:A:1112:C:H1'	3:C:179:ARG:NH1	2.33	0.43
22:A:1601:SRY:HI32	22:A:1601:SRY:C22	2.49	0.43
4:D:190:ASP:HB3	4:D:193:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:100:ASN:HB2	18:R:23:LYS:HD2	1.99	0.43
9:I:89:ASN:HB3	9:I:92:TYR:HB2	2.01	0.43
10:J:88:LEU:HD23	10:J:88:LEU:HA	1.85	0.43
13:M:92:HIS:CD2	13:M:98:VAL:HG21	2.53	0.43
1:A:854:G:H3'	1:A:871:U:O4	2.18	0.43
1:A:927:G:O2'	1:A:1503:A:N7	2.46	0.43
1:A:1326:C:H2'	1:A:1327:C:C6	2.53	0.43
2:B:226:ARG:HE	2:B:226:ARG:HB2	1.64	0.43
4:D:187:ARG:NH2	4:D:188:LEU:O	2.51	0.43
5:E:43:LEU:HD11	5:E:133:TYR:CD2	2.53	0.43
17:Q:89:LEU:HD23	17:Q:89:LEU:HA	1.77	0.43
19:S:75:ALA:HA	19:S:76:PRO:HD2	1.82	0.43
1:A:585:G:C6	1:A:586:C:C4	3.06	0.43
1:A:1157:A:H4'	1:A:1158:C:O4'	2.18	0.43
1:A:1206:G:H4'	3:C:192:THR:O	2.19	0.43
1:A:1384:C:H2'	1:A:1385:G:C8	2.54	0.43
4:D:11:LEU:HD13	4:D:66:ARG:CD	2.49	0.43
9:I:36:TYR:CD2	9:I:37:PHE:CE2	3.07	0.43
9:I:104:ARG:HD2	9:I:105:ASP:N	2.34	0.43
11:K:58:PRO:O	11:K:61:ALA:HB3	2.19	0.43
11:K:101:SER:HG	11:K:103:LEU:H	1.65	0.43
12:L:98:TYR:CD1	12:L:98:TYR:N	2.87	0.43
1:A:24:U:H2'	1:A:25:C:C6	2.54	0.42
1:A:77:G:N1	1:A:93:G:C6	2.87	0.42
1:A:386:C:C2'	1:A:387:U:H5'	2.49	0.42
1:A:474:G:C2	1:A:475:G:N7	2.87	0.42
1:A:865:A:C6	1:A:866:C:C4	3.07	0.42
1:A:1303:C:C2'	1:A:1304:G:H5'	2.44	0.42
1:A:1502:A:H2	1:A:1505:G:H1	1.66	0.42
11:K:33:THR:HB	11:K:39:PRO:HA	2.01	0.42
12:L:115:LYS:HD2	12:L:115:LYS:HA	1.87	0.42
14:N:44:LEU:O	14:N:48:ALA:HB2	2.19	0.42
16:P:41:PRO:O	16:P:43:LYS:HD3	2.19	0.42
1:A:113:G:H2'	1:A:114:U:H6	1.84	0.42
1:A:255:G:H1'	17:Q:16:GLN:OE1	2.19	0.42
1:A:448:A:C4	1:A:487:A:C2	3.07	0.42
1:A:981:U:H2'	1:A:982:U:C6	2.54	0.42
1:A:1060:C:N3	1:A:1198:G:C6	2.87	0.42
3:C:113:ALA:N	3:C:114:PRO:HD2	2.33	0.42
4:D:18:LYS:HB3	4:D:20:TYR:HE2	1.84	0.42
5:E:100:VAL:HG12	5:E:118:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:15:PHE:HE2	15:O:85:LEU:HD21	1.83	0.42
1:A:825:G:H1	1:A:875:C:N4	2.16	0.42
1:A:833:U:H2'	1:A:834:C:H6	1.84	0.42
1:A:1092:A:H1'	1:A:1183:A:N6	2.34	0.42
1:A:1376:U:C2	1:A:1377:A:N7	2.87	0.42
1:A:1518:MA6:H102	1:A:1519:MA6:C6	2.49	0.42
2:B:91:PRO:HA	2:B:154:LEU:HD12	2.01	0.42
5:E:78:HIS:ND1	8:H:104:ARG:HG3	2.33	0.42
5:E:139:LEU:HD23	5:E:139:LEU:HA	1.59	0.42
7:G:136:LYS:HE2	7:G:136:LYS:HB2	1.76	0.42
7:G:152:ALA:HA	7:G:155:ARG:CZ	2.49	0.42
10:J:15:THR:HG21	10:J:93:GLY:HA3	2.00	0.42
16:P:4:ILE:HA	16:P:20:VAL:O	2.19	0.42
20:T:18:GLN:O	20:T:21:LYS:HB2	2.18	0.42
1:A:162:A:H1'	1:A:348:G:O2'	2.19	0.42
1:A:200:G:N2	1:A:218:C:C2	2.87	0.42
1:A:279:A:H5''	1:A:281:G:O4'	2.18	0.42
1:A:945:G:O6	1:A:1236:A:N1	2.52	0.42
1:A:1201:A:H1'	1:A:1202:G:OP2	2.20	0.42
1:A:1213:A:N6	1:A:1215:G:N3	2.67	0.42
1:A:1479:C:H2'	1:A:1480:G:C8	2.52	0.42
2:B:25:ASN:C	2:B:25:ASN:HD22	2.22	0.42
2:B:115:LEU:HD11	2:B:146:GLN:HG3	2.02	0.42
3:C:94:LEU:HA	3:C:94:LEU:HD13	1.73	0.42
3:C:106:VAL:CG1	3:C:109:PRO:HA	2.45	0.42
5:E:11:ILE:HG22	5:E:12:LEU:N	2.33	0.42
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.54	0.42
8:H:39:LEU:HD13	8:H:39:LEU:HA	1.72	0.42
11:K:34:ASP:HA	11:K:35:PRO:HD3	1.81	0.42
13:M:6:GLY:O	13:M:67:GLU:HG2	2.19	0.42
13:M:23:TYR:CZ	13:M:71:ARG:HG2	2.55	0.42
1:A:216:G:H2'	1:A:217:C:C6	2.54	0.42
1:A:217:C:H2'	1:A:218:C:C6	2.54	0.42
1:A:647:C:H2'	1:A:648:A:C8	2.55	0.42
1:A:1241:G:H2'	1:A:1242:C:H6	1.84	0.42
1:A:1249:C:H2'	1:A:1250:A:H5'	2.01	0.42
1:A:1361(A):C:O2'	1:A:1362:C:H6	2.01	0.42
2:B:28:PHE:HD2	2:B:32:ILE:HD11	1.84	0.42
2:B:108:ILE:HD13	2:B:108:ILE:HA	1.83	0.42
3:C:135:LYS:HB3	3:C:135:LYS:HE2	1.84	0.42
4:D:57:ARG:NH1	4:D:202:LEU:HD11	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:ILE:N	5:E:76:ILE:HD12	2.34	0.42
9:I:15:ALA:CB	9:I:65:VAL:HG12	2.48	0.42
10:J:37:PRO:HB2	10:J:70:ARG:HB3	2.02	0.42
17:Q:29:HIS:ND1	17:Q:29:HIS:C	2.73	0.42
18:R:53:ARG:NH1	18:R:59:SER:HA	2.34	0.42
19:S:39:THR:HG22	19:S:40:ILE:O	2.18	0.42
20:T:53:LEU:HD22	20:T:53:LEU:HA	1.79	0.42
20:T:88:VAL:O	20:T:92:LEU:HD23	2.20	0.42
1:A:7:G:O6	5:E:92:LYS:HE3	2.19	0.42
1:A:219:C:C4	1:A:220:G:C8	3.07	0.42
1:A:460:A:C6	1:A:462:G:C5	3.08	0.42
1:A:1328:C:C2	1:A:1329:A:C8	3.08	0.42
2:B:157:ARG:HG2	2:B:158:LEU:N	2.34	0.42
4:D:156:GLU:O	4:D:160:GLN:NE2	2.53	0.42
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.55	0.42
7:G:10:ARG:NH1	7:G:10:ARG:HB2	2.34	0.42
11:K:19:ALA:HB2	11:K:80:VAL:CG1	2.50	0.42
11:K:48:ILE:HD13	11:K:63:LEU:HB3	2.02	0.42
14:N:12:ARG:HD2	14:N:14:PRO:HG3	2.02	0.42
15:O:28:GLN:O	15:O:32:LEU:HB2	2.19	0.42
16:P:38:TYR:O	16:P:49:LEU:HD12	2.20	0.42
19:S:30:LEU:HB3	19:S:31:ILE:H	1.67	0.42
1:A:132:C:O3'	20:T:74:LYS:NZ	2.43	0.42
1:A:809:G:C6	1:A:810:C:C5	3.08	0.42
3:C:175:LEU:HD22	3:C:201:TYR:CE2	2.54	0.42
6:F:79:LEU:HD23	6:F:79:LEU:HA	1.80	0.42
8:H:95:VAL:HB	8:H:99:GLU:HB2	2.01	0.42
9:I:50:LEU:HD21	9:I:85:LEU:HD11	2.02	0.42
9:I:79:LEU:O	9:I:83:ARG:HB2	2.20	0.42
10:J:49:VAL:CG1	14:N:41:ARG:HB2	2.50	0.42
11:K:18:ARG:HB2	11:K:33:THR:HG23	2.01	0.42
16:P:65:GLN:HA	16:P:66:PRO:HD2	1.84	0.42
20:T:33:ILE:HG12	20:T:62:LEU:HD23	2.01	0.42
1:A:33:A:N3	12:L:32:PHE:HE2	2.17	0.42
1:A:1276:G:H2'	1:A:1277:C:C6	2.55	0.42
3:C:17:ASP:O	3:C:54:ARG:NH2	2.53	0.42
11:K:21:ILE:HD12	11:K:95:ILE:HG12	2.02	0.42
13:M:92:HIS:NE2	13:M:98:VAL:HG21	2.35	0.42
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	2.02	0.42
1:A:35:G:C4	1:A:36:C:C5	3.07	0.42
1:A:232:G:H2'	1:A:233:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:C:O3'	11:K:20:TYR:HE2	2.03	0.42
1:A:1138:G:O2'	1:A:1140:C:H5'	2.20	0.42
3:C:134:ILE:HD13	3:C:134:ILE:N	2.34	0.42
3:C:155:GLY:HA3	3:C:163:ALA:HB1	2.02	0.42
13:M:40:ASN:ND2	13:M:43:THR:HG23	2.35	0.42
16:P:53:VAL:HG23	16:P:54:GLU:H	1.84	0.42
1:A:522:C:H5''	12:L:120:TYR:OH	2.19	0.42
1:A:538:G:P	12:L:115:LYS:HB2	2.60	0.42
1:A:980:C:C5	1:A:981:U:C4	3.08	0.42
1:A:1321:C:H5'	13:M:87:TYR:CE2	2.54	0.42
3:C:180:ALA:HB1	3:C:203:PHE:HE1	1.85	0.42
6:F:55:ASP:HA	6:F:56:PRO:HD3	1.83	0.42
18:R:32:ARG:HA	18:R:69:THR:CG2	2.46	0.42
19:S:12:ASP:H	19:S:15:LEU:HD11	1.84	0.42
1:A:460:A:H8	1:A:460:A:OP1	2.03	0.41
1:A:663:A:H5''	18:R:61:LYS:HE3	2.01	0.41
1:A:1474:G:H2'	1:A:1475:G:H8	1.85	0.41
22:A:1601:SRY:HI32	22:A:1601:SRY:H22	2.02	0.41
4:D:11:LEU:HD13	4:D:66:ARG:HD3	2.02	0.41
14:N:41:ARG:HA	14:N:44:LEU:HB2	2.02	0.41
16:P:39:TYR:CZ	16:P:41:PRO:HA	2.55	0.41
1:A:9:G:OP1	5:E:122:GLU:HG3	2.19	0.41
1:A:78:G:C5	1:A:79:G:N7	2.88	0.41
1:A:491:G:C4	1:A:492:G:C8	3.07	0.41
1:A:778:G:C5	1:A:779:C:C5	3.08	0.41
1:A:960:U:H4'	1:A:961:U:O5'	2.21	0.41
1:A:1198:G:H2'	1:A:1199:U:C5	2.56	0.41
1:A:1347:G:H2'	1:A:1373:G:O6	2.20	0.41
2:B:23:ARG:O	2:B:24:TRP:CD1	2.74	0.41
3:C:150:LYS:HG3	3:C:173:VAL:HG21	2.01	0.41
4:D:206:PHE:CE2	4:D:207:TYR:CE2	3.08	0.41
9:I:96:LEU:HA	9:I:99:LEU:HD12	2.01	0.41
16:P:50:LYS:HE2	16:P:50:LYS:HB2	1.81	0.41
16:P:51:VAL:HG12	16:P:52:ASP:C	2.40	0.41
17:Q:26:GLN:HG2	17:Q:37:LYS:HB2	2.01	0.41
18:R:20:ALA:HA	18:R:21:LYS:NZ	2.35	0.41
20:T:10:LEU:HD22	20:T:11:SER:N	2.32	0.41
1:A:881:G:P	12:L:12:ARG:HH22	2.43	0.41
1:A:1060:C:H4'	10:J:51:ARG:HB3	2.01	0.41
1:A:1061:G:C6	1:A:1197:G:C6	3.08	0.41
1:A:1354:C:H2'	1:A:1355:G:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1497:G:H2'	1:A:1498:UR3:H5'	2.01	0.41
2:B:172:ILE:H	2:B:172:ILE:HG13	1.46	0.41
3:C:26:LYS:HG2	10:J:45:ARG:HH22	1.85	0.41
4:D:117:ALA:O	4:D:121:VAL:HG23	2.21	0.41
4:D:199:ASN:ND2	4:D:202:LEU:HD23	2.36	0.41
4:D:205:GLU:CD	5:E:100:VAL:HG23	2.40	0.41
5:E:18:ARG:HE	5:E:18:ARG:HB3	1.45	0.41
12:L:37:CYS:SG	12:L:56:ALA:HB1	2.61	0.41
15:O:38:ARG:O	15:O:41:GLU:HB3	2.20	0.41
1:A:412:A:O2'	1:A:413:G:O4'	2.37	0.41
1:A:929:G:H2'	1:A:930:C:O4'	2.20	0.41
1:A:986:A:C6	1:A:1220:G:C6	3.09	0.41
1:A:1092:A:H5''	7:G:4:ARG:CZ	2.50	0.41
1:A:1098:C:H2'	1:A:1099:G:O4'	2.21	0.41
1:A:1277:C:H1'	1:A:1282:C:H1'	2.02	0.41
1:A:1346:A:C5'	9:I:120:ARG:HH12	2.30	0.41
1:A:1350:A:OP2	9:I:118:LYS:HD3	2.19	0.41
1:A:1516:G:N2	1:A:1519:MA6:OP2	2.47	0.41
2:B:22:LYS:HE2	2:B:22:LYS:HB2	1.90	0.41
2:B:40:HIS:HD1	2:B:190:THR:HG21	1.85	0.41
2:B:135:GLN:HE21	2:B:135:GLN:HB2	1.55	0.41
2:B:189:ASP:N	2:B:189:ASP:OD1	2.53	0.41
3:C:116:VAL:O	3:C:119:ARG:HB3	2.20	0.41
4:D:157:LEU:HD23	4:D:157:LEU:HA	1.81	0.41
5:E:71:LEU:HD11	5:E:113:ALA:O	2.20	0.41
5:E:75:THR:C	5:E:76:ILE:HD12	2.41	0.41
19:S:66:MET:H	19:S:66:MET:HG2	1.63	0.41
1:A:89:C:N3	1:A:90:U:C4	2.89	0.41
1:A:101:A:C2	1:A:102:G:C8	3.09	0.41
1:A:682:G:N2	1:A:708:C:O2	2.51	0.41
1:A:837:G:N2	1:A:850:U:C2	2.89	0.41
1:A:1133:G:N2	1:A:1141:C:C2	2.84	0.41
1:A:1306:A:C6	1:A:1332:A:C8	3.07	0.41
2:B:73:THR:HG22	2:B:73:THR:O	2.21	0.41
2:B:105:PHE:HD1	2:B:105:PHE:HA	1.71	0.41
5:E:11:ILE:HG23	5:E:11:ILE:HD12	1.67	0.41
7:G:30:ILE:HA	7:G:30:ILE:HD13	1.74	0.41
7:G:94:ARG:HA	7:G:97:GLN:HB2	2.02	0.41
10:J:48:THR:HB	10:J:62:HIS:CD2	2.55	0.41
11:K:15:ALA:HA	11:K:77:MET:HA	2.02	0.41
16:P:32:TYR:CD1	16:P:32:TYR:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:73:HIS:HB3	20:T:74:LYS:H	1.56	0.41
1:A:146:G:N2	1:A:147:G:C4	2.88	0.41
1:A:284:G:H2'	1:A:285:G:H8	1.84	0.41
1:A:544:G:C6	1:A:545:C:C4	3.08	0.41
1:A:1277:C:O2'	1:A:1279:A:H1'	2.20	0.41
1:A:1314:C:H2'	1:A:1315:U:C6	2.56	0.41
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.36	0.41
1:A:1372:U:H2'	1:A:1373:G:H5'	2.02	0.41
2:B:220:ASP:HA	2:B:230:VAL:HG21	2.02	0.41
3:C:59:ARG:O	10:J:92:THR:HG23	2.21	0.41
4:D:58:LEU:HA	4:D:58:LEU:HD22	1.74	0.41
4:D:174:LEU:HA	4:D:184:LYS:O	2.20	0.41
9:I:49:PRO:O	9:I:53:VAL:HB	2.21	0.41
10:J:10:GLY:HA3	10:J:16:LEU:HD11	2.02	0.41
10:J:32:ALA:O	10:J:34:VAL:HG23	2.20	0.41
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.21	0.41
18:R:37:VAL:O	18:R:40:LEU:N	2.54	0.41
1:A:79:G:H2'	1:A:80:G:C8	2.55	0.41
1:A:389:A:C5	1:A:390:C:H1'	2.56	0.41
1:A:969:A:H8	1:A:969:A:H5'	1.85	0.41
1:A:986:A:H4'	19:S:55:LYS:NZ	2.36	0.41
1:A:1061:G:H5''	1:A:1062:U:OP2	2.21	0.41
1:A:1109:C:H2'	1:A:1110:A:O4'	2.21	0.41
1:A:1254:C:H2'	1:A:1255:G:H8	1.86	0.41
1:A:1360:A:H8	1:A:1361:G:O4'	2.04	0.41
1:A:1473:A:H2'	1:A:1474:G:O4'	2.21	0.41
2:B:208:ILE:HG12	2:B:211:ILE:HD11	2.03	0.41
3:C:24:ALA:HB1	3:C:28:GLN:HB2	2.03	0.41
4:D:64:LEU:HD22	4:D:64:LEU:HA	1.83	0.41
5:E:9:LYS:NZ	5:E:108:ALA:HA	2.36	0.41
7:G:140:ASP:HA	7:G:143:ARG:CD	2.50	0.41
9:I:89:ASN:O	9:I:92:TYR:HB2	2.21	0.41
9:I:111:ARG:NH1	9:I:113:LYS:HA	2.36	0.41
11:K:92:GLU:HG3	11:K:96:ARG:HH11	1.85	0.41
16:P:58:TYR:CD1	16:P:59:TRP:N	2.88	0.41
20:T:53:LEU:HA	20:T:56:MET:HE2	2.03	0.41
1:A:81:U:C6	1:A:81:U:H3'	2.55	0.41
1:A:144:G:H2'	1:A:145:G:O4'	2.21	0.41
1:A:413:G:H2'	1:A:428:G:N2	2.36	0.41
1:A:426:G:OP1	4:D:38:TYR:OH	2.28	0.41
1:A:1004:A:H1'	1:A:1038:C:H42	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:U:H5'	3:C:163:ALA:HB2	2.02	0.41
3:C:174:PRO:HB2	3:C:177:THR:HG22	2.03	0.41
3:C:195:VAL:O	3:C:196:LEU:HD23	2.21	0.41
4:D:151:LYS:H	4:D:151:LYS:HD2	1.84	0.41
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.69	0.41
11:K:20:TYR:CD1	11:K:83:ILE:HB	2.55	0.41
13:M:108:ARG:HD3	13:M:114:ARG:HH21	1.85	0.41
16:P:78:GLY:HA2	16:P:80:PHE:H	1.86	0.41
1:A:35:G:C4	1:A:550:G:N2	2.88	0.41
1:A:140:A:H2'	1:A:141:A:O4'	2.21	0.41
1:A:363:A:OP2	12:L:61:THR:HG21	2.21	0.41
1:A:363:A:OP2	12:L:34:ARG:HG2	2.20	0.41
1:A:371:G:C2'	1:A:372:C:H5'	2.51	0.41
1:A:669:U:H2'	1:A:670:G:H8	1.86	0.41
1:A:922:G:H5''	1:A:922:G:H8	1.86	0.41
1:A:963:G:N2	1:A:973:G:C5	2.89	0.41
1:A:974:A:P	14:N:41:ARG:HH12	2.44	0.41
1:A:998:G:H1	1:A:1043:C:H42	1.69	0.41
1:A:1060:C:H2'	1:A:1061:G:H8	1.86	0.41
1:A:1091:U:O2	1:A:1093:A:H8	2.03	0.41
1:A:1196:U:OP1	1:A:1197:G:H5'	2.20	0.41
1:A:1287:A:H2'	1:A:1288:A:C8	2.56	0.41
1:A:1351:U:H3	1:A:1371:G:H1	1.67	0.41
1:A:1356:G:H2'	1:A:1357:A:C8	2.56	0.41
1:A:1393:U:HO2'	1:A:1501:C:HO2'	1.69	0.41
1:A:1417:G:O5'	1:A:1417:G:H8	2.04	0.41
1:A:1507:A:H2'	1:A:1508:G:O4'	2.21	0.41
2:B:25:ASN:HD21	2:B:27:LYS:HG3	1.86	0.41
2:B:130:ARG:HD2	2:B:134:GLU:OE2	2.21	0.41
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.73	0.41
3:C:43:LEU:HD13	3:C:47:LEU:CD1	2.51	0.41
3:C:151:VAL:HG12	3:C:152:ILE:N	2.35	0.41
4:D:72:GLU:O	4:D:72:GLU:HG3	2.21	0.41
8:H:95:VAL:O	8:H:131:GLY:N	2.43	0.41
9:I:49:PRO:HD3	9:I:101:PHE:CE2	2.56	0.41
16:P:1:MET:HE3	16:P:1:MET:HB3	1.91	0.41
1:A:114:U:H1'	1:A:353:A:H1'	2.02	0.41
1:A:297:G:N2	1:A:300:A:OP2	2.53	0.41
1:A:406:G:H21	4:D:119:GLN:NE2	2.18	0.41
1:A:830:G:N2	1:A:857:C:C2	2.89	0.41
1:A:837:G:N2	1:A:850:U:O2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:G:H5''	7:G:102:ARG:NH1	2.36	0.41
1:A:946:A:H2'	1:A:947:G:H8	1.85	0.41
1:A:954:G:C6	1:A:955:U:C4	3.09	0.41
1:A:1075:C:H5''	2:B:179:LYS:NZ	2.36	0.41
1:A:1347:G:N2	1:A:1373:G:H2'	2.36	0.41
1:A:1399:C:H4'	1:A:1400:5MC:H5''	2.02	0.41
5:E:131:ILE:HA	5:E:131:ILE:HD13	1.55	0.41
8:H:83:ILE:HG21	8:H:83:ILE:HD13	1.74	0.41
12:L:7:ILE:HD13	12:L:7:ILE:HA	1.40	0.41
14:N:25:VAL:HG12	14:N:38:GLY:O	2.21	0.41
15:O:43:LEU:HD11	15:O:53:HIS:HA	2.02	0.41
16:P:34:GLU:OE2	16:P:55:ARG:HD2	2.21	0.41
17:Q:4:LYS:O	17:Q:60:ILE:HD13	2.22	0.41
17:Q:31:LEU:HD12	17:Q:31:LEU:HA	1.75	0.41
20:T:14:LYS:HA	20:T:17:ARG:NH2	2.36	0.41
20:T:20:LEU:O	20:T:23:ARG:HB3	2.20	0.41
1:A:597:G:C4	1:A:644:G:C2	3.09	0.40
1:A:720:C:H5''	18:R:52:PRO:HA	2.03	0.40
1:A:925:G:C2	1:A:927:G:C8	3.09	0.40
1:A:1425:U:H2'	1:A:1426:C:C6	2.56	0.40
3:C:22:TRP:HH2	3:C:33:LEU:HD21	1.84	0.40
3:C:52:LEU:O	3:C:115:LEU:HD21	2.21	0.40
6:F:4:TYR:CD1	6:F:92:LYS:HA	2.56	0.40
7:G:64:GLN:HA	7:G:67:GLU:HB3	2.03	0.40
10:J:7:LYS:HD3	10:J:9:ARG:HE	1.86	0.40
10:J:49:VAL:HG23	14:N:34:TYR:OH	2.21	0.40
18:R:79:LEU:CD2	18:R:80:PRO:HD2	2.51	0.40
1:A:246:A:O3'	1:A:247:G:H4'	2.21	0.40
1:A:285:G:C4	1:A:286:G:C8	3.09	0.40
1:A:373:A:H1'	1:A:481:G:H1'	2.02	0.40
1:A:775:G:H2'	1:A:776:G:H5'	2.03	0.40
1:A:1090:U:O2'	1:A:1091:U:H5'	2.20	0.40
1:A:1214:C:H3'	1:A:1215:G:H8	1.86	0.40
1:A:1447:G:N3	1:A:1447:G:H2'	2.36	0.40
2:B:144:ARG:HG3	2:B:145:LEU:N	2.36	0.40
4:D:111:ALA:HA	4:D:161:ASN:HD22	1.85	0.40
7:G:70:LYS:NZ	7:G:97:GLN:HA	2.36	0.40
9:I:15:ALA:CA	9:I:65:VAL:HG12	2.51	0.40
11:K:82:VAL:HB	11:K:108:ILE:CD1	2.51	0.40
1:A:820:U:H4'	1:A:821:G:OP2	2.20	0.40
1:A:899:C:H2'	1:A:900:A:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:A:O5'	1:A:919:A:H8	2.04	0.40
1:A:1000:U:H2'	1:A:1001:A:C8	2.56	0.40
1:A:1053:G:O2'	1:A:1199:U:H5	2.04	0.40
1:A:1125:U:P	1:A:1145:C:H41	2.42	0.40
2:B:117:GLU:O	2:B:120:ALA:HB3	2.21	0.40
3:C:20:SER:HB3	3:C:22:TRP:NE1	2.37	0.40
4:D:164:ALA:O	4:D:168:ARG:HD2	2.21	0.40
6:F:39:LYS:NZ	6:F:39:LYS:HB2	2.37	0.40
8:H:39:LEU:HB3	8:H:45:ILE:HG12	2.04	0.40
13:M:40:ASN:HB3	13:M:43:THR:HG23	2.03	0.40
20:T:36:LEU:HA	20:T:36:LEU:HD23	1.68	0.40
1:A:79:G:C2	1:A:80:G:C5	3.10	0.40
1:A:474:G:N2	1:A:475:G:C5	2.90	0.40
1:A:580:U:H2'	1:A:581:G:O4'	2.21	0.40
1:A:633:G:H2'	1:A:634:C:H6	1.86	0.40
1:A:778:G:C6	1:A:779:C:C4	3.10	0.40
1:A:1005:A:N6	1:A:1024:G:O2'	2.55	0.40
1:A:1181:G:C4	1:A:1182:G:N1	2.90	0.40
1:A:1311:G:N2	1:A:1327:C:C2	2.89	0.40
1:A:1311:G:N3	1:A:1311:G:H2'	2.36	0.40
1:A:1519:MA6:H8	1:A:1519:MA6:O5'	2.20	0.40
3:C:34:LEU:HG	14:N:25:VAL:HG11	2.03	0.40
3:C:58:GLU:H	3:C:65:ALA:HB3	1.86	0.40
5:E:61:TYR:HD2	5:E:61:TYR:HA	1.77	0.40
7:G:21:VAL:H	7:G:21:VAL:HG22	1.57	0.40
7:G:75:VAL:HG13	7:G:87:VAL:C	2.41	0.40
9:I:104:ARG:NH1	9:I:105:ASP:O	2.54	0.40
10:J:16:LEU:HB3	10:J:70:ARG:HE	1.85	0.40
13:M:34:LEU:HA	13:M:34:LEU:HD23	1.58	0.40
17:Q:6:LEU:HD13	17:Q:23:VAL:HG11	2.02	0.40
17:Q:29:HIS:CE1	17:Q:32:TYR:H	2.40	0.40
1:A:75:G:O2'	1:A:76:C:H5'	2.21	0.40
1:A:136:C:H1'	16:P:1:MET:HG3	2.03	0.40
1:A:260:G:C6	1:A:261:U:C4	3.10	0.40
1:A:945:G:H2'	1:A:945:G:N3	2.36	0.40
1:A:1047:G:C2'	1:A:1048:G:H5'	2.51	0.40
1:A:1126:U:H2'	1:A:1127:G:H5'	2.03	0.40
1:A:1179:A:OP2	9:I:93:ARG:NH1	2.54	0.40
1:A:1290:G:O2'	1:A:1291:G:H5'	2.21	0.40
1:A:1478:C:O2	1:A:1478:C:H2'	2.22	0.40
3:C:93:LYS:O	3:C:94:LEU:HD13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:203:VAL:O	4:D:206:PHE:HB3	2.21	0.40
18:R:62:GLU:O	18:R:65:ILE:N	2.55	0.40
19:S:74:PHE:CD1	19:S:74:PHE:N	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	200 (86%)	30 (13%)	2 (1%)	14	48
3	C	204/239 (85%)	179 (88%)	25 (12%)	0	100	100
4	D	206/209 (99%)	186 (90%)	20 (10%)	0	100	100
5	E	148/162 (91%)	136 (92%)	11 (7%)	1 (1%)	19	54
6	F	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	13	46
7	G	153/156 (98%)	136 (89%)	16 (10%)	1 (1%)	19	54
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16	51
10	J	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	13	46
11	K	114/129 (88%)	103 (90%)	11 (10%)	0	100	100
12	L	121/135 (90%)	107 (88%)	12 (10%)	2 (2%)	7	36
13	M	116/126 (92%)	103 (89%)	12 (10%)	1 (1%)	14	48
14	N	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
15	O	85/89 (96%)	80 (94%)	4 (5%)	1 (1%)	11	43
16	P	81/88 (92%)	75 (93%)	5 (6%)	1 (1%)	11	43
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	R	68/88 (77%)	59 (87%)	9 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	78/93 (84%)	67 (86%)	10 (13%)	1 (1%)	10	41
20	T	97/106 (92%)	85 (88%)	11 (11%)	1 (1%)	13	46
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2336/2541 (92%)	2089 (89%)	233 (10%)	14 (1%)	22	57

