



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 09:11 am BST

PDB ID : 6S12
EMDB ID : EMD-10078
Title : Erythromycin Resistant Staphylococcus aureus 50S ribosome (delta R88 A89 uL22).
Authors : Halfon, Y.; Matozv, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Kjeldgaard, J.; Ingmer, H.; Yonath, A.
Deposited on : 2019-06-18
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

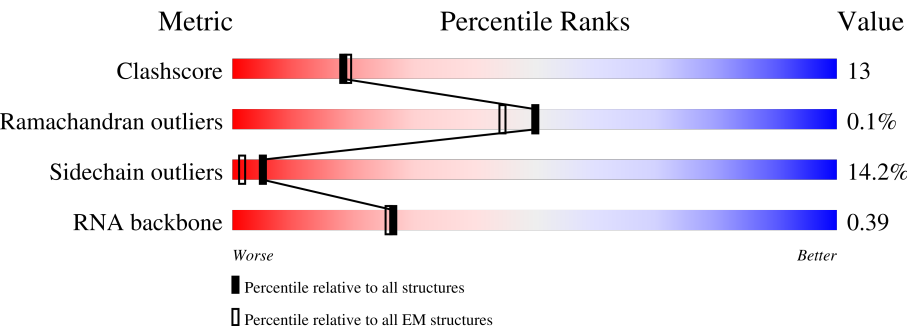
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.














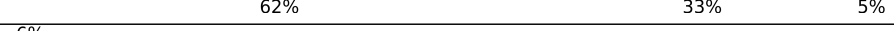

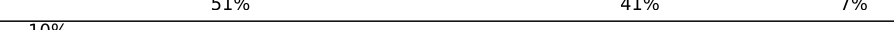







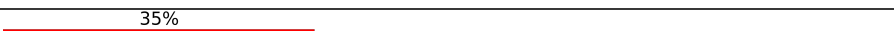

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2905	<div><div>7%</div><div>35%</div><div>40%</div><div>21%</div><div>.</div></div>
2	B	115	<div><div>34%</div><div>40%</div><div>21%</div><div>5%</div></div>
3	C	274	<div><div>.</div><div>63%</div><div>28%</div><div>9%</div></div>
4	D	215	<div><div>67%</div><div>28%</div><div>.</div></div>
5	E	206	<div><div>57%</div><div>39%</div><div>.</div></div>
6	F	175	<div><div>19%</div><div>58%</div><div>37%</div><div>6%</div></div>
7	G	175	<div><div>68%</div><div>70%</div><div>23%</div><div>6%</div></div>

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Mol	Chain	Length	Quality of chain
8	H	145	
9	I	122	
10	J	146	
11	K	137	
12	L	120	
13	M	119	
14	N	114	
15	O	116	
16	P	102	
17	Q	110	
18	R	89	
19	S	103	
20	T	94	
21	U	82	
22	V	58	
23	W	67	
24	X	58	
25	Y	59	
26	Z	48	
27	1	47	
28	2	43	
29	3	64	
30	4	37	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 146017 atoms, of which 57352 are hydrogens and 0 are deuteriums.

In the tables below, 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 ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2905	Total	C	H	N	O	P	0	0
			93573	27803	31296	11387	20182	2905		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	115	Total	C	H	N	O	P	0	0
			3685	1094	1240	436	801	114		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	274	Total	C	H	N	O	S	0	0
			4291	1301	2201	415	369	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	215	Total	C	H	N	O	S	0	0
			3294	1018	1667	299	305	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	206	Total	C	H	N	O	S	0	0
			3192	986	1620	288	296	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	175	Total	C	H	N	O	S	0	0
			2667	837	1342	227	255	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	175	Total	C	H	N	O	S	0	0
			2488	790	1225	239	231	3		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	145	Total	C	H	N	O	S	0	0
			2277	714	1134	208	218	3		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	122	Total	C	H	N	O	S	0	0
			1899	572	981	174	168	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	146	Total	C	H	N	O	S	0	0
			2211	674	1125	214	197	1		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	137	Total	C	H	N	O	S	0	0
			2194	689	1123	203	175	4		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	120	Total	C	H	N	O	S	0	0
			1915	576	983	182	173	1		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	119	Total	C	H	N	O	S	0	0
			1816	557	925	174	159	1		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	114	Total	C	H	N	O	0	0
			1826	563	937	175	151		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	116	Total	C	H	N	O	S	0	0
			1956	593	1014	189	156	4		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	102	Total	C	H	N	O	S	0	0
			1620	503	830	142	144	1		

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	110	Total	C	H	N	O	S	0	0
			1724	523	887	158	153	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	ARG	deletion	UNP A0A077UKF9
Q	?	-	ALA	deletion	UNP A0A077UKF9

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	89	Total	C	H	N	O	S	0	0
			1463	453	748	127	131	4		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	103	Total	C	H	N	O	S	0	0
			1579	486	809	142	141	1		

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	94	Total	C	H	N	O	0	0
			1488	463	766	130	129		

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	82	Total	C	H	N	O	0	0
			1265	385	643	122	115		

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	58	Total	C	H	N	O	0	0
			911	277	466	96	72		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	67	Total	C	H	N	O	0	0
			1104	333	563	102	106		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	58	Total	C	H	N	O	0	0
			940	280	491	85	84		

- Molecule 25 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	59	Total	C	H	N	O	S	0	0
			613	225	243	68	76	1		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
26	Z	48	Total	C	H	N	O	S	0	0
			718	222	358	77	59	2		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	1	47	Total	C	H	N	O	S	0	0
			784	238	394	78	70	4		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	2	43	Total	C	H	N	O	S	0	0
			782	225	415	89	52	1		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	3	64	Total	C	H	N	O	S	0	0
			1107	324	586	113	82	2		

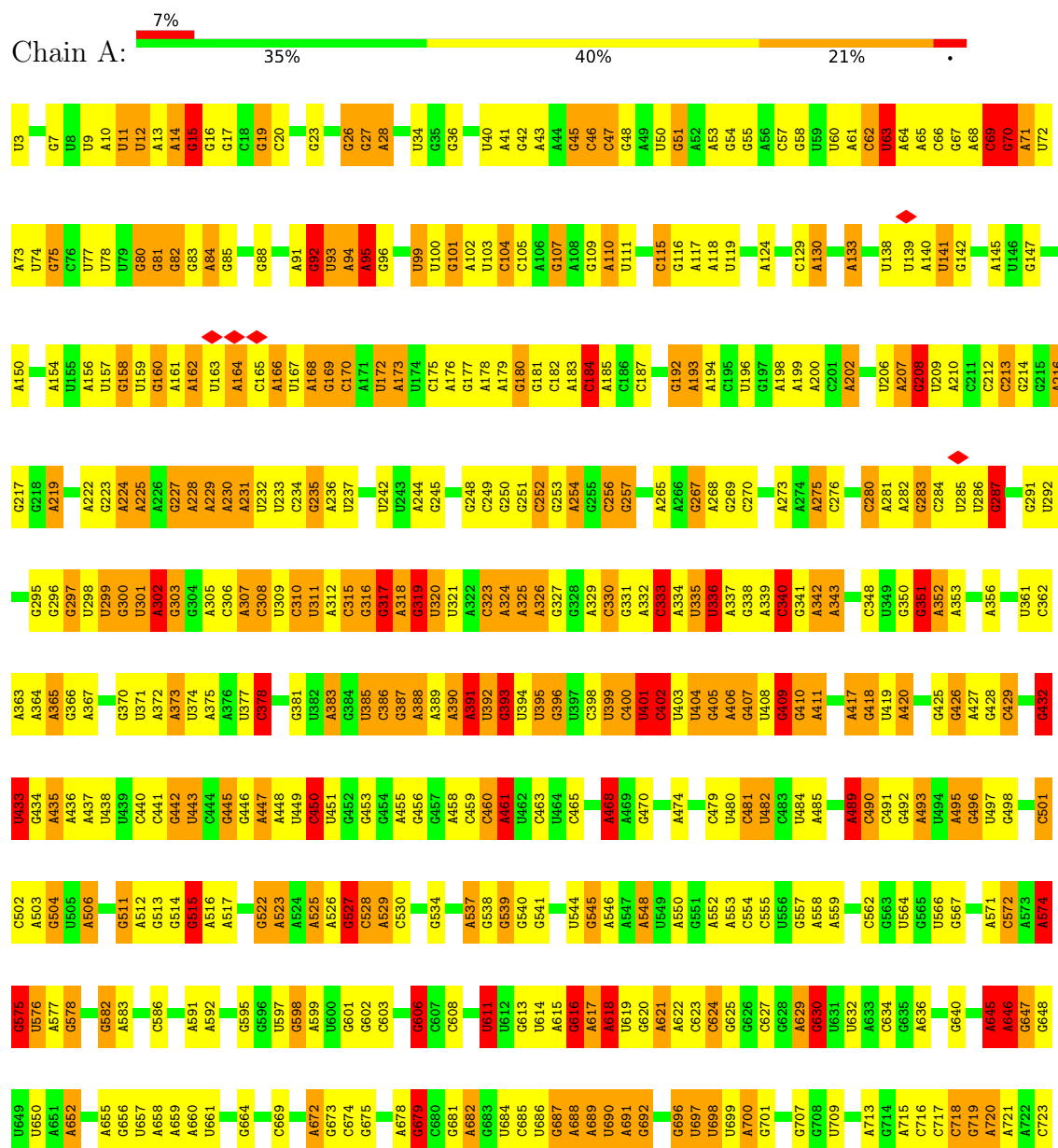
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	4	37	Total	C	H	N	O	S	0	0
			635	186	340	60	44	5		

3 Residue-property plots [i](#)

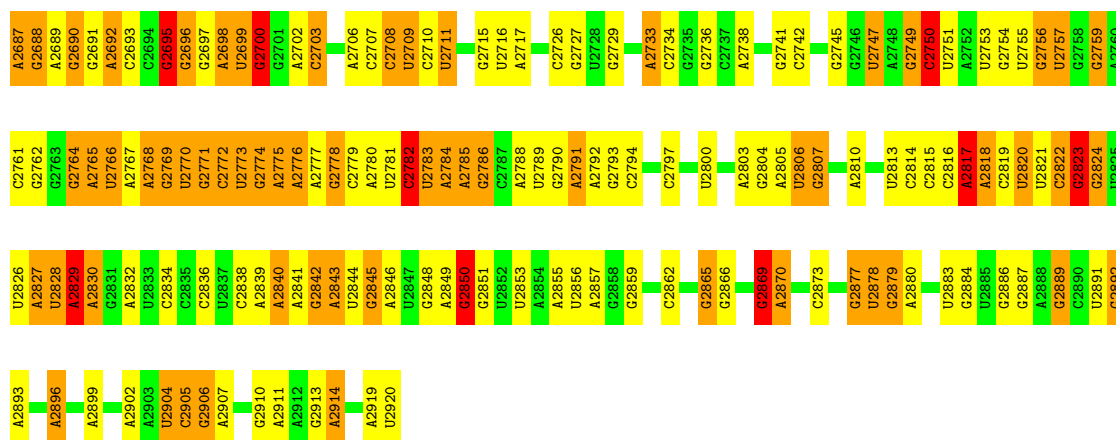
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 ribosomal RNA

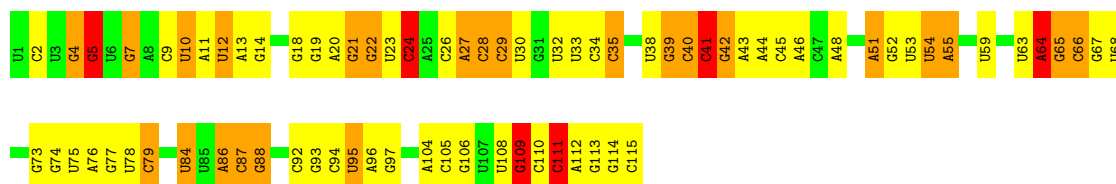


C1622	U1623	C1624	U1625	A1626	C1627	A1628	U1629	A1630	C1631	A1632	A1633	A1634	A1635	U1636	A1637	C1638	C1639	U1640	A1641	C1642	C1643	C1644	A1647	C1648	C1649	U1650	C1651	A1652	A1653	A1654	C1655	A1658	C1659	A1660	C1661	A1662	C1663	U1664	A1665	A1666	C1675	A1678	A1679	A1684	A1690	C1691	C1692	C1693	A1694	U1697	A1698	A1699																																																
G1556	C1557	U1558	G1559	A1560	G1561	C1562	U1563	A1564	U1565	G1566	C1567	U1568	G1569	U1570	C1571	U1572	A1573	G1574	A1575	A1576	U1577	U1578	C1579	A1580	U1581	U1582	U1583	U1584	G1585	U1586	C1587	U1588	U1589	C1590	G1591	A1592	U1593	U1594	C1595	U1598	U1599	A1600	U1601	C1604	A1605	C1606	A1607	G1613	A1614	G1615	A1616	A1617	A1618	A1619	G1620	C1621																																												
U1431	A1432	C1435	U1438	U1439	A1440	C1444	C1445	U1446	U1447	U1448	A1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	A1458	A1459	U1460	C1461	G1462	A1463	U1464	G1465	G1466	U1467	U1468	U1469	U1470	A1471	C1472	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	C1491	G1492	U1493	U1494	U1495																																													
G1496	A1497	U1498	U1499	G1500	G1501	A1502	U1503	U1504	G1505	C1506	A1507	C1508	U1509	U1510	C1511	U1512	A1513	A1514	C1515	C1516	A1517	G1518	U1519	A1520	A1521	G1522	G1523	C1524	U1525	G1526	A1527	U1528	U1529	A1530	U1531	A1532	G1533	U1534	G1535	C1536	A1537	A1538	U1539	U1540	C1541	C1542	G1543	G1544	U1545	C1546	C1547	U1548	C1549	G1550	U1551	U1552	A1553	A1554	G1555																																									
U1556	C1557	U1558	G1559	A1560	G1561	C1562	U1563	A1564	U1565	G1566	C1567	U1568	G1569	U1570	C1571	U1572	A1573	G1574	A1575	A1576	U1577	U1578	C1579	A1580	U1581	U1582	U1583	U1584	G1585	U1586	C1587	U1588	U1589	C1590	G1591	A1592	U1593	U1594	C1595	U1598	U1599	A1600	U1601	C1604	A1605	C1606	A1607	G1613	A1614	G1615	A1616	A1617	A1618	A1619	G1620	C1621																																												
G1496	A1497	U1498	U1499	G1500	G1501	A1502	U1503	U1504	G1505	C1506	A1507	C1508	U1509	U1510	C1511	U1512	A1513	A1514	C1515	C1516	A1517	G1518	U1519	A1520	A1521	G1522	G1523	C1524	U1525	G1526	A1527	U1528	U1529	A1530	U1531	A1532	G1533	U1534	G1535	C1536	A1537	A1538	U1539	U1540	C1541	C1542	G1543	G1544	U1545	C1546	C1547	U1548	C1549	G1550	U1551	U1552	A1553	A1554	G1555																																									
U1431	A1432	C1435	U1438	U1439	A1440	C1444	C1445	U1446	U1447	U1448	A1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	A1458	A1459	U1460	C1461	G1462	A1463	U1464	G1465	G1466	U1467	U1468	U1469	U1470	A1471	C1472	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	C1491	G1492	U1493	U1494	U1495																																													
G1365	U1366	C1367	C1368	G1369	C1370	G1375	U1376	U1377	U1378	A1379	G1380	U1381	C1382	G1383	U1384	U1385	U1386	C1387	A1390	A1391	C1392	A1393	U1394	A1395	A1396	G1397	G1401	A1402	C1403	A1404	G1405	U1406	C1407	U1408	A1409	U1410	A1411	U1412	G1413	G1414	A1415	U1416	G1417	G1418	A1419	A1421	C1422	C1423	A1424	G1425	G1426	U1427	U1428	U1429	A1430																																													
A1282	G1283	A1284	U1285	G1286	U1287	G1290	A1291	A1292	U1293	G1294	C1295	C1296	G1297	G1298	U1301	G1302	A1303	G1304	G1307	C1308	G1309	A1310	A1311	C1312	G1313	A1314	C1315	G1316	G1317	G1320	A1323	A1324	G1336	U1337	U1338	U1339	G1340	A1341	G1342	U1343	A1344	G1347	A1363	G1364	A1365	G1366	G1367	A1368	U1369	U1370	G1375	U1376	U1377	U1378	U1379	G1380	U1381	C1382	G1383	U1384	G1385	U1386	C1387	A1390	A1391	C1392	C1393	U1394	G1395	A1396	G1397	G1401	A1402	C1403	A1404	G1405	G1406	C1407	G1408	U1409	A1410	U1411	U1412	G1413	G1414	A1415	U1416	G1417	G1418	A1419	A1421	C1422	C1423	A1424	G1425	G1426	U1427	U1428	U1429	A1430
U1212	C1213	A1214	C1215	U1216	U1217	G1218	G1219	A1220	C1221	A1222	G1225	U1226	U1227	A1228	G1229	G1230	C1231	G1232	A1233	G1234	U1238	C1239	A1242	G1243	G1244	G1245	U1248	G1249	A1251	C1252	G1257	A1258	U1259	C1260	G1261	U1262	A1263	A1264	G1265	G1266	A1267	C1268	C1269	U1270	G1271	G1274	U1275	G1276	C1279	U1210	G1211																																																	
C1144	U1145	C1146	A1147	C1148	U1149	G1150	C1151	U1152	C1153	G1154	A1155	G1156	U1157	A1158	C1159	C1160	A1161	C1162	U1163	G1164	C1165	G1166	C1167	C1168	A1169	A1170	A1173	U1174	G1175	C1178	U1179	C1180	G1181	C1182	G1183	C1184	U1185	A1186	U1187	A1188	A1192	A1195	C1196	C1197	U1198	A1199	A1200	G1201	C1202	G1207	A1208	U1209	U1210	G1211																																														
U1084	U1085	G1086	C1087	C1088	C1089	A1090	G1091	A1092	C1093	A1094	A1095	C1096	U1097	U1098	G1099	G1100	A1101	U1102	G1103	U1104	U1105	G1106	G1107	C1108	U1109	U1110	A1111	G1112	A1113	A1114	G1115	C1116	A1117	G1118	C1119	C1120	A1121	U1122	C1123	A1124	U1125	U1126	U1127	A1128	A1129	A1130	G1131	A1132	G1133	U1134	G1135	C1136	U1137	U1138	A1139	U1140	A1141	A1142	G1143																																									
A1018	A1019	G1020	G1021	A1022	A1023	C1024	A1025	C1026	A1027	G1028	C1029	C1030	A1031	A1032	C1033	A1034	C1035	C1036	A1037	C1038	C1039	A1040	U1041	C1042	U1043	A1044	A1045	G1046	G1047	U1048	C1049	C1050	C1051	A1052	A1053	A1054	A1055	U1056	A1057	U1063	G1066	U1067	G1068	G1069	A1070	A1071	A1072	A1073	G1074	G1075	A1076	U1077	G1078	U1079	G1080	G1081	C1082	G1083																																										
C942	C943	G944	A945	A946	U947	U948	C949	G950	G951	A952	A955	A956	C957	C958	C959	C960	A962	A963	U964	G965	C966	C967	U970	U971	A972	A973	A977	G983	G984	A985	C986	U987	C988	G989	G990	A991	A992	G997	G998	U999	G1000	A1001	A1002	U1003	A1004	G1005	G1006	U1007	C1008	C1015	U939	A941																																																
A866	U867	A868	U871	U872	U873	A874	G875	G876	G877	C878	A809	A810	C881	C882	C883	A814	G815	G816	G817	U818	A819	G820	C821	C822	G823	A824	G825	A826	A827	G828	U829	U830	C831	C832	A833	C910	A911	C912	U913	G914	U915	A916	U917	U918	U919	A845	A849	G850	C851	C857	U858	G859	U860	C861	C862	A788	G789	U790	A791																																									
C724	A725	U731	C732	U733	A734	C735	C736	U737	U738	U739	G740	C741	U742	C743	G749	A750	A751	G752	U753	U754	C755	G756	G757	U758	U759	A760	A761	C762	A763	C764	U765	G766	A767	A768	U769	G770	G771	A772	G773	G774	A775	C776	C777	G778	A779	C780	C781	C782	A784	C785	A788	G789	U790	A791																																														

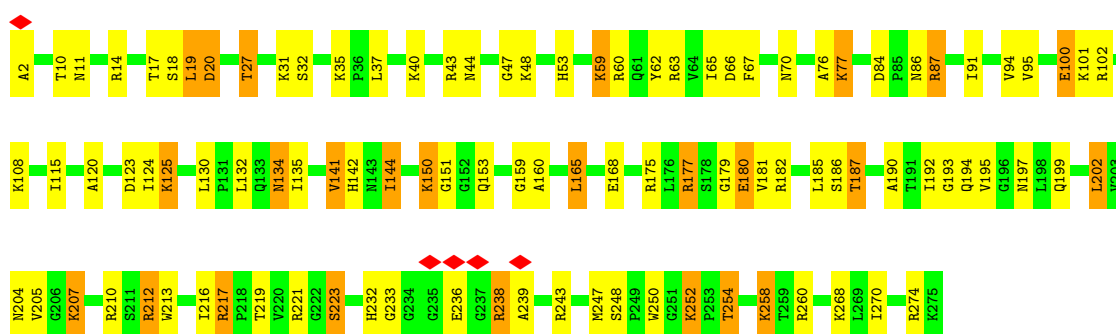




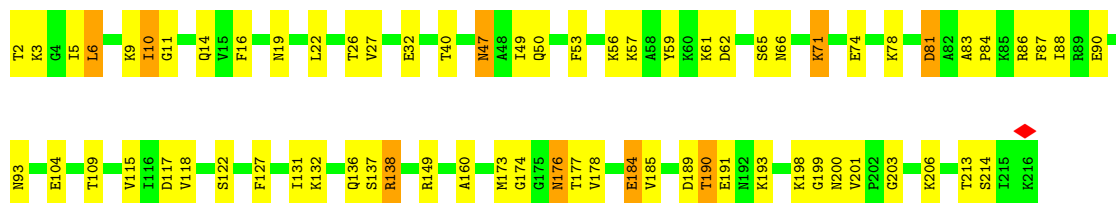
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3



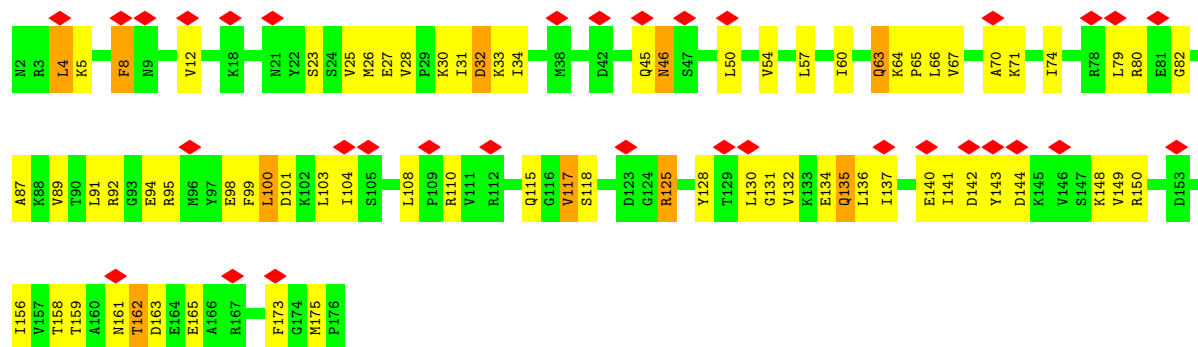
• Molecule 5: 50S ribosomal protein L4

Chain E:  57% 39% .



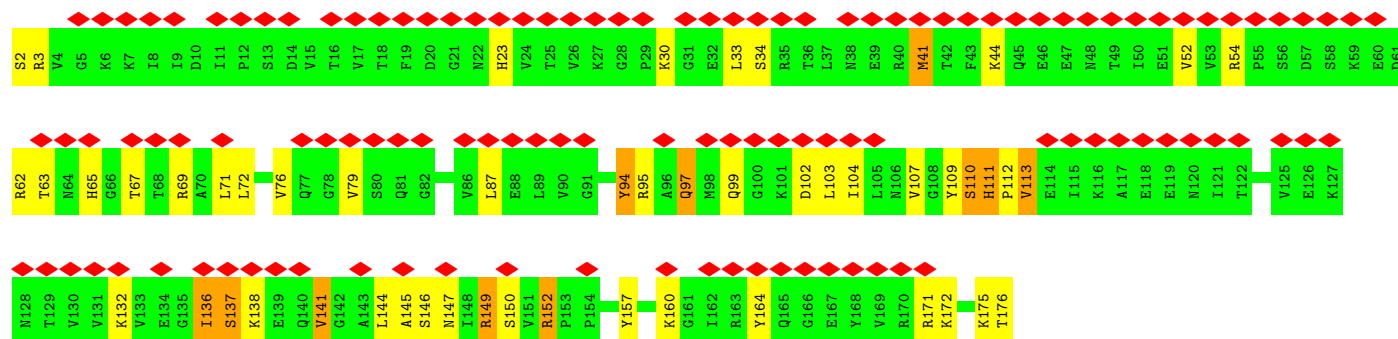
• Molecule 6: 50S ribosomal protein L5

Chain F:  19% 58% 37% 6%



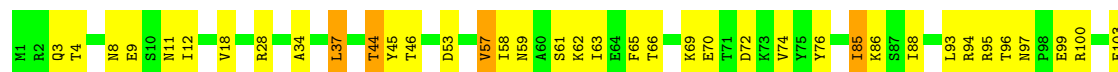
• Molecule 7: 50S ribosomal protein L6

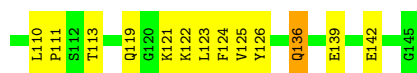
Chain G:  68% 70% 23% 6%



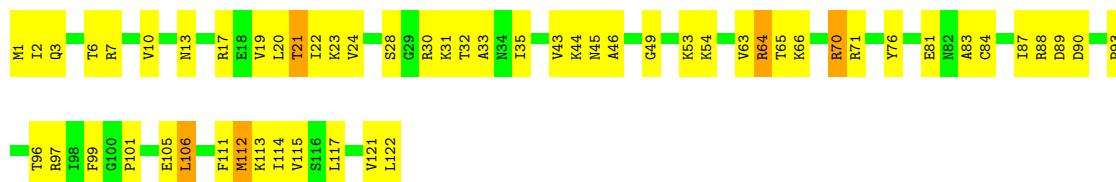
• Molecule 8: 50S ribosomal protein L13

Chain H:  65% 32% .

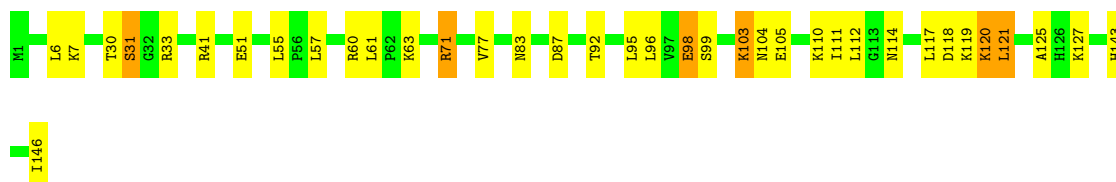
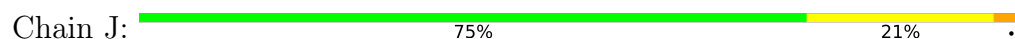




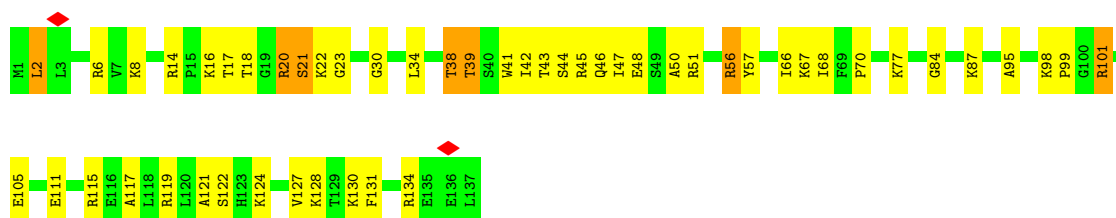
- Molecule 9: 50S ribosomal protein L14



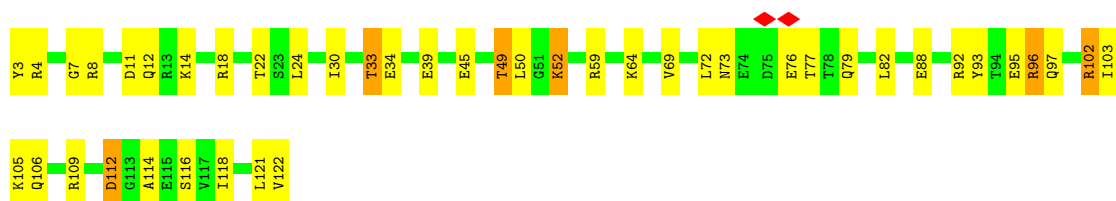
- Molecule 10: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L16

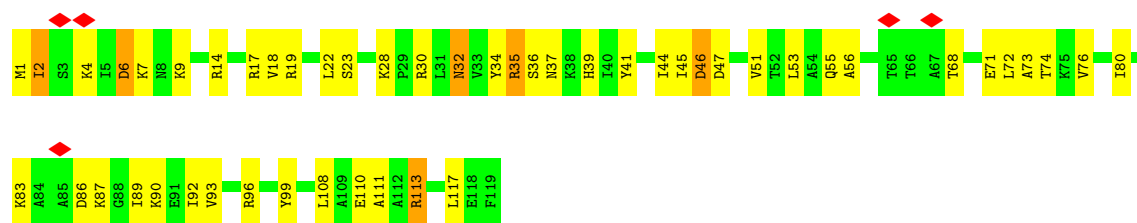


- Molecule 12: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L18





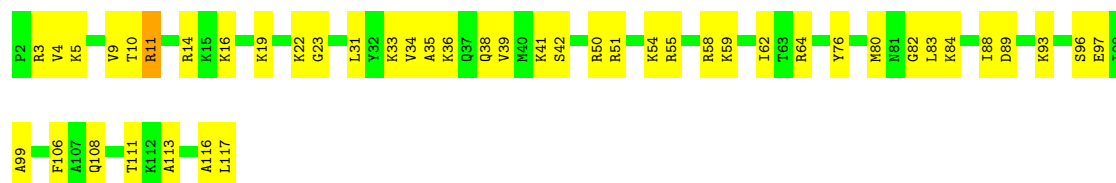
- Molecule 14: 50S ribosomal protein L19

Chain N: 70% 27% .



- Molecule 15: 50S ribosomal protein L20

Chain O: 61% 38% .



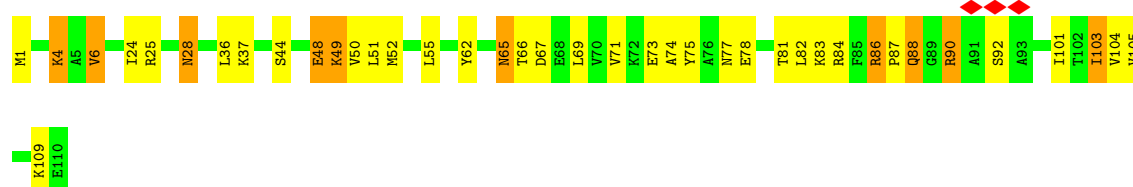
- Molecule 16: 50S ribosomal protein L21

Chain P: 65% 33% .



- Molecule 17: 50S ribosomal protein L22

Chain Q: 64% 27% 9% .

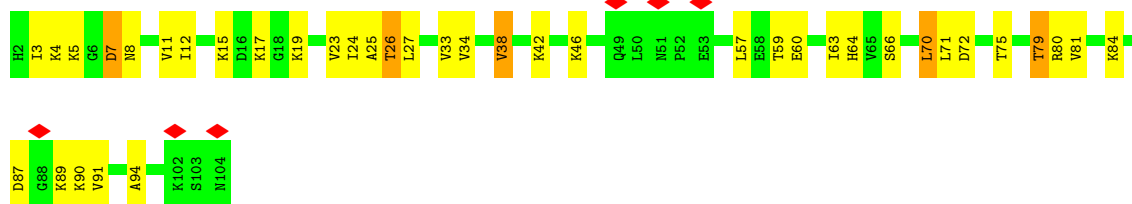


- Molecule 18: 50S ribosomal protein L23

Chain R: 63% 33% .



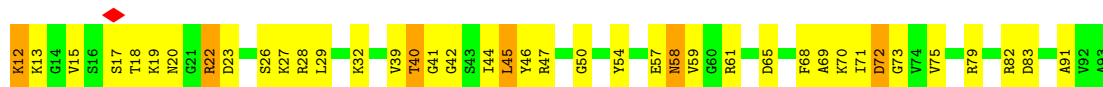
- Molecule 19: 50S ribosomal protein L24



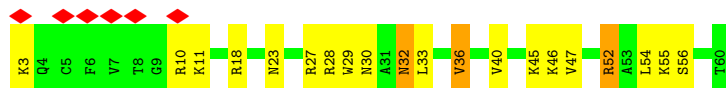
- Molecule 20: 50S ribosomal protein L25



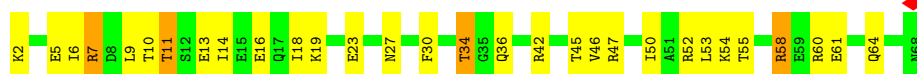
- Molecule 21: 50S ribosomal protein L27



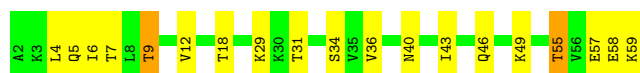
- Molecule 22: 50S ribosomal protein L28



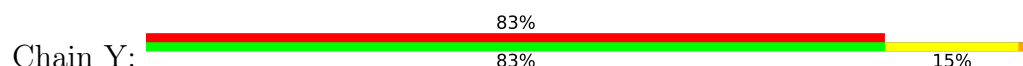
- Molecule 23: 50S ribosomal protein L29

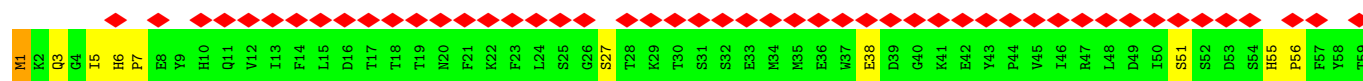


- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L31 type B

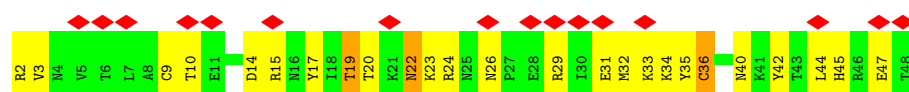




• Molecule 26: 50S ribosomal protein L32



• Molecule 27: 50S ribosomal protein L33



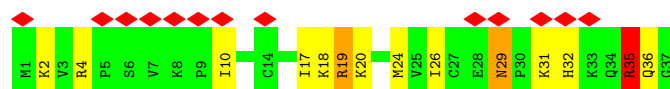
• Molecule 28: 50S ribosomal protein L34



• Molecule 29: 50S ribosomal protein L35



• Molecule 30: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.076	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.288	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	426.80002, 426.80002, 426.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.75	217/69739 (0.3%)	1.56	1126/108751 (1.0%)
2	B	1.05	1/2733 (0.0%)	1.43	37/4257 (0.9%)
3	C	0.73	0/2125	0.75	1/2853 (0.0%)
4	D	0.87	1/1651 (0.1%)	0.71	1/2215 (0.0%)
5	E	0.79	0/1595	0.73	0/2154
6	F	0.35	0/1339	0.61	0/1805
7	G	0.34	0/1281	0.59	0/1736
8	H	0.82	0/1165	0.75	0/1570
9	I	0.78	0/925	0.79	0/1242
10	J	0.73	0/1100	0.73	0/1467
11	K	0.61	0/1095	0.70	1/1472 (0.1%)
12	L	0.73	0/936	0.79	2/1253 (0.2%)
13	M	0.48	0/900	0.69	0/1205
14	N	0.79	0/901	0.74	0/1209
15	O	0.90	0/954	0.76	0/1264
16	P	0.87	0/800	0.75	0/1070
17	Q	0.75	0/845	0.78	0/1140
18	R	0.72	0/723	0.69	0/966
19	S	0.58	0/779	0.66	0/1043
20	T	0.44	0/730	0.61	0/981
21	U	0.84	0/628	0.80	1/833 (0.1%)
22	V	0.54	0/451	0.74	0/603
23	W	0.50	0/542	0.63	0/722
24	X	0.82	0/451	0.70	0/606
25	Y	0.29	0/378	0.55	0/521
26	Z	0.75	0/366	0.86	3/489 (0.6%)
27	1	0.36	0/395	0.68	0/530
28	2	0.86	0/371	0.81	1/484 (0.2%)
29	3	0.67	0/526	0.81	0/690
30	4	0.48	0/298	0.80	0/392
All	All	1.54	219/96722 (0.2%)	1.41	1173/145523 (0.8%)

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	1
16	P	0	2
23	W	0	1
30	4	0	1
All	All	0	6

