



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:36 PM GMT

PDB ID : 3I20  
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting  
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.  
Deposited on : 2009-06-28  
Resolution : 3.71 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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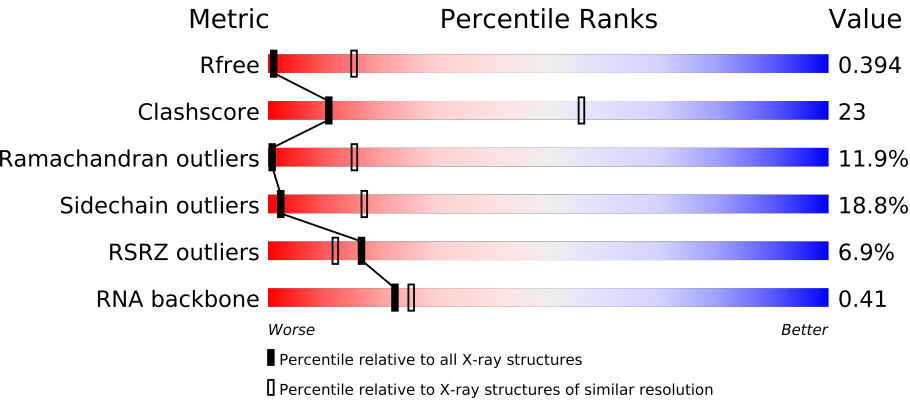
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.71 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 <sub>free</sub>	66092	1103 (4.04-3.40)
Clashscore	79885	1026 (3.98-3.46)
Ramachandran outliers	78287	1082 (4.00-3.44)
Sidechain outliers	78261	1075 (4.00-3.44)
RSRZ outliers	66119	1104 (4.04-3.40)
RNA backbone	1838	1008 (4.52-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	118	
3	C	273	
4	D	209	
5	E	201	
6	F	179	
7	G	177	
8	H	149	
9	I	142	
10	J	142	
11	K	123	
12	L	144	

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Mol	Chain	Length	Quality of chain
13	M	136	
14	N	127	
15	O	117	
16	P	115	
17	Q	118	
18	R	103	
19	S	110	
20	T	100	
21	U	104	
22	V	94	
23	W	85	
24	X	78	
25	Y	63	
26	Z	59	
27	0	57	
28	1	55	
29	2	46	
30	3	65	
31	4	38	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	A	2909	-	X
32	MG	A	2912	-	X
32	MG	A	2914	-	X
32	MG	A	2918	-	X
32	MG	A	2923	-	X
32	MG	A	2924	-	X
32	MG	A	2929	-	X
32	MG	A	2933	-	X
32	MG	A	2934	-	X
32	MG	A	2937	-	X
32	MG	A	2938	-	X
32	MG	A	2961	-	X
32	MG	A	2964	-	X
32	MG	A	2971	-	X
32	MG	A	2974	-	X
32	MG	A	2975	-	X
32	MG	A	2984	-	X
32	MG	A	2988	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	A	3002	-	X
32	MG	A	3006	-	X
32	MG	A	3013	-	X
32	MG	A	3027	-	X
32	MG	A	3034	-	X
32	MG	A	3039	-	X
32	MG	B	120	-	X

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 90740 atoms, of which 0 are hydrogen and 0 are deuterium.

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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	102	Total	C	N	O			
			779	492	146	141	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	W	79	Total	C	N	O	S		
			596	367	120	108	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	X	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Y	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	0	56	Total	C	N	O	S		
			444	269	94	80	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	B	4	Total	Mg	0	0
			4	4		
32	A	136	Total	Mg	0	0
			136	136		
32	D	1	Total	Mg	0	0
			1	1		

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	4	1	Total	Zn	0	0
			1	1		

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	614	Total	O	0	0
			614	614		

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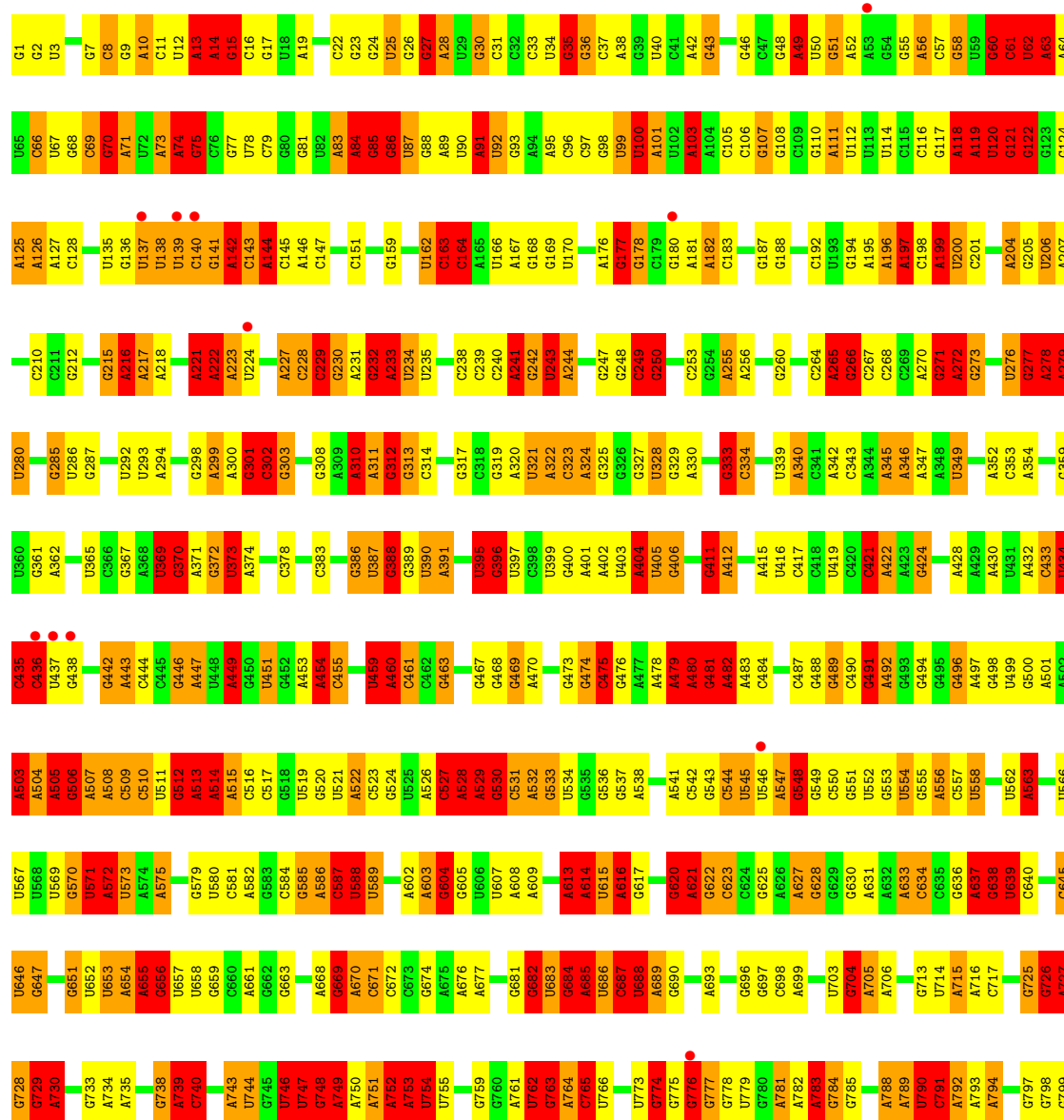
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	B	20	Total 20	O 20	0	0
34	C	8	Total 8	O 8	0	0
34	D	3	Total 3	O 3	0	0
34	E	1	Total 1	O 1	0	0
34	L	4	Total 4	O 4	0	0
34	N	3	Total 3	O 3	0	0
34	T	1	Total 1	O 1	0	0
34	2	1	Total 1	O 1	0	0
34	3	2	Total 2	O 2	0	0
34	4	3	Total 3	O 3	0	0

### 3 Residue-property plots

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

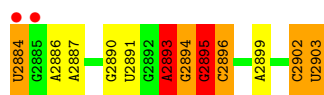
#### • Molecule 1: 23S rRNA

Chain A: 



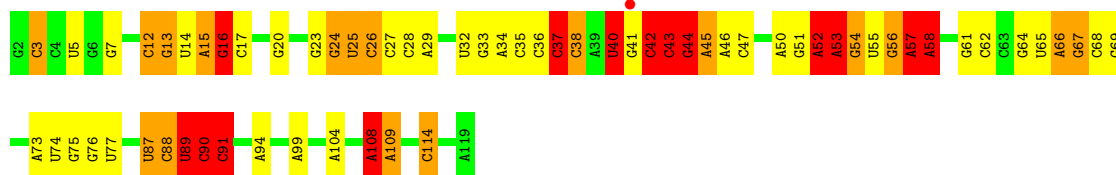
A1763	A1713		C1558	A1490	G1408	A1342	A1276	C1208	G1139	G1075	A1008	A947	U858	A800
A1764	U1714	A1641	U1559	G1491	G1411	G1343	G1277	U1209	C1140	C1076	A1009	C945	G869	G801
A1765	G1715	G1642	G1560	G1492	U1411	U1344	C1278	G1210	A1141	A1077	A1010	G949	U870	A802
A1766	U1716	G1643	C1493	G1493	U1412	C1345		C1211	A1142	U1078	G1011	G950	U871	U803
A1767	A1717	A1494	A1494	A1494	U1415	G1346	G1281	G1212	A1143	C1079	U1012	C951		A804
A1768		G1645	C1565	A1495	U1416	A1347	A1286	A1213	A1144	A1060	C1013	G954	G880	G805
A1769	G1721	C1646	A1566	A1496	C1417	C1348	A1287	G1214	C1145	U1081	A1014	U955	G883	C806
C1790	A1722	G1647	G1567	A1497	U1418	C1349	A1288	G1215	C1146	U1082	U1015	U956	U884	U807
A1791	G1723	U1648	G1568	C1498	G1419	C1350	G1288	G1216	A1147	U1083	G1016	U957	U885	G809
G1792	U1724	G1649	C1499	C1499	A1420	C1351	C1289	U1217	U1148	A1084	G1017	U958	A	G809
	U1725		A1570		G1421	U1352	C1290		G1149	A1085	U1018	U959	U	U810
U1796		A1652	A1571	A1503	G1422	G1356	C1291	G1223	C1150	A1086	U1019	A959	C	U811
G1797	C1728	G1653	A1572	A1504	G1423	C1357	G1292	U1224	A1151	G1087	A1020	A960	C	C812
U1798	U1729	A1654			G1424	C1357	C1293	G1225	C1152	A1088	A1021	C961	C	U813
G1799	C1730	A1655	U1578	A1508	G1425	G1358	U1294	G1226	C1153	A1089	U1022	G962	C	U814
C1800	G1731	C1656	G1581	A1509	G1426	A1359	C1295	A1227	G1154	A1090	G1023	U963	G	
A1801	C1732	U1657	G1582	G1510	A1427	G1360	G1296	G1228	A1155	C1091	G1024	C964	A892	C817
A1802	G1733	C1658	C1582	G1511	C1428	G1361	C1297	C1229	G1156	C1092	G1025	C965	C893	C818
A1803	G1734	G1659	U1583	C1512	G1429	C1362	C1298	G1232	G1157	G1093	G1026	U966	U894	A819
C1804	U1735	G1660	U1584	U1513	G1430	C1363	G1299		C1158		A1027	U967	U895	A820
A1805	A1736	G1661	G1588	G1514	A1431	A1365	G1300	G1233	U1159	A1096	A1028	C968	U896	A821
C1806	G1737	G1662	U1589	A1516	G1435	A1368	A1301	U1234	G1160	U1097	A1029	G969	C897	G822
G1807	G1738	G1663	G1517	G1517	G1436	G1369	A1302	G1235	C1161	A1098		U970		C823
A1808	A1739	A1664	C1518	C1519	G1437	C1370	A1304	A1237	G1162	C1102	U1033	A972	A900	U824
U1809		A1665	G1519		U1438	C1371	C1305	G1288		A1165	U1035	A973	C901	A825
A1810	G1743	G1666	U1520			U1372	G1309	U1239	A1166	C1103	G1036	A974	G907	U826
U1811	A1744	G1667	G1521	G1530	U1442	U1373	G1310	U1240	C1167	C1104	U1037	A975	C908	U827
U1812	A1745	A1668	A1522	C1531	U1443	G1381	G1311	A1241	G1171	C1105	G1037	A976	C915	U828
G1813	U1746	A1669	U1523	G1532	G1444	G1374	U1312		G1172	U1108	A1040	A977	C916	A829
G1814	U1747	U1671	G1524	A1525	G1445	U1375	U1313	G1245	U1173	C1109		A978	A911	C830
A1815		A1672	C1604	A1526			C1319	A1246	U1174	G1109	C1045	A979	C912	C831
C1816	G1753	G1673	C1605	C1526	C1451	A1378	C1314	A1247	U1175	C1110	A1046	A980	C913	U832
A1817	A1754	G1674	C1606		G1452	U1379	C1315	A1248	A1176	C1111	G1047	A981	C914	A833
U1818	G1755	A1675	A1532	G1530	A1453	G1380	U1316	U1249	U1176	G1112	A1048	A982	C915	C834
A1819	G1756	C1675	C1531	C1530	C1454	G1381	G1317	G1250	G1177	C1113	C1049	A983	G916	C835
U1820	A1757	A1676	A1532	C1532	G1455	G1382	U1318	C1251	C1178	C1114	A1050	A984	A917	C836
A1821	U1758	A1677	C1533	C1533	G1456	A1383	C1319	G1252	G1179	G1115	G1051	C985	A918	C837
A1822	A1759	A1678	U1534	U1534	U1457	A1384	C1320	A1253	U1180	C1116		C986	A919	C838
G1823	G1760	G1681	U1535	A1535	U1458	A1385	A1321	A1254	U1181	C1117	A1054	C987	A920	C839
U1824	C1761	G1682	C1536	G1536	G1459	C1386	A1322	U1255	G1182	C1118	G1055	A988	C921	C840
U1825	G1762	U1683	G1537	A1537	U1460	A1387	C1323	G1256	U1183	C1119	G1056	G989	C922	U842
	G1763		G1538	G1538	C1461	G1388	G1324	C1257	U1184	C1120	A1057	A990	G923	
	U1764	U1688	U1539	U1539		G1389	U1325	U1258	G1185	C1121	U1058	C991	G924	A845
U1765	G1765		G1540	G1540	U1468		A1327	G1259	G1186	G1122	G1059	C992		U846
G1766			C1541	C1541		A1392	A1328	A1260	U1187	G1125	U1060	C993	A927	U847
G1767			U1542	U1542	G1471	A1393	U1329	C1261	U1188	C1126	U1061	C994		
C1768			G1543	G1543	C1472	U1394	C1330		A1189	A1127	G1062	C995	U931	C854
U1769			A1544	A1544	G1476	U1395	G1331	A1264	G1190	C1127	G1063	A996	U932	C855
G1770			U1545	U1545	U1476	U1396	G1332	A1265		G1128	C1064	G997	A933	C856
	A1773		A1549	A1549	U1477	U1397	G1333	G1266	A1194	A1129	U1065	C998	U934	G857
	C1774		C1550	C1550	A1477	C1398	U1334	U1267	G1195	U1130	U1066	U999		G858
G1840			A1551	A1551	G1478	C1399	G1335	A1268	C1196	G1131	A1067	A1000	G938	G859
U1841	U1777		G1482	G1482		U1400	C1335	A1269		U1132	G1068	A1001		U860
A1842	U1778		A1552	A1552	G1483	A1403	A1336	G1270	G1203	A1134	A1069	G1002	A941	A861
C1843	U1779		A1553	A1553	U1484	C1404	G1337	G1271	U1202	A1134	A1070	G1003	G942	
C1844	U1780		U1554	U1554		C1404	G1338	A1272	A1284	G1135	G1071	U1004	A943	C864
	U1781		G1555	G1555	U1487	U1405	G1339	U1273	G1196	G1136	C1072	U1005	C944	C865
A1847	U1782		C1557	C1557		U1406	U1340	A1274	G1206	G1137	A1073	C1006	C946	A866
						G1407	G1341	A1275	C1207	G1138	G1074	C1007		C967

G2816	G2747	G2864	G2527	G2465	U2402	C2332	A2199	G2136	C1997	A1848
U2817	A2748	A2665	U2528	A2468	C2403	A2383	C2200	U2137	A1998	G1849
G2818	A2749	G2666	G2529	A2469	U2404	U2334	G2201	G2140	A1932	G1850
G2819	A2750	C2667	A2530	G2470	G2405	A2335	G2202	G2141	A1936	U1851
A2820	G2751	G2668	A2531	A2471	A2406	G2336	A2203	A2142	A1938	U1852
G2821	C2752	U2592	G2532	G2472	U2408	C2337	G2204	C2143	C1941	A1853
G2822	A2753	G2593	U2533	U2473	G2409	C2338	G2205	G2144	C1942	A1854
A2823	G2754	G2594	A2534	U2474	G2410	C2339	C2207	G2145	U1943	U1855
G2824	A2755	G2595	G2535	C2475	A2411	A2340	G2208	C2146	U1944	G1857
G2825	C2756	A2600	G2536	A2476	G2412	G2342	G2209	C2147	U1945	A1858
	A2757	G2601	C2537	U2477	G2413	U2343	U2210	G2148	U1946	U1859
		A2602	C2538	A2478	G2414	U2344	A2211	U2149	C1947	G1860
G2828	C2762	G2603	G2539	U2479	G2415	G2345	U2212	C2150	A2013	G1861
A2829	G2763	G2604	C2540	G2480	C2416	A2346	U2213	U2151	U1950	U1865
G2830	A2764	U2604	A2541	G2481	C2417	C2347	C2214	U2152	U1951	U1951
U2831	A2765	G2607	A2542	G2482	U2418	U2348	C2215	G2155	A1952	A1866
G2832		G2608	G2543	A2483	U2419	G2349	G2216	G2156	A1953	G1867
G2833	U2769	U2609	G2544	G2484	G2420	C2350	G2217	G2157	G1954	G1868
A2834	G2770	G2610	G2545	G2485	G2421	C2351	G2218	A	U1955	G1869
U2835	C2771	G2611	U2546	C2486	C2422	G2352	U2219	C	U1956	C1870
U2836	G2772	G2612	A2547	G2487	U2423	C2353	G2220	G	U1957	A1871
A2837		G2613	U2548	U2488	C2424	A2354	G2221	C	G1958	A1872
	A2776	G2614	G2549	U2489	A2425	G2355	G2222	C	G1959	G1873
G2842	G2777	A2614	G2550	A2490	A2426	G2356	G2223	G	A1960	C1874
G2843	A2778	U2615	G2551	G2491	G2427	A2357	G2224	A	C1961	G1875
U2844	U2779	G2616	U2552	U2492	U2428	G2358	G2225	C	U1962	A1876
G2846	G2780	U2617	G2553	G2493	G2429	G2359	C2226	C	U1963	C1881
U2847	A2781	G2618	U2554	U2494	G2430	G2360	A2227	C	U1964	U1882
G2848	G2782	C2619	U2555	G2495	U2431	C2361	U2228	U	C1965	G1883
U2849	U2783	G2620	G2556	G2496	U2432	G2362	G2229	U	U1966	U1884
A2851			G2557	A2497	G2433	C2363	U2230	G	G1967	A1885
G2852	C2787	G2625	G2558	A2498	A2434	C2364	C2231	A	G1968	
G2853	C2788	U2629	C2559	G2499	A2435	G2365	C2232	A	A1969	
G2854	G2789	G2630	A2560	C2499	A2436	A2366	U2233	A	U1970	A1899
G2855	U2790	U2631	U2561	U2500	G2437	G2367	G2234	U	U1971	A1900
A2856	G2791	A2632	U2562	C2501	A2439	A2368	G2235	A	G1972	A1901
G2857	A2792		U2563	G2502	U2441	U2370	G2236	C	C1973	
	C2793	G2636	A2564	A2503	C2442	G2371	G2237	C	C1974	C1905
A2860	C2794	U2637	A2565	U2504	U2443	U2372	G2238	C	C1975	G1906
U2861	C2795	G2638	U2566	G2505	C2443	G2373	U2240	A	U1976	G1907
G2862	U2796	U2639	G2567	U2506	G2444	A2381	A2241	C	A1977	C1908
G2863	U2797	A2639	U2568	C2507	G2445	G2382	U2242	G	A1978	
G2864	U2798	G2640	G2569	G2508	U2446	G2383	U2243	A	U1979	U1911
U2865	A2799	G2641	G2570	G2509	G2447	U2384	G2244	U	G1980	A1912
U2866			U2571	C2510	A2448	C2385	G2245	A	A1981	A1913
G2867	G2800	G2645	A2572	U2511	U2449	A2386	A2246	G	U1982	C1914
A2868	C2801	C2646	C2573	G2512	A2450	U2387	U2247	G	U1983	U1915
G2869	G2802		G2574	A2513	A2451	G2388	G2248	G	G1984	A1916
	G2803	A2726	G2575	U2514	C2452	G2389	G2249	G	C1985	U1917
	U2804	U2650	G2576	G2515	A2453	U2390	G2250	A	G1986	A1918
A2872	C2805	C2651	G2577	A2516	G2454	G2391	G2251	G	U1987	A1919
G2873	U2806	U2652	A2578	C2517	G2455	A2392	G2252	A	G1988	C1925
G2874	C2807	U2653	G2579	A2518	G2456	U2393	G2253	G	U1991	U1926
C2875	G2808	A2654	U2580	U2519	U2457	G2394	G2254	C	U1992	A1927
G2876	A2809	G2655	G2581	G2520	G2458	C2395	G2255	U	U1993	A1928
	A2810	U2656	G2582	C2521	A2459	G2396	U2256	U	C1994	G1929
A2879	C2811	A2657	G2583	U2522	U2460	U2397	U2257	U	U1995	U1930
G2880	G2812	C2658	U2584	G2525	C2461	U2398	U2258	U	G1996	U1931
U2881	A2813	U2659	G2585	U2526	A2462	G2399	C2260	G		
A2882	A2814		G2586			U2401	U2261			
A2883	C2815		U2586							



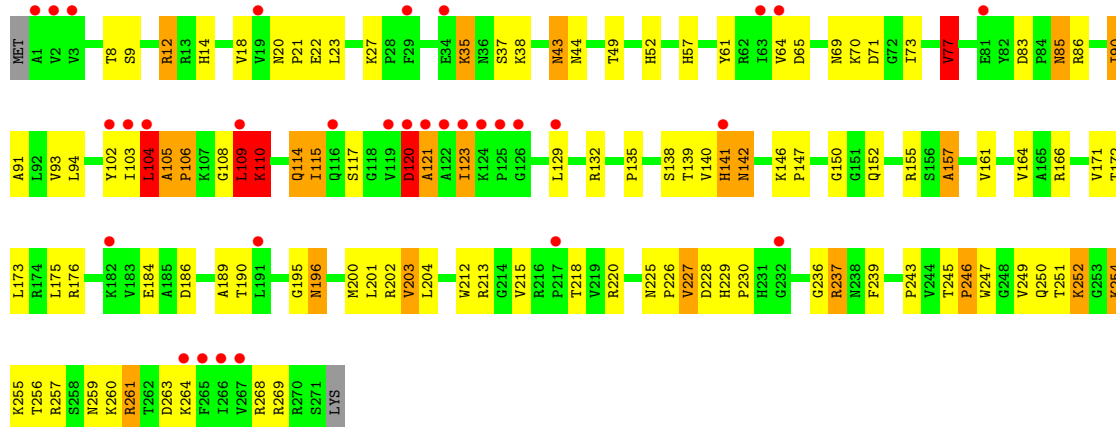
• Molecule 2: 5S rRNA

Chain B:



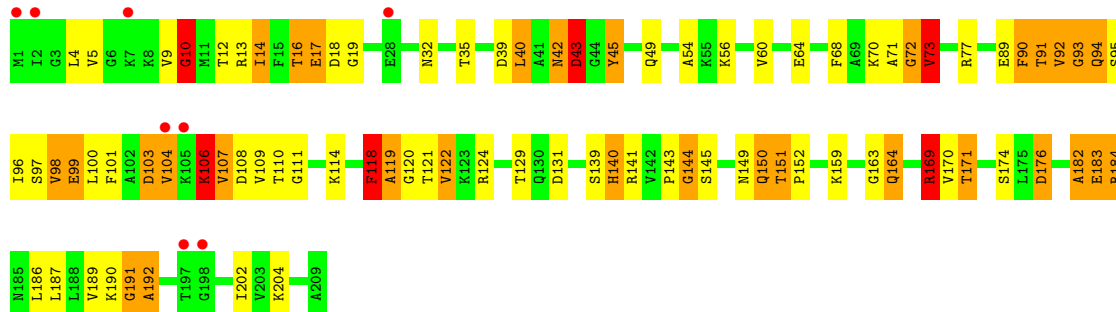
• Molecule 3: 50S ribosomal protein L2

Chain C:



• Molecule 4: 50S ribosomal protein L3

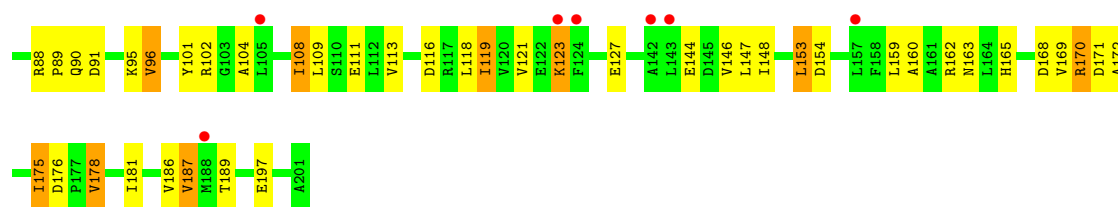
Chain D:



• Molecule 5: 50S ribosomal protein L4

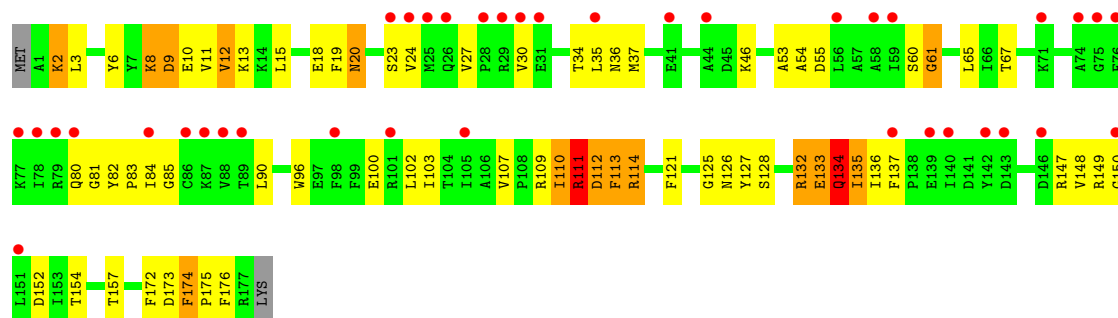
Chain E:





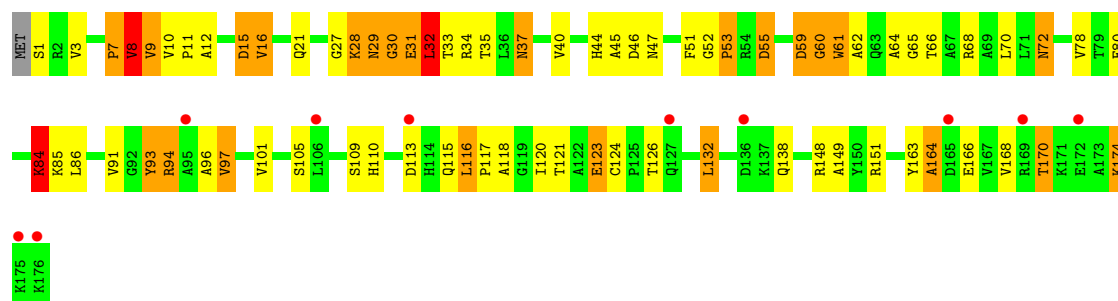
• Molecule 6: 50S ribosomal protein L5

Chain F:



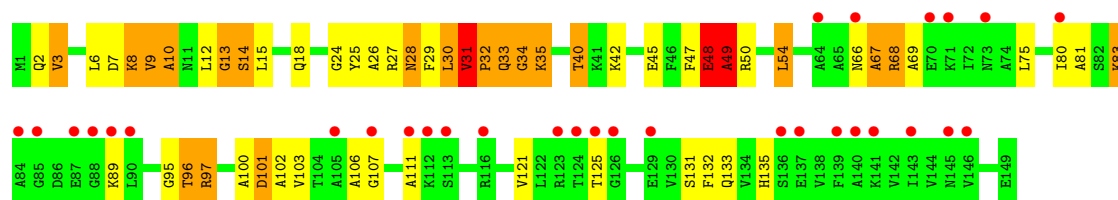
• Molecule 7: 50S ribosomal protein L6

Chain G:



• Molecule 8: 50S ribosomal protein L9

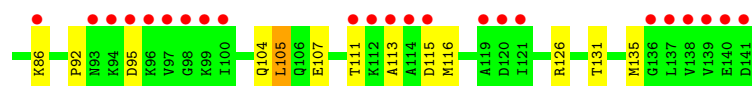
Chain H:



• Molecule 9: 50S ribosomal protein L11

Chain I:





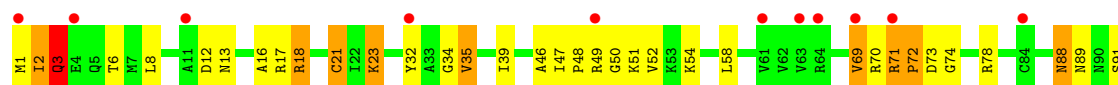
• Molecule 10: 50S ribosomal protein L13

Chain J:



• Molecule 11: 50S ribosomal protein L14

Chain K:



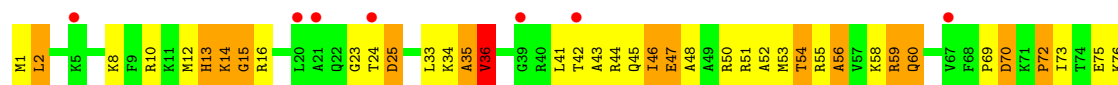
• Molecule 12: 50S ribosomal protein L15

Chain L:



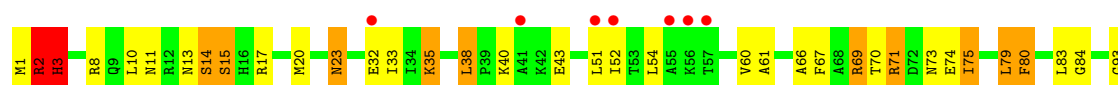
• Molecule 13: 50S ribosomal protein L16

Chain M:

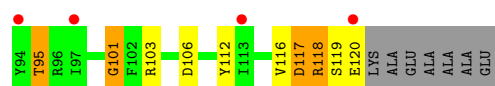


• Molecule 14: 50S ribosomal protein L17

Chain N:







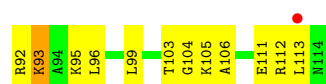
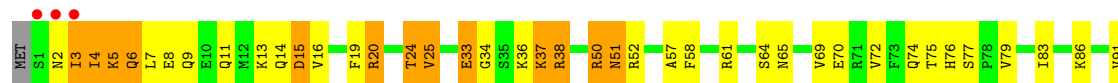
- Molecule 15: 50S ribosomal protein L18

Chain O:



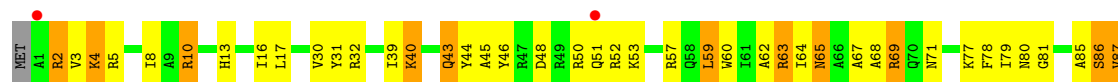
- Molecule 16: 50S ribosomal protein L19

Chain P:



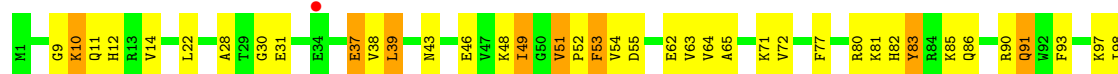
- Molecule 17: 50S ribosomal protein L20

Chain Q:



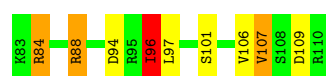
- Molecule 18: 50S ribosomal protein L21

Chain R:

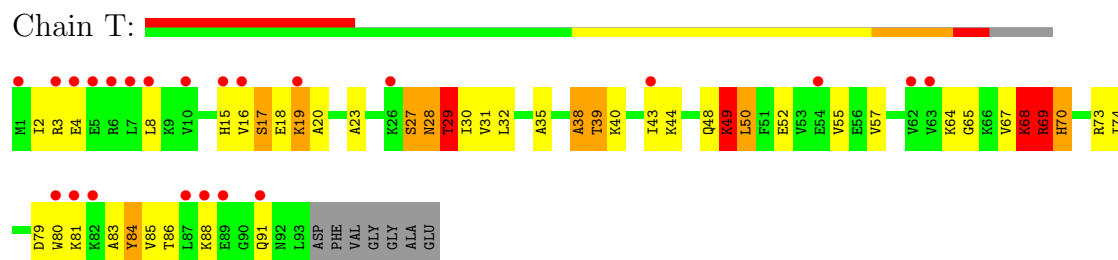


- Molecule 19: 50S ribosomal protein L22

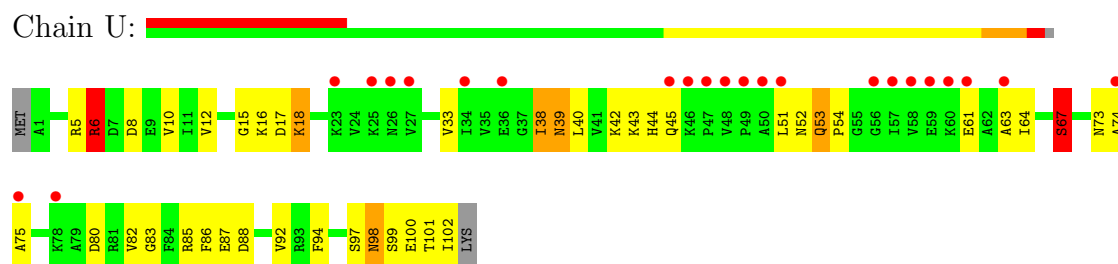
Chain S:



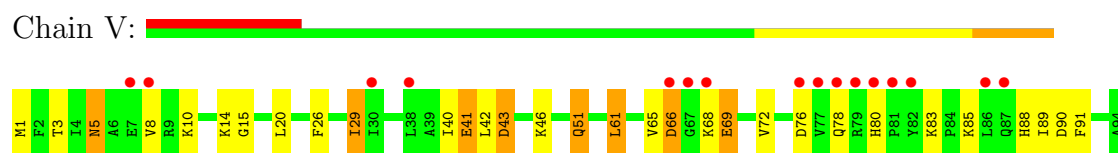
- Molecule 20: 50S ribosomal protein L23



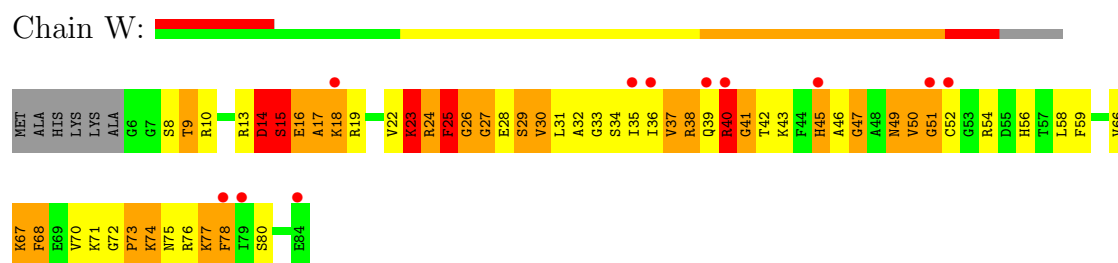
- Molecule 21: 50S ribosomal protein L24



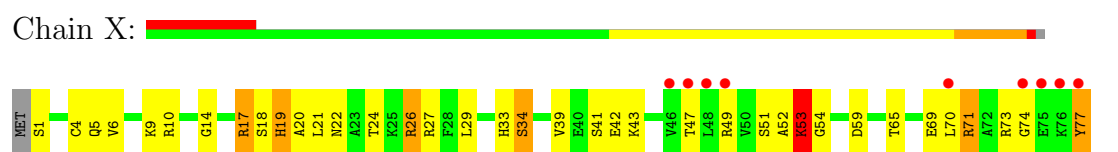
- Molecule 22: 50S ribosomal protein L25



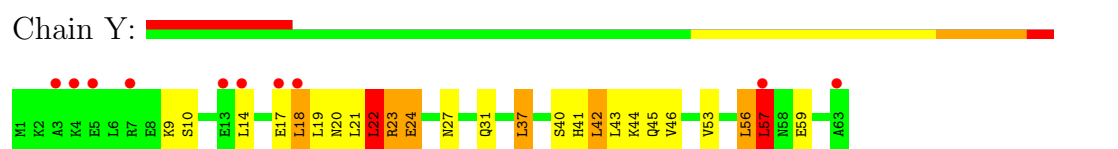
- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L30

Chain Z:



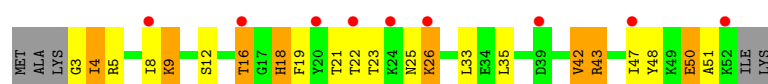
- Molecule 27: 50S ribosomal protein L32

Chain 0:



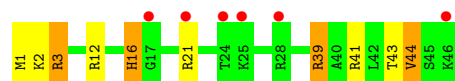
- Molecule 28: 50S ribosomal protein L33

Chain 1:



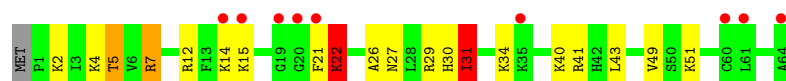
- Molecule 29: 50S ribosomal protein L34

Chain 2:



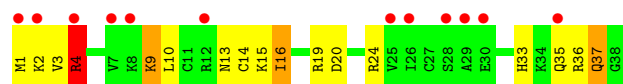
- Molecule 30: 50S ribosomal protein L35

Chain 3:



- Molecule 31: 50S ribosomal protein L36

Chain 4:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.95Å 433.08Å 624.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.44 – 3.71 73.44 – 3.71	Depositor EDS
% Data completeness (in resolution range)	75.7 (73.44-3.71) 75.7 (73.44-3.71)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.227 , 0.268 0.387 , 0.394	Depositor DCC
$R_{free}$ test set	9145 reflections (2.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	109.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 27.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 452802 reflections	Xtriage
$F_o, F_c$ correlation	0.72	EDS
Total number of atoms	90740	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.76	12/68626 (0.0%)	1.69	1758/107056 (1.6%)
2	B	0.66	0/2828	1.67	74/4410 (1.7%)
3	C	0.45	0/2121	0.72	1/2852 (0.0%)
4	D	0.50	0/1586	0.75	1/2134 (0.0%)
5	E	0.44	0/1571	0.67	0/2113
6	F	0.41	0/1434	0.68	3/1926 (0.2%)
7	G	0.43	0/1343	0.65	0/1816
8	H	0.70	6/1122 (0.5%)	0.83	6/1515 (0.4%)
9	I	0.24	0/1046	0.50	0/1410
10	J	0.55	0/1152	0.75	0/1551
11	K	0.55	0/947	0.83	0/1268
12	L	0.42	0/1054	0.77	1/1403 (0.1%)
13	M	0.51	0/1093	0.77	1/1460 (0.1%)
14	N	0.55	0/973	0.79	0/1301
15	O	0.42	0/902	0.63	0/1209
16	P	0.51	0/929	0.77	0/1242
17	Q	0.60	0/960	0.71	0/1278
18	R	0.56	0/829	0.85	1/1107 (0.1%)
19	S	0.50	0/864	0.75	0/1156
20	T	0.48	0/744	0.70	0/994
21	U	0.41	0/787	0.70	0/1051
22	V	0.48	0/766	0.66	0/1025
23	W	0.51	0/603	0.76	0/797
24	X	0.42	0/635	0.67	0/848
25	Y	0.40	0/510	0.66	0/677
26	Z	0.52	0/453	0.77	0/605
27	0	0.45	0/450	0.79	0/599
28	1	0.40	0/416	0.63	0/554
29	2	0.47	0/380	0.73	0/498
30	3	0.51	0/513	0.76	0/676
31	4	0.47	0/303	0.76	0/397
All	All	0.70	18/97940 (0.0%)	1.52	1846/146928 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
8	H	0	2
14	N	0	1
All	All	0	4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1142	A	N9-C4	-13.92	1.29	1.37
8	H	48	GLU	C-O	9.51	1.41	1.23
1	A	2451	A	C8-N7	9.03	1.37	1.31
8	H	48	GLU	CA-CB	6.93	1.69	1.53
8	H	48	GLU	CA-C	-6.56	1.35	1.52
8	H	49	ALA	N-CA	6.50	1.59	1.46
1	A	783	A	N9-C4	-6.32	1.34	1.37
1	A	2447	G	C6-N1	6.31	1.44	1.39
1	A	2860	A	C6-N6	6.00	1.38	1.33
1	A	1086	A	N7-C5	-5.74	1.35	1.39
8	H	47	PHE	CD2-CE2	5.54	1.50	1.39
1	A	1876	A	N7-C5	5.51	1.42	1.39
8	H	48	GLU	CD-OE1	5.45	1.31	1.25
1	A	2275	C	C1'-N1	5.32	1.56	1.48
1	A	1142	A	C8-N7	5.29	1.35	1.31
1	A	528	A	N7-C5	-5.26	1.36	1.39
1	A	2857	G	N3-C4	5.05	1.39	1.35
1	A	2884	U	C1'-N1	5.04	1.56	1.48