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
12	L	28	LYS
2	B	21	ARG
2	B	24	TRP
9	I	119	ALA
20	T	99	LEU
5	E	129	ILE
16	P	53	VAL
7	G	80	VAL
6	F	68	PRO
10	J	34	VAL
13	M	84	ILE
12	L	25	PRO
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%)	158 (78%)	44 (22%)	1	5
3	C	160/188 (85%)	129 (81%)	31 (19%)	1	7
4	D	180/181 (99%)	136 (76%)	44 (24%)	0	4
5	E	115/123 (94%)	83 (72%)	32 (28%)	0	2
6	F	90/90 (100%)	70 (78%)	20 (22%)	1	5
7	G	126/127 (99%)	96 (76%)	30 (24%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	119/119 (100%)	91 (76%)	28 (24%)	0	4
9	I	98/99 (99%)	76 (78%)	22 (22%)	1	5
10	J	87/92 (95%)	71 (82%)	16 (18%)	1	9
11	K	88/99 (89%)	71 (81%)	17 (19%)	1	7
12	L	103/110 (94%)	75 (73%)	28 (27%)	0	3
13	M	94/101 (93%)	74 (79%)	20 (21%)	1	5
14	N	49/50 (98%)	39 (80%)	10 (20%)	1	6
15	O	79/80 (99%)	56 (71%)	23 (29%)	0	2
16	P	72/74 (97%)	57 (79%)	15 (21%)	1	5
17	Q	94/97 (97%)	71 (76%)	23 (24%)	0	3
18	R	61/77 (79%)	47 (77%)	14 (23%)	0	4
19	S	71/80 (89%)	51 (72%)	20 (28%)	0	2
20	T	76/82 (93%)	55 (72%)	21 (28%)	0	2
21	U	19/22 (86%)	16 (84%)	3 (16%)	2	13
All	All	1983/2111 (94%)	1522 (77%)	461 (23%)	0	4