All (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	C	N1-C6	137.42	2.19	1.37
1	A	333	C	N3-C4	117.87	2.16	1.33
1	A	333	C	C2-N3	108.34	2.22	1.35
1	A	333	C	C4-C5	94.04	2.18	1.43
1	A	333	C	C5-C6	87.55	2.04	1.34
1	A	333	C	N1-C2	81.00	2.21	1.40
1	A	393	G	C1'-N9	67.25	2.49	1.48
1	A	393	G	N9-C4	35.55	1.66	1.38
1	A	393	G	N9-C8	34.75	1.62	1.37
1	A	393	G	N7-C5	-21.42	1.26	1.39
1	A	2044	C	N1-C6	-7.44	1.32	1.37
1	A	2477	A	N9-C4	-7.34	1.33	1.37
1	A	554	C	N1-C6	-7.30	1.32	1.37
1	A	2497	G	C8-N7	-7.11	1.26	1.30
1	A	985	A	N9-C4	-7.05	1.33	1.37
1	A	393	G	C8-N7	-6.98	1.26	1.30
1	A	845	A	N9-C4	-6.79	1.33	1.37
1	A	1467	G	C8-N7	-6.73	1.26	1.30
1	A	490	C	N1-C6	-6.57	1.33	1.37
1	A	1692	C	N1-C6	-6.52	1.33	1.37
1	A	629	A	N9-C4	-6.49	1.33	1.37
1	A	2028	A	N9-C4	-6.47	1.33	1.37
1	A	491	C	N3-C4	-6.39	1.29	1.33
1	A	945	A	N9-C4	-6.38	1.34	1.37
1	A	393	G	C2'-C1'	6.38	1.60	1.53
1	A	897	A	C5-C6	-6.32	1.35	1.41
1	A	1042	C	N1-C6	-6.27	1.33	1.37
1	A	219	A	N9-C4	-6.25	1.34	1.37
1	A	1817	C	N1-C6	-6.23	1.33	1.37
1	A	864	A	N9-C4	-6.23	1.34	1.37
1	A	1220	A	N7-C5	-6.23	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2528	C	N1-C6	-6.18	1.33	1.37
1	A	737	C	C4-C5	-6.14	1.38	1.43
1	A	2698	A	N9-C4	-6.13	1.34	1.37
1	A	2677	C	C4-C5	-6.12	1.38	1.43
1	A	2388	A	N9-C4	-6.09	1.34	1.37
1	A	845	A	C5-C6	-6.09	1.35	1.41
1	A	1196	C	C4-C5	-6.07	1.38	1.43
1	A	862	C	N3-C4	-6.05	1.29	1.33
1	A	2849	A	N9-C4	-6.04	1.34	1.37
1	A	1818	A	N9-C4	-6.03	1.34	1.37
1	A	1694	A	N9-C4	-6.01	1.34	1.37
1	A	613	G	N9-C8	-6.01	1.33	1.37
1	A	198	A	N9-C4	-5.95	1.34	1.37
1	A	756	A	N7-C5	-5.95	1.35	1.39
1	A	1467	G	N7-C5	-5.95	1.35	1.39
1	A	2896	A	N9-C4	-5.94	1.34	1.37
1	A	2069	A	N9-C4	-5.93	1.34	1.37
1	A	254	A	N9-C4	-5.92	1.34	1.37
1	A	1031	C	N1-C6	-5.92	1.33	1.37
1	A	559	A	N9-C4	-5.92	1.34	1.37
1	A	2071	C	C4-C5	-5.89	1.38	1.43
1	A	866	A	N9-C4	-5.88	1.34	1.37
1	A	2848	G	N9-C4	-5.88	1.33	1.38
1	A	503	A	N9-C4	-5.84	1.34	1.37
1	A	491	C	N1-C6	-5.83	1.33	1.37
1	A	1026	C	N1-C6	-5.83	1.33	1.37
1	A	1853	C	N1-C6	-5.83	1.33	1.37
1	A	2294	A	N9-C4	-5.82	1.34	1.37
1	A	636	A	C5-C6	-5.82	1.35	1.41
1	A	1415	A	N9-C4	-5.82	1.34	1.37
1	A	2651	G	N9-C4	-5.81	1.33	1.38
1	A	814	A	N9-C4	-5.81	1.34	1.37
1	A	1842	A	N9-C4	-5.78	1.34	1.37
1	A	859	C	C4-C5	-5.77	1.38	1.43
1	A	882	C	N1-C6	-5.75	1.33	1.37
1	A	721	A	N7-C5	-5.75	1.35	1.39
1	A	501	C	N1-C6	-5.74	1.33	1.37
1	A	1537	A	C2-N3	-5.74	1.28	1.33
1	A	1759	G	N9-C8	-5.72	1.33	1.37
1	A	2738	A	C6-N6	-5.70	1.29	1.33
1	A	718	C	N1-C6	-5.68	1.33	1.37
1	A	110	A	N9-C4	-5.67	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2045	A	N9-C4	-5.65	1.34	1.37
1	A	548	A	N9-C4	-5.65	1.34	1.37
1	A	967	C	N1-C6	-5.63	1.33	1.37
1	A	2708	C	N1-C6	-5.62	1.33	1.37
1	A	721	A	C5-C6	-5.61	1.35	1.41
1	A	2734	C	N3-C4	-5.61	1.30	1.33
1	A	777	C	N1-C6	-5.59	1.33	1.37
1	A	1410	A	N9-C4	-5.58	1.34	1.37
1	A	1435	C	C4-C5	-5.58	1.38	1.43
1	A	1296	C	N1-C6	-5.57	1.33	1.37
1	A	192	G	N9-C4	-5.57	1.33	1.38
1	A	627	C	C4-C5	-5.57	1.38	1.43
1	A	511	G	N9-C8	-5.55	1.33	1.37
1	A	2643	C	C4-C5	-5.55	1.38	1.43
1	A	1467	G	C5-C6	-5.54	1.36	1.42
1	A	832	C	N1-C6	-5.53	1.33	1.37
1	A	1954	A	N9-C8	-5.53	1.33	1.37
1	A	2774	G	C6-N1	-5.53	1.35	1.39
1	A	1466	G	N1-C2	-5.51	1.33	1.37
1	A	2810	A	N9-C4	-5.51	1.34	1.37
1	A	1632	A	N7-C5	-5.50	1.35	1.39
1	A	1197	C	C4-C5	-5.50	1.38	1.43
1	A	2029	G	N9-C4	-5.49	1.33	1.38
1	A	194	A	C6-N1	-5.49	1.31	1.35
1	A	1196	C	N3-C4	-5.49	1.30	1.33
1	A	983	G	N9-C4	-5.49	1.33	1.38
1	A	216	A	N9-C4	-5.49	1.34	1.37
1	A	1344	A	N9-C4	-5.49	1.34	1.37
1	A	824	A	N9-C4	-5.48	1.34	1.37
1	A	2293	A	N9-C4	-5.47	1.34	1.37
1	A	2076	A	N9-C4	-5.46	1.34	1.37
1	A	2030	A	N9-C4	-5.46	1.34	1.37
1	A	2845	G	N9-C4	-5.45	1.33	1.38
1	A	950	A	N9-C4	-5.44	1.34	1.37
1	A	1463	A	C5-C6	-5.43	1.36	1.41
1	A	1207	G	N9-C4	-5.42	1.33	1.38
1	A	723	C	C4-C5	-5.41	1.38	1.43
1	A	713	A	N9-C4	-5.41	1.34	1.37
1	A	516	A	N9-C4	-5.39	1.34	1.37
1	A	1415	A	N3-C4	-5.39	1.31	1.34
1	A	2850	G	N9-C4	-5.38	1.33	1.38
1	A	495	A	N9-C4	-5.37	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2454	C	N3-C4	-5.37	1.30	1.33
1	A	154	A	N9-C4	-5.36	1.34	1.37
1	A	2387	A	N9-C4	-5.35	1.34	1.37
1	A	1044	A	N9-C4	-5.35	1.34	1.37
1	A	2644	C	C4-C5	-5.34	1.38	1.43
1	A	781	C	C4-C5	-5.33	1.38	1.43
1	A	608	C	C4-C5	-5.33	1.38	1.43
1	A	1303	A	N9-C4	-5.33	1.34	1.37
1	A	1634	A	C5-C6	-5.32	1.36	1.41
1	A	806	A	C5-C6	-5.32	1.36	1.41
1	A	1015	C	C4-C5	-5.31	1.38	1.43
1	A	1463	A	C8-N7	-5.30	1.27	1.31
1	A	2082	C	N1-C6	-5.29	1.33	1.37
1	A	1036	C	N1-C6	-5.29	1.33	1.37
1	A	14	A	N9-C4	-5.28	1.34	1.37
1	A	616	G	N9-C4	-5.28	1.33	1.38
1	A	2076	A	C6-N1	-5.28	1.31	1.35
1	A	2666	A	N9-C4	-5.27	1.34	1.37
1	A	878	C	N3-C4	-5.25	1.30	1.33
1	A	2604	A	N9-C4	-5.25	1.34	1.37
1	A	623	C	N3-C4	-5.24	1.30	1.33
1	A	1801	C	N3-C4	-5.24	1.30	1.33
1	A	2310	C	N1-C6	-5.24	1.34	1.37
1	A	253	G	N9-C8	-5.24	1.34	1.37
1	A	627	C	N1-C6	-5.24	1.34	1.37
1	A	1700	C	N3-C4	-5.22	1.30	1.33
1	A	839	A	C6-N1	-5.22	1.31	1.35
1	A	2700	G	N9-C4	-5.22	1.33	1.38
1	A	647	G	C6-N1	-5.21	1.35	1.39
1	A	724	C	C4-C5	-5.21	1.38	1.43
1	A	2301	A	N9-C4	-5.21	1.34	1.37
1	A	82	G	N9-C4	-5.21	1.33	1.38
1	A	193	A	C5-C6	-5.20	1.36	1.41
1	A	1772	G	C8-N7	-5.20	1.27	1.30
1	A	2841	A	N9-C4	-5.20	1.34	1.37
1	A	133	A	C5-C6	-5.20	1.36	1.41
1	A	836	C	N1-C6	-5.20	1.34	1.37
1	A	187	C	N3-C4	-5.20	1.30	1.33
1	A	2076	A	C6-N6	-5.20	1.29	1.33
1	A	1051	C	N1-C6	-5.19	1.34	1.37
1	A	1182	G	N9-C8	-5.19	1.34	1.37
1	A	2857	A	N9-C4	-5.18	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1647	A	C6-N1	-5.17	1.31	1.35
1	A	897	A	N7-C5	-5.17	1.36	1.39
1	A	1239	C	N1-C6	-5.17	1.34	1.37
1	A	1800	A	N9-C8	-5.17	1.33	1.37
1	A	839	A	C6-N6	-5.16	1.29	1.33
1	A	342	A	N9-C4	-5.16	1.34	1.37
1	A	2248	G	N9-C4	-5.16	1.33	1.38
1	A	2070	C	N3-C4	-5.15	1.30	1.33
1	A	1049	C	N3-C4	-5.14	1.30	1.33
1	A	555	C	N3-C4	-5.14	1.30	1.33
1	A	2287	C	N3-C4	-5.14	1.30	1.33
1	A	1046	G	N9-C4	-5.14	1.33	1.38
1	A	378	C	C4-C5	-5.13	1.38	1.43
1	A	426	G	C6-N1	-5.13	1.35	1.39
1	A	736	C	N1-C6	-5.13	1.34	1.37
1	A	2919	A	N9-C4	-5.13	1.34	1.37
1	A	1008	C	N1-C6	-5.12	1.34	1.37
1	A	620	G	N9-C8	-5.12	1.34	1.37
1	A	601	G	N9-C4	-5.11	1.33	1.38
1	A	2075	G	N9-C8	-5.11	1.34	1.37
1	A	1693	G	N9-C4	-5.11	1.33	1.38
1	A	2291	C	N1-C6	-5.11	1.34	1.37
1	A	857	C	N1-C6	-5.11	1.34	1.37
1	A	1501	G	N9-C4	-5.11	1.33	1.38
1	A	1622	C	C4-C5	-5.10	1.38	1.43
1	A	1030	C	C4-C5	-5.10	1.38	1.43
1	A	2242	G	C8-N7	-5.10	1.27	1.30
1	A	2247	G	N9-C4	-5.10	1.33	1.38
1	A	2278	G	N7-C5	-5.10	1.36	1.39
1	A	878	C	N1-C6	-5.09	1.34	1.37
1	A	851	C	N3-C4	-5.09	1.30	1.33
1	A	1831	A	C6-N6	-5.08	1.29	1.33
1	A	2000	G	N9-C4	-5.08	1.33	1.38
1	A	455	A	N9-C4	-5.08	1.34	1.37
1	A	71	A	N9-C4	-5.07	1.34	1.37
1	A	1228	A	N7-C5	-5.07	1.36	1.39
1	A	1384	G	N9-C4	-5.07	1.33	1.38
1	A	2310	C	N3-C4	-5.07	1.30	1.33
1	A	1438	G	N9-C4	-5.06	1.33	1.38
1	A	2064	A	N9-C4	-5.06	1.34	1.37
1	A	1040	A	N9-C4	-5.05	1.34	1.37
1	A	717	C	N1-C6	-5.05	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	118	VAL	CB-CG2	-5.05	1.42	1.52
1	A	461	A	C6-N1	-5.05	1.32	1.35
1	A	2742	C	N3-C4	-5.04	1.30	1.33
1	A	249	C	C4-C5	-5.04	1.39	1.43
1	A	624	C	N3-C4	-5.04	1.30	1.33
1	A	897	A	C6-N1	-5.04	1.32	1.35
1	A	1796	A	N9-C4	-5.04	1.34	1.37
1	A	1018	A	N9-C4	-5.03	1.34	1.37
1	A	2497	G	N7-C5	-5.03	1.36	1.39
2	B	86	A	N9-C4	-5.02	1.34	1.37
1	A	859	C	N1-C6	-5.02	1.34	1.37
1	A	2092	C	C4-C5	-5.02	1.39	1.43
1	A	833	A	N9-C4	-5.02	1.34	1.37
1	A	47	C	C2-O2	-5.01	1.20	1.24
1	A	2044	C	C5-C6	-5.01	1.30	1.34
1	A	2742	C	C4-C5	-5.01	1.39	1.43
1	A	95	A	N7-C5	-5.01	1.36	1.39
1	A	861	C	N1-C6	-5.01	1.34	1.37
1	A	1021	G	N9-C4	-5.01	1.33	1.38
1	A	178	A	N9-C4	-5.00	1.34	1.37