All (1846) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2447	G	C6-N1-C2	-22.51	111.59	125.10
1	A	2451	A	C5-N7-C8	-17.23	95.28	103.90
1	A	2347	C	N1-C1'-C2'	-16.79	92.17	114.00
1	A	790	U	P-O3'-C3'	-16.12	100.36	119.70
2	B	88	C	O4'-C1'-N1	-15.24	96.01	108.20
1	A	2447	G	C5-C6-O6	-15.23	119.46	128.60
1	A	2447	G	C5-C6-N1	15.21	119.11	111.50
1	A	1023	U	N1-C1'-C2'	-15.17	94.28	114.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2424	C	N1-C1'-C2'	-15.08	94.40	114.00
1	A	812	C	N1-C1'-C2'	-14.96	94.55	114.00
1	A	740	C	N1-C1'-C2'	-14.69	94.91	114.00
1	A	1022	G	P-O3'-C3'	14.59	137.21	119.70
1	A	206	U	N1-C1'-C2'	-14.54	95.09	114.00
1	A	2752	C	N1-C1'-C2'	-14.37	95.33	114.00
1	A	1675	C	N1-C1'-C2'	-14.18	95.56	114.00
1	A	373	U	N1-C1'-C2'	-14.03	95.77	114.00
1	A	805	G	P-O3'-C3'	14.02	136.52	119.70
6	F	112	ASP	CB-CG-OD2	-13.89	105.80	118.30
1	A	1142	A	C5-N7-C8	-13.73	97.04	103.90
1	A	1681	G	P-O3'-C3'	13.57	135.98	119.70
1	A	1461	C	N1-C1'-C2'	-13.54	96.41	114.00
1	A	946	C	N1-C1'-C2'	-13.52	96.42	114.00
1	A	435	C	N1-C1'-C2'	-13.49	96.47	114.00
1	A	2036	C	N1-C1'-C2'	-13.41	96.57	114.00
1	A	2504	U	N1-C1'-C2'	-13.29	96.72	114.00
1	A	249	C	P-O3'-C3'	13.26	135.62	119.70
1	A	686	U	O4'-C1'-N1	13.24	118.79	108.20
1	A	919	U	N1-C2-O2	13.20	132.04	122.80
1	A	2629	U	P-O3'-C3'	13.16	135.49	119.70
2	B	16	G	P-O3'-C3'	-13.09	103.99	119.70
1	A	1142	A	N3-C4-N9	-13.07	116.95	127.40
1	A	2068	U	N1-C1'-C2'	-12.98	97.12	114.00
1	A	1815	A	P-O3'-C3'	12.96	135.25	119.70
1	A	1760	C	N1-C1'-C2'	-12.90	97.22	114.00
1	A	1082	U	C2-N3-C4	-12.85	119.29	127.00
2	B	90	C	N1-C1'-C2'	-12.82	97.33	114.00
1	A	2575	C	C2-N3-C4	-12.82	113.49	119.90
1	A	2238	G	P-O3'-C3'	12.76	135.01	119.70
1	A	1019	U	C2-N3-C4	-12.72	119.37	127.00
1	A	646	U	N1-C1'-C2'	-12.71	97.47	114.00
1	A	919	U	C2-N1-C1'	12.71	132.95	117.70
1	A	302	C	N1-C1'-C2'	-12.68	97.52	114.00
1	A	919	U	C5-C6-N1	12.66	129.03	122.70
1	A	1210	G	P-O3'-C3'	12.60	134.82	119.70
1	A	2451	A	N7-C8-N9	12.51	120.05	113.80
1	A	1396	U	O4'-C1'-N1	12.49	118.19	108.20
1	A	2833	U	P-O3'-C3'	12.47	134.66	119.70
1	A	2225	A	P-O3'-C3'	12.42	134.61	119.70
1	A	1247	A	P-O3'-C3'	12.42	134.60	119.70
1	A	164	C	P-O3'-C3'	-12.39	104.83	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1965	C	P-O3'-C3'	-12.38	104.85	119.70
1	A	1648	U	N1-C1'-C2'	-12.36	97.93	114.00
1	A	860	U	N1-C1'-C2'	-12.36	97.94	114.00
1	A	1914	C	N1-C1'-C2'	-12.33	97.97	114.00
1	A	2630	G	P-O3'-C3'	-12.32	104.92	119.70
2	B	37	C	N1-C1'-C2'	-12.27	98.05	114.00
1	A	688	U	N1-C1'-C2'	-12.17	98.17	114.00
1	A	1558	C	P-O3'-C3'	12.02	134.12	119.70
1	A	685	A	P-O3'-C3'	11.98	134.08	119.70
1	A	614	A	P-O3'-C3'	11.97	134.07	119.70
1	A	1142	A	N3-C4-C5	11.97	135.18	126.80
1	A	1499	C	N1-C1'-C2'	-11.97	98.44	114.00
1	A	1145	C	P-O5'-C5'	-11.93	101.82	120.90
1	A	1993	U	N1-C1'-C2'	-11.91	98.52	114.00
1	A	2447	G	P-O3'-C3'	11.89	133.97	119.70
1	A	2447	G	N3-C4-C5	-11.87	122.66	128.60
1	A	2023	C	N1-C1'-C2'	-11.85	98.60	114.00
1	A	2857	G	C2-N3-C4	-11.83	105.98	111.90
1	A	2283	C	N1-C1'-C2'	-11.83	98.62	114.00
1	A	1802	A	P-O3'-C3'	-11.66	105.70	119.70
1	A	1965	C	N1-C1'-C2'	-11.64	98.87	114.00
1	A	2425	A	P-O3'-C3'	11.60	133.62	119.70
1	A	1962	C	P-O3'-C3'	11.59	133.60	119.70
1	A	138	U	N1-C1'-C2'	-11.57	98.96	114.00
1	A	2848	G	P-O3'-C3'	11.54	133.55	119.70
1	A	2638	G	P-O3'-C3'	11.53	133.54	119.70
1	A	1956	U	N1-C1'-C2'	-11.53	99.01	114.00
1	A	633	A	N1-C6-N6	11.42	125.45	118.60
1	A	442	G	P-O3'-C3'	11.40	133.38	119.70
1	A	934	U	N1-C1'-C2'	-11.40	99.19	114.00
1	A	1142	A	C4-C5-C6	-11.39	111.30	117.00
1	A	654	A	P-O3'-C3'	-11.33	106.11	119.70
1	A	200	U	N1-C1'-C2'	-11.31	99.30	114.00
1	A	2581	G	P-O3'-C3'	11.29	133.24	119.70
1	A	436	C	N1-C1'-C2'	-11.24	99.39	114.00
1	A	858	G	O4'-C1'-N9	11.24	117.19	108.20
1	A	1380	G	P-O3'-C3'	-11.20	106.26	119.70
1	A	1708	C	P-O3'-C3'	-11.18	106.28	119.70
1	A	489	G	P-O3'-C3'	11.17	133.11	119.70
1	A	303	G	P-O3'-C3'	-11.16	106.31	119.70
1	A	957	C	P-O3'-C3'	11.15	133.09	119.70
1	A	2440	C	N1-C1'-C2'	-11.15	99.50	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1971	U	N1-C1'-C2'	-11.15	99.51	114.00
1	A	2691	C	N1-C1'-C2'	-11.13	99.54	114.00
1	A	1329	U	N1-C1'-C2'	11.09	128.41	114.00
1	A	2645	G	O4'-C1'-N9	11.06	117.05	108.20
1	A	2051	A	P-O3'-C3'	11.05	132.96	119.70
1	A	783	A	P-O3'-C3'	-11.04	106.45	119.70
1	A	2385	C	P-O3'-C3'	-11.03	106.46	119.70
8	H	49	ALA	CB-CA-C	11.02	126.63	110.10
1	A	2458	G	P-O3'-C3'	11.00	132.90	119.70
1	A	1344	U	N1-C1'-C2'	-11.00	99.70	114.00
1	A	671	C	N1-C1'-C2'	-11.00	99.70	114.00
1	A	1816	C	N1-C1'-C2'	-10.98	99.73	114.00
1	A	784	G	P-O3'-C3'	10.96	132.85	119.70
1	A	2866	U	O4'-C1'-N1	10.96	116.96	108.20
1	A	1250	G	P-O3'-C3'	10.95	132.84	119.70
1	A	2498	C	P-O5'-C5'	-10.91	103.45	120.90
1	A	858	G	N1-C6-O6	-10.90	113.36	119.90
1	A	1072	C	N1-C1'-C2'	-10.90	99.83	114.00
1	A	1145	C	P-O3'-C3'	-10.90	106.62	119.70
1	A	1539	U	N1-C1'-C2'	-10.89	99.85	114.00
2	B	88	C	P-O3'-C3'	10.88	132.76	119.70
1	A	621	A	P-O3'-C3'	-10.88	106.64	119.70
1	A	1060	U	C5-C4-O4	-10.88	119.37	125.90
1	A	1265	A	P-O3'-C3'	10.86	132.73	119.70
8	H	48	GLU	CB-CA-C	-10.85	88.70	110.40
1	A	1330	C	N1-C1'-C2'	-10.84	99.90	114.00
1	A	2609	U	O4'-C1'-N1	10.84	116.87	108.20
1	A	2451	A	C8-N9-C4	-10.81	101.48	105.80
1	A	962	G	P-O3'-C3'	-10.79	106.76	119.70
1	A	1865	U	C2-N3-C4	-10.74	120.56	127.00
1	A	1758	U	P-O3'-C3'	10.73	132.58	119.70
1	A	2681	C	P-O3'-C3'	10.66	132.49	119.70
1	A	1126	A	P-O3'-C3'	10.62	132.44	119.70
1	A	1286	A	P-O3'-C3'	10.60	132.41	119.70
1	A	2428	G	P-O3'-C3'	-10.59	106.99	119.70
1	A	491	G	P-O3'-C3'	-10.58	107.01	119.70
1	A	1329	U	P-O3'-C3'	10.57	132.38	119.70
1	A	2383	G	P-O3'-C3'	-10.52	107.07	119.70
1	A	2573	C	N1-C1'-C2'	-10.51	100.33	114.00
1	A	1178	C	O4'-C1'-N1	10.51	116.60	108.20
1	A	1717	A	P-O3'-C3'	-10.50	107.10	119.70
1	A	687	C	N1-C1'-C2'	-10.48	100.38	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1957	C	P-O3'-C3'	-10.47	107.13	119.70
1	A	2214	C	N1-C1'-C2'	-10.47	100.39	114.00
1	A	2333	A	P-O3'-C3'	10.42	132.21	119.70
1	A	2200	C	N1-C1'-C2'	-10.42	100.45	114.00
1	A	100	U	P-O3'-C3'	10.41	132.19	119.70
1	A	781	A	P-O3'-C3'	10.41	132.19	119.70
1	A	726	G	P-O3'-C3'	10.40	132.18	119.70
1	A	164	C	N1-C1'-C2'	-10.39	100.49	114.00
1	A	730	A	P-O3'-C3'	-10.39	107.23	119.70
1	A	1490	A	P-O3'-C3'	10.36	132.14	119.70
1	A	92	U	N1-C1'-C2'	-10.36	100.53	114.00
1	A	2326	C	P-O3'-C3'	10.36	132.13	119.70
1	A	1556	C	N1-C1'-C2'	-10.30	100.61	114.00
1	A	2336	A	P-O3'-C3'	10.27	132.03	119.70
1	A	2447	G	N1-C2-N3	10.25	130.05	123.90
1	A	302	C	O4'-C1'-N1	10.24	116.40	108.20
1	A	1810	A	P-O3'-C3'	-10.24	107.41	119.70
1	A	500	G	C2-N3-C4	-10.22	106.79	111.90
1	A	1478	G	N3-C4-N9	-10.19	119.88	126.00
1	A	630	G	C2-N3-C4	-10.18	106.81	111.90
1	A	2880	C	P-O3'-C3'	-10.18	107.49	119.70
1	A	2451	A	C5-C6-N1	10.15	122.78	117.70
1	A	2210	U	P-O3'-C3'	10.15	131.88	119.70
1	A	2880	C	N1-C1'-C2'	-10.15	100.81	114.00
1	A	86	G	P-O3'-C3'	-10.12	107.55	119.70
1	A	1511	G	P-O3'-C3'	-10.11	107.57	119.70
1	A	1732	C	P-O3'-C3'	10.10	131.82	119.70
1	A	142	A	P-O3'-C3'	-10.10	107.58	119.70
1	A	548	G	P-O3'-C3'	-10.09	107.59	119.70
1	A	1475	G	P-O3'-C3'	10.06	131.77	119.70
1	A	2266	A	P-O3'-C3'	10.05	131.76	119.70
1	A	2645	G	P-O3'-C3'	10.02	131.72	119.70
1	A	279	A	P-O3'-C3'	-10.00	107.70	119.70
1	A	404	A	P-O3'-C3'	9.99	131.69	119.70
1	A	482	A	P-O3'-C3'	-9.96	107.74	119.70
1	A	752	A	P-O3'-C3'	9.96	131.65	119.70
1	A	1276	A	P-O3'-C3'	-9.95	107.76	119.70
1	A	369	U	P-O3'-C3'	9.94	131.63	119.70
1	A	2732	G	P-O3'-C3'	9.94	131.63	119.70
1	A	2712	C	N1-C1'-C2'	9.94	126.92	114.00
1	A	2226	C	N1-C1'-C2'	-9.92	101.08	112.00
1	A	301	G	P-O3'-C3'	9.92	131.60	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	A	P-O3'-C3'	9.91	131.59	119.70
2	B	52	A	P-O3'-C3'	9.89	131.57	119.70
1	A	1865	U	O4'-C1'-N1	9.88	116.10	108.20
1	A	507	A	P-O3'-C3'	-9.82	107.92	119.70
2	B	87	U	P-O3'-C3'	9.81	131.47	119.70
1	A	2613	U	P-O3'-C3'	9.74	131.39	119.70
1	A	2902	C	O4'-C1'-N1	9.74	115.99	108.20
1	A	227	A	P-O3'-C3'	9.73	131.37	119.70
1	A	1156	A	P-O3'-C3'	9.72	131.37	119.70
1	A	2835	A	P-O3'-C3'	9.70	131.34	119.70
1	A	2893	A	P-O3'-C3'	9.68	131.31	119.70
1	A	865	C	P-O3'-C3'	9.67	131.31	119.70
1	A	229	C	N1-C1'-C2'	-9.66	101.37	112.00
1	A	1236	G	P-O3'-C3'	9.65	131.28	119.70
1	A	1498	C	N1-C1'-C2'	-9.65	101.39	112.00
1	A	459	U	N1-C1'-C2'	-9.63	101.40	112.00
1	A	2384	U	P-O3'-C3'	9.62	131.24	119.70
1	A	1045	C	P-O3'-C3'	9.59	131.21	119.70
1	A	125	A	P-O3'-C3'	9.58	131.19	119.70
1	A	1828	G	P-O3'-C3'	9.56	131.17	119.70
1	A	2199	A	P-O3'-C3'	-9.56	108.23	119.70
1	A	861	A	P-O3'-C3'	-9.49	108.31	119.70
1	A	1700	A	P-O3'-C3'	-9.47	108.34	119.70
1	A	669	G	P-O3'-C3'	9.45	131.03	119.70
1	A	1635	A	P-O3'-C3'	-9.45	108.36	119.70
1	A	2860	A	N1-C6-N6	9.43	124.26	118.60
1	A	620	G	P-O3'-C3'	9.43	131.01	119.70
1	A	914	G	P-O3'-C3'	-9.41	108.41	119.70
1	A	2258	C	P-O3'-C3'	9.40	130.98	119.70
1	A	2832	U	P-O3'-C3'	9.37	130.95	119.70
1	A	1082	U	O4'-C1'-N1	9.37	115.69	108.20
1	A	2725	A	P-O3'-C3'	9.37	130.94	119.70
1	A	91	A	P-O3'-C3'	9.36	130.93	119.70
1	A	790	U	N1-C1'-C2'	-9.34	101.72	112.00
1	A	2820	A	P-O3'-C3'	9.34	130.90	119.70
1	A	460	A	P-O3'-C3'	-9.32	108.51	119.70
1	A	2682	A	P-O3'-C3'	-9.32	108.52	119.70
1	A	49	A	P-O3'-C3'	9.31	130.87	119.70
1	A	2296	U	N1-C1'-C2'	9.31	126.10	114.00
2	B	42	C	N1-C1'-C2'	-9.31	101.76	112.00
1	A	788	A	P-O3'-C3'	9.30	130.86	119.70
1	A	1378	A	P-O3'-C3'	9.30	130.86	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	C	P-O3'-C3'	9.29	130.85	119.70
1	A	1716	U	N1-C1'-C2'	-9.28	101.79	112.00
1	A	1127	A	P-O3'-C3'	-9.28	108.57	119.70
1	A	2451	A	C4-C5-N7	9.27	115.33	110.70
1	A	2423	U	P-O3'-C3'	9.27	130.82	119.70
1	A	1158	C	P-O3'-C3'	-9.26	108.58	119.70
1	A	2857	G	N9-C4-C5	-9.26	101.70	105.40
1	A	2728	U	P-O3'-C3'	-9.25	108.59	119.70
1	A	1345	C	N1-C1'-C2'	-9.22	101.85	112.00
1	A	512	G	O4'-C1'-N9	9.22	115.58	108.20
1	A	984	A	P-O3'-C3'	9.21	130.75	119.70
1	A	2689	U	O4'-C1'-N1	9.20	115.56	108.20
1	A	1345	C	P-O3'-C3'	-9.19	108.67	119.70
1	A	1272	A	P-O3'-C3'	9.18	130.72	119.70
2	B	66	A	P-O3'-C3'	9.17	130.71	119.70
2	B	91	C	P-O3'-C3'	-9.16	108.70	119.70
1	A	1799	G	P-O3'-C3'	9.15	130.68	119.70
2	B	13	G	P-O3'-C3'	-9.15	108.72	119.70
1	A	829	A	P-O3'-C3'	9.15	130.68	119.70
1	A	2586	U	N1-C1'-C2'	-9.14	101.94	112.00
1	A	1784	A	P-O3'-C3'	9.14	130.66	119.70
1	A	2520	C	N1-C1'-C2'	-9.13	101.96	112.00
1	A	2689	U	N1-C1'-C2'	9.12	125.86	114.00
1	A	1569	A	P-O3'-C3'	-9.12	108.76	119.70
1	A	915	C	N1-C1'-C2'	-9.09	102.00	112.00
1	A	1993	U	P-O5'-C5'	-9.09	106.36	120.90
1	A	2500	U	O4'-C1'-N1	9.09	115.47	108.20
1	A	1385	A	P-O3'-C3'	9.08	130.59	119.70
1	A	2052	A	P-O3'-C3'	-9.07	108.81	119.70
1	A	753	A	P-O3'-C3'	-9.07	108.82	119.70
1	A	1427	A	P-O3'-C3'	9.06	130.57	119.70
1	A	2451	A	C4-C5-C6	-9.06	112.47	117.00
1	A	1706	C	P-O3'-C3'	9.05	130.56	119.70
1	A	913	U	P-O3'-C3'	9.04	130.54	119.70
1	A	1082	U	C5-C4-O4	-9.02	120.49	125.90
1	A	1566	A	P-O3'-C3'	9.02	130.52	119.70
1	A	747	U	N1-C1'-C2'	-9.00	102.10	112.00
1	A	2468	A	P-O3'-C3'	8.99	130.49	119.70
1	A	1275	A	P-O3'-C3'	8.99	130.48	119.70
1	A	2588	G	P-O3'-C3'	8.97	130.47	119.70
1	A	243	U	N1-C1'-C2'	-8.96	102.14	112.00
1	A	2425	A	O4'-C1'-N9	8.96	115.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2503	A	P-O3'-C3'	8.96	130.45	119.70
1	A	2609	U	P-O3'-C3'	8.95	130.44	119.70
1	A	1142	A	C8-N9-C1'	8.95	143.80	127.70
1	A	2136	G	P-O3'-C3'	-8.94	108.98	119.70
1	A	1522	A	P-O3'-C3'	8.93	130.41	119.70
1	A	1915	U	N1-C1'-C2'	-8.93	102.18	112.00
1	A	140	C	P-O3'-C3'	8.92	130.41	119.70
1	A	14	A	P-O3'-C3'	-8.92	109.00	119.70
1	A	958	U	N1-C1'-C2'	-8.91	102.20	112.00
1	A	647	G	P-O3'-C3'	-8.90	109.02	119.70
1	A	1606	C	P-O3'-C3'	8.90	130.39	119.70
2	B	91	C	N1-C1'-C2'	-8.90	102.20	112.00
1	A	2068	U	P-O3'-C3'	-8.90	109.02	119.70
1	A	2646	C	N1-C1'-C2'	-8.88	102.23	112.00
2	B	88	C	N1-C1'-C2'	8.82	125.47	114.00
1	A	2517	C	P-O3'-C3'	8.81	130.27	119.70
1	A	1816	C	O4'-C1'-N1	8.81	115.25	108.20
1	A	324	A	P-O3'-C3'	-8.80	109.14	119.70
1	A	919	U	C6-N1-C1'	-8.80	108.88	121.20
1	A	1653	G	P-O3'-C3'	8.78	130.24	119.70
1	A	2384	U	N1-C1'-C2'	8.77	125.41	114.00
1	A	1913	A	P-O3'-C3'	8.76	130.22	119.70
1	A	1333	G	P-O3'-C3'	-8.76	109.19	119.70
1	A	1931	U	N1-C1'-C2'	-8.75	102.38	112.00
1	A	120	U	O4'-C1'-N1	-8.74	101.20	108.20
1	A	1812	U	O4'-C1'-N1	8.74	115.19	108.20
1	A	1022	G	N3-C4-N9	-8.73	120.76	126.00
1	A	1303	G	P-O3'-C3'	-8.71	109.25	119.70
1	A	919	U	N3-C2-O2	-8.70	116.11	122.20
1	A	1788	C	O4'-C1'-N1	-8.70	101.24	108.20
1	A	2511	U	C2-N3-C4	-8.69	121.79	127.00
1	A	2781	A	P-O3'-C3'	-8.68	109.28	119.70
1	A	436	C	O4'-C1'-N1	8.68	115.14	108.20
1	A	588	U	N1-C1'-C2'	-8.67	102.46	112.00
1	A	2586	U	P-O3'-C3'	-8.67	109.30	119.70
1	A	1461	C	O4'-C1'-N1	8.66	115.13	108.20
1	A	1398	C	N1-C1'-C2'	-8.65	102.48	112.00
1	A	1997	C	P-O3'-C3'	-8.65	109.32	119.70
1	A	2836	U	N1-C1'-C2'	-8.64	102.50	112.00
1	A	509	C	P-O3'-C3'	-8.62	109.36	119.70
1	A	1539	U	P-O3'-C3'	-8.61	109.36	119.70
1	A	1557	C	N1-C1'-C2'	-8.61	102.53	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1013	C	N1-C1'-C2'	-8.60	102.54	112.00
1	A	1675	C	P-O3'-C3'	-8.59	109.39	119.70
1	A	835	C	N1-C1'-C2'	-8.59	102.55	112.00
1	A	1478	G	C5-C6-O6	8.58	133.75	128.60
1	A	84	A	P-O3'-C3'	8.57	129.99	119.70
1	A	2344	U	P-O3'-C3'	8.57	129.99	119.70
1	A	386	G	P-O3'-C3'	8.57	129.98	119.70
1	A	443	A	P-O3'-C3'	-8.57	109.42	119.70
1	A	2585	U	P-O3'-C3'	8.52	129.93	119.70
1	A	2513	A	C5-C6-N6	8.51	130.51	123.70
1	A	2834	G	P-O5'-C5'	-8.51	107.29	120.90
1	A	645	C	N1-C1'-C2'	8.50	125.05	114.00
1	A	746	U	P-O3'-C3'	8.50	129.90	119.70
1	A	1602	U	P-O3'-C3'	8.49	129.88	119.70
1	A	1856	U	O4'-C1'-N1	8.49	114.99	108.20
1	A	2319	G	P-O3'-C3'	8.47	129.87	119.70
1	A	531	C	N1-C1'-C2'	8.47	125.01	114.00
1	A	1287	A	P-O3'-C3'	-8.46	109.54	119.70
1	A	1635	A	N9-C1'-C2'	-8.46	102.70	112.00
1	A	811	U	P-O3'-C3'	8.46	129.85	119.70
1	A	506	G	P-O3'-C3'	8.45	129.84	119.70
1	A	1174	U	N1-C1'-C2'	-8.43	102.73	112.00
1	A	2866	U	P-O3'-C3'	8.42	129.81	119.70
1	A	2520	C	O4'-C1'-N1	8.42	114.93	108.20
1	A	2322	A	P-O3'-C3'	-8.41	109.61	119.70
1	A	2392	A	P-O3'-C3'	-8.40	109.62	119.70
1	A	996	A	P-O3'-C3'	-8.38	109.64	119.70
1	A	301	G	C4-N9-C1'	-8.38	115.61	126.50
1	A	1020	A	P-O3'-C3'	8.38	129.76	119.70
1	A	1013	C	P-O3'-C3'	-8.37	109.66	119.70
1	A	1141	U	P-O3'-C3'	8.36	129.74	119.70
1	A	2267	A	P-O3'-C3'	-8.36	109.67	119.70
1	A	671	C	O4'-C1'-N1	8.33	114.87	108.20
1	A	1033	U	P-O3'-C3'	8.33	129.70	119.70
1	A	2490	G	P-O3'-C3'	8.31	129.68	119.70
1	A	2873	A	O4'-C1'-N9	8.30	114.84	108.20
1	A	2275	C	P-O3'-C3'	8.30	129.66	119.70
1	A	278	A	P-O3'-C3'	8.29	129.65	119.70
1	A	2447	G	N3-C4-N9	8.29	130.97	126.00
1	A	613	A	P-O3'-C3'	8.28	129.64	119.70
1	A	1721	G	P-O3'-C3'	8.28	129.64	119.70
1	A	1931	U	P-O3'-C3'	-8.28	109.76	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	749	A	P-O3'-C3'	-8.28	109.76	119.70
1	A	1062	G	P-O3'-C3'	-8.27	109.77	119.70
1	A	162	U	P-O3'-C3'	8.27	129.62	119.70
1	A	2035	G	O4'-C1'-N9	8.26	114.80	108.20
1	A	1249	U	N1-C1'-C2'	-8.25	102.93	112.00
1	A	1019	U	N1-C2-N3	8.24	119.85	114.90
1	A	443	A	P-O5'-C5'	-8.24	107.72	120.90
1	A	645	C	P-O3'-C3'	8.23	129.58	119.70
1	A	1668	A	P-O3'-C3'	8.23	129.58	119.70
1	A	688	U	P-O3'-C3'	-8.22	109.83	119.70
1	A	858	G	P-O3'-C3'	8.22	129.57	119.70
1	A	2492	U	N1-C1'-C2'	-8.22	102.96	112.00
1	A	931	U	P-O3'-C3'	8.20	129.54	119.70
1	A	1024	G	P-O3'-C3'	-8.20	109.86	119.70
1	A	1125	G	N9-C4-C5	-8.18	102.13	105.40
1	A	2215	C	N1-C1'-C2'	-8.18	103.00	112.00
1	A	752	A	N1-C6-N6	8.18	123.51	118.60
1	A	748	G	P-O3'-C3'	8.17	129.51	119.70
1	A	2520	C	P-O3'-C3'	-8.17	109.89	119.70
1	A	811	U	O4'-C1'-N1	8.17	114.73	108.20
1	A	1647	U	P-O3'-C3'	8.16	129.50	119.70
1	A	2895	G	P-O3'-C3'	-8.16	109.90	119.70
1	A	2566	A	P-O3'-C3'	8.16	129.49	119.70
1	A	2497	A	P-O3'-C3'	8.15	129.48	119.70
1	A	976	G	P-O3'-C3'	-8.14	109.93	119.70
1	A	1996	C	O4'-C1'-N1	8.14	114.71	108.20
1	A	119	A	P-O3'-C3'	8.14	129.47	119.70
1	A	421	C	P-O3'-C3'	8.14	129.47	119.70
1	A	2424	C	O4'-C1'-N1	8.14	114.71	108.20
1	A	1698	A	P-O3'-C3'	8.13	129.46	119.70
1	A	2251	G	P-O3'-C3'	-8.13	109.94	119.70
1	A	989	G	P-O3'-C3'	8.13	129.45	119.70
1	A	638	G	P-O3'-C3'	-8.12	109.95	119.70
1	A	2611	C	N1-C1'-C2'	-8.12	103.07	112.00
1	A	1008	A	P-O3'-C3'	8.11	129.44	119.70
1	A	2303	G	P-O3'-C3'	-8.11	109.97	119.70
1	A	2283	C	O4'-C1'-N1	8.11	114.69	108.20
1	A	1682	G	P-O3'-C3'	-8.10	109.99	119.70
1	A	945	A	O4'-C1'-N9	8.09	114.67	108.20
1	A	2440	C	O4'-C1'-N1	8.06	114.65	108.20
1	A	2066	C	P-O3'-C3'	-8.06	110.03	119.70
1	A	199	A	O4'-C1'-N9	8.06	114.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1981	A	P-O3'-C3'	-8.06	110.03	119.70
1	A	2447	G	N3-C2-N2	-8.06	114.26	119.90
1	A	1915	U	P-O3'-C3'	-8.05	110.04	119.70
1	A	1876	A	C4-C5-C6	-8.05	112.97	117.00
1	A	2054	A	C8-N9-C4	-8.05	102.58	105.80
1	A	241	A	P-O3'-C3'	8.05	129.36	119.70
1	A	2834	G	P-O3'-C3'	-8.04	110.06	119.70
1	A	959	A	P-O3'-C3'	-8.04	110.06	119.70
1	A	13	A	P-O3'-C3'	8.03	129.34	119.70
1	A	743	A	P-O3'-C3'	8.02	129.32	119.70
1	A	2462	C	P-O3'-C3'	-8.02	110.08	119.70
8	H	48	GLU	CA-C-O	-8.02	103.26	120.10
1	A	571	U	P-O3'-C3'	8.01	129.31	119.70
1	A	1942	C	N1-C1'-C2'	-8.01	103.19	112.00
1	A	310	A	P-O3'-C3'	8.01	129.31	119.70
1	A	1019	U	C5-C4-O4	-8.00	121.10	125.90
1	A	1782	U	N1-C1'-C2'	-8.00	103.20	112.00
1	A	2406	A	P-O3'-C3'	8.00	129.30	119.70
1	A	390	U	P-O3'-C3'	7.99	129.29	119.70
1	A	2386	A	N9-C1'-C2'	-7.99	103.21	112.00
1	A	1602	U	O4'-C1'-N1	7.98	114.59	108.20
1	A	2093	G	N9-C1'-C2'	-7.98	103.22	112.00
1	A	406	G	P-O3'-C3'	-7.98	110.12	119.70
1	A	1857	G	P-O3'-C3'	7.98	129.27	119.70
1	A	1048	A	P-O3'-C3'	-7.97	110.14	119.70
1	A	301	G	N3-C4-N9	-7.96	121.22	126.00
1	A	2062	A	N1-C6-N6	7.96	123.38	118.60
1	A	1954	G	P-O3'-C3'	7.96	129.25	119.70
1	A	1619	G	P-O3'-C3'	-7.96	110.15	119.70
1	A	2239	G	P-O3'-C3'	-7.96	110.15	119.70
1	A	2879	A	P-O3'-C3'	7.95	129.25	119.70
1	A	1967	C	N1-C1'-C2'	-7.95	103.25	112.00
1	A	2593	U	P-O3'-C3'	-7.95	110.16	119.70
1	A	2513	A	N1-C6-N6	-7.93	113.84	118.60
1	A	2734	A	P-O3'-C3'	-7.93	110.19	119.70
1	A	1330	C	O4'-C1'-N1	7.92	114.53	108.20
1	A	1647	U	O4'-C1'-N1	7.92	114.53	108.20
1	A	1111	A	P-O3'-C3'	7.90	129.18	119.70
1	A	1965	C	P-O5'-C5'	-7.89	108.28	120.90
2	B	26	C	O4'-C1'-N1	7.89	114.51	108.20
1	A	776	G	O4'-C1'-N9	-7.88	101.90	108.20
1	A	1971	U	P-O3'-C3'	-7.88	110.25	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1865	U	C5-C4-O4	-7.88	121.17	125.90
1	A	866	A	N9-C1'-C2'	-7.87	103.34	112.00
1	A	1012	U	O4'-C1'-N1	7.87	114.50	108.20
1	A	656	G	P-O3'-C3'	-7.87	110.26	119.70
1	A	1997	C	N1-C1'-C2'	-7.86	103.35	112.00
1	A	2518	A	P-O5'-C5'	-7.86	108.33	120.90
1	A	1029	A	N1-C6-N6	7.85	123.31	118.60
1	A	1266	G	P-O3'-C3'	7.84	129.11	119.70
1	A	2575	C	C5-C6-N1	-7.83	117.08	121.00
1	A	15	G	C5-C6-O6	7.83	133.30	128.60
1	A	1649	G	P-O3'-C3'	-7.83	110.31	119.70
1	A	264	C	O4'-C1'-N1	7.83	114.46	108.20
1	A	1142	A	C4-N9-C1'	-7.81	112.23	126.30
1	A	2060	A	P-O3'-C3'	7.81	129.08	119.70
1	A	1147	A	N1-C6-N6	-7.81	113.91	118.60
1	A	1716	U	O4'-C1'-N1	7.80	114.44	108.20
1	A	1963	U	N1-C1'-C2'	-7.79	103.43	112.00
2	B	25	U	P-O3'-C3'	-7.79	110.35	119.70
1	A	1112	G	P-O3'-C3'	-7.79	110.35	119.70
1	A	531	C	P-O3'-C3'	7.79	129.05	119.70
1	A	1810	A	N9-C1'-C2'	-7.79	103.43	112.00
1	A	1351	C	O4'-C1'-N1	7.78	114.42	108.20
1	A	1872	A	P-O3'-C3'	-7.78	110.36	119.70
2	B	12	C	O4'-C1'-N1	7.78	114.42	108.20
1	A	2275	C	N1-C1'-C2'	7.77	124.10	114.00
1	A	2836	U	P-O5'-C5'	-7.77	108.47	120.90
1	A	449	A	P-O3'-C3'	-7.76	110.39	119.70
1	A	451	U	O4'-C1'-N1	7.76	114.41	108.20
1	A	1272	A	O4'-C1'-N9	7.76	114.41	108.20
1	A	1714	U	N1-C1'-C2'	-7.76	103.47	112.00
1	A	519	U	N1-C1'-C2'	-7.75	103.47	112.00
1	A	2615	U	P-O3'-C3'	-7.75	110.40	119.70
1	A	479	A	O4'-C1'-N9	7.74	114.39	108.20
1	A	2259	U	N1-C1'-C2'	-7.74	103.49	112.00
1	A	266	G	P-O3'-C3'	-7.74	110.42	119.70
1	A	2501	C	N1-C1'-C2'	7.73	124.05	114.00
1	A	2791	G	P-O3'-C3'	-7.73	110.42	119.70
1	A	2035	G	P-O3'-C3'	7.72	128.97	119.70
1	A	474	G	P-O3'-C3'	7.72	128.96	119.70
1	A	1693	U	P-O3'-C3'	7.72	128.96	119.70
1	A	1458	U	P-O3'-C3'	7.71	128.95	119.70
1	A	1957	C	N1-C1'-C2'	-7.71	103.52	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	791	C	O4'-C1'-N1	7.70	114.36	108.20
1	A	2056	G	O4'-C1'-N9	-7.68	102.05	108.20
1	A	2459	A	P-O3'-C3'	-7.68	110.48	119.70
2	B	12	C	P-O3'-C3'	7.68	128.91	119.70
1	A	481	G	P-O3'-C3'	7.67	128.91	119.70
1	A	1180	U	P-O3'-C3'	7.67	128.90	119.70
1	A	2250	G	O4'-C1'-N9	-7.66	102.07	108.20
1	A	2874	C	N1-C1'-C2'	-7.65	103.58	112.00
1	A	1021	A	P-O5'-C5'	-7.64	108.68	120.90
1	A	961	C	P-O3'-C3'	7.63	128.86	119.70
1	A	1022	G	N3-C2-N2	-7.63	114.56	119.90
1	A	1996	C	P-O3'-C3'	7.62	128.85	119.70
1	A	475	C	N1-C1'-C2'	-7.62	103.62	112.00
1	A	2613	U	N1-C1'-C2'	7.62	123.91	114.00
1	A	2439	A	P-O3'-C3'	7.61	128.83	119.70
1	A	1478	G	C8-N9-C1'	7.61	136.89	127.00
1	A	35	G	P-O3'-C3'	-7.60	110.58	119.70
1	A	2733	A	N9-C1'-C2'	-7.60	103.64	112.00
1	A	2259	U	P-O3'-C3'	-7.60	110.58	119.70
1	A	1759	A	P-O3'-C3'	-7.59	110.58	119.70
1	A	1006	C	P-O3'-C3'	-7.58	110.60	119.70
1	A	2757	A	P-O3'-C3'	-7.58	110.61	119.70
1	A	2567	G	P-O3'-C3'	-7.58	110.61	119.70
1	A	1654	A	P-O3'-C3'	-7.57	110.61	119.70
1	A	199	A	P-O3'-C3'	7.57	128.79	119.70
8	H	49	ALA	N-CA-C	-7.57	90.56	111.00
2	B	43	C	O4'-C1'-N1	7.57	114.25	108.20
1	A	2611	C	P-O3'-C3'	-7.57	110.62	119.70
1	A	1839	G	P-O3'-C3'	-7.56	110.62	119.70
1	A	1615	C	P-O3'-C3'	7.56	128.77	119.70
1	A	2791	G	N9-C1'-C2'	-7.56	103.69	112.00
1	A	1964	G	P-O3'-C3'	7.55	128.76	119.70
1	A	2555	U	O4'-C1'-N1	7.54	114.24	108.20
1	A	301	G	C8-N9-C1'	7.54	136.80	127.00
1	A	2542	A	O4'-C1'-N9	7.54	114.23	108.20
1	A	739	A	P-O3'-C3'	7.53	128.74	119.70
1	A	272	A	P-O3'-C3'	-7.53	110.67	119.70
1	A	1478	G	N3-C4-C5	7.52	132.36	128.60
2	B	26	C	N1-C1'-C2'	-7.52	103.73	112.00
2	B	26	C	P-O3'-C3'	-7.52	110.68	119.70
1	A	2777	G	O4'-C1'-N9	-7.50	102.20	108.20
1	A	2884	U	O4'-C1'-N1	7.50	114.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1557	C	P-O3'-C3'	-7.47	110.73	119.70
1	A	1496	A	P-O3'-C3'	-7.46	110.75	119.70
1	A	919	U	C2-N3-C4	7.46	131.47	127.00
1	A	1207	C	P-O3'-C3'	-7.45	110.75	119.70
1	A	1708	C	N1-C1'-C2'	-7.45	103.80	112.00
1	A	588	U	P-O3'-C3'	-7.45	110.77	119.70
1	A	633	A	O4'-C1'-N9	-7.44	102.25	108.20
1	A	764	A	P-O3'-C3'	7.44	128.63	119.70
1	A	139	U	O4'-C1'-N1	7.43	114.15	108.20
1	A	73	A	N9-C1'-C2'	-7.43	103.83	112.00
1	A	1345	C	P-O5'-C5'	-7.43	109.02	120.90
1	A	1011	G	P-O3'-C3'	7.43	128.61	119.70
1	A	2072	C	O4'-C1'-N1	-7.43	102.26	108.20
1	A	2385	C	N1-C1'-C2'	-7.43	103.83	112.00
1	A	2572	A	P-O3'-C3'	7.43	128.61	119.70
1	A	2868	A	P-O3'-C3'	-7.43	110.79	119.70
2	B	43	C	N1-C1'-C2'	-7.42	103.83	112.00
1	A	855	G	C8-N9-C4	-7.41	103.44	106.40
1	A	1086	A	N1-C2-N3	7.41	133.01	129.30
1	A	1499	C	O4'-C1'-N1	7.41	114.13	108.20
1	A	2215	C	P-O3'-C3'	-7.40	110.82	119.70
1	A	913	U	N1-C1'-C2'	7.39	123.61	114.00
1	A	279	A	N9-C1'-C2'	-7.38	103.88	112.00
1	A	1340	U	N1-C1'-C2'	7.38	123.60	114.00
1	A	2822	G	N1-C6-O6	7.38	124.33	119.90
1	A	2603	G	P-O3'-C3'	-7.38	110.84	119.70
1	A	206	U	P-O3'-C3'	-7.37	110.86	119.70
1	A	459	U	P-O5'-C5'	-7.36	109.12	120.90
1	A	2337	G	P-O5'-C5'	-7.36	109.12	120.90
1	A	995	C	P-O3'-C3'	7.36	128.53	119.70
1	A	1268	A	P-O3'-C3'	-7.36	110.87	119.70
1	A	1086	A	C8-N9-C4	-7.35	102.86	105.80
1	A	2903	U	O4'-C1'-N1	7.35	114.08	108.20
1	A	915	C	P-O3'-C3'	-7.33	110.90	119.70
1	A	763	G	C6-C5-N7	-7.33	126.00	130.40
1	A	2211	A	P-O3'-C3'	7.33	128.50	119.70
1	A	454	A	P-O3'-C3'	7.32	128.49	119.70
1	A	391	A	P-O3'-C3'	-7.31	110.93	119.70
1	A	1799	G	O4'-C1'-N9	7.31	114.05	108.20
1	A	2275	C	O4'-C1'-N1	7.30	114.04	108.20
1	A	204	A	P-O3'-C3'	7.30	128.46	119.70
1	A	475	C	P-O5'-C5'	-7.29	109.23	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	A	P-O3'-C3'	7.29	128.45	119.70
1	A	2007	U	P-O3'-C3'	-7.29	110.96	119.70
1	A	221	A	P-O3'-C3'	7.28	128.44	119.70
1	A	1615	C	N1-C1'-C2'	7.28	123.46	114.00
1	A	1072	C	P-O3'-C3'	-7.27	110.97	119.70
2	B	109	A	P-O3'-C3'	-7.26	110.99	119.70
1	A	1372	U	C2-N3-C4	-7.25	122.65	127.00
1	A	1706	C	N1-C1'-C2'	7.25	123.42	114.00
1	A	2307	G	P-O3'-C3'	7.25	128.40	119.70
1	A	1732	C	N1-C2-O2	-7.24	114.56	118.90
1	A	1082	U	N1-C2-N3	7.21	119.23	114.90
1	A	2862	G	P-O3'-C3'	-7.21	111.04	119.70
1	A	1555	G	P-O5'-C5'	-7.21	109.36	120.90
1	A	1634	A	P-O3'-C3'	7.21	128.35	119.70
1	A	233	A	P-O3'-C3'	-7.20	111.06	119.70
1	A	125	A	O4'-C1'-N9	7.20	113.96	108.20
1	A	528	A	P-O3'-C3'	-7.20	111.06	119.70
1	A	1451	C	N1-C1'-C2'	7.20	123.36	114.00
1	A	812	C	P-O3'-C3'	-7.20	111.06	119.70
1	A	616	A	P-O3'-C3'	-7.19	111.07	119.70
1	A	2053	G	P-O3'-C3'	-7.19	111.07	119.70
1	A	1213	A	P-O3'-C3'	-7.19	111.07	119.70
1	A	1714	U	P-O3'-C3'	-7.18	111.09	119.70
1	A	2595	G	P-O3'-C3'	-7.18	111.09	119.70
1	A	2199	A	P-O5'-C5'	-7.17	109.43	120.90
1	A	2427	C	P-O3'-C3'	-7.17	111.10	119.70
1	A	1091	G	P-O3'-C3'	-7.17	111.10	119.70
1	A	974	G	P-O3'-C3'	7.17	128.30	119.70
1	A	2063	C	O4'-C1'-N1	-7.15	102.48	108.20
1	A	1669	A	P-O3'-C3'	-7.14	111.13	119.70
1	A	1060	U	N3-C4-O4	7.14	124.40	119.40
1	A	1238	G	N9-C1'-C2'	-7.14	104.15	112.00
1	A	2772	C	C6-N1-C2	7.14	123.16	120.30
1	A	163	C	P-O3'-C3'	-7.14	111.13	119.70
1	A	1022	G	N3-C4-C5	7.14	132.17	128.60
1	A	704	G	P-O3'-C3'	7.13	128.25	119.70
1	A	2821	A	P-O3'-C3'	-7.13	111.15	119.70
1	A	1779	U	C5-C6-N1	-7.12	119.14	122.70
1	A	301	G	C6-C5-N7	7.12	134.67	130.40
1	A	2857	G	C4-C5-N7	7.12	113.65	110.80
1	A	1633	G	P-O3'-C3'	7.11	128.23	119.70
1	A	1664	A	P-O3'-C3'	7.11	128.23	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1654	A	N9-C1'-C2'	-7.10	104.19	112.00
1	A	1129	A	P-O3'-C3'	-7.10	111.18	119.70
1	A	61	C	P-O5'-C5'	-7.10	109.54	120.90
1	A	628	G	P-O3'-C3'	-7.10	111.18	119.70
1	A	907	G	N3-C4-C5	7.09	132.15	128.60
1	A	1311	G	P-O3'-C3'	7.09	128.20	119.70
1	A	455	C	O4'-C1'-N1	-7.07	102.54	108.20
1	A	685	A	O3'-P-O5'	7.07	117.43	104.00
1	A	1805	A	N9-C4-C5	7.07	108.63	105.80
1	A	2724	U	P-O3'-C3'	7.06	128.18	119.70
1	A	774	G	P-O3'-C3'	7.06	128.18	119.70
1	A	2857	G	C6-C5-N7	-7.06	126.17	130.40
1	A	1499	C	P-O3'-C3'	-7.06	111.23	119.70
1	A	919	U	O4'-C1'-N1	-7.05	102.56	108.20
1	A	2321	U	P-O3'-C3'	-7.05	111.24	119.70
1	A	1298	C	P-O5'-C5'	-7.04	109.63	120.90
1	A	2808	G	P-O3'-C3'	7.04	128.15	119.70
1	A	621	A	N9-C1'-C2'	-7.03	104.27	112.00
1	A	2860	A	C5-C6-N1	-7.03	114.19	117.70
1	A	1326	U	P-O3'-C3'	-7.02	111.27	119.70
1	A	85	G	P-O3'-C3'	-7.02	111.27	119.70
1	A	216	A	N9-C1'-C2'	-7.02	104.28	112.00
1	A	1936	A	P-O3'-C3'	7.02	128.12	119.70
8	H	48	GLU	N-CA-CB	-7.02	97.97	110.60
1	A	2044	C	O4'-C1'-N1	-6.99	102.61	108.20
1	A	299	A	C5-N7-C8	-6.99	100.41	103.90
1	A	1324	G	P-O3'-C3'	6.99	128.09	119.70
1	A	752	A	O4'-C1'-N9	6.97	113.78	108.20
1	A	945	A	P-O3'-C3'	6.97	128.06	119.70
1	A	396	G	N9-C1'-C2'	-6.96	104.34	112.00
1	A	868	U	P-O3'-C3'	6.96	128.06	119.70
1	A	2610	C	P-O3'-C3'	6.96	128.06	119.70
1	A	530	G	C4-N9-C1'	6.96	135.54	126.50
1	A	1073	A	P-O3'-C3'	-6.95	111.36	119.70
2	B	3	C	P-O3'-C3'	-6.95	111.36	119.70
1	A	61	C	N1-C1'-C2'	-6.95	104.36	112.00
1	A	1707	G	P-O3'-C3'	-6.95	111.36	119.70
1	A	2691	C	P-O3'-C3'	-6.94	111.37	119.70
1	A	1523	U	O4'-C1'-N1	6.94	113.75	108.20
1	A	1782	U	P-O3'-C3'	-6.94	111.37	119.70
1	A	2069	G	P-O3'-C3'	-6.94	111.38	119.70
1	A	2034	U	N1-C1'-C2'	-6.93	104.37	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	G	P-O5'-C5'	-6.93	109.81	120.90
1	A	2296	U	O4'-C1'-N1	-6.93	102.66	108.20
1	A	1273	U	N1-C1'-C2'	-6.92	104.39	112.00
1	A	1455	G	P-O3'-C3'	-6.92	111.39	119.70
1	A	2576	G	P-O3'-C3'	6.92	128.00	119.70
1	A	747	U	P-O3'-C3'	-6.92	111.40	119.70
1	A	777	G	N9-C1'-C2'	-6.91	104.39	112.00
1	A	1396	U	P-O3'-C3'	6.91	128.00	119.70
1	A	1526	C	C6-N1-C2	6.91	123.06	120.30
1	A	1654	A	C3'-C2'-C1'	6.91	107.03	101.50
1	A	1073	A	N9-C1'-C2'	-6.91	104.40	112.00
1	A	1478	G	C4-N9-C1'	-6.91	117.52	126.50
1	A	2063	C	P-O3'-C3'	-6.91	111.41	119.70
1	A	504	A	P-O5'-C5'	-6.91	109.85	120.90
1	A	1509	A	O4'-C1'-N9	6.91	113.72	108.20
1	A	2382	G	P-O3'-C3'	6.90	127.98	119.70
1	A	1334	G	P-O3'-C3'	-6.90	111.42	119.70
1	A	1556	C	O4'-C1'-N1	6.90	113.72	108.20
1	A	232	G	P-O3'-C3'	6.89	127.97	119.70
1	A	2062	A	P-O3'-C3'	-6.89	111.43	119.70
1	A	2860	A	C4-C5-C6	6.89	120.44	117.00
1	A	2815	C	P-O3'-C3'	-6.88	111.44	119.70
1	A	1142	A	C4-C5-N7	6.87	114.14	110.70
1	A	1247	A	O4'-C1'-N9	6.87	113.70	108.20
1	A	2513	A	N9-C4-C5	6.87	108.55	105.80
1	A	974	G	N7-C8-N9	6.87	116.53	113.10
2	B	36	C	O4'-C1'-N1	-6.87	102.71	108.20
1	A	2822	G	P-O3'-C3'	-6.86	111.47	119.70
1	A	2229	U	O4'-C1'-N1	6.86	113.69	108.20
1	A	2860	A	N9-C4-C5	-6.86	103.06	105.80
1	A	800	A	P-O3'-C3'	6.85	127.92	119.70
1	A	1019	U	N1-C2-O2	-6.85	118.00	122.80
1	A	70	G	P-O3'-C3'	6.85	127.92	119.70
1	A	137	U	O4'-C1'-N1	-6.85	102.72	108.20
1	A	434	U	P-O3'-C3'	6.85	127.92	119.70
1	A	1274	A	P-O3'-C3'	-6.85	111.48	119.70
1	A	1495	A	P-O3'-C3'	-6.85	111.48	119.70
1	A	1452	G	N3-C4-C5	6.84	132.02	128.60
1	A	802	A	C3'-C2'-C1'	6.84	106.97	101.50
1	A	1805	A	N1-C6-N6	-6.84	114.50	118.60
1	A	2701	U	C2-N3-C4	-6.83	122.90	127.00
1	A	2883	A	N1-C6-N6	6.83	122.70	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1868	C	O4'-C1'-N1	6.83	113.66	108.20
1	A	2542	A	P-O3'-C3'	6.83	127.89	119.70
1	A	1359	A	C5-N7-C8	-6.82	100.49	103.90
1	A	1941	C	N1-C1'-C2'	-6.82	104.50	112.00
1	A	1334	G	P-O5'-C5'	-6.81	110.00	120.90
1	A	250	G	P-O3'-C3'	-6.81	111.53	119.70
1	A	1158	C	P-O5'-C5'	-6.81	110.00	120.90
1	A	1757	A	P-O3'-C3'	6.81	127.87	119.70
1	A	972	A	P-O3'-C3'	6.80	127.86	119.70
1	A	1125	G	C4-C5-N7	6.80	113.52	110.80
1	A	2496	C	O4'-C1'-N1	6.80	113.64	108.20
1	A	215	G	P-O3'-C3'	6.80	127.86	119.70
1	A	2005	A	P-O3'-C3'	6.80	127.86	119.70
1	A	1838	C	P-O3'-C3'	6.79	127.85	119.70
12	L	6	LEU	CA-CB-CG	6.79	130.92	115.30
1	A	411	G	P-O3'-C3'	6.78	127.84	119.70
1	A	459	U	P-O3'-C3'	-6.78	111.56	119.70
1	A	2639	A	N9-C1'-C2'	-6.78	104.54	112.00
1	A	1866	A	P-O3'-C3'	-6.78	111.57	119.70
1	A	373	U	P-O3'-C3'	-6.77	111.57	119.70
1	A	974	G	C5-N7-C8	-6.77	100.92	104.30
1	A	2067	G	P-O3'-C3'	6.76	127.82	119.70
1	A	2273	A	N1-C6-N6	6.76	122.66	118.60
1	A	1452	G	N3-C4-N9	-6.76	121.94	126.00
1	A	1342	A	N1-C6-N6	6.76	122.65	118.60
1	A	403	U	P-O3'-C3'	6.75	127.81	119.70
1	A	509	C	N1-C1'-C2'	-6.75	104.57	112.00
1	A	1118	C	P-O5'-C5'	-6.75	110.09	120.90
1	A	2772	C	P-O3'-C3'	-6.75	111.60	119.70
1	A	1142	A	C2-N3-C4	-6.74	107.23	110.60
1	A	1429	G	C3'-C2'-C1'	6.73	106.89	101.50
1	A	1497	U	N1-C1'-C2'	6.73	122.75	114.00
1	A	27	G	P-O3'-C3'	6.73	127.77	119.70
1	A	2893	A	C8-N9-C4	6.72	108.49	105.80
1	A	2063	C	N1-C1'-C2'	-6.72	104.61	112.00
1	A	121	G	P-O3'-C3'	-6.72	111.64	119.70
1	A	824	U	P-O3'-C3'	-6.72	111.64	119.70
1	A	684	G	N9-C4-C5	-6.71	102.72	105.40
1	A	1901	A	C6-N1-C2	6.71	122.63	118.60
1	A	1325	U	O4'-C1'-N1	6.70	113.56	108.20
1	A	671	C	C3'-C2'-C1'	6.69	106.86	101.50
1	A	800	A	N1-C6-N6	-6.69	114.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1019	U	N3-C4-C5	6.69	118.61	114.60
1	A	1155	A	N1-C2-N3	-6.69	125.96	129.30
1	A	2451	A	N1-C6-N6	-6.68	114.59	118.60
1	A	396	G	P-O3'-C3'	-6.67	111.69	119.70
1	A	73	A	C3'-C2'-C1'	6.67	106.84	101.50
2	B	77	U	P-O3'-C3'	-6.67	111.70	119.70
1	A	2093	G	P-O3'-C3'	-6.66	111.70	119.70
1	A	1731	G	N3-C4-N9	-6.66	122.00	126.00
1	A	634	C	O4'-C1'-N1	-6.66	102.87	108.20
1	A	1255	U	O4'-C1'-N1	6.66	113.52	108.20
1	A	2200	C	P-O3'-C3'	-6.65	111.72	119.70
2	B	89	U	C3'-C2'-C1'	6.65	106.82	101.50
1	A	989	G	O4'-C1'-N9	6.65	113.52	108.20
1	A	142	A	N9-C1'-C2'	-6.64	104.69	112.00
1	A	1174	U	P-O3'-C3'	-6.64	111.73	119.70
1	A	1708	C	P-O5'-C5'	-6.64	110.27	120.90
1	A	2293	G	P-O3'-C3'	-6.64	111.73	119.70
1	A	633	A	C4-C5-C6	6.64	120.32	117.00
1	A	2639	A	N1-C6-N6	6.63	122.58	118.60
1	A	1945	G	C3'-C2'-C1'	6.63	106.81	101.50
1	A	1438	U	C5-C4-O4	-6.63	121.92	125.90
1	A	747	U	O5'-P-OP2	-6.62	99.75	105.70
1	A	1661	G	N3-C4-C5	6.62	131.91	128.60
1	A	567	U	P-O3'-C3'	-6.61	111.77	119.70
1	A	2575	C	C5-C4-N4	-6.61	115.57	120.20
1	A	1145	C	N1-C1'-C2'	-6.60	104.74	112.00
1	A	249	C	N1-C1'-C2'	6.60	122.58	114.00
1	A	1932	A	P-O3'-C3'	-6.59	111.79	119.70
1	A	2297	A	N9-C1'-C2'	-6.59	104.75	112.00
1	A	74	A	P-O3'-C3'	6.59	127.61	119.70
1	A	628	G	N9-C1'-C2'	-6.59	104.75	112.00
1	A	1786	A	O4'-C1'-N9	6.59	113.47	108.20
1	A	633	A	C6-C5-N7	-6.59	127.69	132.30
1	A	268	C	O4'-C1'-N1	-6.58	102.94	108.20
2	B	15	A	P-O5'-C5'	-6.58	110.38	120.90
1	A	349	U	O4'-C1'-N1	-6.58	102.94	108.20
1	A	1478	G	C6-C5-N7	6.58	134.34	130.40
1	A	1942	C	P-O3'-C3'	-6.57	111.81	119.70
1	A	831	G	P-O3'-C3'	-6.57	111.82	119.70
1	A	2391	G	O4'-C1'-N9	6.57	113.45	108.20
1	A	2578	G	N1-C6-O6	-6.56	115.96	119.90
2	B	16	G	N9-C1'-C2'	-6.56	104.78	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2511	U	C5-C4-O4	-6.56	121.97	125.90
1	A	1867	G	P-O3'-C3'	-6.56	111.83	119.70
2	B	58	A	P-O3'-C3'	-6.56	111.83	119.70
1	A	2504	U	O4'-C1'-N1	6.55	113.44	108.20
1	A	2881	U	P-O3'-C3'	-6.55	111.84	119.70
1	A	1554	U	P-O3'-C3'	6.55	127.56	119.70
1	A	2556	C	O4'-C1'-N1	6.55	113.44	108.20
2	B	90	C	P-O5'-C5'	-6.55	110.42	120.90
2	B	57	A	P-O5'-C5'	-6.55	110.42	120.90
1	A	178	G	N9-C1'-C2'	-6.54	104.80	112.00
1	A	975	A	N9-C1'-C2'	-6.54	104.81	112.00
6	F	110	ILE	CB-CA-C	-6.54	98.53	111.60
1	A	957	C	O4'-C1'-N1	6.53	113.42	108.20
1	A	233	A	N9-C1'-C2'	-6.53	104.82	112.00
1	A	1240	U	N1-C1'-C2'	6.53	122.49	114.00
1	A	2779	U	O4'-C1'-N1	6.52	113.42	108.20
1	A	507	A	P-O5'-C5'	-6.52	110.47	120.90
1	A	907	G	N3-C4-N9	-6.52	122.09	126.00
1	A	1695	G	P-O3'-C3'	-6.52	111.88	119.70
1	A	62	U	P-O3'-C3'	6.52	127.52	119.70
1	A	1430	G	C5-C6-O6	6.52	132.51	128.60
1	A	2148	G	P-O3'-C3'	-6.52	111.88	119.70
1	A	2894	G	N9-C1'-C2'	-6.52	104.83	112.00
1	A	510	C	P-O3'-C3'	-6.51	111.89	119.70
1	A	2363	G	N9-C4-C5	6.51	108.00	105.40
1	A	683	U	N1-C2-N3	6.50	118.80	114.90
1	A	528	A	N9-C1'-C2'	-6.50	104.85	112.00
1	A	800	A	C5-C6-N6	6.50	128.90	123.70
1	A	2728	U	O4'-C1'-N1	6.50	113.40	108.20
1	A	687	C	C3'-C2'-C1'	6.50	106.70	101.50
1	A	1213	A	N9-C1'-C2'	-6.50	104.85	112.00
1	A	2335	A	C3'-C2'-C1'	6.50	106.70	101.50
1	A	1876	A	C5-N7-C8	-6.50	100.65	103.90
8	H	47	PHE	C-N-CA	-6.50	105.46	121.70
1	A	2398	U	P-O3'-C3'	-6.49	111.91	119.70
1	A	1247	A	N1-C6-N6	6.49	122.49	118.60
1	A	23	G	N1-C6-O6	-6.49	116.01	119.90
1	A	974	G	C8-N9-C4	-6.49	103.81	106.40
1	A	1611	C	C3'-C2'-C1'	6.48	106.69	101.50
1	A	2347	C	C3'-C2'-C1'	6.48	106.69	101.50
1	A	299	A	N7-C8-N9	6.48	117.04	113.80
1	A	1760	C	O4'-C1'-N1	6.48	113.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1551	A	P-O3'-C3'	-6.48	111.93	119.70
1	A	2030	A	P-O3'-C3'	6.48	127.47	119.70
1	A	2052	A	N9-C1'-C2'	-6.48	104.88	112.00
1	A	1435	G	P-O3'-C3'	-6.47	111.94	119.70
1	A	919	U	P-O3'-C3'	-6.46	111.94	119.70
1	A	556	A	P-O3'-C3'	6.46	127.45	119.70
1	A	1238	G	P-O3'-C3'	-6.46	111.95	119.70
1	A	503	A	P-O3'-C3'	6.45	127.44	119.70
1	A	2656	U	N1-C1'-C2'	-6.45	104.90	112.00
1	A	1818	U	P-O3'-C3'	-6.45	111.96	119.70
1	A	196	A	P-O3'-C3'	6.45	127.44	119.70
1	A	35	G	C3'-C2'-C1'	6.45	106.66	101.50
1	A	2307	G	O4'-C1'-N9	6.45	113.36	108.20
1	A	587	C	C6-N1-C2	6.44	122.88	120.30
1	A	2332	C	O4'-C1'-N1	6.44	113.35	108.20
1	A	2249	U	O4'-C1'-N1	6.44	113.35	108.20
1	A	2447	G	C2-N3-C4	6.44	115.12	111.90
2	B	68	C	O4'-C1'-N1	6.44	113.35	108.20
1	A	1688	U	O4'-C1'-N1	6.44	113.35	108.20
1	A	505	A	C3'-C2'-C1'	6.43	106.65	101.50
1	A	265	A	P-O3'-C3'	6.43	127.42	119.70
1	A	2385	C	O4'-C1'-N1	-6.42	103.06	108.20
1	A	2546	U	O4'-C1'-N1	-6.42	103.06	108.20
1	A	63	A	P-O3'-C3'	-6.42	112.00	119.70
1	A	1731	G	N9-C4-C5	6.42	107.97	105.40
1	A	271	G	P-O3'-C3'	6.42	127.40	119.70
2	B	24	G	P-O3'-C3'	6.42	127.40	119.70
1	A	60	G	P-O3'-C3'	6.42	127.40	119.70
1	A	633	A	C5-C6-N1	-6.42	114.49	117.70
1	A	752	A	C4-C5-N7	6.41	113.90	110.70
1	A	1060	U	C2-N3-C4	-6.41	123.16	127.00
1	A	995	C	O4'-C1'-N1	-6.40	103.08	108.20
1	A	2239	G	P-O5'-C5'	-6.40	110.66	120.90
1	A	1551	A	C6-N1-C2	6.39	122.43	118.60
1	A	2528	U	P-O3'-C3'	6.39	127.37	119.70
1	A	2822	G	C5-C6-O6	-6.39	124.77	128.60
1	A	2543	G	N9-C1'-C2'	-6.38	104.98	112.00
1	A	2427	C	C3'-C2'-C1'	6.38	106.60	101.50
1	A	460	A	P-O5'-C5'	-6.37	110.71	120.90
1	A	1142	A	N7-C8-N9	6.37	116.98	113.80
1	A	1324	G	O4'-C1'-N9	6.37	113.29	108.20
1	A	783	A	C5-N7-C8	-6.36	100.72	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1277	G	P-O3'-C3'	-6.36	112.07	119.70
1	A	2790	U	N1-C1'-C2'	6.36	122.27	114.00
1	A	1491	G	C3'-C2'-C1'	6.36	106.59	101.50
1	A	2857	G	N1-C2-N2	-6.35	110.48	116.20
1	A	1089	A	P-O3'-C3'	6.35	127.32	119.70
1	A	496	G	P-O3'-C3'	-6.35	112.08	119.70
1	A	958	U	P-O3'-C3'	-6.34	112.09	119.70
1	A	968	C	N1-C2-O2	6.34	122.70	118.90
1	A	395	U	P-O3'-C3'	6.34	127.31	119.70
1	A	2575	C	P-O3'-C3'	6.33	127.30	119.70
1	A	243	U	C3'-C2'-C1'	6.33	106.57	101.50
1	A	934	U	P-O3'-C3'	-6.33	112.10	119.70
1	A	1496	A	N9-C1'-C2'	-6.33	105.04	112.00
1	A	1805	A	C5-C6-N6	6.33	128.77	123.70
1	A	1115	G	O4'-C1'-N9	6.33	113.26	108.20
1	A	2492	U	C3'-C2'-C1'	6.33	106.56	101.50
1	A	229	C	C3'-C2'-C1'	6.33	106.56	101.50
1	A	729	G	C3'-C2'-C1'	6.32	106.56	101.50
1	A	2210	U	O4'-C1'-N1	6.32	113.26	108.20
1	A	1619	G	N9-C1'-C2'	-6.32	105.05	112.00
1	A	1858	A	C3'-C2'-C1'	6.31	106.55	101.50
1	A	2272	U	P-O3'-C3'	6.31	127.27	119.70
1	A	2520	C	C3'-C2'-C1'	6.31	106.55	101.50
1	A	2850	A	P-O3'-C3'	-6.31	112.12	119.70
1	A	1125	G	C2-N3-C4	-6.31	108.75	111.90
1	A	2034	U	N3-C2-O2	-6.31	117.78	122.20
1	A	302	C	C3'-C2'-C1'	6.30	106.54	101.50
1	A	1009	A	C3'-C2'-C1'	6.30	106.54	101.50
1	A	212	G	P-O3'-C3'	-6.30	112.14	119.70
1	A	1552	A	P-O3'-C3'	-6.30	112.14	119.70
1	A	1829	A	C3'-C2'-C1'	6.30	106.54	101.50
1	A	1816	C	C3'-C2'-C1'	6.29	106.53	101.50
1	A	759	G	P-O5'-C5'	-6.28	110.85	120.90
1	A	2545	G	C8-N9-C4	-6.28	103.89	106.40
1	A	858	G	C5-C6-N1	6.28	114.64	111.50
1	A	2517	C	O4'-C1'-N1	6.27	113.22	108.20
1	A	740	C	O4'-C1'-N1	6.27	113.22	108.20
1	A	802	A	P-O3'-C3'	-6.27	112.18	119.70
1	A	946	C	C3'-C2'-C1'	6.27	106.51	101.50
1	A	763	G	C4-N9-C1'	6.27	134.65	126.50
1	A	1568	G	O4'-C1'-N9	-6.26	103.19	108.20
1	A	2036	C	C3'-C2'-C1'	6.26	106.51	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2427	C	C6-N1-C2	-6.26	117.80	120.30
1	A	1962	C	O4'-C1'-N1	6.25	113.20	108.20
1	A	1568	G	P-O3'-C3'	-6.25	112.20	119.70
1	A	119	A	O3'-P-O5'	6.25	115.87	104.00
1	A	2511	U	C2-N1-C1'	6.25	125.19	117.70
1	A	763	G	C3'-C2'-C1'	6.24	106.50	101.50
1	A	2001	C	P-O3'-C3'	-6.24	112.21	119.70
1	A	684	G	N3-C2-N2	6.24	124.27	119.90
1	A	2359	C	C6-N1-C2	6.23	122.79	120.30
1	A	1733	G	P-O3'-C3'	-6.23	112.22	119.70
1	A	1137	G	P-O3'-C3'	-6.23	112.23	119.70
1	A	389	G	P-O3'-C3'	-6.22	112.23	119.70
1	A	1142	A	C6-N1-C2	6.22	122.33	118.60
1	A	2800	A	C3'-C2'-C1'	6.22	106.48	101.50
1	A	162	U	O4'-C1'-N1	6.21	113.17	108.20
1	A	967	U	P-O5'-C5'	-6.21	110.96	120.90
1	A	2780	G	P-O5'-C5'	-6.21	110.97	120.90
1	A	75	G	P-O3'-C3'	-6.21	112.25	119.70
1	A	2812	G	C4-N9-C1'	6.21	134.57	126.50
1	A	1809	A	C3'-C2'-C1'	6.20	106.46	101.50
1	A	2801	G	N9-C1'-C2'	-6.20	105.18	112.00
1	A	2750	A	P-O3'-C3'	6.20	127.14	119.70
1	A	1110	G	P-O3'-C3'	6.20	127.14	119.70
1	A	1914	C	C3'-C2'-C1'	6.19	106.45	101.50
1	A	858	G	N3-C4-C5	-6.19	125.50	128.60
1	A	2066	C	C2-N3-C4	6.19	123.00	119.90
1	A	333	G	C3'-C2'-C1'	6.18	106.45	101.50
1	A	449	A	C3'-C2'-C1'	6.18	106.45	101.50
1	A	1915	U	O4'-C1'-N1	6.18	113.15	108.20
1	A	530	G	C3'-C2'-C1'	6.18	106.45	101.50
1	A	1733	G	C3'-C2'-C1'	6.18	106.44	101.50
1	A	1812	U	C5-C4-O4	6.18	129.61	125.90
1	A	858	G	C2-N3-C4	6.17	114.99	111.90
1	A	1644	C	O4'-C1'-N1	-6.17	103.26	108.20
1	A	1663	G	P-O3'-C3'	6.17	127.10	119.70
1	A	2582	G	P-O3'-C3'	-6.17	112.30	119.70
1	A	2654	A	P-O3'-C3'	6.17	127.10	119.70
1	A	2730	C	O4'-C1'-N1	6.17	113.13	108.20
1	A	301	G	N3-C4-C5	6.16	131.68	128.60
1	A	1318	U	O4'-C1'-N1	6.16	113.13	108.20
1	A	1333	G	P-O5'-C5'	-6.16	111.04	120.90
1	A	2498	C	N1-C1'-C2'	-6.16	105.22	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2607	G	P-O3'-C3'	-6.16	112.31	119.70
1	A	38	A	P-O3'-C3'	-6.16	112.31	119.70
1	A	2023	C	P-O3'-C3'	-6.16	112.31	119.70
1	A	1144	A	C3'-C2'-C1'	6.16	106.42	101.50
1	A	2655	G	P-O3'-C3'	6.16	127.09	119.70
1	A	1273	U	O4'-C1'-N1	6.15	113.12	108.20
2	B	5	U	O4'-C1'-N1	6.15	113.12	108.20
1	A	1778	U	C2-N3-C4	-6.15	123.31	127.00
1	A	378	C	C6-N1-C2	6.15	122.76	120.30
1	A	1498	C	C3'-C2'-C1'	6.15	106.42	101.50
1	A	323	C	O4'-C1'-N1	6.14	113.12	108.20
1	A	747	U	C3'-C2'-C1'	6.14	106.42	101.50
1	A	1340	U	P-O3'-C3'	6.14	127.07	119.70
1	A	411	G	O4'-C1'-N9	6.14	113.11	108.20
1	A	2641	G	N3-C4-N9	-6.14	122.32	126.00
1	A	1728	C	O4'-C1'-N1	6.13	113.11	108.20
1	A	1760	C	C3'-C2'-C1'	6.13	106.41	101.50
1	A	1885	A	C3'-C2'-C1'	6.13	106.41	101.50
1	A	1943	U	N1-C1'-C2'	6.13	121.97	114.00
1	A	181	A	P-O5'-C5'	-6.13	111.09	120.90
1	A	1305	C	P-O3'-C3'	-6.13	112.35	119.70
1	A	2046	G	P-O3'-C3'	6.13	127.05	119.70
1	A	1478	G	C6-N1-C2	6.12	128.78	125.10
1	A	2566	A	O4'-C1'-N9	6.12	113.10	108.20
1	A	126	A	P-O3'-C3'	-6.12	112.35	119.70
1	A	1380	G	P-O5'-C5'	-6.12	111.11	120.90
1	A	1944	U	N1-C1'-C2'	6.12	121.95	114.00
1	A	2450	A	C3'-C2'-C1'	6.12	106.39	101.50
1	A	2514	U	C2-N3-C4	-6.12	123.33	127.00
1	A	2812	G	N3-C4-C5	-6.12	125.54	128.60
1	A	812	C	C3'-C2'-C1'	6.12	106.39	101.50
1	A	1643	G	P-O3'-C3'	-6.11	112.37	119.70
1	A	688	U	P-O5'-C5'	-6.11	111.13	120.90
1	A	1060	U	N1-C2-O2	-6.11	118.53	122.80
1	A	2504	U	C3'-C2'-C1'	6.10	106.38	101.50
1	A	1560	G	C3'-C2'-C1'	6.10	106.38	101.50
1	A	1792	G	N9-C1'-C2'	-6.10	105.29	112.00
1	A	2362	C	P-O3'-C3'	-6.10	112.38	119.70
1	A	435	C	P-O3'-C3'	-6.10	112.38	119.70
1	A	2022	U	P-O5'-C5'	-6.10	111.14	120.90
1	A	2327	A	P-O3'-C3'	-6.10	112.38	119.70
1	A	1015	U	P-O3'-C3'	-6.10	112.38	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1359	A	N7-C8-N9	6.10	116.85	113.80
1	A	1956	U	C3'-C2'-C1'	6.10	106.38	101.50
1	A	2347	C	O4'-C1'-N1	6.10	113.08	108.20
1	A	2797	U	P-O3'-C3'	6.10	127.02	119.70
1	A	587	C	O4'-C1'-N1	6.09	113.08	108.20
1	A	1082	U	N3-C4-C5	6.09	118.25	114.60
1	A	627	A	P-O3'-C3'	6.09	127.01	119.70
1	A	2061	G	C6-N1-C2	-6.09	121.45	125.10
1	A	118	A	P-O3'-C3'	6.09	127.00	119.70
1	A	2297	A	P-O3'-C3'	-6.09	112.40	119.70
1	A	1461	C	C3'-C2'-C1'	6.08	106.37	101.50
1	A	2617	U	C5-C4-O4	6.08	129.55	125.90
1	A	2810	A	N9-C1'-C2'	-6.08	105.31	112.00
1	A	2573	C	C3'-C2'-C1'	6.08	106.36	101.50
1	A	2823	A	P-O3'-C3'	6.08	126.99	119.70
1	A	1865	U	N1-C2-N3	6.08	118.55	114.90
1	A	2092	U	N1-C1'-C2'	6.08	121.90	114.00
1	A	1024	G	P-O5'-C5'	-6.08	111.18	120.90
1	A	1760	C	P-O3'-C3'	-6.07	112.41	119.70
1	A	1980	G	P-O3'-C3'	6.07	126.99	119.70
1	A	630	G	N9-C4-C5	-6.07	102.97	105.40
1	A	1182	G	C3'-C2'-C1'	6.07	106.36	101.50
1	A	1259	G	N3-C4-N9	-6.07	122.36	126.00
1	A	962	G	N3-C4-N9	-6.06	122.36	126.00
1	A	2578	G	N9-C4-C5	6.06	107.83	105.40
1	A	1348	C	C6-N1-C2	6.06	122.72	120.30
1	A	2514	U	N1-C2-O2	-6.06	118.56	122.80
1	A	529	A	C4-C5-C6	-6.06	113.97	117.00
1	A	1952	A	C8-N9-C4	-6.06	103.38	105.80
1	A	1611	C	N1-C1'-C2'	-6.05	105.34	112.00
1	A	1731	G	C8-N9-C1'	6.05	134.87	127.00
1	A	1667	G	P-O3'-C3'	6.05	126.96	119.70
1	A	2407	A	P-O3'-C3'	-6.05	112.44	119.70
1	A	58	G	C8-N9-C4	-6.05	103.98	106.40
1	A	1767	G	C8-N9-C4	-6.05	103.98	106.40
1	A	2867	G	N3-C4-N9	-6.05	122.37	126.00
1	A	513	A	P-O3'-C3'	-6.05	112.44	119.70
1	A	1188	U	C2-N3-C4	6.04	130.63	127.00
1	A	661	A	P-O3'-C3'	-6.04	112.45	119.70
3	C	109	LEU	CA-CB-CG	6.03	129.17	115.30
1	A	548	G	N9-C1'-C2'	-6.03	105.37	112.00
1	A	1770	G	C4-C5-N7	6.03	113.21	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	G	P-O3'-C3'	6.03	126.93	119.70
1	A	1732	C	O4'-C1'-N1	6.03	113.02	108.20
1	A	2828	G	P-O3'-C3'	6.02	126.93	119.70
1	A	216	A	C3'-C2'-C1'	6.02	106.31	101.50
1	A	1716	U	C3'-C2'-C1'	6.02	106.31	101.50
1	A	2148	G	C3'-C2'-C1'	6.02	106.31	101.50
1	A	1	G	P-O3'-C3'	-6.02	112.48	119.70
1	A	1787	A	C6-N1-C2	6.02	122.21	118.60
1	A	1267	U	P-O3'-C3'	-6.01	112.48	119.70
1	A	1387	A	P-O3'-C3'	-6.01	112.48	119.70
1	A	389	G	N9-C1'-C2'	-6.01	105.39	112.00
1	A	1606	C	P-O5'-C5'	-6.01	111.28	120.90
1	A	460	A	C3'-C2'-C1'	6.01	106.31	101.50
1	A	121	G	C3'-C2'-C1'	6.01	106.31	101.50
1	A	1040	A	O4'-C1'-N9	6.01	113.01	108.20
2	B	58	A	N9-C1'-C2'	-6.00	105.40	112.00
1	A	934	U	C3'-C2'-C1'	6.00	106.30	101.50
1	A	1817	G	N9-C1'-C2'	-6.00	105.40	112.00
1	A	2441	U	O4'-C1'-N1	6.00	113.00	108.20
1	A	2426	A	P-O3'-C3'	5.99	126.89	119.70
2	B	37	C	P-O3'-C3'	-5.99	112.51	119.70
1	A	994	C	P-O3'-C3'	-5.99	112.51	119.70
1	A	1157	G	P-O3'-C3'	-5.99	112.51	119.70
1	A	1960	A	C6-N1-C2	5.99	122.19	118.60
1	A	1828	G	P-O5'-C5'	5.98	130.47	120.90
1	A	1135	C	C3'-C2'-C1'	5.98	106.28	101.50
1	A	2543	G	C3'-C2'-C1'	5.98	106.28	101.50
1	A	1508	A	P-O3'-C3'	5.97	126.87	119.70
1	A	1963	U	P-O3'-C3'	-5.97	112.53	119.70
2	B	44	G	P-O3'-C3'	5.97	126.87	119.70
1	A	61	C	P-O3'-C3'	-5.97	112.54	119.70
1	A	1241	A	P-O3'-C3'	5.97	126.86	119.70
1	A	1399	C	P-O3'-C3'	5.97	126.86	119.70
1	A	2049	G	C5-C6-O6	5.96	132.18	128.60
1	A	744	U	N1-C2-N3	5.96	118.48	114.90
1	A	2392	A	P-O5'-C5'	-5.96	111.36	120.90
1	A	2727	A	P-O3'-C3'	-5.96	112.55	119.70
2	B	40	U	P-O3'-C3'	5.96	126.85	119.70
1	A	1204	A	O4'-C1'-N9	5.96	112.97	108.20
1	A	1386	C	N1-C1'-C2'	-5.95	105.45	112.00
1	A	1429	G	N9-C1'-C2'	-5.95	105.45	112.00
1	A	1386	C	C3'-C2'-C1'	5.95	106.26	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1585	C	O4'-C1'-N1	-5.95	103.44	108.20
1	A	1919	A	P-O3'-C3'	-5.95	112.56	119.70
1	A	2022	U	P-O3'-C3'	-5.95	112.56	119.70
1	A	2575	C	C6-N1-C2	5.95	122.68	120.30
1	A	61	C	C3'-C2'-C1'	5.95	106.26	101.50
1	A	2197	U	N1-C1'-C2'	5.95	121.73	114.00
1	A	1733	G	N9-C1'-C2'	-5.95	105.46	112.00
1	A	2752	C	C3'-C2'-C1'	5.94	106.25	101.50
1	A	1026	G	C3'-C2'-C1'	5.94	106.25	101.50
1	A	1568	G	P-O5'-C5'	-5.94	111.39	120.90
1	A	1838	C	O4'-C1'-N1	5.94	112.95	108.20
1	A	365	U	C5-C4-O4	-5.93	122.34	125.90
1	A	633	A	N9-C4-C5	-5.93	103.43	105.80
1	A	1161	C	N1-C2-O2	-5.93	115.34	118.90
1	A	1326	U	C3'-C2'-C1'	5.93	106.25	101.50
1	A	1135	C	N1-C1'-C2'	-5.93	105.48	112.00
1	A	1142	A	N1-C2-N3	-5.93	126.34	129.30
1	A	197	A	N9-C1'-C2'	-5.93	105.48	112.00
1	A	2199	A	O4'-C1'-N9	-5.93	103.46	108.20
1	A	2049	G	C5-C6-N1	-5.92	108.54	111.50
1	A	2055	C	O4'-C1'-N1	-5.92	103.46	108.20
1	A	265	A	O4'-C1'-N9	5.92	112.93	108.20
1	A	520	G	P-O3'-C3'	-5.91	112.61	119.70
1	A	140	C	N1-C1'-C2'	5.91	121.68	114.00
1	A	2075	U	C5-C4-O4	5.90	129.44	125.90
1	A	2857	G	C8-N9-C4	5.90	108.76	106.40
1	A	2860	A	O4'-C1'-N9	-5.90	103.48	108.20
1	A	1130	U	C2-N1-C1'	5.90	124.78	117.70
1	A	1303	G	C3'-C2'-C1'	5.89	106.22	101.50
1	A	1800	C	O4'-C1'-N1	-5.89	103.48	108.20
1	A	2574	G	C3'-C2'-C1'	5.89	106.22	101.50
1	A	653	U	P-O3'-C3'	-5.89	112.63	119.70
1	A	1147	A	N9-C4-C5	5.89	108.16	105.80
1	A	2423	U	N1-C1'-C2'	5.89	121.66	114.00
1	A	2440	C	C3'-C2'-C1'	5.89	106.21	101.50
1	A	1478	G	N9-C4-C5	5.89	107.75	105.40
1	A	469	G	P-O3'-C3'	-5.89	112.64	119.70
2	B	89	U	N1-C1'-C2'	-5.88	105.53	112.00
1	A	1956	U	O4'-C1'-N1	5.88	112.90	108.20
1	A	1696	G	P-O3'-C3'	-5.87	112.65	119.70
1	A	572	A	C3'-C2'-C1'	5.87	106.20	101.50
1	A	1238	G	C3'-C2'-C1'	5.87	106.20	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1666	G	O4'-C1'-N9	5.87	112.90	108.20
1	A	1379	U	C3'-C2'-C1'	5.87	106.20	101.50
1	A	111	A	P-O3'-C3'	-5.86	112.67	119.70
1	A	639	U	O4'-C1'-N1	5.86	112.89	108.20
1	A	919	U	C4-C5-C6	-5.86	116.18	119.70
1	A	460	A	N9-C1'-C2'	-5.86	105.56	112.00
1	A	1707	G	C3'-C2'-C1'	5.86	106.19	101.50
1	A	2276	G	P-O3'-C3'	-5.86	112.67	119.70
1	A	2326	C	N1-C1'-C2'	5.86	121.62	114.00
1	A	2792	A	P-O3'-C3'	-5.86	112.67	119.70
1	A	2868	A	C3'-C2'-C1'	5.85	106.18	101.50
1	A	645	C	C2-N1-C1'	5.85	125.24	118.80
2	B	15	A	N1-C6-N6	5.85	122.11	118.60
1	A	1188	U	O4'-C1'-N1	-5.84	103.52	108.20
1	A	1993	U	C3'-C2'-C1'	5.84	106.18	101.50
1	A	86	G	N9-C1'-C2'	-5.84	105.57	112.00
1	A	2712	C	P-O3'-C3'	5.84	126.71	119.70
1	A	860	U	P-O5'-C5'	-5.84	111.56	120.90
1	A	1510	G	C3'-C2'-C1'	5.84	106.17	101.50
1	A	1326	U	N1-C1'-C2'	-5.84	105.58	112.00
1	A	200	U	O4'-C1'-N1	5.84	112.87	108.20
1	A	2580	U	P-O3'-C3'	5.84	126.70	119.70
1	A	1023	U	P-O3'-C3'	-5.83	112.70	119.70
1	A	2281	A	C6-N1-C2	-5.83	115.10	118.60
2	B	32	U	C6-N1-C2	5.83	124.50	121.00
1	A	2424	C	C3'-C2'-C1'	5.83	106.16	101.50
1	A	138	U	P-O3'-C3'	-5.83	112.70	119.70
1	A	813	U	O4'-C1'-N1	-5.83	103.54	108.20
1	A	1942	C	C3'-C2'-C1'	5.83	106.16	101.50
1	A	975	A	C3'-C2'-C1'	5.83	106.16	101.50
1	A	1345	C	O4'-C1'-N1	5.82	112.86	108.20
1	A	1254	A	C3'-C2'-C1'	5.82	106.16	101.50
1	A	1437	C	O4'-C1'-N1	5.82	112.86	108.20
1	A	2309	A	C3'-C2'-C1'	5.82	106.16	101.50
1	A	395	U	N1-C1'-C2'	5.82	121.56	114.00
1	A	1229	C	C5-C6-N1	-5.81	118.09	121.00
1	A	589	U	P-O3'-C3'	-5.81	112.72	119.70
1	A	2282	G	N3-C4-N9	-5.81	122.51	126.00
1	A	2860	A	C6-C5-N7	-5.81	128.23	132.30
1	A	2639	A	C3'-C2'-C1'	5.81	106.14	101.50
1	A	2896	C	C5-C4-N4	5.81	124.26	120.20
1	A	1981	A	C3'-C2'-C1'	5.80	106.14	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	U	N3-C2-O2	-5.80	118.14	122.20
1	A	522	A	P-O3'-C3'	-5.80	112.74	119.70
1	A	2092	U	P-O3'-C3'	5.80	126.66	119.70
1	A	436	C	C3'-C2'-C1'	5.80	106.14	101.50
1	A	2728	U	P-O5'-C5'	-5.80	111.63	120.90
1	A	818	G	P-O3'-C3'	-5.79	112.75	119.70
1	A	1060	U	N1-C1'-C2'	5.79	121.53	114.00
1	A	482	A	C3'-C2'-C1'	5.79	106.13	101.50
1	A	514	A	P-O3'-C3'	-5.79	112.75	119.70
1	A	1330	C	C3'-C2'-C1'	5.79	106.13	101.50
1	A	2052	A	C5-C6-N6	5.79	128.33	123.70
1	A	2797	U	O4'-C1'-N1	5.79	112.83	108.20
1	A	303	G	N9-C1'-C2'	-5.79	105.63	112.00
1	A	750	A	C8-N9-C4	-5.79	103.48	105.80
1	A	2554	U	P-O3'-C3'	5.79	126.65	119.70
1	A	370	G	P-O3'-C3'	5.79	126.64	119.70
2	B	36	C	C2-N1-C1'	5.79	125.17	118.80
1	A	860	U	C3'-C2'-C1'	5.78	106.13	101.50
1	A	200	U	P-O3'-C3'	-5.78	112.77	119.70
1	A	1156	A	N1-C6-N6	5.78	122.07	118.60
1	A	2650	U	P-O5'-C5'	-5.78	111.65	120.90
1	A	860	U	C5'-C4'-O4'	-5.78	102.17	109.10
1	A	2054	A	N1-C2-N3	5.78	132.19	129.30
1	A	1350	C	P-O3'-C3'	-5.78	112.77	119.70
1	A	1238	G	O4'-C1'-N9	5.77	112.82	108.20
1	A	1649	G	C3'-C2'-C1'	5.77	106.11	101.50
1	A	1331	G	P-O3'-C3'	5.77	126.62	119.70
2	B	43	C	P-O3'-C3'	-5.77	112.78	119.70
1	A	554	U	O4'-C1'-N1	5.77	112.81	108.20
1	A	2099	U	O4'-C1'-N1	5.76	112.81	108.20
1	A	2346	A	P-O3'-C3'	5.76	126.62	119.70
1	A	2682	A	C3'-C2'-C1'	5.76	106.11	101.50
2	B	26	C	P-O5'-C5'	-5.76	111.68	120.90
1	A	831	G	N9-C1'-C2'	-5.76	105.67	112.00
1	A	2777	G	P-O5'-C5'	-5.76	111.69	120.90
2	B	56	G	O3'-P-O5'	5.76	114.94	104.00
2	B	90	C	C3'-C2'-C1'	5.76	106.11	101.50
1	A	92	U	P-O3'-C3'	-5.75	112.80	119.70
1	A	528	A	C4-C5-C6	5.75	119.88	117.00
1	A	585	G	O5'-P-OP2	-5.75	100.52	105.70
1	A	1885	A	N9-C4-C5	5.75	108.10	105.80
1	A	2226	C	P-O3'-C3'	-5.75	112.80	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	U	N1-C1'-C2'	5.75	121.47	114.00
1	A	985	C	O4'-C1'-N1	-5.75	103.60	108.20
1	A	2447	G	O4'-C1'-N9	5.75	112.80	108.20
1	A	1289	C	C3'-C2'-C1'	5.74	106.09	101.50
1	A	1204	A	P-O3'-C3'	5.74	126.59	119.70
1	A	2501	C	P-O3'-C3'	5.74	126.59	119.70
1	A	455	C	P-O3'-C3'	5.74	126.59	119.70
1	A	763	G	N3-C4-N9	5.74	129.44	126.00
1	A	1538	G	C3'-C2'-C1'	5.74	106.09	101.50
1	A	2582	G	N9-C1'-C2'	-5.74	105.69	112.00
1	A	1372	U	C5-C4-O4	-5.74	122.46	125.90
1	A	2441	U	C2-N3-C4	-5.74	123.56	127.00
1	A	2575	C	N3-C4-C5	5.74	124.19	121.90
1	A	943	A	C8-N9-C4	-5.73	103.51	105.80
1	A	2727	A	C3'-C2'-C1'	5.73	106.09	101.50
2	B	90	C	P-O3'-C3'	-5.73	112.82	119.70
2	B	42	C	P-O3'-C3'	-5.73	112.82	119.70
1	A	1866	A	C3'-C2'-C1'	5.73	106.08	101.50
1	A	2618	G	N9-C4-C5	5.73	107.69	105.40
1	A	1379	U	N1-C1'-C2'	-5.72	105.70	112.00
1	A	2034	U	C3'-C2'-C1'	5.72	106.08	101.50
1	A	1493	C	O4'-C1'-N1	5.72	112.78	108.20
1	A	1556	C	P-O3'-C3'	-5.72	112.83	119.70
1	A	621	A	C3'-C2'-C1'	5.72	106.08	101.50
1	A	2511	U	N3-C4-C5	5.72	118.03	114.60
1	A	1821	A	C5-C6-N1	-5.72	114.84	117.70
1	A	1829	A	N9-C1'-C2'	-5.72	105.71	112.00
1	A	1287	A	C3'-C2'-C1'	5.72	106.07	101.50
1	A	1884	G	P-O3'-C3'	5.71	126.56	119.70
1	A	1770	G	C5-C6-O6	-5.71	125.17	128.60
1	A	871	U	P-O5'-C5'	-5.71	111.76	120.90
1	A	1731	G	C6-C5-N7	5.71	133.83	130.40
1	A	223	A	C3'-C2'-C1'	5.71	106.07	101.50
1	A	1821	A	N9-C1'-C2'	-5.71	105.72	112.00
1	A	2787	C	N1-C2-O2	-5.71	115.48	118.90
1	A	2778	A	P-O3'-C3'	5.70	126.55	119.70
1	A	866	A	C3'-C2'-C1'	5.70	106.06	101.50
1	A	2249	U	N1-C1'-C2'	5.70	121.41	114.00
2	B	43	C	C3'-C2'-C1'	5.70	106.06	101.50
1	A	965	C	O4'-C1'-N1	-5.70	103.64	108.20
1	A	1385	A	O4'-C1'-N9	5.70	112.76	108.20
1	A	1693	U	O4'-C1'-N1	5.70	112.76	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2135	A	C3'-C2'-C1'	5.69	106.06	101.50
1	A	683	U	O4'-C1'-N1	5.69	112.75	108.20
1	A	806	C	N1-C1'-C2'	-5.69	105.74	112.00
1	A	2324	U	N1-C1'-C2'	5.69	121.40	114.00
1	A	2226	C	C3'-C2'-C1'	5.69	106.05	101.50
1	A	272	A	C3'-C2'-C1'	5.68	106.05	101.50
1	A	435	C	C3'-C2'-C1'	5.68	106.05	101.50
1	A	1798	U	C5-C4-O4	5.68	129.31	125.90
1	A	1254	A	P-O5'-C5'	-5.68	111.82	120.90
1	A	2710	C	O4'-C1'-N1	5.68	112.74	108.20
1	A	1133	A	P-O5'-C5'	-5.67	111.82	120.90
1	A	1617	C	N1-C2-O2	-5.67	115.50	118.90
1	A	2860	A	C8-N9-C1'	-5.67	117.49	127.70
1	A	2035	G	O5'-P-OP2	-5.67	100.59	105.70
1	A	1009	A	P-O3'-C3'	-5.67	112.89	119.70
4	D	10	GLY	N-CA-C	5.67	127.27	113.10
1	A	1027	A	N9-C1'-C2'	-5.67	105.77	112.00
1	A	2517	C	C6-N1-C2	5.67	122.57	120.30
13	M	41	LEU	CA-CB-CG	5.67	128.33	115.30
1	A	1119	U	N1-C1'-C2'	-5.66	105.77	112.00
1	A	765	C	N1-C1'-C2'	-5.66	105.77	112.00
1	A	19	A	P-O5'-C5'	-5.66	111.85	120.90
1	A	858	G	C5-C6-O6	5.66	131.99	128.60
1	A	2575	C	C4-C5-C6	5.65	120.23	117.40
1	A	2023	C	O4'-C1'-N1	5.65	112.72	108.20
1	A	412	A	P-O3'-C3'	-5.65	112.92	119.70
1	A	1782	U	O4'-C1'-N1	5.65	112.72	108.20
1	A	1125	G	C6-C5-N7	-5.65	127.01	130.40
1	A	2297	A	C3'-C2'-C1'	5.65	106.02	101.50
1	A	922	C	P-O3'-C3'	-5.64	112.93	119.70
1	A	1663	G	C4-C5-N7	-5.64	108.54	110.80
1	A	2385	C	C3'-C2'-C1'	5.64	106.01	101.50
1	A	2629	U	N1-C1'-C2'	5.64	121.33	114.00
1	A	2480	C	O4'-C1'-N1	5.64	112.71	108.20
1	A	1525	A	N1-C6-N6	-5.64	115.22	118.60
1	A	1637	A	P-O5'-C5'	-5.63	111.88	120.90
1	A	197	A	C3'-C2'-C1'	5.63	106.01	101.50
1	A	1143	A	P-O3'-C3'	5.63	126.46	119.70
1	A	233	A	C3'-C2'-C1'	5.63	106.00	101.50
1	A	2716	C	O4'-C1'-N1	5.63	112.70	108.20
1	A	1184	U	N1-C1'-C2'	5.63	121.32	114.00
1	A	2846	G	C8-N9-C4	-5.63	104.15	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1082	U	N1-C2-O2	-5.62	118.86	122.80
1	A	2589	A	C5-C6-N6	5.62	128.20	123.70
1	A	2197	U	P-O3'-C3'	5.62	126.45	119.70
1	A	2733	A	N1-C6-N6	5.62	121.97	118.60