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	10	LEU
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	25	ASN
2	B	33	TYR
2	B	39	ILE
2	B	45	GLN
2	B	48	MET
2	B	53	ARG
2	B	61	LEU
2	B	67	THR
2	B	69	LEU
2	B	79	ASP

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Mol	Chain	Res	Type
2	B	87	ARG
2	B	97	TRP
2	B	102	LEU
2	B	107	THR
2	B	112	VAL
2	B	121	LEU
2	B	122	PHE
2	B	126	GLU
2	B	127	ILE
2	B	128	GLU
2	B	135	GLN
2	B	139	LYS
2	B	142	LEU
2	B	144	ARG
2	B	157	ARG
2	B	158	LEU
2	B	160	ASP
2	B	169	LYS
2	B	172	ILE
2	B	178	ARG
2	B	190	THR
2	B	196	LEU
2	B	208	ILE
2	B	212	GLN
2	B	221	LEU
2	B	238	LEU
3	C	3	ASN
3	C	11	ARG
3	C	29	TYR
3	C	30	ARG
3	C	31	HIS
3	C	33	LEU
3	C	34	LEU
3	C	43	LEU
3	C	45	LYS
3	C	48	TYR
3	C	64	VAL
3	C	69	HIS
3	C	79	ARG
3	C	95	THR
3	C	110	ASN
3	C	130	VAL

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Mol	Chain	Res	Type
3	C	131	ARG
3	C	138	VAL
3	C	147	LYS
3	C	156	ARG
3	C	165	THR
3	C	166	GLU
3	C	172	ARG
3	C	175	LEU
3	C	177	THR
3	C	178	LEU
3	C	179	ARG
3	C	183	ASP
3	C	198	VAL
3	C	204	LEU
3	C	206	GLU
4	D	10	ARG
4	D	13	ARG
4	D	14	ARG
4	D	15	GLU
4	D	19	LEU
4	D	21	LEU
4	D	25	ARG
4	D	26	CYS
4	D	36	ARG
4	D	39	PRO
4	D	47	ARG
4	D	50	ARG
4	D	52	SER
4	D	57	ARG
4	D	61	LYS
4	D	64	LEU
4	D	67	ILE
4	D	70	ILE
4	D	71	SER
4	D	78	LEU
4	D	80	GLU
4	D	84	LYS
4	D	120	LEU
4	D	122	ARG
4	D	127	THR
4	D	129	ASN
4	D	135	LEU