All (1173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	G	C8-N9-C4	-101.37	65.85	106.40
1	A	393	G	N7-C8-N9	63.97	145.09	113.10
1	A	393	G	N9-C4-C5	53.72	126.89	105.40
1	A	393	G	N3-C4-C5	-41.56	107.82	128.60
1	A	393	G	C2-N3-C4	26.55	125.18	111.90
1	A	393	G	C4-C5-C6	19.11	130.26	118.80
1	A	393	G	C4-N9-C1'	16.95	148.54	126.50
1	A	393	G	C5-N7-C8	-16.85	95.87	104.30
1	A	393	G	O4'-C1'-N9	15.58	120.67	108.20
1	A	393	G	C8-N9-C1'	14.27	145.56	127.00
1	A	393	G	N9-C1'-C2'	13.14	131.09	114.00
1	A	806	A	N1-C6-N6	13.08	126.45	118.60
1	A	333	C	C6-N1-C2	12.82	125.43	120.30
1	A	333	C	N1-C2-N3	-11.95	110.84	119.20
1	A	2782	C	C2-N1-C1'	11.87	131.86	118.80
1	A	1467	G	C4-C5-N7	11.73	115.49	110.80
1	A	393	G	C6-C5-N7	-11.61	123.44	130.40
1	A	393	G	C4-C5-N7	-11.49	106.20	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1467	G	C6-C5-N7	-11.19	123.69	130.40
1	A	333	C	C5-C4-N4	11.15	128.01	120.20
1	A	1634	A	N1-C6-N6	11.15	125.29	118.60
1	A	333	C	N3-C4-C5	-10.77	117.59	121.90
1	A	265	A	N1-C6-N6	10.53	124.92	118.60
1	A	1461	C	N1-C2-O2	10.51	125.21	118.90
1	A	897	A	N9-C4-C5	-10.38	101.65	105.80
1	A	751	A	C5-C6-N6	-10.15	115.58	123.70
1	A	2782	C	C6-N1-C1'	-10.12	108.66	120.80
1	A	333	C	C2-N3-C4	10.07	124.94	119.90
1	A	806	A	C5-C6-N6	-10.03	115.68	123.70
1	A	396	G	N3-C4-C5	-10.00	123.60	128.60
1	A	1906	C	N1-C2-O2	9.93	124.86	118.90
1	A	2150	A	C5-N7-C8	9.89	108.85	103.90
1	A	1467	G	C5-N7-C8	-9.72	99.44	104.30
1	A	333	C	C4-C5-C6	9.70	122.25	117.40
1	A	1461	C	N3-C2-O2	-9.60	115.18	121.90
2	B	114	G	N7-C8-N9	9.52	117.86	113.10
1	A	1467	G	N7-C8-N9	9.46	117.83	113.10
1	A	851	C	N1-C2-O2	9.41	124.54	118.90
1	A	393	G	C6-N1-C2	-9.34	119.50	125.10
1	A	1634	A	C5-C6-N6	-9.32	116.25	123.70
1	A	2361	U	C2-N1-C1'	9.29	128.85	117.70
1	A	396	G	C4-N9-C1'	9.20	138.46	126.50
1	A	1391	A	N1-C6-N6	9.20	124.12	118.60
1	A	1500	G	C4-C5-N7	9.18	114.47	110.80
1	A	1607	A	N9-C4-C5	-9.10	102.16	105.80
1	A	897	A	C4-C5-N7	9.10	115.25	110.70
1	A	751	A	N1-C6-N6	9.09	124.05	118.60
1	A	265	A	C5-C6-N6	-9.01	116.49	123.70
1	A	2734	C	N1-C2-O2	8.99	124.30	118.90
1	A	608	C	C5-C4-N4	-8.96	113.92	120.20
1	A	1802	U	C5-C4-O4	-8.91	120.56	125.90
1	A	756	A	C6-C5-N7	-8.84	126.11	132.30
1	A	1081	G	N3-C4-N9	-8.81	120.71	126.00
1	A	988	C	N1-C2-O2	8.77	124.16	118.90
1	A	1654	A	N1-C6-N6	8.67	123.80	118.60
1	A	988	C	C2-N1-C1'	8.64	128.31	118.80
1	A	1480	G	N7-C8-N9	8.64	117.42	113.10
1	A	1072	A	N1-C6-N6	8.59	123.75	118.60
1	A	1759	G	N7-C8-N9	8.55	117.38	113.10
1	A	574	A	N1-C6-N6	8.55	123.73	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	C	N1-C2-O2	8.47	123.98	118.90
1	A	574	A	C5-C6-N6	-8.45	116.94	123.70
1	A	1634	A	N9-C4-C5	-8.42	102.43	105.80
1	A	1468	G	C4-C5-N7	8.37	114.15	110.80
1	A	623	C	N1-C2-O2	8.35	123.91	118.90
1	A	1906	C	N3-C2-O2	-8.32	116.08	121.90
1	A	2326	G	C6-C5-N7	-8.28	125.43	130.40
1	A	333	C	N1-C2-O2	8.18	123.81	118.90
1	A	461	A	N9-C4-C5	-8.15	102.54	105.80
1	A	2834	C	N1-C2-O2	8.14	123.78	118.90
1	A	1087	C	C6-N1-C2	-8.14	117.05	120.30
1	A	1463	A	N9-C4-C5	-8.13	102.55	105.80
1	A	757	G	C4-C5-N7	8.12	114.05	110.80
1	A	1467	G	N9-C4-C5	-8.10	102.16	105.40
2	B	24	C	C2-N1-C1'	8.06	127.67	118.80
1	A	575	G	N1-C2-N2	-8.05	108.95	116.20
1	A	1219	G	N3-C2-N2	-8.03	114.28	119.90
1	A	2326	G	C4-C5-N7	8.03	114.01	110.80
1	A	2774	G	N1-C6-O6	-8.02	115.09	119.90
1	A	751	A	N9-C4-C5	-7.99	102.61	105.80
1	A	2782	C	N1-C2-O2	7.99	123.69	118.90
1	A	757	G	C6-C5-N7	-7.93	125.64	130.40
1	A	1538	A	N1-C6-N6	-7.92	113.84	118.60
1	A	1802	U	N3-C4-O4	7.92	124.94	119.40
1	A	1920	C	N3-C2-O2	-7.92	116.36	121.90
1	A	319	G	N9-C4-C5	-7.91	102.24	105.40
1	A	95	A	N1-C6-N6	7.87	123.32	118.60
1	A	2523	C	N3-C2-O2	-7.86	116.40	121.90
1	A	1501	G	N3-C4-N9	-7.85	121.29	126.00
1	A	806	A	C6-C5-N7	-7.84	126.81	132.30
1	A	1024	A	C5-C6-N6	-7.82	117.44	123.70
1	A	1072	A	C5-C6-N6	-7.82	117.44	123.70
1	A	757	G	N7-C8-N9	7.82	117.01	113.10
2	B	21	G	N3-C4-C5	7.79	132.49	128.60
2	B	24	C	N1-C2-O2	7.78	123.57	118.90
1	A	721	A	C5-N7-C8	-7.77	100.01	103.90
1	A	1537	A	C5-C6-N6	7.77	129.92	123.70
1	A	252	C	C5-C4-N4	-7.77	114.76	120.20
1	A	396	G	C8-N9-C4	-7.77	103.29	106.40
1	A	897	A	N1-C6-N6	7.77	123.26	118.60
2	B	114	G	C8-N9-C4	-7.77	103.29	106.40
1	A	897	A	C6-C5-N7	-7.74	126.88	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	G	C2-N3-C4	7.74	115.77	111.90
1	A	317	G	C2-N3-C4	-7.73	108.04	111.90
1	A	2786	G	C4-C5-N7	7.73	113.89	110.80
1	A	2834	C	N3-C2-O2	-7.72	116.50	121.90
1	A	307	A	N9-C4-C5	-7.71	102.72	105.80
1	A	806	A	C4-C5-N7	7.70	114.55	110.70
1	A	92	G	C5-C6-O6	7.67	133.20	128.60
1	A	924	G	C6-C5-N7	-7.66	125.81	130.40
1	A	1075	G	N3-C4-N9	-7.65	121.41	126.00
1	A	1024	A	N1-C6-N6	7.65	123.19	118.60
1	A	752	G	C4-C5-N7	7.63	113.85	110.80
1	A	1625	U	N3-C2-O2	-7.60	116.88	122.20
1	A	759	U	O4'-C1'-N1	7.57	114.26	108.20
1	A	1500	G	C6-C5-N7	-7.57	125.86	130.40
1	A	988	C	C6-N1-C1'	-7.55	111.74	120.80
1	A	756	A	C4-C5-C6	7.54	120.77	117.00
1	A	1719	C	C5-C4-N4	-7.51	114.94	120.20
1	A	2525	C	C6-N1-C2	-7.50	117.30	120.30
1	A	1467	G	N1-C6-O6	7.49	124.39	119.90
1	A	1494	G	N3-C4-N9	-7.48	121.51	126.00
1	A	721	A	C4-C5-N7	7.48	114.44	110.70
1	A	2461	A	N1-C6-N6	7.48	123.09	118.60
1	A	1709	A	N1-C6-N6	7.47	123.08	118.60
1	A	755	C	N1-C2-O2	7.46	123.38	118.90
2	B	76	A	C5-C6-N6	-7.46	117.74	123.70
1	A	47	C	N3-C2-O2	-7.45	116.68	121.90
2	B	24	C	C6-N1-C2	-7.44	117.32	120.30
2	B	76	A	N1-C6-N6	7.43	123.06	118.60
1	A	897	A	C5-C6-N6	-7.41	117.77	123.70
1	A	1500	G	C5-N7-C8	-7.41	100.59	104.30
1	A	806	A	C5-N7-C8	-7.41	100.20	103.90
1	A	751	A	C4-C5-N7	7.41	114.40	110.70
1	A	1759	G	C4-N9-C1'	7.41	136.13	126.50
1	A	133	A	C4-C5-N7	7.40	114.40	110.70
1	A	766	G	N9-C4-C5	-7.38	102.45	105.40
1	A	924	G	C4-N9-C1'	7.35	136.06	126.50
1	A	2774	G	N1-C2-N2	-7.35	109.58	116.20
1	A	806	A	N9-C4-C5	-7.35	102.86	105.80
1	A	2326	G	N7-C8-N9	7.33	116.76	113.10
1	A	489	A	N1-C6-N6	7.32	122.99	118.60
1	A	2212	G	C5-C6-O6	7.30	132.98	128.60
1	A	522	G	C2-N3-C4	-7.29	108.25	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	735	C	N3-C2-O2	-7.27	116.81	121.90
1	A	2651	G	C2-N3-C4	-7.26	108.27	111.90
1	A	575	G	N3-C2-N2	7.26	124.98	119.90
1	A	2047	A	C5-C6-N6	-7.24	117.91	123.70
1	A	721	A	N1-C6-N6	7.23	122.94	118.60
1	A	2613	C	N3-C4-N4	-7.23	112.94	118.00
1	A	2102	U	C5-C4-O4	-7.22	121.57	125.90
1	A	92	G	N1-C6-O6	-7.21	115.58	119.90
1	A	636	A	C5-C6-N6	-7.20	117.94	123.70
1	A	2461	A	C5-C6-N6	-7.20	117.94	123.70
1	A	1410	A	N1-C6-N6	7.20	122.92	118.60
1	A	2845	G	N3-C4-C5	7.20	132.20	128.60
1	A	1422	A	N1-C2-N3	7.19	132.89	129.30
1	A	636	A	N1-C6-N6	7.19	122.91	118.60
1	A	2212	G	N1-C6-O6	-7.18	115.59	119.90
1	A	2734	C	N3-C2-O2	-7.17	116.88	121.90
1	A	1391	A	C5-C6-N6	-7.17	117.96	123.70
1	A	2457	A	C5-C6-N6	-7.17	117.97	123.70
1	A	2786	G	N9-C4-C5	-7.16	102.54	105.40
1	A	396	G	N3-C4-N9	7.15	130.29	126.00
1	A	1991	G	N3-C4-N9	-7.14	121.71	126.00
1	A	819	A	C5-C6-N6	-7.14	117.98	123.70
2	B	24	C	N3-C2-O2	-7.13	116.91	121.90
1	A	2361	U	N3-C2-O2	-7.12	117.21	122.20
1	A	924	G	C4-C5-N7	7.11	113.64	110.80
1	A	1857	C	N1-C2-O2	7.10	123.16	118.90
1	A	1461	C	C6-N1-C2	-7.09	117.46	120.30
1	A	636	A	C4-C5-N7	7.08	114.24	110.70
1	A	1336	G	N3-C4-C5	7.08	132.14	128.60
1	A	2850	G	N3-C4-C5	7.06	132.13	128.60
1	A	1607	A	C4-C5-N7	7.05	114.23	110.70
1	A	2436	G	N3-C4-C5	7.05	132.12	128.60
1	A	2248	G	N3-C4-N9	-7.04	121.77	126.00
1	A	336	U	C5-C6-N1	7.04	126.22	122.70
1	A	1081	G	N3-C2-N2	-7.03	114.98	119.90
1	A	636	A	C5-N7-C8	-7.03	100.38	103.90
1	A	1466	G	C2-N3-C4	-7.03	108.39	111.90
1	A	1370	C	N1-C2-O2	7.01	123.11	118.90
1	A	2150	A	N7-C8-N9	7.00	117.30	113.80
1	A	2884	G	C4-C5-N7	7.00	113.60	110.80
1	A	319	G	C4-C5-N7	7.00	113.60	110.80
1	A	1632	A	N1-C6-N6	6.99	122.79	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1623	U	C5-C6-N1	6.98	126.19	122.70
1	A	1087	C	C6-N1-C1'	6.97	129.16	120.80
1	A	2021	C	N3-C4-N4	6.97	122.88	118.00
1	A	721	A	C5-C6-N6	-6.97	118.13	123.70
1	A	1537	A	N9-C4-C5	6.97	108.59	105.80
1	A	2210	C	N1-C2-O2	6.96	123.08	118.90
1	A	2877	G	N3-C4-C5	6.96	132.08	128.60
1	A	2733	A	N9-C4-C5	-6.95	103.02	105.80
1	A	461	A	C4-C5-N7	6.95	114.17	110.70
1	A	2397	G	N3-C4-N9	-6.95	121.83	126.00
1	A	1537	A	N1-C6-N6	-6.94	114.43	118.60
1	A	2651	G	N3-C4-C5	6.93	132.06	128.60
1	A	1598	U	C5-C6-N1	6.91	126.16	122.70
2	B	21	G	N3-C4-N9	-6.91	121.85	126.00
1	A	1501	G	N3-C2-N2	-6.91	115.06	119.90
1	A	2850	G	N3-C4-N9	-6.91	121.86	126.00
1	A	924	G	C8-N9-C1'	-6.91	118.02	127.00
1	A	1480	G	C8-N9-C4	-6.90	103.64	106.40
1	A	1462	G	N7-C8-N9	6.90	116.55	113.10
1	A	1979	A	N1-C6-N6	6.90	122.74	118.60
1	A	2436	G	C2-N3-C4	-6.90	108.45	111.90
1	A	2419	A	N1-C6-N6	6.89	122.74	118.60
1	A	789	C	N3-C4-C5	6.88	124.65	121.90
1	A	2248	G	N3-C4-C5	6.87	132.04	128.60
1	A	2480	A	C5-C6-N6	-6.87	118.21	123.70
1	A	396	G	C8-N9-C1'	-6.86	118.08	127.00
1	A	717	C	N1-C2-O2	6.86	123.02	118.90
1	A	1004	A	N1-C6-N6	6.86	122.72	118.60
1	A	851	C	N3-C2-O2	-6.86	117.10	121.90
1	A	922	G	N3-C2-N2	-6.86	115.10	119.90
1	A	555	C	N1-C2-O2	6.85	123.01	118.90
1	A	640	G	C2-N3-C4	-6.84	108.48	111.90
1	A	2644	C	C5-C4-N4	-6.84	115.41	120.20
1	A	1393	C	N1-C2-O2	6.84	123.00	118.90
1	A	1021	G	N3-C4-C5	6.83	132.02	128.60
1	A	2677	C	N1-C2-O2	6.83	123.00	118.90
1	A	1979	A	C5-C6-N6	-6.83	118.24	123.70
1	A	19	G	N1-C2-N2	-6.82	110.06	116.20
1	A	757	G	C5-N7-C8	-6.81	100.90	104.30
1	A	1607	A	C8-N9-C4	6.79	108.52	105.80
1	A	1422	A	C6-N1-C2	-6.78	114.53	118.60
1	A	1440	A	C8-N9-C4	6.78	108.51	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1501	G	N3-C4-C5	6.77	131.99	128.60
1	A	2102	U	N3-C4-O4	6.76	124.13	119.40
1	A	2525	C	N1-C2-O2	6.75	122.95	118.90
1	A	608	C	N3-C4-C5	6.75	124.60	121.90
1	A	2099	G	N1-C2-N2	-6.74	110.14	116.20
2	B	76	A	C4-C5-N7	6.74	114.07	110.70
1	A	721	A	C6-C5-N7	-6.73	127.59	132.30
1	A	2259	C	N1-C2-O2	6.73	122.94	118.90
1	A	1538	A	C5-C6-N6	6.73	129.08	123.70
1	A	721	A	N7-C8-N9	6.72	117.16	113.80
1	A	1539	A	N1-C6-N6	-6.72	114.57	118.60
1	A	1268	C	N1-C2-O2	6.72	122.93	118.90
1	A	1837	A	N1-C6-N6	6.71	122.63	118.60
1	A	280	C	C6-N1-C2	-6.71	117.61	120.30
1	A	1438	G	N3-C4-N9	-6.71	121.97	126.00
1	A	2877	G	N3-C4-N9	-6.71	121.98	126.00
1	A	133	A	C5-N7-C8	-6.70	100.55	103.90
1	A	133	A	N9-C4-C5	-6.69	103.12	105.80
1	A	983	G	C2-N3-C4	-6.69	108.56	111.90
1	A	1435	C	C5-C4-N4	-6.68	115.52	120.20
1	A	1506	C	N3-C2-O2	-6.68	117.23	121.90
1	A	2563	G	N3-C4-N9	-6.68	121.99	126.00
1	A	2715	G	C2-N3-C4	-6.67	108.56	111.90
1	A	655	A	N9-C4-C5	-6.66	103.14	105.80
1	A	863	G	C2-N3-C4	-6.66	108.57	111.90
1	A	1500	G	N7-C8-N9	6.66	116.43	113.10
1	A	2021	C	C5-C4-N4	-6.66	115.54	120.20
1	A	2711	U	C5-C4-O4	-6.65	121.91	125.90
1	A	1742	A	C5-C6-N6	-6.64	118.39	123.70
1	A	1742	A	N1-C6-N6	6.64	122.58	118.60
2	B	64	A	C5-C6-N6	-6.63	118.39	123.70
1	A	426	G	C4-C5-N7	6.63	113.45	110.80
1	A	1954	A	N7-C8-N9	6.63	117.11	113.80
1	A	2396	A	C4-C5-N7	6.63	114.01	110.70
1	A	2069	A	N1-C6-N6	6.62	122.57	118.60
1	A	1468	G	C6-C5-N7	-6.62	126.43	130.40
1	A	1438	G	N3-C4-C5	6.61	131.91	128.60
1	A	2326	G	C5-N7-C8	-6.61	100.99	104.30
1	A	623	C	N3-C2-O2	-6.61	117.27	121.90
2	B	64	A	N1-C6-N6	6.61	122.57	118.60
1	A	95	A	C5-C6-N6	-6.60	118.42	123.70
1	A	652	A	N1-C6-N6	6.60	122.56	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2750	C	N1-C2-O2	6.60	122.86	118.90
1	A	1196	C	N1-C2-O2	6.60	122.86	118.90
1	A	2013	G	C8-N9-C4	6.59	109.04	106.40
1	A	2843	A	N1-C6-N6	6.58	122.55	118.60
1	A	1892	U	C2-N1-C1'	6.57	125.58	117.70
1	A	902	A	N1-C6-N6	6.57	122.54	118.60
1	A	522	G	N3-C4-C5	6.56	131.88	128.60
1	A	396	G	N7-C8-N9	6.56	116.38	113.10
1	A	2873	C	N1-C2-O2	6.56	122.84	118.90
1	A	2786	G	C5-C6-O6	-6.55	124.67	128.60
1	A	2247	G	N3-C4-C5	6.54	131.87	128.60
1	A	2298	G	C2-N3-C4	-6.54	108.63	111.90
1	A	735	C	N1-C2-O2	6.53	122.82	118.90
1	A	184	C	C2-N1-C1'	6.53	125.98	118.80
1	A	330	C	N1-C2-O2	6.52	122.81	118.90
1	A	1494	G	N3-C4-C5	6.52	131.86	128.60
1	A	1538	A	N9-C4-C5	6.51	108.41	105.80
1	A	778	G	C2-N3-C4	-6.51	108.64	111.90
1	A	725	A	C5-C6-N6	-6.51	118.49	123.70
1	A	1758	A	N1-C6-N6	6.51	122.51	118.60
1	A	1994	C	C2-N1-C1'	6.51	125.96	118.80
1	A	1701	U	C5-C6-N1	6.50	125.95	122.70
1	A	1634	A	C4-C5-N7	6.50	113.95	110.70
1	A	160	G	N3-C4-C5	-6.50	125.35	128.60
1	A	924	G	N9-C4-C5	-6.50	102.80	105.40
1	A	575	G	O4'-C1'-N9	6.50	113.40	108.20
1	A	2865	G	C2-N3-C4	-6.50	108.65	111.90
1	A	1654	A	C5-C6-N6	-6.49	118.51	123.70
1	A	1906	C	C2-N1-C1'	6.49	125.94	118.80
1	A	46	C	C6-N1-C2	-6.48	117.71	120.30
1	A	576	U	C2-N1-C1'	6.48	125.47	117.70
1	A	1414	G	C2-N3-C4	-6.47	108.67	111.90
1	A	63	U	N3-C2-O2	-6.46	117.68	122.20
1	A	192	G	N3-C4-C5	6.45	131.83	128.60
1	A	988	C	N3-C2-O2	-6.45	117.38	121.90
1	A	1920	C	C6-N1-C2	-6.45	117.72	120.30
1	A	756	A	N3-C4-N9	6.45	132.56	127.40
1	A	2774	G	N3-C2-N2	6.45	124.41	119.90
1	A	862	C	N3-C2-O2	-6.44	117.39	121.90
1	A	1413	C	N1-C2-O2	6.44	122.76	118.90
1	A	2302	C	C6-N1-C2	-6.43	117.73	120.30
1	A	2480	A	N1-C6-N6	6.43	122.46	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	G	N3-C4-N9	-6.42	122.15	126.00
1	A	2480	A	C6-C5-N7	-6.42	127.81	132.30
1	A	95	A	C6-C5-N7	-6.41	127.81	132.30
1	A	1499	U	C5-C6-N1	6.41	125.90	122.70
1	A	2708	C	C5-C4-N4	-6.40	115.72	120.20
1	A	814	A	C5-C6-N6	-6.39	118.59	123.70
1	A	2361	U	N1-C2-O2	6.39	127.27	122.80
1	A	1692	C	C2-N1-C1'	6.38	125.82	118.80
1	A	2326	G	N9-C4-C5	-6.37	102.85	105.40
1	A	2480	A	C4-C5-N7	6.37	113.89	110.70
1	A	53	A	N1-C6-N6	6.37	122.42	118.60
1	A	2819	C	N3-C2-O2	-6.37	117.44	121.90
1	A	2839	A	N9-C4-C5	-6.37	103.25	105.80
1	A	2013	G	N1-C2-N2	-6.37	110.47	116.20
1	A	402	C	C6-N1-C2	-6.36	117.75	120.30
1	A	758	G	C4-N9-C1'	6.36	134.77	126.50
1	A	840	C	N1-C2-O2	6.35	122.71	118.90
1	A	2711	U	N3-C4-O4	6.35	123.85	119.40
2	B	114	G	C4-N9-C1'	6.35	134.76	126.50
1	A	1207	G	N3-C4-C5	6.35	131.78	128.60
1	A	2247	G	N3-C4-N9	-6.34	122.19	126.00
1	A	546	A	N1-C6-N6	6.34	122.40	118.60
1	A	740	G	C2-N3-C4	-6.33	108.73	111.90
1	A	1380	G	C4-N9-C1'	6.33	134.73	126.50
1	A	1179	C	N1-C2-O2	6.32	122.69	118.90
1	A	2361	U	C5-C4-O4	6.32	129.69	125.90
1	A	2131	C	C6-N1-C2	-6.32	117.77	120.30
1	A	283	G	C4-C5-N7	6.32	113.33	110.80
2	B	114	G	C6-C5-N7	-6.31	126.62	130.40
1	A	679	G	C6-C5-N7	-6.30	126.62	130.40
1	A	997	G	N1-C2-N2	-6.30	110.53	116.20
1	A	1384	G	N3-C4-C5	6.29	131.74	128.60
1	A	249	C	C5-C4-N4	-6.28	115.80	120.20
1	A	317	G	N3-C4-C5	6.28	131.74	128.60
1	A	685	C	N1-C2-O2	6.28	122.67	118.90
1	A	545	G	C2-N3-C4	-6.28	108.76	111.90
1	A	2324	C	N1-C2-O2	6.28	122.67	118.90
1	A	2677	C	C5-C6-N1	6.28	124.14	121.00
1	A	1200	A	N1-C6-N6	-6.28	114.83	118.60
1	A	897	A	C5-N7-C8	-6.27	100.77	103.90
1	A	1075	G	N9-C4-C5	6.27	107.91	105.40
1	A	15	G	C2-N3-C4	-6.26	108.77	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1380	G	C8-N9-C1'	-6.26	118.87	127.00
1	A	1468	G	C5-N7-C8	-6.25	101.17	104.30
1	A	2523	C	N1-C2-O2	6.25	122.65	118.90
1	A	2071	C	C5-C4-N4	-6.25	115.83	120.20
1	A	1924	G	N3-C4-N9	-6.25	122.25	126.00
1	A	891	A	O5'-P-OP1	-6.24	100.08	105.70
1	A	2348	G	C4-C5-N7	6.24	113.30	110.80
1	A	1367	C	N1-C2-O2	6.23	122.64	118.90
1	A	883	C	N1-C2-O2	6.23	122.64	118.90
1	A	2848	G	N3-C4-C5	6.23	131.72	128.60
1	A	1440	A	N9-C4-C5	-6.23	103.31	105.80
1	A	2782	C	P-O3'-C3'	6.23	127.17	119.70
1	A	2379	A	N1-C6-N6	6.22	122.33	118.60
1	A	2563	G	N3-C4-C5	6.22	131.71	128.60
1	A	1470	G	C2-N3-C4	-6.21	108.79	111.90
1	A	2210	C	N3-C2-O2	-6.21	117.55	121.90
1	A	924	G	N3-C4-N9	6.21	129.72	126.00
1	A	1072	A	N9-C4-C5	-6.20	103.32	105.80
1	A	1906	C	C6-N1-C2	-6.20	117.82	120.30
1	A	1410	A	C5-C6-N6	-6.20	118.74	123.70
1	A	737	C	C5-C4-N4	-6.20	115.86	120.20
1	A	756	A	C4-N9-C1'	6.20	137.45	126.30
1	A	851	C	N3-C4-C5	6.19	124.38	121.90
1	A	1284	A	C5-C6-N6	-6.19	118.75	123.70
1	A	1834	G	N3-C4-C5	6.19	131.69	128.60
1	A	1799	G	N3-C4-N9	-6.18	122.29	126.00
1	A	863	G	N3-C4-C5	6.18	131.69	128.60
1	A	1406	G	N3-C4-N9	-6.18	122.29	126.00
1	A	724	C	C6-N1-C2	-6.17	117.83	120.30
1	A	862	C	N1-C2-O2	6.17	122.60	118.90
1	A	1655	C	C6-N1-C2	-6.17	117.83	120.30
1	A	1283	G	N3-C4-N9	-6.17	122.30	126.00
1	A	882	C	C6-N1-C1'	-6.16	113.41	120.80
1	A	503	A	C5-N7-C8	-6.15	100.83	103.90
1	A	1421	A	N1-C6-N6	6.15	122.29	118.60
1	A	756	A	N1-C6-N6	6.15	122.29	118.60
1	A	602	G	C2-N3-C4	-6.14	108.83	111.90
1	A	575	G	C4-N9-C1'	6.14	134.49	126.50
1	A	627	C	C5-C4-N4	-6.14	115.90	120.20
1	A	838	A	N1-C6-N6	-6.14	114.92	118.60
1	A	2457	A	C5-C6-N1	6.14	120.77	117.70
1	A	1406	G	N3-C4-C5	6.14	131.67	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	A	C4-C5-N7	6.12	113.76	110.70
1	A	2845	G	C2-N3-C4	-6.12	108.84	111.90
1	A	1283	G	N3-C4-C5	6.12	131.66	128.60
1	A	1465	G	N7-C8-N9	6.12	116.16	113.10
1	A	2677	C	C2-N3-C4	6.12	122.96	119.90
1	A	2413	U	C5-C6-N1	6.11	125.75	122.70
1	A	1975	G	N3-C4-C5	6.10	131.65	128.60
1	A	922	G	N3-C4-N9	-6.10	122.34	126.00
1	A	1396	A	N1-C6-N6	-6.10	114.94	118.60
1	A	2326	G	C4-N9-C1'	6.09	134.42	126.50
1	A	723	C	C5-C4-N4	-6.09	115.94	120.20
1	A	755	C	C2-N1-C1'	6.09	125.50	118.80
1	A	1004	A	C5-C6-N6	-6.09	118.83	123.70
1	A	2000	G	N3-C4-C5	6.08	131.64	128.60
1	A	546	A	C5-C6-N6	-6.07	118.85	123.70
1	A	1393	C	N3-C2-O2	-6.07	117.65	121.90
1	A	2431	C	C5-C4-N4	-6.07	115.95	120.20
1	A	2819	C	N1-C2-O2	6.06	122.53	118.90
1	A	336	U	C5-C4-O4	-6.05	122.27	125.90
1	A	1453	G	N3-C2-N2	6.05	124.14	119.90
1	A	395	U	C6-N1-C1'	6.05	129.67	121.20
1	A	253	G	C2-N3-C4	-6.05	108.88	111.90
1	A	1837	A	C5-C6-N6	-6.05	118.86	123.70
1	A	1268	C	N3-C2-O2	-6.04	117.67	121.90
1	A	378	C	C5-C4-N4	-6.04	115.97	120.20
1	A	897	A	N3-C4-N9	6.04	132.23	127.40
1	A	1467	G	C4-N9-C1'	6.04	134.36	126.50
1	A	2396	A	N9-C4-C5	-6.04	103.38	105.80
1	A	207	A	C5-C6-N6	-6.04	118.87	123.70
1	A	429	C	C6-N1-C2	6.04	122.72	120.30
1	A	1701	U	N3-C4-O4	6.03	123.62	119.40
1	A	2525	C	N3-C2-O2	-6.03	117.68	121.90
1	A	2750	C	N3-C2-O2	-6.03	117.68	121.90
1	A	95	A	C4-C5-N7	6.02	113.71	110.70
1	A	2013	G	N3-C2-N2	6.02	124.12	119.90
1	A	1447	A	N9-C4-C5	-6.02	103.39	105.80
1	A	2698	A	C2-N3-C4	-6.02	107.59	110.60
1	A	1850	G	C2-N3-C4	-6.02	108.89	111.90
1	A	383	A	N1-C6-N6	6.02	122.21	118.60
1	A	1472	C	C6-N1-C2	-6.02	117.89	120.30
2	B	65	G	N3-C2-N2	6.02	124.11	119.90
1	A	429	C	N3-C4-C5	6.01	124.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1759	G	C8-N9-C1'	-6.00	119.20	127.00
1	A	2064	A	C5-C6-N6	-6.00	118.90	123.70
1	A	2636	U	C2-N1-C1'	6.00	124.90	117.70
1	A	2348	G	N9-C4-C5	-5.99	103.00	105.40
1	A	2587	C	C2-N1-C1'	5.99	125.39	118.80
1	A	180	G	C4-C5-N7	5.99	113.20	110.80
1	A	1501	G	C8-N9-C1'	5.99	134.79	127.00
1	A	503	A	C4-C5-N7	5.99	113.69	110.70
1	A	972	A	C4-C5-N7	5.98	113.69	110.70
1	A	1445	C	N1-C2-O2	5.98	122.49	118.90
1	A	468	A	N1-C6-N6	-5.98	115.01	118.60
1	A	679	G	N9-C4-C5	-5.98	103.01	105.40
1	A	1842	A	N1-C6-N6	5.97	122.19	118.60
1	A	2829	A	C5-C6-N6	-5.97	118.92	123.70
2	B	108	U	C2-N1-C1'	5.97	124.87	117.70
1	A	576	U	N1-C2-O2	5.97	126.98	122.80
1	A	1038	C	N1-C2-O2	5.97	122.48	118.90
1	A	1033	G	N1-C2-N2	-5.96	110.83	116.20
1	A	616	G	N3-C4-N9	-5.96	122.42	126.00
1	A	902	A	C5-C6-N6	-5.96	118.93	123.70
1	A	1759	G	C5-N7-C8	-5.96	101.32	104.30
1	A	2056	G	N3-C4-C5	5.96	131.58	128.60
1	A	107	G	N3-C4-C5	5.96	131.58	128.60
1	A	130	A	N9-C4-C5	-5.95	103.42	105.80
1	A	2379	A	C5-C6-N6	-5.95	118.94	123.70
2	B	18	G	N3-C4-C5	5.95	131.58	128.60
21	U	22	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	A	882	C	C2-N1-C1'	5.95	125.34	118.80
1	A	618	A	C5-C6-N6	-5.95	118.94	123.70
1	A	1269	A	C4-C5-N7	5.94	113.67	110.70
1	A	1081	G	N3-C4-C5	5.94	131.57	128.60
1	A	503	A	N1-C6-N6	5.94	122.16	118.60
1	A	283	G	C6-C5-N7	-5.94	126.84	130.40
1	A	1726	A	N9-C4-C5	-5.93	103.43	105.80
1	A	450	C	N3-C4-C5	5.93	124.27	121.90
1	A	737	C	N3-C4-N4	5.93	122.15	118.00
1	A	1033	G	N7-C8-N9	5.93	116.07	113.10
1	A	1404	A	N1-C6-N6	5.93	122.16	118.60
1	A	115	C	N3-C4-C5	5.93	124.27	121.90
1	A	1740	G	N3-C4-C5	5.93	131.56	128.60
1	A	2636	U	N1-C2-O2	5.93	126.95	122.80
1	A	479	C	N3-C4-N4	-5.92	113.85	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1024	A	C4-C5-N7	5.92	113.66	110.70
1	A	1799	G	N3-C4-C5	5.92	131.56	128.60
2	B	76	A	C5-N7-C8	-5.92	100.94	103.90
1	A	575	G	C6-C5-N7	-5.92	126.85	130.40
1	A	522	G	C8-N9-C4	5.92	108.77	106.40
1	A	770	G	N7-C8-N9	5.92	116.06	113.10
1	A	624	C	N1-C2-O2	5.91	122.45	118.90
1	A	1932	C	C2-N1-C1'	5.91	125.31	118.80
1	A	461	A	C6-C5-N7	-5.91	128.16	132.30
1	A	860	U	C5-C4-O4	-5.91	122.36	125.90
1	A	2509	A	N7-C8-N9	5.90	116.75	113.80
1	A	187	C	N3-C2-O2	-5.90	117.77	121.90
1	A	1385	G	N3-C4-C5	5.90	131.55	128.60
1	A	470	G	N3-C4-C5	5.90	131.55	128.60
1	A	2436	G	C4-C5-N7	5.90	113.16	110.80
1	A	1503	U	P-O3'-C3'	5.89	126.77	119.70
1	A	1637	A	N9-C4-C5	-5.89	103.44	105.80
1	A	1202	C	N1-C2-O2	5.89	122.44	118.90
1	A	1317	G	N3-C4-C5	5.89	131.55	128.60
1	A	1361	G	N3-C2-N2	5.89	124.03	119.90
1	A	515	G	N1-C2-N2	-5.89	110.90	116.20
1	A	2036	G	N3-C4-C5	5.89	131.54	128.60
1	A	1088	C	C6-N1-C2	-5.88	117.95	120.30
1	A	1168	C	N3-C2-O2	-5.88	117.78	121.90
1	A	762	C	C6-N1-C1'	5.88	127.86	120.80
1	A	1463	A	C4-C5-N7	5.88	113.64	110.70
1	A	1227	U	C2-N1-C1'	5.88	124.76	117.70
1	A	1541	C	C6-N1-C2	-5.88	117.95	120.30
1	A	1384	G	N3-C4-N9	-5.87	122.48	126.00
1	A	2099	G	N3-C2-N2	5.87	124.01	119.90
1	A	65	A	N9-C4-C5	-5.87	103.45	105.80
1	A	409	G	N3-C2-N2	5.87	124.01	119.90
1	A	1017	A	C5-C6-N6	-5.86	119.01	123.70
1	A	2457	A	C4-C5-N7	5.86	113.63	110.70
1	A	2047	A	C4-C5-N7	5.86	113.63	110.70
1	A	2845	G	N3-C4-N9	-5.86	122.49	126.00
1	A	461	A	C5-N7-C8	-5.85	100.97	103.90
1	A	608	C	C2-N3-C4	-5.85	116.97	119.90
1	A	1537	A	C8-N9-C4	-5.85	103.46	105.80
1	A	2480	A	C5-N7-C8	-5.85	100.98	103.90
1	A	2747	U	N3-C2-O2	-5.85	118.11	122.20
1	A	1391	A	C5-N7-C8	-5.85	100.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	603	C	N3-C4-C5	5.84	124.24	121.90
1	A	1920	C	N1-C2-O2	5.84	122.41	118.90
1	A	755	C	C6-N1-C2	-5.84	117.96	120.30
1	A	825	G	C2-N3-C4	-5.84	108.98	111.90
1	A	2548	C	N1-C2-O2	5.84	122.40	118.90
1	A	961	G	C4-C5-N7	5.83	113.13	110.80
1	A	945	A	N3-C4-N9	-5.83	122.74	127.40
1	A	2734	C	C2-N1-C1'	5.83	125.21	118.80
1	A	1754	C	N1-C2-O2	5.83	122.39	118.90
1	A	1948	G	C4-C5-N7	5.83	113.13	110.80
1	A	302	A	O4'-C1'-N9	5.82	112.86	108.20
1	A	839	A	C5-C6-N1	5.82	120.61	117.70
1	A	2698	A	N1-C2-N3	5.82	132.21	129.30
1	A	2703	C	N1-C2-O2	5.81	122.39	118.90
1	A	1791	G	N1-C2-N2	-5.80	110.98	116.20
1	A	2419	A	C5-C6-N6	-5.80	119.06	123.70
1	A	756	A	N7-C8-N9	5.80	116.70	113.80
1	A	2356	A	C5-C6-N6	-5.80	119.06	123.70
1	A	1081	G	N9-C4-C5	5.79	107.72	105.40
1	A	265	A	N9-C4-C5	-5.79	103.49	105.80
1	A	2361	U	C6-N1-C1'	-5.79	113.10	121.20
1	A	1046	G	N3-C4-C5	5.78	131.49	128.60
1	A	2457	A	N9-C4-C5	-5.78	103.49	105.80
1	A	616	G	C2-N3-C4	-5.78	109.01	111.90
1	A	1033	G	C8-N9-C4	-5.78	104.09	106.40
1	A	1491	C	C6-N1-C1'	5.78	127.73	120.80
1	A	752	G	N9-C4-C5	-5.77	103.09	105.40
1	A	2419	A	C5-N7-C8	-5.77	101.01	103.90
1	A	2497	G	N9-C4-C5	-5.77	103.09	105.40
1	A	208	G	O4'-C1'-N9	5.77	112.81	108.20
1	A	2499	G	N3-C4-N9	-5.77	122.54	126.00
1	A	2218	G	C4-C5-N7	5.76	113.10	110.80
1	A	575	G	C8-N9-C1'	-5.76	119.52	127.00
1	A	2679	U	C5-C6-N1	5.76	125.58	122.70
1	A	2310	C	N3-C4-C5	5.75	124.20	121.90
1	A	1004	A	N9-C4-C5	-5.75	103.50	105.80
1	A	1447	A	C4-C5-N7	5.75	113.58	110.70
1	A	1830	A	N1-C6-N6	5.75	122.05	118.60
1	A	1228	A	C5-N7-C8	-5.75	101.03	103.90
1	A	679	G	C4-C5-N7	5.74	113.10	110.80
1	A	1336	G	N3-C4-N9	-5.74	122.56	126.00
1	A	1413	C	N3-C2-O2	-5.74	117.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2086	A	O4'-C1'-N9	5.74	112.79	108.20
2	B	76	A	N9-C4-C5	-5.74	103.50	105.80
1	A	2036	G	C2-N3-C4	-5.74	109.03	111.90
1	A	527	G	O4'-C1'-N9	5.74	112.79	108.20
1	A	1075	G	C5-C6-O6	5.74	132.04	128.60
1	A	757	G	C5-C6-O6	-5.73	125.16	128.60
1	A	1468	G	N9-C4-C5	-5.73	103.11	105.40
1	A	1030	C	C5-C4-N4	-5.73	116.19	120.20
1	A	1219	G	N1-C2-N2	5.73	121.35	116.20
1	A	193	A	C4-C5-N7	5.72	113.56	110.70
1	A	1370	C	N3-C2-O2	-5.72	117.89	121.90
1	A	1622	C	C5-C4-N4	-5.72	116.19	120.20
1	A	2004	A	N9-C4-C5	-5.72	103.51	105.80
1	A	2570	G	C2-N3-C4	-5.72	109.04	111.90
1	A	2696	G	N3-C4-C5	5.72	131.46	128.60
1	A	2816	C	O4'-C1'-N1	5.72	112.77	108.20
1	A	2830	A	N1-C6-N6	5.72	122.03	118.60
1	A	971	U	C5-C4-O4	-5.72	122.47	125.90
1	A	1087	C	N1-C2-N3	5.71	123.20	119.20
1	A	1051	C	C5-C4-N4	-5.71	116.20	120.20
1	A	212	C	N1-C2-O2	5.71	122.33	118.90
1	A	997	G	C2-N3-C4	-5.71	109.05	111.90
1	A	2587	C	N1-C2-O2	5.71	122.32	118.90
1	A	814	A	C5-N7-C8	-5.71	101.05	103.90
1	A	440	C	N1-C2-O2	5.70	122.32	118.90
1	A	1284	A	N1-C6-N6	5.70	122.02	118.60
1	A	1179	C	C2-N1-C1'	5.70	125.07	118.80
1	A	330	C	N3-C2-O2	-5.70	117.91	121.90
1	A	107	G	C2-N3-C4	-5.69	109.05	111.90
1	A	1286	G	N1-C2-N2	-5.69	111.08	116.20
1	A	184	C	O4'-C1'-N1	5.69	112.75	108.20
1	A	1033	G	C6-C5-N7	-5.69	126.98	130.40
1	A	2061	U	C5-C4-O4	-5.69	122.49	125.90
1	A	1232	G	N1-C2-N2	-5.68	111.08	116.20
1	A	1494	G	C2-N3-C4	-5.68	109.06	111.90
1	A	16	G	N3-C4-C5	5.68	131.44	128.60
1	A	109	G	N3-C4-C5	5.68	131.44	128.60
1	A	182	C	N1-C2-O2	5.68	122.31	118.90
1	A	343	A	N1-C6-N6	5.68	122.01	118.60
1	A	2675	G	C2-N3-C4	-5.68	109.06	111.90
1	A	554	C	N1-C2-O2	5.67	122.31	118.90
1	A	1837	A	C5-N7-C8	-5.67	101.06	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	752	G	C6-C5-N7	-5.67	127.00	130.40
1	A	762	C	C2-N1-C1'	-5.67	112.56	118.80
1	A	630	G	C2-N3-C4	-5.67	109.07	111.90
1	A	2770	U	O4'-C1'-N1	5.67	112.74	108.20
1	A	1232	G	N3-C2-N2	5.67	123.87	119.90
1	A	1634	A	C8-N9-C4	5.67	108.07	105.80
1	A	1283	G	C2-N3-C4	-5.66	109.07	111.90
1	A	1196	C	C5-C4-N4	-5.66	116.24	120.20
1	A	1819	G	C2-N3-C4	-5.66	109.07	111.90
26	Z	6	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	A	2695	G	N3-C4-C5	5.66	131.43	128.60
1	A	2386	C	N1-C2-O2	5.66	122.29	118.90
1	A	962	A	N1-C6-N6	5.65	121.99	118.60
1	A	630	G	O4'-C1'-N9	5.65	112.72	108.20
1	A	816	G	N3-C4-C5	5.65	131.42	128.60
1	A	2290	C	C6-N1-C2	-5.65	118.04	120.30
1	A	70	G	N3-C4-C5	5.65	131.42	128.60
2	B	59	U	C5-C6-N1	5.65	125.52	122.70
1	A	256	C	C5-C4-N4	-5.64	116.25	120.20
1	A	280	C	C5-C6-N1	5.64	123.82	121.00
1	A	1614	A	N9-C4-C5	-5.64	103.54	105.80
1	A	109	G	N3-C4-N9	-5.64	122.62	126.00
1	A	2677	C	N3-C4-N4	5.63	121.94	118.00
1	A	82	G	N3-C4-N9	-5.63	122.62	126.00
1	A	766	G	C4-C5-N7	5.63	113.05	110.80
1	A	1024	A	N9-C4-C5	-5.63	103.55	105.80
1	A	758	G	N7-C8-N9	5.62	115.91	113.10
1	A	574	A	C4-C5-N7	5.62	113.51	110.70
1	A	1748	G	N3-C4-C5	5.62	131.41	128.60
2	B	114	G	C5-N7-C8	-5.62	101.49	104.30
1	A	2073	G	N3-C2-N2	-5.62	115.97	119.90
1	A	1719	C	N3-C4-N4	5.62	121.93	118.00
2	B	86	A	N3-C4-N9	-5.62	122.91	127.40
1	A	1842	A	C5-C6-N6	-5.62	119.21	123.70
1	A	2869	G	N3-C4-C5	5.62	131.41	128.60
1	A	924	G	N7-C8-N9	5.61	115.91	113.10
1	A	2281	C	N3-C4-C5	5.61	124.14	121.90
1	A	2596	G	N3-C4-C5	5.61	131.41	128.60
1	A	1793	C	N3-C4-C5	5.61	124.14	121.90
1	A	2370	U	C6-N1-C1'	5.60	129.04	121.20
1	A	955	A	N1-C6-N6	-5.60	115.24	118.60
1	A	2111	C	N1-C2-O2	5.60	122.26	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1418	G	N3-C4-C5	5.60	131.40	128.60
1	A	319	G	C5-C6-O6	-5.59	125.24	128.60
1	A	640	G	N3-C4-C5	5.59	131.40	128.60
1	A	845	A	C5-C6-N6	-5.59	119.22	123.70
1	A	567	G	C4-C5-N7	5.59	113.04	110.80
1	A	2278	G	C4-N9-C1'	5.59	133.77	126.50
1	A	1467	G	N3-C4-N9	5.59	129.35	126.00
1	A	1758	A	N9-C4-C5	-5.59	103.56	105.80
1	A	2464	C	N1-C2-O2	5.59	122.25	118.90
1	A	282	A	N7-C8-N9	5.59	116.59	113.80
1	A	2604	A	N1-C6-N6	5.59	121.95	118.60
1	A	351	G	N3-C4-C5	5.58	131.39	128.60
1	A	757	G	N1-C6-O6	5.58	123.25	119.90
1	A	2155	C	C6-N1-C2	-5.58	118.07	120.30
1	A	752	G	C5-N7-C8	-5.58	101.51	104.30
1	A	1467	G	C5-C6-O6	-5.58	125.25	128.60
1	A	1890	G	N1-C2-N2	-5.58	111.18	116.20
1	A	192	G	C2-N3-C4	-5.58	109.11	111.90
1	A	1466	G	N1-C2-N3	5.58	127.25	123.90
1	A	2223	C	C5-C4-N4	5.58	124.11	120.20
1	A	1842	A	N9-C4-C5	-5.58	103.57	105.80
1	A	2817	A	N7-C8-N9	5.58	116.59	113.80
1	A	660	A	N1-C6-N6	-5.57	115.26	118.60
1	A	775	A	N9-C4-C5	-5.57	103.57	105.80
1	A	1021	G	C4-C5-N7	5.57	113.03	110.80
1	A	1385	G	N3-C4-N9	-5.57	122.66	126.00
1	A	1231	A	C4-C5-N7	5.57	113.48	110.70
1	A	1017	A	N1-C6-N6	5.57	121.94	118.60
1	A	47	C	N1-C2-N3	5.56	123.09	119.20
1	A	426	G	N3-C2-N2	5.56	123.79	119.90
1	A	2747	U	C6-N1-C2	-5.56	117.67	121.00
1	A	280	C	C2-N1-C1'	5.56	124.91	118.80
1	A	1396	A	C5-C6-N6	5.55	128.14	123.70
2	B	28	C	C6-N1-C2	-5.55	118.08	120.30
1	A	1245	G	N3-C4-C5	5.55	131.38	128.60
1	A	2326	G	N1-C6-O6	5.55	123.23	119.90
1	A	2014	G	N3-C4-C5	5.55	131.37	128.60
1	A	515	G	C4-C5-N7	5.55	113.02	110.80
1	A	661	U	C5-C4-O4	-5.55	122.57	125.90
1	A	1391	A	C4-C5-N7	5.54	113.47	110.70
1	A	1804	U	N1-C2-O2	5.54	126.68	122.80
1	A	1506	C	N1-C2-N3	5.54	123.08	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1842	A	C4-C5-N7	5.54	113.47	110.70
1	A	1087	C	O4'-C1'-N1	5.54	112.63	108.20
1	A	717	C	C5-C4-N4	-5.53	116.33	120.20
1	A	1462	G	C4-N9-C1'	5.53	133.69	126.50
1	A	819	A	C4-C5-N7	5.52	113.46	110.70
1	A	1816	A	C5-N7-C8	-5.52	101.14	103.90
1	A	393	G	O4'-C1'-C2'	-5.52	100.28	105.80
1	A	2762	G	N3-C4-N9	-5.52	122.69	126.00
1	A	428	G	N3-C2-N2	5.52	123.76	119.90
1	A	624	C	C2-N1-C1'	5.52	124.87	118.80
1	A	1815	C	N3-C4-C5	5.52	124.11	121.90
1	A	2013	G	C2-N3-C4	-5.52	109.14	111.90
1	A	2398	G	N3-C4-C5	5.52	131.36	128.60
1	A	2047	A	N1-C6-N6	5.51	121.91	118.60
1	A	822	G	N3-C4-N9	-5.51	122.69	126.00
12	L	8	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	1465	G	C6-C5-N7	-5.51	127.09	130.40
1	A	1615	G	N3-C4-N9	-5.51	122.69	126.00
1	A	809	A	O4'-C1'-N9	5.51	112.61	108.20
1	A	2356	A	C5-N7-C8	-5.51	101.14	103.90
2	B	41	C	C6-N1-C2	5.51	122.50	120.30
1	A	95	A	N9-C4-C5	-5.51	103.60	105.80
1	A	845	A	N1-C6-N6	5.51	121.90	118.60
1	A	1700	C	N1-C2-O2	5.51	122.20	118.90
1	A	2061	U	N3-C4-O4	5.51	123.25	119.40
1	A	2643	C	C5-C4-N4	-5.50	116.35	120.20
1	A	1620	G	N3-C4-N9	-5.50	122.70	126.00
1	A	558	A	N1-C6-N6	5.50	121.90	118.60
1	A	27	G	N3-C4-C5	5.50	131.35	128.60
1	A	193	A	C5-C6-N1	5.50	120.45	117.70
1	A	496	G	C2-N3-C4	-5.50	109.15	111.90
1	A	1438	G	C2-N3-C4	-5.50	109.15	111.90
1	A	2606	C	N1-C2-O2	5.50	122.20	118.90
1	A	2069	A	C5-C6-N6	-5.50	119.30	123.70
1	A	212	C	C2-N1-C1'	5.49	124.84	118.80
1	A	1841	G	N3-C4-C5	5.49	131.35	128.60
1	A	1490	G	C5-C6-O6	-5.49	125.31	128.60
1	A	428	G	N1-C2-N2	-5.49	111.26	116.20
1	A	766	G	N3-C4-N9	5.49	129.29	126.00
1	A	788	A	N9-C4-C5	-5.49	103.61	105.80
1	A	2644	C	N3-C4-C5	5.49	124.09	121.90
1	A	945	A	C2-N3-C4	-5.48	107.86	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1181	G	N3-C4-C5	5.48	131.34	128.60
1	A	1772	G	N3-C4-N9	5.48	129.29	126.00
1	A	1932	C	N1-C2-O2	5.48	122.19	118.90
1	A	66	C	N1-C2-O2	5.47	122.18	118.90
1	A	1196	C	C6-N1-C2	-5.47	118.11	120.30
1	A	2764	G	C4-C5-N7	5.47	112.99	110.80
1	A	348	C	N1-C2-O2	5.47	122.18	118.90
1	A	1834	G	N3-C4-N9	-5.47	122.72	126.00
26	Z	16	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	351	G	N3-C4-N9	-5.47	122.72	126.00
1	A	1069	G	N3-C2-N2	-5.47	116.07	119.90
1	A	2370	U	C2-N1-C1'	-5.47	111.14	117.70
1	A	145	A	N9-C4-C5	-5.47	103.61	105.80
1	A	840	C	N3-C2-O2	-5.47	118.07	121.90
1	A	1908	A	O4'-C1'-N9	5.47	112.57	108.20
1	A	2056	G	C2-N3-C4	-5.47	109.17	111.90
2	B	41	C	O5'-P-OP1	-5.47	100.78	105.70
1	A	283	G	N9-C4-C5	-5.46	103.21	105.40
1	A	1496	G	C5-C6-O6	-5.46	125.32	128.60
1	A	2829	A	N1-C6-N6	5.46	121.88	118.60
1	A	733	U	C5-C6-N1	5.46	125.43	122.70
1	A	1029	C	N1-C2-O2	5.46	122.18	118.90
1	A	1040	A	C5-C6-N6	-5.46	119.33	123.70
1	A	1211	G	C4-C5-N7	5.46	112.98	110.80
1	A	2131	C	C5-C4-N4	5.46	124.02	120.20
1	A	370	G	C4-C5-N7	5.46	112.98	110.80
2	B	109	G	C4-N9-C1'	-5.46	119.40	126.50
1	A	822	G	N3-C4-C5	5.46	131.33	128.60
1	A	992	A	C5-N7-C8	-5.46	101.17	103.90
1	A	395	U	C2-N1-C1'	-5.45	111.16	117.70
1	A	2562	G	N1-C6-O6	5.45	123.17	119.90
1	A	685	C	C6-N1-C2	-5.45	118.12	120.30
1	A	2772	C	N3-C4-C5	5.45	124.08	121.90
1	A	618	A	N1-C6-N6	5.45	121.87	118.60
1	A	196	U	C2-N1-C1'	5.45	124.23	117.70
1	A	1453	G	N1-C2-N2	-5.44	111.30	116.20
1	A	1054	A	C5-C6-N1	5.44	120.42	117.70
1	A	2786	G	C6-C5-N7	-5.44	127.14	130.40
1	A	751	A	C6-C5-N7	-5.44	128.49	132.30
1	A	764	C	C5-C6-N1	5.44	123.72	121.00
1	A	770	G	C8-N9-C4	-5.43	104.23	106.40
1	A	2707	C	C5-C4-N4	-5.43	116.40	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2813	U	C5-C6-N1	5.43	125.42	122.70
1	A	333	C	N3-C4-N4	-5.43	114.20	118.00
1	A	1561	G	N3-C2-N2	-5.43	116.10	119.90
1	A	757	G	C4-N9-C1'	5.42	133.55	126.50
1	A	2496	A	O5'-P-OP1	-5.42	100.82	105.70
1	A	1803	G	C4-N9-C1'	5.42	133.54	126.50
1	A	2025	A	N1-C6-N6	-5.42	115.35	118.60
1	A	515	G	N9-C4-C5	-5.41	103.24	105.40
1	A	1268	C	N3-C4-C5	5.41	124.06	121.90
1	A	2397	G	C8-N9-C1'	5.41	134.03	127.00
1	A	2884	G	N9-C4-C5	-5.41	103.24	105.40
1	A	2819	C	C6-N1-C2	-5.41	118.14	120.30
1	A	2914	A	N9-C4-C5	-5.41	103.64	105.80
1	A	2079	G	C4-C5-N7	5.40	112.96	110.80
1	A	2762	G	N3-C4-C5	5.40	131.30	128.60
1	A	425	G	N3-C4-C5	5.39	131.30	128.60
1	A	85	G	C2-N3-C4	-5.39	109.20	111.90
1	A	574	A	N9-C4-C5	-5.39	103.64	105.80
1	A	1081	G	C8-N9-C1'	5.39	134.01	127.00
1	A	528	C	N3-C4-N4	-5.39	114.23	118.00
1	A	1506	C	C2-N3-C4	-5.39	117.21	119.90
1	A	1828	U	N1-C2-O2	5.39	126.57	122.80
1	A	613	G	N7-C8-N9	5.38	115.79	113.10
1	A	685	C	C2-N1-C1'	5.38	124.72	118.80
1	A	2672	G	N3-C2-N2	5.38	123.67	119.90
1	A	1202	C	C5-C4-N4	-5.38	116.44	120.20
1	A	1447	A	N1-C6-N6	5.38	121.83	118.60
1	A	634	C	N3-C4-C5	5.38	124.05	121.90
1	A	606	G	C2-N3-C4	-5.37	109.21	111.90
1	A	883	C	N3-C2-O2	-5.37	118.14	121.90
1	A	1625	U	N1-C2-O2	5.37	126.56	122.80
1	A	26	G	C2-N3-C4	-5.37	109.22	111.90
1	A	45	G	C2-N3-C4	-5.37	109.22	111.90
1	A	2062	G	C4-N9-C1'	5.37	133.48	126.50
1	A	629	A	C4-C5-C6	-5.37	114.32	117.00
1	A	19	G	C4-N9-C1'	5.36	133.47	126.50
1	A	2727	G	C4-C5-N7	5.36	112.95	110.80
1	A	1962	G	N3-C4-N9	-5.36	122.78	126.00
1	A	2071	C	N3-C4-N4	5.36	121.75	118.00
1	A	2782	C	N3-C2-O2	-5.36	118.15	121.90
1	A	2823	G	C4-N9-C1'	5.36	133.47	126.50
1	A	19	G	N3-C2-N2	5.36	123.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1072	A	C4-C5-N7	5.36	113.38	110.70
1	A	1750	U	C5-C4-O4	-5.36	122.69	125.90
1	A	2028	A	C8-N9-C4	5.36	107.94	105.80
1	A	819	A	N1-C6-N6	5.35	121.81	118.60
1	A	1405	G	N3-C4-C5	5.35	131.28	128.60
1	A	1424	A	C4-C5-N7	5.35	113.38	110.70
1	A	319	G	C8-N9-C4	5.35	108.54	106.40
1	A	2278	G	C8-N9-C1'	-5.35	120.04	127.00
1	A	2892	G	N3-C2-N2	-5.35	116.15	119.90
1	A	2525	C	C2-N1-C1'	5.35	124.68	118.80
1	A	433	U	N3-C4-C5	5.34	117.81	114.60
1	A	757	G	N3-C4-N9	5.34	129.21	126.00
1	A	645	A	C5-N7-C8	-5.34	101.23	103.90
1	A	816	G	N3-C4-N9	-5.34	122.80	126.00
1	A	1480	G	C4-N9-C1'	5.34	133.44	126.50
1	A	2715	G	N3-C4-C5	5.34	131.27	128.60
1	A	751	A	C5-C6-N1	5.33	120.37	117.70
1	A	2324	C	C2-N3-C4	5.33	122.57	119.90
1	A	2634	G	C2-N3-C4	-5.33	109.23	111.90
2	B	28	C	N1-C2-O2	5.33	122.10	118.90
1	A	1476	G	C4-C5-N7	5.33	112.93	110.80
1	A	1495	C	C6-N1-C2	-5.33	118.17	120.30
1	A	2596	G	N3-C4-N9	-5.33	122.80	126.00
28	2	36	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	2436	G	C5-N7-C8	-5.33	101.64	104.30
1	A	972	A	C5-N7-C8	-5.33	101.24	103.90
1	A	2747	U	N1-C2-O2	5.33	126.53	122.80
1	A	15	G	N3-C4-C5	5.32	131.26	128.60
1	A	842	U	C5-C4-O4	-5.32	122.71	125.90
1	A	860	U	N3-C4-O4	5.32	123.13	119.40
1	A	1622	C	N1-C2-O2	5.32	122.09	118.90
1	A	71	A	C8-N9-C4	5.32	107.93	105.80
1	A	576	U	P-O3'-C3'	5.32	126.08	119.70
1	A	69	C	N1-C2-O2	5.32	122.09	118.90
1	A	2846	A	N1-C6-N6	5.32	121.79	118.60
1	A	252	C	N3-C4-C5	5.32	124.03	121.90
1	A	1088	C	N3-C2-O2	-5.32	118.18	121.90
1	A	2675	G	C5-C6-N1	-5.32	108.84	111.50
1	A	755	C	C5-C6-N1	5.31	123.66	121.00
1	A	1405	G	N3-C4-N9	-5.31	122.81	126.00
1	A	27	G	C2-N3-C4	-5.31	109.25	111.90
1	A	887	A	C5-N7-C8	-5.31	101.25	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1226	G	C2-N3-C4	-5.31	109.25	111.90
1	A	2677	C	C6-N1-C2	-5.31	118.18	120.30
1	A	616	G	N3-C4-C5	5.30	131.25	128.60
1	A	997	G	N3-C2-N2	5.30	123.61	119.90
1	A	1742	A	N9-C4-C5	-5.30	103.68	105.80
1	A	2348	G	N3-C2-N2	5.30	123.61	119.90
26	Z	16	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	707	G	C2-N3-C4	-5.30	109.25	111.90
1	A	857	C	N3-C4-C5	5.30	124.02	121.90
1	A	1084	U	C5-C6-N1	5.30	125.35	122.70
1	A	1390	A	C5-C6-N1	5.30	120.35	117.70
1	A	2029	G	N3-C4-C5	5.30	131.25	128.60
1	A	95	A	C5-N7-C8	-5.29	101.25	103.90
1	A	876	G	N3-C2-N2	-5.29	116.20	119.90
1	A	1045	A	C5-C6-N6	-5.29	119.47	123.70
1	A	1279	C	N1-C2-O2	5.29	122.08	118.90
2	B	109	G	N3-C2-N2	5.29	123.60	119.90
1	A	1463	A	C5-C6-N6	-5.29	119.47	123.70
1	A	2448	G	N9-C4-C5	-5.29	103.28	105.40
1	A	2613	C	C5-C4-N4	5.29	123.90	120.20
1	A	1391	A	C6-C5-N7	-5.29	128.60	132.30
1	A	555	C	N3-C2-O2	-5.29	118.20	121.90
1	A	595	G	N3-C4-N9	-5.29	122.83	126.00
1	A	601	G	C2-N3-C4	-5.28	109.26	111.90
1	A	1075	G	N1-C6-O6	-5.28	116.73	119.90
1	A	2747	U	C5-C6-N1	5.28	125.34	122.70
1	A	1991	G	C8-N9-C1'	5.28	133.86	127.00
1	A	2218	G	N1-C6-O6	5.28	123.07	119.90
1	A	646	A	C5-C6-N6	-5.28	119.48	123.70
1	A	2756	G	N1-C2-N2	-5.28	111.45	116.20
1	A	2308	C	N3-C4-C5	5.27	124.01	121.90
1	A	2666	A	N1-C6-N6	5.27	121.76	118.60
1	A	2480	A	N7-C8-N9	5.27	116.44	113.80
1	A	1655	C	N3-C2-O2	-5.27	118.21	121.90
1	A	2839	A	C8-N9-C4	5.27	107.91	105.80
1	A	1480	G	C5-N7-C8	-5.27	101.67	104.30
1	A	1819	G	C8-N9-C4	5.27	108.51	106.40
1	A	1852	G	N3-C4-C5	5.27	131.23	128.60
1	A	1196	C	C2-N1-C1'	5.26	124.59	118.80
1	A	546	A	N9-C4-C5	-5.26	103.69	105.80
1	A	160	G	N3-C4-N9	5.26	129.16	126.00
1	A	645	A	N7-C8-N9	5.26	116.43	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2112	C	N1-C2-O2	5.26	122.06	118.90
1	A	193	A	C5-C6-N6	-5.26	119.49	123.70
1	A	2774	G	C5-C6-O6	5.26	131.76	128.60
1	A	192	G	N3-C4-N9	-5.26	122.84	126.00
1	A	2675	G	N3-C2-N2	5.26	123.58	119.90
1	A	453	G	N3-C4-N9	-5.26	122.85	126.00
1	A	806	A	N7-C8-N9	5.26	116.43	113.80
1	A	1287	U	N1-C2-O2	5.26	126.48	122.80
1	A	1776	A	C5-C6-N1	5.26	120.33	117.70
2	B	68	U	C5-C4-O4	-5.26	122.75	125.90
1	A	130	A	C4-C5-N7	5.25	113.33	110.70
1	A	861	C	N1-C2-O2	5.25	122.05	118.90
1	A	1614	A	C8-N9-C4	5.25	107.90	105.80
1	A	2328	A	C4-C5-N7	5.25	113.33	110.70
1	A	420	A	N1-C6-N6	5.25	121.75	118.60
1	A	814	A	N1-C6-N6	5.25	121.75	118.60
1	A	1516	C	C6-N1-C2	-5.25	118.20	120.30
1	A	523	A	N1-C6-N6	5.25	121.75	118.60
1	A	778	G	C4-C5-N7	5.25	112.90	110.80
1	A	1295	C	C5-C4-N4	-5.25	116.53	120.20
1	A	2131	C	C6-N1-C1'	5.25	127.09	120.80
1	A	1632	A	C5-C6-N6	-5.24	119.51	123.70
1	A	1491	C	C2-N1-C1'	-5.24	113.03	118.80
1	A	409	G	N1-C2-N2	-5.24	111.48	116.20
1	A	983	G	N3-C4-C5	5.24	131.22	128.60
1	A	19	G	C8-N9-C1'	-5.24	120.19	127.00
1	A	307	A	C6-C5-N7	-5.24	128.63	132.30
1	A	2503	A	C2-N3-C4	-5.24	107.98	110.60
1	A	2604	A	C5-C6-N6	-5.24	119.51	123.70
1	A	707	G	N3-C4-C5	5.24	131.22	128.60
1	A	2570	G	N3-C4-N9	-5.24	122.86	126.00
1	A	825	G	N3-C4-C5	5.24	131.22	128.60
1	A	829	U	C5-C4-O4	5.24	129.04	125.90
1	A	1284	A	C4-C5-N7	5.24	113.32	110.70
1	A	2742	C	C5-C4-N4	-5.24	116.54	120.20
1	A	333	C	C5-C6-N1	-5.23	118.38	121.00
1	A	652	A	C5-C6-N6	-5.23	119.51	123.70
1	A	2326	G	C8-N9-C1'	-5.23	120.20	127.00
1	A	1447	A	C6-C5-N7	-5.23	128.64	132.30
1	A	2044	C	C6-N1-C1'	-5.23	114.53	120.80
1	A	557	G	O4'-C1'-N9	5.23	112.38	108.20
1	A	992	A	C4-C5-N7	5.23	113.31	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2846	A	C4-C5-N7	5.23	113.31	110.70
1	A	816	G	C2-N3-C4	-5.22	109.29	111.90
1	A	1632	A	C3'-C2'-C1'	5.22	105.68	101.50
1	A	1378	U	N1-C2-O2	5.22	126.46	122.80
1	A	2604	A	C5-N7-C8	-5.22	101.29	103.90
1	A	742	U	C5-C4-O4	-5.22	122.77	125.90
1	A	1816	A	C4-C5-N7	5.22	113.31	110.70
1	A	647	G	N9-C4-C5	-5.22	103.31	105.40
1	A	1422	A	C5-C6-N1	5.22	120.31	117.70
1	A	1615	G	C8-N9-C1'	5.21	133.78	127.00
1	A	2244	G	N9-C4-C5	5.21	107.49	105.40
1	A	2461	A	C4-C5-N7	5.21	113.31	110.70
1	A	2717	A	N1-C6-N6	5.21	121.73	118.60
1	A	2044	C	C6-N1-C2	5.21	122.39	120.30
1	A	15	G	C8-N9-C4	5.21	108.48	106.40
1	A	1692	C	C6-N1-C1'	-5.21	114.55	120.80
1	A	2013	G	N3-C4-C5	5.21	131.21	128.60
1	A	1816	A	C5-C6-N6	-5.21	119.53	123.70
1	A	2460	A	N1-C6-N6	5.21	121.73	118.60
1	A	129	C	N3-C4-C5	5.21	123.98	121.90
1	A	603	C	C6-N1-C2	5.21	122.38	120.30
1	A	738	U	C5-C6-N1	5.21	125.31	122.70
1	A	1314	A	N9-C4-C5	-5.21	103.72	105.80
2	B	64	A	N9-C4-C5	-5.21	103.72	105.80
1	A	2092	C	C5-C4-N4	-5.21	116.56	120.20
1	A	2356	A	C4-C5-N7	5.21	113.30	110.70
1	A	611	U	N3-C2-O2	-5.20	118.56	122.20
1	A	998	G	C2-N3-C4	-5.20	109.30	111.90
1	A	2497	G	C6-C5-N7	-5.20	127.28	130.40
1	A	267	G	N3-C4-C5	5.19	131.20	128.60
1	A	1537	A	N3-C4-N9	-5.19	123.25	127.40
1	A	1462	G	C6-C5-N7	-5.19	127.28	130.40
1	A	2477	A	N3-C4-C5	5.19	130.44	126.80
1	A	2563	G	C2-N3-C4	-5.19	109.31	111.90
1	A	207	A	N1-C6-N6	5.19	121.71	118.60
1	A	874	A	C5-C6-N6	-5.19	119.55	123.70
1	A	1709	A	C5-C6-N6	-5.19	119.55	123.70
1	A	2321	C	N1-C2-O2	5.19	122.01	118.90
2	B	4	G	C4-C5-N7	5.19	112.88	110.80
1	A	2679	U	C2-N3-C4	5.18	130.11	127.00
1	A	757	G	N9-C4-C5	-5.18	103.33	105.40
1	A	401	U	N3-C2-O2	-5.18	118.57	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1016	G	N7-C8-N9	5.18	115.69	113.10
1	A	1709	A	N9-C4-C5	-5.18	103.73	105.80
1	A	2078	A	C4-C5-N7	5.18	113.29	110.70
1	A	2314	A	C5-N7-C8	-5.18	101.31	103.90
1	A	160	G	C4-N9-C1'	5.18	133.23	126.50
1	A	1462	G	C8-N9-C4	-5.18	104.33	106.40
1	A	2497	G	N3-C4-N9	5.18	129.10	126.00
1	A	2839	A	C4-C5-N7	5.18	113.29	110.70
1	A	257	G	C2-N3-C4	-5.17	109.31	111.90
1	A	1655	C	N1-C2-O2	5.17	122.00	118.90
1	A	2412	C	C6-N1-C2	-5.17	118.23	120.30
1	A	629	A	N1-C6-N6	-5.17	115.50	118.60
1	A	1991	G	N3-C4-C5	5.17	131.19	128.60
1	A	16	G	C2-N3-C4	-5.17	109.31	111.90
1	A	432	G	N3-C4-N9	5.17	129.10	126.00
1	A	1184	C	C5-C4-N4	-5.17	116.58	120.20
1	A	2707	C	N3-C4-C5	5.17	123.97	121.90
1	A	691	A	N7-C8-N9	5.17	116.39	113.80
1	A	2636	U	N3-C2-O2	-5.17	118.58	122.20
1	A	1242	A	C5-C6-N1	5.17	120.28	117.70
1	A	2643	C	N1-C2-O2	5.17	122.00	118.90
1	A	2768	A	N1-C6-N6	5.16	121.70	118.60
1	A	1890	G	N9-C4-C5	-5.16	103.33	105.40
1	A	2750	C	C2-N1-C1'	5.16	124.47	118.80
1	A	1356	G	C2-N3-C4	-5.16	109.32	111.90
1	A	2677	C	C2-N1-C1'	5.16	124.47	118.80
1	A	1410	A	C4-C5-N7	5.16	113.28	110.70
1	A	2840	A	C5-C6-N6	-5.16	119.58	123.70
1	A	402	C	C5-C6-N1	5.15	123.58	121.00
1	A	2675	G	C6-N1-C2	5.15	128.19	125.10
1	A	685	C	N3-C2-O2	-5.15	118.29	121.90
1	A	1307	G	N3-C4-N9	-5.15	122.91	126.00
1	A	2479	C	N3-C4-C5	5.15	123.96	121.90
1	A	181	G	C2-N3-C4	-5.15	109.32	111.90
1	A	1029	C	C5-C4-N4	-5.15	116.60	120.20
1	A	2618	C	N3-C4-N4	-5.15	114.40	118.00
1	A	1196	C	C5-C6-N1	5.14	123.57	121.00
1	A	1410	A	C5-N7-C8	-5.14	101.33	103.90
1	A	1890	G	N3-C2-N2	5.14	123.50	119.90
1	A	874	A	N1-C6-N6	5.14	121.68	118.60
1	A	2078	A	C5-N7-C8	-5.14	101.33	103.90
1	A	2630	G	C2-N3-C4	-5.14	109.33	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2698	A	N3-C4-N9	-5.14	123.29	127.40
1	A	432	G	N3-C4-C5	-5.13	126.03	128.60
1	A	1986	G	N3-C4-C5	5.13	131.17	128.60
1	A	735	C	N3-C4-N4	-5.13	114.41	118.00
1	A	503	A	O4'-C1'-N9	5.13	112.31	108.20
1	A	2817	A	C6-C5-N7	-5.13	128.71	132.30
1	A	2460	A	N9-C4-C5	-5.13	103.75	105.80
4	D	149	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	182	C	O4'-C1'-N1	5.13	112.30	108.20
1	A	881	G	C2-N3-C4	-5.13	109.34	111.90
2	B	5	G	C5-C6-O6	5.13	131.68	128.60
1	A	265	A	C6-C5-N7	-5.13	128.71	132.30
1	A	307	A	N1-C6-N6	5.13	121.67	118.60
1	A	515	G	C2-N3-C4	-5.13	109.34	111.90
1	A	2461	A	N9-C4-C5	-5.13	103.75	105.80
1	A	62	C	N3-C2-O2	-5.12	118.31	121.90
1	A	1435	C	N3-C4-N4	5.12	121.59	118.00
1	A	2647	C	N1-C2-O2	5.12	121.97	118.90
1	A	613	G	C2-N3-C4	-5.12	109.34	111.90
1	A	340	C	N3-C2-O2	-5.12	118.32	121.90
1	A	1316	G	C4-C5-N7	5.12	112.85	110.80
1	A	611	U	C6-N1-C2	-5.12	117.93	121.00
1	A	1411	G	N1-C2-N2	-5.12	111.59	116.20
11	K	101	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	1378	U	C2-N1-C1'	5.12	123.84	117.70
1	A	1495	C	N1-C2-N3	5.12	122.78	119.20
1	A	1607	A	C5-N7-C8	-5.12	101.34	103.90
1	A	2460	A	C5-C6-N6	-5.12	119.61	123.70
1	A	1620	G	N3-C4-C5	5.11	131.16	128.60
2	B	111	C	N3-C2-O2	-5.11	118.32	121.90
1	A	701	G	C2-N3-C4	-5.11	109.35	111.90
1	A	709	U	N3-C4-O4	5.11	122.97	119.40
1	A	2846	A	C5-C6-N6	-5.11	119.62	123.70
1	A	766	G	N3-C2-N2	5.10	123.47	119.90
1	A	2849	A	C4-C5-C6	-5.10	114.45	117.00
1	A	351	G	C4-N9-C1'	-5.10	119.87	126.50
1	A	1287	U	C2-N1-C1'	5.10	123.82	117.70
1	A	945	A	N3-C4-C5	5.10	130.37	126.80
1	A	669	C	N3-C4-C5	5.10	123.94	121.90
1	A	902	A	C5-N7-C8	-5.10	101.35	103.90
1	A	2052	C	N1-C2-O2	5.10	121.96	118.90
1	A	1701	U	C2-N1-C1'	5.10	123.82	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2062	G	C8-N9-C1'	-5.10	120.37	127.00
1	A	2539	C	N1-C2-O2	5.10	121.96	118.90
1	A	2700	G	N3-C4-C5	5.10	131.15	128.60
1	A	1458	A	C4-C5-N7	5.09	113.25	110.70
1	A	1956	G	N3-C4-N9	-5.09	122.94	126.00
1	A	2019	G	N1-C2-N2	-5.09	111.62	116.20
1	A	17	G	C4-C5-N7	5.09	112.84	110.80
1	A	1723	A	C5-N7-C8	-5.09	101.35	103.90
1	A	2129	C	N1-C2-O2	5.09	121.95	118.90
1	A	636	A	N9-C4-C5	-5.09	103.76	105.80
1	A	1604	C	N3-C4-N4	-5.09	114.44	118.00
1	A	1857	C	N3-C2-O2	-5.09	118.34	121.90
1	A	94	A	N7-C8-N9	5.09	116.34	113.80
1	A	2044	C	N1-C2-O2	5.09	121.95	118.90
1	A	287	G	N1-C6-O6	5.09	122.95	119.90
1	A	470	G	N3-C4-N9	-5.09	122.95	126.00
1	A	1747	G	N3-C4-C5	5.08	131.14	128.60
1	A	2829	A	C4-C5-N7	5.08	113.24	110.70
1	A	2884	G	C5-N7-C8	-5.08	101.76	104.30
1	A	208	G	N3-C2-N2	-5.08	116.34	119.90
1	A	2275	C	N1-C2-O2	5.08	121.95	118.90
1	A	2756	G	C2-N3-C4	-5.08	109.36	111.90
1	A	391	A	O4'-C1'-N9	5.08	112.26	108.20
1	A	725	A	C5-C6-N1	5.08	120.24	117.70
1	A	503	A	N9-C4-C5	-5.08	103.77	105.80
1	A	756	A	C8-N9-C1'	-5.08	118.56	127.70
1	A	1008	C	N3-C2-O2	-5.08	118.34	121.90
1	A	1728	C	N1-C2-O2	5.08	121.95	118.90
1	A	1852	G	C2-N3-C4	-5.08	109.36	111.90
1	A	719	G	N1-C2-N2	-5.08	111.63	116.20
1	A	621	A	C5-C6-N1	5.08	120.24	117.70
1	A	62	C	C5-C4-N4	5.07	123.75	120.20
1	A	1807	A	N1-C6-N6	-5.07	115.56	118.60
1	A	2348	G	C6-C5-N7	-5.07	127.36	130.40
1	A	2669	G	N3-C4-N9	-5.07	122.96	126.00
1	A	601	G	N3-C4-C5	5.07	131.13	128.60
1	A	1238	U	N3-C4-O4	5.07	122.95	119.40
1	A	1733	A	N1-C6-N6	5.07	121.64	118.60
1	A	2896	A	N9-C4-C5	-5.07	103.77	105.80
1	A	2076	A	C5-C6-N1	5.07	120.23	117.70
12	L	102	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	1690	A	C2-N3-C4	-5.07	108.07	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	217	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	20	C	N3-C4-C5	5.07	123.93	121.90
1	A	669	C	C5-C4-N4	-5.07	116.65	120.20
1	A	2742	C	N3-C4-C5	5.07	123.93	121.90
1	A	782	C	N3-C4-C5	5.06	123.93	121.90
1	A	2462	A	C5-C6-N1	5.06	120.23	117.70
1	A	1365	G	C2-N3-C4	-5.06	109.37	111.90
1	A	1649	C	C5-C4-N4	-5.06	116.66	120.20
1	A	2218	G	N9-C4-C5	-5.06	103.38	105.40
1	A	636	A	C6-C5-N7	-5.06	128.76	132.30
1	A	1500	G	N9-C4-C5	-5.06	103.38	105.40
1	A	1742	A	C4-C5-N7	5.06	113.23	110.70
1	A	1772	G	C8-N9-C1'	-5.05	120.43	127.00
1	A	2862	C	N3-C4-C5	5.05	123.92	121.90
1	A	2889	G	C2-N3-C4	-5.05	109.37	111.90
1	A	1740	G	N3-C4-N9	-5.05	122.97	126.00
1	A	2436	G	N1-C6-O6	5.05	122.93	119.90
1	A	1654	A	C4-C5-N7	5.05	113.22	110.70
2	B	64	A	C4-C5-N7	5.05	113.22	110.70
1	A	356	A	N9-C4-C5	-5.05	103.78	105.80
2	B	79	C	N3-C4-C5	5.05	123.92	121.90
1	A	1320	G	C2-N3-C4	-5.04	109.38	111.90
1	A	2397	G	C4-N9-C1'	-5.04	119.94	126.50
1	A	1637	A	C4-C5-N7	5.04	113.22	110.70
1	A	2028	A	N9-C4-C5	-5.04	103.78	105.80
1	A	2846	A	C5-N7-C8	-5.04	101.38	103.90
1	A	1733	A	C5-C6-N6	-5.04	119.67	123.70
1	A	1422	A	N1-C6-N6	-5.04	115.58	118.60
1	A	1491	C	N1-C2-O2	-5.04	115.88	118.90
1	A	2098	A	N9-C4-C5	-5.04	103.78	105.80
1	A	991	A	C5-C6-N1	5.03	120.22	117.70
1	A	2495	A	N7-C8-N9	5.03	116.32	113.80
1	A	1994	C	N1-C2-O2	5.03	121.92	118.90
1	A	2738	A	C5-C6-N1	5.03	120.22	117.70
1	A	1387	C	C6-N1-C2	-5.03	118.29	120.30
1	A	1830	A	C5-N7-C8	-5.03	101.39	103.90
1	A	771	G	N3-C4-N9	-5.03	122.98	126.00
1	A	1522	G	C4-N9-C1'	-5.03	119.96	126.50
1	A	2078	A	C5-C6-N6	-5.03	119.68	123.70
1	A	1341	A	N1-C6-N6	5.03	121.61	118.60
1	A	1772	G	C4-N9-C1'	5.03	133.03	126.50
1	A	1202	C	N3-C4-C5	5.02	123.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	582	G	N3-C4-C5	5.02	131.11	128.60
1	A	2383	C	N3-C4-N4	-5.02	114.49	118.00
1	A	2512	G	N3-C4-C5	5.02	131.11	128.60
1	A	523	A	C5-C6-N6	-5.02	119.69	123.70
1	A	352	A	N9-C4-C5	-5.01	103.79	105.80
1	A	1496	G	C5-C6-N1	5.01	114.01	111.50
1	A	2869	G	N3-C4-N9	-5.01	122.99	126.00
1	A	2379	A	N9-C4-C5	-5.01	103.80	105.80
1	A	2817	A	C8-N9-C4	-5.01	103.80	105.80
1	A	719	G	N9-C4-C5	-5.01	103.40	105.40
1	A	1253	G	C4-N9-C1'	5.01	133.01	126.50
1	A	2078	A	N1-C6-N6	5.01	121.60	118.60
2	B	19	G	N3-C4-C5	5.01	131.10	128.60
1	A	42	G	C2-N3-C4	-5.00	109.40	111.90
1	A	758	G	C8-N9-C1'	-5.00	120.50	127.00
1	A	778	G	C5-N7-C8	-5.00	101.80	104.30
1	A	1038	C	N3-C2-O2	-5.00	118.40	121.90
1	A	1694	A	C8-N9-C4	5.00	107.80	105.80
1	A	819	A	C5-C6-N1	5.00	120.20	117.70
1	A	1269	A	N9-C4-C5	-5.00	103.80	105.80
1	A	1961	C	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	4	35	ARG	Peptide
4	D	173	MET	Peptide
8	H	11	ASN	Peptide
16	P	50	ALA	Peptide
16	P	77	LYS	Peptide
23	W	34	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62277	31296	31303	1057	0
2	B	2445	1240	1240	65	0
3	C	2090	2201	2201	73	0
4	D	1627	1667	1667	44	0
5	E	1572	1620	1619	57	0
6	F	1325	1342	1342	52	0
7	G	1263	1225	1225	40	0
8	H	1143	1134	1134	30	0
9	I	918	981	981	39	0
10	J	1086	1125	1125	23	0
11	K	1071	1123	1123	34	0
12	L	932	983	983	29	0
13	M	891	925	925	32	0
14	N	889	937	937	18	0
15	O	942	1014	1014	35	0
16	P	790	830	830	16	0
17	Q	837	887	887	24	0
18	R	715	748	748	23	0
19	S	770	809	809	27	0
20	T	722	766	766	19	0
21	U	622	643	643	26	0
22	V	445	466	466	15	0
23	W	541	563	563	21	0
24	X	449	491	491	9	0
25	Y	370	243	243	12	0
26	Z	360	358	358	21	0
27	1	390	394	394	26	0
28	2	367	415	415	16	0
29	3	521	586	586	23	0
30	4	295	340	340	18	0
All	All	88665	57352	57358	1616	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1616) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:C:C5	1:A:333:C:C6	2.04	1.45
1:A:2432:G:N2	1:A:2439:A:N7	1.69	1.35
1:A:333:C:C5	1:A:333:C:C4	2.18	1.31
1:A:1675:G:N3	1:A:1679:A:N6	1.87	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1663:G:HO2'	28:2:2:VAL:N	1.39	1.18
1:A:2496:A:N7	1:A:2508:G:C2	2.12	1.17
1:A:333:C:N1	1:A:393:G:H1'	1.60	1.15
1:A:333:C:C4	1:A:333:C:N3	2.16	1.14
1:A:2496:A:C8	1:A:2508:G:N2	2.17	1.12
1:A:333:C:C6	1:A:333:C:N1	2.19	1.10
1:A:2379:A:N7	1:A:2392:G:N2	1.97	1.10
1:A:333:C:N1	1:A:333:C:C2	2.21	1.08
1:A:333:C:N3	1:A:333:C:C2	2.22	1.07
1:A:420:A:N7	1:A:446:G:N2	2.02	1.07
1:A:2774:G:C2	1:A:2784:A:N6	2.24	1.06
1:A:159:U:N3	1:A:169:G:O6	1.93	1.01
1:A:2774:G:N2	1:A:2784:A:C6	2.32	0.96
1:A:751:A:N6	1:A:770:G:N3	2.12	0.96
1:A:1731:G:N2	1:A:1745:A:N7	2.14	0.96
1:A:749:G:N2	1:A:772:A:H62	1.62	0.96
1:A:752:G:C6	1:A:769:U:O2	2.22	0.92
1:A:159:U:C4	1:A:169:G:O6	2.21	0.92
1:A:2125:U:O2	1:A:2218:G:N1	2.02	0.92
1:A:333:C:C2	1:A:393:G:N9	2.38	0.92
1:A:1451:U:N3	1:A:1633:A:N7	2.20	0.89
1:A:2618:C:O2	1:A:2630:G:N2	2.06	0.88
1:A:336:U:O4	1:A:388:A:C6	2.25	0.88
1:A:749:G:H21	1:A:772:A:H62	1.19	0.88
30:4:35:ARG:NH1	30:4:36:GLN:O	2.06	0.88
1:A:1725:G:HO2'	1:A:1789:A:HO2'	1.11	0.86
1:A:1450:A:OP2	1:A:1452:C:N4	2.08	0.86
1:A:2774:G:C2	1:A:2784:A:C6	2.64	0.86
1:A:1261:G:OP1	16:P:67:ARG:NH2	2.09	0.86
1:A:2378:G:N7	29:3:42:ARG:NH1	2.23	0.85
1:A:84:A:N6	1:A:101:G:C2	2.44	0.85
1:A:2736:G:OP1	12:L:14:LYS:NZ	2.10	0.85
29:3:32:LEU:O	29:3:36:LYS:NZ	2.10	0.85
1:A:1301:U:HO2'	26:Z:8:THR:HG1	1.23	0.85
1:A:790:G:N2	1:A:795:A:H61	1.74	0.85
1:A:2496:A:N6	1:A:2508:G:C4	2.45	0.85
1:A:562:C:OP2	26:Z:10:LYS:NZ	2.09	0.84
1:A:2499:G:N2	1:A:2504:C:OP1	2.10	0.84
1:A:1709:A:O2'	9:I:1:MET:N	2.10	0.84
1:A:749:G:O2'	1:A:771:G:N2	2.10	0.84
1:A:1538:A:N3	1:A:1625:U:O2'	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:56:ALA:HB2	13:M:80:ILE:HD13	1.59	0.83
1:A:1466:G:N2	1:A:1541:C:O2	2.11	0.83
1:A:1725:G:O2'	1:A:1789:A:O2'	1.93	0.83
1:A:2124:U:O4	1:A:2219:C:N4	2.08	0.83
2:B:77:G:N1	2:B:95:U:O2	2.11	0.83
1:A:1215:U:O2'	1:A:1217:U:OP2	1.95	0.83
1:A:679:G:N7	10:J:71:ARG:NH2	2.26	0.83
1:A:1083:G:N2	1:A:1160:C:O2	2.12	0.82
1:A:1708:A:H61	1:A:2023:C:H42	1.25	0.82
1:A:1708:A:H61	1:A:2023:C:N4	1.76	0.82
1:A:2361:U:O4	1:A:2363:A:N7	2.12	0.82
11:K:18:THR:O	11:K:98:LYS:NZ	2.10	0.82
1:A:333:C:C5	1:A:393:G:N9	2.47	0.82
1:A:574:A:N3	1:A:575:G:N2	2.27	0.82
1:A:1887:G:N2	1:A:1909:C:O2	2.12	0.82
1:A:1854:U:OP1	1:A:1998:A:O2'	1.98	0.81
22:V:45:LYS:NZ	22:V:46:LYS:O	2.13	0.81
1:A:333:C:OP2	1:A:393:G:N2	2.13	0.81
1:A:2125:U:N3	1:A:2218:G:O6	2.13	0.81
1:A:2772:C:N4	1:A:2782:C:O2'	2.14	0.81
1:A:333:C:C4	1:A:393:G:N9	2.47	0.81
1:A:1263:A:O3'	16:P:85:LYS:NZ	2.14	0.81
1:A:333:C:N1	1:A:393:G:N9	2.29	0.81
1:A:1229:G:OP1	10:J:30:THR:OG1	1.99	0.81
1:A:2628:C:O2'	1:A:2629:A:O4'	1.97	0.81
1:A:333:C:C2	1:A:393:G:C1'	2.63	0.81
1:A:1404:A:O3'	28:2:26:LYS:NZ	2.14	0.81
1:A:2088:G:OP1	5:E:68:LYS:NZ	2.14	0.81
1:A:142:G:N2	18:R:40:MET:SD	2.52	0.81
1:A:336:U:O4	1:A:388:A:C5	2.34	0.80
1:A:916:U:O2	1:A:951:G:N2	2.14	0.80
1:A:2279:G:N7	21:U:12:LYS:N	2.29	0.80
1:A:2292:U:O2	1:A:2301:A:N6	2.14	0.80
4:D:56:LYS:NZ	4:D:66:ASN:O	2.12	0.80
11:K:20:ARG:NH1	11:K:99:PRO:O	2.14	0.80
1:A:829:U:O2'	1:A:837:G:N7	2.13	0.80
1:A:1880:A:N6	1:A:2114:G:O2'	2.13	0.80
1:A:333:C:C6	1:A:393:G:N9	2.50	0.80
1:A:333:C:C4	1:A:393:G:C1'	2.65	0.80
1:A:606:G:O3'	15:O:41:LYS:NZ	2.14	0.80
22:V:27:ARG:NH1	22:V:28:ARG:O	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2555:U:O2	1:A:2562:G:O6	1.99	0.80
16:P:99:LYS:NZ	16:P:100:ILE:O	2.11	0.80
1:A:333:C:N3	1:A:393:G:N9	2.30	0.80
1:A:2278:G:N7	21:U:12:LYS:NZ	2.29	0.80
1:A:351:G:O2'	19:S:15:LYS:NZ	2.15	0.80
1:A:790:G:H21	1:A:795:A:N6	1.78	0.80
1:A:1827:C:OP2	3:C:182:ARG:NH2	2.15	0.80
1:A:540:G:OP1	17:Q:4:LYS:NZ	2.14	0.80
15:O:50:ARG:O	15:O:54:LYS:NZ	2.15	0.80
1:A:493:A:OP1	15:O:5:LYS:NZ	2.14	0.80
2:B:78:U:O4	20:T:15:ARG:NH2	2.15	0.79
1:A:1890:G:O2'	1:A:2438:A:O2'	1.97	0.79
1:A:1935:C:O2	1:A:1949:G:N2	2.15	0.79
1:A:1495:C:N3	1:A:1504:U:O4	2.16	0.79
2:B:29:C:O2	2:B:51:A:N6	2.15	0.79
1:A:184:C:N4	1:A:214:G:N7	2.29	0.79
11:K:130:LYS:NZ	11:K:131:PHE:O	2.16	0.79
1:A:230:A:H61	1:A:456:G:H21	1.28	0.79
1:A:333:C:C6	1:A:393:G:C1'	2.66	0.79
2:B:41:C:O2'	25:Y:1:MET:SD	2.40	0.79
1:A:1828:U:OP2	3:C:150:LYS:NZ	2.16	0.78
1:A:1916:A:N3	1:A:2113:U:O2'	2.16	0.78
1:A:306:C:O2	1:A:411:A:N6	2.15	0.78
1:A:1222:A:O3'	24:X:29:LYS:NZ	2.16	0.78
1:A:1324:A:O4'	12:L:109:ARG:NH1	2.15	0.78
1:A:1979:A:OP1	9:I:44:LYS:NZ	2.14	0.78
1:A:2775:A:N6	30:4:18:LYS:O	2.15	0.78
1:A:9:U:O2	1:A:2656:A:N7	2.16	0.78
1:A:2113:U:N3	1:A:2261:G:C6	2.52	0.78
1:A:1889:G:O6	1:A:1907:U:N3	2.17	0.78
1:A:2678:C:O2	1:A:2696:G:N2	2.16	0.78
2:B:5:G:O2'	13:M:32:ASN:ND2	2.17	0.78
9:I:112:MET:N	9:I:112:MET:SD	2.56	0.78
1:A:158:G:O6	1:A:170:C:N4	2.16	0.78
1:A:352:A:N6	1:A:1248:U:O2	2.16	0.78
1:A:752:G:O6	1:A:769:U:O2	2.01	0.78
1:A:1087:C:O2'	1:A:1092:A:O3'	2.01	0.78
1:A:1522:G:O3'	1:A:1607:A:O2'	2.02	0.78
1:A:1891:U:O2'	1:A:2436:G:N2	2.17	0.78
1:A:2372:G:O6	1:A:2398:G:N2	2.14	0.78
1:A:1520:A:O2'	1:A:1561:G:O6	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2558:A:N6	1:A:2688:G:O6	2.16	0.78
2:B:53:U:O2'	2:B:55:A:N7	2.16	0.78
1:A:446:G:N7	22:V:55:LYS:NZ	2.31	0.78
1:A:2425:U:O2	27:1:15:ARG:NH2	2.17	0.77
1:A:273:A:N7	1:A:298:U:O2	2.16	0.77
1:A:460:C:O2	1:A:1891:U:O2'	2.03	0.77
1:A:752:G:O6	1:A:769:U:C2	2.38	0.77
1:A:1024:A:OP1	1:A:1026:C:N4	2.17	0.77
1:A:2905:C:N4	26:Z:29:GLU:O	2.18	0.77
1:A:674:C:O2	1:A:684:U:O2'	2.03	0.77
1:A:675:G:N2	1:A:678:A:OP2	2.15	0.77
1:A:1761:G:N2	1:A:1767:G:OP2	2.18	0.77
1:A:2126:C:O2	1:A:2217:G:N2	2.14	0.77
1:A:2817:A:N3	1:A:2818:A:N6	2.33	0.77
1:A:2828:U:O2	1:A:2911:A:N6	2.15	0.77
1:A:2130:A:O2'	1:A:2213:U:O4	2.01	0.77
2:B:42:G:OP1	25:Y:3:GLN:NE2	2.18	0.77
1:A:1035:C:O2'	16:P:84:ARG:NH1	2.18	0.77
1:A:61:A:N6	1:A:93:U:O2	2.18	0.77
1:A:429:C:N4	1:A:432:G:OP2	2.18	0.77
11:K:30:GLY:O	11:K:134:ARG:NH1	2.18	0.77
1:A:1968:C:N4	1:A:1992:C:O4'	2.18	0.77
1:A:2392:G:N7	29:3:39:LYS:NZ	2.33	0.77
1:A:2776:A:N7	1:A:2780:A:N6	2.31	0.77
1:A:445:G:N7	22:V:52:ARG:NH2	2.33	0.76
1:A:2692:A:N6	7:G:107:VAL:O	2.18	0.76
23:W:23:GLU:O	23:W:27:ASN:ND2	2.18	0.76
1:A:1424:A:O2'	1:A:1571:G:N2	2.17	0.76
1:A:332:A:N6	1:A:333:C:O2	2.19	0.76
1:A:928:C:N4	1:A:938:G:OP2	2.18	0.76
1:A:1708:A:N6	1:A:2023:C:H42	1.83	0.76
1:A:1966:U:OP1	1:A:2631:U:O2'	2.04	0.76
1:A:309:U:O2	1:A:406:A:O2'	2.04	0.76
1:A:1464:U:O2'	1:A:1465:G:O4'	2.03	0.76
1:A:1658:A:N6	17:Q:86:ARG:O	2.18	0.76
1:A:2766:U:O2	1:A:2791:A:N6	2.19	0.76
1:A:333:C:C2	1:A:393:G:H1'	2.21	0.76
1:A:418:G:O2'	1:A:446:G:O6	2.03	0.76
1:A:1463:A:N6	1:A:1537:A:N1	2.31	0.76
1:A:375:A:O2'	1:A:377:U:OP2	2.04	0.76
1:A:2044:C:O2'	26:Z:6:ARG:NH1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2334:G:O2'	1:A:2337:A:OP2	2.04	0.76
13:M:55:GLN:O	13:M:83:LYS:NZ	2.19	0.76
18:R:9:ARG:NH1	18:R:10:PRO:O	2.19	0.76
1:A:441:C:O3'	22:V:10:ARG:NH1	2.19	0.76
1:A:2305:A:OP2	21:U:20:ASN:ND2	2.19	0.76
1:A:2747:U:O4	1:A:2893:A:N6	2.19	0.76
6:F:60:ILE:O	6:F:95:ARG:NH1	2.18	0.76
1:A:230:A:N6	1:A:456:G:H21	1.83	0.75
1:A:1448:U:O3'	1:A:1449:A:OP1	2.04	0.75
2:B:29:C:O2'	2:B:51:A:N1	2.19	0.75
1:A:1875:A:O2'	1:A:1876:G:N7	2.16	0.75
1:A:62:C:O2	1:A:92:G:N2	2.19	0.75
1:A:333:C:N3	1:A:393:G:C1'	2.49	0.75
1:A:1470:G:OP2	1:A:1471:A:O2'	2.02	0.75
1:A:2497:G:O6	1:A:2503:A:O2'	2.03	0.75
14:N:16:ARG:NH2	14:N:80:THR:O	2.20	0.75
1:A:897:A:N6	1:A:971:U:O4	2.18	0.75
1:A:1763:U:O2	1:A:1765:A:O2'	2.03	0.75
1:A:2046:U:OP2	26:Z:6:ARG:NH1	2.20	0.75
1:A:2142:G:N2	1:A:2188:C:OP1	2.19	0.75
1:A:2313:A:N6	27:1:19:THR:OG1	2.20	0.75
1:A:2818:A:N6	1:A:2826:U:O4	2.20	0.75
12:L:73:ASN:N	12:L:77:THR:O	2.20	0.75
1:A:302:A:O2'	1:A:410:G:N1	2.19	0.75
1:A:2324:C:O2	1:A:2348:G:N2	2.19	0.75
2:B:84:U:O2	2:B:88:G:N2	2.19	0.75
1:A:393:G:N9	1:A:393:G:C1'	2.49	0.75
1:A:1490:G:O2'	1:A:1491:C:O4'	2.05	0.75
1:A:1490:G:O2'	1:A:1491:C:O5'	2.03	0.75
1:A:1865:C:N4	1:A:1926:A:O4'	2.20	0.75
1:A:2783:U:O2'	1:A:2785:A:OP2	2.05	0.75
7:G:95:ARG:O	7:G:97:GLN:NE2	2.20	0.75
1:A:749:G:H21	1:A:772:A:N6	1.84	0.75
1:A:809:A:N3	3:C:212:ARG:NH1	2.35	0.75
1:A:43:A:N6	1:A:482:U:O4	2.13	0.75
1:A:1096:C:O2	1:A:1151:G:N2	2.20	0.75
1:A:752:G:N1	1:A:769:U:O2	2.19	0.74
1:A:914:G:O2'	11:K:8:LYS:NZ	2.20	0.74
17:Q:83:LYS:O	17:Q:84:ARG:NE	2.20	0.74
1:A:1085:U:O2	1:A:1158:G:O6	2.05	0.74
1:A:1095:A:N6	1:A:1153:C:O2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:C:O3'	18:R:24:LYS:NZ	2.19	0.74