1	A	1045	C	N1-C1'-C2'	5.62	121.30	114.00
1	A	2747	G	C2-N3-C4	-5.62	109.09	111.90
1	A	676	A	N1-C6-N6	5.62	121.97	118.60
1	A	2200	C	C3'-C2'-C1'	5.61	105.99	101.50
1	A	528	A	O4'-C1'-N9	-5.61	103.71	108.20
1	A	2689	U	C2-N1-C1'	-5.61	110.97	117.70
1	A	1817	G	C3'-C2'-C1'	5.60	105.98	101.50
1	A	604	G	P-O3'-C3'	-5.60	112.98	119.70
1	A	1476	U	C2-N3-C4	-5.60	123.64	127.00
1	A	2214	C	C3'-C2'-C1'	5.60	105.98	101.50
1	A	2287	A	P-O3'-C3'	5.60	126.42	119.70
1	A	1669	A	N9-C4-C5	5.60	108.04	105.80
1	A	468	G	C5-C6-N1	5.60	114.30	111.50
1	A	1034	G	N9-C1'-C2'	-5.60	105.84	112.00
1	A	2656	U	N3-C2-O2	-5.60	118.28	122.20
1	A	763	G	C4-C5-N7	5.59	113.04	110.80
1	A	1131	G	O4'-C1'-N9	-5.59	103.72	108.20
1	A	2798	U	O4'-C1'-N1	5.59	112.68	108.20
1	A	2894	G	C4-N9-C1'	5.59	133.77	126.50
1	A	373	U	C3'-C2'-C1'	5.59	105.97	101.50
1	A	2220	U	N1-C1'-C2'	-5.59	105.85	112.00
1	A	2397	G	P-O3'-C3'	-5.59	112.99	119.70
1	A	783	A	C4-C5-N7	5.59	113.49	110.70
1	A	30	G	P-O5'-C5'	-5.58	111.97	120.90
1	A	676	A	C4-C5-N7	5.58	113.49	110.70
1	A	1820	U	O4'-C1'-N1	5.58	112.67	108.20
1	A	2273	A	P-O3'-C3'	-5.58	113.01	119.70
1	A	85	G	N9-C1'-C2'	-5.58	105.87	112.00
1	A	2136	G	N9-C1'-C2'	-5.58	105.87	112.00
1	A	2003	A	C6-N1-C2	-5.57	115.26	118.60
1	A	1128	G	P-O3'-C3'	5.57	126.38	119.70
1	A	1154	G	C8-N9-C4	-5.57	104.17	106.40
1	A	2189	U	O4'-C1'-N1	5.57	112.66	108.20
1	A	2894	G	C3'-C2'-C1'	5.57	105.95	101.50
1	A	1524	G	P-O3'-C3'	-5.56	113.02	119.70
2	B	13	G	C3'-C2'-C1'	5.56	105.95	101.50
2	B	67	G	P-O5'-C5'	-5.56	112.00	120.90
1	A	325	G	P-O3'-C3'	-5.56	113.03	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1495	A	C3'-C2'-C1'	5.56	105.95	101.50
1	A	2541	A	C8-N9-C4	5.56	108.03	105.80
1	A	2631	G	N1-C6-O6	-5.56	116.56	119.90
1	A	1759	A	C3'-C2'-C1'	5.56	105.95	101.50
1	A	1206	G	C3'-C2'-C1'	5.55	105.94	101.50
1	A	1695	G	C3'-C2'-C1'	5.55	105.94	101.50
1	A	1373	A	N1-C6-N6	5.55	121.93	118.60
1	A	2273	A	P-O5'-C5'	-5.55	112.02	120.90
1	A	73	A	P-O3'-C3'	-5.55	113.04	119.70
1	A	1428	C	P-O3'-C3'	5.55	126.36	119.70
1	A	1158	C	N3-C4-C5	-5.55	119.68	121.90
1	A	1499	C	C3'-C2'-C1'	5.55	105.94	101.50
1	A	980	A	C8-N9-C4	-5.55	103.58	105.80
1	A	1663	G	N1-C6-O6	-5.55	116.57	119.90
1	A	1022	G	C2-N3-C4	-5.54	109.13	111.90
1	A	2339	C	O4'-C1'-N1	5.54	112.63	108.20
1	A	544	C	P-O3'-C3'	5.54	126.35	119.70
1	A	2224	G	C2-N3-C4	-5.54	109.13	111.90
1	A	753	A	N1-C6-N6	-5.54	115.28	118.60
1	A	1568	G	C3'-C2'-C1'	5.54	105.93	101.50
1	A	2809	A	P-O3'-C3'	-5.54	113.06	119.70
1	A	1386	C	C6-N1-C2	-5.53	118.09	120.30
1	A	2023	C	C3'-C2'-C1'	5.53	105.93	101.50
1	A	831	G	P-O5'-C5'	-5.53	112.05	120.90
1	A	1457	U	N1-C1'-C2'	5.53	121.19	114.00
1	A	2578	G	C4-C5-N7	-5.53	108.59	110.80
1	A	85	G	C3'-C2'-C1'	5.53	105.92	101.50
1	A	271	G	C4-N9-C1'	-5.53	119.31	126.50
1	A	846	U	O4'-C1'-N1	5.53	112.62	108.20
1	A	2799	A	C3'-C2'-C1'	5.53	105.92	101.50
1	A	794	A	C3'-C2'-C1'	5.53	105.92	101.50
1	A	1021	A	C3'-C2'-C1'	5.53	105.92	101.50
1	A	312	G	P-O3'-C3'	-5.53	113.07	119.70
1	A	2551	C	O4'-C1'-N1	5.53	112.62	108.20
1	A	2857	G	N1-C2-N3	5.52	127.21	123.90
1	A	1408	G	P-O3'-C3'	5.52	126.33	119.70
1	A	1127	A	C3'-C2'-C1'	5.52	105.92	101.50
1	A	1537	G	C3'-C2'-C1'	5.52	105.92	101.50
1	A	1838	C	N1-C1'-C2'	5.52	121.18	114.00
1	A	2361	G	P-O3'-C3'	-5.52	113.08	119.70
1	A	2452	C	O4'-C1'-N1	-5.52	103.78	108.20
1	A	1144	A	P-O3'-C3'	-5.52	113.08	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	762	U	P-O3'-C3'	5.52	126.32	119.70
2	B	23	G	N3-C4-N9	5.52	129.31	126.00
1	A	1309	G	P-O3'-C3'	-5.52	113.08	119.70
1	A	1865	U	N3-C4-C5	5.52	117.91	114.60
1	A	2255	G	P-O3'-C3'	-5.51	113.09	119.70
1	A	674	G	P-O3'-C3'	-5.51	113.09	119.70
1	A	1206	G	P-O3'-C3'	-5.51	113.09	119.70
1	A	1478	G	N1-C6-O6	-5.51	116.60	119.90
1	A	2337	G	P-O3'-C3'	-5.51	113.09	119.70
1	A	2630	G	N9-C1'-C2'	-5.50	105.94	112.00
1	A	2283	C	C3'-C2'-C1'	5.50	105.90	101.50
1	A	250	G	C3'-C2'-C1'	5.50	105.90	101.50
1	A	1090	A	O4'-C1'-N9	5.50	112.60	108.20
1	A	2460	U	O4'-C1'-N1	5.50	112.60	108.20
1	A	2266	A	C5-N7-C8	-5.50	101.15	103.90
1	A	1022	G	C8-N9-C1'	5.50	134.14	127.00
1	A	312	G	N9-C1'-C2'	-5.49	105.96	112.00
1	A	1019	U	O4'-C1'-N1	5.49	112.59	108.20
1	A	1143	A	N1-C6-N6	5.49	121.90	118.60
1	A	1411	U	O4'-C1'-N1	5.49	112.59	108.20
1	A	861	A	C3'-C2'-C1'	5.49	105.89	101.50
1	A	2372	U	P-O5'-C5'	-5.49	112.12	120.90
1	A	1129	A	C3'-C2'-C1'	5.49	105.89	101.50
1	A	1027	A	C3'-C2'-C1'	5.49	105.89	101.50
1	A	1112	G	C3'-C2'-C1'	5.48	105.89	101.50
1	A	2625	G	C8-N9-C4	-5.48	104.21	106.40
1	A	2656	U	C3'-C2'-C1'	5.48	105.89	101.50
1	A	944	C	C6-N1-C2	5.48	122.49	120.30
1	A	2295	C	N1-C1'-C2'	5.48	121.12	114.00
1	A	1091	G	C3'-C2'-C1'	5.48	105.88	101.50
1	A	1343	G	C3'-C2'-C1'	5.48	105.88	101.50
1	A	1876	A	O4'-C1'-N9	5.48	112.58	108.20
1	A	1316	U	O4'-C1'-N1	-5.48	103.82	108.20
1	A	2494	G	C4-C5-N7	-5.48	108.61	110.80
1	A	765	C	P-O3'-C3'	-5.47	113.13	119.70
1	A	1491	G	N9-C1'-C2'	-5.47	105.98	112.00
1	A	1804	C	P-O3'-C3'	-5.47	113.13	119.70
1	A	2574	G	N1-C6-O6	-5.47	116.62	119.90
2	B	29	A	P-O5'-C5'	-5.47	112.14	120.90
1	A	500	G	N3-C4-C5	5.47	131.34	128.60
1	A	1295	C	C5-C4-N4	5.47	124.03	120.20
1	A	503	A	O4'-C1'-N9	5.47	112.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	819	A	P-O3'-C3'	-5.47	113.14	119.70
1	A	1288	G	O5'-P-OP2	-5.47	100.78	105.70
1	A	1430	G	C6-N1-C2	5.47	128.38	125.10
1	A	1560	G	N9-C1'-C2'	-5.47	105.99	112.00
1	A	1881	C	O4'-C1'-N1	5.47	112.57	108.20
1	A	2407	A	N1-C6-N6	-5.47	115.32	118.60
2	B	57	A	O5'-P-OP2	-5.47	100.78	105.70
2	B	75	G	P-O3'-C3'	-5.47	113.14	119.70
1	A	434	U	N1-C1'-C2'	5.46	121.10	114.00
1	A	1682	G	C3'-C2'-C1'	5.46	105.87	101.50
1	A	228	C	O4'-C1'-N1	5.46	112.57	108.20
1	A	2482	A	N1-C6-N6	5.46	121.88	118.60
1	A	533	G	C3'-C2'-C1'	5.46	105.87	101.50
1	A	777	G	P-O3'-C3'	-5.46	113.15	119.70
1	A	1525	A	C5-C6-N6	5.46	128.07	123.70
1	A	2894	G	P-O3'-C3'	-5.46	113.15	119.70
1	A	746	U	N1-C1'-C2'	5.46	121.09	114.00
1	A	1805	A	C8-N9-C4	-5.45	103.62	105.80
1	A	2061	G	N3-C4-C5	-5.45	125.87	128.60
1	A	2386	A	P-O5'-C5'	-5.45	112.18	120.90
1	A	114	U	O4'-C1'-N1	-5.45	103.84	108.20
1	A	1661	G	P-O5'-C5'	-5.45	112.18	120.90
1	A	2063	C	C3'-C2'-C1'	5.45	105.86	101.50
1	A	22	C	C2-N3-C4	-5.45	117.17	119.90
1	A	1946	U	C5-C4-O4	5.45	129.17	125.90
1	A	2791	G	C3'-C2'-C1'	5.45	105.86	101.50
1	A	1885	A	N1-C6-N6	-5.45	115.33	118.60
2	B	74	U	P-O5'-C5'	-5.45	112.19	120.90
1	A	1427	A	O4'-C1'-N9	5.44	112.56	108.20
1	A	2589	A	P-O5'-C5'	-5.44	112.19	120.90
1	A	137	U	P-O3'-C3'	5.44	126.23	119.70
1	A	907	G	C2-N3-C4	-5.44	109.18	111.90
1	A	421	C	N1-C1'-C2'	5.44	121.07	114.00
1	A	693	A	P-O3'-C3'	-5.44	113.17	119.70
1	A	1875	G	P-O3'-C3'	-5.44	113.18	119.70
2	B	25	U	C3'-C2'-C1'	5.44	105.85	101.50
1	A	103	A	C3'-C2'-C1'	5.43	105.85	101.50
1	A	670	A	C8-N9-C4	5.43	107.97	105.80
1	A	1956	U	P-O3'-C3'	-5.43	113.18	119.70
1	A	1965	C	C2-N1-C1'	5.43	124.78	118.80
1	A	1091	G	O4'-C1'-N9	5.43	112.55	108.20
1	A	765	C	C3'-C2'-C1'	5.43	105.84	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1872	A	C3'-C2'-C1'	5.43	105.84	101.50
1	A	302	C	P-O3'-C3'	-5.43	113.19	119.70
1	A	1320	C	P-O3'-C3'	5.43	126.21	119.70
1	A	2217	G	P-O3'-C3'	-5.43	113.19	119.70
1	A	653	U	O4'-C1'-N1	-5.42	103.86	108.20
1	A	1452	G	O4'-C1'-N9	-5.42	103.86	108.20
1	A	2582	G	N1-C6-O6	-5.42	116.64	119.90
1	A	2585	U	N1-C1'-C2'	5.42	121.05	114.00
1	A	480	A	C2-N3-C4	5.42	113.31	110.60
1	A	1148	U	C5-C4-O4	5.42	129.15	125.90
1	A	752	A	OP2-P-O3'	5.42	117.11	105.20
1	A	829	A	N7-C8-N9	-5.41	111.09	113.80
1	A	677	A	C6-N1-C2	-5.41	115.36	118.60
1	A	1359	A	C8-N9-C4	-5.41	103.64	105.80
1	A	2210	U	N1-C1'-C2'	5.41	121.03	114.00
1	A	563	A	P-O3'-C3'	-5.40	113.22	119.70
1	A	1062	G	C3'-C2'-C1'	5.40	105.82	101.50
2	B	94	A	P-O5'-C5'	-5.40	112.26	120.90
1	A	144	A	C6-N1-C2	-5.40	115.36	118.60
1	A	530	G	C8-N9-C1'	-5.40	119.98	127.00
1	A	1841	U	C2-N3-C4	5.39	130.23	127.00
1	A	1009	A	P-O5'-C5'	-5.39	112.28	120.90
1	A	1455	G	N9-C1'-C2'	-5.39	106.07	112.00
1	A	1964	G	C4-C5-N7	-5.39	108.64	110.80
1	A	752	A	C5-N7-C8	-5.39	101.21	103.90
1	A	1621	U	N1-C1'-C2'	5.39	121.00	114.00
1	A	1004	U	O4'-C1'-N1	5.38	112.51	108.20
1	A	1311	G	N3-C4-C5	5.38	131.29	128.60
1	A	703	U	C5-C6-N1	-5.38	120.01	122.70
1	A	1557	C	C3'-C2'-C1'	5.38	105.81	101.50
1	A	491	G	N9-C1'-C2'	-5.38	106.08	112.00
1	A	1109	C	C6-N1-C2	-5.38	118.15	120.30
1	A	791	C	N1-C2-O2	5.38	122.13	118.90
1	A	2874	C	P-O3'-C3'	-5.38	113.25	119.70
1	A	2679	A	C5-C6-N6	5.38	128.00	123.70
2	B	45	A	C3'-C2'-C1'	5.38	105.80	101.50
1	A	2883	A	C5-C6-N1	-5.37	115.01	117.70
1	A	2619	C	C5-C4-N4	5.37	123.96	120.20
1	A	676	A	C5-N7-C8	-5.37	101.22	103.90
1	A	1635	A	C3'-C2'-C1'	5.37	105.79	101.50
1	A	2454	G	P-O3'-C3'	-5.37	113.26	119.70
1	A	2474	U	O4'-C1'-N1	5.36	112.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1947	C	P-O3'-C3'	-5.36	113.27	119.70
1	A	2337	G	C3'-C2'-C1'	5.36	105.79	101.50
1	A	2450	A	N1-C2-N3	-5.36	126.62	129.30
1	A	725	G	P-O3'-C3'	5.36	126.13	119.70
1	A	962	G	N3-C4-C5	5.36	131.28	128.60
1	A	277	G	P-O3'-C3'	5.35	126.12	119.70
1	A	2260	C	P-O3'-C3'	-5.35	113.28	119.70
1	A	2498	C	C3'-C2'-C1'	5.35	105.78	101.50
2	B	17	C	O4'-C1'-N1	5.35	112.48	108.20
1	A	2305	U	P-O3'-C3'	-5.35	113.28	119.70
1	A	783	A	O5'-P-OP2	-5.35	100.89	105.70
1	A	2751	G	P-O5'-C5'	-5.35	112.34	120.90
1	A	521	U	P-O3'-C3'	-5.35	113.28	119.70
1	A	2650	U	C6-N1-C2	5.35	124.21	121.00
1	A	809	G	P-O5'-C5'	-5.34	112.35	120.90
1	A	1871	A	C3'-C2'-C1'	5.34	105.78	101.50
1	A	2489	U	C2-N3-C4	-5.34	123.79	127.00
1	A	727	A	N1-C6-N6	5.34	121.81	118.60
1	A	1606	C	O4'-C1'-N1	-5.34	103.93	108.20
1	A	979	A	P-O5'-C5'	-5.34	112.36	120.90
1	A	2639	A	C4-C5-N7	5.33	113.37	110.70
1	A	505	A	P-O5'-C5'	-5.33	112.37	120.90
1	A	1970	A	P-O3'-C3'	5.33	126.10	119.70
1	A	19	A	P-O3'-C3'	-5.33	113.31	119.70
1	A	2756	U	C6-N1-C2	5.33	124.20	121.00
1	A	1261	C	N1-C2-O2	-5.33	115.70	118.90
1	A	1304	A	C6-N1-C2	5.33	121.80	118.60
1	A	2062	A	C5-C6-N6	-5.33	119.44	123.70
1	A	56	A	P-O3'-C3'	-5.32	113.31	119.70
1	A	958	U	C3'-C2'-C1'	5.32	105.76	101.50
1	A	558	U	P-O3'-C3'	-5.32	113.32	119.70
1	A	984	A	N1-C6-N6	5.32	121.79	118.60
1	A	312	G	C3'-C2'-C1'	5.32	105.75	101.50
1	A	178	G	P-O3'-C3'	-5.32	113.32	119.70
1	A	1293	C	P-O5'-C5'	-5.32	112.39	120.90
1	A	1960	A	P-O3'-C3'	-5.31	113.33	119.70
1	A	964	C	O4'-C1'-N1	-5.31	103.95	108.20
1	A	2902	C	C6-N1-C2	5.31	122.42	120.30
1	A	459	U	C3'-C2'-C1'	5.31	105.75	101.50
1	A	1313	U	N1-C1'-C2'	-5.31	106.16	112.00
1	A	1416	G	P-O3'-C3'	5.31	126.07	119.70
1	A	1521	G	C4-N9-C1'	5.31	133.40	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2068	U	C3'-C2'-C1'	5.31	105.75	101.50
1	A	2282	G	N9-C4-C5	5.31	107.52	105.40
1	A	339	U	C2-N3-C4	-5.30	123.82	127.00
1	A	1979	U	P-O5'-C5'	-5.30	112.41	120.90
1	A	2574	G	P-O3'-C3'	-5.30	113.34	119.70
2	B	17	C	P-O3'-C3'	-5.30	113.33	119.70
1	A	1492	G	O4'-C1'-N9	5.30	112.44	108.20
1	A	2391	G	P-O3'-C3'	5.30	126.06	119.70
1	A	2389	G	P-O5'-C5'	-5.30	112.42	120.90
1	A	2679	A	C6-N1-C2	5.30	121.78	118.60
1	A	829	A	C8-N9-C4	5.30	107.92	105.80
1	A	1206	G	N9-C1'-C2'	-5.30	106.17	112.00
1	A	2025	C	N1-C1'-C2'	5.30	120.89	114.00
1	A	1659	G	P-O5'-C5'	-5.30	112.42	120.90
1	A	2354	C	N3-C2-O2	-5.30	118.19	121.90
1	A	2430	A	O4'-C1'-N9	5.30	112.44	108.20
1	A	933	A	C3'-C2'-C1'	5.29	105.73	101.50
1	A	962	G	C6-N1-C2	5.29	128.28	125.10
1	A	1362	C	O4'-C1'-N1	-5.29	103.97	108.20
1	A	1978	A	C8-N9-C4	5.29	107.92	105.80
1	A	1292	G	P-O3'-C3'	-5.29	113.35	119.70
1	A	1313	U	C3'-C2'-C1'	5.29	105.73	101.50
1	A	206	U	C3'-C2'-C1'	5.29	105.73	101.50
1	A	1144	A	P-O5'-C5'	-5.29	112.44	120.90
1	A	1905	C	O4'-C1'-N1	5.29	112.43	108.20
1	A	1946	U	O4'-C1'-N1	-5.29	103.97	108.20
1	A	749	A	C3'-C2'-C1'	5.28	105.73	101.50
1	A	1731	G	C4-C5-N7	-5.28	108.69	110.80
1	A	1882	U	O4'-C1'-N1	5.28	112.42	108.20
1	A	2823	A	P-O5'-C5'	-5.28	112.45	120.90
1	A	919	U	P-O5'-C5'	5.28	129.35	120.90
1	A	1769	U	O4'-C1'-N1	5.28	112.42	108.20
1	A	107	G	N9-C4-C5	5.28	107.51	105.40
1	A	945	A	N9-C1'-C2'	5.28	120.86	114.00
1	A	1521	G	N3-C4-N9	5.28	129.17	126.00
1	A	25	U	P-O3'-C3'	-5.28	113.37	119.70
1	A	481	G	O4'-C1'-N9	5.28	112.42	108.20
1	A	388	G	P-O5'-C5'	-5.27	112.46	120.90
1	A	2713	U	N1-C1'-C2'	5.27	120.86	114.00
1	A	588	U	C3'-C2'-C1'	5.27	105.72	101.50
1	A	2511	U	C6-N1-C1'	-5.27	113.82	121.20
1	A	2777	G	C3'-C2'-C1'	5.27	105.72	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	G	P-O5'-C5'	-5.27	112.47	120.90
2	B	114	C	C6-N1-C2	5.27	122.41	120.30
1	A	806	C	N1-C2-O2	-5.27	115.74	118.90
1	A	1156	A	O3'-P-O5'	-5.26	94.00	104.00
1	A	2812	G	N3-C4-N9	5.26	129.16	126.00
1	A	2809	A	C3'-C2'-C1'	5.26	105.71	101.50
1	A	415	A	N1-C2-N3	-5.26	126.67	129.30
1	A	1700	A	C3'-C2'-C1'	5.26	105.71	101.50
1	A	1941	C	C3'-C2'-C1'	5.26	105.71	101.50
1	A	475	C	C3'-C2'-C1'	5.25	105.70	101.50
1	A	1051	G	C5-C6-O6	-5.25	125.45	128.60
1	A	1112	G	N9-C1'-C2'	-5.25	106.22	112.00
1	A	1289	C	P-O3'-C3'	-5.25	113.40	119.70
1	A	1694	C	O4'-C1'-N1	5.25	112.40	108.20
1	A	1759	A	N9-C1'-C2'	-5.25	106.22	112.00
1	A	2382	G	N3-C4-C5	5.25	131.23	128.60
1	A	1022	G	C4-N9-C1'	-5.25	119.67	126.50
1	A	1510	G	N9-C1'-C2'	-5.25	106.23	112.00
1	A	1311	G	N3-C4-N9	-5.25	122.85	126.00
1	A	907	G	C5-C6-O6	5.24	131.75	128.60
1	A	918	A	N1-C6-N6	5.24	121.74	118.60
1	A	2899	A	P-O5'-C5'	-5.24	112.52	120.90
1	A	1276	A	C8-N9-C4	-5.24	103.70	105.80
1	A	2241	A	P-O3'-C3'	-5.24	113.41	119.70
1	A	509	C	C6-N1-C2	-5.24	118.21	120.30
1	A	544	C	O4'-C1'-N1	-5.24	104.01	108.20
1	A	1027	A	P-O3'-C3'	-5.23	113.42	119.70
1	A	2369	A	N9-C4-C5	5.23	107.89	105.80
1	A	2615	U	C3'-C2'-C1'	5.23	105.68	101.50
2	B	42	C	C3'-C2'-C1'	5.23	105.68	101.50
1	A	2268	A	C8-N9-C4	-5.23	103.71	105.80
1	A	2491	U	O4'-C1'-N1	5.23	112.38	108.20
1	A	142	A	C3'-C2'-C1'	5.22	105.68	101.50
1	A	2054	A	N9-C4-C5	5.22	107.89	105.80
1	A	682	G	O4'-C1'-N9	-5.22	104.02	108.20
1	A	1228	G	C2-N3-C4	-5.22	109.29	111.90
1	A	2383	G	N9-C1'-C2'	-5.22	106.26	112.00
1	A	529	A	C8-N9-C4	5.22	107.89	105.80
1	A	753	A	P-O5'-C5'	-5.22	112.55	120.90
1	A	1007	C	O4'-C1'-N1	5.22	112.38	108.20
1	A	1971	U	C3'-C2'-C1'	5.22	105.68	101.50
2	B	109	A	N9-C1'-C2'	-5.22	106.26	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2250	G	P-O3'-C3'	5.22	125.96	119.70
1	A	2652	C	O4'-C1'-N1	5.22	112.37	108.20
1	A	2757	A	N1-C6-N6	5.22	121.73	118.60
1	A	509	C	C2-N1-C1'	5.21	124.53	118.80
1	A	651	G	P-O3'-C3'	-5.21	113.44	119.70
1	A	1521	G	C6-C5-N7	-5.21	127.27	130.40
1	A	806	C	C6-N1-C2	-5.21	118.22	120.30
1	A	1967	C	C3'-C2'-C1'	5.21	105.67	101.50
1	A	637	A	O4'-C1'-N9	5.21	112.37	108.20
1	A	548	G	P-O5'-C5'	-5.21	112.57	120.90
1	A	1644	C	C6-N1-C2	5.21	122.38	120.30
1	A	124	G	P-O3'-C3'	5.21	125.95	119.70
1	A	391	A	N9-C1'-C2'	-5.21	106.27	112.00
1	A	570	G	P-O3'-C3'	5.21	125.95	119.70
1	A	858	G	C6-N1-C2	-5.21	121.98	125.10
1	A	1180	U	N1-C1'-C2'	5.20	120.77	114.00
1	A	1476	U	C5-C4-O4	-5.20	122.78	125.90
1	A	2639	A	C5-N7-C8	-5.20	101.30	103.90
1	A	575	A	P-O3'-C3'	-5.20	113.46	119.70
1	A	2714	G	N9-C1'-C2'	-5.20	106.28	112.00
1	A	470	A	C8-N9-C4	-5.20	103.72	105.80
1	A	2497	A	O3'-P-O5'	5.20	113.88	104.00
1	A	1147	A	C4-C5-N7	-5.20	108.10	110.70
1	A	2890	G	O4'-C1'-N9	-5.20	104.04	108.20
1	A	654	A	N9-C1'-C2'	-5.20	106.28	112.00
1	A	2269	G	P-O5'-C5'	-5.20	112.59	120.90
1	A	1555	G	C3'-C2'-C1'	5.19	105.66	101.50
1	A	2570	G	C5-C6-O6	5.19	131.72	128.60
1	A	14	A	P-O5'-C5'	-5.19	112.59	120.90
1	A	2543	G	C5-C6-O6	5.19	131.72	128.60
2	B	91	C	N3-C2-O2	-5.19	118.27	121.90
1	A	919	U	N3-C4-O4	5.19	123.03	119.40
1	A	1663	G	C5-C6-O6	5.19	131.71	128.60
1	A	2656	U	N1-C2-O2	5.19	126.43	122.80
1	A	1459	G	P-O3'-C3'	-5.19	113.47	119.70
1	A	1821	A	C6-N1-C2	5.19	121.71	118.60
6	F	112	ASP	OD1-CG-OD2	5.19	133.16	123.30
1	A	1669	A	N1-C6-N6	-5.19	115.49	118.60
1	A	1809	A	P-O3'-C3'	-5.19	113.47	119.70
1	A	1944	U	O4'-C1'-N1	5.19	112.35	108.20
1	A	1959	G	P-O5'-C5'	-5.19	112.60	120.90
1	A	2691	C	C3'-C2'-C1'	5.19	105.65	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1955	U	O4'-C1'-N1	5.18	112.35	108.20
1	A	1379	U	O4'-C1'-N1	-5.18	104.06	108.20
1	A	2282	G	C8-N9-C1'	5.18	133.74	127.00
1	A	333	G	P-O3'-C3'	-5.18	113.48	119.70
1	A	484	C	O4'-C1'-N1	-5.18	104.06	108.20
1	A	727	A	C3'-C2'-C1'	5.18	105.64	101.50
1	A	1142	A	N9-C4-C5	5.18	107.87	105.80
1	A	1698	A	N1-C6-N6	5.18	121.71	118.60
1	A	1821	A	C3'-C2'-C1'	5.18	105.64	101.50
1	A	1086	A	C6-N1-C2	-5.17	115.50	118.60
1	A	2052	A	C6-N1-C2	5.17	121.70	118.60
1	A	340	A	N1-C6-N6	5.17	121.70	118.60
1	A	655	A	P-O3'-C3'	5.17	125.91	119.70
1	A	1957	C	N1-C2-O2	5.17	122.00	118.90
1	A	1675	C	C3'-C2'-C1'	5.17	105.64	101.50
1	A	1731	G	C4-N9-C1'	-5.17	119.78	126.50
1	A	2135	A	P-O3'-C3'	-5.17	113.50	119.70
1	A	2136	G	C3'-C2'-C1'	5.17	105.63	101.50
1	A	2451	A	C6-N1-C2	-5.17	115.50	118.60
2	B	66	A	P-O5'-C5'	5.17	129.17	120.90
1	A	100	U	N1-C1'-C2'	5.17	120.71	114.00
1	A	66	C	O4'-C1'-N1	5.16	112.33	108.20
1	A	299	A	C8-N9-C4	-5.16	103.73	105.80
1	A	791	C	N3-C2-O2	-5.16	118.29	121.90
1	A	813	U	O5'-P-OP2	-5.16	101.06	105.70
1	A	752	A	N9-C4-C5	-5.16	103.74	105.80
1	A	324	A	C3'-C2'-C1'	5.16	105.63	101.50
1	A	2071	A	P-O3'-C3'	5.16	125.89	119.70
1	A	2322	A	C3'-C2'-C1'	5.16	105.62	101.50
1	A	2513	A	C8-N9-C4	-5.16	103.74	105.80
1	A	12	U	C2-N1-C1'	5.16	123.89	117.70
1	A	1925	C	O4'-C1'-N1	5.16	112.32	108.20
1	A	1144	A	N9-C1'-C2'	-5.15	106.33	112.00
1	A	663	G	C5-C6-O6	5.15	131.69	128.60
1	A	2363	G	C8-N9-C4	-5.15	104.34	106.40
1	A	1058	U	O4'-C1'-N1	5.15	112.32	108.20
1	A	1370	C	N1-C2-O2	-5.15	115.81	118.90
1	A	2822	G	C4-C5-N7	5.15	112.86	110.80
1	A	1867	G	C3'-C2'-C1'	5.14	105.61	101.50
1	A	753	A	C3'-C2'-C1'	5.14	105.61	101.50
1	A	86	G	C3'-C2'-C1'	5.14	105.61	101.50
1	A	2676	C	N1-C2-O2	-5.14	115.82	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2894	G	C8-N9-C1'	-5.14	120.32	127.00
1	A	1249	U	O4'-C1'-N1	-5.14	104.09	108.20
1	A	645	C	C6-N1-C1'	-5.13	114.64	120.80
1	A	1247	A	C1'-O4'-C4'	-5.13	105.79	109.90
1	A	2273	A	C5-N7-C8	-5.13	101.33	103.90
1	A	727	A	N9-C1'-C2'	-5.13	106.35	112.00
1	A	752	A	C5-C6-N6	-5.13	119.59	123.70
1	A	271	G	C8-N9-C1'	5.13	133.67	127.00
1	A	43	G	P-O5'-C5'	-5.13	112.69	120.90
1	A	2513	A	C4-C5-N7	-5.13	108.14	110.70
1	A	1952	A	N9-C4-C5	5.13	107.85	105.80
1	A	2225	A	N1-C6-N6	5.13	121.68	118.60
1	A	1681	G	O4'-C1'-N9	5.12	112.30	108.20
1	A	1183	U	N1-C2-O2	5.12	126.39	122.80
1	A	1476	U	C3'-C2'-C1'	5.12	105.60	101.50
1	A	1554	U	O3'-P-O5'	-5.12	94.26	104.00
1	A	2211	A	P-O5'-C5'	5.12	129.10	120.90
1	A	1033	U	N1-C1'-C2'	5.12	120.66	114.00
1	A	2250	G	N7-C8-N9	5.12	115.66	113.10
1	A	1294	U	O4'-C1'-N1	-5.12	104.11	108.20
1	A	1693	U	O3'-P-O5'	-5.12	94.28	104.00
1	A	2371	G	N3-C2-N2	-5.12	116.32	119.90
1	A	2631	G	C5-C6-O6	5.12	131.67	128.60
1	A	800	A	N9-C4-C5	5.12	107.85	105.80
1	A	1313	U	P-O3'-C3'	-5.12	113.56	119.70
1	A	1657	U	P-O3'-C3'	-5.12	113.56	119.70
1	A	688	U	C3'-C2'-C1'	5.11	105.59	101.50
1	A	1566	A	O4'-C1'-N9	-5.11	104.11	108.20
1	A	1865	U	C5-C6-N1	-5.11	120.14	122.70
1	A	2812	G	C8-N9-C1'	-5.11	120.35	127.00
1	A	1521	G	C8-N9-C1'	-5.11	120.35	127.00
1	A	763	G	C8-N9-C1'	-5.11	120.36	127.00
1	A	2451	A	N9-C4-C5	5.11	107.84	105.80
1	A	1681	G	O3'-P-O5'	-5.11	94.29	104.00
1	A	2262	U	O4'-C1'-N1	5.11	112.29	108.20
1	A	2752	C	O4'-C1'-N1	5.11	112.28	108.20
1	A	2893	A	N7-C8-N9	-5.11	111.25	113.80
1	A	763	G	N7-C8-N9	5.11	115.65	113.10
1	A	962	G	C3'-C2'-C1'	5.11	105.58	101.50
1	A	1649	G	N9-C1'-C2'	-5.11	106.39	112.00
1	A	1915	U	C3'-C2'-C1'	5.10	105.58	101.50
1	A	241	A	O4'-C1'-N9	5.10	112.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1375	U	C5-C4-O4	5.10	128.96	125.90
1	A	1915	U	C2-N1-C1'	5.10	123.82	117.70
1	A	2294	G	C4-C5-N7	5.10	112.84	110.80
2	B	87	U	N1-C1'-C2'	5.10	120.63	114.00
1	A	1682	G	N9-C1'-C2'	-5.10	106.39	112.00
1	A	1019	U	P-O3'-C3'	5.10	125.82	119.70
1	A	1332	G	C4-N9-C1'	5.10	133.13	126.50
1	A	2603	G	N9-C1'-C2'	-5.10	106.39	112.00
18	R	9	GLY	N-CA-C	-5.10	100.35	113.10
1	A	444	C	P-O3'-C3'	-5.10	113.58	119.70
1	A	446	G	P-O3'-C3'	5.10	125.82	119.70
1	A	984	A	O4'-C1'-N9	-5.10	104.12	108.20
1	A	985	C	C2-N1-C1'	5.09	124.40	118.80
1	A	1245	G	N9-C4-C5	5.09	107.44	105.40
1	A	2650	U	C5-C6-N1	-5.09	120.15	122.70
1	A	1787	A	N9-C1'-C2'	-5.09	106.40	112.00
1	A	919	U	N1-C2-N3	-5.09	111.84	114.90
1	A	2075	U	C2-N3-C4	5.09	130.06	127.00
1	A	548	G	C4-N9-C1'	5.09	133.12	126.50
1	A	1442	U	P-O3'-C3'	-5.09	113.59	119.70
1	A	222	A	N1-C6-N6	5.09	121.65	118.60
1	A	1003	G	C8-N9-C4	-5.09	104.36	106.40
1	A	1957	C	N3-C2-O2	-5.09	118.34	121.90
1	A	1208	C	C5-C6-N1	-5.09	118.46	121.00
1	A	1344	U	O4'-C1'-N1	5.09	112.27	108.20
1	A	988	A	P-O3'-C3'	5.08	125.80	119.70
1	A	2312	U	P-O3'-C3'	-5.08	113.60	119.70
1	A	604	G	C3'-C2'-C1'	5.08	105.57	101.50
1	A	2066	C	N1-C2-N3	-5.08	115.64	119.20
1	A	122	G	C3'-C2'-C1'	5.08	105.56	101.50
1	A	1171	G	N9-C4-C5	5.08	107.43	105.40
1	A	1029	A	N9-C4-C5	-5.08	103.77	105.80
1	A	2259	U	C2-N3-C4	-5.08	123.95	127.00
1	A	1380	G	N1-C6-O6	-5.08	116.85	119.90
1	A	2224	G	N9-C4-C5	-5.08	103.37	105.40
1	A	2792	A	C3'-C2'-C1'	5.08	105.56	101.50
1	A	434	U	C5-C6-N1	-5.08	120.16	122.70
1	A	1669	A	C3'-C2'-C1'	5.08	105.56	101.50
1	A	1865	U	N1-C1'-C2'	5.08	120.60	114.00
1	A	2359	C	C5-C6-N1	-5.08	118.46	121.00
1	A	1286	A	C5-N7-C8	5.07	106.44	103.90
1	A	1648	U	C3'-C2'-C1'	5.07	105.56	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2311	A	P-O3'-C3'	5.07	125.78	119.70
1	A	2326	C	C6-N1-C2	5.07	122.33	120.30
1	A	1809	A	N9-C1'-C2'	-5.06	106.43	112.00
2	B	88	C	C6-N1-C2	5.06	122.33	120.30
1	A	2093	G	C3'-C2'-C1'	5.06	105.55	101.50
1	A	1782	U	C3'-C2'-C1'	5.06	105.55	101.50
1	A	58	G	N9-C4-C5	5.05	107.42	105.40
1	A	463	G	O4'-C1'-N9	5.05	112.24	108.20
1	A	807	U	P-O5'-C5'	-5.05	112.81	120.90
1	A	1406	U	N1-C1'-C2'	5.05	120.57	114.00
1	A	1796	U	O4'-C1'-N1	5.05	112.24	108.20
1	A	2520	C	N3-C4-C5	-5.05	119.88	121.90
1	A	1029	A	O4'-C1'-N9	-5.05	104.16	108.20
2	B	53	A	N9-C1'-C2'	-5.05	106.44	112.00
1	A	729	G	P-O3'-C3'	-5.05	113.64	119.70
1	A	1070	A	P-O3'-C3'	5.05	125.76	119.70
1	A	1777	U	C2-N3-C4	5.05	130.03	127.00
1	A	2849	U	C5'-C4'-O4'	-5.05	103.04	109.10
1	A	1958	C	C6-N1-C2	5.05	122.32	120.30
1	A	2818	U	P-O3'-C3'	-5.05	113.64	119.70
1	A	2213	U	P-O3'-C3'	-5.04	113.65	119.70
1	A	2822	G	C6-C5-N7	-5.04	127.37	130.40
1	A	105	C	N1-C2-O2	5.04	121.93	118.90
1	A	1947	C	N1-C2-O2	-5.04	115.87	118.90
1	A	2491	U	O5'-P-OP2	-5.04	101.16	105.70
1	A	1497	U	P-O3'-C3'	5.04	125.75	119.70
1	A	2494	G	P-O3'-C3'	-5.04	113.65	119.70
1	A	2219	U	O4'-C1'-N1	5.04	112.23	108.20
2	B	25	U	N1-C1'-C2'	-5.04	106.46	112.00
1	A	12	U	N1-C2-O2	5.04	126.33	122.80
1	A	1511	G	C3'-C2'-C1'	5.04	105.53	101.50
1	A	1844	C	O4'-C1'-N1	-5.04	104.17	108.20
1	A	8	C	P-O5'-C5'	-5.03	112.85	120.90
1	A	1695	G	C8-N9-C4	-5.03	104.39	106.40
2	B	26	C	C3'-C2'-C1'	5.03	105.53	101.50
2	B	53	A	C3'-C2'-C1'	5.03	105.53	101.50
1	A	461	C	C2-N3-C4	-5.03	117.38	119.90
1	A	2246	G	C6-C5-N7	-5.03	127.38	130.40
1	A	628	G	C3'-C2'-C1'	5.03	105.52	101.50
1	A	1781	U	P-O5'-C5'	-5.03	112.85	120.90
1	A	2268	A	P-O3'-C3'	-5.03	113.67	119.70
1	A	754	U	P-O3'-C3'	-5.03	113.67	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	53	A	P-O3'-C3'	-5.03	113.67	119.70
1	A	2451	A	C8-N9-C1'	5.02	136.74	127.70
1	A	2801	G	P-O3'-C3'	-5.02	113.67	119.70
1	A	60	G	OP1-P-O3'	5.02	116.25	105.20
1	A	1782	U	P-O5'-C5'	-5.02	112.86	120.90
1	A	1872	A	N9-C1'-C2'	-5.02	106.47	112.00
1	A	2867	G	C8-N9-C1'	5.02	133.53	127.00
1	A	1779	U	O4'-C1'-N1	5.02	112.22	108.20
1	A	69	C	C2-N3-C4	5.02	122.41	119.90
1	A	71	A	O5'-P-OP2	-5.02	101.18	105.70
1	A	468	G	C6-N1-C2	-5.02	122.09	125.10
1	A	682	G	C4-N9-C1'	5.02	133.02	126.50
1	A	1667	G	O4'-C1'-N9	5.02	112.21	108.20
1	A	514	A	P-O5'-C5'	-5.01	112.88	120.90
1	A	1539	U	O4'-C1'-N1	5.01	112.21	108.20
1	A	141	G	C3'-C2'-C1'	5.01	105.51	101.50
1	A	334	C	O4'-C1'-N1	5.01	112.21	108.20
1	A	415	A	C6-N1-C2	5.01	121.61	118.60
1	A	2589	A	N1-C6-N6	-5.01	115.59	118.60
1	A	200	U	C3'-C2'-C1'	5.01	105.51	101.50
1	A	623	C	C6-N1-C2	5.01	122.30	120.30
1	A	783	A	N9-C1'-C2'	-5.01	106.49	112.00
1	A	1496	A	P-O5'-C5'	-5.01	112.89	120.90
1	A	2076	U	P-O3'-C3'	-5.01	113.69	119.70
1	A	1908	C	O4'-C1'-N1	5.00	112.20	108.20
1	A	2249	U	C4'-C3'-C2'	5.00	107.61	102.60
1	A	684	G	C4-C5-N7	5.00	112.80	110.80
1	A	1082	U	P-O3'-C3'	5.00	125.70	119.70
1	A	1565	C	O4'-C1'-N1	5.00	112.20	108.20
1	A	2770	G	C2-N3-C4	-5.00	109.40	111.90
1	A	686	U	O5'-P-OP2	-5.00	101.20	105.70
1	A	1985	C	P-O5'-C5'	-5.00	112.90	120.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	10	GLY	Peptide
8	H	48	GLU	Mainchain
8	H	49	ALA	Mainchain
14	N	101	GLY	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61274	0	0	1337	0
2	B	2529	0	0	36	0
3	C	2082	0	0	61	0
4	D	1565	0	0	66	0
5	E	1552	0	0	40	0
6	F	1410	0	0	36	0
7	G	1323	0	0	36	0
8	H	1111	0	0	21	0
9	I	1032	0	0	6	0
10	J	1129	0	0	49	0
11	K	938	0	0	26	0
12	L	1045	0	0	36	0
13	M	1074	0	0	37	0
14	N	960	0	0	25	0
15	O	892	0	0	28	0
16	P	917	0	0	31	0
17	Q	947	0	0	45	0
18	R	816	0	0	18	0
19	S	857	0	0	25	0
20	T	738	0	0	21	0
21	U	779	0	0	18	0
22	V	753	0	0	19	0
23	W	596	0	0	52	0
24	X	625	0	0	22	0
25	Y	509	0	0	14	0
26	Z	449	0	0	6	0
27	0	444	0	0	10	0
28	1	409	0	0	10	0
29	2	377	0	0	6	0
30	3	504	0	0	12	0
31	4	302	0	0	11	0
32	A	136	0	0	0	0
32	B	4	0	0	0	0
32	D	1	0	0	0	0
33	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	2	1	0	0	0	0
34	3	2	0	0	0	0
34	4	3	0	0	0	0
34	A	614	0	0	11	0
34	B	20	0	0	0	0
34	C	8	0	0	1	0
34	D	3	0	0	3	0
34	E	1	0	0	0	0
34	L	4	0	0	0	0
34	N	3	0	0	0	0
34	T	1	0	0	0	0
All	All	90740	0	0	2029	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (2029) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:118:A:C8	1:A:119:A:C8	2.61	0.89
1:A:1509:A:O2'	1:A:1510:G:O5'	1.92	0.88
1:A:954:G:C5	1:A:955:U:C5	2.61	0.87
1:A:370:G:O2'	1:A:424:G:OP1	1.92	0.87
1:A:13:A:O2'	1:A:15:G:N7	2.10	0.85
1:A:931:U:O4	1:A:1166:G:N2	2.09	0.84
1:A:404:A:O2'	1:A:405:U:OP2	1.96	0.83
1:A:1509:A:O2'	1:A:1510:G:P	2.36	0.82
12:L:29:LYS:O	12:L:31:GLY:N	2.12	0.82
23:W:72:GLY:O	23:W:74:LYS:N	2.13	0.82
1:A:1998:A:OP2	4:D:141:ARG:NH2	2.13	0.81
1:A:1818:U:O2'	3:C:152:GLN:O	1.99	0.80
4:D:140:HIS:NE2	34:D:613:HOH:O	2.13	0.80
1:A:2093:G:C6	1:A:2225:A:C8	2.70	0.80
1:A:1269:A:OP2	34:A:3227:HOH:O	2.00	0.79
1:A:1783:A:C2	1:A:2587:A:C4	2.70	0.79
17:Q:63:ARG:NH1	17:Q:96:ASP:CA	2.46	0.79
1:A:996:A:N6	1:A:1160:G:C6	2.51	0.78
1:A:1091:G:O2'	1:A:1092:C:C6	2.37	0.78
1:A:859:G:C8	1:A:859:G:OP2	2.38	0.77
1:A:1079:C:N4	1:A:1088:A:C2	2.52	0.77
1:A:734:A:C5	1:A:735:A:C8	2.73	0.77
31:4:3:VAL:O	31:4:4:ARG:O	2.03	0.75
1:A:2013:A:N3	19:S:88:ARG:NH1	2.34	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2707:U:O2	14:N:71:ARG:NH1	2.20	0.74
1:A:2673:G:C2	1:A:2674:G:C8	2.76	0.74
1:A:734:A:C5	1:A:735:A:N7	2.55	0.74
1:A:395:U:O2'	1:A:396:G:C8	2.40	0.74
1:A:1027:A:C6	1:A:1126:A:N3	2.56	0.74
6:F:134:GLN:O	6:F:136:ILE:N	2.21	0.73
17:Q:85:ALA:O	17:Q:86:SER:C	2.24	0.73
1:A:1181:U:O2'	1:A:1182:G:O5'	2.06	0.73
1:A:1286:A:O2'	1:A:1288:G:OP2	2.05	0.73
1:A:63:A:C2	1:A:64:A:N7	2.56	0.73
21:U:15:GLY:O	21:U:17:ASP:N	2.21	0.73
1:A:2305:U:C4	1:A:2306:C:C4	2.76	0.73
4:D:45:TYR:CD1	4:D:45:TYR:N	2.57	0.72
1:A:395:U:O2'	1:A:396:G:N7	2.22	0.72
1:A:1962:C:O2'	1:A:1964:G:OP2	2.07	0.72
1:A:1681:G:O2'	1:A:1762:A:O2'	2.06	0.72
3:C:141:HIS:N	3:C:190:THR:O	2.23	0.72
10:J:30:THR:CG2	10:J:31:GLU:N	2.53	0.72
1:A:811:U:C4	12:L:21:ARG:NH2	2.57	0.72
10:J:21:THR:CG2	10:J:22:GLY:N	2.51	0.72
1:A:265:A:C8	1:A:428:A:C2	2.77	0.72
6:F:112:ASP:OD1	6:F:113:PHE:N	2.23	0.72
1:A:321:U:O2'	1:A:340:A:O2'	2.06	0.72
1:A:734:A:C4	1:A:735:A:C8	2.77	0.72
1:A:825:A:C1'	12:L:54:GLN:NE2	2.52	0.72
19:S:73:LYS:O	19:S:106:VAL:N	2.23	0.72
4:D:140:HIS:CE1	34:D:614:HOH:O	2.42	0.71
1:A:1027:A:C2	1:A:1126:A:C4	2.78	0.71
1:A:738:G:C6	1:A:739:A:C2	2.79	0.71
29:2:43:THR:O	29:2:44:VAL:CB	2.37	0.71
1:A:1553:A:N7	1:A:1555:G:C5	2.59	0.71
4:D:93:GLY:O	4:D:95:SER:N	2.24	0.71
1:A:1062:G:O2'	1:A:1063:G:O4'	2.08	0.71
1:A:2200:C:N4	1:A:2224:G:N2	2.38	0.71
1:A:811:U:C2	1:A:1251:C:C5	2.79	0.70
1:A:1090:A:C2	1:A:1091:G:C8	2.79	0.70
1:A:2532:G:C5	1:A:2533:U:C5	2.79	0.70
1:A:2583:G:OP2	34:A:3553:HOH:O	2.09	0.70
1:A:1253:A:N7	34:A:3176:HOH:O	2.23	0.70
1:A:1210:G:O2'	1:A:1211:C:OP2	2.07	0.70
1:A:811:U:N3	12:L:21:ARG:NH2	2.40	0.70
1:A:90:U:C2	1:A:91:A:N7	2.60	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1789:A:OP2	3:C:220:ARG:NH1	2.25	0.70
13:M:14:LYS:O	13:M:15:GLY:O	2.09	0.70
1:A:747:U:C4	1:A:2613:U:C5	2.79	0.70
15:O:67:ASN:O	15:O:69:ASP:N	2.24	0.70
3:C:12:ARG:NH1	3:C:12:ARG:CG	2.55	0.70
1:A:528:A:OP2	10:J:116:ARG:NH2	2.24	0.69
1:A:868:U:C4	1:A:869:G:N7	2.60	0.69
1:A:1538:G:N2	1:A:1539:U:C2	2.61	0.69
12:L:77:ILE:O	12:L:110:VAL:O	2.10	0.69
15:O:16:ARG:O	15:O:19:GLN:N	2.26	0.69
1:A:2197:U:O2'	1:A:2198:A:C2'	2.40	0.69
1:A:1943:U:O2	1:A:1943:U:O4'	2.10	0.69
1:A:496:G:C5	1:A:497:A:C8	2.80	0.69
1:A:1385:A:C4	1:A:1386:C:C5	2.81	0.69
23:W:26:GLY:O	23:W:27:GLY:O	2.11	0.69
16:P:50:ARG:CB	16:P:57:ALA:N	2.56	0.68
1:A:1475:G:O2'	1:A:1476:U:OP2	2.10	0.68
1:A:88:G:C2	1:A:89:A:C8	2.82	0.68
17:Q:65:ASN:ND2	17:Q:69:ARG:NH2	2.41	0.68
1:A:1022:G:N2	1:A:1142:A:C2	2.62	0.68
1:A:370:G:C6	1:A:424:G:N7	2.62	0.68
7:G:93:TYR:O	7:G:105:SER:O	2.11	0.68
1:A:2276:G:OP2	13:M:83:GLY:O	2.12	0.68
4:D:107:VAL:O	4:D:174:SER:O	2.11	0.68
1:A:1364:G:OP2	24:X:1:SER:N	2.26	0.68
1:A:725:G:C6	1:A:726:G:N1	2.62	0.68
1:A:522:A:C6	1:A:523:C:C4	2.82	0.68
1:A:704:G:O2'	1:A:726:G:N2	2.27	0.68
1:A:976:G:C2	1:A:977:G:N7	2.61	0.68
1:A:2813:A:C2	1:A:2887:A:N6	2.62	0.67
23:W:14:ASP:OD2	23:W:16:GLU:OE1	2.11	0.67
2:B:52:A:N7	15:O:64:TYR:OH	2.27	0.67
1:A:1783:A:C2	1:A:2587:A:C5	2.83	0.67
13:M:83:GLY:O	13:M:85:GLY:N	2.28	0.67
26:Z:26:LEU:O	26:Z:37:ARG:NH1	2.27	0.67
1:A:373:U:OP2	1:A:400:G:N1	2.28	0.67
1:A:2297:A:N1	1:A:2321:U:C5	2.63	0.67
1:A:1322:A:O3'	19:S:84:ARG:NH1	2.27	0.67
1:A:1997:C:OP2	4:D:129:THR:OG1	2.13	0.67
1:A:1361:G:C5	1:A:1371:G:N2	2.63	0.67
1:A:2848:G:O2'	1:A:2867:G:N2	2.27	0.67
2:B:7:G:O2'	15:O:38:GLN:NE2	2.28	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1181:U:O2'	1:A:1182:G:C8	2.48	0.66
10:J:43:GLU:O	10:J:44:TYR:C	2.33	0.66
23:W:50:VAL:O	23:W:52:CYS:N	2.27	0.66
1:A:1731:G:C4	1:A:1733:G:N7	2.64	0.66
1:A:1652:A:C2	1:A:2006:C:N3	2.63	0.66
1:A:478:A:C6	1:A:480:A:C6	2.83	0.66
1:A:614:A:O2'	1:A:615:U:OP2	2.13	0.66
6:F:107:VAL:CG1	6:F:113:PHE:CZ	2.79	0.66
1:A:994:C:O2	18:R:10:LYS:NZ	2.29	0.66
1:A:1980:G:O2'	1:A:1982:U:OP2	2.14	0.66
13:M:54:THR:O	13:M:56:ALA:N	2.29	0.66
1:A:459:U:O2'	1:A:460:A:C5'	2.44	0.66
1:A:1071:G:C8	1:A:1089:A:N6	2.65	0.65
10:J:43:GLU:O	10:J:45:THR:N	2.29	0.65
1:A:1266:G:OP2	27:O:16:ARG:NE	2.28	0.65
1:A:532:A:C8	1:A:2021:C:C6	2.85	0.65
1:A:763:G:N7	1:A:765:C:C5	2.65	0.65
12:L:93:ASN:ND2	12:L:94:THR:N	2.45	0.65
17:Q:48:ASP:O	17:Q:51:GLN:N	2.30	0.65
13:M:35:ALA:O	13:M:36:VAL:CB	2.45	0.65
1:A:2629:U:O2'	1:A:2630:G:OP2	2.15	0.65
1:A:1422:G:C4	1:A:1423:G:C8	2.85	0.65
1:A:1125:G:C6	1:A:1126:A:N6	2.65	0.64
1:A:9:G:C6	1:A:2629:U:C6	2.85	0.64
1:A:2020:A:C2	1:A:2022:U:O4'	2.50	0.64
1:A:541:A:C2	1:A:553:G:C2	2.85	0.64
1:A:842:U:O4	34:A:3432:HOH:O	2.10	0.64
1:A:272:A:O2'	1:A:273:G:O4'	2.15	0.64
18:R:49:ILE:CB	18:R:51:VAL:O	2.45	0.64
2:B:57:A:C2	2:B:58:A:C4	2.85	0.64
1:A:1436:G:N2	1:A:1557:C:C2	2.65	0.64
1:A:672:C:C2	1:A:809:G:N2	2.65	0.64
1:A:1131:G:C8	10:J:77:HIS:CE1	2.86	0.64
1:A:1721:G:O2'	1:A:1722:A:C8	2.50	0.64
1:A:63:A:C2	1:A:64:A:C8	2.86	0.64
1:A:1057:A:C8	1:A:1086:A:C8	2.85	0.64
1:A:276:U:O2'	1:A:278:A:N7	2.31	0.64
19:S:88:ARG:NE	19:S:94:ASP:OD1	2.30	0.64
1:A:1553:A:N7	1:A:1555:G:C6	2.66	0.64
1:A:77:G:C5	1:A:78:U:C5	2.86	0.64
1:A:1508:A:O2'	1:A:1509:A:O4'	2.17	0.63
1:A:522:A:C5	1:A:523:C:C5	2.86	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1059:G:C6	1:A:1060:U:N3	2.65	0.63
1:A:1517:G:C2	1:A:1518:C:C2	2.86	0.63
1:A:822:G:C5	1:A:836:G:N2	2.67	0.63
16:P:50:ARG:CD	16:P:51:ASN:N	2.61	0.63
1:A:2725:A:O2'	1:A:2726:A:O5'	2.16	0.63
1:A:1847:A:C8	1:A:1848:A:N7	2.66	0.63
1:A:1062:G:C8	1:A:1088:A:C8	2.87	0.63
1:A:2308:G:O2'	1:A:2310:C:C5	2.51	0.63
1:A:2728:U:O2'	1:A:2729:G:C8	2.52	0.63
19:S:96:ILE:CG1	19:S:96:ILE:O	2.47	0.63
17:Q:86:SER:O	17:Q:88:GLU:N	2.31	0.63
1:A:1247:A:C4	1:A:1249:U:C5	2.87	0.63
14:N:106:ASP:OD1	14:N:106:ASP:C	2.37	0.63
19:S:2:GLU:O	19:S:107:VAL:O	2.16	0.63
1:A:945:A:C4	1:A:2448:A:C2	2.86	0.63
1:A:84:A:N1	1:A:103:A:C5	2.67	0.63
1:A:2532:G:N7	1:A:2533:U:C5	2.66	0.62
8:H:31:VAL:CB	8:H:32:PRO:CD	2.76	0.62
1:A:58:G:N2	1:A:70:G:C4	2.67	0.62
1:A:1166:G:C2	1:A:1184:U:O2	2.53	0.62
1:A:2673:G:N3	1:A:2674:G:C8	2.67	0.62
1:A:954:G:C4	1:A:955:U:C6	2.87	0.62
1:A:747:U:C2	1:A:2613:U:O4	2.52	0.62
1:A:9:G:C6	1:A:2629:U:C5	2.87	0.62
1:A:1136:G:N2	1:A:1137:G:C4	2.68	0.62
20:T:27:SER:O	20:T:28:ASN:OD1	2.18	0.62
7:G:61:TRP:O	7:G:65:GLY:N	2.32	0.62
1:A:391:A:C6	1:A:411:G:C2	2.87	0.62
1:A:1082:U:N3	1:A:1086:A:C6	2.67	0.62
1:A:826:U:O2'	12:L:53:GLY:CA	2.47	0.62
1:A:1973:G:C5	1:A:1974:C:C5	2.88	0.62
1:A:2383:G:C4	1:A:2384:U:C5	2.88	0.62
1:A:1082:U:N3	1:A:1086:A:C5	2.68	0.62
7:G:29:ASN:CG	7:G:30:GLY:N	2.51	0.62
13:M:45:GLN:O	13:M:46:ILE:C	2.37	0.62
12:L:87:GLY:O	12:L:89:VAL:N	2.31	0.62
1:A:231:A:C6	1:A:232:G:C2	2.88	0.62
1:A:1456:G:C5	1:A:1457:U:C5	2.88	0.62
1:A:2794:C:C2	1:A:2803:G:N2	2.68	0.62
17:Q:43:GLN:NE2	18:R:77:PHE:CB	2.62	0.61
1:A:2521:C:C2	1:A:2545:G:N2	2.68	0.61
1:A:2209:G:C6	1:A:2210:U:C4	2.87	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:12:THR:CG2	4:D:13:ARG:N	2.63	0.61
1:A:2305:U:C4	1:A:2306:C:N3	2.69	0.61
1:A:572:A:C2	1:A:2033:A:C2	2.88	0.61
1:A:2279:G:N7	23:W:10:ARG:NH2	2.48	0.61
1:A:322:A:C2	1:A:340:A:C6	2.88	0.61
1:A:541:A:N1	1:A:553:G:C6	2.69	0.61
1:A:1649:G:O6	1:A:2009:A:N6	2.33	0.61
1:A:799:G:N1	1:A:800:A:N6	2.48	0.61
1:A:2683:C:O2	11:K:70:ARG:NH2	2.33	0.61
1:A:2796:U:C4	1:A:2798:U:C4	2.89	0.61
1:A:1131:G:C4	10:J:77:HIS:ND1	2.68	0.61
1:A:1179:G:C2	1:A:1180:U:O2'	2.53	0.61
1:A:687:C:O2'	1:A:1780:A:N1	2.33	0.61
7:G:52:GLY:O	7:G:53:PRO:O	2.19	0.61
2:B:20:G:C2	2:B:64:G:C2	2.89	0.61
1:A:1027:A:N1	1:A:1126:A:C4	2.69	0.61
1:A:2287:A:N7	1:A:2289:G:C8	2.69	0.61
1:A:2331:G:O2'	23:W:39:GLN:O	2.19	0.61
23:W:39:GLN:NE2	23:W:43:LYS:N	2.49	0.61
1:A:2733:A:C8	1:A:2733:A:O5'	2.54	0.61
1:A:1429:G:C4	1:A:1568:G:C2	2.88	0.60
30:3:30:HIS:O	30:3:31:ILE:C	2.39	0.60
24:X:52:ALA:O	24:X:53:LYS:CB	2.48	0.60
1:A:854:C:O2	1:A:924:G:C2	2.54	0.60
1:A:27:G:N2	1:A:512:G:O2'	2.34	0.60
5:E:44:ARG:NH2	5:E:44:ARG:CG	2.61	0.60
14:N:23:ASN:ND2	14:N:23:ASN:N	2.50	0.60
1:A:1779:U:C5	1:A:1784:A:N7	2.69	0.60
17:Q:68:ALA:O	17:Q:71:ASN:N	2.34	0.60
11:K:118:LEU:O	11:K:119:ALA:O	2.19	0.60
1:A:528:A:C3'	1:A:528:A:C8	2.83	0.60
8:H:31:VAL:O	8:H:32:PRO:C	2.37	0.60
1:A:604:G:O6	1:A:625:G:C6	2.54	0.60
1:A:1271:G:OP2	34:A:3230:HOH:O	2.16	0.60
1:A:2762:C:N4	1:A:2763:G:C6	2.70	0.60
8:H:40:THR:O	8:H:42:LYS:N	2.35	0.60
1:A:1073:A:C3'	1:A:1074:G:C5'	2.80	0.60
24:X:33:HIS:O	24:X:34:SER:O	2.19	0.60
1:A:2832:U:O2	1:A:2834:G:N1	2.34	0.60
1:A:1195:G:N2	1:A:1196:C:C2	2.69	0.60
1:A:2287:A:C8	1:A:2289:G:C8	2.90	0.60
23:W:37:VAL:CG1	23:W:38:ARG:N	2.65	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2063:C:C4	1:A:2064:C:C5	2.89	0.60
1:A:1315:C:C2	1:A:1338:G:N2	2.69	0.60
1:A:2404:U:O2	1:A:2414:G:C2	2.54	0.60
1:A:2725:A:O2'	1:A:2726:A:C2'	2.50	0.60
4:D:110:THR:N	4:D:202:ILE:O	2.34	0.60
30:3:40:LYS:O	30:3:43:LEU:N	2.35	0.60
1:A:547:A:C8	1:A:548:G:N3	2.70	0.60
11:K:121:GLU:OE2	16:P:64:SER:OG	2.19	0.60
1:A:2134:A:N6	1:A:2157:G:C5	2.70	0.60
1:A:2331:G:N2	1:A:2385:C:C2	2.70	0.60
1:A:1429:G:N3	1:A:1568:G:C2	2.70	0.60
1:A:1681:G:O2'	1:A:1762:A:C2'	2.50	0.59
3:C:85:ASN:OD1	3:C:85:ASN:N	2.35	0.59
1:A:1408:G:C2	1:A:1595:C:O2	2.55	0.59
1:A:14:A:N6	1:A:15:G:C2	2.69	0.59
1:A:1027:A:N1	1:A:1126:A:N3	2.50	0.59
1:A:1083:U:O2	1:A:1086:A:N6	2.36	0.59
1:A:811:U:C4	12:L:21:ARG:CZ	2.85	0.59
1:A:26:G:C2	1:A:27:G:N2	2.71	0.59
1:A:142:A:O2'	1:A:143:C:O4'	2.19	0.59
1:A:447:A:C2	1:A:454:A:C8	2.89	0.59
1:A:2485:G:N2	1:A:2486:C:C2	2.70	0.59
10:J:4:PHE:O	10:J:44:TYR:CE1	2.56	0.59
17:Q:63:ARG:CZ	17:Q:95:ALA:O	2.51	0.59
17:Q:96:ASP:C	17:Q:98:ALA:N	2.54	0.59
4:D:191:GLY:O	4:D:192:ALA:CB	2.50	0.59
1:A:571:U:O3'	18:R:80:ARG:NH2	2.36	0.59
1:A:1079:C:C4	1:A:1080:A:N7	2.70	0.59
25:Y:42:LEU:O	25:Y:45:GLN:O	2.20	0.59
13:M:1:MET:O	13:M:2:LEU:CB	2.49	0.59
1:A:2400:G:C5	1:A:2401:U:C5	2.91	0.59
1:A:1539:U:O2'	1:A:1540:G:O4'	2.20	0.59
1:A:822:G:C6	1:A:836:G:C2	2.91	0.59
1:A:2307:G:C2	1:A:2311:A:N7	2.71	0.59
1:A:2795:C:C2	1:A:2802:G:N2	2.71	0.59
19:S:12:SER:OG	19:S:13:SER:N	2.35	0.59
1:A:995:C:O2'	1:A:996:A:P	2.60	0.59
1:A:1555:G:C6	1:A:1556:C:N4	2.71	0.59
1:A:1050:A:C2	1:A:2751:G:C5	2.90	0.59
1:A:2023:C:O2'	1:A:2024:G:C5'	2.50	0.59
1:A:637:A:C4'	1:A:638:G:O5'	2.51	0.59
1:A:1343:G:C4	1:A:1344:U:C5	2.90	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1361:G:C4	1:A:1371:G:N2	2.71	0.59
23:W:35:ILE:O	23:W:37:VAL:N	2.36	0.59
4:D:118:PHE:O	4:D:120:GLY:N	2.36	0.59
1:A:554:U:C4	1:A:555:G:C6	2.90	0.59
1:A:1140:C:OP1	10:J:25:LEU:O	2.21	0.58
4:D:91:THR:O	4:D:93:GLY:N	2.35	0.58
1:A:2297:A:N7	1:A:2320:U:N3	2.51	0.58
23:W:9:THR:OG1	23:W:10:ARG:N	2.35	0.58
14:N:79:LEU:O	14:N:80:PHE:CB	2.50	0.58
1:A:222:A:C6	1:A:224:U:O2	2.56	0.58
1:A:2714:G:P	34:A:3394:HOH:O	2.61	0.58
1:A:1553:A:C8	1:A:1555:G:C6	2.91	0.58
15:O:111:ARG:O	15:O:113:ALA:N	2.36	0.58
16:P:19:PHE:O	16:P:20:ARG:CB	2.50	0.58
1:A:1106:G:C2	1:A:1107:G:C8	2.91	0.58
13:M:72:PRO:O	13:M:91:TYR:O	2.21	0.58
10:J:42:ALA:O	10:J:43:GLU:C	2.40	0.58
1:A:1422:G:N3	1:A:1423:G:C8	2.71	0.58
4:D:118:PHE:CD2	4:D:119:ALA:N	2.71	0.58
11:K:34:GLY:O	11:K:35:VAL:C	2.41	0.58
1:A:522:A:C6	1:A:523:C:N4	2.72	0.58
1:A:976:G:C2	1:A:977:G:C8	2.91	0.58
30:3:21:PHE:O	30:3:22:LYS:O	2.21	0.58
1:A:1333:G:N3	1:A:1334:G:C8	2.71	0.58
1:A:2665:A:C2	1:A:2666:C:C6	2.92	0.58
1:A:2850:A:C2	1:A:2851:A:C4	2.90	0.58
1:A:684:G:OP1	29:2:16:HIS:CD2	2.57	0.58
1:A:2052:A:N6	1:A:2618:G:C2	2.72	0.58
1:A:1257:C:O2'	5:E:79:ARG:N	2.36	0.58
23:W:72:GLY:C	23:W:74:LYS:N	2.54	0.58
1:A:2636:C:O2'	4:D:45:TYR:OH	2.21	0.58
1:A:522:A:N6	1:A:523:C:N4	2.51	0.58
1:A:638:G:C5	1:A:651:G:N2	2.72	0.58
1:A:2391:G:O6	1:A:2425:A:C8	2.56	0.58
1:A:856:G:N2	1:A:857:G:C2	2.71	0.58
4:D:140:HIS:CE1	34:D:613:HOH:O	2.53	0.58
1:A:2581:G:C8	1:A:2610:C:N4	2.71	0.58
1:A:633:A:C8	1:A:633:A:O5'	2.57	0.58
1:A:1416:G:O2'	1:A:1417:C:O5'	2.22	0.58
1:A:860:U:O2'	1:A:861:A:C5'	2.52	0.58
1:A:2776:A:O2'	1:A:2777:G:OP2	2.20	0.58
1:A:1060:U:O4'	1:A:1062:G:C5'	2.52	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:655:A:O2'	1:A:656:G:C8	2.57	0.58
5:E:79:ARG:CG	5:E:80:SER:N	2.67	0.58
21:U:53:GLN:N	21:U:54:PRO:CD	2.67	0.58
1:A:176:A:N7	1:A:177:G:C6	2.72	0.57
1:A:60:G:N3	1:A:74:A:C2	2.72	0.57
6:F:30:VAL:CG1	6:F:96:TRP:CH2	2.87	0.57
10:J:101:ILE:O	10:J:105:VAL:CG1	2.51	0.57
22:V:80:HIS:CD2	22:V:83:LYS:N	2.72	0.57
1:A:747:U:C4	1:A:2613:U:C4	2.92	0.57
19:S:25:ARG:NE	19:S:73:LYS:NZ	2.52	0.57
10:J:73:VAL:CG2	10:J:74:TYR:N	2.67	0.57
1:A:954:G:N7	1:A:955:U:C5	2.72	0.57
15:O:103:VAL:O	15:O:105:ALA:O	2.22	0.57
1:A:51:G:N2	1:A:120:U:O2	2.37	0.57
1:A:838:C:C5	1:A:941:A:N6	2.72	0.57
1:A:827:U:OP2	1:A:828:U:N3	2.37	0.57
3:C:103:ILE:O	3:C:104:LEU:O	2.23	0.57
1:A:2297:A:C5	1:A:2320:U:C2	2.92	0.57
1:A:447:A:N1	1:A:454:A:C8	2.72	0.57
10:J:56:VAL:CG1	10:J:57:LEU:N	2.67	0.57
13:M:78:LEU:O	13:M:80:VAL:N	2.37	0.57
1:A:31:C:O3'	1:A:1238:G:C5'	2.52	0.57
1:A:1782:U:C4	1:A:2587:A:C2	2.92	0.57
1:A:300:A:N1	1:A:333:G:O2'	2.38	0.57
16:P:4:ILE:CG2	16:P:5:LYS:N	2.68	0.57
1:A:1165:A:C2	1:A:1185:G:C2	2.92	0.57
1:A:475:C:N3	1:A:481:G:C6	2.72	0.57
1:A:2049:G:N2	1:A:2620:C:C2	2.73	0.57
1:A:1050:A:C2	1:A:2751:G:C4	2.93	0.57
4:D:184:ARG:NH1	16:P:6:GLN:OE1	2.37	0.57
28:1:8:ILE:CG2	28:1:9:LYS:N	2.68	0.57
14:N:69:ARG:O	14:N:70:THR:OG1	2.23	0.57
1:A:1063:G:C6	1:A:1064:C:N3	2.72	0.57
1:A:2383:G:C5	1:A:2384:U:C5	2.93	0.57
1:A:2592:G:C6	1:A:2593:U:C4	2.93	0.57
13:M:13:HIS:O	13:M:14:LYS:CB	2.53	0.57
1:A:1022:G:O2'	1:A:1023:U:OP2	2.23	0.57
1:A:2307:G:N2	1:A:2311:A:C8	2.72	0.57
1:A:638:G:O2'	1:A:639:U:O4'	2.23	0.57
1:A:163:C:O2'	1:A:164:C:C5'	2.52	0.57
15:O:31:THR:CG2	15:O:34:HIS:N	2.68	0.57
1:A:1115:G:O2'	1:A:1116:G:O5'	2.23	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1253:A:C5	34:A:3176:HOH:O	2.58	0.57
2:B:53:A:C2	2:B:54:G:C8	2.93	0.57
1:A:2860:A:C8	1:A:2860:A:C3'	2.88	0.57
1:A:84:A:N1	1:A:103:A:C6	2.72	0.56
1:A:974:G:C2	1:A:1186:G:N1	2.73	0.56
7:G:84:LYS:CG	7:G:132:LEU:N	2.68	0.56
17:Q:91:ARG:N	18:R:11:GLN:OE1	2.38	0.56
1:A:532:A:C8	1:A:2021:C:C5	2.93	0.56
11:K:78:ARG:NH1	16:P:70:GLU:OE2	2.38	0.56
1:A:2792:A:C2	1:A:2793:C:C2	2.93	0.56
23:W:8:SER:O	23:W:9:THR:CB	2.53	0.56
2:B:51:G:N2	2:B:53:A:N6	2.53	0.56
1:A:2548:U:O2	11:K:23:LYS:NZ	2.38	0.56
1:A:2397:G:C2	1:A:2420:C:O2	2.58	0.56
25:Y:56:LEU:O	25:Y:57:LEU:CB	2.53	0.56
1:A:570:G:OP1	1:A:972:A:O2'	2.23	0.56
1:A:919:U:N3	1:A:920:A:N7	2.54	0.56
1:A:83:A:N6	1:A:101:A:C4	2.74	0.56
3:C:106:PRO:CA	3:C:141:HIS:CE1	2.87	0.56
6:F:148:VAL:O	6:F:150:GLY:N	2.38	0.56
1:A:950:G:C5	1:A:951:C:C5	2.93	0.56
10:J:38:GLY:O	10:J:40:HIS:N	2.39	0.56
1:A:2135:A:C2'	1:A:2136:G:C8	2.88	0.56
1:A:2391:G:O2'	1:A:2424:C:N4	2.37	0.56
20:T:19:LYS:O	20:T:23:ALA:N	2.37	0.56
1:A:2656:U:C5	1:A:2664:G:N2	2.73	0.56
1:A:831:G:C6	1:A:832:U:C4	2.93	0.56
1:A:1509:A:O2'	1:A:1510:G:OP2	2.23	0.56
1:A:1653:G:O6	14:N:11:ASN:N	2.39	0.56
1:A:27:G:O2'	1:A:28:A:P	2.64	0.56
25:Y:45:GLN:O	25:Y:46:VAL:CB	2.51	0.56
1:A:1021:A:N6	1:A:1142:A:N6	2.54	0.56
1:A:1419:A:N7	1:A:1421:G:C6	2.74	0.56
1:A:271:G:O2'	1:A:272:A:C5'	2.53	0.56
1:A:100:U:C2	1:A:101:A:N6	2.73	0.56
1:A:2516:A:C4	1:A:2569:G:N2	2.73	0.56
1:A:2816:G:C4	1:A:2817:U:C5	2.93	0.56
1:A:864:G:C6	1:A:865:C:N4	2.74	0.56
4:D:99:GLU:CG	4:D:100:LEU:N	2.69	0.56
3:C:263:ASP:O	3:C:264:LYS:C	2.44	0.56
26:Z:29:ARG:NH2	26:Z:29:ARG:CG	2.69	0.56
31:4:9:LYS:CD	31:4:9:LYS:N	2.68	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:231:A:N6	1:A:232:G:N2	2.54	0.56
1:A:35:G:O2'	1:A:36:G:O5'	2.23	0.56
1:A:1383:A:C6	1:A:1384:A:N1	2.74	0.56
24:X:14:GLY:O	24:X:26:ARG:N	2.39	0.56
1:A:463:G:N1	1:A:467:G:C6	2.74	0.56
1:A:960:A:N7	1:A:962:G:C8	2.74	0.56
10:J:112:GLY:O	10:J:113:PRO:C	2.45	0.56
10:J:13:ARG:O	10:J:14:ASP:CB	2.54	0.56
1:A:2305:U:C5	1:A:2306:C:C4	2.94	0.55
1:A:1649:G:O2'	14:N:106:ASP:OD2	2.23	0.55
1:A:503:A:C2	1:A:505:A:C4	2.95	0.55
1:A:1313:U:C6	1:A:1610:A:N3	2.74	0.55
1:A:1468:U:C2	1:A:1522:A:C2	2.95	0.55
1:A:2144:G:C2'	1:A:2148:G:O6	2.54	0.55
1:A:1998:A:P	4:D:141:ARG:NH2	2.79	0.55
1:A:1026:G:C2'	1:A:1027:A:C8	2.89	0.55
1:A:2657:A:C2	1:A:2665:A:C4	2.94	0.55
1:A:1831:G:C4	1:A:1832:C:C5	2.94	0.55
1:A:2697:G:C5	1:A:2698:U:C5	2.94	0.55
3:C:184:GLU:O	3:C:186:ASP:N	2.39	0.55
1:A:977:G:C2	1:A:978:G:C8	2.94	0.55
1:A:1006:C:C6	1:A:1138:G:N2	2.74	0.55
3:C:69:ASN:O	3:C:117:SER:OG	2.25	0.55
1:A:1734:G:C4	1:A:1735:A:C8	2.94	0.55
1:A:7:G:C6	1:A:8:C:C4	2.94	0.55
12:L:81:ASP:O	12:L:83:ALA:N	2.39	0.55
1:A:1079:C:C4	1:A:1088:A:C2	2.95	0.55
1:A:860:U:C5'	1:A:860:U:C6	2.89	0.55
1:A:1833:C:C2	1:A:1834:U:C6	2.95	0.55
1:A:370:G:C6	1:A:424:G:C8	2.94	0.55
1:A:1495:A:O2'	1:A:1496:A:C8	2.58	0.55
1:A:77:G:C6	1:A:78:U:C4	2.95	0.55
1:A:983:A:C6	1:A:984:A:C2	2.95	0.55
1:A:949:G:N2	1:A:969:G:C4	2.75	0.55
21:U:97:SER:O	21:U:98:ASN:CB	2.54	0.55
1:A:1805:A:N3	3:C:49:THR:CG2	2.70	0.55
1:A:790:U:O2'	1:A:791:C:O5'	2.24	0.55
1:A:2417:C:C2	1:A:2418:A:C8	2.94	0.55
1:A:85:G:O6	1:A:98:G:C6	2.59	0.55
13:M:70:ASP:OD1	13:M:70:ASP:C	2.45	0.55
1:A:60:G:O2'	1:A:61:C:P	2.64	0.55
1:A:2304:G:N2	6:F:152:ASP:OD1	2.40	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1797:G:C6	1:A:1798:U:C4	2.94	0.55
1:A:2037:A:C2	1:A:2038:G:C4	2.94	0.55
1:A:1649:G:C6	1:A:2009:A:C6	2.94	0.55
1:A:2484:G:C2	1:A:2485:G:C8	2.94	0.55
3:C:90:ILE:CG2	3:C:102:TYR:CD1	2.90	0.55
1:A:432:A:C5	1:A:433:C:C5	2.94	0.55
1:A:469:G:O6	29:2:39:ARG:NH1	2.39	0.55
1:A:60:G:C2	1:A:74:A:C2	2.95	0.55
1:A:1385:A:C6	1:A:1403:A:C5	2.95	0.55
9:I:104:GLN:O	9:I:105:LEU:CB	2.55	0.55
1:A:242:G:N2	1:A:255:A:OP2	2.39	0.55
1:A:1017:G:C5	1:A:1018:U:C5	2.95	0.55
3:C:104:LEU:O	3:C:105:ALA:CB	2.54	0.55
1:A:88:G:C6	1:A:89:A:N7	2.75	0.55
1:A:229:C:C5	1:A:230:G:C8	2.95	0.55
1:A:1944:U:O4	1:A:2557:G:N2	2.40	0.55
1:A:10:A:C5	1:A:2800:A:C6	2.95	0.55
1:A:1641:A:N6	1:A:1642:G:C2	2.74	0.55
6:F:134:GLN:CG	6:F:135:ILE:N	2.70	0.55
1:A:2209:G:C5	1:A:2210:U:C4	2.95	0.55
1:A:515:A:C8	1:A:516:C:C5	2.95	0.55
1:A:2063:C:O2	1:A:2450:A:N1	2.40	0.55
1:A:639:U:C2	1:A:640:C:C5	2.95	0.55
1:A:1820:U:O2	3:C:200:MET:N	2.40	0.55
1:A:195:A:C6	1:A:198:C:C5	2.95	0.55
1:A:1667:G:O2'	1:A:1991:U:O4	2.24	0.54
22:V:51:GLN:O	22:V:51:GLN:NE2	2.40	0.54
29:2:3:ARG:NH2	29:2:3:ARG:CG	2.70	0.54
4:D:14:ILE:CG1	4:D:14:ILE:O	2.55	0.54
1:A:2305:U:C2'	1:A:2306:C:O4'	2.55	0.54
1:A:2287:A:C5	1:A:2289:G:C8	2.96	0.54
1:A:2808:G:N2	1:A:2891:U:C6	2.76	0.54
1:A:187:G:C2	1:A:210:C:O2	2.61	0.54
1:A:1995:U:O2	11:K:3:GLN:NE2	2.40	0.54
1:A:1274:A:C2	1:A:1645:G:O4'	2.60	0.54
3:C:254:LYS:O	3:C:256:THR:N	2.40	0.54
1:A:1965:C:C6	1:A:1965:C:C5'	2.90	0.54
1:A:1019:U:C4	1:A:1020:A:N6	2.75	0.54
1:A:1817:G:O2'	1:A:1818:U:C5'	2.56	0.54
1:A:1385:A:C6	1:A:1403:A:C6	2.96	0.54
1:A:1416:G:O2'	1:A:1417:C:O4'	2.25	0.54
1:A:1017:G:C6	1:A:1018:U:C5	2.95	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1900:A:C2	1:A:1970:A:C4	2.96	0.54
1:A:685:A:C2	1:A:689:A:C6	2.95	0.54
2:B:37:C:C5	2:B:38:C:C4	2.96	0.54
1:A:976:G:C2	1:A:977:G:C5	2.96	0.54
1:A:2289:G:O2'	1:A:2346:A:OP2	2.25	0.54
1:A:2720:U:C2	1:A:2872:A:C5	2.95	0.54
2:B:61:G:C6	2:B:62:C:C4	2.96	0.54
1:A:2602:A:C4'	1:A:2603:G:OP2	2.56	0.54
1:A:1298:C:C2	1:A:1643:G:N2	2.75	0.54
8:H:8:LYS:O	8:H:9:VAL:CB	2.55	0.54
11:K:18:ARG:CG	11:K:18:ARG:NH1	2.69	0.54
1:A:151:C:O2	1:A:176:A:C2	2.61	0.54
1:A:1088:A:O4'	1:A:1088:A:N3	2.39	0.54
1:A:827:U:C4	1:A:2430:A:C6	2.95	0.54
1:A:243:U:OP1	30:3:5:THR:CG2	2.55	0.54
7:G:15:ASP:CG	7:G:16:VAL:N	2.61	0.54
4:D:16:THR:O	4:D:19:GLY:N	2.40	0.54
1:A:2846:G:OP1	16:P:50:ARG:O	2.25	0.54
19:S:13:SER:O	19:S:14:ALA:CB	2.55	0.54
1:A:1797:G:O3'	3:C:255:LYS:O	2.25	0.54
1:A:776:G:C5	1:A:793:A:C8	2.95	0.54
1:A:1380:G:C2	1:A:1381:G:C8	2.95	0.54
1:A:1779:U:C5	1:A:1783:A:C8	2.95	0.54
14:N:71:ARG:NH2	14:N:71:ARG:CG	2.71	0.54
1:A:1555:G:N2	1:A:1556:C:C2	2.75	0.54
23:W:24:ARG:CD	23:W:25:PHE:N	2.71	0.54
1:A:2091:C:O2	24:X:33:HIS:CE1	2.61	0.54
1:A:136:G:C6	1:A:142:A:N6	2.75	0.54
1:A:2018:G:C2	1:A:2019:A:C4	2.96	0.54
1:A:369:U:O2'	1:A:370:G:OP2	2.26	0.54
1:A:734:A:N7	1:A:735:A:N7	2.56	0.54
1:A:265:A:N7	1:A:428:A:N3	2.55	0.54
1:A:1555:G:N1	1:A:1556:C:C4	2.76	0.54
1:A:479:A:C2	1:A:480:A:C4	2.95	0.54
16:P:4:ILE:O	16:P:6:GLN:N	2.41	0.54
1:A:2100:G:C6	1:A:2190:G:C6	2.95	0.54
4:D:143:PRO:O	4:D:144:GLY:O	2.26	0.54
18:R:90:ARG:O	18:R:91:GLN:CB	2.56	0.54
1:A:63:A:N3	1:A:64:A:C8	2.76	0.54
1:A:554:U:O4	1:A:555:G:C6	2.61	0.54
5:E:104:ALA:O	5:E:108:ILE:CG2	2.56	0.54
1:A:1387:A:O2'	1:A:1388:G:O4'	2.25	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1394:U:C4	1:A:1395:A:C6	2.96	0.54
1:A:2508:G:C4	1:A:2509:G:C8	2.96	0.54
19:S:97:LEU:N	19:S:97:LEU:CD2	2.70	0.54
16:P:50:ARG:CG	16:P:57:ALA:N	2.71	0.54
2:B:20:G:C2	2:B:64:G:N3	2.76	0.54
1:A:790:U:O2'	1:A:791:C:C5'	2.56	0.54
14:N:35:LYS:NZ	14:N:112:TYR:OH	2.41	0.54
7:G:7:PRO:O	7:G:8:VAL:CB	2.54	0.54
1:A:669:G:C2'	1:A:669:G:N3	2.71	0.54
1:A:401:A:C2	1:A:402:A:C4	2.96	0.54
1:A:1142:A:C8	1:A:1144:A:N6	2.76	0.53
1:A:1805:A:C5	1:A:1806:C:C5	2.96	0.53
1:A:1867:G:O2'	1:A:1868:C:C5'	2.56	0.53
1:A:1659:G:C6	1:A:1660:G:N7	2.76	0.53
5:E:169:VAL:O	5:E:170:ARG:CD	2.56	0.53
1:A:1964:G:C2	1:A:1967:C:C5	2.96	0.53
1:A:9:G:N1	1:A:2629:U:C6	2.76	0.53
1:A:2545:G:C6	1:A:2546:U:N3	2.76	0.53
1:A:1677:A:N6	1:A:1678:A:C6	2.76	0.53
1:A:1677:A:C6	1:A:1678:A:C5	2.97	0.53
18:R:12:HIS:CE1	18:R:22:LEU:CD2	2.91	0.53
17:Q:57:ARG:NH2	17:Q:92:LYS:CE	2.71	0.53
1:A:2555:U:C5	1:A:2556:C:C6	2.97	0.53
1:A:2503:A:O2'	1:A:2505:G:OP2	2.26	0.53
1:A:2013:A:C2	19:S:88:ARG:NH1	2.76	0.53
1:A:2532:G:C5	1:A:2533:U:C6	2.97	0.53
1:A:1770:G:C5	1:A:1983:G:C6	2.97	0.53
1:A:1483:G:C2	1:A:1484:U:C2	2.96	0.53
13:M:25:ASP:OD2	13:M:25:ASP:N	2.42	0.53
1:A:1062:G:C6	1:A:1063:G:C6	2.96	0.53
22:V:83:LYS:O	22:V:85:LYS:N	2.41	0.53
1:A:1522:A:O2'	1:A:1523:U:OP2	2.27	0.53
5:E:7:ASP:O	5:E:9:GLN:N	2.42	0.53
1:A:1062:G:C4	1:A:1088:A:N7	2.77	0.53
1:A:866:A:O2'	1:A:867:C:C5'	2.57	0.53
10:J:44:TYR:O	10:J:45:THR:CB	2.56	0.53
1:A:1071:G:C5	1:A:1089:A:N1	2.76	0.53
1:A:1422:G:C2	1:A:1423:G:C8	2.97	0.53
7:G:61:TRP:O	7:G:62:ALA:C	2.46	0.53
1:A:1813:G:N3	3:C:49:THR:CG2	2.71	0.53
1:A:17:G:C6	1:A:524:G:C6	2.96	0.53
3:C:146:LYS:O	3:C:147:PRO:C	2.45	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1275:A:OP2	1:A:1646:C:N4	2.42	0.53
14:N:117:ASP:OD2	14:N:118:ARG:N	2.42	0.53
1:A:954:G:OP2	13:M:16:ARG:NH2	2.42	0.53
1:A:463:G:C6	1:A:467:G:C6	2.96	0.53
1:A:374:A:C2	1:A:401:A:C4	2.96	0.53
6:F:125:GLY:O	6:F:157:THR:OG1	2.26	0.53
1:A:1142:A:C5	1:A:1144:A:C5	2.96	0.53
1:A:2297:A:C5	1:A:2320:U:N3	2.77	0.53
1:A:1333:G:C2	1:A:1334:G:C8	2.96	0.53
15:O:34:HIS:CD2	15:O:53:THR:O	2.61	0.53
1:A:1224:U:C4	1:A:1225:G:C6	2.97	0.53
1:A:2070:A:C2	1:A:2442:C:C2	2.96	0.53
2:B:73:A:C4	2:B:104:A:C2	2.96	0.53
1:A:1202:G:C6	1:A:1203:U:N3	2.76	0.53
1:A:1850:G:C6	1:A:1851:U:C4	2.97	0.53
1:A:747:U:C5	1:A:2613:U:C5	2.96	0.53
1:A:2209:G:C2	1:A:2216:G:C2	2.97	0.53
1:A:216:A:N7	1:A:432:A:C5	2.77	0.53
1:A:958:U:C2	2:B:89:U:O2'	2.62	0.53
1:A:2527:C:C5	1:A:2528:U:C5	2.96	0.53
1:A:1421:G:C2	1:A:1422:G:C8	2.97	0.53
20:T:39:THR:CG2	20:T:39:THR:O	2.57	0.53
10:J:67:ASN:O	10:J:69:ARG:N	2.42	0.52
1:A:1964:G:C6	1:A:1967:C:N4	2.77	0.52
1:A:435:C:O2'	1:A:436:C:C5'	2.57	0.52
4:D:149:ASN:OD1	4:D:150:GLN:N	2.42	0.52
1:A:615:U:C4	5:E:35:TYR:CE1	2.97	0.52
1:A:1179:G:C5	1:A:1180:U:C1'	2.92	0.52
1:A:2135:A:O2'	1:A:2136:G:O4'	2.27	0.52
31:4:36:ARG:CG	31:4:37:GLN:N	2.71	0.52
12:L:101:ILE:CG2	12:L:102:GLY:N	2.73	0.52
1:A:855:G:N3	23:W:23:LYS:CD	2.72	0.52
1:A:2216:G:C6	1:A:2217:G:C6	2.97	0.52
1:A:197:A:C6	1:A:2430:A:C2	2.97	0.52
1:A:1468:U:N3	1:A:1522:A:C2	2.78	0.52
1:A:2553:G:N1	1:A:2554:U:O2	2.42	0.52
1:A:498:G:N2	1:A:499:U:C2	2.78	0.52
1:A:449:A:C4'	17:Q:2:ARG:NH1	2.73	0.52
1:A:1915:U:O2'	1:A:1916:A:O4'	2.27	0.52
27:0:30:ASP:O	27:0:33:SER:O	2.26	0.52
6:F:132:ARG:O	6:F:133:GLU:CB	2.57	0.52
1:A:1142:A:N7	1:A:1144:A:C6	2.78	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:9:G:C5	1:A:2629:U:C5	2.97	0.52
1:A:1600:C:OP1	20:T:81:LYS:NZ	2.42	0.52
1:A:2291:U:N3	1:A:2292:U:O4	2.43	0.52
1:A:1171:G:C6	1:A:1172:C:C4	2.97	0.52
1:A:2756:U:C4'	1:A:2757:A:O5'	2.57	0.52
1:A:1000:A:C6	1:A:1001:A:C6	2.98	0.52
7:G:10:VAL:O	7:G:10:VAL:CG2	2.58	0.52
10:J:31:GLU:O	10:J:32:LEU:C	2.48	0.52
1:A:2856:A:N6	1:A:2857:G:C6	2.78	0.52
2:B:33:G:C2	2:B:50:A:C2	2.98	0.52
1:A:1048:A:C4	1:A:1049:C:C5	2.97	0.52
1:A:1857:G:O2'	1:A:1858:A:P	2.68	0.52
23:W:45:HIS:N	23:W:45:HIS:ND1	2.57	0.52
12:L:27:LEU:N	12:L:27:LEU:CD1	2.72	0.52
7:G:93:TYR:O	7:G:94:ARG:O	2.27	0.52
4:D:98:VAL:O	4:D:99:GLU:C	2.47	0.52
1:A:2856:A:C6	1:A:2857:G:C5	2.97	0.52
1:A:1549:A:C6	1:A:1550:C:C4	2.97	0.52
1:A:86:G:O2'	1:A:87:U:C5'	2.58	0.52
1:A:1287:A:O2'	1:A:1288:G:C5'	2.58	0.52
19:S:24:ILE:O	19:S:25:ARG:C	2.47	0.52
1:A:231:A:N6	1:A:232:G:C2	2.77	0.52
1:A:2400:G:C6	1:A:2401:U:C4	2.97	0.52
1:A:2816:G:N2	1:A:2831:G:C4	2.77	0.52
1:A:1824:G:C6	1:A:1825:U:C4	2.98	0.52
1:A:1693:U:O4	1:A:1977:A:C5	2.63	0.52
15:O:7:ARG:CD	15:O:97:PHE:CE1	2.92	0.52
20:T:68:LYS:O	20:T:69:ARG:O	2.28	0.52
1:A:1344:U:O2'	1:A:1345:C:OP1	2.28	0.52
1:A:1385:A:N3	1:A:1386:C:C5	2.78	0.52
4:D:106:LYS:O	4:D:107:VAL:CB	2.58	0.52
2:B:37:C:C4	2:B:38:C:C4	2.98	0.52
21:U:73:ASN:O	21:U:75:ALA:N	2.42	0.52
1:A:2550:G:C6	1:A:2551:C:C4	2.97	0.52
1:A:2478:A:OP2	31:4:2:LYS:NZ	2.43	0.52
3:C:245:THR:O	3:C:247:TRP:N	2.42	0.52
1:A:1014:A:C4	1:A:1149:G:N2	2.78	0.52
14:N:38:LEU:CD1	14:N:38:LEU:O	2.58	0.52
1:A:1784:A:C4'	1:A:1785:A:O5'	2.58	0.52
1:A:1421:G:C2	1:A:1422:G:N7	2.77	0.52
1:A:541:A:C2	1:A:553:G:C4	2.97	0.52
1:A:1008:A:N6	1:A:1136:G:C6	2.78	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:799:G:C6	1:A:800:A:C6	2.97	0.52
1:A:42:A:C2	1:A:438:G:C6	2.97	0.52
22:V:14:LYS:O	22:V:15:GLY:C	2.48	0.52
1:A:1140:C:P	10:J:68:LYS:NZ	2.83	0.52
1:A:2832:U:O2	1:A:2834:G:C2	2.63	0.52
1:A:2816:G:C5	1:A:2817:U:C5	2.98	0.52
11:K:91:SER:O	11:K:92:GLU:C	2.48	0.52
1:A:2243:U:O2	1:A:2434:A:C2	2.62	0.52
23:W:39:GLN:O	23:W:40:ARG:C	2.48	0.51
1:A:1333:G:C2	1:A:1334:G:N7	2.78	0.51
4:D:9:VAL:CG2	4:D:10:GLY:N	2.72	0.51
1:A:2585:U:O2'	1:A:2586:U:C5'	2.58	0.51
21:U:17:ASP:O	21:U:18:LYS:C	2.49	0.51
22:V:51:GLN:CD	22:V:51:GLN:C	2.69	0.51
1:A:1223:G:C5	1:A:1225:G:OP2	2.64	0.51
1:A:1045:C:C2	1:A:1047:G:N2	2.78	0.51
1:A:1346:G:C2	1:A:1601:G:C4	2.98	0.51
1:A:451:U:C2	1:A:453:A:N7	2.78	0.51
1:A:2782:G:N2	1:A:2783:U:C2	2.78	0.51
1:A:1487:U:C2	1:A:1503:A:C2	2.97	0.51
1:A:1268:A:C2	1:A:2013:A:C4	2.99	0.51
17:Q:39:ILE:O	17:Q:43:GLN:N	2.44	0.51
1:A:2354:C:O2'	23:W:32:ALA:N	2.44	0.51
20:T:15:HIS:O	20:T:17:SER:N	2.43	0.51
1:A:2489:U:O2	1:A:2491:U:C4	2.63	0.51
1:A:1369:G:C2	1:A:1370:C:C2	2.99	0.51
4:D:163:GLY:O	4:D:164:GLN:C	2.48	0.51
1:A:111:A:C2	1:A:112:U:C2	2.97	0.51
3:C:105:ALA:O	3:C:106:PRO:O	2.29	0.51
1:A:1419:A:N6	1:A:1494:A:N1	2.58	0.51
1:A:84:A:C2	1:A:103:A:C6	2.99	0.51
1:A:555:G:O2'	1:A:556:A:OP2	2.28	0.51
1:A:919:U:C6	1:A:919:U:C4'	2.94	0.51
1:A:195:A:N7	34:A:3607:HOH:O	2.33	0.51
1:A:2577:A:O4'	1:A:2612:C:N4	2.44	0.51
1:A:1918:A:O2'	1:A:1919:A:N7	2.44	0.51
1:A:2:G:C6	1:A:3:U:C4	2.99	0.51
1:A:1019:U:O4	1:A:1020:A:N6	2.43	0.51
29:2:43:THR:O	29:2:44:VAL:CG2	2.58	0.51
18:R:49:ILE:CD1	18:R:52:PRO:CA	2.88	0.51
17:Q:13:HIS:CD2	17:Q:31:TYR:CD1	2.99	0.51
1:A:182:A:C6	1:A:183:C:C4	2.98	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2047:C:O2'	1:A:2823:A:N1	2.43	0.51
28:1:42:VAL:O	28:1:42:VAL:CG1	2.58	0.51
10:J:131:ASN:N	10:J:131:ASN:OD1	2.42	0.51
1:A:151:C:C2	1:A:176:A:C2	2.99	0.51
1:A:14:A:C6	1:A:526:A:C2	2.98	0.51
1:A:1815:A:C5	1:A:1817:G:C6	2.99	0.51
1:A:60:G:C8	1:A:62:U:C6	2.98	0.51
7:G:27:GLY:O	7:G:28:LYS:C	2.48	0.51
1:A:2720:U:OP1	16:P:52:ARG:NH2	2.43	0.51
1:A:2555:U:C6	1:A:2556:C:C6	2.98	0.51
20:T:83:ALA:O	20:T:84:TYR:O	2.28	0.51
25:Y:20:ASN:O	25:Y:21:LEU:C	2.49	0.51
3:C:166:ARG:O	3:C:166:ARG:CG	2.58	0.51
1:A:60:G:C4	1:A:74:A:C2	2.98	0.51
1:A:2198:A:O2'	1:A:2224:G:N2	2.44	0.51
1:A:522:A:C4	1:A:523:C:C5	2.99	0.51
1:A:1494:A:C2	1:A:1495:A:C4	2.99	0.51
1:A:28:A:C8	1:A:513:A:C6	2.99	0.51
16:P:20:ARG:CD	16:P:112:ARG:NH1	2.74	0.51
1:A:1857:G:O2'	1:A:1858:A:OP2	2.29	0.51
1:A:508:A:C6	19:S:9:HIS:CE1	2.99	0.51