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Mol	Chain	Res	Type
4	D	137	SER
4	D	141	ARG
4	D	145	GLU
4	D	151	LYS
4	D	158	ILE
4	D	176	LEU
4	D	178	VAL
4	D	179	GLU
4	D	185	PHE
4	D	186	LEU
4	D	187	ARG
4	D	188	LEU
4	D	194	LEU
4	D	198	VAL
4	D	202	LEU
4	D	203	VAL
4	D	209	ARG
5	E	5	ASP
5	E	12	LEU
5	E	14	ARG
5	E	15	ARG
5	E	18	ARG
5	E	19	MET
5	E	24	ARG
5	E	32	VAL
5	E	34	VAL
5	E	53	LEU
5	E	55	VAL
5	E	60	TYR
5	E	61	TYR
5	E	67	VAL
5	E	69	VAL
5	E	75	THR
5	E	78	HIS
5	E	79	GLU
5	E	80	ILE
5	E	81	GLU
5	E	87	SER
5	E	100	VAL
5	E	107	ARG
5	E	112	LEU
5	E	118	ILE

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Mol	Chain	Res	Type
5	E	125	SER
5	E	131	ILE
5	E	136	MET
5	E	137	GLU
5	E	141	GLN
5	E	144	THR
5	E	147	ASP
6	F	15	ASP
6	F	19	LEU
6	F	24	GLU
6	F	28	ARG
6	F	30	LEU
6	F	39	LYS
6	F	43	LEU
6	F	45	LEU
6	F	46	ARG
6	F	47	ARG
6	F	65	VAL
6	F	73	ASN
6	F	74	ASP
6	F	75	LEU
6	F	77	ARG
6	F	82	ARG
6	F	87	ARG
6	F	88	VAL
6	F	94	GLN
6	F	98	LEU
7	G	3	ARG
7	G	8	GLU
7	G	22	LEU
7	G	30	ILE
7	G	31	MET
7	G	33	ASP
7	G	38	LEU
7	G	45	ASP
7	G	48	LYS
7	G	50	ILE
7	G	52	GLU
7	G	53	LYS
7	G	56	GLN
7	G	57	GLU
7	G	59	LEU

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Mol	Chain	Res	Type
7	G	77	SER
7	G	80	VAL
7	G	85	TYR
7	G	91	VAL
7	G	92	SER
7	G	94	ARG
7	G	97	GLN
7	G	98	SER
7	G	99	LEU
7	G	109	ASN
7	G	110	GLN
7	G	113	GLU
7	G	124	LEU
7	G	126	ASP
7	G	146	GLU
8	H	6	ILE
8	H	11	THR
8	H	12	ARG
8	H	14	ARG
8	H	22	GLU
8	H	23	SER
8	H	29	SER
8	H	39	LEU
8	H	51	VAL
8	H	63	LEU
8	H	65	TYR
8	H	81	HIS
8	H	82	HIS
8	H	83	ILE
8	H	84	ARG
8	H	85	ARG
8	H	91	ARG
8	H	97	VAL
8	H	102	ARG
8	H	104	ARG
8	H	105	ARG
8	H	112	LEU
8	H	113	SER
8	H	118	VAL
8	H	120	THR
8	H	123	GLU
8	H	127	LEU

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Mol	Chain	Res	Type
8	H	136	GLU
9	I	3	GLN
9	I	14	VAL
9	I	16	ARG
9	I	29	ASN
9	I	35	GLU
9	I	38	GLN
9	I	48	GLU
9	I	53	VAL
9	I	58	HIS
9	I	70	LYS
9	I	79	LEU
9	I	83	ARG
9	I	87	GLN
9	I	91	ASP
9	I	92	TYR
9	I	104	ARG
9	I	109	VAL
9	I	111	ARG
9	I	113	LYS
9	I	114	TYR
9	I	118	LYS
9	I	121	ARG
10	J	5	ARG
10	J	43	ARG
10	J	47	PHE
10	J	48	THR
10	J	49	VAL
10	J	54	PHE
10	J	57	LYS
10	J	63	PHE
10	J	64	GLU
10	J	68	HIS
10	J	71	LEU
10	J	74	ILE
10	J	83	GLU
10	J	85	LEU
10	J	88	LEU
10	J	96	ILE
11	K	11	LYS
11	K	13	GLN
11	K	18	ARG

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Mol	Chain	Res	Type
11	K	29	ILE
11	K	33	THR
11	K	47	VAL
11	K	59	TYR
11	K	75	TYR
11	K	81	ASP
11	K	91	ARG
11	K	95	ILE
11	K	98	LEU
11	K	101	SER
11	K	109	VAL
11	K	116	HIS
11	K	119	CYS
11	K	126	ARG
12	L	7	ILE
12	L	11	VAL
12	L	27	LEU
12	L	33	ARG
12	L	34	ARG
12	L	39	VAL
12	L	41	ARG
12	L	42	THR
12	L	43	VAL
12	L	44	THR
12	L	53	ARG
12	L	55	VAL
12	L	60	LEU
12	L	61	THR
12	L	64	TYR
12	L	65	GLU
12	L	66	VAL
12	L	67	THR
12	L	76	ASN
12	L	80	HIS
12	L	96	VAL
12	L	97	ARG
12	L	99	HIS
12	L	101	VAL
12	L	104	VAL
12	L	120	TYR
12	L	122	THR
12	L	127	GLU

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Mol	Chain	Res	Type
13	M	3	ARG
13	M	9	ILE
13	M	19	LEU
13	M	35	GLU
13	M	39	ILE
13	M	49	THR
13	M	53	VAL
13	M	54	VAL
13	M	56	LEU
13	M	57	ARG
13	M	63	THR
13	M	66	LEU
13	M	73	GLU
13	M	77	ASN
13	M	80	ARG
13	M	93	ARG
13	M	101	GLN
13	M	102	ARG
13	M	110	ARG
13	M	115	LYS
14	N	18	VAL
14	N	21	TYR
14	N	22	THR
14	N	25	VAL
14	N	27	CYS
14	N	31	ARG
14	N	41	ARG
14	N	44	LEU
14	N	47	LEU
14	N	58	LYS
15	O	4	THR
15	O	5	LYS
15	O	9	GLN
15	O	26	GLU
15	O	27	VAL
15	O	32	LEU
15	O	33	THR
15	O	38	ARG
15	O	42	HIS
15	O	44	LYS
15	O	45	VAL
15	O	47	LYS

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Mol	Chain	Res	Type
15	O	56	LEU
15	O	64	ARG
15	O	67	LEU
15	O	68	ARG
15	O	70	LEU
15	O	71	GLN
15	O	73	GLU
15	O	78	TYR
15	O	81	LEU
15	O	87	ILE
15	O	88	ARG
16	P	1	MET
16	P	5	ARG
16	P	6	LEU
16	P	18	ARG
16	P	27	LYS
16	P	33	ILE
16	P	45	THR
16	P	50	LYS
16	P	53	VAL
16	P	55	ARG
16	P	61	SER
16	P	62	VAL
16	P	68	ASP
16	P	69	THR
16	P	79	VAL
17	Q	12	SER
17	Q	15	MET
17	Q	19	VAL
17	Q	21	VAL
17	Q	34	LYS
17	Q	35	VAL
17	Q	36	ILE
17	Q	45	HIS
17	Q	53	LEU
17	Q	58	GLU
17	Q	59	ILE
17	Q	60	ILE
17	Q	63	ARG
17	Q	72	ARG
17	Q	74	LEU
17	Q	75	ARG

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Mol	Chain	Res	Type
17	Q	77	VAL
17	Q	84	LEU
17	Q	86	GLU
17	Q	89	LEU
17	Q	92	ARG
17	Q	94	ASN
17	Q	98	LEU
18	R	21	LYS
18	R	28	GLU
18	R	31	LEU
18	R	35	ARG
18	R	37	VAL
18	R	40	LEU
18	R	42	ARG
18	R	46	GLU
18	R	47	THR
18	R	56	THR
18	R	58	LEU
18	R	82	THR
18	R	86	VAL
18	R	88	LYS
19	S	3	ARG
19	S	6	LYS
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	17	GLU
19	S	20	LEU
19	S	23	ASN
19	S	28	LYS
19	S	29	ARG
19	S	41	VAL
19	S	43	GLU
19	S	55	LYS
19	S	58	VAL
19	S	62	ILE
19	S	63	THR
19	S	64	GLU
19	S	66	MET
19	S	77	THR
19	S	81	ARG
20	T	10	LEU

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Mol	Chain	Res	Type
20	T	13	LEU
20	T	19	SER
20	T	20	LEU
20	T	24	LEU
20	T	34	LYS
20	T	36	LEU
20	T	38	LYS
20	T	42	GLN
20	T	43	LEU
20	T	46	GLU
20	T	53	LEU
20	T	64	ASP
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	79	ARG
20	T	85	MET
20	T	86	ARG
20	T	90	GLN
20	T	91	LEU
21	U	8	THR
21	U	12	LYS
21	U	13	ILE

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

Mol	Chain	Res	Type
2	B	25	ASN
3	C	6	HIS
4	D	119	GLN
6	F	73	ASN
6	F	100	ASN
7	G	110	GLN
9	I	73	GLN
15	O	46	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	390 (25%)	45 (2%)

All (390) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	19	C
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	41	G
1	A	45	U
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	58	C
1	A	66	G
1	A	68	G
1	A	69	G
1	A	76	C
1	A	81	U
1	A	89	C
1	A	91	C
1	A	92	C
1	A	97	G
1	A	99	C
1	A	106	C
1	A	107	G
1	A	108	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	141	A
1	A	145	G
1	A	157	G
1	A	163	C
1	A	175	C
1	A	178	C
1	A	182	U

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Mol	Chain	Res	Type
1	A	183	G
1	A	190(D)	U
1	A	190(E)	U
1	A	190(G)	G
1	A	195	A
1	A	197	A
1	A	199	G
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	217	C
1	A	220	G
1	A	231	G
1	A	243	A
1	A	244	U
1	A	246	A
1	A	247	G
1	A	251	G
1	A	252	U
1	A	254	G
1	A	257	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	299	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	324	G
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A

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Mol	Chain	Res	Type
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	384	G
1	A	388	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	405	U
1	A	406	G
1	A	412	A
1	A	413	G
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	455	C
1	A	460	A
1	A	461	C
1	A	475	G
1	A	476	G
1	A	478	A
1	A	481	G
1	A	482	A
1	A	485	G
1	A	486	U
1	A	487	A
1	A	497	A
1	A	498	U
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	513	C
1	A	518	C

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Mol	Chain	Res	Type
1	A	519	C
1	A	524	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	541	G
1	A	547	A
1	A	558	G
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	597	G
1	A	598	U
1	A	607	A
1	A	615	C
1	A	618	C
1	A	624	C
1	A	630	G
1	A	631	G
1	A	652	U
1	A	653	A
1	A	656	C
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	694	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	718	G
1	A	722	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	749	C
1	A	755	G
1	A	759	A
1	A	760	G
1	A	773	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	784	C
1	A	787	A
1	A	788	U
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	818	G
1	A	821	G
1	A	826	C
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	855	G
1	A	858	G
1	A	869	G
1	A	872	A
1	A	873	A
1	A	876	G
1	A	889	A
1	A	902	G
1	A	910	C
1	A	914	A
1	A	919	A