1:A:1933:G:N2	1:A:1951:C:O2	2.18	0.74
12:L:52:LYS:NZ	12:L:93:TYR:O	2.18	0.74
1:A:84:A:N6	1:A:101:G:N2	2.34	0.74
1:A:2530:A:O2'	1:A:2532:G:OP2	2.05	0.74
1:A:2686:G:N2	1:A:2689:A:OP2	2.20	0.74
1:A:2830:A:H62	1:A:2910:G:H21	1.32	0.74
2:B:24:C:OP1	2:B:26:C:N4	2.19	0.74
11:K:67:LYS:NZ	11:K:105:GLU:OE2	2.20	0.74
1:A:2313:A:OP2	27:1:22:ASN:ND2	2.20	0.74
29:3:9:GLY:O	29:3:13:ARG:NH1	2.20	0.74
1:A:1360:G:OP1	17:Q:84:ARG:NH1	2.21	0.74
1:A:1648:C:O2'	1:A:1654:A:N6	2.20	0.74
7:G:145:ALA:O	7:G:164:TYR:OH	2.03	0.74
1:A:299:U:O2	1:A:300:G:N2	2.21	0.74
1:A:1091:G:H1	1:A:1154:G:HO2'	1.33	0.74
5:E:3:ASN:ND2	5:E:17:ILE:O	2.21	0.74
1:A:1977:G:N2	1:A:1983:U:O4	2.18	0.74
1:A:2685:C:OP1	7:G:160:LYS:NZ	2.20	0.74
1:A:1780:G:N2	1:A:1783:G:OP2	2.17	0.74
1:A:2496:A:C5	1:A:2508:G:C2	2.76	0.74
1:A:2555:U:O2	1:A:2562:G:C6	2.40	0.74
11:K:21:SER:OG	11:K:99:PRO:O	2.06	0.74
1:A:159:U:O4	1:A:169:G:O6	2.05	0.74
1:A:2366:G:O3'	2:B:39:G:N2	2.21	0.74
13:M:6:ASP:OD1	13:M:9:LYS:NZ	2.19	0.74
1:A:1979:A:N3	1:A:2587:C:O2'	2.16	0.73
1:A:2877:G:N2	1:A:2880:A:OP2	2.20	0.73
2:B:46:A:OP1	13:M:35:ARG:NH1	2.21	0.73
30:4:17:ILE:O	30:4:24:MET:N	2.21	0.73
1:A:333:C:N4	1:A:393:G:OP2	2.20	0.73
1:A:1915:G:N2	1:A:1915:G:OP2	2.20	0.73
1:A:2495:A:N1	1:A:2508:G:O2'	2.19	0.73
5:E:137:LYS:O	5:E:141:ASN:ND2	2.22	0.73
1:A:301:U:O2'	1:A:302:A:O5'	2.03	0.73
1:A:1793:C:O2	1:A:2013:G:N2	2.20	0.73
1:A:1885:G:O4'	1:A:1911:A:N6	2.21	0.73
1:A:2022:U:O2'	9:I:31:LYS:NZ	2.14	0.73
8:H:53:ASP:O	8:H:122:LYS:NZ	2.21	0.73
1:A:350:G:O2'	1:A:352:A:N7	2.19	0.73
5:E:158:ASN:O	5:E:177:THR:OG1	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:111:GLU:OE2	11:K:115:ARG:NE	2.22	0.73
1:A:160:G:O2'	1:A:168:A:N1	2.18	0.73
1:A:162:A:O4'	1:A:2235:A:O2'	2.04	0.73
1:A:1579:C:OP2	1:A:1587:C:N4	2.21	0.73
1:A:2398:G:N2	27:1:42:TYR:OH	2.20	0.73
1:A:2865:G:N2	1:A:2891:U:O2	2.19	0.73
1:A:2421:C:N3	1:A:2459:A:N6	2.36	0.73
1:A:2675:G:N1	1:A:2699:U:O2	2.20	0.73
1:A:2783:U:O2'	1:A:2786:G:OP2	2.07	0.73
1:A:1033:G:OP1	24:X:31:THR:OG1	2.07	0.73
1:A:248:G:N7	29:3:8:ARG:NH2	2.36	0.73
1:A:1085:U:O2	1:A:1158:G:C6	2.42	0.73
1:A:1261:G:N7	16:P:70:LYS:NZ	2.36	0.73
1:A:1301:U:O2'	26:Z:8:THR:OG1	2.06	0.73
1:A:1478:A:O2'	1:A:1522:G:OP1	2.05	0.73
1:A:2499:G:C2	1:A:2505:A:N6	2.57	0.73
1:A:1826:G:N2	1:A:1846:A:OP2	2.20	0.72
1:A:495:A:O2'	15:O:3:ARG:NH1	2.21	0.72
1:A:2347:A:O2'	1:A:2349:A:N6	2.21	0.72
1:A:1480:G:N2	1:A:1561:G:N3	2.37	0.72
1:A:515:G:N7	28:2:38:LYS:NZ	2.35	0.72
1:A:1489:A:N1	1:A:1506:C:N4	2.37	0.72
1:A:1796:A:O2'	1:A:1985:C:OP1	2.07	0.72
4:D:26:THR:OG1	4:D:199:GLY:O	2.07	0.72
1:A:341:G:O2'	1:A:365:A:N1	2.20	0.72
1:A:688:A:O2'	1:A:689:A:O5'	2.08	0.72
1:A:823:G:OP1	3:C:48:LYS:NZ	2.23	0.72
1:A:2178:U:OP1	1:A:2187:G:N2	2.22	0.72
1:A:2137:G:OP1	1:A:2170:C:O2'	2.07	0.72
1:A:2324:C:N3	1:A:2348:G:N1	2.38	0.72
1:A:2622:G:N2	1:A:2625:A:OP2	2.19	0.72
1:A:834:A:N6	1:A:1658:A:OP2	2.22	0.72
1:A:1763:U:O2'	1:A:1767:G:O6	2.08	0.72
1:A:1455:U:O2'	1:A:1631:G:OP2	2.08	0.72
1:A:1520:A:N6	1:A:1562:C:O4'	2.23	0.72
1:A:2129:C:O2'	1:A:2130:A:O3'	2.08	0.72
1:A:1039:C:O2'	15:O:93:LYS:NZ	2.22	0.72
1:A:1402:A:O4'	22:V:28:ARG:NH2	2.22	0.72
1:A:2851:G:N2	1:A:2904:U:OP2	2.22	0.72
1:A:1869:G:O6	1:A:1925:U:O2	2.08	0.71
1:A:2153:A:O2'	1:A:2189:G:N2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2709:U:O2'	4:D:14:GLN:OE1	2.08	0.71
1:A:165:C:OP2	1:A:166:A:N6	2.23	0.71
1:A:273:A:OP2	1:A:297:G:N2	2.23	0.71
1:A:365:A:OP1	5:E:168:ARG:NE	2.21	0.71
1:A:378:C:OP2	19:S:80:ARG:NH1	2.24	0.71
29:3:54:ASP:OD1	29:3:57:ARG:NH1	2.24	0.71
1:A:60:U:O4	1:A:63:U:O2'	2.09	0.71
1:A:284:C:O2'	1:A:287:G:N2	2.14	0.71
1:A:795:A:OP2	17:Q:88:GLN:NE2	2.24	0.71
1:A:2450:U:O2'	1:A:2451:C:O5'	2.08	0.71
9:I:64:ARG:NH1	9:I:101:PRO:O	2.24	0.71
13:M:96:ARG:NH2	13:M:99:TYR:O	2.24	0.71
1:A:1000:G:N7	11:K:14:ARG:NH2	2.38	0.71
1:A:1759:G:N2	1:A:1771:A:O3'	2.24	0.71
1:A:229:A:O2'	1:A:231:A:O4'	2.07	0.70
1:A:448:A:N1	1:A:468:A:N6	2.39	0.70
1:A:630:G:N1	10:J:31:SER:OG	2.23	0.70
1:A:1470:G:N7	3:C:31:LYS:NZ	2.30	0.70
1:A:2113:U:C2	1:A:2261:G:N1	2.58	0.70
27:1:19:THR:OG1	27:1:20:THR:N	2.24	0.70
1:A:342:A:N3	1:A:362:C:O2'	2.23	0.70
1:A:1053:A:O2'	1:A:1054:A:O4'	2.07	0.70
1:A:1448:U:N3	1:A:1635:A:C6	2.59	0.70
1:A:2195:G:N2	1:A:2197:G:O6	2.24	0.70
14:N:95:ARG:O	14:N:96:ARG:NH1	2.25	0.70
1:A:230:A:H61	1:A:456:G:N2	1.88	0.70
1:A:1068:G:O2'	1:A:1188:A:O2'	2.08	0.70
1:A:1376:G:O3'	18:R:15:LYS:NZ	2.25	0.70
1:A:2134:C:N4	1:A:2208:A:OP2	2.24	0.70
20:T:14:THR:N	20:T:17:ASP:OD1	2.25	0.70
1:A:1074:G:OP2	11:K:128:LYS:NZ	2.20	0.70
1:A:162:A:O2'	1:A:2234:C:O2	2.10	0.70
1:A:794:A:O2'	1:A:1309:G:N2	2.25	0.70
1:A:1448:U:N3	1:A:1635:A:N1	2.39	0.70
1:A:1449:A:O2'	1:A:1450:A:O4'	2.10	0.70
1:A:2005:A:N3	3:C:11:ASN:ND2	2.39	0.70
1:A:1616:A:O5'	3:C:59:LYS:NZ	2.25	0.70
3:C:35:LYS:O	3:C:62:TYR:N	2.25	0.70
29:3:16:ARG:NH1	29:3:20:GLY:O	2.25	0.70
1:A:1091:G:O2'	1:A:1155:A:N6	2.25	0.69
1:A:2504:C:OP2	30:4:4:ARG:NH2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:GLY:O	3:C:177:ARG:NH2	2.24	0.69
1:A:333:C:C5	1:A:393:G:C1'	2.75	0.69
1:A:743:C:O2'	1:A:779:A:N6	2.24	0.69
1:A:2499:G:O2'	1:A:2505:A:N1	2.18	0.69
2:B:112:A:O2'	13:M:55:GLN:NE2	2.25	0.69
12:L:92:ARG:NH2	12:L:93:TYR:OH	2.25	0.69
1:A:2251:G:OP1	3:C:268:LYS:NZ	2.26	0.69
3:C:18:SER:OG	3:C:19:LEU:N	2.25	0.69
23:W:45:THR:HG23	23:W:46:VAL:HG23	1.75	0.69
1:A:2175:G:O2'	1:A:2176:C:O4'	2.10	0.69
1:A:1466:G:O2'	1:A:1535:G:N3	2.26	0.69
1:A:252:C:O2	10:J:63:LYS:NZ	2.25	0.69
27:1:22:ASN:OD1	27:1:22:ASN:N	2.25	0.69
1:A:9:U:C2	1:A:2656:A:N7	2.61	0.69
1:A:442:G:O4'	22:V:10:ARG:NH2	2.25	0.69
1:A:1555:G:N2	1:A:1556:G:O6	2.26	0.69
1:A:2113:U:C2	1:A:2261:G:C2	2.81	0.69
5:E:40:GLN:O	5:E:43:SER:OG	2.10	0.69
2:B:109:G:O2'	2:B:110:C:O4'	2.08	0.69
1:A:1501:G:N2	1:A:1504:U:O4'	2.26	0.69
1:A:1757:U:O2'	1:A:1758:A:O5'	2.11	0.69
1:A:2869:G:O3'	1:A:2886:G:N2	2.26	0.69
18:R:7:LEU:HA	18:R:29:VAL:HG12	1.74	0.69
1:A:28:A:N3	15:O:11:ARG:NH2	2.41	0.68
1:A:1422:A:O4'	1:A:1513:A:O2'	2.10	0.68
1:A:2496:A:C5	1:A:2508:G:N3	2.61	0.68
1:A:2559:G:N1	1:A:2689:A:N1	2.40	0.68
1:A:562:C:O2'	17:Q:78:GLU:OE2	2.04	0.68
4:D:2:THR:O	4:D:213:THR:OG1	2.06	0.68
5:E:20:SER:N	5:E:203:GLU:OE2	2.25	0.68
14:N:64:ARG:NH1	14:N:73:GLU:OE2	2.25	0.68
1:A:1248:U:O4'	1:A:1275:A:N6	2.27	0.68
1:A:1756:U:O4	1:A:1774:A:N6	2.26	0.68
3:C:100:GLU:OE2	3:C:102:ARG:NH2	2.26	0.68
1:A:1077:U:O4	1:A:1162:C:N4	2.26	0.68
1:A:2780:A:C2	30:4:17:ILE:HG21	2.28	0.68
1:A:1427:U:O2	1:A:1432:A:N7	2.27	0.68
10:J:118:ASP:O	10:J:119:LYS:NZ	2.26	0.68
23:W:60:ARG:O	23:W:64:GLN:NE2	2.27	0.68
1:A:316:G:O6	1:A:403:U:O2'	2.08	0.68
1:A:699:U:HO2'	1:A:700:A:P	2.17	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1448:U:O3'	1:A:1449:A:O4'	2.10	0.68
1:A:1509:G:O2'	1:A:1595:C:N4	2.26	0.68
1:A:2212:G:O2'	1:A:2213:U:O4'	2.12	0.68
1:A:2312:C:OP2	27:1:24:ARG:NH2	2.27	0.68
1:A:2314:A:O2'	1:A:2315:A:OP2	2.12	0.68
1:A:697:U:O2'	1:A:698:U:OP1	2.11	0.68
1:A:1491:C:O2'	1:A:1492:G:O4'	2.06	0.68
4:D:19:ASN:O	14:N:82:LYS:NZ	2.26	0.68
1:A:418:G:N2	1:A:447:A:OP2	2.26	0.68
1:A:2144:A:N6	1:A:2188:C:OP2	2.27	0.68
17:Q:74:ALA:HB2	17:Q:103:ILE:HD13	1.74	0.68
1:A:2078:A:O2'	1:A:2079:G:OP2	2.12	0.68
1:A:2608:G:N2	1:A:2608:G:OP2	2.23	0.68
1:A:383:A:O2'	5:E:168:ARG:NH1	2.28	0.67
1:A:409:G:H22	1:A:411:A:H62	1.41	0.67
1:A:1378:U:O2'	18:R:54:ASN:OD1	2.05	0.67
11:K:16:LYS:NZ	11:K:18:THR:OG1	2.27	0.67
21:U:26:SER:O	21:U:28:ARG:NH2	2.27	0.67
1:A:2044:C:O3'	26:Z:6:ARG:NH1	2.27	0.67
1:A:1663:G:O2'	28:2:2:VAL:N	2.20	0.67
1:A:2817:A:O4'	1:A:2827:A:N6	2.28	0.67
1:A:1347:G:OP2	28:2:10:LYS:NZ	2.20	0.67
9:I:88:ARG:NH1	9:I:93:PRO:O	2.28	0.67
1:A:303:G:OP2	1:A:410:G:N1	2.27	0.67
1:A:350:G:OP2	1:A:350:G:N2	2.24	0.67
13:M:68:THR:OG1	13:M:71:GLU:N	2.28	0.67
1:A:1196:C:OP1	15:O:84:LYS:NZ	2.23	0.67
1:A:1501:G:H22	1:A:2729:G:H22	1.43	0.67
1:A:1698:A:O2'	4:D:127:PHE:O	2.10	0.67
7:G:147:ASN:O	7:G:150:SER:OG	2.10	0.67
1:A:2618:C:OP1	3:C:238:ARG:NH1	2.28	0.67
1:A:1379:A:O2'	1:A:1381:U:OP2	2.12	0.67
1:A:1401:G:O2'	1:A:1404:A:N6	2.28	0.67
1:A:2859:G:N2	12:L:97:GLN:O	2.24	0.67
1:A:80:G:N2	1:A:105:C:O2	2.20	0.66
1:A:750:A:N6	1:A:771:G:O4'	2.27	0.66
1:A:1214:C:O2	1:A:1219:G:N2	2.26	0.66
1:A:1710:G:N3	9:I:3:GLN:NE2	2.42	0.66
2:B:73:G:N2	20:T:78:GLN:OE1	2.28	0.66
10:J:83:ASN:ND2	10:J:117:LEU:O	2.28	0.66
1:A:213:C:O2'	1:A:1403:C:O2	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2135:U:OP2	1:A:2205:C:N4	2.28	0.66
1:A:2695:G:O4'	7:G:111:HIS:NE2	2.29	0.66
18:R:13:THR:OG1	18:R:14:GLU:OE1	2.10	0.66
1:A:333:C:N1	1:A:393:G:C1'	2.49	0.66
1:A:775:A:OP1	1:A:1802:U:O2'	2.13	0.66
2:B:27:A:OP2	13:M:37:ASN:ND2	2.28	0.66
1:A:12:U:O2	1:A:571:A:N7	2.28	0.66
1:A:2842:G:O2'	1:A:2844:U:OP2	2.04	0.66
3:C:199:GLN:HA	3:C:202:LEU:HD21	1.78	0.66
5:E:132:GLU:OE1	5:E:132:GLU:N	2.28	0.66
1:A:458:A:N1	1:A:1890:G:O2'	2.29	0.66
1:A:162:A:C1'	1:A:2235:A:HO2'	2.07	0.66
1:A:336:U:C4	1:A:388:A:C6	2.83	0.66
1:A:496:G:OP1	1:A:1286:G:N2	2.28	0.66
2:B:42:G:OP2	2:B:44:A:N6	2.29	0.66
4:D:174:GLY:O	4:D:176:ASN:ND2	2.28	0.66
1:A:386:C:N4	1:A:387:G:O6	2.29	0.66
19:S:79:THR:OG1	19:S:80:ARG:O	2.14	0.66
24:X:6:ILE:O	24:X:34:SER:OG	2.05	0.66
1:A:410:G:O2'	1:A:411:A:N7	2.28	0.66
1:A:480:U:O2	1:A:481:C:N4	2.28	0.66
1:A:2312:C:OP2	27:1:2:ARG:NH2	2.29	0.66
3:C:130:LEU:HB2	3:C:135:ILE:HD11	1.78	0.66
6:F:30:LYS:N	6:F:159:THR:OG1	2.28	0.66
1:A:1889:G:O6	1:A:1907:U:C4	2.49	0.66
1:A:2757:U:OP1	4:D:198:LYS:NZ	2.29	0.66
1:A:138:U:N3	1:A:141:U:OP2	2.28	0.65
1:A:2147:G:N2	1:A:2205:C:O2	2.28	0.65
1:A:2329:U:O2	6:F:125:ARG:NH1	2.28	0.65
1:A:2499:G:N2	1:A:2505:A:N6	2.45	0.65
1:A:2684:A:HO2'	7:G:94:TYR:HH	1.45	0.65
4:D:117:ASP:OD1	4:D:214:SER:OG	2.06	0.65
11:K:119:ARG:O	11:K:122:SER:OG	2.14	0.65
2:B:77:G:C2	2:B:95:U:O2	2.50	0.65
9:I:88:ARG:NH2	9:I:90:ASP:OD2	2.30	0.65
1:A:1886:A:C5	1:A:1910:G:N2	2.65	0.65
15:O:99:ALA:HB2	15:O:106:PHE:CE1	2.31	0.65
1:A:1149:U:O2'	1:A:1150:A:O4'	2.10	0.65
1:A:1448:U:C2	1:A:1635:A:N6	2.64	0.65
2:B:53:U:O2	2:B:55:A:N6	2.29	0.65
29:3:54:ASP:O	29:3:58:VAL:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:147:GLU:OE1	5:E:147:GLU:N	2.30	0.65
1:A:2496:A:O2'	11:K:56:ARG:NH1	2.30	0.65
1:A:2498:A:N6	1:A:2503:A:O2'	2.29	0.65
1:A:2555:U:OP1	7:G:172:LYS:NZ	2.18	0.65
2:B:64:A:O2'	2:B:104:A:N6	2.30	0.65
4:D:56:LYS:N	4:D:84:PRO:O	2.29	0.65
8:H:99:GLU:OE1	8:H:99:GLU:N	2.30	0.65
21:U:57:GLU:N	21:U:57:GLU:OE1	2.29	0.65
1:A:1024:A:O2'	1:A:1025:A:OP1	2.13	0.64
1:A:1304:G:O2'	1:A:2039:G:O6	2.14	0.64
1:A:2561:C:N4	1:A:2562:G:O6	2.29	0.64
1:A:1312:A:O4'	12:L:12:GLN:NE2	2.30	0.64
1:A:1496:G:OP1	1:A:1497:A:N6	2.30	0.64
5:E:157:GLU:OE1	5:E:198:ALA:N	2.31	0.64
10:J:33:ARG:NH1	10:J:41:ARG:O	2.30	0.64
19:S:79:THR:OG1	19:S:94:ALA:O	2.15	0.64
29:3:16:ARG:NE	29:3:65:LYS:O	2.30	0.64
1:A:3:U:O2	1:A:2920:U:O2'	2.13	0.64
1:A:333:C:C5	1:A:393:G:O4'	2.51	0.64
2:B:77:G:N2	2:B:95:U:O2	2.31	0.64
1:A:1072:A:H61	1:A:1169:G:H2'	1.62	0.64
1:A:1369:G:N7	1:A:1653:A:O2'	2.30	0.64
1:A:1440:A:O2'	1:A:1514:A:O4'	2.13	0.64
9:I:30:ARG:NE	9:I:32:THR:O	2.27	0.64
1:A:300:G:O2'	1:A:301:U:OP2	2.15	0.64
12:L:79:GLN:NE2	12:L:88:GLU:OE2	2.29	0.64
1:A:865:A:N3	1:A:987:U:O2'	2.28	0.64
1:A:1465:G:O2'	1:A:1536:C:O2'	2.02	0.64
1:A:335:U:O2'	1:A:336:U:O5'	2.15	0.64
1:A:1472:C:O2'	1:A:1616:A:OP2	2.08	0.64
1:A:2510:C:N3	11:K:124:LYS:NZ	2.34	0.64
1:A:250:G:OP2	1:A:252:C:N4	2.31	0.64
1:A:1079:U:O2	1:A:1164:G:O6	2.16	0.64
1:A:1485:G:O2'	1:A:1599:G:N1	2.31	0.64
1:A:2089:A:N6	1:A:2530:A:N7	2.45	0.64
21:U:45:LEU:HD21	21:U:69:ALA:H	1.63	0.64
1:A:319:G:O4'	1:A:325:A:N6	2.30	0.63
1:A:1615:G:OP2	3:C:63:ARG:NH2	2.31	0.63
1:A:2711:U:OP2	14:N:53:ARG:NH2	2.32	0.63
1:A:2883:U:OP1	14:N:93:LYS:NZ	2.22	0.63
5:E:135:LYS:N	5:E:166:SER:OG	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:G:N7	10:J:103:LYS:NZ	2.46	0.63
1:A:687:G:N1	1:A:690:U:OP2	2.30	0.63
1:A:2302:C:O2'	11:K:84:GLY:O	2.15	0.63
1:A:2667:G:OP1	8:H:100:ARG:NH1	2.30	0.63
1:A:206:U:OP2	1:A:207:A:O2'	2.17	0.63
1:A:1496:G:O2'	1:A:1497:A:O5'	2.16	0.63
1:A:2261:G:O2'	1:A:2262:G:OP1	2.10	0.63
2:B:12:U:O2'	2:B:104:A:O2'	2.12	0.63
4:D:59:TYR:N	4:D:74:GLU:OE2	2.30	0.63
5:E:182:ASN:OD1	5:E:184:LEU:N	2.32	0.63
25:Y:51:SER:O	25:Y:55:HIS:NE2	2.32	0.63
1:A:1800:A:N6	3:C:11:ASN:O	2.30	0.63
2:B:35:C:N3	2:B:46:A:O2'	2.23	0.63
3:C:243:ARG:NH2	3:C:247:MET:SD	2.71	0.63
1:A:1451:U:C2	1:A:1633:A:N7	2.66	0.63
23:W:5:GLU:OE1	23:W:5:GLU:N	2.32	0.63
30:4:10:ILE:HD12	30:4:29:ASN:HB2	1.81	0.63
1:A:84:A:H62	1:A:101:G:N2	1.96	0.63
1:A:301:U:HO2'	1:A:302:A:P	2.22	0.63
1:A:311:U:O2	1:A:405:G:O2'	2.13	0.63
1:A:1217:U:O2	1:A:1218:G:N1	2.32	0.63
1:A:2448:G:N7	29:3:31:HIS:NE2	2.47	0.63
1:A:2499:G:N2	1:A:2505:A:H62	1.96	0.63
12:L:95:GLU:O	12:L:97:GLN:NE2	2.32	0.63
1:A:1521:A:N6	1:A:1560:A:O2'	2.32	0.62
3:C:120:ALA:O	3:C:134:ASN:ND2	2.31	0.62
5:E:141:ASN:O	5:E:145:THR:HG23	1.98	0.62
1:A:202:A:O3'	22:V:23:ASN:ND2	2.32	0.62
1:A:753:U:N3	1:A:769:U:O2	2.32	0.62
1:A:1478:A:N6	1:A:1605:A:N7	2.37	0.62
1:A:1962:G:N1	1:A:1989:C:O2'	2.31	0.62
1:A:2324:C:O2	1:A:2348:G:C2	2.52	0.62
19:S:11:VAL:HG23	19:S:17:LYS:HA	1.82	0.62
6:F:70:ALA:N	6:F:82:GLY:O	2.32	0.62
1:A:583:A:O3'	8:H:8:ASN:ND2	2.31	0.62
24:X:9:THR:OG1	24:X:55:THR:OG1	2.14	0.62
1:A:1505:G:O4'	1:A:2729:G:N2	2.27	0.62
1:A:299:U:O2'	1:A:300:G:N2	2.32	0.62
1:A:1213:C:H42	1:A:1219:G:H22	1.46	0.62
1:A:1485:G:HO2'	1:A:1599:G:H1	1.46	0.62
1:A:2851:G:OP2	4:D:65:SER:OG	2.05	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:G:O2'	1:A:515:G:O6	2.08	0.62
1:A:2060:A:O2'	1:A:2062:G:OP2	2.17	0.62
1:A:2196:G:O2'	1:A:2197:G:O4'	2.13	0.62
1:A:2546:U:O2'	1:A:2568:A:N6	2.33	0.62
13:M:74:THR:HG23	13:M:111:ALA:HB2	1.82	0.62
1:A:1199:A:O3'	15:O:55:ARG:NH2	2.32	0.62
1:A:2171:G:N2	1:A:2173:U:O4'	2.33	0.62
6:F:32:ASP:N	6:F:32:ASP:OD1	2.33	0.62
8:H:37:LEU:HD12	8:H:37:LEU:O	1.99	0.62
8:H:85:ILE:HD12	8:H:86:LYS:N	2.14	0.61
1:A:227:G:H22	1:A:235:G:H21	1.46	0.61
1:A:1448:U:C2	1:A:1635:A:C6	2.87	0.61
1:A:2558:A:N7	1:A:2687:A:N6	2.48	0.61
1:A:2800:U:O3'	4:D:177:THR:OG1	2.18	0.61
4:D:16:PHE:O	14:N:14:GLN:NE2	2.33	0.61
19:S:5:LYS:O	19:S:23:VAL:HG13	1.99	0.61
1:A:333:C:N3	1:A:393:G:C8	2.68	0.61
1:A:442:G:O2'	22:V:30:ASN:O	2.18	0.61
1:A:517:A:OP1	5:E:84:ARG:NH1	2.33	0.61
1:A:1652:A:N7	1:A:1665:U:O2	2.33	0.61
1:A:2684:A:O2'	7:G:94:TYR:OH	2.17	0.61
10:J:51:GLU:OE2	29:3:57:ARG:NE	2.33	0.61
1:A:1067:U:OP2	1:A:1069:G:O2'	2.18	0.61
1:A:1079:U:C2	1:A:1164:G:O6	2.53	0.61
23:W:11:THR:OG1	23:W:60:ARG:NH2	2.33	0.61
1:A:318:A:O2'	1:A:402:C:N4	2.33	0.61
1:A:2557:U:OP1	1:A:2562:G:N2	2.32	0.61
1:A:2672:G:O2'	1:A:2673:C:OP1	2.11	0.61
12:L:4:ARG:NH1	12:L:39:GLU:OE2	2.33	0.61
1:A:84:A:N6	1:A:99:U:O4'	2.34	0.61
1:A:2224:U:O2'	1:A:2225:A:N3	2.21	0.61
1:A:2259:C:OP2	22:V:27:ARG:NH2	2.33	0.61
1:A:2555:U:C2	1:A:2562:G:O6	2.53	0.61
1:A:2774:G:N3	1:A:2784:A:N6	2.49	0.61
1:A:2906:G:O2'	26:Z:29:GLU:OE1	2.11	0.61
2:B:10:U:O5'	2:B:13:A:N6	2.34	0.61
15:O:89:ASP:O	16:P:11:GLN:NE2	2.34	0.61
1:A:1476:G:O6	1:A:1607:A:N6	2.34	0.61
1:A:2682:G:O2'	1:A:2691:G:O6	2.09	0.61
1:A:2776:A:OP1	7:G:3:ARG:N	2.34	0.61
1:A:333:C:C6	1:A:393:G:H1'	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:G:O2'	1:A:435:A:O5'	2.15	0.61
11:K:70:PRO:HA	11:K:95:ALA:HB2	1.81	0.61
1:A:963:A:OP2	1:A:2295:A:N6	2.34	0.60
1:A:335:U:HO2'	1:A:336:U:H6	1.48	0.60
1:A:1039:C:N3	8:H:4:THR:OG1	2.28	0.60
1:A:2433:C:OP1	1:A:2438:A:N6	2.34	0.60
2:B:64:A:N6	2:B:105:C:O5'	2.32	0.60
1:A:1185:U:OP2	8:H:66:THR:OG1	2.19	0.60
1:A:1462:G:N2	1:A:1463:A:N7	2.49	0.60
1:A:672:A:N6	1:A:682:A:O4'	2.33	0.60
1:A:1486:C:O2	1:A:1598:U:N3	2.35	0.60
6:F:4:LEU:HD22	6:F:100:LEU:HD11	1.83	0.60
6:F:108:LEU:HD21	25:Y:56:PRO:HD2	1.84	0.60
7:G:157:TYR:O	7:G:171:ARG:NH1	2.35	0.60
1:A:1963:A:N6	1:A:1990:C:O2	2.20	0.60
1:A:111:U:OP1	23:W:58:ARG:NH1	2.35	0.60
1:A:461:A:O2'	1:A:1892:U:O3'	2.19	0.60
1:A:621:A:OP1	1:A:1293:U:O2'	2.18	0.60
1:A:1874:A:N6	1:A:1876:G:O6	2.35	0.60
5:E:80:ALA:HB1	5:E:81:PRO:HD2	1.84	0.60
1:A:1533:A:N7	3:C:100:GLU:N	2.44	0.60
1:A:84:A:N6	1:A:101:G:H21	1.98	0.60
6:F:140:GLU:HB2	6:F:141:ILE:HD12	1.83	0.60
11:K:44:SER:HA	11:K:47:ILE:HD11	1.83	0.60
21:U:50:GLY:N	21:U:65:ASP:OD2	2.35	0.60
19:S:3:ILE:HD12	19:S:4:LYS:N	2.17	0.60
5:E:101:MET:O	5:E:106:ARG:NH1	2.35	0.59
1:A:7:G:O4'	8:H:136:GLN:NE2	2.35	0.59
1:A:78:U:O2	1:A:107:G:N2	2.24	0.59
1:A:2774:G:H2'	7:G:67:THR:HG22	1.84	0.59
3:C:141:VAL:HG12	3:C:192:ILE:HA	1.82	0.59
17:Q:36:LEU:O	17:Q:44:SER:OG	2.17	0.59
1:A:526:A:O2'	19:S:42:LYS:O	2.18	0.59
1:A:1712:A:H61	1:A:1720:A:H61	1.48	0.59
1:A:1952:C:N4	1:A:1956:G:H22	2.00	0.59
1:A:2496:A:C6	1:A:2508:G:N3	2.70	0.59
6:F:94:GLU:OE1	6:F:94:GLU:N	2.34	0.59
9:I:87:ILE:HD12	9:I:89:ASP:H	1.66	0.59
5:E:33:LEU:HD21	5:E:183:VAL:HG21	1.83	0.59
1:A:1081:G:N2	1:A:1163:U:O2'	2.36	0.59
1:A:1086:G:N2	1:A:1157:U:O2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:G:O2'	1:A:1227:U:O2	2.20	0.59
1:A:2771:G:O2'	7:G:149:ARG:NH1	2.35	0.59
3:C:179:GLY:O	3:C:274:ARG:NH1	2.35	0.59
1:A:522:G:N1	1:A:525:A:OP2	2.36	0.59
19:S:25:ALA:HB3	19:S:34:VAL:HG12	1.84	0.59
1:A:1085:U:C2	1:A:1158:G:O6	2.55	0.59
1:A:1257:G:O5'	15:O:19:LYS:NZ	2.36	0.59
1:A:1356:G:H21	1:A:1358:A:N6	2.01	0.59
1:A:1712:A:N6	1:A:1720:A:H61	2.01	0.59
1:A:2113:U:O2	1:A:2261:G:C2	2.56	0.59
1:A:124:A:O4'	28:2:15:LYS:NZ	2.34	0.59
6:F:161:ASN:ND2	6:F:165:GLU:OE2	2.36	0.59
1:A:1076:A:N6	1:A:1163:U:O4	2.31	0.59
7:G:2:SER:O	7:G:54:ARG:NH1	2.35	0.59
1:A:72:U:OP1	23:W:54:LYS:NZ	2.33	0.58
1:A:2306:G:N7	21:U:22:ARG:NH1	2.51	0.58
3:C:65:ILE:HD11	3:C:67:PHE:CE2	2.38	0.58
27:1:36:CYS:SG	27:1:45:HIS:NE2	2.75	0.58
1:A:751:A:H61	1:A:770:G:C1'	2.16	0.58
3:C:65:ILE:HD11	3:C:67:PHE:CD2	2.38	0.58
1:A:460:C:O4'	1:A:1890:G:N2	2.36	0.58
1:A:1173:A:O2'	1:A:2542:C:O2	2.20	0.58
1:A:1963:A:OP2	1:A:1989:C:N4	2.36	0.58
13:M:28:LYS:HB3	13:M:93:VAL:HG23	1.84	0.58
1:A:489:A:N6	1:A:1283:G:O2'	2.37	0.58
1:A:514:G:O2'	5:E:62:ARG:NH1	2.35	0.58
1:A:1764:A:N7	1:A:1765:A:N6	2.52	0.58
23:W:50:ILE:HA	23:W:53:LEU:HD12	1.86	0.58
13:M:44:ILE:O	13:M:53:LEU:N	2.35	0.58
27:1:9:CYS:SG	27:1:10:THR:N	2.76	0.58
1:A:69:C:O2'	1:A:70:G:OP1	2.19	0.58
1:A:1282:A:OP1	10:J:7:LYS:NZ	2.36	0.58
1:A:333:C:C4	1:A:393:G:C8	2.91	0.58
1:A:418:G:N7	22:V:56:SER:OG	2.26	0.58
1:A:427:A:OP1	22:V:18:ARG:NH2	2.36	0.58
10:J:87:ASP:OD1	10:J:120:LYS:N	2.36	0.58
1:A:1096:C:O2'	1:A:1151:G:N2	2.36	0.57
1:A:1301:U:OP1	26:Z:13:LYS:NZ	2.37	0.57
1:A:1385:G:H22	1:A:1642:C:H42	1.52	0.57
1:A:2785:A:N1	7:G:71:LEU:HD11	2.18	0.57
3:C:233:GLY:HA2	3:C:239:ALA:HB1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:58:VAL:HB	29:3:61:LEU:HD12	1.85	0.57
1:A:1063:U:H3	1:A:1186:A:H62	1.52	0.57
1:A:1737:U:O2	3:C:14:ARG:NH2	2.37	0.57
1:A:2618:C:C2	1:A:2630:G:N2	2.65	0.57
2:B:77:G:O6	20:T:15:ARG:NH2	2.37	0.57
1:A:427:A:N6	1:A:433:U:O4	2.37	0.57
6:F:134:GLU:CB	6:F:137:ILE:HD11	2.34	0.57
1:A:1066:G:O6	8:H:69:LYS:NZ	2.25	0.57
1:A:1981:G:O2'	1:A:1983:U:O4	2.13	0.57
9:I:49:GLY:O	9:I:53:LYS:NZ	2.36	0.57
1:A:310:C:O3'	1:A:405:G:N2	2.35	0.57
1:A:1397:G:N2	1:A:2241:C:C4	2.73	0.57
1:A:1466:G:N3	1:A:1535:G:N2	2.52	0.57
1:A:1887:G:N1	1:A:1909:C:N3	2.52	0.57
3:C:151:GLY:O	3:C:153:GLN:NE2	2.37	0.57
19:S:72:ASP:OD2	19:S:75:THR:N	2.38	0.57
1:A:223:G:O2'	1:A:236:A:N3	2.29	0.57
1:A:228:A:N6	1:A:465:C:O2'	2.38	0.57
1:A:351:G:O3'	19:S:15:LYS:NZ	2.34	0.57
1:A:1002:U:C2	11:K:17:THR:HG21	2.40	0.57
1:A:1489:A:P	1:A:1492:G:H22	2.28	0.57
1:A:1832:C:OP1	3:C:252:LYS:NZ	2.31	0.57
1:A:2104:A:OP1	1:A:2265:G:N2	2.34	0.57
1:A:2807:G:OP1	8:H:121:LYS:NZ	2.26	0.57
1:A:332:A:O5'	1:A:393:G:N2	2.38	0.57
1:A:1079:U:O2	1:A:1164:G:C6	2.58	0.57
1:A:1173:A:N1	1:A:2596:G:O2'	2.36	0.57
20:T:4:LEU:HD23	20:T:5:LYS:H	1.69	0.57
3:C:100:GLU:OE1	3:C:101:LYS:N	2.38	0.57
1:A:13:A:O2'	1:A:15:G:N7	2.37	0.57
1:A:678:A:OP1	10:J:71:ARG:NE	2.31	0.57
1:A:681:G:O6	10:J:110:LYS:NZ	2.37	0.57
1:A:795:A:OP1	1:A:1659:C:N4	2.38	0.57
1:A:2093:C:N4	1:A:2094:G:O6	2.38	0.57
1:A:2285:C:O2'	1:A:2454:C:OP2	2.21	0.57
1:A:2511:G:OP1	11:K:45:ARG:NH2	2.38	0.57
3:C:204:ASN:OD1	3:C:205:VAL:N	2.36	0.57
5:E:195:THR:OG1	5:E:196:GLU:N	2.37	0.57
9:I:115:VAL:HG13	9:I:121:VAL:HG21	1.86	0.57
1:A:2342:U:H5''	13:M:2:ILE:HD12	1.86	0.57
1:A:2710:C:OP1	14:N:53:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2672:G:HO2'	1:A:2673:C:P	2.26	0.56
19:S:33:VAL:O	19:S:63:ILE:N	2.38	0.56
1:A:1458:A:H2	1:A:1631:G:H21	1.52	0.56
1:A:2113:U:N3	1:A:2261:G:N1	2.52	0.56
17:Q:65:ASN:ND2	17:Q:67:ASP:OD1	2.39	0.56
1:A:1094:A:N1	1:A:1153:C:O2'	2.27	0.56
1:A:1957:G:N2	1:A:1958:U:O4	2.34	0.56
3:C:223:SER:O	3:C:239:ALA:HB2	2.06	0.56
14:N:31:HIS:NE2	14:N:87:GLU:OE2	2.37	0.56
18:R:82:LEU:HD12	18:R:83:LYS:N	2.21	0.56
1:A:1956:G:O2'	1:A:1957:G:OP2	2.20	0.56
1:A:2485:U:O2'	1:A:2487:U:O4	2.15	0.56
3:C:27:THR:O	3:C:27:THR:OG1	2.18	0.56
18:R:84:GLU:OE1	18:R:84:GLU:N	2.38	0.56
4:D:81:ASP:N	4:D:81:ASP:OD1	2.36	0.56
1:A:2769:G:N2	1:A:2789:U:O2	2.35	0.56
3:C:168:GLU:N	3:C:168:GLU:OE1	2.38	0.56
4:D:14:GLN:HB2	4:D:22:LEU:HD11	1.88	0.56
19:S:66:SER:O	19:S:66:SER:OG	2.21	0.56
1:A:1467:G:H21	1:A:1542:C:C4'	2.19	0.56
2:B:32:U:O2'	2:B:42:G:N7	2.34	0.56
24:X:5:GLN:HB2	24:X:36:VAL:HG22	1.87	0.56
1:A:332:A:N6	1:A:395:U:O2	2.39	0.56
1:A:2499:G:H2'	1:A:2505:A:H61	1.69	0.56
1:A:2649:U:O3'	1:A:2845:G:N2	2.33	0.56
3:C:254:THR:O	3:C:254:THR:OG1	2.24	0.56
17:Q:25:ARG:NH1	17:Q:74:ALA:O	2.35	0.56
23:W:6:ILE:HG23	23:W:9:LEU:HD12	1.88	0.56
1:A:2380:G:N2	21:U:42:GLY:O	2.33	0.56
1:A:2662:U:O2'	4:D:50:GLN:NE2	2.39	0.56
1:A:2830:A:H62	1:A:2910:G:N2	2.04	0.56
15:O:59:LYS:HA	15:O:62:ILE:HD12	1.88	0.56
17:Q:103:ILE:HD12	17:Q:104:VAL:N	2.21	0.56
18:R:24:LYS:HG2	18:R:81:THR:HG23	1.88	0.56
1:A:1073:A:H61	1:A:1169:G:H1'	1.70	0.55
1:A:1086:G:N1	1:A:1157:U:C2	2.74	0.55
19:S:89:LYS:O	19:S:91:VAL:HG13	2.06	0.55
1:A:193:A:H61	1:A:210:A:H1'	1.70	0.55
1:A:2359:C:OP1	21:U:54:TYR:OH	2.25	0.55
1:A:1869:G:C6	1:A:1925:U:O2	2.59	0.55
4:D:27:VAL:HG11	14:N:7:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:C:O2	1:A:317:G:N2	2.40	0.55
1:A:320:U:OP1	1:A:323:C:N4	2.40	0.55
1:A:926:G:H21	1:A:941:A:H62	1.55	0.55
1:A:2048:G:OP1	26:Z:9:SER:OG	2.17	0.55
1:A:2896:A:OP1	14:N:3:ASN:ND2	2.40	0.55
9:I:114:ILE:HA	9:I:117:LEU:HD12	1.87	0.55
1:A:458:A:OP2	1:A:2433:C:N4	2.39	0.55
1:A:928:C:N4	1:A:937:G:OP1	2.40	0.55
1:A:1187:A:OP1	8:H:28:ARG:NH1	2.39	0.55
1:A:2313:A:N6	27:1:19:THR:HG1	2.04	0.55
27:1:22:ASN:O	27:1:26:ASN:N	2.39	0.55
1:A:1039:C:O2	15:O:93:LYS:NZ	2.32	0.55
1:A:1086:G:C2	1:A:1157:U:O2	2.60	0.55
1:A:1080:G:H1	1:A:1163:U:HO2'	1.55	0.55
1:A:2276:U:N3	1:A:2280:G:OP2	2.38	0.55
5:E:60:GLY:HA2	5:E:78:ILE:HG22	1.87	0.55
21:U:72:ASP:N	21:U:72:ASP:OD1	2.38	0.55
29:3:31:HIS:CG	29:3:32:LEU:HD23	2.42	0.55
1:A:227:G:N2	1:A:235:G:H21	2.05	0.55
1:A:1302:G:N1	1:A:2041:A:OP2	2.38	0.55
1:A:2374:C:O3'	27:1:17:TYR:OH	2.18	0.55
1:A:2774:G:N7	30:4:19:ARG:NE	2.55	0.55
19:S:70:LEU:HD23	19:S:71:LEU:H	1.71	0.55
1:A:1103:G:O6	1:A:1124:A:N6	2.39	0.55
2:B:53:U:O2'	2:B:54:U:O4'	2.24	0.55
1:A:751:A:H61	1:A:770:G:C2'	2.20	0.55
1:A:2558:A:OP1	7:G:176:THR:OG1	2.25	0.55
1:A:2612:U:O2'	1:A:2613:C:OP2	2.19	0.55
10:J:55:LEU:HD23	10:J:60:ARG:HG2	1.88	0.55
1:A:1520:A:H62	1:A:1562:C:C1'	2.19	0.54
1:A:1931:G:O2'	1:A:1955:A:N1	2.31	0.54
1:A:2782:C:O2'	1:A:2783:U:OP2	2.15	0.54
9:I:81:GLU:OE1	9:I:81:GLU:N	2.39	0.54
1:A:790:G:N2	1:A:795:A:N6	2.40	0.54
1:A:11:U:O2'	1:A:12:U:OP1	2.21	0.54
1:A:1134:U:O4	1:A:1145:U:N3	2.41	0.54
1:A:1579:C:O2	1:A:1580:A:N6	2.31	0.54
1:A:1715:U:O2'	1:A:1717:G:N7	2.34	0.54
11:K:38:THR:HG22	11:K:39:THR:H	1.71	0.54
1:A:1448:U:O2	1:A:1450:A:N6	2.40	0.54
1:A:2129:C:H42	1:A:2213:U:H3'	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2558:A:OP2	7:G:176:THR:N	2.40	0.54
2:B:52:G:N2	6:F:26:MET:SD	2.77	0.54
3:C:185:LEU:HD13	3:C:186:SER:N	2.23	0.54
13:M:110:GLU:OE2	13:M:113:ARG:NH1	2.40	0.54
1:A:625:G:OP1	15:O:14:ARG:NH1	2.41	0.54
1:A:2374:C:C3'	27:1:17:TYR:HH	2.19	0.54
1:A:2546:U:O4'	1:A:2569:A:N6	2.40	0.54
1:A:333:C:N3	1:A:393:G:C2'	2.70	0.54
1:A:1466:G:H2'	1:A:1467:G:C8	2.43	0.54
1:A:2397:G:O2'	27:1:35:TYR:OH	2.25	0.54
5:E:157:GLU:CD	5:E:197:ALA:HB3	2.28	0.54
1:A:94:A:OP2	1:A:95:A:N6	2.41	0.54
1:A:1869:G:O6	1:A:1925:U:C2	2.60	0.54
1:A:2815:C:O2'	1:A:2829:A:N3	2.37	0.54
4:D:184:GLU:OE1	4:D:185:VAL:N	2.41	0.54
7:G:99:GLN:OE1	7:G:104:ILE:HD11	2.07	0.54
17:Q:52:MET:N	17:Q:52:MET:SD	2.81	0.54
1:A:652:A:N6	1:A:664:G:O2'	2.33	0.54
1:A:1884:G:O2'	1:A:1912:A:N6	2.38	0.54
1:A:1265:G:N7	15:O:16:LYS:NZ	2.56	0.54
1:A:2026:C:OP1	4:D:132:LYS:NZ	2.41	0.54
2:B:73:G:O2'	20:T:88:HIS:NE2	2.32	0.54
4:D:6:LEU:HD12	4:D:53:PHE:HB2	1.89	0.54
8:H:74:VAL:HG23	8:H:76:TYR:HE2	1.72	0.54
1:A:47:C:N4	1:A:48:G:O6	2.41	0.54
1:A:447:A:H61	1:A:468:A:H61	1.55	0.54
1:A:922:G:H22	1:A:945:A:H2	1.54	0.54
1:A:1459:A:N6	1:A:1631:G:O4'	2.41	0.54
10:J:111:ILE:O	10:J:112:LEU:HD23	2.07	0.54
13:M:14:ARG:O	13:M:18:VAL:HG23	2.07	0.54
1:A:443:U:O3'	22:V:32:ASN:ND2	2.41	0.53
1:A:527:G:O2'	1:A:552:A:N6	2.41	0.53
1:A:529:A:O5'	19:S:46:LYS:NZ	2.40	0.53
1:A:2618:C:N3	1:A:2630:G:N1	2.51	0.53
14:N:55:GLY:O	14:N:58:SER:OG	2.24	0.53
1:A:1153:C:O3'	1:A:2778:G:O6	2.11	0.53
1:A:2680:U:N3	7:G:110:SER:OG	2.41	0.53
1:A:2878:U:O2'	1:A:2879:G:OP1	2.23	0.53
3:C:65:ILE:HD12	3:C:66:ASP:N	2.23	0.53
4:D:104:GLU:N	4:D:104:GLU:OE1	2.42	0.53
1:A:333:C:C6	1:A:393:G:C4	2.95	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2354:A:N7	1:A:2415:A:N6	2.56	0.53
2:B:4:G:O6	2:B:111:C:N4	2.41	0.53
6:F:66:LEU:HD13	25:Y:5:ILE:HG21	1.91	0.53
1:A:970:U:H3'	1:A:971:U:H4'	1.90	0.53
2:B:42:G:O4'	2:B:45:C:N4	2.42	0.53
29:3:22:LEU:O	29:3:49:LEU:HD23	2.08	0.53
1:A:1261:G:N2	1:A:1264:A:OP2	2.40	0.53
1:A:1440:A:HO2'	1:A:1514:A:C4'	2.20	0.53
1:A:1465:G:C2'	1:A:1537:A:H62	2.22	0.53
1:A:1697:G:O6	12:L:7:GLY:N	2.40	0.53
1:A:250:G:O6	29:3:12:LYS:NZ	2.26	0.53
1:A:736:C:O4'	3:C:43:ARG:NH2	2.40	0.53
1:A:564:U:O2'	17:Q:73:GLU:OE2	2.25	0.53
1:A:797:A:OP1	28:2:4:ARG:NH2	2.40	0.53
1:A:1561:G:O4'	1:A:1604:C:O2'	2.26	0.53
1:A:1864:C:O3'	1:A:1954:A:O2'	2.23	0.53
1:A:1935:C:N3	1:A:1949:G:N1	2.47	0.53
4:D:10:ILE:HG12	4:D:27:VAL:HG13	1.90	0.53
1:A:388:A:O2'	1:A:390:A:N6	2.40	0.53
1:A:2566:C:O2'	1:A:2768:A:O2'	2.25	0.53
4:D:9:LYS:NZ	4:D:203:GLY:O	2.40	0.53
12:L:109:ARG:NH2	12:L:112:ASP:OD2	2.41	0.53
29:3:37:SER:O	29:3:41:LYS:NZ	2.39	0.53
1:A:632:U:O3'	5:E:95:ARG:NH1	2.42	0.53
1:A:1395:G:O2'	1:A:1410:A:N6	2.39	0.53
1:A:2324:C:C2	1:A:2348:G:N2	2.77	0.53
1:A:2495:A:N7	1:A:2504:C:C4	2.77	0.53
21:U:44:ILE:C	21:U:45:LEU:HD23	2.28	0.53
1:A:1088:C:N4	1:A:1156:G:O6	2.42	0.52
1:A:2674:U:O4	1:A:2700:G:O6	2.26	0.52
13:M:28:LYS:CB	13:M:93:VAL:HG23	2.39	0.52
18:R:34:ASN:OD1	18:R:36:THR:N	2.42	0.52
23:W:61:GLU:OE1	23:W:61:GLU:N	2.42	0.52
1:A:688:A:O2'	1:A:689:A:O4'	2.28	0.52
1:A:750:A:H61	1:A:771:G:C4'	2.22	0.52
1:A:2141:A:N3	1:A:2193:G:O2'	2.42	0.52
6:F:99:PHE:CE2	6:F:103:LEU:HD22	2.44	0.52
17:Q:66:THR:HA	17:Q:69:LEU:HD12	1.91	0.52
1:A:791:U:H1'	1:A:793:G:H21	1.74	0.52
1:A:1723:A:O4'	1:A:2017:C:O2'	2.25	0.52
1:A:2496:A:N6	1:A:2508:G:N9	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2778:G:H21	1:A:2778:G:P	2.32	0.52
7:G:23:HIS:NE2	7:G:34:SER:OG	2.33	0.52
12:L:52:LYS:NZ	12:L:96:ARG:O	2.43	0.52
27:1:29:ARG:NH2	27:1:47:GLU:O	2.41	0.52
1:A:1018:A:O4'	1:A:1225:G:N2	2.43	0.52
1:A:1080:G:N1	1:A:1164:G:N7	2.57	0.52
1:A:1957:G:O2'	1:A:1995:G:O6	2.12	0.52
5:E:21:ASP:O	5:E:25:GLY:N	2.38	0.52
8:H:37:LEU:HD11	8:H:119:GLN:HB3	1.91	0.52
18:R:6:ILE:CG1	18:R:7:LEU:HD12	2.40	0.52
1:A:302:A:N7	1:A:450:C:O2'	2.40	0.52
1:A:904:G:O2'	1:A:961:G:O6	2.24	0.52
1:A:2417:U:N3	1:A:2452:A:N7	2.57	0.52
1:A:2662:U:O2'	4:D:90:GLU:OE2	2.11	0.52
1:A:2706:A:N3	4:D:200:ASN:ND2	2.56	0.52
3:C:44:ASN:O	3:C:47:GLY:N	2.41	0.52
5:E:157:GLU:OE2	5:E:195:THR:OG1	2.23	0.52
1:A:352:A:N6	1:A:1248:U:C2	2.68	0.52
1:A:2125:U:C2	1:A:2218:G:N1	2.69	0.52
1:A:2783:U:O2'	1:A:2783:U:O2	2.28	0.52
1:A:84:A:C5	1:A:101:G:N2	2.78	0.52
1:A:616:G:N2	1:A:2058:A:OP1	2.43	0.52
9:I:17:ARG:NH2	9:I:46:ALA:O	2.41	0.52
15:O:99:ALA:HB2	15:O:106:PHE:HE1	1.75	0.52
1:A:207:A:O2'	1:A:208:G:OP2	2.27	0.52
1:A:228:A:O2'	1:A:229:A:O4'	2.28	0.52
1:A:1336:G:N1	1:A:1684:A:OP2	2.40	0.52
1:A:333:C:C2	1:A:393:G:C2'	2.93	0.52
1:A:2905:C:H42	26:Z:37:LYS:NZ	2.08	0.52
5:E:77:THR:OG1	5:E:78:ILE:N	2.42	0.52
6:F:30:LYS:O	6:F:159:THR:OG1	2.21	0.52
6:F:108:LEU:HD21	25:Y:56:PRO:CD	2.40	0.52
23:W:45:THR:HG23	23:W:46:VAL:CG2	2.39	0.52
1:A:2774:G:N2	1:A:2784:A:N1	2.58	0.52
1:A:2822:C:O2'	1:A:2824:G:O6	2.11	0.52
13:M:36:SER:OG	13:M:37:ASN:N	2.41	0.52
18:R:24:LYS:CG	18:R:81:THR:HG23	2.40	0.52
1:A:1072:A:H62	1:A:1170:A:H62	1.57	0.51
1:A:1385:G:N2	1:A:1642:C:H42	2.08	0.51
1:A:1470:G:O2'	1:A:1619:A:N6	2.37	0.51
1:A:2421:C:H42	1:A:2459:A:H62	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2817:A:N7	1:A:2822:C:O2'	2.43	0.51
7:G:33:LEU:HD11	7:G:136:ILE:HG13	1.91	0.51
19:S:7:ASP:O	19:S:23:VAL:HG12	2.09	0.51
20:T:22:ARG:NE	20:T:87:THR:O	2.36	0.51
1:A:84:A:O5'	19:S:4:LYS:NZ	2.32	0.51
1:A:2907:A:H1'	26:Z:28:THR:HG22	1.93	0.51
4:D:14:GLN:OE1	4:D:14:GLN:N	2.43	0.51
23:W:7:ARG:O	23:W:60:ARG:NH1	2.43	0.51
1:A:75:G:H22	1:A:110:A:H2	1.58	0.51
1:A:2019:G:N2	1:A:2023:C:O2'	2.42	0.51
4:D:11:GLY:O	4:D:27:VAL:HG12	2.10	0.51
11:K:43:THR:OG1	11:K:46:GLN:OE1	2.25	0.51
12:L:18:ARG:NH2	12:L:64:LYS:O	2.43	0.51
21:U:12:LYS:HA	21:U:12:LYS:HZ2	1.76	0.51
1:A:1675:G:H1'	1:A:1679:A:H61	1.75	0.51
1:A:2092:C:H5'	1:A:2278:G:H21	1.75	0.51
12:L:72:LEU:HD21	12:L:76:GLU:HA	1.92	0.51
16:P:68:GLY:O	16:P:89:ARG:NE	2.41	0.51
1:A:1880:A:N6	1:A:2114:G:HO2'	2.09	0.51
1:A:2702:A:N6	1:A:2759:G:N1	2.57	0.51
3:C:159:GLY:H	3:C:195:VAL:HG23	1.75	0.51
9:I:24:VAL:HG11	9:I:33:ALA:HB2	1.92	0.51
9:I:112:MET:SD	9:I:113:LYS:N	2.81	0.51
28:2:33:ALA:O	28:2:37:ARG:N	2.43	0.51
1:A:254:A:OP1	29:3:7:HIS:NE2	2.41	0.51
1:A:1710:G:OP1	9:I:66:LYS:NZ	2.44	0.51
1:A:2418:G:O2'	1:A:2419:A:OP2	2.22	0.51
5:E:117:LYS:CD	5:E:192:LEU:HD23	2.40	0.51
17:Q:28:ASN:N	17:Q:28:ASN:OD1	2.44	0.51
1:A:1592:A:O2'	1:A:1593:G:O4'	2.28	0.51
16:P:31:ASP:N	16:P:31:ASP:OD1	2.44	0.51
18:R:90:PHE:HD2	23:W:34:THR:HG21	1.74	0.51
25:Y:38:GLU:OE1	25:Y:38:GLU:N	2.43	0.51
5:E:138:GLU:O	5:E:142:VAL:HG23	2.10	0.51
8:H:34:ALA:HB1	8:H:110:LEU:HD21	1.92	0.51
8:H:123:LEU:HD12	8:H:124:PHE:H	1.76	0.51
1:A:84:A:C6	1:A:101:G:N2	2.73	0.51
1:A:297:G:O2'	1:A:298:U:O5'	2.27	0.51
1:A:928:C:O2'	1:A:939:U:O4	2.09	0.51
1:A:1293:U:N3	5:E:72:ARG:O	2.41	0.51
4:D:87:PHE:C	4:D:88:ILE:HD12	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:59:ARG:CD	12:L:82:LEU:HD21	2.41	0.51
14:N:27:THR:C	14:N:28:LEU:HD12	2.31	0.51
1:A:81:G:H1	1:A:104:C:H42	1.56	0.51
1:A:1213:C:N4	1:A:1219:G:H22	2.09	0.51
1:A:1396:A:OP2	1:A:1408:G:N1	2.43	0.51
1:A:1440:A:HO2'	1:A:1514:A:C1'	2.23	0.51
1:A:1731:G:H21	1:A:1745:A:H62	1.57	0.51
1:A:2052:C:HO2'	1:A:2053:U:H5'	1.76	0.51
1:A:2479:C:N3	1:A:2531:U:O4	2.44	0.51
17:Q:86:ARG:O	17:Q:92:SER:OG	2.29	0.51
1:A:252:C:O2'	10:J:63:LYS:NZ	2.21	0.50
1:A:1251:A:OP2	1:A:1274:G:N2	2.38	0.50
1:A:2324:C:C2	1:A:2348:G:N1	2.79	0.50
1:A:2499:G:H21	1:A:2505:A:N6	2.08	0.50
1:A:2710:C:N3	1:A:2754:G:O2'	2.32	0.50
2:B:7:G:H1'	2:B:110:C:H42	1.76	0.50
1:A:23:G:H21	17:Q:77:ASN:ND2	2.08	0.50
1:A:1891:U:C5'	1:A:2437:G:H21	2.24	0.50
6:F:45:GLN:O	6:F:45:GLN:NE2	2.42	0.50
6:F:162:THR:OG1	6:F:163:ASP:N	2.44	0.50
8:H:9:GLU:HA	8:H:12:ILE:HD11	1.92	0.50
1:A:909:G:N7	11:K:22:LYS:NZ	2.57	0.50
1:A:1833:C:OP1	3:C:250:TRP:NE1	2.39	0.50
1:A:1891:U:H5'	1:A:2437:G:H21	1.76	0.50
9:I:3:GLN:O	9:I:6:THR:OG1	2.30	0.50
1:A:774:G:O4'	3:C:207:LYS:NZ	2.42	0.50
1:A:1613:G:OP1	3:C:210:ARG:NE	2.43	0.50
7:G:146:SER:O	7:G:149:ARG:NH1	2.43	0.50
8:H:63:ILE:O	8:H:94:ARG:NH2	2.44	0.50
12:L:22:THR:HG21	12:L:69:VAL:HG21	1.92	0.50
1:A:1490:G:N2	1:A:1490:G:OP1	2.45	0.50
1:A:2499:G:N2	1:A:2506:U:O4	2.45	0.50
4:D:47:ASN:OD1	4:D:47:ASN:N	2.45	0.50
21:U:58:ASN:N	21:U:58:ASN:OD1	2.43	0.50
7:G:99:GLN:N	7:G:102:ASP:O	2.40	0.50
9:I:70:ARG:NH1	9:I:76:TYR:OH	2.44	0.50
1:A:224:A:O2'	1:A:269:G:N7	2.33	0.50
1:A:2102:U:OP2	1:A:2265:G:O2'	2.27	0.50
5:E:9:LEU:HD11	5:E:129:PHE:HD1	1.77	0.50
12:L:33:THR:OG1	12:L:34:GLU:N	2.44	0.50
15:O:82:GLY:HA2	15:O:117:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1401:G:N2	1:A:1404:A:OP2	2.39	0.50
1:A:1472:C:N4	1:A:1617:A:OP2	2.25	0.50
1:A:1879:U:O2	1:A:1916:A:N7	2.44	0.50
3:C:134:ASN:N	3:C:134:ASN:OD1	2.45	0.50
5:E:33:LEU:HD21	5:E:183:VAL:CG2	2.42	0.50
9:I:17:ARG:NH2	9:I:45:ASN:OD1	2.45	0.50
1:A:583:A:O2'	8:H:8:ASN:OD1	2.26	0.50
1:A:1353:A:O4'	1:A:1429:G:N2	2.41	0.50
1:A:1397:G:N2	1:A:2241:C:N3	2.59	0.50
1:A:2749:G:O2'	1:A:2750:C:OP1	2.26	0.50
12:L:72:LEU:HD22	12:L:77:THR:O	2.11	0.50
15:O:35:ALA:O	15:O:39:VAL:HG23	2.12	0.50
1:A:340:C:OP1	19:S:90:LYS:NZ	2.31	0.49
1:A:1889:G:C6	1:A:1907:U:N3	2.79	0.49
4:D:189:ASP:OD1	4:D:190:THR:N	2.45	0.49
17:Q:48:GLU:OE1	17:Q:49:LYS:N	2.44	0.49
2:B:64:A:H1'	2:B:66:C:H41	1.77	0.49
5:E:123:LEU:HD12	5:E:124:THR:N	2.28	0.49
10:J:125:ALA:O	10:J:146:ILE:N	2.44	0.49
1:A:1465:G:H2'	1:A:1537:A:H62	1.77	0.49
4:D:213:THR:HG22	4:D:214:SER:O	2.12	0.49
6:F:50:LEU:O	6:F:54:VAL:HG23	2.11	0.49
6:F:142:ASP:OD1	6:F:143:TYR:N	2.42	0.49
6:F:156:ILE:CG2	6:F:158:THR:HG23	2.42	0.49
9:I:20:LEU:HD12	9:I:21:THR:N	2.28	0.49
1:A:434:G:HO2'	1:A:435:A:P	2.34	0.49
1:A:1302:G:O2'	1:A:2042:A:N6	2.34	0.49
1:A:1067:U:O2'	1:A:1166:G:OP1	2.29	0.49
1:A:1467:G:O5'	1:A:1535:G:O2'	2.26	0.49
2:B:40:C:C1'	6:F:66:LEU:HD22	2.43	0.49
1:A:673:G:O2'	1:A:696:G:O2'	2.31	0.49
1:A:2780:A:H2	30:4:17:ILE:HG21	1.72	0.49
5:E:121:ASN:OD1	5:E:121:ASN:N	2.45	0.49
6:F:33:LYS:C	6:F:34:ILE:HD12	2.33	0.49
1:A:1175:G:O2'	1:A:2052:C:O2'	2.24	0.49
1:A:1198:G:OP2	15:O:58:ARG:NH2	2.44	0.49
4:D:9:LYS:NZ	4:D:201:VAL:O	2.45	0.49
11:K:41:TRP:C	11:K:42:ILE:HD12	2.32	0.49
14:N:107:GLY:O	14:N:110:ALA:N	2.45	0.49
1:A:1091:G:N1	1:A:1154:G:O2'	2.33	0.49
1:A:1885:G:N2	1:A:1911:A:OP2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1952:C:H42	1:A:1956:G:N2	2.11	0.49
1:A:2185:A:O2'	1:A:2186:G:O5'	2.28	0.49
1:A:2770:U:O5'	1:A:2782:C:N4	2.46	0.49
3:C:205:VAL:HG13	3:C:210:ARG:HD3	1.94	0.49
23:W:19:LYS:NZ	23:W:23:GLU:OE2	2.45	0.49
1:A:82:G:N1	1:A:101:G:O3'	2.43	0.49
1:A:302:A:O2'	1:A:303:G:N7	2.27	0.49
1:A:333:C:N1	1:A:393:G:C4	2.81	0.49
1:A:2176:C:HO2'	1:A:2199:U:H3	1.58	0.49
3:C:160:ALA:H	3:C:195:VAL:HG22	1.78	0.49
11:K:57:TYR:CD2	11:K:117:ALA:HB2	2.48	0.49
27:1:14:ASP:N	27:1:14:ASP:OD1	2.46	0.49
1:A:1448:U:C4	1:A:1635:A:N1	2.80	0.49
1:A:1731:G:N2	1:A:1745:A:H62	2.10	0.49
1:A:2189:G:O2'	1:A:2200:A:N7	2.40	0.49
1:A:2557:U:O2'	1:A:2561:C:N4	2.45	0.49
3:C:108:LYS:N	3:C:194:GLN:O	2.41	0.49
3:C:123:ASP:OD1	3:C:125:LYS:NZ	2.42	0.49
1:A:82:G:H22	1:A:102:A:P	2.35	0.48
1:A:1000:G:OP2	11:K:87:LYS:NZ	2.46	0.48
1:A:2161:A:H61	1:A:2184:G:C2'	2.25	0.48
1:A:2672:G:H1	1:A:2797:C:H42	1.60	0.48
6:F:8:PHE:O	6:F:12:VAL:HG22	2.13	0.48
7:G:111:HIS:O	7:G:113:VAL:HG13	2.12	0.48
13:M:73:ALA:HB1	13:M:108:LEU:HB2	1.95	0.48
17:Q:1:MET:SD	17:Q:1:MET:N	2.85	0.48
1:A:2703:C:O2	1:A:2759:G:N2	2.43	0.48
8:H:142:GLU:N	8:H:142:GLU:OE1	2.46	0.48
9:I:35:ILE:HD11	9:I:65:THR:H	1.77	0.48
18:R:47:ASN:O	18:R:47:ASN:ND2	2.46	0.48
1:A:1504:U:O2'	1:A:1505:G:OP2	2.26	0.48
1:A:672:A:O2'	1:A:681:G:N2	2.42	0.48
1:A:749:G:N2	1:A:772:A:N6	2.43	0.48
1:A:751:A:H61	1:A:770:G:H1'	1.77	0.48
3:C:77:LYS:N	3:C:95:VAL:O	2.46	0.48
15:O:108:GLN:O	15:O:111:THR:OG1	2.29	0.48
1:A:352:A:C2'	1:A:372:A:HO2'	2.23	0.48
1:A:1953:U:O2'	1:A:1954:A:N7	2.34	0.48
1:A:2361:U:O4	1:A:2363:A:C5	2.66	0.48
6:F:110:ARG:O	6:F:135:GLN:NE2	2.47	0.48
7:G:72:LEU:O	7:G:76:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:58:ASN:O	21:U:70:LYS:N	2.42	0.48
1:A:19:G:OP1	15:O:23:GLY:N	2.42	0.48
1:A:392:U:N3	1:A:393:G:O6	2.47	0.48
1:A:918:G:N7	11:K:2:LEU:HD23	2.28	0.48
1:A:1501:G:N2	1:A:2729:G:H22	2.09	0.48
1:A:2044:C:HO2'	26:Z:6:ARG:HH11	1.60	0.48
1:A:2559:G:N3	1:A:2690:G:N2	2.57	0.48
5:E:111:ARG:HG2	5:E:206:LEU:HD23	1.95	0.48
21:U:39:VAL:HG22	21:U:73:GLY:O	2.12	0.48
1:A:821:C:O2'	1:A:822:G:OP1	2.28	0.48
1:A:973:A:O2'	24:X:40:ASN:ND2	2.47	0.48
1:A:1396:A:N7	1:A:1409:U:O4	2.46	0.48
1:A:1881:A:N1	1:A:2114:G:O2'	2.32	0.48
1:A:2281:C:H42	21:U:15:VAL:CG2	2.26	0.48
5:E:201:LYS:O	5:E:205:VAL:HG23	2.13	0.48
17:Q:55:LEU:CD2	17:Q:105:VAL:HG11	2.44	0.48
1:A:513:G:OP1	28:2:34:ARG:NH2	2.47	0.48
1:A:616:G:O2'	1:A:618:A:OP1	2.20	0.48
1:A:2421:C:N4	1:A:2459:A:H62	2.10	0.48
1:A:2485:U:O2	1:A:2486:A:N6	2.45	0.48
1:A:2784:A:N1	7:G:67:THR:HG21	2.28	0.48
3:C:144:ILE:HG23	3:C:190:ALA:HB2	1.95	0.48
18:R:34:ASN:N	18:R:37:GLN:OE1	2.45	0.48
1:A:390:A:H3'	1:A:391:A:H4'	1.96	0.48
1:A:2559:G:N2	1:A:2690:G:N3	2.62	0.48
8:H:123:LEU:HD12	8:H:124:PHE:N	2.28	0.48
15:O:62:ILE:HG23	15:O:76:TYR:CE1	2.49	0.48
1:A:364:A:OP2	5:E:135:LYS:NZ	2.39	0.48
1:A:774:G:O5'	3:C:207:LYS:NZ	2.47	0.48
1:A:882:C:H5	1:A:986:G:H22	1.61	0.48
1:A:2171:G:N2	1:A:2174:A:N7	2.62	0.48
5:E:170:ILE:HG22	5:E:171:PRO:O	2.13	0.48
12:L:59:ARG:HD2	12:L:82:LEU:HD21	1.96	0.48
1:A:545:G:N1	1:A:548:A:OP2	2.43	0.47
1:A:1083:G:N2	1:A:1160:C:C2	2.63	0.47
1:A:1290:G:O4'	15:O:33:LYS:NZ	2.25	0.47
1:A:1892:U:P	1:A:2436:G:H21	2.36	0.47
1:A:2780:A:O2'	30:4:26:ILE:HG21	2.14	0.47
5:E:37:ILE:HG23	5:E:184:LEU:CD1	2.43	0.47
5:E:123:LEU:HD12	5:E:124:THR:H	1.77	0.47
29:3:63:ALA:HB3	29:3:64:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:G:N1	1:A:474:A:OP2	2.44	0.47
1:A:915:U:OP1	11:K:6:ARG:NH1	2.47	0.47
6:F:130:LEU:HD23	6:F:131:GLY:N	2.29	0.47
30:4:31:LYS:O	30:4:32:HIS:ND1	2.47	0.47
1:A:40:U:O4	1:A:41:A:N6	2.47	0.47
1:A:1536:C:O2'	1:A:1537:A:N7	2.43	0.47
1:A:1731:G:H21	1:A:1745:A:N6	2.11	0.47
1:A:2499:G:H22	30:4:2:LYS:HZ1	1.62	0.47
3:C:66:ASP:N	3:C:66:ASP:OD1	2.47	0.47
8:H:45:TYR:O	15:O:64:ARG:NH2	2.41	0.47
9:I:21:THR:OG1	9:I:22:ILE:N	2.48	0.47
13:M:73:ALA:O	13:M:108:LEU:HD13	2.14	0.47
19:S:38:VAL:N	19:S:60:GLU:OE1	2.47	0.47
24:X:4:LEU:HD23	24:X:58:GLU:HA	1.96	0.47
1:A:323:C:O2	1:A:324:A:N6	2.47	0.47
1:A:1339:U:HO2'	1:A:1340:G:P	2.37	0.47
1:A:2593:A:N1	9:I:28:SER:OG	2.31	0.47
6:F:31:ILE:HA	6:F:158:THR:HG22	1.97	0.47
6:F:134:GLU:HB2	6:F:137:ILE:HD11	1.95	0.47
23:W:14:ILE:HG22	23:W:18:ILE:HD11	1.96	0.47
1:A:1141:U:O2'	1:A:1142:A:O4'	2.24	0.47
1:A:2774:G:OP1	7:G:138:LYS:NZ	2.31	0.47
3:C:2:ALA:N	3:C:20:ASP:OD1	2.47	0.47
4:D:3:LYS:HE3	4:D:109:THR:HG22	1.96	0.47
9:I:111:PHE:O	9:I:114:ILE:N	2.47	0.47
26:Z:18:THR:HG23	26:Z:19:HIS:H	1.79	0.47
1:A:699:U:O2'	1:A:700:A:O5'	2.26	0.47
1:A:1320:G:N2	1:A:1323:A:OP2	2.47	0.47
1:A:1496:G:HO2'	1:A:1497:A:C5'	2.25	0.47
1:A:2125:U:N3	1:A:2218:G:C6	2.77	0.47
1:A:2338:A:OP1	1:A:2340:C:N4	2.45	0.47
1:A:2710:C:H42	1:A:2754:G:C2'	2.28	0.47
4:D:83:ALA:HB1	4:D:84:PRO:CD	2.45	0.47
26:Z:28:THR:HG21	26:Z:39:SER:OG	2.15	0.47
1:A:1034:A:O2'	1:A:1036:C:OP2	2.32	0.47
1:A:1726:A:P	1:A:1743:G:H22	2.37	0.47
2:B:74:G:OP1	20:T:9:ARG:NH2	2.47	0.47
6:F:104:ILE:HD12	6:F:173:PHE:CB	2.45	0.47
1:A:333:C:H41	1:A:392:U:H3'	1.79	0.47
1:A:2775:A:H62	1:A:2781:U:H3	1.63	0.47
1:A:2870:A:P	1:A:2886:G:H22	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:120:LYS:C	10:J:121:LEU:HD23	2.35	0.47
13:M:56:ALA:CB	13:M:80:ILE:HD13	2.37	0.47
1:A:1636:U:O4	1:A:1637:A:N6	2.48	0.47
1:A:1758:A:O2'	1:A:1759:G:OP2	2.25	0.47
1:A:2775:A:O2'	7:G:62:ARG:O	2.32	0.47
1:A:2878:U:HO2'	1:A:2879:G:P	2.39	0.47
13:M:92:ILE:HD12	13:M:93:VAL:N	2.30	0.47
1:A:19:G:O3'	15:O:22:LYS:NZ	2.49	0.46
1:A:943:C:N4	1:A:944:G:O6	2.49	0.46
1:A:1712:A:O2'	1:A:1718:G:N7	2.45	0.46
1:A:2142:G:O2'	1:A:2192:G:N2	2.46	0.46
1:A:2774:G:C2'	7:G:67:THR:HG22	2.45	0.46
3:C:142:HIS:ND1	3:C:193:GLY:O	2.48	0.46
12:L:11:ASP:OD1	12:L:12:GLN:N	2.48	0.46
1:A:275:A:H61	1:A:296:G:C2'	2.29	0.46
1:A:762:C:O2	1:A:763:A:O2'	2.16	0.46
1:A:1675:G:N2	1:A:1679:A:H62	2.11	0.46
1:A:2313:A:H62	27:1:19:THR:HG1	1.60	0.46
1:A:2776:A:N6	30:4:18:LYS:O	2.45	0.46
3:C:124:ILE:HD12	3:C:124:ILE:N	2.30	0.46
4:D:189:ASP:OD1	4:D:191:GLU:N	2.47	0.46
6:F:117:VAL:HG13	6:F:175:MET:HE2	1.96	0.46
15:O:116:ALA:C	15:O:117:LEU:HD23	2.35	0.46
19:S:7:ASP:OD1	19:S:7:ASP:N	2.44	0.46
1:A:1397:G:C2	1:A:2241:C:N3	2.84	0.46
1:A:1425:G:C4'	1:A:1571:G:H21	2.28	0.46
1:A:275:A:H61	1:A:296:G:H2'	1.80	0.46
1:A:1250:G:O2'	1:A:1274:G:N1	2.48	0.46
1:A:1699:A:N6	1:A:2032:A:O2'	2.43	0.46
1:A:2311:U:H3	1:A:2411:A:H62	1.62	0.46
1:A:2698:A:H3'	1:A:2699:U:H5''	1.96	0.46
1:A:2710:C:O2	9:I:76:TYR:OH	2.33	0.46
1:A:2828:U:N3	1:A:2911:A:N7	2.60	0.46
3:C:202:LEU:N	3:C:202:LEU:HD23	2.31	0.46
7:G:52:VAL:O	7:G:65:HIS:NE2	2.48	0.46
12:L:106:GLN:NE2	12:L:118:ILE:HD12	2.30	0.46
1:A:385:U:O2'	1:A:386:C:OP1	2.29	0.46
1:A:2496:A:C6	1:A:2508:G:C4	3.03	0.46
2:B:74:G:O2'	20:T:78:GLN:NE2	2.42	0.46
3:C:165:LEU:HD21	3:C:175:ARG:NH1	2.31	0.46
1:A:333:C:C2	1:A:393:G:H2'	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1526:G:N2	1:A:1552:U:O4	2.48	0.46
1:A:1844:G:OP1	3:C:87:ARG:NH2	2.49	0.46
1:A:2866:G:OP1	14:N:54:GLY:N	2.49	0.46
1:A:1539:A:N3	1:A:1624:C:O2'	2.28	0.46
1:A:1827:C:OP1	3:C:260:ARG:NH2	2.46	0.46
6:F:23:SER:N	6:F:27:GLU:OE2	2.49	0.46
8:H:58:ILE:HD12	8:H:59:ASN:N	2.30	0.46
19:S:11:VAL:HG22	19:S:19:LYS:O	2.16	0.46
1:A:1834:G:N2	1:A:1837:A:OP2	2.39	0.46
4:D:9:LYS:O	4:D:206:LYS:N	2.46	0.46
19:S:25:ALA:HB3	19:S:34:VAL:CG1	2.45	0.46
1:A:163:U:O2'	1:A:164:A:OP2	2.25	0.46
1:A:245:G:O2'	1:A:257:G:O6	2.27	0.46
1:A:1962:G:H22	1:A:1991:G:P	2.39	0.46
23:W:14:ILE:HG22	23:W:18:ILE:CD1	2.46	0.46
1:A:82:G:N2	1:A:102:A:OP2	2.49	0.46
9:I:106:LEU:N	9:I:106:LEU:HD23	2.31	0.46
1:A:394:U:O2'	1:A:395:U:O2	2.25	0.45
1:A:2048:G:OP2	26:Z:12:ARG:NH2	2.49	0.45
1:A:2774:G:O6	30:4:20:LYS:NZ	2.45	0.45
2:B:43:A:O4'	6:F:92:ARG:NE	2.49	0.45
2:B:64:A:H61	2:B:105:C:C5'	2.29	0.45
6:F:4:LEU:HD21	6:F:173:PHE:CB	2.46	0.45
16:P:53:VAL:HG21	16:P:56:ALA:HB3	1.97	0.45
1:A:373:A:H2	1:A:1248:U:HO2'	1.62	0.45
5:E:185:ASP:OD1	5:E:186:ILE:N	2.49	0.45
6:F:118:SER:OG	6:F:128:TYR:OH	2.33	0.45
23:W:11:THR:HA	23:W:14:ILE:HD12	1.98	0.45
1:A:611:U:N3	1:A:614:U:OP2	2.48	0.45
1:A:1475:A:N6	1:A:1606:C:O2	2.49	0.45
1:A:2782:C:O5'	30:4:19:ARG:NH1	2.46	0.45
5:E:141:ASN:O	5:E:144:SER:OG	2.28	0.45
6:F:46:ASN:OD1	6:F:46:ASN:N	2.49	0.45
1:A:1644:C:OP1	18:R:76:ARG:NH1	2.49	0.45
2:B:12:U:OP2	21:U:82:ARG:NH1	2.50	0.45
2:B:21:G:N1	2:B:22:G:O6	2.50	0.45
3:C:180:GLU:OE1	3:C:180:GLU:N	2.49	0.45
5:E:5:ASP:HB2	5:E:7:LEU:HD21	1.98	0.45
5:E:33:LEU:HD22	5:E:37:ILE:HD11	1.97	0.45
7:G:137:SER:O	7:G:141:VAL:N	2.45	0.45
8:H:93:LEU:HD23	8:H:96:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:18:THR:HG22	24:X:49:LYS:NZ	2.32	0.45
1:A:572:C:N4	1:A:2806:U:OP2	2.50	0.45
1:A:1304:G:OP1	26:Z:16:ARG:NE	2.44	0.45
1:A:2507:C:N4	1:A:2508:G:O6	2.49	0.45
1:A:2686:G:O2'	1:A:2688:G:N7	2.37	0.45
1:A:2767:A:OP2	1:A:2790:G:N1	2.47	0.45
1:A:2773:U:O4	30:4:20:LYS:NZ	2.50	0.45
1:A:2820:U:O2'	1:A:2823:G:N7	2.45	0.45
5:E:108:LEU:HD12	5:E:108:LEU:O	2.16	0.45
6:F:98:GLU:OE1	6:F:98:GLU:N	2.50	0.45
6:F:148:LYS:NZ	6:F:149:VAL:O	2.46	0.45
1:A:213:C:OP2	28:2:30:LYS:NZ	2.48	0.45
1:A:333:C:C6	1:A:393:G:N3	2.85	0.45
1:A:2091:C:O2'	1:A:2278:G:N2	2.49	0.45
1:A:2177:U:OP2	1:A:2187:G:O2'	2.29	0.45
1:A:2338:A:O3'	6:F:74:ILE:HD12	2.17	0.45
9:I:13:ASN:OD1	9:I:96:THR:N	2.50	0.45
1:A:923:A:H2	1:A:944:G:H22	1.65	0.45
2:B:77:G:N1	2:B:95:U:C2	2.77	0.45
6:F:134:GLU:OE2	6:F:150:ARG:N	2.50	0.45
23:W:34:THR:O	23:W:36:GLN:N	2.44	0.45
1:A:64:A:O2'	18:R:68:TYR:O	2.34	0.45
1:A:222:A:N3	1:A:237:U:O2'	2.45	0.45
1:A:862:C:N3	1:A:1230:G:N1	2.65	0.45
1:A:1375:G:O6	18:R:61:LYS:NZ	2.21	0.45
1:A:1891:U:C4'	1:A:2437:G:H21	2.30	0.45
1:A:2125:U:O2	1:A:2218:G:C2	2.69	0.45
1:A:319:G:C4'	1:A:325:A:H62	2.30	0.45
1:A:2709:U:O4	1:A:2755:U:O2'	2.20	0.45
2:B:29:C:OP1	13:M:4:LYS:NZ	2.41	0.45
3:C:185:LEU:HD12	3:C:187:THR:O	2.17	0.45
6:F:142:ASP:O	6:F:144:ASP:N	2.49	0.45
21:U:45:LEU:HD23	21:U:45:LEU:N	2.32	0.45
1:A:777:C:H2'	1:A:778:G:O4'	2.17	0.45
1:A:1284:A:O2'	5:E:45:ARG:NH1	2.49	0.45
1:A:2017:C:H2'	1:A:2018:U:O4'	2.17	0.45
2:B:87:C:H1'	11:K:18:THR:HG22	1.99	0.45
20:T:92:LEU:HD13	20:T:93:ALA:N	2.32	0.45
1:A:988:C:O2'	1:A:989:A:OP1	2.32	0.44
1:A:1518:G:HO2'	1:A:1519:U:H6	1.65	0.44
1:A:2044:C:O2'	1:A:2046:U:OP2	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:114:ALA:O	12:L:116:SER:N	2.50	0.44
13:M:89:ILE:HA	13:M:117:LEU:HD22	1.98	0.44
15:O:39:VAL:O	15:O:42:SER:OG	2.32	0.44
1:A:312:A:O2'	1:A:404:U:OP2	2.20	0.44
1:A:336:U:C4	1:A:388:A:N1	2.85	0.44
1:A:401:U:H2'	1:A:402:C:H6	1.81	0.44
2:B:109:G:HO2'	2:B:110:C:C1'	2.25	0.44
25:Y:6:HIS:ND1	25:Y:7:PRO:O	2.50	0.44
1:A:225:A:O2'	1:A:227:G:N7	2.49	0.44
1:A:417:A:H61	1:A:447:A:H3'	1.80	0.44
1:A:534:G:N2	1:A:537:A:OP2	2.50	0.44
1:A:1290:G:N3	15:O:33:LYS:NZ	2.66	0.44
1:A:1965:A:N3	1:A:2632:U:O2'	2.40	0.44
1:A:2726:C:N4	1:A:2736:G:O6	2.50	0.44
3:C:132:LEU:HD12	3:C:185:LEU:O	2.17	0.44
6:F:63:GLN:CG	6:F:89:VAL:HG13	2.47	0.44
13:M:30:ARG:NH2	13:M:47:ASP:OD1	2.50	0.44
1:A:842:U:OP1	5:E:62:ARG:NH2	2.50	0.44
1:A:1094:A:H62	1:A:2778:G:H2'	1.81	0.44
1:A:1733:A:OP2	1:A:1742:A:N6	2.43	0.44
1:A:2424:G:N2	1:A:2446:U:O2	2.44	0.44
1:A:2682:G:N2	1:A:2683:U:O4	2.36	0.44
1:A:2781:U:H1'	30:4:26:ILE:HD11	1.98	0.44
2:B:38:U:H1'	2:B:43:A:H61	1.81	0.44
1:A:1479:G:H2'	1:A:1480:G:C8	2.53	0.44
1:A:2580:G:H21	1:A:2609:G:N2	2.16	0.44
2:B:40:C:N1	6:F:66:LEU:HD22	2.33	0.44
16:P:65:GLN:HG2	16:P:93:THR:HG22	1.99	0.44
29:3:21:GLN:HB3	29:3:49:LEU:HD22	1.98	0.44
1:A:1452:C:O2'	1:A:1631:G:N2	2.50	0.44
1:A:2113:U:C4	1:A:2261:G:O6	2.70	0.44
1:A:2765:A:N1	1:A:2793:G:C6	2.86	0.44
5:E:136:THR:HG22	5:E:170:ILE:HD11	2.00	0.44
6:F:60:ILE:HG22	6:F:99:PHE:CE1	2.53	0.44
7:G:107:VAL:HG23	7:G:109:TYR:CD1	2.53	0.44
9:I:101:PRO:HD2	14:N:70:VAL:HG21	2.00	0.44
21:U:83:ASP:N	21:U:83:ASP:OD1	2.49	0.44
1:A:2710:C:H42	1:A:2754:G:H2'	1.81	0.44
2:B:73:G:H1'	20:T:30:VAL:HG21	2.00	0.44
6:F:50:LEU:HD13	6:F:54:VAL:HG23	1.99	0.44
9:I:7:ARG:HE	9:I:20:LEU:HD23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:113:LYS:CE	9:I:117:LEU:HD11	2.47	0.44
10:J:55:LEU:HD23	10:J:60:ARG:CG	2.47	0.44
11:K:34:LEU:HD12	11:K:130:LYS:O	2.18	0.44
1:A:905:U:OP2	1:A:961:G:N1	2.44	0.44
1:A:1076:A:C8	30:4:36:GLN:HB3	2.52	0.44
1:A:1397:G:C2	1:A:2241:C:C2	3.06	0.44
1:A:1449:A:O2'	1:A:1450:A:N3	2.41	0.44
1:A:1964:A:H62	1:A:1967:U:H5	1.65	0.44
1:A:1989:C:HO2'	1:A:1991:G:P	2.37	0.44
1:A:2382:C:O3'	21:U:32:LYS:NZ	2.42	0.44
1:A:2775:A:H1'	7:G:67:THR:HG23	2.00	0.44
1:A:2814:C:O3'	4:D:71:LYS:NZ	2.47	0.44
2:B:27:A:H2'	2:B:28:C:C2	2.52	0.44
28:2:10:LYS:O	28:2:14:SER:OG	2.36	0.44
1:A:921:C:H42	1:A:946:A:N6	2.16	0.44
1:A:1457:U:OP2	1:A:1628:A:N6	2.42	0.44
1:A:2430:C:H2'	1:A:2431:C:C6	2.53	0.44
1:A:2850:G:OP2	4:D:86:ARG:NH1	2.47	0.44
6:F:57:LEU:HD12	6:F:65:PRO:HG3	1.99	0.44
15:O:88:ILE:HD13	15:O:88:ILE:N	2.33	0.44
16:P:57:THR:OG1	16:P:58:VAL:N	2.50	0.44
1:A:334:A:H3'	1:A:335:U:C4'	2.48	0.43
1:A:443:U:O5'	22:V:32:ASN:ND2	2.51	0.43
1:A:1537:A:H2	1:A:1626:A:H1'	1.83	0.43
1:A:1816:A:OP2	3:C:221:ARG:NH2	2.49	0.43
1:A:1980:A:O2'	1:A:2586:C:O2'	2.22	0.43
1:A:2374:C:HO2'	27:1:17:TYR:HH	1.47	0.43
2:B:34:C:H42	2:B:48:A:C1'	2.30	0.43
2:B:79:C:H41	2:B:92:C:H42	1.65	0.43
2:B:94:C:OP2	20:T:12:LYS:NZ	2.50	0.43
9:I:43:VAL:HG23	9:I:54:LYS:HA	1.99	0.43
9:I:87:ILE:HD12	9:I:88:ARG:N	2.33	0.43
12:L:24:LEU:HD13	12:L:24:LEU:C	2.38	0.43
1:A:544:U:H2'	1:A:545:G:O4'	2.18	0.43
1:A:617:A:H62	1:A:2081:A:H4'	1.82	0.43
1:A:2290:C:N4	21:U:23:ASP:OD2	2.51	0.43
1:A:2902:A:OP1	12:L:102:ARG:NH1	2.46	0.43
2:B:7:G:H21	2:B:110:C:H41	1.66	0.43
5:E:16:SER:OG	5:E:17:ILE:N	2.51	0.43
11:K:50:ALA:HB1	11:K:121:ALA:HB1	2.00	0.43
1:A:318:A:H1'	1:A:402:C:H42	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:A:H2'	1:A:326:A:C4	2.53	0.43
1:A:1316:G:H5'	12:L:30:ILE:HG22	2.00	0.43
1:A:1533:A:H62	3:C:100:GLU:N	2.16	0.43
15:O:116:ALA:O	15:O:117:LEU:HD23	2.18	0.43
21:U:71:ILE:HD13	21:U:91:ALA:HB2	2.00	0.43
25:Y:1:MET:O	25:Y:3:GLN:N	2.51	0.43
1:A:401:U:O2'	1:A:402:C:O4'	2.30	0.43
1:A:718:C:OP1	5:E:54:ARG:NH2	2.44	0.43
1:A:1024:A:HO2'	1:A:1025:A:P	2.37	0.43
1:A:1465:G:O2'	1:A:1537:A:N7	2.51	0.43
1:A:1761:G:O2'	1:A:1763:U:O4'	2.35	0.43
1:A:2431:C:H42	1:A:2440:G:H1	1.66	0.43
2:B:29:C:H1'	2:B:51:A:H61	1.83	0.43
20:T:4:LEU:HD23	20:T:5:LYS:N	2.32	0.43
27:1:32:MET:O	27:1:44:LEU:HD12	2.18	0.43
1:A:597:U:H2'	1:A:598:G:O4'	2.19	0.43
1:A:794:A:C3'	1:A:1309:G:H21	2.32	0.43
1:A:2557:U:HO2'	1:A:2561:C:N4	2.17	0.43
7:G:94:TYR:OH	7:G:152:ARG:NH2	2.51	0.43
18:R:6:ILE:HG12	18:R:7:LEU:HD12	1.99	0.43
20:T:51:VAL:O	20:T:55:VAL:HG12	2.18	0.43
1:A:889:U:H2'	1:A:890:G:O4'	2.19	0.43
1:A:1463:A:O2'	1:A:1464:U:O5'	2.30	0.43
1:A:1875:A:N1	1:A:1919:C:N4	2.67	0.43
1:A:2449:C:N4	1:A:2450:U:O4	2.51	0.43
2:B:73:G:H2'	2:B:74:G:O4'	2.18	0.43
18:R:87:ILE:HG22	18:R:89:LEU:HD21	2.01	0.43
19:S:26:THR:HA	19:S:33:VAL:HG12	2.01	0.43
1:A:1767:G:OP2	1:A:1768:C:N4	2.50	0.43
1:A:2024:A:OP1	4:D:137:SER:OG	2.32	0.43
1:A:2399:G:O3'	27:1:33:LYS:NZ	2.51	0.43
5:E:179:GLN:OE1	5:E:180:GLY:N	2.51	0.43
6:F:140:GLU:OE1	25:Y:27:SER:N	2.51	0.43
11:K:39:THR:HG23	11:K:98:LYS:HA	2.01	0.43
1:A:162:A:H2'	1:A:2244:G:H21	1.83	0.43
1:A:908:A:O3'	2:B:97:G:N2	2.44	0.43
1:A:1074:G:H2'	1:A:1075:G:C1'	2.48	0.43
1:A:1168:C:H3'	1:A:1169:G:C8	2.54	0.43
1:A:1816:A:P	3:C:221:ARG:HE	2.41	0.43
30:4:19:ARG:HD3	30:4:20:LYS:HZ3	1.83	0.43
1:A:193:A:H61	1:A:210:A:C1'	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1447:A:N6	1:A:1637:A:N1	2.67	0.43
1:A:1760:G:O6	1:A:1761:G:N2	2.45	0.43
1:A:2629:A:O2'	1:A:2631:U:OP2	2.34	0.43
3:C:84:ASP:OD2	3:C:86:ASN:N	2.50	0.43
8:H:57:VAL:O	8:H:126:TYR:N	2.48	0.43
1:A:308:C:O2'	1:A:407:G:N2	2.48	0.43
1:A:1018:A:O2'	1:A:1033:G:N2	2.50	0.43
6:F:134:GLU:HB3	6:F:137:ILE:HD11	2.00	0.43
1:A:26:G:H2'	1:A:27:G:O4'	2.19	0.42
1:A:796:A:OP2	17:Q:90:ARG:NE	2.52	0.42
1:A:1465:G:N3	1:A:1537:A:N6	2.67	0.42
1:A:1632:A:H2'	1:A:1633:A:N3	2.34	0.42
13:M:46:ASP:N	13:M:51:VAL:O	2.50	0.42
28:2:31:VAL:HG12	28:2:34:ARG:NH2	2.34	0.42
1:A:645:A:O2'	1:A:646:A:O5'	2.37	0.42
1:A:719:G:H2'	1:A:849:A:H61	1.84	0.42
1:A:1079:U:N3	1:A:1080:G:N7	2.67	0.42
1:A:1829:A:OP2	1:A:1841:G:N1	2.47	0.42
2:B:40:C:O5'	25:Y:5:ILE:HG23	2.19	0.42
3:C:185:LEU:HD13	3:C:187:THR:N	2.34	0.42
8:H:97:ASN:OD1	8:H:100:ARG:NE	2.48	0.42
13:M:19:ARG:NH2	13:M:23:SER:OG	2.48	0.42
26:Z:15:LYS:O	26:Z:18:THR:HG22	2.19	0.42
1:A:10:A:N6	1:A:2656:A:O4'	2.52	0.42
1:A:362:C:H2'	1:A:363:A:O4'	2.19	0.42
1:A:926:G:N1	1:A:939:U:OP1	2.52	0.42
1:A:1174:U:N3	4:D:160:ALA:HB2	2.34	0.42
1:A:1309:G:O6	1:A:1659:C:O2	2.37	0.42
1:A:1614:A:OP1	3:C:60:ARG:NH2	2.52	0.42
1:A:2349:A:H2'	1:A:2350:G:O4'	2.19	0.42
1:A:2496:A:N6	1:A:2508:G:O4'	2.52	0.42
2:B:75:U:H3	2:B:96:A:H62	1.67	0.42
3:C:165:LEU:HD21	3:C:175:ARG:HH12	1.84	0.42
4:D:93:ASN:OD1	4:D:93:ASN:N	2.51	0.42
7:G:41:MET:N	7:G:41:MET:SD	2.92	0.42
9:I:19:VAL:HG23	9:I:43:VAL:HA	2.01	0.42
16:P:4:ILE:HG22	16:P:39:LEU:HD12	2.00	0.42
18:R:18:GLU:O	18:R:21:ALA:HB3	2.19	0.42
23:W:6:ILE:HA	23:W:9:LEU:HD12	2.00	0.42
28:2:9:ASN:OD1	28:2:12:LYS:N	2.46	0.42
1:A:1290:G:N7	15:O:36:LYS:NZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1455:U:O2	1:A:1457:U:N3	2.46	0.42
1:A:1503:U:O2'	1:A:1504:U:OP2	2.36	0.42
1:A:1633:A:H1'	1:A:1634:A:C8	2.55	0.42
1:A:2307:G:N7	21:U:22:ARG:NH2	2.67	0.42
27:1:31:GLU:HB2	27:1:44:LEU:HD11	2.01	0.42
1:A:50:U:O2'	1:A:51:G:OP1	2.35	0.42
1:A:172:U:O4	1:A:173:A:N6	2.53	0.42
1:A:284:C:HO2'	1:A:287:G:H22	1.54	0.42
1:A:317:G:H22	1:A:402:C:H2'	1.85	0.42
1:A:333:C:N4	1:A:392:U:H3'	2.34	0.42
1:A:484:U:O4	1:A:485:A:N6	2.53	0.42
1:A:2362:A:O5'	13:M:17:ARG:NH2	2.52	0.42
1:A:578:G:O2'	15:O:38:GLN:OE1	2.35	0.42
1:A:912:C:N3	1:A:957:C:O2'	2.52	0.42
1:A:1039:C:O2'	1:A:1040:A:OP2	2.25	0.42
2:B:7:G:N2	2:B:109:G:N7	2.67	0.42
6:F:74:ILE:N	6:F:79:LEU:HD21	2.34	0.42
8:H:37:LEU:HD11	8:H:119:GLN:CB	2.50	0.42
8:H:44:THR:O	8:H:44:THR:OG1	2.27	0.42
9:I:13:ASN:OD1	9:I:13:ASN:N	2.53	0.42
24:X:43:ILE:HD13	24:X:46:GLN:OE1	2.20	0.42
1:A:54:G:H1	1:A:115:C:H42	1.67	0.42
1:A:208:G:HO2'	1:A:209:U:P	2.42	0.42
1:A:248:G:O6	29:3:8:ARG:NE	2.52	0.42
1:A:926:G:N2	1:A:941:A:H62	2.16	0.42
1:A:1854:U:H2'	1:A:1855:G:O4'	2.19	0.42
1:A:1866:G:O2'	1:A:1954:A:OP1	2.20	0.42
1:A:2042:A:C2	26:Z:3:VAL:HG12	2.55	0.42
1:A:2836:C:O3'	12:L:105:LYS:NZ	2.49	0.42
1:A:2844:U:H2'	1:A:2845:G:O4'	2.20	0.42
5:E:155:VAL:HG12	5:E:156:THR:O	2.20	0.42
13:M:86:ASP:N	13:M:86:ASP:OD1	2.53	0.42
1:A:506:A:H2	1:A:515:G:H21	1.68	0.42
1:A:624:C:H5'	15:O:31:LEU:HD22	2.01	0.42
1:A:1090:A:O2'	1:A:1091:G:OP1	2.37	0.42
1:A:2371:U:O2'	27:1:32:MET:SD	2.66	0.42
1:A:2372:G:O6	1:A:2398:G:C2	2.71	0.42
1:A:2378:G:N2	1:A:2393:A:OP2	2.51	0.42
2:B:40:C:O2'	25:Y:5:ILE:HD11	2.20	0.42
8:H:57:VAL:HG23	8:H:125:VAL:HG23	2.02	0.42
8:H:111:PRO:HB2	8:H:113:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:61:LEU:O	29:3:13:ARG:NE	2.48	0.42
17:Q:88:GLN:O	17:Q:90:ARG:NE	2.53	0.42
19:S:3:ILE:HD12	19:S:4:LYS:O	2.20	0.42
1:A:116:G:OP2	1:A:118:A:O2'	2.38	0.42
1:A:1952:C:H42	1:A:1956:G:H22	1.65	0.42
1:A:399:U:H3'	1:A:400:C:O4'	2.19	0.42
1:A:1359:A:H2	1:A:1370:C:HO2'	1.67	0.42
1:A:2347:A:H4'	1:A:2348:G:O5'	2.19	0.42
1:A:2684:A:N6	1:A:2691:G:O2'	2.52	0.42
12:L:45:GLU:O	12:L:49:THR:OG1	2.38	0.42
1:A:323:C:H2'	1:A:324:A:C5	2.55	0.41
1:A:1092:A:N6	1:A:1155:A:O4'	2.52	0.41
1:A:1226:G:O2'	1:A:1227:U:O5'	2.37	0.41
1:A:2225:A:C5'	1:A:2227:C:H41	2.33	0.41
1:A:2371:U:H2'	27:1:32:MET:HB2	2.01	0.41
3:C:216:ILE:HG22	3:C:217:ARG:N	2.35	0.41
4:D:131:ILE:HG22	4:D:136:GLN:O	2.19	0.41
5:E:21:ASP:O	5:E:25:GLY:CA	2.68	0.41
6:F:65:PRO:CB	6:F:87:ALA:HB1	2.50	0.41
21:U:18:THR:OG1	21:U:19:LYS:N	2.53	0.41
1:A:343:A:O2'	1:A:361:U:O2	2.31	0.41
1:A:575:G:N2	1:A:2050:A:OP2	2.53	0.41
1:A:1078:G:H2'	1:A:1079:U:O4'	2.20	0.41
1:A:2397:G:O3'	27:1:40:ASN:ND2	2.48	0.41
3:C:53:HIS:CD2	3:C:219:THR:HG22	2.55	0.41
6:F:89:VAL:CG1	6:F:91:LEU:HD21	2.49	0.41
15:O:96:SER:OG	15:O:97:GLU:N	2.53	0.41
16:P:97:ILE:H	16:P:97:ILE:HD12	1.86	0.41
20:T:44:ASP:N	20:T:44:ASP:OD1	2.53	0.41
1:A:9:U:O2	1:A:2656:A:C5	2.74	0.41
1:A:622:A:O2'	1:A:2046:U:OP1	2.38	0.41
1:A:958:U:O2	1:A:959:C:N4	2.50	0.41
1:A:2080:G:N7	1:A:2604:A:N6	2.68	0.41
1:A:2082:C:OP1	26:Z:5:LYS:NZ	2.53	0.41
1:A:2350:G:H2'	1:A:2351:U:O4'	2.20	0.41
16:P:25:LEU:HD22	16:P:93:THR:HG21	2.01	0.41
1:A:2479:C:C4	1:A:2531:U:O4	2.73	0.41
1:A:2693:C:N4	7:G:109:TYR:HA	2.35	0.41
6:F:25:VAL:O	6:F:28:VAL:HG13	2.21	0.41
11:K:66:ILE:HG22	11:K:68:ILE:H	1.85	0.41
15:O:83:LEU:HD12	15:O:113:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:89:LYS:O	19:S:91:VAL:N	2.53	0.41
26:Z:18:THR:HG23	26:Z:19:HIS:N	2.35	0.41
1:A:720:A:OP1	5:E:63:LYS:NZ	2.43	0.41
6:F:60:ILE:HG22	6:F:99:PHE:HE1	1.85	0.41
7:G:136:ILE:H	7:G:141:VAL:HG11	1.85	0.41
9:I:105:GLU:N	9:I:106:LEU:HD23	2.36	0.41
13:M:32:ASN:HB3	13:M:45:ILE:HD12	2.01	0.41
17:Q:50:VAL:CG1	17:Q:103:ILE:HG21	2.51	0.41
1:A:678:A:P	10:J:71:ARG:HE	2.41	0.41
1:A:794:A:H61	1:A:798:G:H1'	1.85	0.41
2:B:22:G:N7	2:B:54:U:H2'	2.35	0.41
5:E:156:THR:OG1	5:E:157:GLU:N	2.52	0.41
7:G:30:LYS:O	7:G:79:VAL:HG13	2.20	0.41
20:T:6:SER:C	20:T:7:ILE:HD12	2.41	0.41
21:U:40:THR:HG22	21:U:41:GLY:H	1.86	0.41
1:A:73:A:O5'	23:W:47:ARG:NH1	2.54	0.41
1:A:342:A:N6	1:A:365:A:O2'	2.48	0.41
1:A:2828:U:H3	1:A:2911:A:H62	1.68	0.41
1:A:2851:G:H21	1:A:2904:U:P	2.42	0.41
9:I:63:VAL:HG23	9:I:83:ALA:HB3	2.02	0.41
1:A:77:U:OP1	23:W:52:ARG:NE	2.47	0.41
1:A:1957:G:N1	1:A:1996:A:OP2	2.48	0.41
1:A:2024:A:OP2	4:D:138:ARG:NH1	2.53	0.41
2:B:64:A:O2'	2:B:67:G:O6	2.33	0.41
5:E:136:THR:CG2	5:E:170:ILE:HD11	2.51	0.41
7:G:94:TYR:HH	7:G:152:ARG:HH22	1.67	0.41
16:P:88:HIS:NE2	16:P:90:GLN:OE1	2.47	0.41
20:T:90:ASP:OD1	20:T:90:ASP:N	2.52	0.41
29:3:19:SER:OG	29:3:20:GLY:N	2.53	0.41
1:A:200:A:H2	1:A:2461:A:H61	1.68	0.41
1:A:325:A:N1	1:A:402:C:N4	2.69	0.41
1:A:606:G:H1	1:A:621:A:H61	1.69	0.41
1:A:686:U:O4	1:A:692:G:O6	2.38	0.41
1:A:774:G:C4'	3:C:207:LYS:HZ2	2.34	0.41
1:A:818:U:O2	1:A:823:G:O2'	2.38	0.41
1:A:1002:U:H3	2:B:87:C:H41	1.68	0.41
1:A:1073:A:H62	1:A:1169:G:N2	2.19	0.41
1:A:1488:A:N7	1:A:1490:G:N1	2.69	0.41
1:A:1488:A:H2'	1:A:1489:A:H3'	2.03	0.41
1:A:1502:A:N3	1:A:1504:U:N3	2.69	0.41
1:A:1504:U:O2'	1:A:1505:G:N7	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2313:A:C5	1:A:2373:A:C6	3.09	0.41
1:A:2348:G:OP1	1:A:2359:C:N4	2.54	0.41
1:A:2676:U:N3	1:A:2699:U:O2	2.54	0.41
1:A:2829:A:H62	1:A:2910:G:H2'	1.85	0.41
7:G:103:LEU:O	7:G:104:ILE:HD13	2.21	0.41
22:V:36:VAL:O	22:V:47:VAL:N	2.48	0.41
28:2:15:LYS:HZ2	28:2:15:LYS:HA	1.85	0.41
1:A:192:G:H21	1:A:210:A:H62	1.68	0.41
1:A:690:U:O2'	1:A:690:U:O2	2.39	0.41
1:A:760:A:O2'	1:A:761:A:OP2	2.28	0.41
1:A:909:G:H2'	1:A:910:C:C6	2.56	0.41
1:A:1162:C:H3'	1:A:1163:U:H5''	2.02	0.41
1:A:1462:G:H22	1:A:1625:U:H2'	1.86	0.41
1:A:1652:A:N7	1:A:1665:U:C2	2.89	0.41
1:A:1759:G:H21	1:A:1772:G:P	2.44	0.41
1:A:2397:G:O2'	27:1:40:ASN:OD1	2.21	0.41
2:B:9:C:H3'	2:B:10:U:C5'	2.51	0.41
10:J:95:LEU:HD13	10:J:96:LEU:HD12	2.02	0.41
10:J:98:GLU:OE1	10:J:99:SER:N	2.54	0.41
11:K:48:GLU:O	11:K:51:ARG:NH2	2.54	0.41
16:P:35:PHE:O	16:P:57:THR:OG1	2.39	0.41
18:R:87:ILE:HG22	18:R:89:LEU:CD2	2.51	0.41
29:3:52:LYS:HA	29:3:55:MET:HB2	2.03	0.41
1:A:1500:G:H2'	1:A:1501:G:O4'	2.21	0.40
1:A:1911:A:O2'	1:A:1912:A:OP2	2.33	0.40
1:A:2628:C:H2'	1:A:2629:A:C8	2.56	0.40
5:E:123:LEU:HD11	5:E:194:ILE:HD11	2.03	0.40
11:K:23:GLY:O	11:K:101:ARG:NE	2.54	0.40
13:M:74:THR:CG2	13:M:111:ALA:HB2	2.50	0.40
28:2:16:VAL:HG23	28:2:17:HIS:CD2	2.55	0.40
28:2:31:VAL:HG12	28:2:34:ARG:HH21	1.87	0.40
1:A:1304:G:N2	1:A:2040:A:OP2	2.54	0.40
1:A:1824:C:O3'	3:C:258:LYS:HB3	2.22	0.40
1:A:2137:G:O6	1:A:2206:C:N4	2.54	0.40
14:N:49:VAL:O	14:N:99:LEU:HD12	2.21	0.40
1:A:921:C:H42	1:A:946:A:H61	1.68	0.40
1:A:2555:U:O2'	1:A:2557:U:OP1	2.25	0.40
1:A:2678:C:H2'	1:A:2679:U:C6	2.57	0.40
1:A:2902:A:OP1	12:L:102:ARG:NH2	2.51	0.40
5:E:54:ARG:O	5:E:57:VAL:HG22	2.21	0.40
9:I:76:TYR:HB2	14:N:75:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:92:ILE:HD12	13:M:93:VAL:C	2.42	0.40
20:T:29:ALA:HB2	20:T:89:ILE:HG23	2.04	0.40
1:A:193:A:H62	1:A:209:U:H3	1.70	0.40
1:A:539:G:H4'	17:Q:6:VAL:HG23	2.03	0.40
1:A:1758:A:H2	1:A:1766:C:HO2'	1.69	0.40
1:A:2772:C:H3'	1:A:2773:U:C5	2.57	0.40
3:C:76:ALA:O	3:C:115:ILE:HG22	2.20	0.40
13:M:76:VAL:O	13:M:80:ILE:HG22	2.22	0.40
1:A:371:U:O2'	19:S:64:HIS:ND1	2.41	0.40
1:A:1003:A:N6	1:A:2522:G:O2'	2.51	0.40
1:A:1243:G:H2'	1:A:1244:G:O4'	2.22	0.40
1:A:1891:U:HO2'	1:A:2436:G:H22	1.69	0.40
2:B:73:G:O3'	20:T:9:ARG:NH1	2.43	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 PDB entries followed by that with respect to all EM entries.