6:F:19:PHE:O	6:F:20:ASN:C	2.49	0.51
1:A:167:A:C5	1:A:168:G:C8	2.99	0.51
8:H:67:ALA:O	8:H:69:ALA:N	2.44	0.51
1:A:1277:G:C6	1:A:1278:C:C4	2.99	0.51
1:A:1287:A:OP2	14:N:103:ARG:CG	2.59	0.51
1:A:855:G:N3	23:W:23:LYS:CG	2.73	0.51
23:W:25:PHE:O	23:W:26:GLY:C	2.49	0.51
1:A:2136:G:C2'	1:A:2137:U:C5	2.94	0.51
1:A:2581:G:N2	1:A:2581:G:OP2	2.43	0.51
1:A:176:A:C6	1:A:177:G:N7	2.79	0.51
1:A:931:U:O2'	1:A:932:U:P	2.69	0.51
1:A:194:G:N7	34:A:3607:HOH:O	2.34	0.51
16:P:37:LYS:N	16:P:37:LYS:CD	2.74	0.51
1:A:1963:U:O5'	1:A:1963:U:C6	2.64	0.51
12:L:94:THR:CG2	12:L:95:LEU:N	2.74	0.51
1:A:1972:G:OP2	3:C:237:ARG:NH1	2.44	0.51
1:A:1315:C:C2	1:A:1338:G:C2	2.99	0.51
1:A:638:G:C5	1:A:651:G:C2	2.99	0.51
5:E:79:ARG:O	5:E:80:SER:C	2.49	0.51
1:A:1135:C:N4	1:A:1139:G:C6	2.79	0.51
12:L:66:PHE:CG	12:L:66:PHE:O	2.64	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:115:GLN:N	7:G:115:GLN:CD	2.65	0.51
1:A:1954:G:O2'	1:A:1955:U:OP2	2.29	0.50
4:D:64:GLU:O	4:D:68:PHE:CD1	2.64	0.50
1:A:2140:G:C6	1:A:2152:G:N1	2.79	0.50
13:M:46:ILE:CG1	13:M:47:GLU:N	2.74	0.50
1:A:2656:U:C4	1:A:2664:G:N2	2.79	0.50
7:G:8:VAL:CG1	7:G:9:VAL:N	2.74	0.50
1:A:2631:G:C4	1:A:2632:A:C8	2.99	0.50
1:A:2468:A:O2'	1:A:2469:A:OP2	2.28	0.50
1:A:1809:A:O2'	1:A:1810:A:C5'	2.59	0.50
1:A:2472:G:C8	1:A:2475:C:N4	2.79	0.50
1:A:957:C:O2'	1:A:959:A:O5'	2.28	0.50
1:A:2789:C:N4	1:A:2893:A:C2	2.79	0.50
22:V:43:ASP:C	22:V:43:ASP:OD1	2.50	0.50
1:A:1817:G:OP1	3:C:86:ARG:NH2	2.45	0.50
1:A:90:U:C6	1:A:91:A:C8	2.99	0.50
1:A:2552:U:O2	1:A:2554:U:C5'	2.59	0.50
25:Y:21:LEU:O	25:Y:22:LEU:O	2.28	0.50
1:A:2652:C:C4	1:A:2653:U:C4	2.99	0.50
1:A:1176:U:C4	1:A:1177:G:C6	2.99	0.50
1:A:1839:G:C4	1:A:1927:A:C8	2.99	0.50
13:M:97:GLN:N	13:M:97:GLN:CD	2.65	0.50
1:A:1385:A:C5	1:A:1403:A:C6	2.99	0.50
1:A:2020:A:C6	1:A:2022:U:C2	2.99	0.50
1:A:28:A:C5	1:A:513:A:N7	2.79	0.50
2:B:53:A:O2'	2:B:54:G:C5'	2.60	0.50
1:A:980:A:C6	1:A:981:A:N1	2.80	0.50
1:A:814:C:C2	1:A:1194:A:C2	2.99	0.50
1:A:996:A:C2	1:A:997:G:C8	3.00	0.50
1:A:1090:A:N6	1:A:1102:C:N3	2.59	0.50
13:M:14:LYS:O	13:M:15:GLY:C	2.50	0.50
1:A:822:G:C5	1:A:836:G:C2	3.00	0.50
1:A:538:A:C2	1:A:556:A:C4	3.00	0.50
1:A:2663:G:C2'	1:A:2664:G:O5'	2.60	0.50
16:P:8:GLU:O	16:P:11:GLN:CB	2.60	0.50
1:A:993:G:C6	1:A:1162:G:C6	2.99	0.50
1:A:2250:G:O5'	1:A:2250:G:C8	2.64	0.50
1:A:1062:G:N9	1:A:1088:A:N7	2.60	0.50
1:A:1973:G:C4	1:A:1974:C:C6	3.00	0.50
24:X:51:SER:O	24:X:54:GLY:N	2.45	0.50
13:M:78:LEU:C	13:M:80:VAL:N	2.64	0.50
1:A:1317:G:C2	1:A:1336:A:C2	3.00	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2204:G:C5	1:A:2221:G:C2	3.00	0.50
1:A:1759:A:O2'	1:A:1760:C:C5'	2.60	0.50
1:A:63:A:C2	1:A:64:A:C5	3.00	0.50
1:A:1942:C:C4	1:A:1943:U:C5	2.98	0.50
1:A:809:G:C2'	1:A:810:U:O5'	2.59	0.50
14:N:66:ALA:O	14:N:70:THR:OG1	2.30	0.50
1:A:920:A:C5	1:A:921:C:C5	2.99	0.50
6:F:37:MET:CE	6:F:150:GLY:O	2.60	0.50
1:A:1820:U:O2'	3:C:157:ALA:O	2.28	0.50
12:L:65:GLY:O	12:L:66:PHE:CB	2.58	0.50
1:A:2456:C:C5	1:A:2457:U:C5	3.00	0.50
5:E:42:GLY:O	5:E:43:THR:O	2.30	0.50
23:W:67:LYS:O	23:W:68:PHE:CB	2.60	0.50
1:A:818:G:N1	1:A:1188:U:OP2	2.44	0.50
1:A:866:A:N7	1:A:914:G:C6	2.80	0.50
1:A:276:U:O2'	1:A:277:G:O5'	2.30	0.50
1:A:821:A:N7	1:A:946:C:C2	2.80	0.50
1:A:858:G:C2	1:A:2268:A:C4	2.99	0.50
1:A:974:G:N1	1:A:1186:G:C6	2.80	0.50
1:A:1154:G:OP2	17:Q:57:ARG:NH1	2.45	0.50
12:L:23:ILE:O	12:L:24:GLY:C	2.50	0.50
4:D:103:ASP:O	4:D:104:VAL:O	2.30	0.50
3:C:225:ASN:O	3:C:228:ASP:N	2.44	0.50
24:X:5:GLN:NE2	24:X:49:ARG:N	2.59	0.50
15:O:67:ASN:O	15:O:68:LYS:C	2.49	0.50
1:A:704:G:C2'	1:A:726:G:N2	2.75	0.50
1:A:687:C:C4	1:A:688:U:C4	3.00	0.50
1:A:2816:G:C6	1:A:2817:U:C4	3.00	0.50
17:Q:13:HIS:CD2	17:Q:31:TYR:CG	2.99	0.50
1:A:883:G:C2	1:A:894:U:O2	2.65	0.50
1:A:1297:C:O2'	1:A:1302:A:N1	2.44	0.50
6:F:110:ILE:O	6:F:111:ARG:O	2.29	0.50
2:B:40:U:O2'	2:B:43:C:C5	2.65	0.50
1:A:954:G:C5	1:A:955:U:C6	2.99	0.49
1:A:792:A:C6	1:A:2440:C:C6	3.00	0.49
1:A:1724:G:C5	1:A:1725:U:C4	2.99	0.49
1:A:1569:A:N1	1:A:1570:A:C2	2.80	0.49
3:C:77:VAL:O	3:C:77:VAL:CG2	2.60	0.49
1:A:2093:G:C6	1:A:2225:A:N7	2.80	0.49
1:A:747:U:N3	1:A:2613:U:C4	2.80	0.49
1:A:825:A:C6	1:A:833:A:N1	2.80	0.49
1:A:1403:A:C5	1:A:1404:C:C5	3.00	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1322:A:C5	1:A:1323:C:C5	3.00	0.49
1:A:319:G:C4	1:A:333:G:N2	2.80	0.49
28:1:3:GLY:O	28:1:5:ARG:N	2.46	0.49
11:K:105:ARG:NE	11:K:106:GLU:OE2	2.45	0.49
1:A:733:G:C8	1:A:761:A:N6	2.80	0.49
24:X:39:VAL:O	24:X:41:SER:N	2.46	0.49
1:A:192:C:O2'	1:A:802:A:N3	2.45	0.49
17:Q:10:ARG:NH1	17:Q:10:ARG:CB	2.75	0.49
1:A:270:A:C2	1:A:370:G:C6	3.01	0.49
1:A:1079:C:C2	1:A:1080:A:C8	3.00	0.49
23:W:22:VAL:O	23:W:23:LYS:O	2.30	0.49
10:J:45:THR:O	10:J:45:THR:CG2	2.60	0.49
1:A:1083:U:C6	1:A:1085:A:OP2	2.65	0.49
1:A:2727:A:O2'	1:A:2728:U:C5'	2.61	0.49
22:V:80:HIS:CD2	22:V:83:LYS:CB	2.95	0.49
26:Z:8:GLN:O	26:Z:10:ARG:N	2.45	0.49
1:A:1669:A:C2'	1:A:1669:A:N3	2.74	0.49
1:A:2636:C:O2'	4:D:45:TYR:CZ	2.65	0.49
23:W:41:GLY:O	23:W:42:THR:C	2.51	0.49
1:A:1392:A:C6	1:A:1393:A:N6	2.81	0.49
1:A:919:U:C2	1:A:920:A:N7	2.80	0.49
1:A:1522:A:O2'	1:A:1523:U:P	2.70	0.49
1:A:1805:A:C4	1:A:1806:C:C5	3.01	0.49
2:B:42:C:O2'	2:B:43:C:C5'	2.61	0.49
1:A:696:G:C4	1:A:697:G:C8	2.99	0.49
1:A:1255:U:C5	5:E:67:ARG:O	2.66	0.49
1:A:2578:G:N2	1:A:2579:C:C2	2.81	0.49
1:A:1083:U:C5	1:A:1085:A:OP2	2.65	0.49
22:V:40:ILE:CG2	22:V:41:GLU:N	2.76	0.49
5:E:119:ILE:O	5:E:187:VAL:O	2.30	0.49
20:T:29:THR:N	20:T:91:GLN:NE2	2.61	0.49
16:P:13:LYS:N	16:P:76:HIS:ND1	2.61	0.49
5:E:48:THR:O	5:E:50:ALA:N	2.46	0.49
27:0:53:VAL:O	27:0:54:ILE:O	2.30	0.49
1:A:517:C:OP1	27:0:12:ARG:NH1	2.45	0.49
6:F:67:THR:N	6:F:85:GLY:O	2.46	0.49
4:D:101:PHE:CD1	4:D:101:PHE:N	2.81	0.49
1:A:1071:G:C5	1:A:1089:A:C6	3.00	0.49
1:A:1435:G:C2	1:A:1558:C:N4	2.81	0.49
1:A:2868:A:O2'	1:A:2869:G:O4'	2.30	0.49
1:A:2868:A:C2	1:A:2869:G:C4	3.01	0.49
1:A:562:U:C4	1:A:2036:C:O4'	2.66	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2571:U:C4	1:A:2574:G:C8	3.01	0.49
1:A:117:G:C6	1:A:119:A:N6	2.81	0.49
1:A:396:G:OP2	24:X:9:LYS:NZ	2.46	0.49
23:W:13:ARG:O	23:W:14:ASP:C	2.51	0.49
1:A:2679:A:C2	1:A:2729:G:C2	3.00	0.49
1:A:513:A:C2	1:A:514:A:C5	3.00	0.49
1:A:604:G:C6	1:A:625:G:C2	3.00	0.49
1:A:2816:G:C2	1:A:2831:G:C4	3.01	0.49
1:A:2800:A:C2	1:A:2895:G:C1'	2.96	0.49
1:A:1865:U:C5	1:A:1875:G:N1	2.81	0.49
5:E:15:SER:N	5:E:197:GLU:OE2	2.46	0.49
10:J:81:ILE:CG2	10:J:82:GLY:N	2.76	0.49
1:A:1498:C:O2'	1:A:1499:C:O4'	2.30	0.49
1:A:221:A:C4	1:A:266:G:N7	2.81	0.49
23:W:25:PHE:O	23:W:27:GLY:N	2.45	0.49
7:G:60:GLY:O	7:G:61:TRP:CB	2.61	0.49
1:A:1452:G:C8	1:A:1457:U:N3	2.81	0.49
1:A:2231:U:C4	1:A:2232:C:C5	3.01	0.49
12:L:80:SER:C	12:L:81:ASP:O	2.49	0.49
1:A:2468:A:O2'	1:A:2469:A:P	2.71	0.49
1:A:1781:U:O2'	1:A:1782:U:P	2.71	0.49
1:A:1638:C:O2	1:A:2698:U:O2'	2.30	0.49
27:O:9:ARG:NH2	27:O:9:ARG:CG	2.76	0.49
1:A:301:G:C5	1:A:302:C:C4	3.01	0.49
10:J:65:THR:CG2	10:J:66:GLY:N	2.74	0.49
1:A:778:G:C6	1:A:779:U:N3	2.81	0.49
1:A:995:C:OP2	17:Q:53:LYS:CE	2.61	0.48
1:A:1059:G:C6	1:A:1080:A:C6	3.01	0.48
1:A:2200:C:N4	1:A:2224:G:C2	2.80	0.48
1:A:1252:G:C2	1:A:1253:A:C2	3.01	0.48
10:J:44:TYR:CD1	17:Q:59:LEU:CD1	2.96	0.48
1:A:2063:C:C5	1:A:2064:C:C5	3.01	0.48
4:D:16:THR:CG2	4:D:18:ASP:OD1	2.61	0.48
1:A:563:A:C6	1:A:2018:G:C4	3.01	0.48
1:A:1520:U:C4	1:A:1521:G:C6	3.01	0.48
1:A:2842:G:C4	1:A:2843:G:C8	3.01	0.48
1:A:728:G:C4	1:A:730:A:C8	3.01	0.48
1:A:726:G:O2'	1:A:727:A:P	2.71	0.48
1:A:976:G:N3	1:A:977:G:C8	2.80	0.48
7:G:59:ASP:O	7:G:60:GLY:C	2.51	0.48
6:F:9:ASP:O	6:F:10:GLU:CB	2.61	0.48
1:A:715:A:C6	1:A:716:A:C6	3.01	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1356:G:C5	1:A:1357:C:C5	3.01	0.48
1:A:1005:C:C2	1:A:1143:A:C6	3.01	0.48
1:A:754:U:C2	1:A:755:U:C5	3.01	0.48
1:A:2276:G:P	13:M:83:GLY:O	2.71	0.48
4:D:182:ALA:O	4:D:184:ARG:N	2.46	0.48
1:A:1351:C:N3	1:A:1381:G:C6	2.81	0.48
1:A:1549:A:C6	1:A:1550:C:N3	2.82	0.48
1:A:752:A:O2'	1:A:753:A:OP2	2.31	0.48
1:A:2444:G:C6	1:A:2445:G:C5	3.01	0.48
1:A:2740:A:C6	1:A:2741:A:C6	3.01	0.48
4:D:70:LYS:O	4:D:71:ALA:CB	2.61	0.48
1:A:1374:G:C5	1:A:1375:U:C5	3.01	0.48
1:A:2318:G:C6	1:A:2319:G:C6	3.01	0.48
1:A:2093:G:C5	1:A:2225:A:C8	3.01	0.48
1:A:1553:A:C5	1:A:1555:G:C5	3.00	0.48
1:A:2020:A:N1	1:A:2022:U:C2	2.81	0.48
1:A:77:G:C4	1:A:78:U:C5	3.01	0.48
1:A:2725:A:C4	1:A:2727:A:C8	3.01	0.48
1:A:684:G:C6	1:A:774:G:C4	3.01	0.48
1:A:797:G:C2	1:A:798:G:C4	3.01	0.48
1:A:49:A:C2	1:A:118:A:C2	3.01	0.48
1:A:49:A:C2	1:A:118:A:N1	2.82	0.48
1:A:1142:A:C4	1:A:1144:A:N7	2.82	0.48
1:A:1517:G:C6	1:A:1518:C:C4	3.01	0.48
1:A:2232:C:OP1	24:X:26:ARG:NH2	2.47	0.48
1:A:2689:U:C2	1:A:2713:U:C6	3.02	0.48
6:F:15:LEU:O	6:F:18:GLU:N	2.46	0.48
19:S:63:GLY:O	19:S:64:ALA:CB	2.61	0.48
1:A:48:G:N2	1:A:177:G:N2	2.61	0.48
1:A:2209:G:N1	1:A:2210:U:O4	2.46	0.48
1:A:2415:G:C2	1:A:2416:C:C2	3.01	0.48
1:A:95:A:N1	1:A:96:C:C2	2.81	0.48
1:A:959:A:N6	13:M:82:MET:CE	2.76	0.48
1:A:1250:G:N7	12:L:18:ARG:NH1	2.62	0.48
3:C:251:THR:CG2	3:C:252:LYS:N	2.76	0.48
1:A:1147:A:C6	1:A:1148:U:C4	3.02	0.48
13:M:101:VAL:CG1	13:M:101:VAL:O	2.61	0.48
7:G:27:GLY:O	7:G:29:ASN:O	2.32	0.48
4:D:110:THR:OG1	4:D:171:THR:CG2	2.61	0.48
1:A:1054:A:C6	1:A:1106:G:O6	2.67	0.48
1:A:475:C:C4	1:A:481:G:O6	2.67	0.48
1:A:668:A:C2'	1:A:669:G:OP1	2.62	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:147:LEU:O	5:E:168:ASP:O	2.31	0.48
1:A:2488:G:C2	1:A:2489:U:C2	3.02	0.48
1:A:2691:C:O2'	1:A:2692:G:C5'	2.60	0.48
14:N:60:VAL:O	14:N:61:ALA:C	2.51	0.48
14:N:67:PHE:CE1	14:N:73:ASN:OD1	2.66	0.48
1:A:1022:G:C6	1:A:1141:U:C5	3.01	0.48
1:A:783:A:C4'	1:A:1779:U:O2	2.62	0.48
1:A:2291:U:C2	1:A:2292:U:C4	3.01	0.48
1:A:2692:G:C4	1:A:2718:G:N2	2.82	0.48
8:H:100:ALA:O	8:H:102:ALA:N	2.47	0.48
1:A:1905:C:O2'	1:A:1929:G:O2'	2.32	0.48
8:H:2:GLN:O	8:H:3:VAL:CG2	2.62	0.48
1:A:947:A:O2'	1:A:984:A:C2	2.67	0.48
6:F:110:ILE:O	6:F:111:ARG:C	2.50	0.48
1:A:966:G:C6	1:A:967:U:N3	2.82	0.48
4:D:35:THR:N	4:D:49:GLN:O	2.47	0.48
1:A:1232:G:C6	1:A:1233:C:C4	3.01	0.48
14:N:2:ARG:O	14:N:3:HIS:C	2.52	0.48
1:A:995:C:O2'	1:A:996:A:OP2	2.32	0.48
4:D:93:GLY:O	4:D:94:GLN:C	2.51	0.48
10:J:44:TYR:C	10:J:44:TYR:CD1	2.87	0.48
1:A:684:G:C6	1:A:774:G:C5	3.02	0.48
1:A:950:G:C6	1:A:951:C:C4	3.02	0.48
5:E:168:ASP:OD1	5:E:169:VAL:N	2.47	0.48
1:A:1570:A:C6	1:A:1571:A:C6	3.02	0.48
16:P:33:GLU:OE2	16:P:38:ARG:NH1	2.47	0.48
1:A:55:G:N2	1:A:116:C:C2	2.81	0.48
1:A:1403:A:C4	1:A:1404:C:C6	3.02	0.47
12:L:93:ASN:O	12:L:95:LEU:N	2.47	0.47
1:A:27:G:C4	1:A:512:G:N2	2.82	0.47
1:A:30:G:C5	1:A:31:C:C4	3.02	0.47
1:A:974:G:C6	1:A:1186:G:C6	3.02	0.47
7:G:84:LYS:CG	7:G:85:LYS:N	2.76	0.47
14:N:117:ASP:O	14:N:119:SER:N	2.47	0.47
1:A:199:A:C2	1:A:2434:A:C2	3.02	0.47
5:E:48:THR:C	5:E:50:ALA:N	2.67	0.47
1:A:249:C:O2'	1:A:250:G:OP2	2.32	0.47
27:O:50:GLY:O	27:O:51:ARG:O	2.32	0.47
1:A:2309:A:O2'	1:A:2310:C:O4'	2.32	0.47
1:A:1798:U:O2'	1:A:1802:A:O2'	2.32	0.47
1:A:10:A:C8	1:A:2800:A:N6	2.83	0.47
1:A:1188:U:C2	1:A:1189:A:C8	3.01	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1471:G:C5	1:A:1472:C:C5	3.02	0.47
1:A:2407:A:C4	1:A:2408:U:C5	3.02	0.47
1:A:880:G:C8	1:A:880:G:O5'	2.67	0.47
20:T:52:GLU:O	20:T:52:GLU:CG	2.61	0.47
10:J:67:ASN:O	10:J:68:LYS:C	2.53	0.47
4:D:97:SER:CB	4:D:99:GLU:OE1	2.63	0.47
1:A:1223:G:N2	1:A:1226:A:OP2	2.47	0.47
1:A:1005:C:N3	1:A:1143:A:C2	2.82	0.47
8:H:132:PHE:CG	8:H:133:GLN:N	2.82	0.47
7:G:66:THR:O	7:G:70:LEU:N	2.47	0.47
15:O:36:TYR:CD2	15:O:36:TYR:N	2.82	0.47
19:S:73:LYS:CE	19:S:74:ILE:N	2.77	0.47
1:A:271:G:C2	1:A:272:A:C5	3.02	0.47
1:A:243:U:OP2	30:3:7:ARG:NE	2.47	0.47
1:A:1987:A:C2	1:A:1988:G:C8	3.02	0.47
24:X:69:GLU:O	24:X:71:ARG:N	2.47	0.47
20:T:50:LEU:N	20:T:50:LEU:CD1	2.77	0.47
1:A:1786:A:O2'	1:A:1938:A:N6	2.48	0.47
1:A:1556:C:O2'	1:A:1557:C:C5'	2.63	0.47
1:A:1936:A:C2	1:A:1943:U:O4	2.67	0.47
28:1:9:LYS:NZ	28:1:50:GLU:OE2	2.47	0.47
1:A:920:A:C6	1:A:921:C:C4	3.02	0.47
1:A:2018:G:N1	1:A:2019:A:C5	2.83	0.47
25:Y:21:LEU:O	25:Y:22:LEU:C	2.52	0.47
1:A:301:G:C5	1:A:302:C:N4	2.81	0.47
10:J:64:VAL:CG1	10:J:65:THR:N	2.77	0.47
1:A:773:U:O2	1:A:778:G:O2'	2.32	0.47
1:A:2740:A:C6	1:A:2764:A:C8	3.03	0.47
4:D:111:GLY:O	4:D:169:ARG:O	2.32	0.47
1:A:608:A:C4	1:A:621:A:C6	3.02	0.47
3:C:229:HIS:CD2	3:C:246:PRO:CB	2.97	0.47
1:A:2599:G:C2	1:A:2600:A:C8	3.02	0.47
7:G:1:SER:O	7:G:3:VAL:N	2.47	0.47
1:A:581:C:C2	1:A:582:A:N7	2.82	0.47
1:A:487:C:N4	1:A:494:G:C6	2.82	0.47
1:A:636:G:C6	12:L:111:ILE:CD1	2.98	0.47
17:Q:59:LEU:O	17:Q:60:TRP:C	2.51	0.47
1:A:1422:G:C5	1:A:1423:G:N7	2.83	0.47
1:A:27:G:O2'	1:A:28:A:OP2	2.33	0.47
1:A:2657:A:C6	1:A:2665:A:C8	3.02	0.47
1:A:197:A:C6	1:A:2430:A:N3	2.82	0.47
1:A:2526:G:C6	1:A:2527:C:N3	2.83	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1005:C:O2	1:A:1143:A:C6	2.67	0.47
14:N:1:MET:O	14:N:2:ARG:CB	2.61	0.47
1:A:241:A:N6	1:A:256:A:OP2	2.47	0.47
25:Y:27:ASN:O	25:Y:31:GLN:N	2.48	0.47
1:A:841:G:C4	1:A:938:G:N2	2.82	0.47
1:A:1672:A:N6	1:A:1673:G:C6	2.83	0.47
23:W:28:GLU:CG	23:W:29:SER:N	2.78	0.47
22:V:26:PHE:CD1	22:V:26:PHE:C	2.87	0.47
1:A:1663:G:C6	1:A:1998:A:C6	3.03	0.47
1:A:1027:A:N3	1:A:1027:A:C2'	2.78	0.47
1:A:62:U:C4'	1:A:63:A:OP1	2.62	0.47
1:A:1553:A:C8	1:A:1555:G:C5	3.02	0.47
1:A:1539:U:O2'	1:A:1540:G:O5'	2.32	0.47
1:A:1247:A:C5	1:A:1249:U:C4	3.03	0.47
1:A:639:U:C2'	1:A:640:C:C6	2.97	0.47
1:A:2776:A:C2	1:A:2778:A:C4	3.02	0.47
1:A:960:A:C8	1:A:962:G:C8	3.02	0.47
1:A:2513:A:C6	1:A:2574:G:C6	3.02	0.47
1:A:752:A:N6	1:A:2609:U:N3	2.63	0.47
1:A:2595:G:N2	1:A:2599:G:C5	2.83	0.47
1:A:241:A:O2'	30:3:2:LYS:NZ	2.48	0.47
3:C:109:LEU:CD2	3:C:110:LYS:N	2.77	0.47
1:A:2748:A:N6	1:A:2749:A:C6	2.82	0.47
1:A:829:A:N7	1:A:2247:A:O2'	2.47	0.47
1:A:2510:C:C4	1:A:2511:U:C4	3.03	0.47
18:R:83:TYR:CD1	18:R:83:TYR:C	2.87	0.47
1:A:2525:G:C2	1:A:2539:C:C2	3.02	0.47
5:E:58:LYS:O	5:E:59:PRO:C	2.52	0.47
13:M:24:THR:O	13:M:34:LYS:CE	2.63	0.47
1:A:387:U:C5	1:A:388:G:O6	2.68	0.47
1:A:2058:A:C5'	1:A:2059:A:OP2	2.63	0.47
1:A:84:A:C6	1:A:103:A:N6	2.83	0.47
1:A:1654:A:C4'	4:D:118:PHE:CZ	2.98	0.47
1:A:1048:A:C6	1:A:1049:C:C4	3.03	0.47
1:A:1809:A:O2'	1:A:1810:A:O5'	2.32	0.47
3:C:229:HIS:CD2	3:C:246:PRO:CA	2.98	0.47
1:A:2076:U:OP2	1:A:2238:G:N2	2.47	0.47
11:K:71:ARG:CB	11:K:72:PRO:CD	2.93	0.47
1:A:2492:U:C2	1:A:2493:U:C5	3.03	0.47
1:A:2410:G:C2	1:A:2411:A:C1'	2.98	0.47
1:A:990:A:C5'	1:A:990:A:C8	2.98	0.47
11:K:6:THR:CG2	11:K:6:THR:O	2.63	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:12:LYS:O	10:J:13:ARG:CB	2.61	0.47
3:C:14:HIS:O	3:C:203:VAL:CG1	2.63	0.47
27:O:53:VAL:O	27:O:54:ILE:C	2.53	0.47
1:A:2330:G:C2	1:A:2386:A:C2	3.03	0.47
16:P:24:THR:O	16:P:25:VAL:O	2.33	0.47
1:A:1060:U:C6	1:A:1060:U:OP1	2.68	0.47
1:A:479:A:C2	1:A:480:A:C5	3.03	0.47
1:A:2549:G:N2	1:A:2560:A:C4	2.83	0.47
8:H:8:LYS:O	8:H:13:GLY:CA	2.62	0.47
1:A:2691:C:C4	1:A:2719:G:N2	2.82	0.47
7:G:163:TYR:O	7:G:164:ALA:CB	2.63	0.47
23:W:72:GLY:N	23:W:73:PRO:CD	2.78	0.46
1:A:1779:U:C6	1:A:1783:A:N7	2.83	0.46
1:A:1475:G:O2'	1:A:1476:U:P	2.73	0.46
1:A:1179:G:C6	1:A:1180:U:O2'	2.68	0.46
1:A:7:G:C5	1:A:8:C:C4	3.03	0.46
3:C:90:ILE:CG2	3:C:91:ALA:N	2.78	0.46
1:A:2902:C:O2'	1:A:2903:U:C5'	2.63	0.46
5:E:101:TYR:O	5:E:102:ARG:C	2.51	0.46
3:C:259:ASN:C	3:C:261:ARG:N	2.68	0.46
1:A:1835:G:C4	1:A:1931:U:C4	3.03	0.46
10:J:49:ASP:C	10:J:49:ASP:OD2	2.54	0.46
1:A:397:U:OP2	24:X:9:LYS:NZ	2.48	0.46
1:A:855:G:N2	23:W:23:LYS:CG	2.78	0.46
1:A:2856:A:C6	1:A:2857:G:C6	3.03	0.46
5:E:57:LYS:CG	5:E:58:LYS:N	2.78	0.46
4:D:42:ASN:ND2	4:D:42:ASN:O	2.48	0.46
5:E:37:ALA:O	5:E:39:ALA:N	2.47	0.46
1:A:2273:A:C2	1:A:2274:A:C5	3.03	0.46
22:V:68:LYS:O	22:V:69:GLU:C	2.53	0.46
2:B:90:C:C2'	2:B:91:C:O5'	2.63	0.46
1:A:279:A:O2'	1:A:280:U:C5'	2.63	0.46
13:M:59:ARG:O	13:M:60:GLN:O	2.33	0.46
1:A:1020:A:C2	1:A:1141:U:O2	2.69	0.46
1:A:1657:U:OP1	4:D:141:ARG:N	2.48	0.46
1:A:1090:A:C6	1:A:1102:C:C2	3.03	0.46
1:A:1964:G:O2'	1:A:1967:C:OP2	2.34	0.46
23:W:51:GLY:CA	23:W:59:PHE:CE2	2.99	0.46
1:A:1659:G:C5	1:A:1660:G:C8	3.03	0.46
1:A:2492:U:O2'	1:A:2493:U:C5'	2.63	0.46
1:A:2077:A:C8	1:A:2435:A:C4	3.04	0.46
9:I:115:ASP:O	9:I:116:MET:CG	2.63	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:172:PHE:O	6:F:173:ASP:C	2.53	0.46
13:M:42:THR:O	13:M:44:ARG:N	2.48	0.46
1:A:292:U:C4	1:A:293:U:C5	3.03	0.46
13:M:133:LYS:O	13:M:134:THR:CB	2.63	0.46
1:A:2536:G:C5	1:A:2537:U:C5	3.03	0.46
4:D:121:THR:O	4:D:122:VAL:CG2	2.64	0.46
12:L:4:ASN:N	12:L:4:ASN:ND2	2.63	0.46
1:A:747:U:O2'	19:S:88:ARG:NH2	2.49	0.46
1:A:945:A:C5	1:A:2448:A:C2	3.04	0.46
4:D:182:ALA:C	4:D:184:ARG:N	2.68	0.46
1:A:2555:U:C5	1:A:2556:C:N1	2.83	0.46
31:4:36:ARG:O	31:4:37:GLN:C	2.54	0.46
1:A:778:G:C6	1:A:779:U:C4	3.03	0.46
7:G:166:GLU:OE2	7:G:166:GLU:C	2.53	0.46
6:F:173:ASP:O	6:F:174:PHE:C	2.53	0.46
30:3:14:LYS:O	30:3:15:LYS:C	2.54	0.46
3:C:114:GLN:O	3:C:115:ILE:CD1	2.64	0.46
1:A:16:C:O3'	27:0:10:SER:OG	2.33	0.46
1:A:66:C:C4	1:A:67:U:C4	3.04	0.46
28:1:25:ASN:O	28:1:26:LYS:C	2.53	0.46
4:D:32:ASN:O	4:D:96:ILE:N	2.48	0.46
1:A:2673:G:C2	1:A:2674:G:N7	2.83	0.46
18:R:49:ILE:CG1	18:R:51:VAL:O	2.63	0.46
1:A:1429:G:N3	1:A:1568:G:N2	2.63	0.46
12:L:80:SER:O	12:L:81:ASP:O	2.34	0.46
1:A:111:A:N1	1:A:112:U:C2	2.84	0.46
1:A:1569:A:N6	1:A:1570:A:N1	2.64	0.46
23:W:17:ALA:O	23:W:18:LYS:CB	2.64	0.46
1:A:1235:G:C2	1:A:1236:G:N2	2.84	0.46
1:A:2106:U:C4	1:A:2107:G:N7	2.84	0.46
1:A:551:G:C6	1:A:552:U:C4	3.03	0.46
15:O:10:ARG:NH2	15:O:96:GLY:O	2.49	0.46
19:S:54:ALA:O	19:S:58:ALA:N	2.49	0.46
11:K:12:ASP:C	11:K:12:ASP:OD1	2.53	0.46
21:U:67:SER:O	21:U:67:SER:OG	2.33	0.46
17:Q:86:SER:O	17:Q:87:VAL:C	2.54	0.46
1:A:1320:C:C6	1:A:1329:U:OP2	2.69	0.46
1:A:68:G:C5	1:A:69:C:C5	3.04	0.46
1:A:763:G:C8	1:A:765:C:C6	3.04	0.46
1:A:272:A:O2'	1:A:273:G:C5'	2.64	0.46
1:A:2404:U:C2	1:A:2414:G:N1	2.83	0.46
1:A:1310:G:N2	1:A:1313:U:C5	2.83	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2805:C:C5	1:A:2806:C:C5	3.04	0.46
1:A:1425:G:N1	1:A:1426:G:C2	2.83	0.46
1:A:1746:A:C4	1:A:1747:U:C5	3.04	0.46
21:U:38:ILE:O	21:U:40:LEU:N	2.49	0.46
1:A:2233:U:C2'	1:A:2234:G:C8	2.98	0.46
10:J:128:ASN:CG	10:J:128:ASN:O	2.54	0.46
10:J:38:GLY:C	10:J:40:HIS:N	2.69	0.46
1:A:503:A:C6	1:A:506:G:C6	3.04	0.46
1:A:96:C:C2	1:A:97:C:C5	3.04	0.46
1:A:1900:A:N1	1:A:1970:A:C5	2.83	0.46
1:A:1839:G:C8	1:A:1927:A:C1'	2.98	0.46
1:A:1005:C:C2	1:A:1143:A:C5	3.03	0.46
21:U:38:ILE:CG2	21:U:39:ASN:N	2.75	0.46
5:E:178:VAL:O	5:E:181:ILE:N	2.49	0.46
14:N:13:ASN:O	14:N:14:SER:C	2.54	0.46
1:A:2394:C:OP1	30:3:29:ARG:NH2	2.48	0.46
1:A:491:G:C2	1:A:492:A:C1'	2.99	0.46
1:A:1997:C:O2'	1:A:1998:A:C5'	2.64	0.46
1:A:802:A:C2'	1:A:803:U:C6	2.99	0.46
1:A:517:C:OP2	27:0:9:ARG:NH2	2.49	0.46
5:E:176:ASP:OD1	5:E:178:VAL:CG1	2.64	0.46
7:G:123:GLU:CD	7:G:124:CYS:N	2.70	0.46
17:Q:91:ARG:NH2	17:Q:93:ILE:CD1	2.79	0.46
1:A:1059:G:OP2	1:A:1060:U:O3'	2.35	0.46
1:A:74:A:C4'	1:A:75:G:O5'	2.64	0.46
1:A:1071:G:C8	1:A:1089:A:C6	3.04	0.46
1:A:1423:G:C2	1:A:1424:G:C8	3.05	0.46
1:A:1131:G:C5	10:J:77:HIS:CE1	3.04	0.46
2:B:54:G:C4	2:B:55:U:C5	3.04	0.46
1:A:831:G:C5	1:A:832:U:C5	3.03	0.46
1:A:2318:G:C6	1:A:2319:G:N1	2.84	0.46
22:V:61:LEU:O	22:V:72:VAL:N	2.49	0.46
19:S:37:THR:CG2	19:S:37:THR:O	2.64	0.46
1:A:49:A:N6	1:A:177:G:C4	2.84	0.45
23:W:24:ARG:O	23:W:25:PHE:CB	2.63	0.45
1:A:821:A:N7	1:A:946:C:N3	2.64	0.45
1:A:24:G:C6	1:A:25:U:C4	3.04	0.45
1:A:2413:G:C4	1:A:2414:G:C8	3.04	0.45
1:A:919:U:C2	1:A:920:A:C8	3.03	0.45
1:A:1224:U:O4	1:A:1225:G:C6	2.69	0.45
25:Y:22:LEU:O	25:Y:23:ARG:O	2.34	0.45
1:A:957:C:C5	1:A:959:A:C5	3.04	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:65:VAL:O	22:V:66:ASP:OD1	2.34	0.45
1:A:1399:C:C2	1:A:1400:U:C5	3.05	0.45
16:P:15:ASP:OD1	16:P:15:ASP:C	2.52	0.45
1:A:404:A:O2'	1:A:405:U:P	2.74	0.45
1:A:923:G:C4'	23:W:25:PHE:CZ	2.99	0.45
1:A:2061:G:C2	1:A:2063:C:C4	3.04	0.45
1:A:2418:A:C2	1:A:2419:U:C2	3.05	0.45
1:A:1369:G:C6	1:A:1370:C:C4	3.05	0.45
16:P:8:GLU:O	16:P:11:GLN:N	2.49	0.45
10:J:80:HIS:O	10:J:81:ILE:C	2.54	0.45
1:A:812:C:C2	1:A:1250:G:N1	2.84	0.45
5:E:37:ALA:C	5:E:39:ALA:N	2.69	0.45
17:Q:40:LYS:O	17:Q:44:TYR:N	2.49	0.45
3:C:52:HIS:NE2	3:C:218:THR:CG2	2.79	0.45
19:S:28:LYS:O	19:S:29:VAL:C	2.54	0.45
7:G:31:GLU:O	7:G:32:LEU:C	2.54	0.45
1:A:1060:U:C5'	1:A:1061:U:OP1	2.64	0.45
1:A:1342:A:C6	1:A:1345:C:C2	3.05	0.45
1:A:1322:A:N7	1:A:1323:C:C5	2.85	0.45
24:X:33:HIS:O	24:X:34:SER:C	2.55	0.45
15:O:104:GLN:C	15:O:105:ALA:O	2.54	0.45
1:A:1724:G:C6	1:A:1725:U:C4	3.04	0.45
1:A:1471:G:C6	1:A:1472:C:C4	3.05	0.45
1:A:1565:C:O2'	1:A:1566:A:O5'	2.34	0.45
1:A:14:A:C5'	1:A:15:G:OP2	2.65	0.45
1:A:1059:G:C2'	9:I:131:THR:OG1	2.64	0.45
1:A:2297:A:C8	1:A:2320:U:N3	2.84	0.45
1:A:994:C:O2	18:R:10:LYS:CE	2.64	0.45
1:A:2679:A:C2	1:A:2729:G:N1	2.84	0.45
1:A:1315:C:N3	1:A:1338:G:C2	2.85	0.45
1:A:919:U:C4	1:A:920:A:N7	2.84	0.45
3:C:65:ASP:N	3:C:102:TYR:O	2.50	0.45
2:B:37:C:C5	2:B:38:C:C5	3.04	0.45
1:A:2603:G:C6	1:A:2604:U:C4	3.05	0.45
1:A:669:G:C5	1:A:801:G:C6	3.05	0.45
1:A:608:A:N6	1:A:609:A:C6	2.84	0.45
23:W:30:VAL:O	23:W:30:VAL:CG2	2.64	0.45
6:F:174:PHE:CD1	6:F:176:PHE:CE1	3.05	0.45
1:A:1872:A:C2'	1:A:1873:G:O4'	2.65	0.45
1:A:1544:A:C6	1:A:1545:A:C6	3.04	0.45
4:D:90:PHE:C	4:D:92:VAL:N	2.70	0.45
1:A:527:C:C5	1:A:2779:U:C5	3.04	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:3:LYS:CG	15:O:4:LYS:N	2.79	0.45
18:R:53:PHE:CD1	18:R:53:PHE:N	2.80	0.45
1:A:1509:A:C4	1:A:1510:G:C8	3.04	0.45
1:A:1419:A:C8	1:A:1421:G:C6	3.05	0.45
1:A:1179:G:N1	1:A:1180:U:O2'	2.50	0.45
1:A:1331:G:C2	1:A:1333:G:C8	3.05	0.45
1:A:1264:A:OP1	27:O:15:ARG:NH1	2.49	0.45
1:A:1016:G:N2	1:A:1147:A:C4	2.84	0.45
23:W:46:ALA:O	23:W:47:GLY:O	2.33	0.45
1:A:1216:G:C5	1:A:1217:U:C5	3.05	0.45
1:A:1190:G:OP1	12:L:32:GLY:CA	2.64	0.45
22:V:76:ASP:O	22:V:90:ASP:N	2.49	0.45
21:U:82:VAL:O	21:U:94:PHE:O	2.34	0.45
1:A:529:A:C4'	1:A:530:G:OP1	2.64	0.45
1:A:536:G:C6	1:A:537:G:C4	3.05	0.45
26:Z:22:THR:O	26:Z:23:LEU:C	2.54	0.45
22:V:29:ILE:O	22:V:91:PHE:N	2.49	0.45
1:A:909:A:C6	1:A:912:C:C2	3.05	0.45
1:A:2863:C:C2	1:A:2864:G:C8	3.05	0.45
20:T:40:LYS:O	20:T:44:LYS:N	2.50	0.45
1:A:1670:C:O2	1:A:1670:C:C2'	2.63	0.45
13:M:96:ILE:C	13:M:96:ILE:CD1	2.85	0.45
1:A:1063:G:C2	1:A:1064:C:C2	3.05	0.45
1:A:746:U:O2'	1:A:747:U:P	2.75	0.45
19:S:25:ARG:CD	19:S:73:LYS:NZ	2.80	0.45
1:A:602:A:N3	1:A:655:A:C2	2.85	0.45
4:D:97:SER:OG	4:D:98:VAL:N	2.50	0.45
1:A:2148:G:C2'	1:A:2149:U:O4'	2.65	0.45
31:4:19:ARG:O	31:4:20:ASP:C	2.54	0.45
1:A:1549:A:C5	1:A:1550:C:C4	3.05	0.45
10:J:64:VAL:O	10:J:65:THR:CB	2.65	0.45
23:W:28:GLU:O	23:W:30:VAL:N	2.50	0.45
1:A:2543:G:O2'	1:A:2544:G:O4'	2.35	0.45
1:A:2824:C:C5	1:A:2825:G:C6	3.05	0.45
1:A:2824:C:C5	1:A:2825:G:C5	3.05	0.45
1:A:1615:C:O2'	1:A:1616:A:P	2.74	0.45
1:A:2561:U:O2'	1:A:2562:U:O5'	2.35	0.45
1:A:729:G:C4	1:A:1775:U:C2	3.04	0.45
8:H:34:GLY:O	8:H:35:LYS:CG	2.65	0.45
1:A:106:C:O2'	1:A:294:A:O2'	2.34	0.45
1:A:56:A:C2	1:A:57:C:C2	3.05	0.45
18:R:81:LYS:O	18:R:82:HIS:C	2.54	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:522:A:C5	1:A:523:C:C4	3.04	0.45
8:H:31:VAL:O	8:H:33:GLN:N	2.50	0.45
1:A:2287:A:C6	1:A:2289:G:C5	3.05	0.45
4:D:13:ARG:NH1	16:P:74:GLN:NE2	2.65	0.45
1:A:35:G:C4	1:A:454:A:C2	3.05	0.45
1:A:2581:G:C5	1:A:2610:C:C4	3.04	0.45
1:A:563:A:C6	1:A:2018:G:C5	3.05	0.45
17:Q:57:ARG:NH2	17:Q:92:LYS:CD	2.79	0.45
1:A:973:A:O4'	1:A:1188:U:C6	2.69	0.45
22:V:41:GLU:OE1	22:V:41:GLU:O	2.35	0.45
1:A:841:G:C2	1:A:938:G:C2	3.05	0.45
1:A:2333:A:C6	1:A:2335:A:N6	2.85	0.45
16:P:104:GLY:O	16:P:106:ALA:N	2.50	0.45
20:T:65:GLY:N	20:T:79:ASP:OD1	2.50	0.45
12:L:55:MET:O	12:L:60:ARG:NE	2.50	0.45
1:A:373:U:C5	1:A:400:G:N2	2.85	0.45
1:A:1247:A:C2	1:A:1249:U:C6	3.05	0.45
1:A:2548:U:C2'	1:A:2549:G:O5'	2.65	0.45
1:A:2662:A:N6	1:A:2663:G:C2	2.85	0.45
1:A:1276:A:C2	1:A:1277:G:C5	3.04	0.45
1:A:2520:C:C4	1:A:2567:G:C8	3.05	0.45
2:B:65:U:O4	2:B:108:A:O2'	2.34	0.45
1:A:1204:A:C8	1:A:1206:G:C2	3.05	0.45
1:A:1166:G:C5	1:A:1167:C:C5	3.05	0.45
1:A:1555:G:C6	1:A:1556:C:C4	3.05	0.45
1:A:727:A:OP1	1:A:1431:A:O2'	2.35	0.45
1:A:704:G:O2'	1:A:705:A:P	2.75	0.45
10:J:42:ALA:O	10:J:44:TYR:O	2.35	0.45
1:A:478:A:N6	1:A:480:A:C6	2.85	0.45
23:W:39:GLN:C	23:W:41:GLY:N	2.68	0.45
1:A:969:G:C2	1:A:970:U:C2	3.05	0.45
1:A:216:A:C8	1:A:432:A:C6	3.05	0.45
1:A:829:A:O2'	1:A:830:G:P	2.75	0.45
22:V:68:LYS:O	22:V:69:GLU:O	2.34	0.45
1:A:239:C:C4	1:A:240:C:N3	2.85	0.45
17:Q:45:ALA:O	17:Q:46:TYR:C	2.54	0.45
1:A:1956:U:O2'	1:A:1957:C:O4'	2.35	0.45
1:A:658:U:C2'	1:A:659:G:O5'	2.65	0.45
1:A:1055:G:N2	1:A:1105:U:O2	2.50	0.45
1:A:1063:G:C5	1:A:1064:C:C4	3.05	0.45
21:U:12:VAL:O	21:U:18:LYS:O	2.34	0.45
23:W:23:LYS:NZ	23:W:24:ARG:CG	2.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:572:A:OP1	1:A:573:U:C5	2.70	0.45
21:U:98:ASN:C	21:U:98:ASN:OD1	2.55	0.45
1:A:1912:A:C2	1:A:1919:A:C6	3.05	0.45
1:A:1300:G:C2	1:A:1626:A:C6	3.05	0.45
24:X:19:HIS:C	24:X:21:LEU:N	2.71	0.45
1:A:1341:G:O2'	1:A:1397:U:O2'	2.35	0.45
15:O:15:ARG:NE	15:O:93:ASP:OD1	2.49	0.45
3:C:236:GLY:O	34:C:778:HOH:O	2.21	0.45
16:P:111:GLU:N	16:P:111:GLU:CD	2.69	0.45
7:G:37:ASN:OD1	7:G:37:ASN:N	2.50	0.45
1:A:2532:G:C4	1:A:2533:U:C6	3.04	0.44
1:A:867:C:C4	1:A:868:U:C4	3.05	0.44
1:A:1404:C:O2	1:A:1405:U:C6	2.70	0.44
1:A:271:G:C4	1:A:272:A:N7	2.85	0.44
1:A:946:C:O2'	1:A:947:A:C5'	2.65	0.44
1:A:2331:G:O2'	1:A:2336:A:N1	2.50	0.44
1:A:463:G:C6	1:A:467:G:O6	2.70	0.44
1:A:555:G:O2'	1:A:556:A:P	2.74	0.44
8:H:9:VAL:O	8:H:10:ALA:O	2.35	0.44
7:G:8:VAL:O	7:G:9:VAL:O	2.34	0.44
1:A:86:G:C2	1:A:87:U:C5	3.05	0.44
1:A:1212:G:C2	1:A:1236:G:C5	3.05	0.44
1:A:2567:G:N2	1:A:2568:U:C2	2.85	0.44
12:L:14:LYS:CG	12:L:15:ALA:N	2.79	0.44
4:D:108:ASP:N	4:D:204:LYS:O	2.49	0.44
1:A:2819:G:C5	1:A:2821:A:C6	3.06	0.44
1:A:2564:A:N1	1:A:2646:C:O2'	2.50	0.44
1:A:2531:A:OP1	7:G:174:LYS:CG	2.65	0.44
1:A:488:G:O2'	19:S:49:LYS:NZ	2.50	0.44
1:A:2054:A:OP1	1:A:2055:C:O2'	2.34	0.44
6:F:134:GLN:C	6:F:136:ILE:N	2.70	0.44
1:A:28:A:C8	1:A:513:A:N6	2.86	0.44
1:A:2762:C:C4	1:A:2763:G:C5	3.05	0.44
1:A:1383:A:C6	1:A:1384:A:C6	3.04	0.44
1:A:2756:U:OP2	31:4:19:ARG:NE	2.50	0.44
1:A:1327:A:C2'	1:A:1328:A:C5'	2.96	0.44
1:A:2345:G:O2'	1:A:2381:A:O2'	2.36	0.44
1:A:1063:G:C2'	1:A:1064:C:O4'	2.65	0.44
1:A:310:A:O2'	1:A:311:A:P	2.75	0.44
1:A:2305:U:N3	1:A:2306:C:C2	2.85	0.44
1:A:233:A:N6	1:A:428:A:N6	2.65	0.44
1:A:923:G:N3	23:W:23:LYS:CE	2.80	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:23:LYS:CG	23:W:24:ARG:N	2.80	0.44
23:W:14:ASP:O	23:W:15:SER:CB	2.65	0.44
3:C:259:ASN:O	3:C:260:LYS:CB	2.65	0.44
19:S:29:VAL:O	19:S:33:LEU:CD2	2.65	0.44
30:3:26:ALA:O	30:3:27:ASN:CB	2.66	0.44
1:A:1816:C:C5	3:C:61:TYR:CE1	3.05	0.44
12:L:67:THR:CG2	12:L:68:SER:N	2.80	0.44
9:I:61:TYR:N	9:I:61:TYR:CD2	2.85	0.44
1:A:545:U:C3'	1:A:545:U:C6	3.00	0.44
1:A:2146:C:O4'	1:A:2146:C:O2	2.35	0.44
1:A:1510:G:O2'	1:A:1511:G:O5'	2.36	0.44
1:A:1343:G:N2	1:A:1405:U:C6	2.85	0.44
1:A:2813:A:C2	1:A:2814:A:C5	3.06	0.44
1:A:372:G:O2'	1:A:373:U:P	2.75	0.44
1:A:513:A:C2	1:A:514:A:C4	3.06	0.44
1:A:1392:A:C6	1:A:1393:A:C6	3.05	0.44
1:A:2592:G:C5	1:A:2593:U:C4	3.06	0.44
1:A:919:U:N3	1:A:920:A:C5	2.86	0.44
2:B:42:C:O2'	2:B:43:C:O4'	2.36	0.44
4:D:151:THR:CB	4:D:152:PRO:CD	2.95	0.44
20:T:57:VAL:O	20:T:85:VAL:O	2.36	0.44
1:A:2723:C:C4	1:A:2724:U:C4	3.05	0.44
24:X:42:GLU:O	24:X:43:LYS:C	2.55	0.44
1:A:1096:A:N6	1:A:1097:U:C4	2.86	0.44
1:A:285:G:N2	1:A:286:U:C2	2.85	0.44
1:A:1753:G:C2	1:A:1756:G:C2	3.05	0.44
1:A:2093:G:C4	1:A:2225:A:C5	3.05	0.44
1:A:89:A:N1	1:A:90:U:C4	2.85	0.44
1:A:867:C:N4	1:A:868:U:O4	2.51	0.44
1:A:2297:A:N7	1:A:2320:U:C4	2.85	0.44
1:A:10:A:N7	1:A:11:C:C5	2.86	0.44
1:A:2720:U:C2	1:A:2872:A:C6	3.05	0.44
1:A:1660:G:N3	1:A:1661:G:C8	2.85	0.44
1:A:2554:U:C4	1:A:2555:U:O4	2.70	0.44
4:D:149:ASN:CG	4:D:150:GLN:N	2.70	0.44
1:A:1927:A:C2	1:A:1928:A:C4	3.06	0.44
1:A:2864:G:C2	1:A:2865:U:C2	3.06	0.44
17:Q:3:VAL:O	17:Q:4:LYS:C	2.55	0.44
1:A:253:C:OP2	30:3:4:LYS:NZ	2.50	0.44
1:A:1036:G:C6	1:A:1120:G:C5	3.05	0.44
6:F:60:SER:O	6:F:61:GLY:C	2.55	0.44
8:H:45:GLU:O	8:H:49:ALA:CB	2.65	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:82:LEU:C	12:L:84:LYS:N	2.71	0.44
2:B:114:C:O4'	15:O:47:VAL:CG2	2.66	0.44
12:L:28:GLY:C	12:L:29:LYS:O	2.55	0.44
1:A:603:A:C4'	1:A:604:G:O5'	2.65	0.44
10:J:111:LYS:CD	10:J:112:GLY:N	2.81	0.44
1:A:1746:A:C2'	1:A:1747:U:C6	3.01	0.44
1:A:2353:G:O2'	23:W:31:LEU:CD2	2.65	0.44
1:A:2365:G:O2'	1:A:2366:A:C8	2.71	0.44
1:A:1181:U:O2'	1:A:1182:G:P	2.75	0.44
1:A:762:U:C4'	1:A:763:G:O5'	2.66	0.44
1:A:77:G:C4	1:A:78:U:C6	3.06	0.44
1:A:945:A:C5'	1:A:946:C:OP2	2.65	0.44
1:A:2033:A:O2'	1:A:2035:G:OP2	2.36	0.44
1:A:789:A:OP1	1:A:790:U:C5	2.70	0.44
1:A:2074:U:C6	1:A:2436:G:N2	2.86	0.44
1:A:2805:C:C4	1:A:2806:C:C5	3.05	0.44
5:E:31:VAL:O	5:E:34:ALA:N	2.51	0.44
1:A:2654:A:C4'	1:A:2655:G:OP1	2.66	0.44
1:A:1458:U:O4'	1:A:1459:G:C2	2.71	0.44
10:J:17:VAL:N	10:J:138:GLN:O	2.50	0.44
24:X:70:LEU:O	24:X:74:GLY:N	2.51	0.44
3:C:21:PRO:O	3:C:23:LEU:N	2.50	0.44
6:F:84:ILE:CG1	6:F:84:ILE:O	2.66	0.44
1:A:1062:G:C5	1:A:1088:A:C8	3.06	0.44
1:A:738:G:N1	1:A:739:A:C2	2.86	0.44
1:A:1475:G:O2'	1:A:1514:G:O6	2.36	0.44
1:A:975:A:C4	1:A:976:G:C8	3.06	0.44
1:A:2813:A:N1	1:A:2814:A:C6	2.85	0.44
1:A:763:G:C5	1:A:765:C:C5	3.05	0.44
1:A:1973:G:C4	1:A:1974:C:C5	3.06	0.44
1:A:637:A:N1	1:A:651:G:O2'	2.51	0.44
1:A:858:G:N2	1:A:2269:G:OP2	2.51	0.44
1:A:1724:G:C6	1:A:1725:U:N3	2.86	0.44
1:A:2446:G:N2	1:A:2449:U:O2	2.51	0.44
10:J:70:THR:C	10:J:71:ASP:OD2	2.56	0.44
10:J:133:ALA:O	10:J:136:GLN:N	2.51	0.44
1:A:1738:G:O2'	1:A:1739:A:C8	2.71	0.44
28:1:22:THR:OG1	28:1:23:THR:N	2.50	0.44
1:A:2290:G:O6	1:A:2341:G:O6	2.35	0.44
1:A:1510:G:O2'	1:A:1511:G:C8	2.70	0.44
17:Q:85:ALA:O	17:Q:87:VAL:C	2.56	0.44
1:A:89:A:C2	1:A:90:U:C2	3.05	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2346:A:C5	1:A:2383:G:C2	3.06	0.44
30:3:40:LYS:O	30:3:41:ARG:C	2.55	0.44
1:A:2134:A:O2'	1:A:2135:A:O4'	2.36	0.44
1:A:683:U:C2	1:A:684:G:C8	3.05	0.44
1:A:319:G:C5	1:A:333:G:C2	3.05	0.44
1:A:503:A:C2	1:A:505:A:C5	3.06	0.44
1:A:243:U:O2'	1:A:244:A:C5'	2.66	0.44
25:Y:23:ARG:O	25:Y:24:GLU:C	2.57	0.44
1:A:2455:G:C2	1:A:2456:C:C2	3.06	0.44
8:H:100:ALA:O	8:H:101:ASP:C	2.56	0.44
1:A:699:A:C4'	1:A:1634:A:N7	2.81	0.44
1:A:1975:G:C6	1:A:1976:U:C4	3.06	0.44
1:A:169:G:C4	1:A:170:U:C5	3.05	0.44
1:A:900:A:C4	1:A:901:C:C6	3.06	0.44
1:A:823:C:C4	1:A:824:U:C4	3.05	0.44
7:G:51:PHE:CD2	7:G:51:PHE:N	2.86	0.44
17:Q:63:ARG:CD	17:Q:64:ILE:N	2.81	0.43
1:A:1436:G:C2	1:A:1557:C:C2	3.06	0.43
4:D:91:THR:C	4:D:93:GLY:N	2.71	0.43
1:A:726:G:O2'	1:A:727:A:C8	2.71	0.43
1:A:1652:A:N6	1:A:1653:G:N2	2.66	0.43
1:A:1071:G:N7	1:A:1089:A:N6	2.66	0.43
1:A:820:A:N1	1:A:821:A:C2	2.86	0.43
1:A:1972:G:C2	1:A:1973:G:N7	2.86	0.43
1:A:1833:C:C2	1:A:1834:U:C5	3.06	0.43
1:A:1914:C:O2'	1:A:1915:U:C5'	2.66	0.43
1:A:1048:A:C5	1:A:1049:C:C5	3.06	0.43
21:U:73:ASN:C	21:U:75:ALA:N	2.70	0.43
5:E:172:ALA:O	5:E:175:ILE:CG2	2.66	0.43
1:A:308:G:C8	1:A:501:A:O4'	2.71	0.43
1:A:323:C:O2'	1:A:1205:A:N6	2.51	0.43
17:Q:79:ILE:O	17:Q:80:ASN:C	2.57	0.43
1:A:1842:G:C5	1:A:1843:C:C5	3.06	0.43
1:A:586:A:N1	1:A:809:G:O2'	2.51	0.43
1:A:919:U:C3'	1:A:919:U:C6	3.00	0.43
2:B:33:G:N3	2:B:50:A:C2	2.86	0.43
1:A:301:G:C6	1:A:317:G:C6	3.06	0.43
24:X:19:HIS:O	24:X:21:LEU:N	2.51	0.43
1:A:2079:U:O2'	24:X:22:ASN:ND2	2.51	0.43
1:A:1950:G:C8	1:A:1951:U:C5	3.06	0.43
1:A:1769:U:N3	1:A:1984:G:C6	2.87	0.43
1:A:2576:G:C8	1:A:2580:U:O4	2.71	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1588:G:C2	1:A:1589:U:C6	3.07	0.43
22:V:5:ASN:ND2	22:V:5:ASN:N	2.66	0.43
23:W:75:ASN:O	23:W:76:ARG:CB	2.66	0.43
1:A:587:C:OP2	12:L:21:ARG:NH1	2.51	0.43
1:A:482:A:C6	1:A:506:G:C4	3.06	0.43
1:A:1608:A:O2'	1:A:1610:A:OP1	2.36	0.43
1:A:195:A:C5	34:A:3607:HOH:O	2.70	0.43
25:Y:18:LEU:O	25:Y:22:LEU:CB	2.66	0.43
1:A:1759:A:N7	1:A:2696:U:O2'	2.51	0.43
3:C:225:ASN:O	3:C:227:VAL:N	2.51	0.43
1:A:2410:G:C6	1:A:2411:A:C4	3.07	0.43
4:D:121:THR:O	4:D:122:VAL:CB	2.66	0.43
1:A:1670:C:N4	1:A:1674:G:O5'	2.51	0.43
1:A:2286:G:O6	28:1:22:THR:CG2	2.66	0.43
14:N:93:GLY:C	14:N:95:THR:N	2.71	0.43
1:A:2747:G:N1	1:A:2754:U:C2	2.87	0.43
5:E:72:SER:C	5:E:74:LYS:N	2.72	0.43
2:B:27:C:C5	2:B:28:C:C5	3.05	0.43
19:S:50:VAL:O	19:S:51:LEU:C	2.57	0.43
1:A:588:U:C1'	5:E:85:PHE:CD1	3.01	0.43
11:K:111:LYS:CE	11:K:111:LYS:N	2.81	0.43
1:A:1286:A:N6	1:A:1329:U:O2'	2.51	0.43
7:G:61:TRP:O	7:G:64:ALA:N	2.51	0.43
1:A:2287:A:C6	1:A:2289:G:C4	3.07	0.43
1:A:2287:A:C4	1:A:2289:G:N7	2.87	0.43
1:A:514:A:O2'	1:A:515:A:O4'	2.36	0.43
1:A:2832:U:C2	1:A:2834:G:C2	3.06	0.43
1:A:1048:A:N7	1:A:1111:A:C6	2.85	0.43
1:A:696:G:C2	1:A:697:G:C8	3.06	0.43
1:A:250:G:OP1	30:3:12:ARG:NH1	2.52	0.43
1:A:2365:G:C2'	1:A:2366:A:C8	3.02	0.43
1:A:987:C:C4	1:A:988:A:C5	3.06	0.43
22:V:78:GLN:N	22:V:88:HIS:O	2.51	0.43
1:A:2275:C:O2	13:M:84:LYS:NZ	2.51	0.43
7:G:46:ASP:OD1	7:G:47:ASN:N	2.52	0.43
3:C:142:ASN:CG	3:C:142:ASN:O	2.56	0.43
17:Q:59:LEU:O	17:Q:62:ALA:N	2.52	0.43
1:A:24:G:C6	1:A:25:U:N3	2.86	0.43
1:A:1069:A:O2'	1:A:1070:A:C5'	2.66	0.43
11:K:92:GLU:O	11:K:93:GLN:O	2.37	0.43
1:A:1277:G:C6	1:A:1278:C:N4	2.86	0.43
1:A:1216:G:C2	1:A:1234:U:O2	2.71	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1204:A:C1'	1:A:1206:G:C5	3.01	0.43
1:A:313:G:C4	1:A:314:C:C5	3.07	0.43
1:A:1712:U:C4	1:A:1713:A:C6	3.06	0.43
4:D:72:GLY:O	4:D:73:VAL:O	2.37	0.43
14:N:40:LYS:O	14:N:43:GLU:N	2.52	0.43
18:R:39:LEU:CD2	18:R:39:LEU:N	2.82	0.43
24:X:77:TYR:O	24:X:77:TYR:CG	2.71	0.43
1:A:587:C:N3	12:L:33:ARG:NH2	2.66	0.43
23:W:22:VAL:O	23:W:23:LYS:C	2.57	0.43
1:A:1731:G:C4	1:A:1733:G:C8	3.06	0.43
1:A:1495:A:O2'	1:A:1496:A:O5'	2.37	0.43
1:A:2282:G:C6	1:A:2425:A:C2	3.07	0.43
1:A:1238:G:O2'	1:A:1239:G:C5'	2.66	0.43
2:B:55:U:O2'	6:F:23:SER:OG	2.36	0.43
2:B:27:C:C6	2:B:28:C:C5	3.06	0.43
1:A:313:G:C5	1:A:314:C:C5	3.07	0.43
1:A:1776:G:C6	1:A:1777:U:C4	3.06	0.43
5:E:82:GLY:O	5:E:83:VAL:CB	2.67	0.43
17:Q:88:GLU:C	17:Q:88:GLU:OE1	2.57	0.43
1:A:923:G:C5'	23:W:25:PHE:CZ	3.01	0.43
25:Y:40:SER:O	25:Y:42:LEU:N	2.52	0.43
1:A:222:A:C5	1:A:224:U:C2	3.07	0.43
1:A:1312:U:C4'	1:A:1313:U:O2	2.67	0.43
1:A:95:A:O2'	25:Y:41:HIS:CD2	2.71	0.43
1:A:1274:A:N1	1:A:1644:C:O2'	2.52	0.43
2:B:33:G:N2	2:B:50:A:C4	2.87	0.43
16:P:37:LYS:CG	16:P:37:LYS:O	2.66	0.43
1:A:2472:G:C5	1:A:2475:C:C4	3.06	0.43
1:A:301:G:N1	1:A:317:G:C5	2.87	0.43
1:A:1151:A:C6	1:A:1152:C:C4	3.07	0.43
3:C:120:ASP:O	3:C:121:ALA:O	2.37	0.43
1:A:159:G:N2	1:A:166:U:C5	2.87	0.43
1:A:2482:A:C5	1:A:2483:C:C5	3.07	0.43
1:A:2674:G:C4	1:A:2675:A:C8	3.06	0.43
17:Q:88:GLU:C	17:Q:88:GLU:CD	2.78	0.43
23:W:22:VAL:CG1	23:W:25:PHE:CE2	3.01	0.43
2:B:20:G:N2	2:B:64:G:N3	2.66	0.43
24:X:4:CYS:SG	24:X:51:SER:N	2.92	0.43
1:A:1048:A:OP2	1:A:1110:G:N2	2.52	0.43
1:A:2842:G:C2	1:A:2876:G:C2	3.07	0.43
1:A:2748:A:C6	1:A:2749:A:C5	3.06	0.43
1:A:536:G:O6	1:A:537:G:C2	2.71	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2824:C:C4	1:A:2825:G:C5	3.07	0.43
1:A:1206:G:C2	1:A:1207:C:C2	3.07	0.43
1:A:416:U:C4	1:A:417:C:C4	3.07	0.43
13:M:52:ALA:O	13:M:53:MET:C	2.57	0.43
18:R:62:GLU:CG	18:R:62:GLU:O	2.66	0.43
1:A:954:G:C6	1:A:955:U:C4	3.06	0.43
1:A:265:A:O2'	1:A:266:G:O4'	2.37	0.43
3:C:245:THR:N	3:C:249:VAL:O	2.52	0.43
15:O:94:ARG:O	15:O:95:SER:C	2.57	0.43
10:J:16:TYR:CA	10:J:138:GLN:O	2.67	0.43
1:A:421:C:O2'	1:A:422:A:OP2	2.37	0.43
1:A:613:A:C8	1:A:616:A:N1	2.86	0.43
1:A:1860:G:C2	1:A:1861:G:C8	3.07	0.43
1:A:2026:U:C2	1:A:2027:G:C8	3.06	0.43
31:4:24:ARG:NH2	31:4:24:ARG:CG	2.78	0.43
1:A:176:A:C5	1:A:177:G:C5	3.07	0.43
1:A:1967:C:C2	1:A:1968:G:C8	3.07	0.43
1:A:825:A:C2	1:A:833:A:C2	3.06	0.43
1:A:1342:A:OP2	1:A:1602:U:O4	2.36	0.43
1:A:460:A:OP1	29:2:41:ARG:NH1	2.52	0.43
1:A:541:A:C5	1:A:542:C:C5	3.07	0.43
24:X:51:SER:O	24:X:52:ALA:C	2.55	0.43
1:A:1381:G:O2'	1:A:1572:A:N1	2.52	0.43
1:A:1110:G:O2'	1:A:1111:A:C8	2.72	0.43
5:E:42:GLY:O	5:E:43:THR:OG1	2.37	0.43
1:A:1569:A:C6	1:A:1570:A:C2	3.07	0.43
1:A:1034:G:C6	1:A:1035:U:N3	2.87	0.43
8:H:24:GLY:O	8:H:26:ALA:N	2.52	0.43
26:Z:3:THR:C	26:Z:4:ILE:CG2	2.87	0.43
17:Q:63:ARG:CZ	17:Q:96:ASP:CA	2.97	0.42
1:A:310:A:OP1	21:U:15:GLY:N	2.52	0.42
1:A:1252:G:N3	17:Q:32:ARG:CG	2.82	0.42
1:A:541:A:C2	1:A:553:G:N3	2.87	0.42
1:A:2209:G:C6	1:A:2210:U:N3	2.87	0.42
17:Q:67:ALA:O	17:Q:68:ALA:C	2.57	0.42
1:A:638:G:C6	1:A:651:G:C2	3.07	0.42
1:A:1654:A:C4'	4:D:118:PHE:CE1	3.02	0.42
2:B:73:A:C5	2:B:104:A:C2	3.07	0.42
1:A:992:C:O2	1:A:993:G:C8	2.72	0.42
14:N:73:ASN:O	14:N:74:GLU:C	2.56	0.42
1:A:1716:U:O2'	1:A:1717:A:C5'	2.67	0.42
1:A:1444:G:C6	1:A:1445:G:C6	3.07	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:77:ILE:C	5:E:78:TRP:O	2.57	0.42
5:E:95:LYS:O	5:E:96:VAL:CB	2.66	0.42
10:J:35:ARG:O	10:J:37:ARG:N	2.52	0.42
2:B:46:A:C5	2:B:47:C:C5	3.07	0.42
15:O:57:ALA:O	15:O:59:ALA:N	2.52	0.42
18:R:37:GLU:OE1	18:R:37:GLU:O	2.36	0.42
23:W:26:GLY:O	23:W:27:GLY:C	2.58	0.42
11:K:117:SER:C	11:K:118:LEU:O	2.58	0.42
1:A:683:U:C2'	1:A:684:G:O5'	2.67	0.42
1:A:858:G:C5	1:A:2268:A:C2	3.07	0.42
16:P:5:LYS:O	16:P:9:GLN:N	2.52	0.42
1:A:991:C:C2	1:A:1185:G:C6	3.08	0.42
1:A:85:G:C5	1:A:98:G:C2	3.07	0.42
1:A:1659:G:C2	1:A:2002:G:N3	2.87	0.42
1:A:1677:A:C6	1:A:1678:A:C6	3.07	0.42
1:A:2555:U:C5	1:A:2556:C:C2	3.07	0.42
4:D:103:ASP:CG	4:D:104:VAL:N	2.72	0.42
1:A:2074:U:N3	1:A:2075:U:C4	2.87	0.42
1:A:1799:G:C4'	1:A:1800:C:O5'	2.67	0.42
1:A:988:A:C2	1:A:989:G:C2	3.07	0.42
1:A:1996:C:C5	11:K:32:TYR:OH	2.72	0.42
6:F:100:GLU:C	6:F:102:LEU:N	2.73	0.42
13:M:109:PRO:O	13:M:110:GLU:C	2.57	0.42
2:B:76:G:C8	2:B:76:G:O5'	2.72	0.42
1:A:68:G:N3	1:A:74:A:C8	2.87	0.42
1:A:2287:A:C5	1:A:2289:G:C5	3.07	0.42
3:C:83:ASP:OD1	3:C:85:ASN:OD1	2.36	0.42
1:A:1331:G:C5	1:A:1333:G:N7	2.87	0.42
1:A:860:U:C6	1:A:2268:A:O4'	2.73	0.42
1:A:434:U:C4'	1:A:435:C:OP1	2.68	0.42
12:L:66:PHE:C	12:L:66:PHE:CD1	2.91	0.42
1:A:715:A:N6	1:A:716:A:C6	2.87	0.42
1:A:1931:U:O2'	1:A:1932:A:C5'	2.66	0.42
1:A:2854:G:C6	1:A:2864:G:C6	3.07	0.42
1:A:1615:C:O2'	1:A:1616:A:O5'	2.37	0.42
1:A:1397:U:OP2	1:A:1398:C:N4	2.52	0.42
10:J:35:ARG:C	10:J:37:ARG:N	2.72	0.42
1:A:345:A:O2'	1:A:346:A:N7	2.53	0.42
2:B:34:A:N6	2:B:44:G:O2'	2.52	0.42
3:C:44:ASN:C	3:C:44:ASN:OD1	2.57	0.42
17:Q:93:ILE:CG2	17:Q:94:LEU:N	2.83	0.42
1:A:555:G:C2'	1:A:556:A:OP2	2.67	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:30:G:C6	1:A:31:C:C4	3.07	0.42
1:A:319:G:C5	1:A:333:G:N2	2.88	0.42
20:T:38:ALA:O	20:T:39:THR:OG1	2.37	0.42
1:A:1346:G:N2	1:A:1601:G:C4	2.88	0.42
1:A:1808:A:C5'	1:A:1809:A:OP2	2.68	0.42
1:A:2075:U:C4	1:A:2238:G:C6	3.07	0.42
9:I:115:ASP:C	9:I:115:ASP:OD1	2.58	0.42
1:A:2357:G:C2	1:A:2361:G:C6	3.07	0.42
1:A:1437:C:C4	1:A:1438:U:C4	3.07	0.42
8:H:27:ARG:NH1	24:X:59:ASP:O	2.52	0.42
8:H:66:ASN:O	8:H:68:ARG:N	2.53	0.42
1:A:749:A:N7	1:A:1618:A:C6	2.87	0.42
6:F:80:GLN:OE1	6:F:81:GLY:N	2.53	0.42
16:P:72:VAL:CG2	16:P:72:VAL:O	2.67	0.42
11:K:88:ASN:C	11:K:88:ASN:ND2	2.73	0.42
1:A:1532:A:C6	1:A:1540:G:C6	3.08	0.42
13:M:47:GLU:OE2	13:M:51:ARG:NH1	2.53	0.42
11:K:121:GLU:O	11:K:122:VAL:C	2.58	0.42
1:A:1408:G:N1	1:A:1595:C:C2	2.87	0.42
1:A:1006:C:C5	1:A:1138:G:N2	2.87	0.42
3:C:69:ASN:O	3:C:70:LYS:C	2.56	0.42
1:A:7:G:C6	1:A:8:C:N4	2.87	0.42
8:H:67:ALA:C	8:H:69:ALA:N	2.73	0.42
8:H:66:ASN:C	8:H:68:ARG:N	2.72	0.42
1:A:238:C:O2	1:A:260:G:C2	2.73	0.42
1:A:2830:C:O3'	4:D:56:LYS:NZ	2.53	0.42
3:C:139:THR:O	3:C:161:VAL:O	2.38	0.42
1:A:1791:A:N6	1:A:1828:G:O2'	2.52	0.42
12:L:120:VAL:CG1	12:L:121:THR:N	2.82	0.42
6:F:114:ARG:N	6:F:114:ARG:CD	2.83	0.42
1:A:117:G:C6	1:A:119:A:C6	3.08	0.42
1:A:1781:U:O2'	1:A:1782:U:OP2	2.37	0.42
15:O:31:THR:O	15:O:102:ARG:NH1	2.53	0.42
1:A:10:A:C5	1:A:2800:A:N6	2.87	0.42
11:K:2:ILE:O	11:K:3:GLN:O	2.38	0.42
1:A:2552:U:C2	1:A:2554:U:C5'	3.02	0.42
6:F:121:PHE:CD1	6:F:126:ASN:O	2.73	0.42
1:A:42:A:C2	1:A:438:G:C5	3.08	0.42
1:A:1177:G:C5	1:A:1178:C:C5	3.08	0.42
1:A:753:A:O2'	1:A:754:U:C5'	2.68	0.42
4:D:42:ASN:O	4:D:43:ASP:O	2.38	0.42
1:A:2253:G:C4	1:A:2254:C:C5	3.07	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:21:CYS:CB	11:K:39:ILE:CD1	2.96	0.42
1:A:1530:G:C2	1:A:1542:U:O2	2.72	0.42
28:1:12:SER:CB	28:1:48:TYR:CZ	3.03	0.42
4:D:176:ASP:OD2	4:D:176:ASP:N	2.53	0.42
1:A:1511:G:C2'	1:A:1512:C:OP2	2.65	0.42
1:A:2197:U:O2'	1:A:2198:A:P	2.78	0.42
1:A:569:U:OP1	1:A:945:A:C4	2.73	0.42
1:A:2414:G:C2	1:A:2415:G:C8	3.08	0.42
1:A:2024:G:C6	1:A:2025:C:N3	2.88	0.42
1:A:1313:U:O2'	1:A:1610:A:N1	2.53	0.42
1:A:1831:G:C5	1:A:1832:C:C5	3.07	0.42
7:G:115:GLN:O	7:G:116:LEU:C	2.57	0.42
1:A:121:G:O2'	1:A:122:G:C8	2.73	0.42
3:C:135:PRO:O	3:C:138:SER:OG	2.38	0.42
1:A:1754:A:N1	1:A:2716:C:O2'	2.53	0.42
1:A:2327:A:C2'	1:A:2328:A:C8	3.03	0.42
13:M:76:LYS:O	13:M:77:PRO:O	2.37	0.42
1:A:2267:A:N3	1:A:2267:A:C2'	2.82	0.42
6:F:27:VAL:O	6:F:27:VAL:CG1	2.67	0.42
5:E:154:ASP:C	5:E:154:ASP:OD2	2.58	0.42
1:A:1063:G:N2	1:A:1076:C:C2	2.88	0.42
1:A:64:A:O2'	20:T:70:HIS:CE1	2.73	0.42
15:O:67:ASN:O	15:O:67:ASN:CG	2.58	0.42
23:W:23:LYS:CD	23:W:24:ARG:N	2.83	0.42
1:A:2549:G:C2	1:A:2560:A:C5	3.08	0.42
1:A:2418:A:C4	1:A:2419:U:C6	3.06	0.42
1:A:98:G:N1	1:A:99:U:C4	2.87	0.42
3:C:255:LYS:O	3:C:257:ARG:N	2.53	0.42
5:E:7:ASP:N	5:E:7:ASP:OD2	2.53	0.42
11:K:72:PRO:O	11:K:74:GLY:N	2.53	0.42
12:L:68:SER:OG	12:L:71:ALA:N	2.53	0.42
1:A:1959:G:N1	1:A:1960:A:C4	2.88	0.42
1:A:2259:U:C2	1:A:2427:C:C4	3.08	0.42
26:Z:24:LEU:O	26:Z:27:GLY:N	2.52	0.42
5:E:88:ARG:O	5:E:89:PRO:C	2.56	0.42
1:A:1815:A:C4	1:A:1817:G:C5	3.07	0.42
17:Q:85:ALA:O	17:Q:87:VAL:O	2.37	0.42
8:H:30:LEU:C	8:H:31:VAL:O	2.58	0.42
20:T:27:SER:O	20:T:28:ASN:CG	2.58	0.42
23:W:9:THR:CG2	23:W:10:ARG:CD	2.98	0.42
15:O:105:ALA:O	15:O:107:ALA:N	2.53	0.42
1:A:2656:U:OP2	1:A:2664:G:N1	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1805:A:C6	1:A:1806:C:C5	3.07	0.42
1:A:1798:U:OP1	3:C:255:LYS:O	2.38	0.42
1:A:999:U:C5	1:A:1154:G:C5	3.08	0.42
4:D:5:VAL:N	4:D:32:ASN:ND2	2.67	0.42
1:A:2373:G:C6	1:A:2381:A:N1	2.88	0.42
1:A:1715:G:O2'	1:A:1743:G:O6	2.37	0.42
1:A:817:C:O2'	1:A:839:U:OP1	2.38	0.42
15:O:21:LEU:O	15:O:22:GLY:O	2.38	0.42
1:A:740:C:C6	1:A:740:C:O5'	2.73	0.42
1:A:1510:G:O2'	1:A:1511:G:C5'	2.67	0.42
17:Q:81:GLY:O	17:Q:85:ALA:N	2.53	0.42
1:A:1423:G:C2	1:A:1424:G:N9	2.88	0.42
1:A:2209:G:C6	1:A:2210:U:O4	2.72	0.42
1:A:25:U:C5	1:A:26:G:C6	3.08	0.42
1:A:1654:A:O3'	4:D:118:PHE:CE2	2.73	0.42
1:A:919:U:C2	1:A:920:A:C5	3.08	0.42
1:A:2478:A:N9	1:A:2529:G:N7	2.66	0.42
1:A:608:A:C6	1:A:609:A:C6	3.08	0.42
3:C:229:HIS:CG	3:C:230:PRO:CD	3.02	0.42
13:M:132:THR:CG2	13:M:133:LYS:N	2.83	0.42
1:A:2095:A:C2	1:A:2195:U:O2	2.73	0.42
1:A:2828:G:N2	1:A:2829:A:C4	2.88	0.42
1:A:2837:A:N1	1:A:2882:A:C6	2.88	0.42
1:A:846:U:O4	1:A:927:A:OP2	2.38	0.42
5:E:73:ILE:O	5:E:73:ILE:CG1	2.67	0.42
1:A:954:G:C6	1:A:955:U:C5	3.08	0.41
1:A:1342:A:C6	1:A:1345:C:N3	2.88	0.41
1:A:977:G:C4	1:A:978:G:C8	3.08	0.41
13:M:47:GLU:O	13:M:50:ARG:N	2.53	0.41
1:A:2077:A:C2	1:A:2078:C:C5	3.09	0.41
1:A:536:G:C2	1:A:558:U:O2	2.73	0.41
1:A:1328:A:C2'	1:A:1330:C:C5	3.02	0.41
22:V:88:HIS:CG	22:V:89:ILE:N	2.88	0.41
1:A:2081:U:C5	1:A:2237:G:N1	2.88	0.41
1:A:1304:A:C2	1:A:1305:C:C2	3.08	0.41
17:Q:16:ILE:O	17:Q:17:LEU:C	2.58	0.41
8:H:95:GLY:C	8:H:97:ARG:N	2.73	0.41
31:4:33:HIS:O	31:4:35:GLN:CG	2.68	0.41
14:N:52:ILE:O	14:N:54:LEU:N	2.53	0.41
15:O:5:SER:O	15:O:6:ALA:C	2.59	0.41
10:J:114:LEU:O	10:J:114:LEU:CD2	2.68	0.41
1:A:1080:A:C2	1:A:1081:U:C6	3.08	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:51:GLN:O	17:Q:52:ARG:C	2.59	0.41
1:A:1082:U:C2	1:A:1086:A:N6	2.87	0.41
1:A:1257:C:C4	1:A:1258:U:C5	3.08	0.41
25:Y:53:VAL:O	25:Y:56:LEU:O	2.38	0.41
1:A:1608:A:C5	1:A:1611:C:C4	3.08	0.41
1:A:1313:U:O2'	1:A:1610:A:C2	2.73	0.41
1:A:1911:U:C4	1:A:1918:A:C5	3.07	0.41
7:G:96:ALA:O	7:G:97:VAL:CB	2.68	0.41
1:A:1853:A:N1	1:A:1854:A:C2	2.89	0.41
17:Q:63:ARG:NH2	17:Q:96:ASP:CA	2.83	0.41
1:A:1286:A:C6	1:A:1329:U:C2	3.09	0.41
1:A:825:A:O2'	12:L:54:GLN:NE2	2.53	0.41
1:A:1343:G:C6	1:A:1344:U:O4	2.73	0.41
2:B:20:G:N2	2:B:64:G:C4	2.89	0.41
16:P:5:LYS:C	16:P:7:LEU:N	2.73	0.41
1:A:991:C:N3	1:A:1185:G:C6	2.88	0.41
1:A:1900:A:C2	1:A:1970:A:C5	3.08	0.41
4:D:151:THR:O	4:D:152:PRO:C	2.58	0.41
1:A:2357:G:N2	1:A:2361:G:C5	2.88	0.41
1:A:1959:G:C6	1:A:1960:A:C5	3.08	0.41
3:C:195:GLY:O	3:C:196:ASN:CB	2.68	0.41
1:A:579:G:C8	1:A:2017:U:C4	3.08	0.41
1:A:1723:G:O6	1:A:1737:G:O2'	2.38	0.41
1:A:1037:G:C2	1:A:1119:U:O2	2.73	0.41
16:P:3:ILE:O	16:P:3:ILE:CD1	2.69	0.41
1:A:698:C:C4	1:A:762:U:C4	3.09	0.41
1:A:391:A:C5	1:A:411:G:C2	3.08	0.41
7:G:29:ASN:OD1	7:G:30:GLY:N	2.53	0.41
11:K:118:LEU:N	11:K:118:LEU:CD1	2.84	0.41
14:N:75:ILE:O	14:N:79:LEU:CD1	2.68	0.41
1:A:2390:U:O2	1:A:2391:G:C8	2.73	0.41
20:T:19:LYS:O	20:T:23:ALA:CB	2.68	0.41
1:A:2557:G:C4	1:A:2558:C:C5	3.08	0.41
1:A:2799:A:O2'	1:A:2800:A:C4'	2.69	0.41
1:A:1000:A:C4	1:A:1155:A:C6	3.08	0.41
1:A:1276:A:C2	1:A:1277:G:N7	2.88	0.41
1:A:778:G:C5	1:A:779:U:C5	3.09	0.41
1:A:146:A:C2	1:A:147:C:C2	3.09	0.41
1:A:2097:A:C2	1:A:2193:G:C2	3.08	0.41
1:A:584:C:N4	1:A:585:G:C6	2.89	0.41
18:R:93:PHE:CD1	18:R:93:PHE:C	2.93	0.41
1:A:1021:A:N3	1:A:1021:A:C2'	2.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:748:G:OP2	19:S:88:ARG:NH2	2.53	0.41
6:F:135:ILE:C	6:F:137:PHE:N	2.74	0.41
1:A:542:C:C2'	1:A:542:C:O2	2.67	0.41
1:A:2851:A:N6	1:A:2852:G:C6	2.88	0.41
1:A:97:C:C2	1:A:98:G:C8	3.09	0.41
1:A:1829:A:N6	1:A:1977:A:N6	2.69	0.41
1:A:992:C:C2	1:A:993:G:C8	3.08	0.41
7:G:164:ALA:C	7:G:166:GLU:N	2.74	0.41
1:A:1866:A:C4	1:A:1876:A:C6	3.09	0.41
11:K:99:ILE:CG2	11:K:100:PHE:N	2.82	0.41
1:A:622:G:C6	1:A:623:C:N4	2.88	0.41
1:A:107:G:C2	1:A:108:G:C8	3.09	0.41
10:J:140:LEU:CD1	10:J:140:LEU:C	2.89	0.41
23:W:74:LYS:O	23:W:75:ASN:C	2.58	0.41
17:Q:94:LEU:O	17:Q:96:ASP:N	2.54	0.41
1:A:1062:G:N7	1:A:1088:A:C8	2.88	0.41
1:A:78:U:C2	1:A:79:C:C5	3.09	0.41
1:A:2287:A:C5	1:A:2289:G:N7	2.89	0.41
13:M:46:ILE:O	13:M:47:GLU:C	2.59	0.41
25:Y:42:LEU:O	25:Y:43:LEU:C	2.58	0.41
1:A:1654:A:N3	1:A:1655:A:C8	2.88	0.41
1:A:971:G:C6	1:A:972:A:C4	3.09	0.41
20:T:19:LYS:O	20:T:20:ALA:C	2.58	0.41
1:A:1798:U:P	3:C:255:LYS:O	2.79	0.41
11:K:2:ILE:N	11:K:2:ILE:CD1	2.82	0.41
5:E:7:ASP:CG	5:E:8:ALA:N	2.74	0.41
6:F:125:GLY:O	6:F:126:ASN:OD1	2.39	0.41
1:A:247:G:OP1	1:A:388:G:N2	2.54	0.41
1:A:987:C:N4	1:A:988:A:C5	2.89	0.41
1:A:312:G:N3	1:A:313:G:C8	2.89	0.41
16:P:3:ILE:C	16:P:3:ILE:CD1	2.89	0.41
1:A:607:U:O4	1:A:620:G:O4'	2.38	0.41
31:4:15:LYS:O	31:4:16:ILE:O	2.38	0.41
1:A:342:A:N1	1:A:343:C:C2	2.88	0.41
23:W:77:LYS:O	23:W:78:PHE:CB	2.67	0.41
1:A:1122:G:N3	1:A:1122:G:C2'	2.84	0.41
20:T:32:LEU:N	20:T:32:LEU:CD2	2.83	0.41
1:A:1125:G:N1	1:A:1126:A:N6	2.69	0.41
1:A:705:A:C2	1:A:706:A:C4	3.08	0.41
1:A:300:A:C2	1:A:333:G:O2'	2.74	0.41
1:A:2516:A:C6	1:A:2517:C:C4	3.09	0.41
1:A:2291:U:N3	1:A:2292:U:C4	2.89	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1753:G:N1	1:A:1756:G:OP2	2.53	0.41
1:A:988:A:C2	1:A:989:G:N2	2.88	0.41
10:J:34:ARG:O	10:J:37:ARG:N	2.54	0.41
1:A:217:A:C4	1:A:218:A:C8	3.08	0.41
1:A:681:G:C4	1:A:682:G:C8	3.09	0.41
1:A:2207:C:C2	1:A:2218:G:C2	3.09	0.41
16:P:58:PHE:N	16:P:58:PHE:CD2	2.88	0.41
1:A:1421:G:N3	1:A:1422:G:C8	2.88	0.41
1:A:36:G:C5	1:A:37:C:C5	3.08	0.41
16:P:112:ARG:O	16:P:113:LEU:C	2.58	0.41
1:A:2037:A:C6	1:A:2038:G:C6	3.09	0.41
1:A:2808:G:C2	1:A:2891:U:C6	3.08	0.41
1:A:1838:C:N4	1:A:1899:A:C4	2.88	0.41
1:A:1809:A:O2'	1:A:1810:A:O4'	2.39	0.41
1:A:301:G:C6	1:A:302:C:N4	2.89	0.41
1:A:752:A:O2'	1:A:753:A:P	2.79	0.41
15:O:57:ALA:C	15:O:59:ALA:N	2.74	0.41
1:A:2534:A:C5	1:A:2535:G:C8	3.09	0.41
1:A:1022:G:C6	1:A:1140:C:C4	3.09	0.41
4:D:91:THR:O	4:D:91:THR:OG1	2.38	0.41
1:A:1253:A:C3'	1:A:1254:A:C5'	2.99	0.41
12:L:110:VAL:O	12:L:111:ILE:CB	2.69	0.41
1:A:705:A:N6	1:A:726:G:C1'	2.83	0.41
1:A:1071:G:C4	1:A:1089:A:C6	3.09	0.41
1:A:1179:G:C4	1:A:1180:U:O2'	2.74	0.41
1:A:447:A:C8	1:A:473:G:C6	3.09	0.41
4:D:189:VAL:O	4:D:191:GLY:N	2.54	0.41
1:A:556:A:C8	1:A:557:C:C5	3.09	0.41
16:P:19:PHE:N	16:P:19:PHE:CD2	2.85	0.41
1:A:1416:G:O2'	1:A:1417:C:P	2.78	0.41
2:B:54:G:N3	2:B:55:U:C6	2.89	0.41
1:A:864:G:C6	1:A:865:C:C4	3.09	0.41
3:C:255:LYS:C	3:C:257:ARG:N	2.73	0.41
14:N:116:VAL:O	14:N:117:ASP:CB	2.69	0.41
1:A:1623:G:C2	1:A:1624:U:C6	3.09	0.41
1:A:2550:G:C6	1:A:2551:C:N4	2.89	0.41
1:A:2455:G:N2	1:A:2456:C:C2	2.89	0.41
20:T:49:LYS:O	20:T:50:LEU:C	2.58	0.41
3:C:108:GLY:O	3:C:109:LEU:C	2.59	0.41
23:W:47:GLY:C	23:W:49:ASN:N	2.75	0.41
21:U:94:PHE:O	21:U:94:PHE:CD1	2.73	0.41
15:O:93:ASP:C	15:O:95:SER:N	2.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1205:A:C6	5:E:165:HIS:CG	3.08	0.41
5:E:72:SER:O	5:E:74:LYS:N	2.54	0.41
10:J:35:ARG:O	10:J:36:LEU:C	2.57	0.41
2:B:46:A:C5	2:B:47:C:C4	3.09	0.41
13:M:108:VAL:CG1	13:M:109:PRO:CD	2.99	0.41
1:A:1406:U:O2'	1:A:1407:G:O5'	2.39	0.41
9:I:111:THR:O	9:I:113:ALA:N	2.54	0.41
6:F:53:ALA:C	6:F:55:ASP:N	2.74	0.41
1:A:1755:A:N6	1:A:2694:G:O2'	2.53	0.41
3:C:123:ILE:CG1	3:C:123:ILE:O	2.68	0.41
7:G:72:ASN:C	7:G:72:ASN:ND2	2.74	0.41
1:A:235:U:O2	1:A:430:A:C5	2.74	0.41
17:Q:114:ALA:C	17:Q:116:LEU:N	2.74	0.41
5:E:24:ASN:ND2	5:E:24:ASN:C	2.74	0.41
10:J:43:GLU:O	10:J:45:THR:CG2	2.69	0.41
1:A:1649:G:C6	1:A:2009:A:N6	2.89	0.41
1:A:2521:C:C4	1:A:2522:U:C4	3.09	0.41
1:A:1429:G:C2	1:A:1430:G:C5	3.09	0.41
1:A:858:G:C4	1:A:2268:A:C2	3.08	0.41
1:A:1677:A:N6	1:A:1678:A:N6	2.69	0.41
7:G:149:ALA:O	7:G:151:ARG:N	2.53	0.41
1:A:60:G:O2'	1:A:61:C:O5'	2.39	0.40
1:A:1404:C:C2	1:A:1405:U:C5	3.09	0.40
1:A:1065:U:O4	1:A:1074:G:N3	2.54	0.40
1:A:919:U:C6	1:A:919:U:C5'	3.03	0.40
1:A:1735:A:C4	1:A:1736:U:C5	3.09	0.40
1:A:2799:A:C5	1:A:2801:G:C8	3.09	0.40
1:A:1388:G:C4	1:A:1389:G:C8	3.09	0.40
1:A:1661:G:C6	1:A:1662:U:C4	3.10	0.40
1:A:498:G:N3	1:A:499:U:C6	2.89	0.40
20:T:80:TRP:CE3	20:T:81:LYS:O	2.74	0.40
1:A:110:G:C2	1:A:111:A:C8	3.09	0.40
1:A:2525:G:N2	1:A:2539:C:C2	2.89	0.40
3:C:259:ASN:O	3:C:261:ARG:N	2.55	0.40
1:A:292:U:N3	1:A:293:U:C5	2.89	0.40
1:A:81:G:C2	1:A:106:C:C2	3.09	0.40
10:J:132:HIS:O	10:J:133:ALA:C	2.59	0.40
1:A:2194:U:C4	1:A:2195:U:C4	3.08	0.40
1:A:2255:G:N7	1:A:2256:G:N7	2.69	0.40
4:D:39:ASP:OD2	4:D:40:LEU:N	2.54	0.40
21:U:5:ARG:O	21:U:6:ARG:C	2.59	0.40
28:1:18:HIS:CG	28:1:19:PHE:N	2.89	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:13:LYS:CD	6:F:13:LYS:C	2.90	0.40
1:A:2358:A:N6	12:L:54:GLN:NE2	2.69	0.40
1:A:1403:A:C4	1:A:1404:C:C5	3.09	0.40
2:B:16:G:C5	2:B:69:G:C2	3.09	0.40
13:M:47:GLU:O	13:M:48:ALA:C	2.60	0.40
1:A:1392:A:C2'	1:A:1393:A:C8	3.05	0.40
1:A:2282:G:C6	1:A:2425:A:N1	2.90	0.40
1:A:827:U:OP2	1:A:828:U:C2	2.74	0.40
1:A:1829:A:O2'	3:C:14:HIS:CE1	2.74	0.40
1:A:2204:G:C6	1:A:2205:A:C5	3.10	0.40
1:A:1800:C:OP1	3:C:259:ASN:ND2	2.54	0.40
1:A:2343:U:O2'	1:A:2373:G:O2'	2.40	0.40
6:F:8:LYS:O	6:F:12:VAL:CG1	2.70	0.40
1:A:1427:A:C4	1:A:1428:C:N4	2.89	0.40
31:4:10:LEU:N	31:4:14:CYS:SG	2.94	0.40
1:A:2186:G:C6	1:A:2187:U:C2	3.10	0.40
17:Q:77:LYS:O	17:Q:78:PHE:C	2.59	0.40
21:U:100:GLU:O	21:U:101:THR:CB	2.69	0.40
1:A:233:A:O2'	1:A:234:U:C5'	2.70	0.40
18:R:49:ILE:O	18:R:49:ILE:CG1	2.68	0.40
13:M:43:ALA:C	13:M:45:GLN:N	2.74	0.40
1:A:1899:A:C2'	1:A:1900:A:OP2	2.70	0.40
1:A:1380:G:C2	1:A:1381:G:N7	2.90	0.40
1:A:1839:G:C8	1:A:1927:A:O4'	2.75	0.40
21:U:94:PHE:O	21:U:94:PHE:CG	2.75	0.40
1:A:1327:A:OP2	34:A:3457:HOH:O	2.21	0.40
1:A:144:A:C6	1:A:145:C:C4	3.10	0.40
1:A:1340:U:C5	1:A:1603:A:C8	3.08	0.40
1:A:1688:U:O2'	1:A:1700:A:N7	2.54	0.40
21:U:44:HIS:O	21:U:45:GLN:C	2.59	0.40
1:A:2093:G:C5	1:A:2225:A:C5	3.09	0.40
1:A:996:A:C6	1:A:1160:G:C6	3.08	0.40
1:A:1538:G:O2'	1:A:1539:U:C5'	2.69	0.40
23:W:23:LYS:O	23:W:66:VAL:CB	2.70	0.40
1:A:725:G:O6	1:A:726:G:N1	2.54	0.40
23:W:51:GLY:O	23:W:52:CYS:C	2.58	0.40
1:A:30:G:C6	1:A:511:U:O2	2.75	0.40
15:O:34:HIS:CD2	15:O:53:THR:OG1	2.74	0.40
1:A:2791:G:C4	1:A:2792:A:C8	3.09	0.40
3:C:245:THR:C	3:C:247:TRP:N	2.74	0.40
1:A:1569:A:C6	1:A:1570:A:N1	2.90	0.40
1:A:2571:U:O3'	4:D:151:THR:OG1	2.39	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:96:ILE:O	13:M:96:ILE:CD1	2.70	0.40
6:F:100:GLU:O	6:F:102:LEU:N	2.55	0.40
1:A:2255:G:C5	1:A:2256:G:C8	3.09	0.40
1:A:1129:A:O2'	1:A:1130:U:OP2	2.39	0.40
1:A:2182:U:C2'	1:A:2183:A:OP1	2.69	0.40
1:A:2283:C:N4	1:A:2389:G:C5	2.90	0.40
6:F:2:LYS:O	6:F:6:TYR:N	2.54	0.40
1:A:287:G:N2	1:A:354:A:C4	2.89	0.40
5:E:160:ALA:O	5:E:162:ARG:N	2.55	0.40
1:A:1491:G:O2'	1:A:1492:G:O4'	2.38	0.40
1:A:320:A:O2'	1:A:322:A:C8	2.75	0.40
15:O:67:ASN:O	15:O:70:ALA:N	2.54	0.40
1:A:541:A:C6	1:A:553:G:C6	3.09	0.40
1:A:27:G:C2	1:A:512:G:O2'	2.74	0.40
1:A:1315:C:O2'	1:A:1392:A:N3	2.55	0.40
19:S:13:SER:OG	19:S:16:LYS:CD	2.69	0.40
1:A:556:A:N7	1:A:557:C:C5	2.90	0.40
1:A:2282:G:O2'	1:A:2390:U:O4	2.40	0.40
1:A:827:U:C4	1:A:2430:A:C5	3.09	0.40
1:A:30:G:O2'	1:A:1214:A:N3	2.55	0.40
15:O:53:THR:O	15:O:53:THR:OG1	2.39	0.40
1:A:751:A:C2	1:A:789:A:C4	3.09	0.40
4:D:90:PHE:O	4:D:92:VAL:N	2.55	0.40
11:K:1:MET:CE	11:K:32:TYR:CE1	3.04	0.40
1:A:1853:A:C6	1:A:1854:A:N1	2.89	0.40
1:A:327:G:C5	1:A:328:U:C4	3.09	0.40
7:G:11:PRO:O	7:G:12:ALA:C	2.60	0.40
6:F:127:TYR:O	6:F:128:SER:CB	2.69	0.40
1:A:1767:G:C2	1:A:1768:C:C6	3.10	0.40
1:A:580:U:O3'	17:Q:30:VAL:CG1	2.69	0.40
28:1:47:ILE:N	28:1:47:ILE:CD1	2.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/273 (98%)	192 (71%)	48 (18%)	29 (11%)	1	18
4	D	207/209 (99%)	141 (68%)	35 (17%)	31 (15%)	0	9
5	E	199/201 (99%)	138 (69%)	41 (21%)	20 (10%)	1	21
6	F	175/179 (98%)	133 (76%)	26 (15%)	16 (9%)	1	25
7	G	174/177 (98%)	114 (66%)	34 (20%)	26 (15%)	0	9
8	H	147/149 (99%)	63 (43%)	53 (36%)	31 (21%)	0	3
9	I	139/142 (98%)	84 (60%)	42 (30%)	13 (9%)	1	24
10	J	140/142 (99%)	100 (71%)	22 (16%)	18 (13%)	0	13
11	K	120/123 (98%)	86 (72%)	17 (14%)	17 (14%)	0	11
12	L	141/144 (98%)	106 (75%)	23 (16%)	12 (8%)	1	27
13	M	134/136 (98%)	95 (71%)	16 (12%)	23 (17%)	0	7
14	N	118/127 (93%)	85 (72%)	23 (20%)	10 (8%)	1	27
15	O	114/117 (97%)	84 (74%)	20 (18%)	10 (9%)	1	26
16	P	112/115 (97%)	74 (66%)	23 (20%)	15 (13%)	0	12
17	Q	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	2	39
18	R	101/103 (98%)	75 (74%)	14 (14%)	12 (12%)	1	15
19	S	108/110 (98%)	81 (75%)	20 (18%)	7 (6%)	2	37
20	T	91/100 (91%)	55 (60%)	20 (22%)	16 (18%)	0	6
21	U	100/104 (96%)	68 (68%)	16 (16%)	16 (16%)	0	8
22	V	92/94 (98%)	76 (83%)	15 (16%)	1 (1%)	21	79
23	W	77/85 (91%)	32 (42%)	18 (23%)	27 (35%)	0	0
24	X	75/78 (96%)	58 (77%)	12 (16%)	5 (7%)	2	36
25	Y	61/63 (97%)	39 (64%)	15 (25%)	7 (12%)	1	16
26	Z	56/59 (95%)	43 (77%)	10 (18%)	3 (5%)	3	43
27	0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	13
28	1	48/55 (87%)	32 (67%)	9 (19%)	7 (15%)	0	10
29	2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	4	48
30	3	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	6	58
31	4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	1	28
All	All	3309/3409 (97%)	2291 (69%)	625 (19%)	393 (12%)	1	15