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Mol	Chain	Res	Type
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	941	G
1	A	944	G
1	A	950	U
1	A	954	G
1	A	957	U
1	A	960	U
1	A	961	U
1	A	964	A
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	973	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	980	C
1	A	985	C
1	A	989	C
1	A	990	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1003	G
1	A	1003(A)	G
1	A	1005	A
1	A	1006	C
1	A	1007	C
1	A	1008	C
1	A	1020	U
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1030(B)	C
1	A	1032	G
1	A	1038	C

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Mol	Chain	Res	Type
1	A	1045	C
1	A	1047	G
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1059	C
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1079	G
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1104	G
1	A	1115	C
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1144	G
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1161	C
1	A	1171	G
1	A	1174	G
1	A	1176	A
1	A	1177	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1196	U

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Mol	Chain	Res	Type
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1207	2MG
1	A	1209	C
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1243	C
1	A	1245	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1261	A
1	A	1263	C
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1297	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1311	G
1	A	1312	G
1	A	1320	C

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Mol	Chain	Res	Type
1	A	1322	C
1	A	1323	G
1	A	1326	C
1	A	1327	C
1	A	1334	G
1	A	1336	C
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1351	U
1	A	1353	G
1	A	1359	C
1	A	1360	A
1	A	1362	C
1	A	1364	U
1	A	1370	G
1	A	1371	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1393	U
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1414	U
1	A	1441	G
1	A	1442	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1453	G
1	A	1454	G
1	A	1469	G
1	A	1487	G
1	A	1490	C
1	A	1493	A
1	A	1495	U
1	A	1496	C
1	A	1497	G
1	A	1498	UR3
1	A	1499	A

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Mol	Chain	Res	Type
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1515	C
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
1	A	1533	C

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	65	U
1	A	115	G
1	A	129(A)	G
1	A	173	U
1	A	181	G
1	A	243	A
1	A	250	A
1	A	251	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	509	A
1	A	518	C
1	A	559	A
1	A	597	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	975	A

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Mol	Chain	Res	Type
1	A	992	U
1	A	1004	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1183	A
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1301	U
1	A	1333	A
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

15 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	PSU	A	1540	1	18,21,22	1.41	1 (5%)	21,30,33	1.64	4 (19%)
1	5MC	A	1404	1	19,22,23	1.54	4 (21%)	26,32,35	1.45	5 (19%)
1	5MC	A	967	1	19,22,23	1.09	2 (10%)	26,32,35	0.90	1 (3%)
1	MA6	A	1519	1	19,26,27	2.25	5 (26%)	18,38,41	0.94	0
1	2MG	A	1207	1	18,26,27	1.70	4 (22%)	16,38,41	1.31	2 (12%)
1	PSU	A	1541	1	18,21,22	1.27	1 (5%)	21,30,33	1.91	4 (19%)
1	7MG	A	527	1	23,26,27	3.80	7 (30%)	27,39,42	2.62	9 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1407	1	19,22,23	2.27	5 (26%)	26,32,35	1.29	4 (15%)
1	UR3	A	1498	1	19,22,23	1.18	1 (5%)	26,32,35	1.14	1 (3%)
1	4OC	A	1402	1	20,23,24	1.25	1 (5%)	25,32,35	0.72	0
12	0TD	L	92	12	8,9,10	1.02	0	6,11,13	3.36	3 (50%)
1	MA6	A	1518	1	19,26,27	1.70	3 (15%)	18,38,41	1.41	2 (11%)
1	5MC	A	1400	1	19,22,23	1.56	4 (21%)	26,32,35	1.09	4 (15%)
1	PSU	A	516	1	18,21,22	1.39	3 (16%)	21,30,33	1.39	4 (19%)
1	M2G	A	966	1	20,27,28	1.40	4 (20%)	19,40,43	1.34	2 (10%)

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	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	5/7/29/30	0/3/3/3
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
1	PSU	A	1541	1	-	2/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
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	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
12	0TD	L	92	12	-	4/7/12/14	-
1	MA6	A	1518	1	-	5/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-16.09	1.35	1.45
1	A	1407	5MC	C5-C4	6.98	1.49	1.44
1	A	1519	MA6	C6-N1	6.11	1.40	1.32
1	A	527	7MG	C5-N7	5.84	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1540	PSU	C6-C5	5.05	1.40	1.35
1	A	1541	PSU	C6-C5	4.68	1.40	1.35
1	A	1519	MA6	C2-N1	4.36	1.41	1.33
1	A	516	PSU	C6-C5	4.35	1.40	1.35
1	A	1407	5MC	C2-N1	4.22	1.48	1.40
1	A	1518	MA6	C6-N1	4.06	1.38	1.32
1	A	1518	MA6	C4-N3	4.04	1.41	1.35
1	A	1519	MA6	C6-N6	4.00	1.46	1.37
1	A	1400	5MC	C2-N1	3.93	1.48	1.40
1	A	1402	4OC	C2-N3	3.88	1.44	1.36
1	A	1207	2MG	C6-N1	3.83	1.43	1.37
1	A	1518	MA6	C9-N6	3.76	1.54	1.45
1	A	1404	5MC	C5-C4	3.74	1.46	1.44
1	A	966	M2G	C5-C6	-3.66	1.40	1.47
1	A	1404	5MC	C1'-N1	-3.55	1.37	1.47
1	A	1207	2MG	C5-C6	-3.39	1.40	1.47
1	A	1498	UR3	C4-N3	-3.36	1.33	1.40
1	A	1207	2MG	C2-N2	3.32	1.40	1.33
1	A	1407	5MC	C2-N3	3.30	1.42	1.36
1	A	1207	2MG	C2-N1	3.19	1.41	1.36
1	A	1404	5MC	C6-N1	-2.91	1.33	1.38
1	A	1400	5MC	C1'-N1	2.83	1.55	1.47
1	A	1400	5MC	C6-C5	2.83	1.39	1.34
1	A	1400	5MC	C2-N3	2.78	1.41	1.36
1	A	1519	MA6	C9-N6	2.76	1.51	1.45
1	A	527	7MG	C2-N1	-2.68	1.31	1.37
1	A	966	M2G	C2-N2	2.62	1.39	1.35
1	A	527	7MG	C2-N2	2.51	1.40	1.34
1	A	1519	MA6	C4-N3	2.48	1.39	1.35
1	A	527	7MG	O6-C6	-2.44	1.18	1.23
1	A	967	5MC	C4-N4	2.42	1.40	1.34
1	A	527	7MG	C4-N3	2.38	1.39	1.34
1	A	967	5MC	C2-N3	2.34	1.41	1.36
1	A	1407	5MC	C1'-N1	2.32	1.54	1.47
1	A	1407	5MC	C4-N4	2.14	1.39	1.34
1	A	966	M2G	O6-C6	-2.13	1.18	1.23
1	A	516	PSU	O4'-C1'	-2.04	1.41	1.43
1	A	1404	5MC	C2-N3	2.04	1.40	1.36
1	A	516	PSU	C2-N1	2.03	1.39	1.36
1	A	966	M2G	C6-N1	2.01	1.40	1.37
1	A	527	7MG	C8-N7	-2.00	1.32	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	6.42	122.24	110.94
12	L	92	0TD	CSB-SB-CB	-6.04	91.51	102.36
1	A	527	7MG	N9-C4-N3	5.74	133.87	125.46
1	A	1541	PSU	N1-C2-N3	5.03	120.48	115.17
1	A	1518	MA6	C1'-N9-C4	-4.96	117.92	126.64
1	A	527	7MG	C5-C4-N3	-4.51	119.67	128.13
1	A	966	M2G	O6-C6-N1	-4.39	115.41	120.62
1	A	527	7MG	N9-C8-N7	4.31	109.47	103.37
1	A	527	7MG	C2-N3-C4	4.19	119.52	112.30
1	A	527	7MG	C2-N1-C6	-3.91	118.02	125.11
1	A	1541	PSU	C4-N3-C2	-3.85	121.07	126.37
1	A	1540	PSU	N1-C2-N3	3.82	119.20	115.17
1	A	1540	PSU	C4-N3-C2	-3.80	121.14	126.37
12	L	92	0TD	CB-CA-N	-3.63	101.75	109.10
1	A	1541	PSU	O2-C2-N1	-3.58	119.10	122.79
1	A	527	7MG	O6-C6-C5	-3.58	118.84	127.62
1	A	1541	PSU	C6-N1-C2	-3.55	119.39	122.69
1	A	1404	5MC	N4-C4-N3	-3.53	112.12	118.51
1	A	527	7MG	C6-C5-C4	-3.38	116.45	122.40
1	A	516	PSU	C4-N3-C2	-3.38	121.72	126.37
1	A	1207	2MG	O6-C6-N1	-3.37	116.62	120.62
1	A	1498	UR3	C6-N1-C2	-3.34	119.07	121.80
12	L	92	0TD	OD1-CG-CB	-3.22	115.69	122.44
1	A	966	M2G	O6-C6-C5	3.05	130.37	124.32
1	A	1207	2MG	O6-C6-C5	2.99	130.24	124.32
1	A	1540	PSU	C6-N1-C2	-2.91	119.99	122.69
1	A	1404	5MC	C5-C4-N3	2.91	124.73	121.75
1	A	1404	5MC	C5-C6-N1	-2.83	120.24	123.31
1	A	1404	5MC	C4-N3-C2	-2.81	116.90	120.81
1	A	527	7MG	C6-C5-N7	2.63	136.01	131.93
1	A	1407	5MC	N4-C4-N3	-2.52	113.94	118.51
1	A	1407	5MC	C4-N3-C2	-2.51	117.32	120.81
1	A	1540	PSU	O4'-C1'-C2'	2.37	108.43	105.15
1	A	516	PSU	N1-C2-N3	2.33	117.63	115.17
1	A	1404	5MC	C6-N1-C2	2.32	124.05	120.95
1	A	1400	5MC	O2-C2-N3	-2.32	118.67	122.33
1	A	1407	5MC	O2-C2-N3	-2.31	118.68	122.33
1	A	516	PSU	O4'-C1'-C2'	2.26	108.28	105.15
1	A	516	PSU	O2-C2-N1	-2.23	120.49	122.79
1	A	1400	5MC	N4-C4-N3	-2.19	114.55	118.51
1	A	1400	5MC	C6-N1-C2	-2.17	118.06	120.95
1	A	1407	5MC	CM5-C5-C6	-2.16	119.93	122.85
1	A	967	5MC	N4-C4-N3	-2.13	114.65	118.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1518	MA6	N1-C6-N6	-2.12	114.38	116.83
1	A	1400	5MC	C5-C4-N3	2.07	123.88	121.75

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C9
1	A	1541	PSU	C2'-C1'-C5-C4
1	A	1541	PSU	C2'-C1'-C5-C6
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	1518	MA6	N1-C6-N6-C9
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9
1	A	1518	MA6	C5-C6-N6-C10
1	A	1519	MA6	C5-C6-N6-C9
12	L	92	0TD	SB-CB-CG-OD1
1	A	527	7MG	O4'-C4'-C5'-O5'
12	L	92	0TD	CA-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD2
1	A	1540	PSU	O4'-C1'-C5-C6
1	A	967	5MC	C2'-C1'-N1-C6
12	L	92	0TD	CG-CB-SB-CSB
1	A	1519	MA6	N1-C6-N6-C10
1	A	967	5MC	C2'-C1'-N1-C2