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	272/274 (99%)	218 (80%)	54 (20%)	0	100	100
4	D	213/215 (99%)	179 (84%)	34 (16%)	0	100	100
5	E	204/206 (99%)	176 (86%)	28 (14%)	0	100	100
6	F	173/175 (99%)	142 (82%)	31 (18%)	0	100	100
7	G	173/175 (99%)	155 (90%)	18 (10%)	0	100	100
8	H	143/145 (99%)	126 (88%)	17 (12%)	0	100	100
9	I	120/122 (98%)	102 (85%)	18 (15%)	0	100	100
10	J	144/146 (99%)	123 (85%)	21 (15%)	0	100	100
11	K	135/137 (98%)	117 (87%)	18 (13%)	0	100	100
12	L	118/120 (98%)	105 (89%)	13 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	117/119 (98%)	100 (86%)	17 (14%)	0	100	100
14	N	112/114 (98%)	97 (87%)	14 (12%)	1 (1%)	14	49
15	O	114/116 (98%)	107 (94%)	7 (6%)	0	100	100
16	P	100/102 (98%)	89 (89%)	10 (10%)	1 (1%)	13	47
17	Q	108/110 (98%)	94 (87%)	13 (12%)	1 (1%)	14	49
18	R	87/89 (98%)	72 (83%)	15 (17%)	0	100	100
19	S	101/103 (98%)	83 (82%)	18 (18%)	0	100	100
20	T	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
21	U	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
22	V	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
23	W	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
24	X	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
25	Y	57/59 (97%)	48 (84%)	9 (16%)	0	100	100
26	Z	46/48 (96%)	33 (72%)	13 (28%)	0	100	100
27	1	45/47 (96%)	41 (91%)	4 (9%)	0	100	100
28	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	52 (84%)	10 (16%)	0	100	100
30	4	35/37 (95%)	25 (71%)	10 (29%)	0	100	100
All	All	3069/3125 (98%)	2632 (86%)	434 (14%)	3 (0%)	50	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Q	87	PRO
16	P	51	PRO
14	N	54	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 PDB entries followed by that with respect to all EM entries.