All (393) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	35	LYS
3	C	77	VAL
3	C	104	LEU
3	C	106	PRO
3	C	110	LYS
3	C	120	ASP
3	C	121	ALA
3	C	196	ASN
4	D	43	ASP
4	D	54	ALA
4	D	73	VAL
4	D	99	GLU
4	D	103	ASP
4	D	104	VAL
4	D	119	ALA
4	D	122	VAL
4	D	169	ARG
4	D	192	ALA
5	E	6	LYS
5	E	8	ALA
5	E	46	GLN
5	E	153	LEU
5	E	175	ILE
6	F	8	LYS
6	F	111	ARG
6	F	134	GLN
7	G	7	PRO
7	G	8	VAL
7	G	9	VAL
7	G	33	THR
7	G	53	PRO
7	G	84	LYS
7	G	94	ARG
7	G	118	ALA
7	G	170	THR
8	H	3	VAL
8	H	8	LYS
8	H	9	VAL
8	H	10	ALA
8	H	14	SER
8	H	28	ASN
8	H	30	LEU
8	H	31	VAL

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Mol	Chain	Res	Type
8	H	32	PRO
8	H	33	GLN
8	H	35	LYS
8	H	121	VAL
9	I	65	SER
9	I	92	PRO
10	J	2	LYS
10	J	4	PHE
10	J	14	ASP
10	J	21	THR
10	J	44	TYR
10	J	45	THR
10	J	73	VAL
10	J	81	ILE
10	J	111	LYS
11	K	13	ASN
11	K	16	ALA
11	K	35	VAL
11	K	49	ARG
11	K	71	ARG
11	K	72	PRO
11	K	118	LEU
11	K	119	ALA
12	L	15	ALA
12	L	66	PHE
12	L	81	ASP
12	L	88	GLY
13	M	2	LEU
13	M	13	HIS
13	M	15	GLY
13	M	35	ALA
13	M	36	VAL
13	M	54	THR
13	M	55	ARG
13	M	60	GLN
13	M	69	PRO
13	M	77	PRO
14	N	2	ARG
14	N	15	SER
15	O	3	LYS
15	O	68	LYS
16	P	25	VAL