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1540	PSU	1	0
1	A	1404	5MC	3	0
1	A	967	5MC	1	0
1	A	1519	MA6	4	0
1	A	1207	2MG	1	0
1	A	1541	PSU	1	0
1	A	527	7MG	1	0
1	A	1498	UR3	3	0
12	L	92	0TD	2	0
1	A	1518	MA6	2	0
1	A	1400	5MC	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 250 ligands modelled in this entry, 249 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	SRY	A	1601	-	40,42,42	2.42	13 (32%)	49,63,63	2.32	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	SRY	A	1601	-	-	5/20/87/87	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	9.49	1.49	1.33
22	A	1601	SRY	CA1-N11	6.03	1.43	1.33
22	A	1601	SRY	C11-N11	-3.42	1.40	1.45
22	A	1601	SRY	O53-C53	-3.38	1.36	1.44
22	A	1601	SRY	CA1-NB1	3.10	1.45	1.34
22	A	1601	SRY	C21-C11	-2.91	1.47	1.53
22	A	1601	SRY	C23-N23	-2.87	1.42	1.47
22	A	1601	SRY	CD1-NE1	2.82	1.44	1.34
22	A	1601	SRY	C32-CG2	-2.42	1.48	1.52
22	A	1601	SRY	C21-C31	-2.27	1.48	1.53
22	A	1601	SRY	O51-C51	-2.25	1.37	1.43
22	A	1601	SRY	O32-C32	-2.21	1.40	1.44
22	A	1601	SRY	O43-C43	-2.11	1.37	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	C13-O13-C22	-6.04	105.98	116.26
22	A	1601	SRY	C61-C11-N11	-6.02	99.52	110.62
22	A	1601	SRY	C12-O42-C42	-5.83	99.07	108.48
22	A	1601	SRY	O41-C12-O42	-4.52	106.75	111.37
22	A	1601	SRY	CI3-N23-C23	-4.51	108.41	114.23
22	A	1601	SRY	C43-C33-C23	-4.20	104.28	110.40
22	A	1601	SRY	O13-C13-C23	3.93	114.44	108.07
22	A	1601	SRY	C12-O41-C41	-3.18	110.45	117.98
22	A	1601	SRY	C21-C31-N31	3.07	116.27	110.62
22	A	1601	SRY	O13-C13-O53	-2.28	104.69	110.69
22	A	1601	SRY	C61-C51-C41	2.02	114.27	109.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

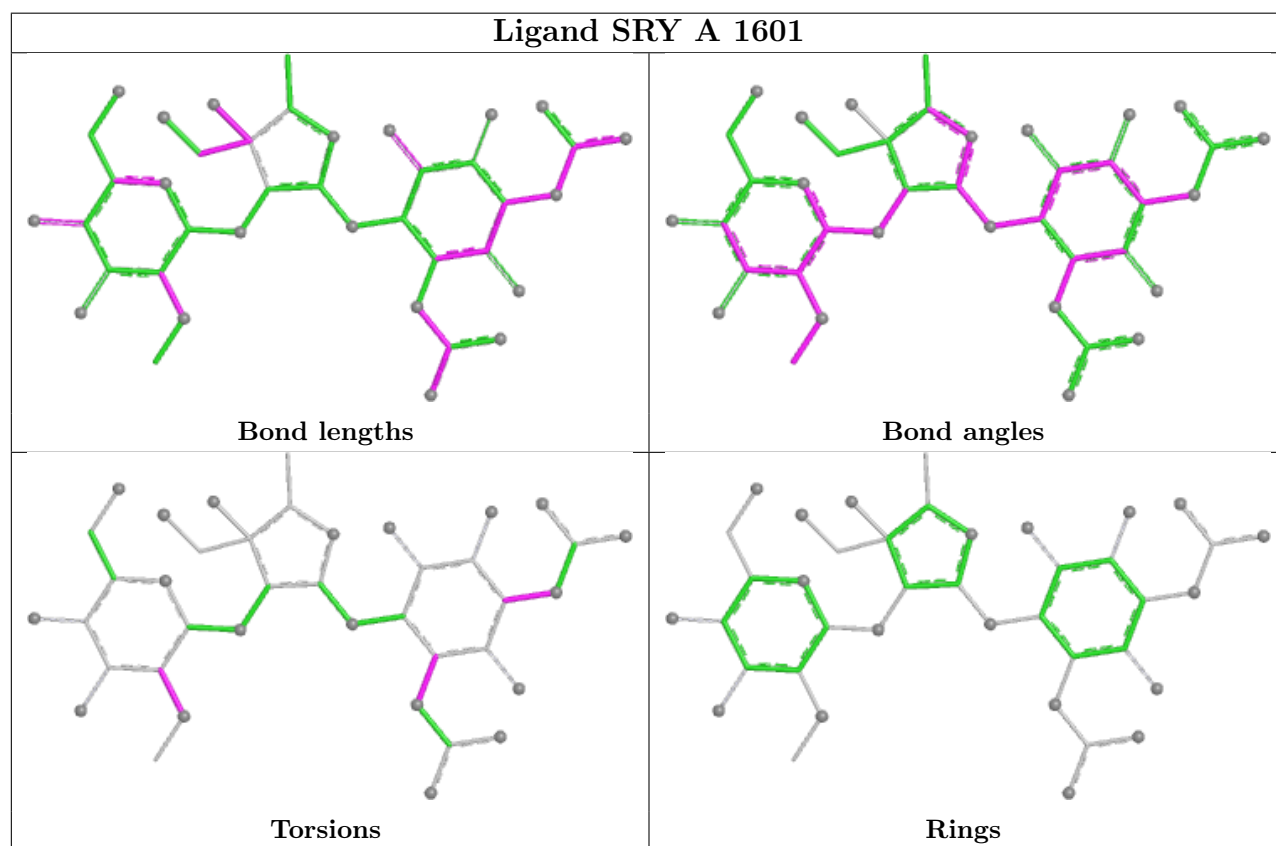
Mol	Chain	Res	Type	Atoms
22	A	1601	SRY	C13-C23-N23-CI3
22	A	1601	SRY	C41-C31-N31-CD1
22	A	1601	SRY	C21-C31-N31-CD1
22	A	1601	SRY	C21-C11-N11-CA1
22	A	1601	SRY	C61-C11-N11-CA1