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	220/221 (100%)	181 (82%)	39 (18%)	1	8
4	D	173/173 (100%)	152 (88%)	21 (12%)	4	19
5	E	168/168 (100%)	145 (86%)	23 (14%)	3	14
6	F	141/154 (92%)	122 (86%)	19 (14%)	3	15
7	G	124/153 (81%)	105 (85%)	19 (15%)	2	11
8	H	122/123 (99%)	105 (86%)	17 (14%)	3	14
9	I	100/100 (100%)	87 (87%)	13 (13%)	3	16
10	J	109/112 (97%)	94 (86%)	15 (14%)	3	14
11	K	108/114 (95%)	100 (93%)	8 (7%)	11	40
12	L	96/101 (95%)	86 (90%)	10 (10%)	5	25
13	M	86/95 (90%)	71 (83%)	15 (17%)	1	8
14	N	93/100 (93%)	82 (88%)	11 (12%)	4	20
15	O	96/96 (100%)	89 (93%)	7 (7%)	11	41
16	P	84/86 (98%)	72 (86%)	12 (14%)	2	13
17	Q	88/90 (98%)	68 (77%)	20 (23%)	0	3
18	R	78/80 (98%)	68 (87%)	10 (13%)	3	17
19	S	81/88 (92%)	67 (83%)	14 (17%)	1	8
20	T	78/82 (95%)	69 (88%)	9 (12%)	4	21
21	U	63/64 (98%)	47 (75%)	16 (25%)	0	2
22	V	44/49 (90%)	35 (80%)	9 (20%)	1	5
23	W	58/60 (97%)	48 (83%)	10 (17%)	1	8
24	X	52/52 (100%)	46 (88%)	6 (12%)	4	21
25	Y	23/56 (41%)	22 (96%)	1 (4%)	25	57
26	Z	35/44 (80%)	28 (80%)	7 (20%)	1	5
27	1	44/45 (98%)	38 (86%)	6 (14%)	3	15
28	2	39/39 (100%)	33 (85%)	6 (15%)	2	11
29	3	55/55 (100%)	48 (87%)	7 (13%)	3	17
30	4	35/35 (100%)	32 (91%)	3 (9%)	8	33
All	All	2493/2635 (95%)	2140 (86%)	353 (14%)	5	13