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Mol	Chain	Res	Type
16	P	50	ARG
16	P	103	THR
16	P	105	LYS
17	Q	87	VAL
18	R	55	ASP
18	R	91	GLN
19	S	3	THR
19	S	14	ALA
19	S	19	LEU
20	T	16	VAL
20	T	27	SER
20	T	29	THR
20	T	49	LYS
20	T	69	ARG
20	T	88	LYS
21	U	6	ARG
21	U	18	LYS
21	U	51	LEU
21	U	88	ASP
21	U	98	ASN
22	V	69	GLU
23	W	9	THR
23	W	23	LYS
23	W	30	VAL
23	W	36	ILE
23	W	51	GLY
24	X	34	SER
25	Y	22	LEU
25	Y	23	ARG
26	Z	3	THR
27	0	35	GLU
27	0	54	ILE
28	1	4	ILE
29	2	44	VAL
30	3	22	LYS
30	3	31	ILE
31	4	4	ARG
3	C	9	SER
3	C	22	GLU
3	C	43	ASN
3	C	57	HIS
3	C	140	VAL

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Mol	Chain	Res	Type
3	C	141	HIS
3	C	239	PHE
4	D	72	GLY
4	D	77	ARG
4	D	92	VAL
4	D	94	GLN
4	D	107	VAL
4	D	144	GLY
4	D	183	GLU
4	D	191	GLY
5	E	11	ALA
5	E	43	THR
5	E	78	TRP
6	F	113	PHE
6	F	149	ARG
6	F	175	PRO
7	G	28	LYS
7	G	30	GLY
7	G	31	GLU
7	G	44	HIS
7	G	45	ALA
7	G	60	GLY
7	G	164	ALA
7	G	168	VAL
8	H	25	TYR
8	H	34	GLY
8	H	54	LEU
8	H	81	ALA
8	H	83	LYS
8	H	101	ASP
8	H	131	SER
9	I	30	GLN
9	I	59	THR
10	J	13	ARG
10	J	39	LYS
10	J	41	LYS
11	K	3	GLN
11	K	93	GLN
11	K	108	ARG
12	L	65	GLY
12	L	111	ILE
13	M	14	LYS