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	7	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.19	22 (1%) 71 55	106, 179, 327, 407	0
2	B	234/256 (91%)	-0.32	6 (2%) 57 44	145, 211, 332, 358	0
3	C	206/239 (86%)	-0.07	7 (3%) 48 39	181, 265, 316, 365	0
4	D	208/209 (99%)	0.04	9 (4%) 40 34	124, 193, 249, 283	0
5	E	150/162 (92%)	-0.47	0 100 100	104, 150, 199, 232	0
6	F	101/101 (100%)	-0.43	0 100 100	155, 212, 246, 277	0
7	G	155/156 (99%)	-0.19	2 (1%) 74 58	172, 228, 288, 335	0
8	H	138/138 (100%)	-0.42	1 (0%) 84 71	94, 135, 187, 218	0
9	I	127/128 (99%)	-0.07	5 (3%) 44 36	201, 250, 303, 322	0
10	J	98/105 (93%)	0.28	6 (6%) 28 25	220, 277, 355, 391	0
11	K	116/129 (89%)	-0.33	2 (1%) 69 52	130, 171, 224, 258	0
12	L	123/135 (91%)	0.02	4 (3%) 49 39	107, 175, 218, 248	0
13	M	118/126 (93%)	0.10	8 (6%) 25 23	162, 214, 254, 309	0
14	N	60/61 (98%)	-0.01	2 (3%) 49 39	187, 249, 314, 329	0
15	O	87/89 (97%)	-0.09	1 (1%) 77 63	113, 171, 213, 232	0
16	P	83/88 (94%)	-0.12	3 (3%) 46 38	130, 180, 220, 274	0
17	Q	99/105 (94%)	-0.10	3 (3%) 52 41	116, 150, 201, 232	0
18	R	70/88 (79%)	-0.26	0 100 100	116, 183, 244, 259	0
19	S	80/93 (86%)	0.36	7 (8%) 17 17	234, 284, 341, 352	0
20	T	99/106 (93%)	-0.24	2 (2%) 64 49	124, 172, 240, 267	0
21	U	24/27 (88%)	0.35	1 (4%) 41 34	198, 248, 286, 302	0
All	All	3874/4063 (95%)	-0.16	91 (2%) 61 46	94, 194, 306, 407	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	4	TYR	5.5
20	T	106	ALA	5.2
7	G	154	TYR	5.0
3	C	2	GLY	4.7
1	A	532	A	4.5
10	J	37	PRO	4.4
12	L	47	LYS	4.4
1	A	984	C	4.4
1	A	353	A	4.1
13	M	8	GLU	4.1
1	A	1361(A)	C	4.0
2	B	208	ILE	4.0
4	D	6	GLY	4.0
21	U	25	LYS	3.9
1	A	1129	C	3.8
19	S	68	GLY	3.7
13	M	94	ARG	3.6
10	J	34	VAL	3.6
1	A	81	U	3.5
1	A	760	G	3.5
1	A	1042	G	3.5
3	C	76	VAL	3.5
9	I	102	LEU	3.5
1	A	202	U	3.3
1	A	792	A	3.2
4	D	5	ILE	3.2
8	H	1	MET	3.2
1	A	723	U	3.1
1	A	805	C	3.1
19	S	2	PRO	3.1
12	L	32	PHE	3.1
2	B	19	HIS	3.1
2	B	14	GLY	3.0
1	A	793	U	3.0
10	J	100	THR	3.0
19	S	32	LYS	2.9
9	I	99	LEU	2.9
2	B	239	VAL	2.9
13	M	102	ARG	2.9
1	A	985	C	2.8
13	M	6	GLY	2.8
2	B	238	LEU	2.8
10	J	38	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	209	ARG	2.7
4	D	31	CYS	2.7
4	D	7	PRO	2.7
2	B	169	LYS	2.7
4	D	54	TYR	2.6
10	J	54	PHE	2.6
13	M	96	LEU	2.6
3	C	100	ALA	2.6
20	T	56	MET	2.6
4	D	42	GLN	2.6
9	I	110	GLU	2.6
17	Q	32	TYR	2.6
16	P	59	TRP	2.6
14	N	4	LYS	2.6
7	G	74	GLU	2.5
10	J	24	VAL	2.5
3	C	66	VAL	2.5
9	I	96	LEU	2.5
19	S	79	THR	2.5
14	N	55	GLY	2.5
19	S	35	SER	2.5
1	A	1482	G	2.4
4	D	9	CYS	2.4
3	C	178	LEU	2.4
11	K	102	GLY	2.4
1	A	1178	G	2.4
1	A	1362	C	2.3
13	M	22	ILE	2.3
12	L	48	PRO	2.3
19	S	37	ARG	2.3
1	A	1124	G	2.2
16	P	25	ARG	2.2
19	S	78	ARG	2.2
13	M	113	PRO	2.2
15	O	54	ARG	2.2
17	Q	19	VAL	2.1
11	K	118	GLY	2.1
13	M	91	ARG	2.1
1	A	82	U	2.1
12	L	94	PRO	2.1
9	I	126	SER	2.1
3	C	175	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	201	TYR	2.1
16	P	23	ASP	2.0
17	Q	45	HIS	2.0
1	A	60	A	2.0
1	A	190(B)	C	2.0
1	A	1200	C	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1541	20/21	0.73	0.18	297,305,321,325	0
1	PSU	A	1540	20/21	0.75	0.21	235,263,334,335	0
1	MA6	A	1518	24/25	0.92	0.10	151,187,221,227	0
1	M2G	A	966	25/26	0.93	0.11	177,182,207,211	0
1	PSU	A	516	20/21	0.93	0.10	163,188,214,220	0
1	7MG	A	527	24/25	0.94	0.13	125,146,165,180	0
1	MA6	A	1519	24/25	0.96	0.13	144,181,202,206	0
1	5MC	A	1407	21/22	0.96	0.09	171,191,202,207	0
1	5MC	A	1400	21/22	0.96	0.11	142,169,178,182	0
12	0TD	L	92	10/11	0.96	0.10	121,166,173,350	0
1	UR3	A	1498	21/22	0.97	0.09	160,183,204,223	0
1	4OC	A	1402	22/23	0.97	0.11	150,156,180,192	0
1	2MG	A	1207	24/25	0.97	0.15	231,289,310,316	0
1	5MC	A	1404	21/22	0.98	0.08	166,182,196,204	0
1	5MC	A	967	21/22	0.98	0.07	182,192,200,205	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
23	MG	A	1681	1/1	0.36	0.20	243,243,243,243	0
23	MG	A	1831	1/1	0.40	0.18	484,484,484,484	0
23	MG	K	201	1/1	0.44	0.23	181,181,181,181	0
23	MG	S	102	1/1	0.52	0.33	156,156,156,156	0
23	MG	B	301	1/1	0.60	0.27	181,181,181,181	0
23	MG	N	103	1/1	0.60	0.25	156,156,156,156	0
23	MG	E	201	1/1	0.60	0.14	435,435,435,435	0
23	MG	A	1757	1/1	0.62	1.04	143,143,143,143	0
23	MG	A	1659	1/1	0.64	0.32	142,142,142,142	0
23	MG	P	101	1/1	0.67	0.44	122,122,122,122	0
23	MG	A	1778	1/1	0.71	0.33	156,156,156,156	0
23	MG	A	1712	1/1	0.72	0.55	138,138,138,138	0
23	MG	A	1788	1/1	0.72	0.27	156,156,156,156	0
23	MG	A	1773	1/1	0.72	0.32	162,162,162,162	0
23	MG	A	1817	1/1	0.73	0.10	197,197,197,197	0
23	MG	A	1763	1/1	0.74	0.37	181,181,181,181	0
23	MG	A	1696	1/1	0.74	0.12	245,245,245,245	0
23	MG	A	1710	1/1	0.74	0.23	161,161,161,161	0
23	MG	A	1693	1/1	0.78	0.35	179,179,179,179	0
23	MG	A	1730	1/1	0.79	0.70	134,134,134,134	0
23	MG	A	1695	1/1	0.80	0.63	245,245,245,245	0
23	MG	A	1714	1/1	0.80	0.22	143,143,143,143	0
23	MG	A	1736	1/1	0.81	0.53	125,125,125,125	0
23	MG	H	201	1/1	0.81	0.21	131,131,131,131	0
23	MG	A	1751	1/1	0.81	0.43	133,133,133,133	0
23	MG	A	1692	1/1	0.81	0.62	142,142,142,142	0
23	MG	A	1728	1/1	0.81	0.16	150,150,150,150	0
23	MG	A	1668	1/1	0.81	0.49	173,173,173,173	0
23	MG	A	1784	1/1	0.82	0.32	145,145,145,145	0
23	MG	A	1819	1/1	0.82	0.22	483,483,483,483	0
23	MG	A	1765	1/1	0.83	0.16	372,372,372,372	0
23	MG	A	1782	1/1	0.83	0.34	131,131,131,131	0
23	MG	A	1787	1/1	0.84	0.40	102,102,102,102	0
23	MG	M	202	1/1	0.84	0.31	148,148,148,148	0
23	MG	A	1739	1/1	0.84	0.27	162,162,162,162	0
23	MG	A	1770	1/1	0.84	0.41	141,141,141,141	0
23	MG	A	1718	1/1	0.84	0.64	144,144,144,144	0
23	MG	A	1783	1/1	0.85	0.32	133,133,133,133	0
23	MG	A	1755	1/1	0.85	0.54	190,190,190,190	0
23	MG	A	1727	1/1	0.85	0.27	138,138,138,138	0
23	MG	A	1744	1/1	0.85	0.17	176,176,176,176	0
23	MG	A	1623	1/1	0.85	0.32	170,170,170,170	0
23	MG	A	1771	1/1	0.86	0.43	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1785	1/1	0.86	0.55	142,142,142,142	0
23	MG	A	1758	1/1	0.86	0.52	128,128,128,128	0
23	MG	A	1774	1/1	0.86	0.37	128,128,128,128	0
23	MG	A	1802	1/1	0.86	0.14	457,457,457,457	0
23	MG	A	1738	1/1	0.86	0.45	123,123,123,123	0
23	MG	A	1636	1/1	0.86	0.29	186,186,186,186	0
23	MG	A	1706	1/1	0.86	0.41	163,163,163,163	0
23	MG	A	1704	1/1	0.87	0.20	118,118,118,118	0
23	MG	A	1746	1/1	0.87	0.21	282,282,282,282	0
23	MG	A	1720	1/1	0.87	0.34	139,139,139,139	0
23	MG	M	201	1/1	0.87	0.43	163,163,163,163	0
23	MG	A	1750	1/1	0.88	0.18	125,125,125,125	0
23	MG	A	1822	1/1	0.88	0.25	374,374,374,374	0
23	MG	A	1795	1/1	0.88	0.38	457,457,457,457	0
23	MG	A	1672	1/1	0.89	0.26	102,102,102,102	0
23	MG	A	1661	1/1	0.89	0.49	124,124,124,124	0
23	MG	A	1626	1/1	0.89	0.57	118,118,118,118	0
23	MG	A	1772	1/1	0.89	0.14	121,121,121,121	0
23	MG	A	1667	1/1	0.90	0.47	143,143,143,143	0
23	MG	D	302	1/1	0.90	0.15	186,186,186,186	0
23	MG	A	1777	1/1	0.90	0.25	107,107,107,107	0
23	MG	A	1768	1/1	0.90	0.06	550,550,550,550	0
23	MG	A	1781	1/1	0.90	0.21	145,145,145,145	0
23	MG	A	1813	1/1	0.90	0.58	146,146,146,146	0
23	MG	A	1643	1/1	0.90	0.27	135,135,135,135	0
23	MG	A	1618	1/1	0.90	0.22	152,152,152,152	0
23	MG	A	1679	1/1	0.90	0.64	133,133,133,133	0
23	MG	A	1637	1/1	0.90	0.39	143,143,143,143	0
23	MG	A	1747	1/1	0.91	0.15	296,296,296,296	0
23	MG	A	1725	1/1	0.91	0.21	153,153,153,153	0
23	MG	A	1737	1/1	0.91	0.24	140,140,140,140	0
23	MG	A	1794	1/1	0.91	0.23	206,206,206,206	0
23	MG	A	1658	1/1	0.91	0.13	146,146,146,146	0
23	MG	I	201	1/1	0.91	0.16	204,204,204,204	0
23	MG	A	1656	1/1	0.92	0.27	173,173,173,173	0
23	MG	A	1682	1/1	0.92	0.08	365,365,365,365	0
23	MG	A	1754	1/1	0.92	0.07	177,177,177,177	0
23	MG	A	1697	1/1	0.92	0.29	135,135,135,135	0
23	MG	A	1701	1/1	0.92	0.22	129,129,129,129	0
23	MG	A	1721	1/1	0.92	0.20	135,135,135,135	0
23	MG	A	1760	1/1	0.92	0.06	130,130,130,130	0
23	MG	A	1779	1/1	0.92	0.52	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1677	1/1	0.92	0.24	191,191,191,191	0
23	MG	A	1818	1/1	0.92	0.42	483,483,483,483	0
23	MG	A	1638	1/1	0.92	0.18	170,170,170,170	0
23	MG	A	1694	1/1	0.92	0.22	180,180,180,180	0
23	MG	A	1769	1/1	0.93	0.15	209,209,209,209	0
23	MG	A	1732	1/1	0.93	0.53	131,131,131,131	0
23	MG	A	1715	1/1	0.93	0.33	151,151,151,151	0
23	MG	A	1759	1/1	0.93	0.16	161,161,161,161	0
23	MG	A	1651	1/1	0.93	0.49	140,140,140,140	0
23	MG	A	1647	1/1	0.93	0.23	180,180,180,180	0
23	MG	A	1820	1/1	0.93	0.13	265,265,265,265	0
23	MG	A	1776	1/1	0.93	0.26	111,111,111,111	0
23	MG	A	1700	1/1	0.93	0.12	134,134,134,134	0
23	MG	A	1731	1/1	0.93	0.42	148,148,148,148	0
23	MG	A	1713	1/1	0.94	0.10	133,133,133,133	0
23	MG	A	1829	1/1	0.94	0.09	323,323,323,323	0
23	MG	A	1752	1/1	0.94	0.32	147,147,147,147	0
23	MG	A	1699	1/1	0.94	0.11	135,135,135,135	0
23	MG	A	1735	1/1	0.94	0.22	155,155,155,155	0
23	MG	A	1676	1/1	0.94	0.32	133,133,133,133	0
23	MG	A	1654	1/1	0.94	0.30	201,201,201,201	0
23	MG	A	1702	1/1	0.94	0.09	126,126,126,126	0
23	MG	A	1811	1/1	0.94	0.16	346,346,346,346	0
23	MG	A	1621	1/1	0.94	0.17	166,166,166,166	0
23	MG	A	1648	1/1	0.94	0.14	230,230,230,230	0
23	MG	A	1707	1/1	0.94	0.56	120,120,120,120	0
23	MG	A	1633	1/1	0.94	0.22	125,125,125,125	0
23	MG	A	1683	1/1	0.94	0.11	422,422,422,422	0
23	MG	A	1660	1/1	0.95	0.06	194,194,194,194	0
23	MG	A	1745	1/1	0.95	0.44	235,235,235,235	0
23	MG	A	1723	1/1	0.95	0.25	109,109,109,109	0
23	MG	A	1734	1/1	0.95	0.29	163,163,163,163	0
23	MG	A	1809	1/1	0.95	0.22	281,281,281,281	0
23	MG	A	1724	1/1	0.95	0.34	176,176,176,176	0
23	MG	A	1670	1/1	0.95	0.28	173,173,173,173	0
23	MG	A	1645	1/1	0.95	0.09	146,146,146,146	0
23	MG	A	1673	1/1	0.95	0.12	118,118,118,118	0
22	SRY	A	1601	40/40	0.95	0.09	123,154,201,206	0
23	MG	A	1756	1/1	0.95	0.10	213,213,213,213	0
23	MG	A	1741	1/1	0.95	0.15	145,145,145,145	0
23	MG	A	1827	1/1	0.95	0.13	391,391,391,391	0
23	MG	T	201	1/1	0.95	0.09	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1786	1/1	0.96	0.76	145,145,145,145	0
23	MG	A	1663	1/1	0.96	0.15	138,138,138,138	0
23	MG	A	1825	1/1	0.96	0.12	377,377,377,377	0
23	MG	A	1616	1/1	0.96	0.22	107,107,107,107	0
23	MG	A	1789	1/1	0.96	0.11	152,152,152,152	0
23	MG	A	1790	1/1	0.96	0.16	148,148,148,148	0
23	MG	A	1619	1/1	0.96	0.19	253,253,253,253	0
23	MG	A	1617	1/1	0.96	0.08	129,129,129,129	0
23	MG	A	1764	1/1	0.96	0.14	308,308,308,308	0
23	MG	A	1803	1/1	0.96	0.14	342,342,342,342	0
23	MG	A	1807	1/1	0.96	0.15	427,427,427,427	0
23	MG	A	1639	1/1	0.96	0.23	126,126,126,126	0
23	MG	A	1686	1/1	0.96	0.11	150,150,150,150	0
23	MG	A	1641	1/1	0.96	0.05	134,134,134,134	0
23	MG	A	1816	1/1	0.96	0.04	262,262,262,262	0
23	MG	A	1652	1/1	0.96	0.09	141,141,141,141	0
23	MG	A	1742	1/1	0.96	0.05	134,134,134,134	0
23	MG	A	1703	1/1	0.96	0.10	180,180,180,180	0
23	MG	A	1666	1/1	0.97	0.39	187,187,187,187	0
23	MG	A	1603	1/1	0.97	0.10	128,128,128,128	0
23	MG	A	1740	1/1	0.97	0.27	123,123,123,123	0
23	MG	A	1622	1/1	0.97	0.06	138,138,138,138	0
23	MG	A	1716	1/1	0.97	0.10	121,121,121,121	0
23	MG	A	1653	1/1	0.97	0.11	185,185,185,185	0
23	MG	A	1604	1/1	0.97	0.19	133,133,133,133	0
23	MG	A	1775	1/1	0.97	0.09	123,123,123,123	0
23	MG	A	1624	1/1	0.97	0.16	210,210,210,210	0
23	MG	A	1675	1/1	0.97	0.18	121,121,121,121	0
23	MG	A	1749	1/1	0.97	0.35	126,126,126,126	0
23	MG	A	1657	1/1	0.97	0.22	177,177,177,177	0
23	MG	A	1780	1/1	0.97	0.11	111,111,111,111	0
23	MG	A	1608	1/1	0.97	0.15	118,118,118,118	0
23	MG	A	1726	1/1	0.97	0.32	130,130,130,130	0
23	MG	A	1628	1/1	0.97	0.28	191,191,191,191	0
23	MG	A	1632	1/1	0.97	0.07	91,91,91,91	0
23	MG	A	1610	1/1	0.97	0.23	193,193,193,193	0
23	MG	A	1705	1/1	0.97	0.24	153,153,153,153	0
23	MG	A	1635	1/1	0.97	0.13	214,214,214,214	0
23	MG	H	202	1/1	0.97	0.04	137,137,137,137	0
23	MG	A	1733	1/1	0.97	0.07	126,126,126,126	0
23	MG	A	1684	1/1	0.97	0.15	124,124,124,124	0
23	MG	A	1709	1/1	0.97	0.13	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1791	1/1	0.97	0.05	144,144,144,144	0
23	MG	N	102	1/1	0.97	0.16	214,214,214,214	0
23	MG	A	1793	1/1	0.97	0.06	302,302,302,302	0
23	MG	A	1665	1/1	0.97	0.12	247,247,247,247	0
23	MG	S	101	1/1	0.97	0.11	138,138,138,138	0
23	MG	A	1691	1/1	0.97	0.10	187,187,187,187	0
23	MG	A	1800	1/1	0.97	0.34	400,400,400,400	0
23	MG	A	1640	1/1	0.98	0.17	129,129,129,129	0
23	MG	A	1743	1/1	0.98	0.17	183,183,183,183	0
23	MG	A	1805	1/1	0.98	0.25	426,426,426,426	0
23	MG	A	1806	1/1	0.98	0.19	392,392,392,392	0
23	MG	A	1606	1/1	0.98	0.40	126,126,126,126	0
23	MG	A	1808	1/1	0.98	0.15	444,444,444,444	0
23	MG	A	1722	1/1	0.98	0.09	116,116,116,116	0
23	MG	A	1810	1/1	0.98	0.05	117,117,117,117	0
23	MG	A	1629	1/1	0.98	0.06	125,125,125,125	0
23	MG	A	1812	1/1	0.98	0.06	226,226,226,226	0
23	MG	A	1631	1/1	0.98	0.33	127,127,127,127	0
23	MG	A	1814	1/1	0.98	0.20	128,128,128,128	0
23	MG	A	1815	1/1	0.98	0.15	190,190,190,190	0
23	MG	A	1611	1/1	0.98	0.07	223,223,223,223	0
23	MG	A	1662	1/1	0.98	0.13	162,162,162,162	0
23	MG	A	1620	1/1	0.98	0.42	197,197,197,197	0
23	MG	A	1664	1/1	0.98	0.22	226,226,226,226	0
23	MG	A	1753	1/1	0.98	0.13	118,118,118,118	0
23	MG	A	1685	1/1	0.98	0.09	263,263,263,263	0
23	MG	A	1823	1/1	0.98	0.08	194,194,194,194	0
23	MG	A	1708	1/1	0.98	0.14	119,119,119,119	0
23	MG	A	1650	1/1	0.98	0.13	155,155,155,155	0
23	MG	A	1613	1/1	0.98	0.11	126,126,126,126	0
23	MG	A	1830	1/1	0.98	0.13	494,494,494,494	0
23	MG	A	1711	1/1	0.98	0.14	187,187,187,187	0
23	MG	A	1614	1/1	0.98	0.08	94,94,94,94	0
23	MG	A	1615	1/1	0.98	0.08	129,129,129,129	0
23	MG	A	1761	1/1	0.98	0.20	158,158,158,158	0
23	MG	A	1762	1/1	0.98	0.10	109,109,109,109	0
23	MG	A	1669	1/1	0.98	0.27	138,138,138,138	0
23	MG	A	1607	1/1	0.98	0.10	161,161,161,161	0
23	MG	J	201	1/1	0.98	0.14	138,138,138,138	0
23	MG	A	1655	1/1	0.98	0.29	181,181,181,181	0
23	MG	A	1766	1/1	0.98	0.04	220,220,220,220	0
23	MG	A	1717	1/1	0.98	0.09	110,110,110,110	0