All (353) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	10	THR
3	C	17	THR
3	C	19	LEU
3	C	20	ASP
3	C	27	THR
3	C	32	SER
3	C	37	LEU
3	C	40	LYS
3	C	59	LYS
3	C	70	ASN
3	C	77	LYS
3	C	87	ARG
3	C	91	ILE
3	C	94	VAL
3	C	100	GLU
3	C	125	LYS
3	C	134	ASN
3	C	141	VAL
3	C	144	ILE
3	C	150	LYS
3	C	165	LEU
3	C	177	ARG
3	C	180	GLU
3	C	181	VAL
3	C	187	THR
3	C	197	ASN
3	C	202	LEU
3	C	207	LYS
3	C	212	ARG
3	C	213	TRP
3	C	223	SER
3	C	232	HIS
3	C	236	GLU
3	C	238	ARG
3	C	248	SER
3	C	252	LYS
3	C	254	THR
3	C	258	LYS
3	C	270	ILE
4	D	5	ILE
4	D	6	LEU
4	D	10	ILE
4	D	32	GLU

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Mol	Chain	Res	Type
4	D	40	THR
4	D	47	ASN
4	D	49	ILE
4	D	57	LYS
4	D	61	LYS
4	D	62	ASP
4	D	71	LYS
4	D	78	LYS
4	D	81	ASP
4	D	115	VAL
4	D	122	SER
4	D	138	ARG
4	D	176	ASN
4	D	178	VAL
4	D	184	GLU
4	D	190	THR
4	D	193	LYS
5	E	13	LYS
5	E	27	GLU
5	E	33	LEU
5	E	35	GLU
5	E	46	GLN
5	E	49	HIS
5	E	55	SER
5	E	101	MET
5	E	112	SER
5	E	114	LEU
5	E	116	PHE
5	E	117	LYS
5	E	119	GLN
5	E	121	ASN
5	E	130	ASN
5	E	139	PHE
5	E	140	LYS
5	E	150	LYS
5	E	156	THR
5	E	187	THR
5	E	192	LEU
5	E	193	VAL
5	E	194	ILE
6	F	4	LEU
6	F	5	LYS

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Mol	Chain	Res	Type
6	F	8	PHE
6	F	32	ASP
6	F	46	ASN
6	F	63	GLN
6	F	64	LYS
6	F	67	VAL
6	F	71	LYS
6	F	80	ARG
6	F	100	LEU
6	F	101	ASP
6	F	115	GLN
6	F	117	VAL
6	F	125	ARG
6	F	132	VAL
6	F	135	GLN
6	F	136	LEU
6	F	162	THR
7	G	41	MET
7	G	44	LYS
7	G	63	THR
7	G	69	ARG
7	G	87	LEU
7	G	94	TYR
7	G	97	GLN
7	G	110	SER
7	G	111	HIS
7	G	112	PRO
7	G	113	VAL
7	G	132	LYS
7	G	136	ILE
7	G	137	SER
7	G	141	VAL
7	G	144	LEU
7	G	149	ARG
7	G	152	ARG
7	G	175	LYS
8	H	3	GLN
8	H	18	VAL
8	H	37	LEU
8	H	44	THR
8	H	46	THR
8	H	57	VAL