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Mol	Chain	Res	Type
13	M	56	ALA
14	N	3	HIS
14	N	101	GLY
14	N	117	ASP
14	N	118	ARG
15	O	22	GLY
15	O	95	SER
15	O	100	HIS
15	O	112	GLU
16	P	2	ASN
16	P	4	ILE
16	P	15	ASP
16	P	65	ASN
16	P	93	LYS
17	Q	86	SER
19	S	64	ALA
20	T	35	ALA
20	T	68	LYS
20	T	70	HIS
20	T	84	TYR
20	T	86	THR
21	U	16	LYS
21	U	87	GLU
23	W	15	SER
23	W	17	ALA
23	W	18	LYS
23	W	25	PHE
23	W	26	GLY
23	W	27	GLY
23	W	33	GLY
23	W	47	GLY
23	W	50	VAL
24	X	18	SER
24	X	53	LYS
25	Y	24	GLU
25	Y	37	LEU
25	Y	44	LYS
27	0	34	GLY
27	0	51	ARG
28	1	51	ALA
31	4	16	ILE
3	C	8	THR

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Mol	Chain	Res	Type
3	C	94	LEU
3	C	105	ALA
3	C	157	ALA
3	C	189	ALA
3	C	237	ARG
3	C	243	PRO
4	D	17	GLU
4	D	106	LYS
4	D	118	PHE
4	D	184	ARG
4	D	190	LYS
5	E	79	ARG
5	E	80	SER
6	F	11	VAL
6	F	20	ASN
6	F	133	GLU
6	F	147	ARG
6	F	174	PHE
7	G	61	TRP
8	H	40	THR
8	H	106	ALA
8	H	111	ALA
9	I	105	LEU
10	J	65	THR
10	J	68	LYS
11	K	17	ARG
11	K	46	ALA
11	K	50	GLY
12	L	29	LYS
12	L	30	THR
13	M	59	ARG
13	M	79	ALA
13	M	81	ARG
14	N	80	PHE
15	O	58	ILE
15	O	94	ARG
15	O	113	ALA
16	P	5	LYS
16	P	20	ARG
16	P	34	GLY
16	P	51	ASN
16	P	86	LYS

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Mol	Chain	Res	Type
17	Q	5	ARG
17	Q	90	ASP
18	R	31	GLU
18	R	53	PHE
19	S	18	ARG
20	T	38	ALA
20	T	39	THR
21	U	38	ILE
21	U	39	ASN
21	U	74	ALA
21	U	83	GLY
21	U	92	VAL
23	W	16	GLU
23	W	29	SER
23	W	34	SER
23	W	74	LYS
24	X	17	ARG
24	X	20	ALA
25	Y	57	LEU
26	Z	34	THR
27	0	12	ARG
28	1	18	HIS
28	1	26	LYS
28	1	43	ARG
28	1	50	GLU
3	C	109	LEU
3	C	204	LEU
3	C	246	PRO
4	D	164	GLN
4	D	170	VAL
4	D	182	ALA
4	D	187	LEU
5	E	45	ALA
5	E	49	ARG
5	E	73	ILE
6	F	2	LYS
6	F	54	ALA
7	G	55	ASP
7	G	97	VAL
7	G	113	ASP
7	G	117	PRO
8	H	7	ASP

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Mol	Chain	Res	Type
8	H	29	PHE
8	H	67	ALA
8	H	89	LYS
8	H	96	THR
9	I	6	ALA
10	J	36	LEU
10	J	102	GLU
10	J	125	TYR
11	K	48	PRO
11	K	69	VAL
12	L	25	SER
12	L	64	PHE
13	M	84	LYS
13	M	134	THR
14	N	17	ARG
15	O	77	ALA
16	P	33	GLU
17	Q	4	LYS
18	R	49	ILE
18	R	71	LYS
19	S	96	ILE
20	T	18	GLU
23	W	14	ASP
23	W	56	HIS
27	0	3	GLN
28	1	16	THR
29	2	2	LYS
31	4	37	GLN
3	C	37	SER
3	C	64	VAL
3	C	150	GLY
4	D	109	VAL
4	D	145	SER
4	D	151	THR
5	E	59	PRO
5	E	71	GLY
5	E	83	VAL
5	E	96	VAL
7	G	16	VAL
7	G	32	LEU
7	G	109	SER
8	H	103	VAL

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Mol	Chain	Res	Type
9	I	3	LYS
9	I	7	TYR
9	I	20	SER
9	I	64	ARG
9	I	83	ALA
11	K	92	GLU
13	M	47	GLU
13	M	73	ILE
20	T	28	ASN
20	T	55	VAL
21	U	63	ALA
21	U	67	SER
21	U	85	ARG
23	W	40	ARG
23	W	78	PHE
25	Y	17	GLU
26	Z	4	ILE
3	C	226	PRO
5	E	123	LYS
5	E	148	ILE
6	F	61	GLY
6	F	83	PRO
8	H	13	GLY
8	H	107	GLY
10	J	96	ARG
12	L	23	ILE
12	L	40	SER
13	M	46	ILE
13	M	133	LYS
14	N	32	GLU
17	Q	43	GLN
17	Q	115	ALA
18	R	28	ALA
18	R	51	VAL
18	R	65	ALA
18	R	98	ILE
19	S	29	VAL
21	U	53	GLN
23	W	68	PHE
5	E	187	VAL
7	G	110	HIS
9	I	31	GLY

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Mol	Chain	Res	Type
13	M	72	PRO
18	R	64	VAL
23	W	41	GLY
4	D	93	GLY
23	W	37	VAL
23	W	73	PRO
8	H	80	ILE
6	F	135	ILE
9	I	23	VAL
13	M	23	GLY
14	N	84	GLY
23	W	70	VAL
27	O	53	VAL
18	R	30	GLY

### 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	
3	C	216/218 (99%)	173 (80%)	43 (20%)	2	14
4	D	164/164 (100%)	136 (83%)	28 (17%)	3	23
5	E	165/165 (100%)	130 (79%)	35 (21%)	1	12
6	F	148/150 (99%)	130 (88%)	18 (12%)	7	41
7	G	137/138 (99%)	107 (78%)	30 (22%)	1	11
8	H	114/114 (100%)	97 (85%)	17 (15%)	4	31
9	I	109/110 (99%)	94 (86%)	15 (14%)	5	35
10	J	116/116 (100%)	90 (78%)	26 (22%)	1	10
11	K	103/104 (99%)	84 (82%)	19 (18%)	2	18
12	L	102/103 (99%)	81 (79%)	21 (21%)	2	13
13	M	109/109 (100%)	90 (83%)	19 (17%)	3	21
14	N	100/103 (97%)	81 (81%)	19 (19%)	2	16
15	O	86/87 (99%)	69 (80%)	17 (20%)	2	15
16	P	99/100 (99%)	79 (80%)	20 (20%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	89/90 (99%)	73 (82%)	16 (18%)	2	19
18	R	84/84 (100%)	69 (82%)	15 (18%)	2	20
19	S	93/93 (100%)	73 (78%)	20 (22%)	1	11
20	T	80/84 (95%)	61 (76%)	19 (24%)	1	8
21	U	83/85 (98%)	69 (83%)	14 (17%)	3	24
22	V	78/78 (100%)	64 (82%)	14 (18%)	2	20
23	W	59/63 (94%)	43 (73%)	16 (27%)	1	6
24	X	67/68 (98%)	53 (79%)	14 (21%)	1	12
25	Y	55/55 (100%)	44 (80%)	11 (20%)	2	14
26	Z	48/49 (98%)	34 (71%)	14 (29%)	0	5
27	0	47/48 (98%)	42 (89%)	5 (11%)	10	49
28	1	45/49 (92%)	37 (82%)	8 (18%)	2	20
29	2	38/38 (100%)	32 (84%)	6 (16%)	4	28
30	3	51/52 (98%)	44 (86%)	7 (14%)	5	35
31	4	34/34 (100%)	30 (88%)	4 (12%)	8	43
All	All	2719/2751 (99%)	2209 (81%)	510 (19%)	2	17

All (510) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	12	ARG
3	C	18	VAL
3	C	20	ASN
3	C	27	LYS
3	C	35	LYS
3	C	38	LYS
3	C	43	ASN
3	C	71	ASP
3	C	73	ILE
3	C	77	VAL
3	C	85	ASN
3	C	90	ILE
3	C	93	VAL
3	C	104	LEU
3	C	109	LEU
3	C	110	LYS
3	C	114	GLN

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Mol	Chain	Res	Type
3	C	115	ILE
3	C	120	ASP
3	C	123	ILE
3	C	129	LEU
3	C	132	ARG
3	C	142	ASN
3	C	155	ARG
3	C	164	VAL
3	C	171	VAL
3	C	172	THR
3	C	173	LEU
3	C	175	LEU
3	C	176	ARG
3	C	201	LEU
3	C	202	ARG
3	C	203	VAL
3	C	212	TRP
3	C	213	ARG
3	C	215	VAL
3	C	227	VAL
3	C	250	GLN
3	C	252	LYS
3	C	254	LYS
3	C	261	ARG
3	C	268	ARG
3	C	269	ARG
4	D	4	LEU
4	D	14	ILE
4	D	16	THR
4	D	17	GLU
4	D	40	LEU
4	D	42	ASN
4	D	43	ASP
4	D	45	TYR
4	D	60	VAL
4	D	73	VAL
4	D	89	GLU
4	D	90	PHE
4	D	91	THR
4	D	98	VAL
4	D	106	LYS
4	D	114	LYS

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Mol	Chain	Res	Type
4	D	118	PHE
4	D	124	ARG
4	D	131	ASP
4	D	139	SER
4	D	140	HIS
4	D	150	GLN
4	D	159	LYS
4	D	169	ARG
4	D	171	THR
4	D	176	ASP
4	D	183	GLU
4	D	186	LEU
5	E	12	LEU
5	E	14	VAL
5	E	24	ASN
5	E	44	ARG
5	E	48	THR
5	E	61	ARG
5	E	65	THR
5	E	69	ARG
5	E	70	SER
5	E	77	ILE
5	E	78	TRP
5	E	80	SER
5	E	84	THR
5	E	90	GLN
5	E	91	ASP
5	E	108	ILE
5	E	109	LEU
5	E	111	GLU
5	E	113	VAL
5	E	116	ASP
5	E	118	LEU
5	E	119	ILE
5	E	121	VAL
5	E	123	LYS
5	E	127	GLU
5	E	144	GLU
5	E	146	VAL
5	E	153	LEU
5	E	159	LEU
5	E	163	ASN

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Mol	Chain	Res	Type
5	E	170	ARG
5	E	171	ASP
5	E	178	VAL
5	E	186	VAL
5	E	189	THR
6	F	3	LEU
6	F	9	ASP
6	F	12	VAL
6	F	24	VAL
6	F	34	THR
6	F	35	LEU
6	F	36	ASN
6	F	46	LYS
6	F	65	LEU
6	F	82	TYR
6	F	90	LEU
6	F	103	ILE
6	F	109	ARG
6	F	111	ARG
6	F	114	ARG
6	F	132	ARG
6	F	134	GLN
6	F	154	THR
7	G	8	VAL
7	G	15	ASP
7	G	21	GLN
7	G	29	ASN
7	G	32	LEU
7	G	34	ARG
7	G	35	THR
7	G	37	ASN
7	G	40	VAL
7	G	55	ASP
7	G	59	ASP
7	G	68	ARG
7	G	72	ASN
7	G	78	VAL
7	G	80	GLU
7	G	84	LYS
7	G	86	LEU
7	G	91	VAL
7	G	93	TYR

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Mol	Chain	Res	Type
7	G	101	VAL
7	G	116	LEU
7	G	120	ILE
7	G	121	THR
7	G	123	GLU
7	G	126	THR
7	G	132	LEU
7	G	138	GLN
7	G	148	ARG
7	G	170	THR
7	G	174	LYS
8	H	6	LEU
8	H	12	LEU
8	H	14	SER
8	H	15	LEU
8	H	18	GLN
8	H	28	ASN
8	H	31	VAL
8	H	48	GLU
8	H	50	ARG
8	H	54	LEU
8	H	68	ARG
8	H	75	LEU
8	H	83	LYS
8	H	96	THR
8	H	97	ARG
8	H	125	THR
8	H	135	HIS
9	I	2	LYS
9	I	10	LEU
9	I	11	GLN
9	I	23	VAL
9	I	37	PHE
9	I	39	LYS
9	I	49	GLU
9	I	61	TYR
9	I	71	LYS
9	I	81	LYS
9	I	86	LYS
9	I	95	ASP
9	I	107	GLU
9	I	126	ARG

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Mol	Chain	Res	Type
9	I	135	MET
10	J	1	MET
10	J	2	LYS
10	J	3	THR
10	J	7	LYS
10	J	24	THR
10	J	25	LEU
10	J	30	THR
10	J	31	GLU
10	J	36	LEU
10	J	40	HIS
10	J	41	LYS
10	J	43	GLU
10	J	44	TYR
10	J	54	ILE
10	J	55	ILE
10	J	65	THR
10	J	72	LYS
10	J	86	GLN
10	J	88	THR
10	J	90	GLU
10	J	103	ILE
10	J	111	LYS
10	J	114	LEU
10	J	129	GLU
10	J	139	VAL
10	J	140	LEU
11	K	2	ILE
11	K	3	GLN
11	K	8	LEU
11	K	18	ARG
11	K	21	CYS
11	K	23	LYS
11	K	47	ILE
11	K	51	LYS
11	K	52	VAL
11	K	54	LYS
11	K	58	LEU
11	K	69	VAL
11	K	73	ASP
11	K	88	ASN
11	K	89	ASN

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Mol	Chain	Res	Type
11	K	93	GLN
11	K	105	ARG
11	K	111	LYS
11	K	114	LYS
12	L	3	LEU
12	L	4	ASN
12	L	6	LEU
12	L	13	LYS
12	L	14	LYS
12	L	19	LEU
12	L	21	ARG
12	L	27	LEU
12	L	46	VAL
12	L	47	ARG
12	L	55	MET
12	L	61	LEU
12	L	66	PHE
12	L	91	ASP
12	L	93	ASN
12	L	94	THR
12	L	101	ILE
12	L	112	LEU
12	L	121	THR
12	L	122	VAL
12	L	135	ILE
13	M	8	LYS
13	M	10	ARG
13	M	12	MET
13	M	25	ASP
13	M	33	LEU
13	M	36	VAL
13	M	58	LYS
13	M	70	ASP
13	M	75	GLU
13	M	90	GLU
13	M	95	LEU
13	M	96	ILE
13	M	97	GLN
13	M	100	LYS
13	M	102	LEU
13	M	110	GLU
13	M	131	VAL

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Mol	Chain	Res	Type
13	M	133	LYS
13	M	134	THR
14	N	2	ARG
14	N	3	HIS
14	N	8	ARG
14	N	10	LEU
14	N	14	SER
14	N	15	SER
14	N	20	MET
14	N	23	ASN
14	N	33	ILE
14	N	35	LYS
14	N	38	LEU
14	N	51	LEU
14	N	69	ARG
14	N	71	ARG
14	N	75	ILE
14	N	79	LEU
14	N	83	LEU
14	N	95	THR
14	N	120	GLU
15	O	4	LYS
15	O	9	ARG
15	O	16	ARG
15	O	17	LYS
15	O	28	VAL
15	O	31	THR
15	O	36	TYR
15	O	52	SER
15	O	53	THR
15	O	65	THR
15	O	80	GLU
15	O	83	LEU
15	O	84	GLU
15	O	94	ARG
15	O	100	HIS
15	O	103	VAL
15	O	111	ARG
16	P	3	ILE
16	P	6	GLN
16	P	14	GLN
16	P	16	VAL

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Mol	Chain	Res	Type
16	P	24	THR
16	P	36	LYS
16	P	37	LYS
16	P	38	ARG
16	P	61	ARG
16	P	69	VAL
16	P	75	THR
16	P	77	SER
16	P	79	VAL
16	P	83	ILE
16	P	91	VAL
16	P	92	ARG
16	P	93	LYS
16	P	95	LYS
16	P	96	LEU
16	P	99	LEU
17	Q	2	ARG
17	Q	8	ILE
17	Q	10	ARG
17	Q	40	LYS
17	Q	50	ARG
17	Q	59	LEU
17	Q	63	ARG
17	Q	65	ASN
17	Q	69	ARG
17	Q	88	GLU
17	Q	91	ARG
17	Q	93	ILE
17	Q	94	LEU
17	Q	96	ASP
17	Q	97	ILE
17	Q	103	VAL
18	R	10	LYS
18	R	14	VAL
18	R	37	GLU
18	R	38	VAL
18	R	39	LEU
18	R	43	ASN
18	R	46	GLU
18	R	48	LYS
18	R	54	VAL
18	R	63	VAL

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Mol	Chain	Res	Type
18	R	72	VAL
18	R	83	TYR
18	R	85	LYS
18	R	86	GLN
18	R	97	LYS
19	S	3	THR
19	S	4	ILE
19	S	7	HIS
19	S	30	SER
19	S	36	LEU
19	S	41	LYS
19	S	45	VAL
19	S	48	LYS
19	S	66	ILE
19	S	68	ASP
19	S	70	LYS
19	S	71	VAL
19	S	73	LYS
19	S	76	VAL
19	S	84	ARG
19	S	88	ARG
19	S	96	ILE
19	S	101	SER
19	S	107	VAL
19	S	109	ASP
20	T	2	ILE
20	T	3	ARG
20	T	4	GLU
20	T	8	LEU
20	T	17	SER
20	T	19	LYS
20	T	29	THR
20	T	30	ILE
20	T	31	VAL
20	T	43	ILE
20	T	48	GLN
20	T	49	LYS
20	T	50	LEU
20	T	64	LYS
20	T	67	VAL
20	T	68	LYS
20	T	69	ARG

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Mol	Chain	Res	Type
20	T	73	ARG
20	T	74	ILE
21	U	6	ARG
21	U	8	ASP
21	U	10	VAL
21	U	33	VAL
21	U	42	LYS
21	U	43	LYS
21	U	52	ASN
21	U	61	GLU
21	U	64	ILE
21	U	67	SER
21	U	80	ASP
21	U	86	PHE
21	U	99	SER
21	U	102	ILE
22	V	1	MET
22	V	3	THR
22	V	5	ASN
22	V	8	VAL
22	V	10	LYS
22	V	20	LEU
22	V	29	ILE
22	V	41	GLU
22	V	42	LEU
22	V	43	ASP
22	V	46	LYS
22	V	51	GLN
22	V	61	LEU
22	V	66	ASP
23	W	14	ASP
23	W	15	SER
23	W	19	ARG
23	W	23	LYS
23	W	24	ARG
23	W	25	PHE
23	W	38	ARG
23	W	40	ARG
23	W	45	HIS
23	W	49	ASN
23	W	54	ARG
23	W	58	LEU

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Mol	Chain	Res	Type
23	W	67	LYS
23	W	71	LYS
23	W	77	LYS
23	W	80	SER
24	X	6	VAL
24	X	10	ARG
24	X	17	ARG
24	X	19	HIS
24	X	24	THR
24	X	26	ARG
24	X	27	ARG
24	X	29	LEU
24	X	47	THR
24	X	53	LYS
24	X	65	THR
24	X	71	ARG
24	X	73	ARG
24	X	77	TYR
25	Y	9	LYS
25	Y	10	SER
25	Y	14	LEU
25	Y	18	LEU
25	Y	19	LEU
25	Y	22	LEU
25	Y	37	LEU
25	Y	42	LEU
25	Y	56	LEU
25	Y	57	LEU
25	Y	59	GLU
26	Z	2	LYS
26	Z	3	THR
26	Z	4	ILE
26	Z	5	LYS
26	Z	8	GLN
26	Z	9	THR
26	Z	15	ARG
26	Z	23	LEU
26	Z	29	ARG
26	Z	30	ARG
26	Z	37	ARG
26	Z	38	GLU
26	Z	43	ILE

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Mol	Chain	Res	Type
26	Z	58	GLU
27	0	9	ARG
27	0	27	LEU
27	0	28	SER
27	0	39	ARG
27	0	42	ILE
28	1	4	ILE
28	1	9	LYS
28	1	16	THR
28	1	21	THR
28	1	33	LEU
28	1	35	LEU
28	1	42	VAL
28	1	43	ARG
29	2	1	MET
29	2	3	ARG
29	2	12	ARG
29	2	16	HIS
29	2	21	ARG
29	2	39	ARG
30	3	5	THR
30	3	7	ARG
30	3	22	LYS
30	3	31	ILE
30	3	34	LYS
30	3	49	VAL
30	3	51	LYS
31	4	1	MET
31	4	4	ARG
31	4	9	LYS
31	4	13	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2850/2903 (98%)	925 (32%)	497 (17%)
2	B	117/118 (99%)	32 (27%)	22 (18%)
All	All	2967/3021 (98%)	957 (32%)	519 (17%)

All (957) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	13	A
1	A	14	A
1	A	15	G
1	A	28	A
1	A	34	U
1	A	35	G
1	A	36	G
1	A	40	U
1	A	43	G
1	A	46	G
1	A	49	A
1	A	50	U
1	A	51	G
1	A	61	C
1	A	62	U
1	A	63	A
1	A	70	G
1	A	71	A
1	A	73	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	85	G
1	A	86	G
1	A	87	U
1	A	91	A
1	A	92	U
1	A	93	G
1	A	99	U
1	A	101	A
1	A	103	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	121	G
1	A	122	G
1	A	125	A
1	A	126	A
1	A	127	A
1	A	128	C
1	A	135	U

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Mol	Chain	Res	Type
1	A	137	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	143	C
1	A	144	A
1	A	162	U
1	A	163	C
1	A	164	C
1	A	177	G
1	A	178	G
1	A	180	G
1	A	182	A
1	A	188	G
1	A	196	A
1	A	197	A
1	A	199	A
1	A	200	U
1	A	201	C
1	A	204	A
1	A	205	G
1	A	206	U
1	A	207	A
1	A	215	G
1	A	216	A
1	A	217	A
1	A	221	A
1	A	222	A
1	A	223	A
1	A	227	A
1	A	228	C
1	A	229	C
1	A	230	G
1	A	232	G
1	A	233	A
1	A	234	U
1	A	241	A
1	A	242	G
1	A	243	U
1	A	244	A

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Mol	Chain	Res	Type
1	A	248	G
1	A	249	C
1	A	250	G
1	A	255	A
1	A	265	A
1	A	266	G
1	A	267	C
1	A	272	A
1	A	273	G
1	A	276	U
1	A	277	G
1	A	278	A
1	A	279	A
1	A	280	U
1	A	285	G
1	A	298	G
1	A	299	A
1	A	301	G
1	A	302	C
1	A	303	G
1	A	310	A
1	A	311	A
1	A	312	G
1	A	313	G
1	A	322	A
1	A	329	G
1	A	330	A
1	A	333	G
1	A	334	C
1	A	346	A
1	A	347	A
1	A	349	U
1	A	352	A
1	A	353	C
1	A	359	G
1	A	361	G
1	A	362	A
1	A	367	G
1	A	370	G
1	A	371	A
1	A	372	G
1	A	383	C

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Mol	Chain	Res	Type
1	A	387	U
1	A	388	G
1	A	390	U
1	A	395	U
1	A	396	G
1	A	399	U
1	A	404	A
1	A	405	U
1	A	412	A
1	A	419	U
1	A	422	A
1	A	424	G
1	A	433	C
1	A	435	C
1	A	436	C
1	A	437	U
1	A	443	A
1	A	446	G
1	A	447	A
1	A	449	A
1	A	454	A
1	A	455	C
1	A	459	U
1	A	460	A
1	A	461	C
1	A	475	C
1	A	476	G
1	A	479	A
1	A	480	A
1	A	481	G
1	A	482	A
1	A	483	A
1	A	490	C
1	A	491	G
1	A	492	A
1	A	504	A
1	A	505	A
1	A	506	G
1	A	507	A
1	A	508	A
1	A	509	C
1	A	510	C

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Mol	Chain	Res	Type
1	A	512	G
1	A	513	A
1	A	514	A
1	A	515	A
1	A	528	A
1	A	529	A
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	534	U
1	A	543	G
1	A	544	C
1	A	545	U
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	550	C
1	A	563	A
1	A	566	U
1	A	572	A
1	A	573	U
1	A	575	A
1	A	586	A
1	A	587	C
1	A	588	U
1	A	589	U
1	A	603	A
1	A	604	G
1	A	605	G
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	617	G
1	A	621	A
1	A	622	G
1	A	627	A
1	A	628	G
1	A	631	A
1	A	634	C

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Mol	Chain	Res	Type
1	A	637	A
1	A	638	G
1	A	639	U
1	A	645	C
1	A	646	U
1	A	647	G
1	A	653	U
1	A	654	A
1	A	655	A
1	A	656	G
1	A	657	U
1	A	669	G
1	A	670	A
1	A	682	G
1	A	684	G
1	A	685	A
1	A	686	U
1	A	687	C
1	A	688	U
1	A	689	A
1	A	690	G
1	A	705	A
1	A	713	G
1	A	714	U
1	A	715	A
1	A	717	C
1	A	727	A
1	A	728	G
1	A	729	G
1	A	730	A
1	A	738	G
1	A	740	C
1	A	743	A
1	A	744	U
1	A	747	U
1	A	748	G
1	A	749	A
1	A	751	A
1	A	753	A
1	A	754	U
1	A	763	G
1	A	764	A

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Mol	Chain	Res	Type
1	A	765	C
1	A	766	U
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	783	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	790	U
1	A	791	C
1	A	792	A
1	A	800	A
1	A	801	G
1	A	802	A
1	A	803	U
1	A	805	G
1	A	806	C
1	A	810	U
1	A	811	U
1	A	812	C
1	A	813	U
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	856	G
1	A	858	G
1	A	859	G
1	A	860	U
1	A	865	C
1	A	866	A
1	A	867	C
1	A	868	U
1	A	896	A
1	A	897	C
1	A	900	A
1	A	910	A