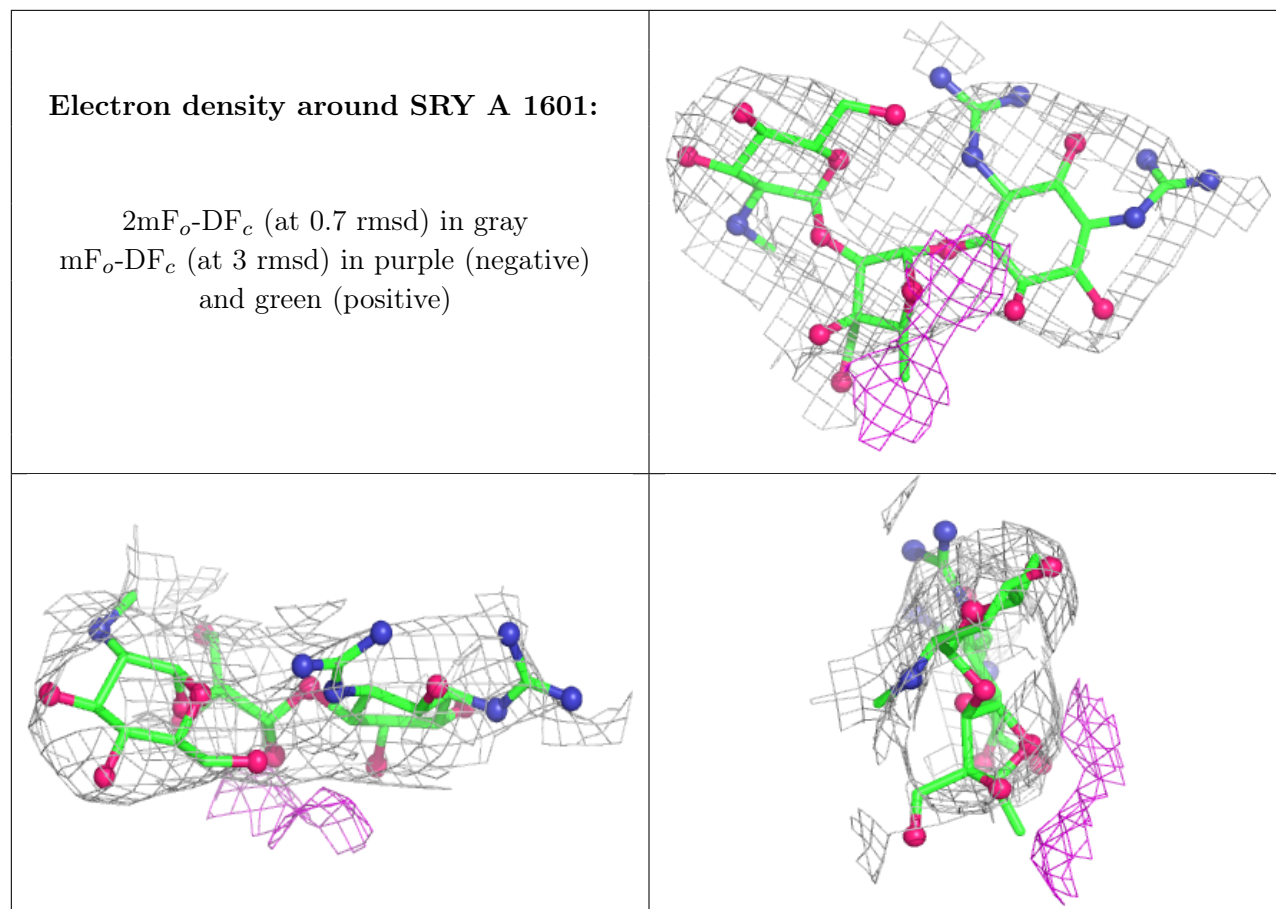
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1796	1/1	0.98	0.23	372,372,372,372	0
23	MG	A	1797	1/1	0.98	0.15	429,429,429,429	0
23	MG	A	1798	1/1	0.98	0.11	454,454,454,454	0
23	MG	A	1799	1/1	0.98	0.12	242,242,242,242	0
23	MG	A	1605	1/1	0.98	0.10	148,148,148,148	0
23	MG	A	1801	1/1	0.98	0.29	423,423,423,423	0
23	MG	T	202	1/1	0.98	0.13	450,450,450,450	0
23	MG	A	1821	1/1	0.99	0.09	236,236,236,236	0
23	MG	A	1687	1/1	0.99	0.04	96,96,96,96	0
23	MG	A	1729	1/1	0.99	0.34	123,123,123,123	0
23	MG	A	1824	1/1	0.99	0.10	366,366,366,366	0
23	MG	A	1688	1/1	0.99	0.20	301,301,301,301	0
23	MG	A	1826	1/1	0.99	0.16	458,458,458,458	0
23	MG	A	1689	1/1	0.99	0.12	151,151,151,151	0
23	MG	A	1828	1/1	0.99	0.19	356,356,356,356	0
23	MG	A	1690	1/1	0.99	0.10	216,216,216,216	0
23	MG	A	1649	1/1	0.99	0.05	192,192,192,192	0
23	MG	A	1602	1/1	0.99	0.20	180,180,180,180	0
23	MG	A	1804	1/1	0.99	0.14	420,420,420,420	0
23	MG	A	1674	1/1	0.99	0.14	112,112,112,112	0
23	MG	A	1627	1/1	0.99	0.12	160,160,160,160	0
23	MG	A	1634	1/1	0.99	0.02	112,112,112,112	0
23	MG	A	1642	1/1	0.99	0.11	107,107,107,107	0
23	MG	A	1678	1/1	0.99	0.07	136,136,136,136	0
23	MG	A	1698	1/1	0.99	0.11	131,131,131,131	0
23	MG	A	1609	1/1	0.99	0.13	155,155,155,155	0
23	MG	A	1680	1/1	0.99	0.11	306,306,306,306	0
23	MG	A	1644	1/1	0.99	0.11	175,175,175,175	0
23	MG	A	1612	1/1	0.99	0.07	123,123,123,123	0
23	MG	A	1767	1/1	0.99	0.09	327,327,327,327	0
23	MG	A	1646	1/1	0.99	0.05	131,131,131,131	0
23	MG	A	1630	1/1	0.99	0.11	92,92,92,92	0
23	MG	A	1625	1/1	0.99	0.11	134,134,134,134	0
23	MG	A	1748	1/1	0.99	0.18	204,204,204,204	0
23	MG	A	1671	1/1	0.99	0.16	208,208,208,208	0
24	ZN	D	301	1/1	0.99	0.20	159,159,159,159	0
24	ZN	N	101	1/1	0.99	0.08	336,336,336,336	0
23	MG	A	1719	1/1	1.00	0.17	105,105,105,105	0
23	MG	A	1792	1/1	1.00	0.08	127,127,127,127	0

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

orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.