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Mol	Chain	Res	Type
1	A	914	G
1	A	915	C
1	A	916	G
1	A	927	A
1	A	931	U
1	A	932	U
1	A	933	A
1	A	934	U
1	A	941	A
1	A	945	A
1	A	946	C
1	A	947	A
1	A	950	G
1	A	957	C
1	A	958	U
1	A	959	A
1	A	961	C
1	A	962	G
1	A	963	U
1	A	973	A
1	A	974	G
1	A	975	A
1	A	976	G
1	A	983	A
1	A	984	A
1	A	985	C
1	A	990	A
1	A	991	C
1	A	995	C
1	A	996	A
1	A	997	G
1	A	1005	C
1	A	1006	C
1	A	1008	A
1	A	1009	A
1	A	1010	A
1	A	1011	G
1	A	1012	U
1	A	1013	C
1	A	1017	G
1	A	1021	A
1	A	1022	G

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Mol	Chain	Res	Type
1	A	1023	U
1	A	1024	G
1	A	1025	G
1	A	1026	G
1	A	1027	A
1	A	1028	A
1	A	1033	U
1	A	1034	G
1	A	1035	U
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1063	G
1	A	1065	U
1	A	1066	U
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1073	A
1	A	1074	G
1	A	1078	U
1	A	1083	U
1	A	1084	A
1	A	1088	A
1	A	1091	G
1	A	1092	C
1	A	1098	A
1	A	1104	C
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1113	U
1	A	1126	A
1	A	1127	A
1	A	1128	G
1	A	1129	A
1	A	1130	U
1	A	1132	U
1	A	1133	A

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Mol	Chain	Res	Type
1	A	1135	C
1	A	1136	G
1	A	1137	G
1	A	1139	G
1	A	1142	A
1	A	1144	A
1	A	1145	C
1	A	1154	G
1	A	1155	A
1	A	1157	G
1	A	1158	C
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1180	U
1	A	1181	U
1	A	1204	A
1	A	1205	A
1	A	1206	G
1	A	1207	C
1	A	1210	G
1	A	1211	C
1	A	1215	G
1	A	1236	G
1	A	1237	A
1	A	1238	G
1	A	1240	U
1	A	1247	A
1	A	1248	G
1	A	1249	U
1	A	1250	G
1	A	1251	C
1	A	1253	A
1	A	1254	A
1	A	1256	G
1	A	1265	A
1	A	1266	G
1	A	1268	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1274	A

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Mol	Chain	Res	Type
1	A	1275	A
1	A	1276	A
1	A	1277	G
1	A	1281	G
1	A	1287	A
1	A	1288	G
1	A	1289	C
1	A	1290	C
1	A	1300	G
1	A	1301	A
1	A	1303	G
1	A	1310	G
1	A	1320	C
1	A	1321	A
1	A	1324	G
1	A	1325	U
1	A	1326	U
1	A	1327	A
1	A	1329	U
1	A	1330	C
1	A	1332	G
1	A	1333	G
1	A	1334	G
1	A	1340	U
1	A	1341	G
1	A	1343	G
1	A	1344	U
1	A	1345	C
1	A	1352	U
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1380	G
1	A	1383	A
1	A	1385	A
1	A	1386	C
1	A	1387	A
1	A	1396	U
1	A	1397	U
1	A	1398	C
1	A	1403	A

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Mol	Chain	Res	Type
1	A	1416	G
1	A	1419	A
1	A	1420	A
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1430	G
1	A	1451	C
1	A	1452	G
1	A	1453	A
1	A	1455	G
1	A	1458	U
1	A	1459	G
1	A	1460	U
1	A	1461	C
1	A	1476	U
1	A	1477	A
1	A	1482	G
1	A	1490	A
1	A	1491	G
1	A	1492	G
1	A	1493	C
1	A	1496	A
1	A	1497	U
1	A	1498	C
1	A	1499	C
1	A	1504	A
1	A	1508	A
1	A	1509	A
1	A	1510	G
1	A	1511	G
1	A	1515	A
1	A	1522	A
1	A	1523	U
1	A	1531	C
1	A	1533	C
1	A	1534	U
1	A	1536	C
1	A	1537	G
1	A	1538	G
1	A	1539	U

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Mol	Chain	Res	Type
1	A	1540	G
1	A	1555	G
1	A	1556	C
1	A	1557	C
1	A	1558	C
1	A	1559	U
1	A	1560	G
1	A	1561	C
1	A	1568	G
1	A	1569	A
1	A	1578	U
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1602	U
1	A	1603	A
1	A	1604	C
1	A	1607	C
1	A	1608	A
1	A	1610	A
1	A	1611	C
1	A	1612	C
1	A	1616	A
1	A	1619	G
1	A	1625	C
1	A	1635	A
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1654	A
1	A	1655	A
1	A	1669	A
1	A	1670	C
1	A	1674	G
1	A	1675	C
1	A	1677	A
1	A	1682	G
1	A	1683	U
1	A	1694	C
1	A	1695	G
1	A	1696	G

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Mol	Chain	Res	Type
1	A	1697	G
1	A	1698	A
1	A	1699	G
1	A	1700	A
1	A	1701	A
1	A	1706	C
1	A	1707	G
1	A	1708	C
1	A	1713	A
1	A	1714	U
1	A	1715	G
1	A	1716	U
1	A	1717	A
1	A	1723	G
1	A	1729	U
1	A	1730	C
1	A	1731	G
1	A	1732	C
1	A	1733	G
1	A	1738	G
1	A	1743	G
1	A	1744	A
1	A	1746	A
1	A	1758	U
1	A	1759	A
1	A	1760	C
1	A	1761	C
1	A	1764	C
1	A	1770	G
1	A	1773	A
1	A	1776	G
1	A	1780	A
1	A	1782	U
1	A	1784	A
1	A	1785	A
1	A	1786	A
1	A	1787	A
1	A	1788	C
1	A	1791	A
1	A	1800	C
1	A	1802	A
1	A	1803	A

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Mol	Chain	Res	Type
1	A	1806	C
1	A	1808	A
1	A	1809	A
1	A	1810	A
1	A	1813	G
1	A	1815	A
1	A	1816	C
1	A	1817	G
1	A	1818	U
1	A	1821	A
1	A	1822	C
1	A	1825	U
1	A	1828	G
1	A	1829	A
1	A	1830	C
1	A	1833	C
1	A	1838	C
1	A	1839	G
1	A	1847	A
1	A	1858	A
1	A	1859	U
1	A	1866	A
1	A	1867	G
1	A	1871	A
1	A	1872	A
1	A	1876	A
1	A	1884	G
1	A	1885	A
1	A	1900	A
1	A	1906	G
1	A	1913	A
1	A	1914	C
1	A	1915	U
1	A	1918	A
1	A	1919	A
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1932	A
1	A	1937	A
1	A	1938	A

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Mol	Chain	Res	Type
1	A	1941	C
1	A	1942	C
1	A	1943	U
1	A	1944	U
1	A	1945	G
1	A	1946	U
1	A	1955	U
1	A	1956	U
1	A	1957	C
1	A	1960	A
1	A	1963	U
1	A	1965	C
1	A	1966	A
1	A	1967	C
1	A	1968	G
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1977	A
1	A	1981	A
1	A	1982	U
1	A	1992	G
1	A	1993	U
1	A	1994	C
1	A	1996	C
1	A	1997	C
1	A	2006	C
1	A	2021	C
1	A	2022	U
1	A	2023	C
1	A	2024	G
1	A	2030	A
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2035	G
1	A	2036	C
1	A	2037	A
1	A	2043	C
1	A	2051	A
1	A	2052	A
1	A	2055	C

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Mol	Chain	Res	Type
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	C
1	A	2064	C
1	A	2068	U
1	A	2069	G
1	A	2072	C
1	A	2092	U
1	A	2093	G
1	A	2095	A
1	A	2104	C
1	A	2106	U
1	A	2107	G
1	A	2109	U
1	A	2110	G
1	A	2134	A
1	A	2135	A
1	A	2136	G
1	A	2137	U
1	A	2140	G
1	A	2143	C
1	A	2144	G
1	A	2145	C
1	A	2146	C
1	A	2147	A
1	A	2148	G
1	A	2149	U
1	A	2150	C
1	A	2151	U
1	A	2155	U
1	A	2156	G
1	A	2180	U
1	A	2181	U
1	A	2183	A
1	A	2184	A
1	A	2185	U
1	A	2187	U
1	A	2197	U
1	A	2198	A

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Mol	Chain	Res	Type
1	A	2199	A
1	A	2200	C
1	A	2201	G
1	A	2204	G
1	A	2210	U
1	A	2211	A
1	A	2212	A
1	A	2214	C
1	A	2215	C
1	A	2225	A
1	A	2226	C
1	A	2227	A
1	A	2228	G
1	A	2238	G
1	A	2239	G
1	A	2249	U
1	A	2250	G
1	A	2252	G
1	A	2253	G
1	A	2256	G
1	A	2259	U
1	A	2266	A
1	A	2267	A
1	A	2268	A
1	A	2269	G
1	A	2273	A
1	A	2275	C
1	A	2278	A
1	A	2283	C
1	A	2284	A
1	A	2286	G
1	A	2287	A
1	A	2288	A
1	A	2296	U
1	A	2297	A
1	A	2298	A
1	A	2305	U
1	A	2307	G
1	A	2308	G
1	A	2309	A
1	A	2310	C
1	A	2312	U

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Mol	Chain	Res	Type
1	A	2313	C
1	A	2319	G
1	A	2320	U
1	A	2321	U
1	A	2323	G
1	A	2325	G
1	A	2327	A
1	A	2328	A
1	A	2333	A
1	A	2334	U
1	A	2335	A
1	A	2336	A
1	A	2337	G
1	A	2345	G
1	A	2347	C
1	A	2348	U
1	A	2350	C
1	A	2354	C
1	A	2361	G
1	A	2372	U
1	A	2382	G
1	A	2383	G
1	A	2384	U
1	A	2385	C
1	A	2386	A
1	A	2388	A
1	A	2389	G
1	A	2391	G
1	A	2392	A
1	A	2402	U
1	A	2406	A
1	A	2407	A
1	A	2423	U
1	A	2424	C
1	A	2425	A
1	A	2426	A
1	A	2427	C
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A

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Mol	Chain	Res	Type
1	A	2439	A
1	A	2440	C
1	A	2441	U
1	A	2447	G
1	A	2448	A
1	A	2450	A
1	A	2459	A
1	A	2465	C
1	A	2469	A
1	A	2470	G
1	A	2476	A
1	A	2477	U
1	A	2490	G
1	A	2491	U
1	A	2492	U
1	A	2493	U
1	A	2498	C
1	A	2499	C
1	A	2502	G
1	A	2503	A
1	A	2504	U
1	A	2505	G
1	A	2506	U
1	A	2517	C
1	A	2518	A
1	A	2520	C
1	A	2521	C
1	A	2529	G
1	A	2542	A
1	A	2543	G
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2568	U
1	A	2573	C
1	A	2574	G
1	A	2579	C
1	A	2581	G
1	A	2582	G
1	A	2583	G
1	A	2585	U
1	A	2586	U

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Mol	Chain	Res	Type
1	A	2589	A
1	A	2603	G
1	A	2609	U
1	A	2610	C
1	A	2611	C
1	A	2612	C
1	A	2613	U
1	A	2614	A
1	A	2615	U
1	A	2630	G
1	A	2631	G
1	A	2639	A
1	A	2640	G
1	A	2646	C
1	A	2654	A
1	A	2655	G
1	A	2658	C
1	A	2663	G
1	A	2664	G
1	A	2668	G
1	A	2681	C
1	A	2682	A
1	A	2683	C
1	A	2689	U
1	A	2690	U
1	A	2691	C
1	A	2692	G
1	A	2714	G
1	A	2724	U
1	A	2727	A
1	A	2728	U
1	A	2729	G
1	A	2732	G
1	A	2733	A
1	A	2748	A
1	A	2750	A
1	A	2751	G
1	A	2753	A
1	A	2756	U
1	A	2757	A
1	A	2765	A
1	A	2769	U

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Mol	Chain	Res	Type
1	A	2777	G
1	A	2778	A
1	A	2779	U
1	A	2781	A
1	A	2791	G
1	A	2792	A
1	A	2793	C
1	A	2798	U
1	A	2799	A
1	A	2800	A
1	A	2801	G
1	A	2808	G
1	A	2809	A
1	A	2810	A
1	A	2812	G
1	A	2820	A
1	A	2821	A
1	A	2822	G
1	A	2824	C
1	A	2825	G
1	A	2833	U
1	A	2834	G
1	A	2835	A
1	A	2836	U
1	A	2837	A
1	A	2848	G
1	A	2849	U
1	A	2850	A
1	A	2851	A
1	A	2861	U
1	A	2866	U
1	A	2867	G
1	A	2868	A
1	A	2869	G
1	A	2874	C
1	A	2879	A
1	A	2880	C
1	A	2883	A
1	A	2884	U
1	A	2886	A
1	A	2894	G
1	A	2895	G

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Mol	Chain	Res	Type
1	A	2896	C
2	B	3	C
2	B	12	C
2	B	13	G
2	B	14	U
2	B	15	A
2	B	16	G
2	B	24	G
2	B	25	U
2	B	26	C
2	B	35	C
2	B	37	C
2	B	38	C
2	B	41	G
2	B	42	C
2	B	43	C
2	B	44	G
2	B	45	A
2	B	52	A
2	B	53	A
2	B	54	G
2	B	57	A
2	B	58	A
2	B	66	A
2	B	67	G
2	B	87	U
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	99	A
2	B	108	A
2	B	109	A

All (519) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	27	G
1	A	33	C
1	A	35	G
1	A	49	A

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Mol	Chain	Res	Type
1	A	52	A
1	A	60	G
1	A	61	C
1	A	62	U
1	A	63	A
1	A	70	G
1	A	73	A
1	A	74	A
1	A	75	G
1	A	83	A
1	A	84	A
1	A	85	G
1	A	86	G
1	A	91	A
1	A	92	U
1	A	100	U
1	A	103	A
1	A	119	A
1	A	121	G
1	A	125	A
1	A	126	A
1	A	137	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	162	U
1	A	164	C
1	A	177	G
1	A	178	G
1	A	196	A
1	A	197	A
1	A	199	A
1	A	200	U
1	A	204	A
1	A	206	U
1	A	215	G
1	A	216	A
1	A	221	A
1	A	223	A
1	A	227	A

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Mol	Chain	Res	Type
1	A	229	C
1	A	232	G
1	A	233	A
1	A	241	A
1	A	243	U
1	A	249	C
1	A	250	G
1	A	265	A
1	A	266	G
1	A	271	G
1	A	272	A
1	A	301	G
1	A	302	C
1	A	310	A
1	A	312	G
1	A	321	U
1	A	324	A
1	A	328	U
1	A	329	G
1	A	333	G
1	A	345	A
1	A	369	U
1	A	370	G
1	A	373	U
1	A	386	G
1	A	388	G
1	A	390	U
1	A	395	U
1	A	404	A
1	A	406	G
1	A	411	G
1	A	421	C
1	A	434	U
1	A	435	C
1	A	436	C
1	A	442	G
1	A	446	G
1	A	449	A
1	A	454	A
1	A	459	U
1	A	460	A
1	A	474	G

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Mol	Chain	Res	Type
1	A	475	C
1	A	479	A
1	A	480	A
1	A	481	G
1	A	482	A
1	A	489	G
1	A	491	G
1	A	503	A
1	A	505	A
1	A	506	G
1	A	507	A
1	A	508	A
1	A	509	C
1	A	512	G
1	A	513	A
1	A	527	C
1	A	529	A
1	A	530	G
1	A	531	C
1	A	533	G
1	A	571	U
1	A	572	A
1	A	575	A
1	A	587	C
1	A	588	U
1	A	603	A
1	A	604	G
1	A	614	A
1	A	616	A
1	A	620	G
1	A	621	A
1	A	627	A
1	A	628	G
1	A	637	A
1	A	638	G
1	A	645	C
1	A	646	U
1	A	652	U
1	A	653	U
1	A	654	A
1	A	655	A
1	A	656	G

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Mol	Chain	Res	Type
1	A	669	G
1	A	671	C
1	A	685	A
1	A	687	C
1	A	688	U
1	A	704	G
1	A	726	G
1	A	727	A
1	A	729	G
1	A	739	A
1	A	746	U
1	A	747	U
1	A	752	A
1	A	753	A
1	A	762	U
1	A	763	G
1	A	764	A
1	A	765	C
1	A	774	G
1	A	781	A
1	A	788	A
1	A	790	U
1	A	794	A
1	A	800	A
1	A	802	A
1	A	805	G
1	A	806	C
1	A	811	U
1	A	812	C
1	A	829	A
1	A	858	G
1	A	860	U
1	A	865	C
1	A	866	A
1	A	913	U
1	A	914	G
1	A	915	C
1	A	931	U
1	A	933	A
1	A	934	U
1	A	945	A
1	A	946	C

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Mol	Chain	Res	Type
1	A	957	C
1	A	958	U
1	A	959	A
1	A	961	C
1	A	962	G
1	A	975	A
1	A	984	A
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	1008	A
1	A	1009	A
1	A	1011	G
1	A	1020	A
1	A	1022	G
1	A	1023	U
1	A	1025	G
1	A	1026	G
1	A	1033	U
1	A	1034	G
1	A	1045	C
1	A	1060	U
1	A	1062	G
1	A	1070	A
1	A	1072	C
1	A	1091	G
1	A	1110	G
1	A	1112	G
1	A	1126	A
1	A	1127	A
1	A	1128	G
1	A	1129	A
1	A	1135	C
1	A	1141	U
1	A	1144	A
1	A	1156	A
1	A	1157	G
1	A	1174	U
1	A	1180	U
1	A	1204	A
1	A	1206	G

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Mol	Chain	Res	Type
1	A	1210	G
1	A	1236	G
1	A	1247	A
1	A	1249	U
1	A	1250	G
1	A	1254	A
1	A	1265	A
1	A	1267	U
1	A	1272	A
1	A	1274	A
1	A	1275	A
1	A	1276	A
1	A	1286	A
1	A	1287	A
1	A	1289	C
1	A	1300	G
1	A	1303	G
1	A	1311	G
1	A	1324	G
1	A	1326	U
1	A	1329	U
1	A	1330	C
1	A	1332	G
1	A	1333	G
1	A	1340	U
1	A	1343	G
1	A	1378	A
1	A	1379	U
1	A	1385	A
1	A	1386	C
1	A	1396	U
1	A	1398	C
1	A	1427	A
1	A	1429	G
1	A	1451	C
1	A	1458	U
1	A	1459	G
1	A	1461	C
1	A	1475	G
1	A	1476	U
1	A	1490	A
1	A	1491	G

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Mol	Chain	Res	Type
1	A	1495	A
1	A	1497	U
1	A	1498	C
1	A	1499	C
1	A	1508	A
1	A	1509	A
1	A	1510	G
1	A	1522	A
1	A	1535	A
1	A	1537	G
1	A	1538	G
1	A	1539	U
1	A	1554	U
1	A	1555	G
1	A	1556	C
1	A	1557	C
1	A	1558	C
1	A	1560	G
1	A	1568	G
1	A	1602	U
1	A	1603	A
1	A	1606	C
1	A	1611	C
1	A	1615	C
1	A	1634	A
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1653	G
1	A	1654	A
1	A	1674	G
1	A	1675	C
1	A	1681	G
1	A	1682	G
1	A	1693	U
1	A	1695	G
1	A	1696	G
1	A	1698	A
1	A	1700	A
1	A	1706	C
1	A	1707	G
1	A	1713	A

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Mol	Chain	Res	Type
1	A	1714	U
1	A	1716	U
1	A	1732	C
1	A	1733	G
1	A	1758	U
1	A	1759	A
1	A	1760	C
1	A	1780	A
1	A	1782	U
1	A	1784	A
1	A	1785	A
1	A	1786	A
1	A	1787	A
1	A	1799	G
1	A	1808	A
1	A	1809	A
1	A	1815	A
1	A	1816	C
1	A	1817	G
1	A	1821	A
1	A	1828	G
1	A	1829	A
1	A	1838	C
1	A	1839	G
1	A	1857	G
1	A	1858	A
1	A	1865	U
1	A	1866	A
1	A	1870	C
1	A	1871	A
1	A	1884	G
1	A	1885	A
1	A	1900	A
1	A	1913	A
1	A	1914	C
1	A	1918	A
1	A	1919	A
1	A	1929	G
1	A	1931	U
1	A	1936	A
1	A	1941	C
1	A	1942	C

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Mol	Chain	Res	Type
1	A	1943	U
1	A	1945	G
1	A	1954	G
1	A	1956	U
1	A	1962	C
1	A	1964	G
1	A	1965	C
1	A	1966	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1980	G
1	A	1981	A
1	A	1992	G
1	A	1993	U
1	A	1996	C
1	A	1997	C
1	A	2021	C
1	A	2023	C
1	A	2030	A
1	A	2034	U
1	A	2035	G
1	A	2036	C
1	A	2051	A
1	A	2052	A
1	A	2060	A
1	A	2062	A
1	A	2063	C
1	A	2067	G
1	A	2068	U
1	A	2092	U
1	A	2093	G
1	A	2134	A
1	A	2135	A
1	A	2136	G
1	A	2146	C
1	A	2148	G
1	A	2197	U
1	A	2199	A
1	A	2200	C
1	A	2210	U
1	A	2214	C

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Mol	Chain	Res	Type
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2249	U
1	A	2258	C
1	A	2266	A
1	A	2272	U
1	A	2273	A
1	A	2275	C
1	A	2282	G
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2296	U
1	A	2297	A
1	A	2307	G
1	A	2309	A
1	A	2319	G
1	A	2321	U
1	A	2326	C
1	A	2327	A
1	A	2333	A
1	A	2335	A
1	A	2336	A
1	A	2344	U
1	A	2347	C
1	A	2382	G
1	A	2383	G
1	A	2384	U
1	A	2385	C
1	A	2391	G
1	A	2406	A
1	A	2407	A
1	A	2423	U
1	A	2424	C
1	A	2425	A
1	A	2427	C
1	A	2428	G
1	A	2439	A
1	A	2447	G
1	A	2450	A
1	A	2458	G

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Mol	Chain	Res	Type
1	A	2459	A
1	A	2468	A
1	A	2490	G
1	A	2492	U
1	A	2497	A
1	A	2498	C
1	A	2503	A
1	A	2504	U
1	A	2517	C
1	A	2520	C
1	A	2542	A
1	A	2543	G
1	A	2566	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2574	G
1	A	2581	G
1	A	2582	G
1	A	2585	U
1	A	2602	A
1	A	2603	G
1	A	2609	U
1	A	2611	C
1	A	2613	U
1	A	2615	U
1	A	2629	U
1	A	2630	G
1	A	2638	G
1	A	2639	A
1	A	2645	G
1	A	2654	A
1	A	2663	G
1	A	2681	C
1	A	2682	A
1	A	2689	U
1	A	2691	C
1	A	2712	C
1	A	2725	A
1	A	2727	A
1	A	2728	U
1	A	2732	G

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Mol	Chain	Res	Type
1	A	2750	A
1	A	2752	C
1	A	2756	U
1	A	2757	A
1	A	2776	A
1	A	2777	G
1	A	2778	A
1	A	2781	A
1	A	2790	U
1	A	2791	G
1	A	2792	A
1	A	2797	U
1	A	2799	A
1	A	2800	A
1	A	2808	G
1	A	2809	A
1	A	2820	A
1	A	2833	U
1	A	2835	A
1	A	2836	U
1	A	2848	G
1	A	2850	A
1	A	2866	U
1	A	2868	A
1	A	2873	A
1	A	2879	A
1	A	2880	C
1	A	2893	A
1	A	2894	G
1	A	2895	G
2	B	12	C
2	B	13	G
2	B	16	G
2	B	24	G
2	B	25	U
2	B	37	C
2	B	40	U
2	B	42	C
2	B	43	C
2	B	44	G
2	B	45	A
2	B	52	A

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Mol	Chain	Res	Type
2	B	53	A
2	B	56	G
2	B	57	A
2	B	66	A
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	108	A
2	B	109	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 142 ligands modelled in this entry, 142 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2854/2903 (98%)	-0.26	53 (1%) 64 41	52, 81, 194, 355	0
2	B	118/118 (100%)	-0.27	1 (0%) 83 63	66, 101, 133, 171	0
3	C	271/273 (99%)	0.67	32 (11%) 5 6	60, 99, 129, 161	0
4	D	209/209 (100%)	0.30	8 (3%) 38 25	55, 75, 114, 129	0
5	E	201/201 (100%)	0.43	7 (3%) 42 26	56, 96, 129, 157	0
6	F	177/179 (98%)	1.04	38 (21%) 1 2	120, 166, 201, 215	0
7	G	176/177 (99%)	0.51	10 (5%) 23 15	83, 108, 134, 152	0
8	H	149/149 (100%)	1.18	31 (20%) 1 2	110, 239, 259, 264	0
9	I	141/142 (99%)	2.54	60 (42%) 1 1	243, 307, 359, 366	0
10	J	142/142 (100%)	0.27	6 (4%) 35 22	59, 76, 102, 132	0
11	K	122/123 (99%)	0.83	20 (16%) 2 3	55, 73, 113, 169	0
12	L	143/144 (99%)	0.54	10 (6%) 16 11	55, 93, 124, 136	0
13	M	136/136 (100%)	0.59	10 (7%) 14 11	58, 81, 111, 138	0
14	N	120/127 (94%)	0.67	11 (9%) 9 8	61, 76, 96, 141	0
15	O	116/117 (99%)	0.52	7 (6%) 21 15	96, 105, 123, 147	0
16	P	114/115 (99%)	0.33	4 (3%) 42 26	64, 81, 119, 134	0
17	Q	117/118 (99%)	0.24	2 (1%) 67 44	56, 77, 99, 120	0
18	R	103/103 (100%)	0.16	1 (0%) 79 57	55, 87, 114, 131	0
19	S	110/110 (100%)	0.20	2 (1%) 65 43	55, 70, 105, 159	0
20	T	93/100 (93%)	1.20	23 (24%) 1 2	65, 105, 142, 151	0
21	U	102/104 (98%)	1.22	23 (22%) 1 2	89, 114, 136, 158	0
22	V	94/94 (100%)	0.74	16 (17%) 2 3	71, 90, 116, 126	0
23	W	79/85 (92%)	0.99	11 (13%) 4 4	68, 86, 136, 156	0
24	X	77/78 (98%)	0.99	9 (11%) 5 6	65, 101, 124, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	63/63 (100%)	0.73	10 (15%) 3 3	101, 123, 149, 159	0
26	Z	58/59 (98%)	0.78	4 (6%) 17 12	64, 74, 111, 141	0
27	0	56/57 (98%)	-0.21	0 100 100	54, 77, 113, 132	0
28	1	50/55 (90%)	1.19	9 (18%) 2 3	76, 100, 118, 132	0
29	2	46/46 (100%)	0.87	6 (13%) 4 5	62, 75, 103, 137	0
30	3	64/65 (98%)	0.91	9 (14%) 3 4	58, 73, 96, 120	0
31	4	38/38 (100%)	1.54	12 (31%) 1 2	69, 84, 110, 120	0
All	All	6339/6430 (98%)	0.26	445 (7%) 17 11	52, 89, 233, 366	0

All (445) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	10	LEU	27.7
8	H	112	LYS	13.0
9	I	13	ALA	11.0
9	I	7	TYR	10.0
9	I	11	GLN	9.4
9	I	96	LYS	9.2
9	I	70	THR	8.9
9	I	9	LYS	8.7
1	A	2885	G	8.2
9	I	1	ALA	8.1
9	I	54	ILE	8.1
9	I	55	PRO	8.0
9	I	12	VAL	7.8
9	I	94	LYS	7.6
9	I	114	ALA	7.4
1	A	2179	C	7.2
9	I	98	GLY	7.0
9	I	97	VAL	6.5
9	I	71	LYS	6.5
3	C	124	LYS	6.3
9	I	8	VAL	5.9
8	H	88	GLY	5.9
28	1	52	LYS	5.8
1	A	2146	C	5.8
8	H	87	GLU	5.7
1	A	2133	G	5.7
9	I	67	THR	5.7
6	F	76	PHE	5.7

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Mol	Chain	Res	Type	RSRZ
9	I	139	VAL	5.6
9	I	72	THR	5.6
9	I	6	ALA	5.6
1	A	892	A	5.5
1	A	1093	G	5.4
6	F	25	MET	5.4
9	I	95	ASP	5.3
8	H	85	GLY	5.1
9	I	113	ALA	5.0
3	C	125	PRO	5.0
1	A	2180	U	5.0
8	H	84	ALA	4.9
9	I	138	VAL	4.9
9	I	59	THR	4.9
9	I	2	LYS	4.8
22	V	78	GLN	4.7
7	G	176	LYS	4.7
23	W	84	GLU	4.7
15	O	63	LYS	4.7
9	I	99	LYS	4.7
3	C	1	ALA	4.6
3	C	121	ALA	4.6
9	I	121	ILE	4.6
9	I	4	VAL	4.6
6	F	59	ILE	4.5
24	X	75	GLU	4.5
9	I	119	ALA	4.5
11	K	103	VAL	4.5
21	U	56	GLY	4.5
9	I	5	GLN	4.5
8	H	141	LYS	4.5
21	U	49	PRO	4.4
20	T	4	GLU	4.3
9	I	53	PRO	4.3
21	U	74	ALA	4.3
6	F	75	GLY	4.3
9	I	111	THR	4.2
1	A	2310	C	4.1
8	H	124	THR	4.1
1	A	438	G	4.1
3	C	122	ALA	4.1
22	V	66	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
9	I	140	GLU	4.0
6	F	77	LYS	4.0
9	I	52	LEU	4.0
20	T	8	LEU	4.0
20	T	6	ARG	3.9
25	Y	17	GLU	3.9
6	F	78	ILE	3.9
21	U	47	PRO	3.9
11	K	107	LEU	3.9
6	F	26	GLN	3.9
9	I	64	ARG	3.9
6	F	71	LYS	3.9
8	H	139	PHE	3.9
1	A	2147	A	3.8
1	A	2309	A	3.8
25	Y	13	GLU	3.8
8	H	71	LYS	3.8
30	3	20	GLY	3.8
1	A	2402	U	3.8
20	T	88	LYS	3.7
9	I	136	GLY	3.7
9	I	69	VAL	3.7
9	I	65	SER	3.7
23	W	39	GLN	3.7
9	I	3	LYS	3.7
6	F	79	ARG	3.7
11	K	84	CYS	3.7
14	N	56	LYS	3.7
25	Y	14	LEU	3.7
23	W	40	ARG	3.6
20	T	7	LEU	3.6
11	K	104	THR	3.6
11	K	71	ARG	3.6
31	4	28	SER	3.6
21	U	57	ILE	3.6
8	H	146	VAL	3.6
7	G	172	GLU	3.6
9	I	120	ASP	3.6
21	U	59	GLU	3.5
20	T	3	ARG	3.5
22	V	87	GLN	3.5
6	F	31	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
14	N	57	THR	3.5
8	H	73	ASN	3.5
20	T	5	GLU	3.5
23	W	45	HIS	3.5
9	I	66	PHE	3.4
23	W	36	ILE	3.4
6	F	143	ASP	3.4
3	C	120	ASP	3.4
21	U	50	ALA	3.4
9	I	112	LYS	3.4
1	A	224	U	3.4
9	I	68	PHE	3.4
10	J	1	MET	3.4
22	V	80	HIS	3.3
1	A	437	U	3.3
20	T	87	LEU	3.3
25	Y	18	LEU	3.3
7	G	165	ASP	3.3
1	A	2150	C	3.3
25	Y	4	LYS	3.3
1	A	2143	C	3.3
31	4	29	ALA	3.3
31	4	2	LYS	3.3
21	U	51	LEU	3.3
6	F	41	GLU	3.3
6	F	142	TYR	3.2
24	X	48	LEU	3.2
6	F	140	ILE	3.2
8	H	89	LYS	3.2
14	N	52	ILE	3.2
1	A	2602	A	3.2
13	M	90	GLU	3.2
23	W	52	CYS	3.2
21	U	34	ILE	3.2
24	X	46	VAL	3.2
13	M	21	ALA	3.2
21	U	48	VAL	3.1
1	A	1490	A	3.1
20	T	91	GLN	3.1
8	H	137	GLU	3.1
3	C	2	VAL	3.1
10	J	9	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
20	T	43	ILE	3.1
1	A	53	A	3.1
1	A	2135	A	3.1
12	L	101	ILE	3.1
11	K	102	PRO	3.1
4	D	105	LYS	3.0
1	A	1078	U	3.0
6	F	58	ALA	3.0
31	4	1	MET	3.0
6	F	139	GLU	3.0
12	L	92	LEU	3.0
22	V	67	GLY	3.0
1	A	1493	C	3.0
9	I	141	ASP	3.0
11	K	108	ARG	3.0
12	L	144	GLU	3.0
30	3	60	CYS	3.0
7	G	175	LYS	3.0
6	F	74	ALA	3.0
3	C	103	ILE	3.0
24	X	49	ARG	3.0
1	A	139	U	3.0
29	2	21	ARG	3.0
5	E	143	LEU	3.0
1	A	1065	U	2.9
20	T	89	GLU	2.9
30	3	64	ALA	2.9
8	H	111	ALA	2.9
1	A	2141	G	2.9
24	X	74	GLY	2.9
29	2	17	GLY	2.9
30	3	19	GLY	2.9
31	4	35	GLN	2.9
10	J	142	ILE	2.9
4	D	198	GLY	2.9
6	F	80	GLN	2.9
1	A	2110	G	2.9
9	I	21	PRO	2.9
3	C	126	GLY	2.9
20	T	81	LYS	2.9
11	K	106	GLU	2.9
21	U	60	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	776	G	2.8
4	D	1	MET	2.8
14	N	120	GLU	2.8
12	L	2	ARG	2.8
23	W	78	PHE	2.8
6	F	137	PHE	2.8
1	A	546	U	2.8
31	4	7	VAL	2.8
11	K	63	VAL	2.8
22	V	38	LEU	2.8
31	4	25	VAL	2.8
9	I	86	LYS	2.8
30	3	61	LEU	2.8
30	3	15	LYS	2.8
1	A	2142	A	2.8
4	D	28	GLU	2.8
22	V	79	ARG	2.7
9	I	29	GLN	2.7
5	E	124	PHE	2.7
31	4	4	ARG	2.7
7	G	106	LEU	2.7
20	T	16	VAL	2.7
1	A	893	C	2.7
3	C	104	LEU	2.7
1	A	1731	G	2.7
28	1	20	TYR	2.7
6	F	35	LEU	2.7
3	C	232	GLY	2.7
13	M	24	THR	2.7
3	C	123	ILE	2.7
1	A	2308	G	2.7
8	H	136	SER	2.7
13	M	20	LEU	2.7
10	J	6	ALA	2.7
21	U	26	ASN	2.7
12	L	126	ARG	2.7
1	A	2799	A	2.7
11	K	32	TYR	2.7
3	C	109	LEU	2.7
8	H	90	LEU	2.7
3	C	116	GLN	2.7
6	F	24	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
13	M	5	LYS	2.7
29	2	25	LYS	2.7
29	2	28	ARG	2.6
15	O	115	LEU	2.6
20	T	82	LYS	2.6
8	H	64	ALA	2.6
13	M	95	LEU	2.6
3	C	34	GLU	2.6
9	I	93	ASN	2.6
8	H	125	THR	2.6
28	1	22	THR	2.6
19	S	82	MET	2.6
16	P	3	ILE	2.6
24	X	47	THR	2.6
6	F	151	LEU	2.6
1	A	2504	U	2.6
1	A	2032	G	2.6
11	K	11	ALA	2.6
3	C	182	LYS	2.6
8	H	105	ALA	2.6
6	F	86	CYS	2.6
11	K	115	ILE	2.6
1	A	1172	C	2.6
6	F	150	GLY	2.6
5	E	123	LYS	2.6
22	V	7	GLU	2.6
1	A	2136	G	2.5
16	P	1	SER	2.5
9	I	115	ASP	2.5
7	G	136	ASP	2.5
8	H	66	ASN	2.5
25	Y	5	GLU	2.5
18	R	34	GLU	2.5
20	T	54	GLU	2.5
20	T	62	VAL	2.5
23	W	79	ILE	2.5
24	X	76	LYS	2.5
9	I	137	LEU	2.5
13	M	39	GLY	2.5
6	F	87	LYS	2.5
10	J	7	LYS	2.5
8	H	145	ASN	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
24	X	77	TYR	2.5
13	M	67	VAL	2.5
17	Q	51	GLN	2.5
14	N	55	ALA	2.5
26	Z	21	ALA	2.5
13	M	98	PRO	2.5
29	2	24	THR	2.5
6	F	88	VAL	2.5
11	K	64	ARG	2.5
28	1	8	ILE	2.5
14	N	32	GLU	2.5
14	N	94	TYR	2.5
20	T	26	LYS	2.5
31	4	8	LYS	2.4
6	F	56	LEU	2.4
1	A	2422	C	2.4
9	I	57	VAL	2.4
28	1	39	ASP	2.4
21	U	25	LYS	2.4
21	U	45	GLN	2.4
6	F	28	PRO	2.4
8	H	143	ILE	2.4
8	H	140	ALA	2.4
22	V	77	VAL	2.4
3	C	19	VAL	2.4
7	G	113	ASP	2.4
3	C	266	ILE	2.4
22	V	68	LYS	2.4
1	A	1415	U	2.4
12	L	100	ILE	2.4
21	U	61	GLU	2.4
3	C	141	HIS	2.4
12	L	27	LEU	2.4
29	2	46	LYS	2.4
11	K	105	ARG	2.4
1	A	180	G	2.4
1	A	1766	G	2.4
26	Z	1	ALA	2.4
1	A	1058	U	2.4
4	D	7	LYS	2.4
15	O	64	TYR	2.3
25	Y	7	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	3	VAL	2.3
12	L	115	GLU	2.3
6	F	105	ILE	2.3
9	I	25	PRO	2.3
3	C	264	LYS	2.3
21	U	78	LYS	2.3
6	F	30	VAL	2.3
28	1	47	ILE	2.3
12	L	18	ARG	2.3
30	3	35	LYS	2.3
3	C	119	VAL	2.3
20	T	15	HIS	2.3
15	O	114	GLY	2.3
3	C	191	LEU	2.3
9	I	48	ILE	2.3
23	W	51	GLY	2.3
6	F	84	ILE	2.3
31	4	26	ILE	2.3
6	F	101	ARG	2.3
8	H	123	ARG	2.3
23	W	18	LYS	2.3
3	C	64	VAL	2.3
1	A	2884	U	2.3
9	I	16	MET	2.3
20	T	10	VAL	2.3
21	U	36	GLU	2.3
21	U	58	VAL	2.3
5	E	142	ALA	2.3
14	N	51	LEU	2.3
22	V	81	PRO	2.3
20	T	19	LYS	2.3
25	Y	3	ALA	2.3
1	A	1067	A	2.3
8	H	126	GLY	2.3
20	T	80	TRP	2.2
21	U	27	VAL	2.2
23	W	35	ILE	2.2
21	U	75	ALA	2.2
4	D	104	VAL	2.2
6	F	89	THR	2.2
20	T	63	VAL	2.2
8	H	107	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
8	H	116	ARG	2.2
15	O	2	ASP	2.2
3	C	265	PHE	2.2
7	G	95	ALA	2.2
1	A	1987	A	2.2
1	A	2275	C	2.2
8	H	80	ILE	2.2
17	Q	1	ALA	2.2
1	A	1311	G	2.2
14	N	97	ILE	2.2
28	1	16	THR	2.2
11	K	61	VAL	2.2
2	B	41	G	2.2
3	C	29	PHE	2.2
8	H	113	SER	2.2
9	I	58	ILE	2.2
4	D	197	THR	2.2
6	F	98	PHE	2.2
22	V	30	ILE	2.2
3	C	102	TYR	2.1
25	Y	63	ALA	2.1
9	I	81	LYS	2.1
7	G	169	ARG	2.1
16	P	2	ASN	2.1
14	N	41	ALA	2.1
30	3	21	PHE	2.1
1	A	1789	A	2.1
6	F	146	ASP	2.1
26	Z	14	GLY	2.1
3	C	217	PRO	2.1
7	G	127	GLN	2.1
1	A	1061	U	2.1
6	F	29	ARG	2.1
1	A	140	C	2.1
11	K	1	MET	2.1
11	K	69	VAL	2.1
21	U	23	LYS	2.1
11	K	4	GLU	2.1
31	4	12	ARG	2.1
22	V	82	TYR	2.1
21	U	46	LYS	2.1
24	X	70	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
12	L	19	LEU	2.1
22	V	8	VAL	2.1
9	I	28	GLY	2.1
1	A	436	C	2.1
1	A	2182	U	2.1
11	K	49	ARG	2.1
3	C	63	ILE	2.1
4	D	2	ILE	2.1
15	O	117	PHE	2.1
22	V	86	LEU	2.1
19	S	44	ALA	2.1
11	K	100	PHE	2.1
3	C	81	GLU	2.1
8	H	70	GLU	2.1
13	M	42	THR	2.1
6	F	23	SER	2.1
28	1	24	LYS	2.1
15	O	55	GLU	2.1
16	P	113	LEU	2.1
31	4	30	GLU	2.1
20	T	1	MET	2.0
9	I	22	PRO	2.0
22	V	76	ASP	2.0
1	A	137	U	2.0
3	C	129	LEU	2.0
6	F	44	ALA	2.0
5	E	188	MET	2.0
5	E	157	LEU	2.0
14	N	113	ILE	2.0
21	U	63	ALA	2.0
9	I	100	ILE	2.0
30	3	14	LYS	2.0
10	J	10	THR	2.0
3	C	267	VAL	2.0
8	H	129	GLU	2.0
5	E	105	LEU	2.0
26	Z	20	LYS	2.0
28	1	26	LYS	2.0
25	Y	57	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	2914	1/1	0.79	31.90	62,62,62,62	0
32	MG	A	2929	1/1	0.39	29.98	59,59,59,59	0
32	MG	A	2933	1/1	0.30	13.22	58,58,58,58	0
32	MG	A	3002	1/1	0.41	11.92	58,58,58,58	0
32	MG	A	2988	1/1	0.30	9.09	59,59,59,59	0
32	MG	A	2937	1/1	0.28	8.96	57,57,57,57	0
32	MG	A	3013	1/1	0.31	8.92	61,61,61,61	0
32	MG	B	120	1/1	0.26	7.74	118,118,118,118	0
32	MG	A	3027	1/1	0.73	7.53	59,59,59,59	0
32	MG	A	3034	1/1	1.06	6.91	68,68,68,68	0
32	MG	A	3039	1/1	0.37	6.62	64,64,64,64	0
32	MG	A	2974	1/1	0.37	6.32	55,55,55,55	0
32	MG	A	2912	1/1	0.26	5.61	61,61,61,61	0
32	MG	A	2918	1/1	0.32	5.60	55,55,55,55	0
32	MG	A	2964	1/1	0.67	4.97	56,56,56,56	0
32	MG	A	2975	1/1	0.54	3.80	55,55,55,55	0
32	MG	A	2938	1/1	0.20	3.62	72,72,72,72	0
32	MG	A	2934	1/1	0.26	3.60	59,59,59,59	0
32	MG	A	2961	1/1	0.39	3.50	63,63,63,63	0
32	MG	A	3006	1/1	0.23	2.87	81,81,81,81	0
32	MG	A	2909	1/1	0.25	2.87	101,101,101,101	0
32	MG	A	2984	1/1	0.23	2.62	56,56,56,56	0
32	MG	A	2971	1/1	0.22	2.58	65,65,65,65	0
32	MG	A	2923	1/1	0.29	2.57	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	2924	1/1	0.30	2.44	59,59,59,59	0
32	MG	A	2968	1/1	0.35	1.99	55,55,55,55	0
32	MG	A	2940	1/1	0.20	1.96	58,58,58,58	0
32	MG	A	2936	1/1	0.24	1.76	56,56,56,56	0
32	MG	A	3038	1/1	0.21	1.64	60,60,60,60	0
32	MG	A	2960	1/1	0.31	1.62	61,61,61,61	0
32	MG	A	2948	1/1	0.32	1.37	80,80,80,80	0
32	MG	A	2919	1/1	0.18	1.26	56,56,56,56	0
32	MG	A	2999	1/1	0.18	1.21	61,61,61,61	0
32	MG	A	2972	1/1	0.17	1.08	65,65,65,65	0
32	MG	A	3028	1/1	0.20	1.07	58,58,58,58	0
32	MG	A	3023	1/1	0.17	0.99	59,59,59,59	0
32	MG	A	3036	1/1	0.28	0.67	73,73,73,73	0
32	MG	A	3004	1/1	0.27	0.61	54,54,54,54	0
32	MG	A	2963	1/1	0.25	0.59	56,56,56,56	0
32	MG	A	3025	1/1	0.23	0.56	57,57,57,57	0
32	MG	D	210	1/1	0.18	0.55	55,55,55,55	0
32	MG	A	2916	1/1	0.22	0.53	55,55,55,55	0
32	MG	A	2925	1/1	0.16	0.40	55,55,55,55	0
32	MG	A	3022	1/1	0.18	0.33	68,68,68,68	0
32	MG	A	2955	1/1	0.16	0.29	54,54,54,54	0
32	MG	A	3012	1/1	0.18	0.17	60,60,60,60	0
32	MG	A	3008	1/1	0.24	0.11	55,55,55,55	0
32	MG	A	2962	1/1	0.13	0.03	69,69,69,69	0
32	MG	A	2973	1/1	0.20	-0.15	158,158,158,158	0
32	MG	B	122	1/1	0.17	-0.27	69,69,69,69	0
32	MG	A	3035	1/1	0.21	-0.30	61,61,61,61	0
32	MG	A	2920	1/1	0.16	-0.30	56,56,56,56	0
32	MG	A	3019	1/1	0.14	-0.41	55,55,55,55	0
32	MG	A	3003	1/1	0.18	-0.54	74,74,74,74	0
32	MG	A	2995	1/1	0.10	-0.64	127,127,127,127	0
32	MG	A	2907	1/1	0.13	-0.66	86,86,86,86	0
32	MG	A	2954	1/1	0.13	-0.79	57,57,57,57	0
32	MG	A	2991	1/1	0.10	-0.82	77,77,77,77	0
32	MG	A	3018	1/1	0.21	-0.83	65,65,65,65	0
32	MG	A	3024	1/1	0.16	-0.84	64,64,64,64	0
32	MG	A	2998	1/1	0.10	-0.89	92,92,92,92	0
32	MG	A	2950	1/1	0.15	-0.91	78,78,78,78	0
32	MG	A	2932	1/1	0.13	-0.92	54,54,54,54	0
32	MG	A	2943	1/1	0.12	-0.95	58,58,58,58	0
32	MG	A	2910	1/1	0.14	-0.97	111,111,111,111	0
32	MG	A	2942	1/1	0.14	-0.99	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	2922	1/1	0.08	-1.06	86,86,86,86	0
32	MG	A	3017	1/1	0.11	-1.06	88,88,88,88	0
32	MG	A	2917	1/1	0.15	-1.18	55,55,55,55	0
32	MG	A	2966	1/1	0.15	-1.19	54,54,54,54	0
32	MG	A	2994	1/1	0.14	-1.21	88,88,88,88	0
32	MG	A	2915	1/1	0.12	-1.29	54,54,54,54	0
32	MG	A	2986	1/1	0.13	-1.29	59,59,59,59	0
32	MG	A	2982	1/1	0.08	-1.30	110,110,110,110	0
32	MG	A	2987	1/1	0.12	-1.32	61,61,61,61	0
32	MG	A	3032	1/1	0.12	-1.34	55,55,55,55	0
32	MG	A	3015	1/1	0.15	-1.35	64,64,64,64	0
32	MG	A	3029	1/1	0.08	-1.35	70,70,70,70	0
32	MG	A	2951	1/1	0.09	-1.38	91,91,91,91	0
32	MG	A	2945	1/1	0.12	-1.39	68,68,68,68	0
32	MG	A	2927	1/1	0.12	-1.55	60,60,60,60	0
32	MG	A	2946	1/1	0.06	-1.58	68,68,68,68	0
32	MG	A	2913	1/1	0.09	-1.64	64,64,64,64	0
32	MG	A	2931	1/1	0.11	-1.68	57,57,57,57	0
32	MG	A	2996	1/1	0.09	-1.74	104,104,104,104	0
32	MG	A	2957	1/1	0.12	-1.75	62,62,62,62	0
32	MG	A	2949	1/1	0.12	-1.78	77,77,77,77	0
32	MG	A	2997	1/1	0.13	-1.81	92,92,92,92	0
32	MG	A	2941	1/1	0.07	-1.86	59,59,59,59	0
32	MG	A	3037	1/1	0.12	-1.88	55,55,55,55	0
32	MG	A	2935	1/1	0.09	-1.88	57,57,57,57	0
32	MG	A	2908	1/1	0.07	-1.89	91,91,91,91	0
32	MG	A	3014	1/1	0.08	-1.92	55,55,55,55	0
32	MG	A	3026	1/1	0.12	-1.92	79,79,79,79	0
32	MG	A	2939	1/1	0.08	-1.92	65,65,65,65	0
32	MG	A	2959	1/1	0.09	-2.08	64,64,64,64	0
33	ZN	4	802	1/1	0.04	-2.08	99,99,99,99	0
32	MG	A	3021	1/1	0.11	-2.10	60,60,60,60	0
32	MG	A	3007	1/1	0.13	-2.15	55,55,55,55	0
32	MG	A	2983	1/1	0.06	-2.25	93,93,93,93	0
32	MG	A	2977	1/1	0.09	-2.28	54,54,54,54	0
32	MG	A	2989	1/1	0.14	-2.31	60,60,60,60	0
32	MG	A	2979	1/1	0.12	-2.32	62,62,62,62	0
32	MG	A	2978	1/1	0.09	-2.35	58,58,58,58	0
32	MG	A	2905	1/1	0.08	-2.38	61,61,61,61	0
32	MG	A	2976	1/1	0.05	-2.40	61,61,61,61	0
32	MG	A	3033	1/1	0.12	-2.55	68,68,68,68	0
32	MG	A	2958	1/1	0.10	-2.61	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3030	1/1	0.10	-2.62	57,57,57,57	0
32	MG	B	121	1/1	0.07	-2.63	127,127,127,127	0
32	MG	A	2965	1/1	0.20	-2.66	55,55,55,55	0
32	MG	A	3010	1/1	0.09	-2.70	67,67,67,67	0
32	MG	A	2981	1/1	0.10	-2.73	100,100,100,100	0
32	MG	A	2928	1/1	0.10	-2.75	59,59,59,59	0
32	MG	A	3000	1/1	0.06	-2.76	65,65,65,65	0
32	MG	A	2993	1/1	0.07	-2.95	63,63,63,63	0
32	MG	A	3005	1/1	0.08	-3.01	57,57,57,57	0
32	MG	A	2944	1/1	0.12	-3.03	60,60,60,60	0
32	MG	A	2969	1/1	0.07	-3.23	61,61,61,61	0
32	MG	A	3011	1/1	0.09	-3.25	58,58,58,58	0
32	MG	A	2985	1/1	0.08	-3.26	55,55,55,55	0
32	MG	A	2926	1/1	0.06	-3.41	59,59,59,59	0
32	MG	A	2930	1/1	0.04	-3.50	59,59,59,59	0
32	MG	A	2967	1/1	0.08	-3.55	55,55,55,55	0
32	MG	A	2970	1/1	0.07	-3.70	57,57,57,57	0
32	MG	A	3009	1/1	0.09	-3.73	58,58,58,58	0
32	MG	A	3016	1/1	0.10	-3.79	54,54,54,54	0
32	MG	A	2990	1/1	0.08	-3.88	61,61,61,61	0
32	MG	A	2911	1/1	0.07	-4.02	59,59,59,59	0
32	MG	A	2953	1/1	0.11	-4.21	56,56,56,56	0
32	MG	A	2906	1/1	0.04	-4.29	90,90,90,90	0
32	MG	A	2921	1/1	0.05	-4.37	80,80,80,80	0
32	MG	A	3001	1/1	0.12	-4.52	72,72,72,72	0
32	MG	A	2947	1/1	0.12	-4.84	88,88,88,88	0
32	MG	A	2952	1/1	0.06	-5.25	61,61,61,61	0
32	MG	B	123	1/1	0.05	-5.93	74,74,74,74	0
32	MG	A	3031	1/1	0.06	-6.43	64,64,64,64	0
32	MG	A	3020	1/1	0.07	-7.52	67,67,67,67	0
32	MG	A	2956	1/1	0.06	-7.76	57,57,57,57	0
32	MG	A	2980	1/1	0.10	-7.84	63,63,63,63	0
32	MG	A	2904	1/1	0.08	-10.66	61,61,61,61	0
32	MG	A	2992	1/1	0.07	-13.78	66,66,66,66	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.