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Mol	Chain	Res	Type
8	H	61	SER
8	H	62	LYS
8	H	65	PHE
8	H	70	GLU
8	H	72	ASP
8	H	85	ILE
8	H	88	ILE
8	H	95	ARG
8	H	103	GLU
8	H	136	GLN
8	H	139	GLU
9	I	2	ILE
9	I	10	VAL
9	I	21	THR
9	I	23	LYS
9	I	64	ARG
9	I	70	ARG
9	I	71	ARG
9	I	84	CYS
9	I	97	ARG
9	I	99	PHE
9	I	106	LEU
9	I	112	MET
9	I	122	LEU
10	J	6	LEU
10	J	31	SER
10	J	57	LEU
10	J	71	ARG
10	J	77	VAL
10	J	92	THR
10	J	98	GLU
10	J	103	LYS
10	J	104	ASN
10	J	105	GLU
10	J	114	ASN
10	J	120	LYS
10	J	121	LEU
10	J	127	LYS
10	J	143	HIS
11	K	2	LEU
11	K	20	ARG
11	K	21	SER

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Mol	Chain	Res	Type
11	K	38	THR
11	K	39	THR
11	K	56	ARG
11	K	77	LYS
11	K	127	VAL
12	L	3	TYR
12	L	33	THR
12	L	49	THR
12	L	50	LEU
12	L	52	LYS
12	L	96	ARG
12	L	103	ILE
12	L	112	ASP
12	L	121	LEU
12	L	122	VAL
13	M	1	MET
13	M	2	ILE
13	M	6	ASP
13	M	7	LYS
13	M	22	LEU
13	M	32	ASN
13	M	34	TYR
13	M	35	ARG
13	M	39	HIS
13	M	41	TYR
13	M	46	ASP
13	M	72	LEU
13	M	87	LYS
13	M	90	LYS
13	M	113	ARG
14	N	2	THR
14	N	6	LEU
14	N	32	VAL
14	N	42	ILE
14	N	43	GLN
14	N	52	ARG
14	N	53	ARG
14	N	78	LEU
14	N	80	THR
14	N	89	LYS
14	N	98	LYS
15	O	4	VAL

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Mol	Chain	Res	Type
15	O	9	VAL
15	O	10	THR
15	O	11	ARG
15	O	34	VAL
15	O	51	ARG
15	O	80	MET
16	P	2	PHE
16	P	10	LYS
16	P	13	LYS
16	P	21	PHE
16	P	24	LYS
16	P	25	LEU
16	P	31	ASP
16	P	34	THR
16	P	59	THR
16	P	75	THR
16	P	76	TYR
16	P	96	THR
17	Q	4	LYS
17	Q	6	VAL
17	Q	24	ILE
17	Q	28	ASN
17	Q	37	LYS
17	Q	48	GLU
17	Q	49	LYS
17	Q	51	LEU
17	Q	62	TYR
17	Q	65	ASN
17	Q	71	VAL
17	Q	75	TYR
17	Q	81	THR
17	Q	82	LEU
17	Q	86	ARG
17	Q	88	GLN
17	Q	90	ARG
17	Q	101	ILE
17	Q	103	ILE
17	Q	109	LYS
18	R	9	ARG
18	R	31	THR
18	R	33	VAL
18	R	35	LYS

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Mol	Chain	Res	Type
18	R	53	VAL
18	R	56	MET
18	R	74	LYS
18	R	83	LYS
18	R	84	GLU
18	R	90	PHE
19	S	7	ASP
19	S	8	ASN
19	S	12	ILE
19	S	24	ILE
19	S	26	THR
19	S	27	LEU
19	S	38	VAL
19	S	57	LEU
19	S	59	THR
19	S	70	LEU
19	S	79	THR
19	S	81	VAL
19	S	84	LYS
19	S	87	ASP
20	T	4	LEU
20	T	31	VAL
20	T	32	TYR
20	T	37	LYS
20	T	42	LYS
20	T	63	LEU
20	T	88	HIS
20	T	89	ILE
20	T	92	LEU
21	U	12	LYS
21	U	13	LYS
21	U	17	SER
21	U	27	LYS
21	U	29	LEU
21	U	40	THR
21	U	45	LEU
21	U	46	TYR
21	U	47	ARG
21	U	58	ASN
21	U	59	VAL
21	U	61	ARG
21	U	68	PHE

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Mol	Chain	Res	Type
21	U	72	ASP
21	U	75	VAL
21	U	79	ARG
22	V	3	LYS
22	V	11	LYS
22	V	29	TRP
22	V	32	ASN
22	V	33	LEU
22	V	36	VAL
22	V	40	VAL
22	V	52	ARG
22	V	54	LEU
23	W	2	LYS
23	W	7	ARG
23	W	10	THR
23	W	11	THR
23	W	13	GLU
23	W	16	GLU
23	W	30	PHE
23	W	42	ARG
23	W	55	THR
23	W	58	ARG
24	X	7	THR
24	X	9	THR
24	X	12	VAL
24	X	55	THR
24	X	57	GLU
24	X	59	LYS
25	Y	1	MET
26	Z	8	THR
26	Z	11	THR
26	Z	16	ARG
26	Z	22	ILE
26	Z	29	GLU
26	Z	30	CYS
26	Z	37	LYS
27	1	3	VAL
27	1	19	THR
27	1	22	ASN
27	1	23	LYS
27	1	34	LYS
27	1	36	CYS

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Mol	Chain	Res	Type
28	2	11	ARG
28	2	14	SER
28	2	15	LYS
28	2	22	ARG
28	2	25	THR
28	2	37	ARG
29	3	3	LYS
29	3	6	THR
29	3	31	HIS
29	3	32	LEU
29	3	44	LEU
29	3	52	LYS
29	3	55	MET
30	4	19	ARG
30	4	29	ASN
30	4	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	15	ASN
3	C	54	HIS
3	C	90	ASN
3	C	153	GLN
3	C	226	ASN
4	D	50	GLN
4	D	176	ASN
5	E	46	GLN
5	E	130	ASN
5	E	148	GLN
8	H	11	ASN
8	H	68	ASN
10	J	83	ASN
10	J	114	ASN
12	L	106	GLN
13	M	32	ASN
13	M	55	GLN
15	O	72	HIS
17	Q	65	ASN
20	T	84	ASN
22	V	23	ASN
24	X	40	ASN

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Mol	Chain	Res	Type
29	3	43	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2896/2905 (99%)	1040 (35%)	36 (1%)
2	B	114/115 (99%)	38 (33%)	0
All	All	3010/3020 (99%)	1078 (35%)	36 (1%)

All (1078) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	U
1	A	14	A
1	A	15	G
1	A	28	A
1	A	34	U
1	A	36	G
1	A	45	G
1	A	46	C
1	A	51	G
1	A	55	G
1	A	57	C
1	A	58	G
1	A	63	U
1	A	67	G
1	A	68	A
1	A	70	G
1	A	71	A
1	A	74	U
1	A	75	G
1	A	80	G
1	A	81	G
1	A	83	G
1	A	84	A
1	A	88	G
1	A	91	A
1	A	92	G
1	A	93	U
1	A	95	A
1	A	96	G

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Mol	Chain	Res	Type
1	A	99	U
1	A	100	U
1	A	101	G
1	A	103	U
1	A	104	C
1	A	117	A
1	A	119	U
1	A	130	A
1	A	133	A
1	A	139	U
1	A	140	A
1	A	141	U
1	A	147	G
1	A	150	A
1	A	156	A
1	A	157	U
1	A	158	G
1	A	161	A
1	A	162	A
1	A	164	A
1	A	166	A
1	A	167	U
1	A	168	A
1	A	169	G
1	A	170	C
1	A	172	U
1	A	173	A
1	A	175	C
1	A	176	A
1	A	177	G
1	A	179	A
1	A	180	G
1	A	183	A
1	A	184	C
1	A	185	A
1	A	199	A
1	A	202	A
1	A	208	G
1	A	213	C
1	A	216	A
1	A	217	G
1	A	219	A

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Mol	Chain	Res	Type
1	A	224	A
1	A	225	A
1	A	227	G
1	A	228	A
1	A	229	A
1	A	230	A
1	A	231	A
1	A	232	U
1	A	233	U
1	A	234	C
1	A	235	G
1	A	242	U
1	A	244	A
1	A	251	G
1	A	256	C
1	A	268	A
1	A	270	C
1	A	275	A
1	A	276	C
1	A	280	C
1	A	281	A
1	A	283	G
1	A	285	U
1	A	286	U
1	A	287	G
1	A	292	U
1	A	295	G
1	A	297	G
1	A	299	U
1	A	300	G
1	A	301	U
1	A	302	A
1	A	303	G
1	A	305	A
1	A	307	A
1	A	308	C
1	A	310	C
1	A	311	U
1	A	315	C
1	A	316	G
1	A	317	G
1	A	318	A

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Mol	Chain	Res	Type
1	A	319	G
1	A	320	U
1	A	321	U
1	A	323	C
1	A	324	A
1	A	325	A
1	A	326	A
1	A	327	G
1	A	329	A
1	A	330	C
1	A	331	G
1	A	333	C
1	A	335	U
1	A	336	U
1	A	338	G
1	A	339	A
1	A	340	C
1	A	351	G
1	A	353	A
1	A	365	A
1	A	366	G
1	A	367	A
1	A	373	A
1	A	374	U
1	A	378	C
1	A	381	G
1	A	386	C
1	A	387	G
1	A	388	A
1	A	389	A
1	A	390	A
1	A	391	A
1	A	392	U
1	A	393	G
1	A	396	G
1	A	398	C
1	A	399	U
1	A	400	C
1	A	401	U
1	A	402	C
1	A	404	U
1	A	405	G

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Mol	Chain	Res	Type
1	A	406	A
1	A	407	G
1	A	408	U
1	A	409	G
1	A	410	G
1	A	411	A
1	A	417	A
1	A	418	G
1	A	419	U
1	A	426	G
1	A	432	G
1	A	433	U
1	A	435	A
1	A	436	A
1	A	437	A
1	A	438	U
1	A	442	G
1	A	443	U
1	A	445	G
1	A	447	A
1	A	449	U
1	A	450	C
1	A	451	U
1	A	459	C
1	A	460	C
1	A	461	A
1	A	463	C
1	A	468	A
1	A	481	C
1	A	482	U
1	A	489	A
1	A	490	C
1	A	492	G
1	A	493	A
1	A	497	U
1	A	498	G
1	A	501	C
1	A	502	C
1	A	504	G
1	A	506	A
1	A	511	G
1	A	512	A

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Mol	Chain	Res	Type
1	A	515	G
1	A	523	A
1	A	525	A
1	A	527	G
1	A	528	C
1	A	529	A
1	A	530	C
1	A	537	A
1	A	538	G
1	A	539	G
1	A	541	G
1	A	550	A
1	A	553	A
1	A	566	U
1	A	572	C
1	A	574	A
1	A	575	G
1	A	576	U
1	A	577	A
1	A	578	G
1	A	582	G
1	A	586	C
1	A	591	A
1	A	592	A
1	A	598	G
1	A	599	A
1	A	606	G
1	A	611	U
1	A	615	A
1	A	616	G
1	A	617	A
1	A	618	A
1	A	619	U
1	A	629	A
1	A	630	G
1	A	645	A
1	A	646	A
1	A	647	G
1	A	650	U
1	A	656	G
1	A	657	U
1	A	658	A

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Mol	Chain	Res	Type
1	A	659	A
1	A	672	A
1	A	679	G
1	A	682	A
1	A	687	G
1	A	688	A
1	A	689	A
1	A	690	U
1	A	691	A
1	A	692	G
1	A	696	G
1	A	697	U
1	A	698	U
1	A	700	A
1	A	715	A
1	A	716	C
1	A	720	A
1	A	731	U
1	A	735	C
1	A	749	G
1	A	750	A
1	A	751	A
1	A	754	U
1	A	755	C
1	A	759	U
1	A	761	A
1	A	762	C
1	A	763	A
1	A	765	U
1	A	766	G
1	A	768	A
1	A	775	A
1	A	779	A
1	A	783	G
1	A	785	C
1	A	792	U
1	A	793	G
1	A	794	A
1	A	797	A
1	A	802	G
1	A	805	G
1	A	809	A

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Mol	Chain	Res	Type
1	A	810	A
1	A	816	G
1	A	820	G
1	A	821	C
1	A	822	G
1	A	826	A
1	A	827	A
1	A	828	A
1	A	829	U
1	A	830	U
1	A	833	A
1	A	834	A
1	A	836	C
1	A	841	C
1	A	842	U
1	A	845	A
1	A	850	G
1	A	851	C
1	A	857	C
1	A	862	C
1	A	868	A
1	A	871	U
1	A	872	U
1	A	873	U
1	A	875	G
1	A	887	A
1	A	891	A
1	A	897	A
1	A	899	U
1	A	900	G
1	A	904	G
1	A	908	A
1	A	911	A
1	A	914	G
1	A	916	U
1	A	918	G
1	A	920	A
1	A	923	A
1	A	925	G
1	A	926	G
1	A	927	G
1	A	928	C

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Mol	Chain	Res	Type
1	A	939	U
1	A	940	U
1	A	943	C
1	A	948	U
1	A	952	A
1	A	955	A
1	A	957	C
1	A	959	C
1	A	960	C
1	A	965	G
1	A	970	U
1	A	971	U
1	A	972	A
1	A	977	A
1	A	985	A
1	A	986	G
1	A	989	A
1	A	990	G
1	A	997	G
1	A	1001	A
1	A	1003	A
1	A	1005	G
1	A	1006	G
1	A	1017	A
1	A	1018	A
1	A	1019	A
1	A	1024	A
1	A	1025	A
1	A	1027	A
1	A	1028	G
1	A	1033	G
1	A	1034	A
1	A	1040	A
1	A	1043	U
1	A	1047	G
1	A	1048	U
1	A	1053	A
1	A	1056	U
1	A	1057	A
1	A	1070	A
1	A	1074	G
1	A	1076	A

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Mol	Chain	Res	Type
1	A	1077	U
1	A	1078	G
1	A	1080	G
1	A	1082	C
1	A	1083	G
1	A	1086	G
1	A	1087	C
1	A	1089	C
1	A	1090	A
1	A	1091	G
1	A	1092	A
1	A	1093	C
1	A	1094	A
1	A	1095	A
1	A	1098	A
1	A	1100	G
1	A	1101	A
1	A	1105	U
1	A	1106	G
1	A	1109	U
1	A	1111	A
1	A	1113	A
1	A	1114	A
1	A	1115	G
1	A	1116	C
1	A	1117	A
1	A	1118	G
1	A	1119	C
1	A	1120	C
1	A	1125	U
1	A	1126	U
1	A	1127	U
1	A	1132	A
1	A	1133	G
1	A	1137	G
1	A	1138	U
1	A	1140	A
1	A	1141	U
1	A	1143	G
1	A	1147	A
1	A	1148	C
1	A	1149	U

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Mol	Chain	Res	Type
1	A	1150	A
1	A	1151	G
1	A	1153	C
1	A	1156	G
1	A	1161	A
1	A	1163	U
1	A	1164	G
1	A	1165	C
1	A	1168	C
1	A	1174	U
1	A	1175	G
1	A	1178	C
1	A	1179	C
1	A	1183	G
1	A	1185	U
1	A	1186	A
1	A	1192	A
1	A	1195	A
1	A	1201	G
1	A	1208	A
1	A	1210	U
1	A	1213	C
1	A	1216	U
1	A	1217	U
1	A	1218	G
1	A	1225	G
1	A	1234	G
1	A	1258	A
1	A	1259	U
1	A	1265	G
1	A	1267	A
1	A	1271	G
1	A	1274	G
1	A	1275	A
1	A	1276	G
1	A	1284	A
1	A	1290	G
1	A	1291	A
1	A	1293	U
1	A	1294	G
1	A	1297	G
1	A	1298	G

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Mol	Chain	Res	Type
1	A	1304	G
1	A	1309	G
1	A	1310	A
1	A	1311	A
1	A	1312	A
1	A	1320	G
1	A	1337	A
1	A	1338	U
1	A	1339	U
1	A	1340	G
1	A	1341	A
1	A	1342	C
1	A	1344	A
1	A	1355	A
1	A	1357	G
1	A	1358	A
1	A	1359	A
1	A	1366	U
1	A	1370	C
1	A	1379	A
1	A	1382	C
1	A	1384	G
1	A	1387	C
1	A	1392	G
1	A	1401	G
1	A	1402	A
1	A	1412	G
1	A	1416	U
1	A	1421	A
1	A	1422	A
1	A	1423	C
1	A	1429	G
1	A	1431	U
1	A	1432	A
1	A	1435	C
1	A	1440	A
1	A	1444	C
1	A	1445	C
1	A	1447	A
1	A	1450	A
1	A	1453	G
1	A	1454	U

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Mol	Chain	Res	Type
1	A	1455	U
1	A	1456	U
1	A	1457	U
1	A	1459	A
1	A	1460	U
1	A	1461	C
1	A	1462	G
1	A	1463	A
1	A	1464	U
1	A	1466	G
1	A	1469	G
1	A	1471	A
1	A	1472	C
1	A	1479	G
1	A	1481	A
1	A	1483	A
1	A	1486	C
1	A	1487	G
1	A	1488	A
1	A	1491	C
1	A	1493	U
1	A	1495	C
1	A	1496	G
1	A	1497	A
1	A	1498	U
1	A	1499	U
1	A	1503	U
1	A	1504	U
1	A	1505	G
1	A	1506	C
1	A	1507	A
1	A	1509	G
1	A	1510	U
1	A	1512	U
1	A	1513	A
1	A	1516	C
1	A	1517	A
1	A	1519	U
1	A	1520	A
1	A	1521	A
1	A	1522	G
1	A	1524	C

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Mol	Chain	Res	Type
1	A	1526	G
1	A	1527	A
1	A	1533	A
1	A	1534	G
1	A	1536	C
1	A	1537	A
1	A	1538	A
1	A	1540	U
1	A	1541	C
1	A	1543	G
1	A	1545	U
1	A	1550	G
1	A	1551	U
1	A	1552	U
1	A	1553	A
1	A	1555	G
1	A	1556	G
1	A	1560	A
1	A	1561	G
1	A	1565	U
1	A	1568	U
1	A	1569	G
1	A	1570	G
1	A	1571	G
1	A	1572	G
1	A	1573	A
1	A	1575	A
1	A	1578	A
1	A	1579	C
1	A	1580	A
1	A	1581	U
1	A	1582	U
1	A	1583	G
1	A	1584	U
1	A	1585	G
1	A	1586	U
1	A	1590	C
1	A	1591	G
1	A	1592	A
1	A	1594	U
1	A	1595	C
1	A	1598	U

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Mol	Chain	Res	Type
1	A	1599	G
1	A	1600	A
1	A	1601	U
1	A	1604	C
1	A	1605	A
1	A	1606	C
1	A	1607	A
1	A	1613	G
1	A	1616	A
1	A	1623	U
1	A	1625	U
1	A	1626	A
1	A	1627	G
1	A	1629	U
1	A	1630	A
1	A	1631	G
1	A	1632	A
1	A	1633	A
1	A	1634	A
1	A	1635	A
1	A	1636	U
1	A	1639	G
1	A	1641	G
1	A	1651	C
1	A	1653	A
1	A	1654	A
1	A	1658	A
1	A	1659	C
1	A	1660	A
1	A	1661	C
1	A	1662	A
1	A	1666	A
1	A	1675	G
1	A	1678	A
1	A	1679	A
1	A	1690	A
1	A	1691	G
1	A	1692	C
1	A	1693	G
1	A	1698	A
1	A	1701	U
1	A	1707	U

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Mol	Chain	Res	Type
1	A	1718	G
1	A	1732	U
1	A	1737	U
1	A	1738	C
1	A	1739	G
1	A	1740	G
1	A	1741	G
1	A	1742	A
1	A	1743	G
1	A	1747	G
1	A	1757	U
1	A	1758	A
1	A	1759	G
1	A	1760	G
1	A	1761	G
1	A	1762	U
1	A	1763	U
1	A	1764	A
1	A	1765	A
1	A	1767	G
1	A	1768	C
1	A	1771	A
1	A	1772	G
1	A	1773	A
1	A	1777	G
1	A	1783	G
1	A	1785	G
1	A	1790	G
1	A	1791	G
1	A	1797	G
1	A	1800	A
1	A	1806	U
1	A	1808	U
1	A	1811	A
1	A	1812	A
1	A	1814	A
1	A	1816	A
1	A	1818	A
1	A	1820	G
1	A	1825	U
1	A	1826	G
1	A	1827	C

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Mol	Chain	Res	Type
1	A	1828	U
1	A	1829	A
1	A	1830	A
1	A	1835	U
1	A	1838	G
1	A	1843	U
1	A	1846	A
1	A	1856	A
1	A	1866	G
1	A	1867	G
1	A	1870	C
1	A	1871	U
1	A	1875	A
1	A	1876	G
1	A	1877	G
1	A	1878	U
1	A	1884	G
1	A	1888	U
1	A	1890	G
1	A	1892	U
1	A	1893	A
1	A	1895	C
1	A	1897	U
1	A	1898	C
1	A	1899	U
1	A	1900	G
1	A	1902	G
1	A	1903	A
1	A	1904	A
1	A	1906	C
1	A	1907	U
1	A	1908	A
1	A	1911	A
1	A	1912	A
1	A	1913	U
1	A	1914	C
1	A	1916	A
1	A	1923	A
1	A	1926	A
1	A	1927	A
1	A	1933	G
1	A	1935	C

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Mol	Chain	Res	Type
1	A	1938	U
1	A	1939	A
1	A	1945	A
1	A	1946	A
1	A	1950	U
1	A	1954	A
1	A	1956	G
1	A	1957	G
1	A	1958	U
1	A	1961	C
1	A	1963	A
1	A	1964	A
1	A	1965	A
1	A	1966	U
1	A	1967	U
1	A	1968	C
1	A	1970	U
1	A	1971	U
1	A	1972	G
1	A	1979	A
1	A	1982	U
1	A	1990	C
1	A	1996	A
1	A	1997	A
1	A	1998	A
1	A	1999	G
1	A	2008	A
1	A	2009	U
1	A	2012	G
1	A	2018	U
1	A	2019	G
1	A	2020	U
1	A	2023	C
1	A	2024	A
1	A	2029	G
1	A	2045	A
1	A	2047	A
1	A	2048	G
1	A	2057	A
1	A	2058	A
1	A	2059	G
1	A	2060	A

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Mol	Chain	Res	Type
1	A	2061	U
1	A	2062	G
1	A	2070	C
1	A	2075	G
1	A	2076	A
1	A	2079	G
1	A	2082	C
1	A	2083	G
1	A	2085	A
1	A	2086	A
1	A	2087	A
1	A	2088	G
1	A	2096	G
1	A	2107	G
1	A	2109	A
1	A	2111	C
1	A	2114	G
1	A	2117	A
1	A	2118	U
1	A	2119	U
1	A	2120	G
1	A	2127	G
1	A	2128	G
1	A	2129	C
1	A	2130	A
1	A	2131	C
1	A	2132	A
1	A	2133	G
1	A	2134	C
1	A	2135	U
1	A	2139	A
1	A	2140	C
1	A	2143	G
1	A	2144	A
1	A	2145	U
1	A	2146	A
1	A	2147	G
1	A	2153	A
1	A	2154	G
1	A	2155	C
1	A	2156	C
1	A	2157	U

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Mol	Chain	Res	Type
1	A	2158	U
1	A	2159	U
1	A	2161	A
1	A	2163	A
1	A	2164	C
1	A	2168	A
1	A	2173	U
1	A	2175	G
1	A	2180	C
1	A	2185	A
1	A	2186	G
1	A	2188	C
1	A	2190	C
1	A	2193	G
1	A	2194	U
1	A	2195	G
1	A	2198	A
1	A	2204	C
1	A	2209	G
1	A	2211	U
1	A	2215	U
1	A	2219	C
1	A	2221	U
1	A	2224	U
1	A	2225	A
1	A	2231	C
1	A	2232	A
1	A	2234	C
1	A	2235	A
1	A	2236	C
1	A	2237	U
1	A	2238	U
1	A	2239	A
1	A	2240	U
1	A	2244	G
1	A	2252	A
1	A	2254	A
1	A	2261	G
1	A	2262	G
1	A	2265	G
1	A	2266	G
1	A	2273	G

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Mol	Chain	Res	Type
1	A	2278	G
1	A	2290	C
1	A	2293	A
1	A	2296	A
1	A	2306	G
1	A	2310	C
1	A	2313	A
1	A	2315	A
1	A	2323	U
1	A	2324	C
1	A	2325	A
1	A	2328	A
1	A	2331	G
1	A	2333	U
1	A	2334	G
1	A	2335	G
1	A	2337	A
1	A	2338	A
1	A	2339	U
1	A	2345	A
1	A	2346	U
1	A	2347	A
1	A	2348	G
1	A	2349	A
1	A	2352	G
1	A	2354	A
1	A	2356	A
1	A	2357	G
1	A	2358	G
1	A	2362	A
1	A	2363	A
1	A	2364	G
1	A	2369	C
1	A	2370	U
1	A	2371	U
1	A	2372	G
1	A	2374	C
1	A	2377	C
1	A	2385	A
1	A	2388	A
1	A	2396	A
1	A	2399	G

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Mol	Chain	Res	Type
1	A	2406	G
1	A	2407	A
1	A	2409	G
1	A	2410	G
1	A	2412	C
1	A	2415	A
1	A	2417	U
1	A	2418	G
1	A	2419	A
1	A	2427	G
1	A	2429	U
1	A	2433	C
1	A	2434	A
1	A	2438	A
1	A	2439	A
1	A	2440	G
1	A	2441	G
1	A	2449	C
1	A	2450	U
1	A	2451	C
1	A	2456	G
1	A	2457	A
1	A	2459	A
1	A	2460	A
1	A	2461	A
1	A	2463	G
1	A	2468	C
1	A	2474	G
1	A	2475	A
1	A	2479	C
1	A	2486	A
1	A	2492	C
1	A	2495	A
1	A	2496	A
1	A	2497	G
1	A	2502	C
1	A	2503	A
1	A	2505	A
1	A	2506	U
1	A	2508	G
1	A	2509	A
1	A	2511	G

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Mol	Chain	Res	Type
1	A	2518	U
1	A	2519	U
1	A	2521	G
1	A	2525	C
1	A	2528	C
1	A	2529	G
1	A	2530	A
1	A	2531	U
1	A	2533	U
1	A	2540	A
1	A	2545	A
1	A	2552	G
1	A	2553	G
1	A	2556	G
1	A	2558	A
1	A	2559	G
1	A	2562	G
1	A	2568	A
1	A	2570	G
1	A	2574	U
1	A	2581	U
1	A	2582	U
1	A	2583	C
1	A	2589	U
1	A	2592	A
1	A	2593	A
1	A	2594	G
1	A	2599	A
1	A	2600	C
1	A	2601	G
1	A	2605	G
1	A	2609	G
1	A	2610	G
1	A	2613	C
1	A	2626	G
1	A	2629	A
1	A	2630	G
1	A	2636	U
1	A	2637	C
1	A	2640	U
1	A	2641	A
1	A	2642	U

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Mol	Chain	Res	Type
1	A	2648	G
1	A	2650	G
1	A	2656	A
1	A	2657	G
1	A	2667	G
1	A	2671	A
1	A	2673	C
1	A	2674	U
1	A	2679	U
1	A	2683	U
1	A	2687	A
1	A	2688	G
1	A	2690	G
1	A	2692	A
1	A	2695	G
1	A	2697	G
1	A	2699	U
1	A	2700	G
1	A	2708	C
1	A	2709	U
1	A	2716	U
1	A	2733	A
1	A	2741	G
1	A	2745	G
1	A	2750	C
1	A	2751	U
1	A	2753	U
1	A	2756	G
1	A	2757	U
1	A	2759	G
1	A	2761	C
1	A	2764	G
1	A	2765	A
1	A	2766	U
1	A	2769	G
1	A	2771	G
1	A	2773	U
1	A	2775	A
1	A	2776	A
1	A	2777	A
1	A	2778	G
1	A	2779	C

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Mol	Chain	Res	Type
1	A	2782	C
1	A	2783	U
1	A	2784	A
1	A	2785	A
1	A	2788	A
1	A	2791	A
1	A	2792	A
1	A	2794	C
1	A	2803	A
1	A	2804	G
1	A	2805	A
1	A	2806	U
1	A	2807	G
1	A	2817	A
1	A	2818	A
1	A	2820	U
1	A	2821	U
1	A	2822	C
1	A	2823	G
1	A	2824	G
1	A	2827	A
1	A	2828	U
1	A	2829	A
1	A	2832	A
1	A	2838	C
1	A	2840	A
1	A	2842	G
1	A	2843	A
1	A	2850	G
1	A	2853	U
1	A	2855	A
1	A	2856	U
1	A	2869	G
1	A	2870	A
1	A	2878	U
1	A	2879	G
1	A	2887	G
1	A	2889	G
1	A	2892	G
1	A	2899	A
1	A	2904	U
1	A	2905	C

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Mol	Chain	Res	Type
1	A	2906	G
1	A	2913	G
1	A	2914	A
2	B	2	C
2	B	5	G
2	B	7	G
2	B	10	U
2	B	11	A
2	B	12	U
2	B	14	G
2	B	20	A
2	B	22	G
2	B	23	U
2	B	24	C
2	B	27	A
2	B	29	C
2	B	30	U
2	B	33	U
2	B	35	C
2	B	39	G
2	B	40	C
2	B	41	C
2	B	42	G
2	B	51	A
2	B	54	U
2	B	55	A
2	B	63	U
2	B	64	A
2	B	65	G
2	B	66	C
2	B	84	U
2	B	86	A
2	B	87	C
2	B	88	G
2	B	93	G
2	B	95	U
2	B	106	G
2	B	109	G
2	B	111	C
2	B	113	G
2	B	115	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	11	U
1	A	69	C
1	A	157	U
1	A	169	G
1	A	227	G
1	A	267	G
1	A	291	G
1	A	335	U
1	A	337	A
1	A	385	U
1	A	576	U
1	A	657	U
1	A	688	A
1	A	697	U
1	A	809	A
1	A	840	C
1	A	890	G
1	A	1024	A
1	A	1026	C
1	A	1503	U
1	A	1520	A
1	A	1521	A
1	A	1632	A
1	A	1658	A
1	A	1756	U
1	A	2117	A
1	A	2127	G
1	A	2237	U
1	A	2261	G
1	A	2428	U
1	A	2450	U
1	A	2455	G
1	A	2462	A
1	A	2749	G
1	A	2782	C
1	A	2878	U

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	8

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2207:U	O3'	2208:A	P	11.16
1	A	1939:A	O3'	1944:U	P	10.86
1	A	929:C	O3'	937:G	P	10.36
1	A	1096:C	O3'	1097:U	P	7.19
1	A	1153:C	O3'	1154:G	P	7.11
1	A	770:G	O3'	771:G	P	3.87
1	A	2217:G	O3'	2218:G	P	3.68
1	A	1448:U	O3'	1449:A	P	3.05

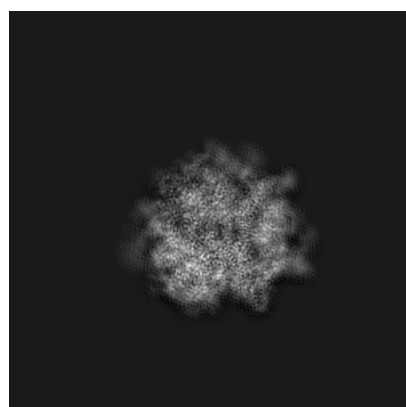
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10078. These allow visual inspection of the internal detail of the map and identification of artifacts.

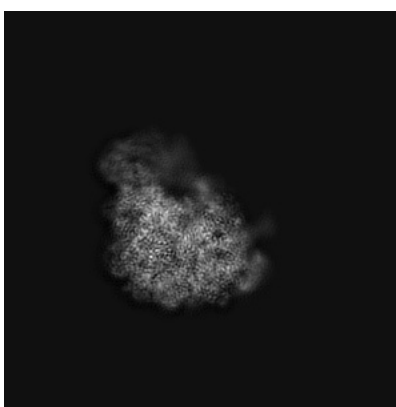
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

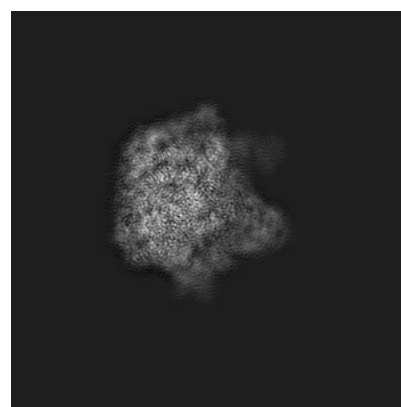
6.1.1 Primary map



X



Y

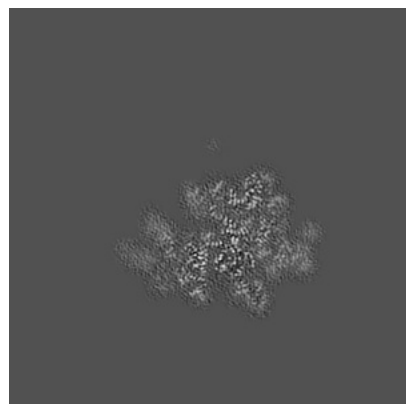


Z

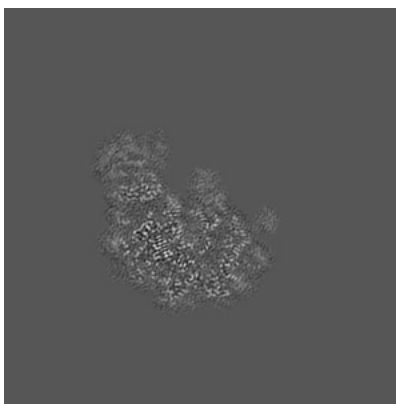
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

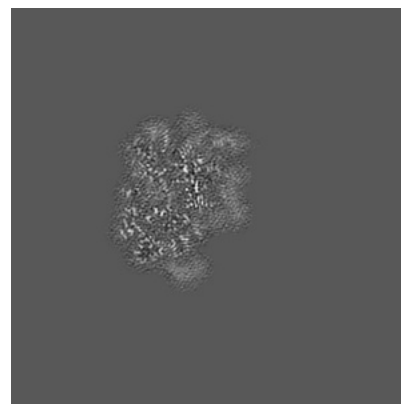
6.2.1 Primary map



X Index: 200



Y Index: 200

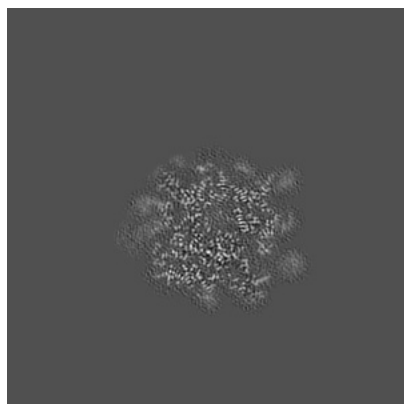


Z Index: 200

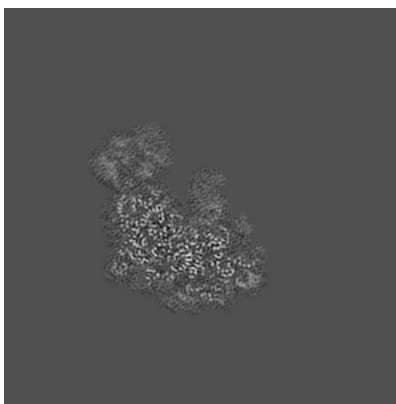
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

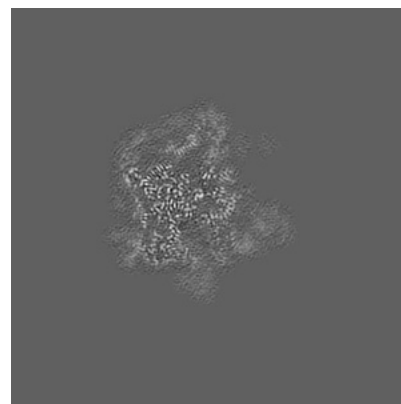
6.3.1 Primary map



X Index: 164



Y Index: 185

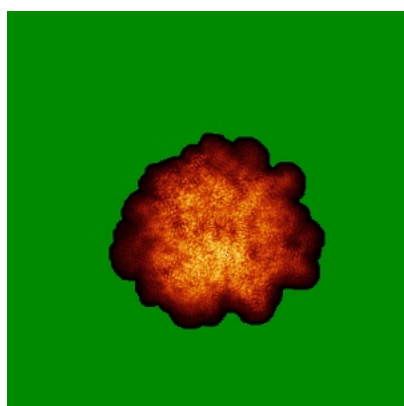


Z Index: 154

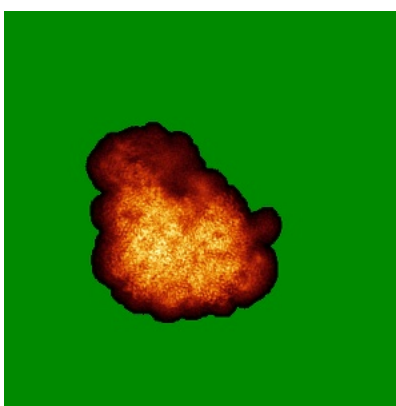
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

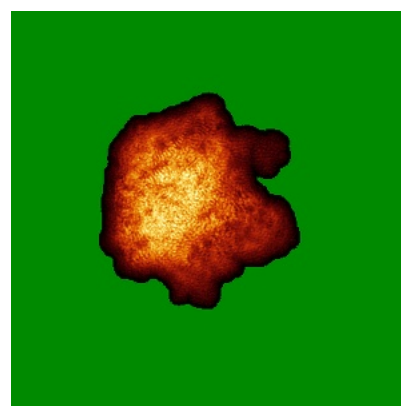
6.4.1 Primary map



X



Y

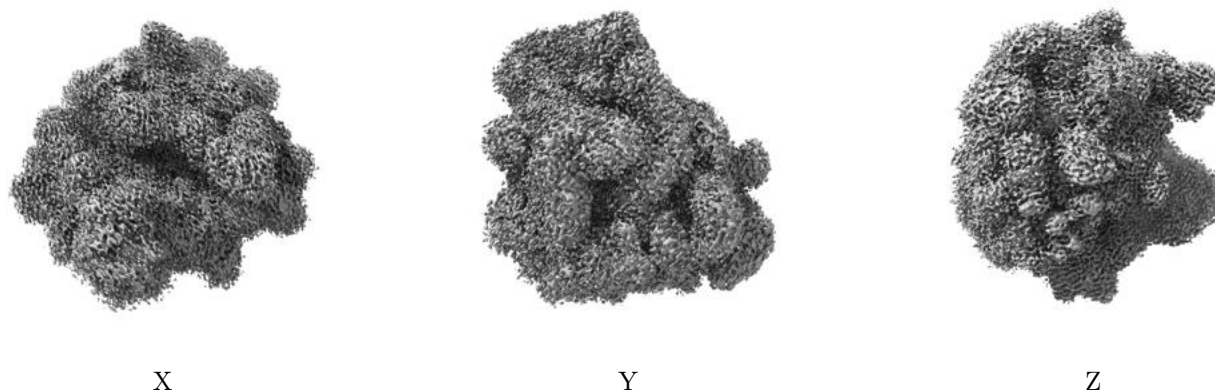


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

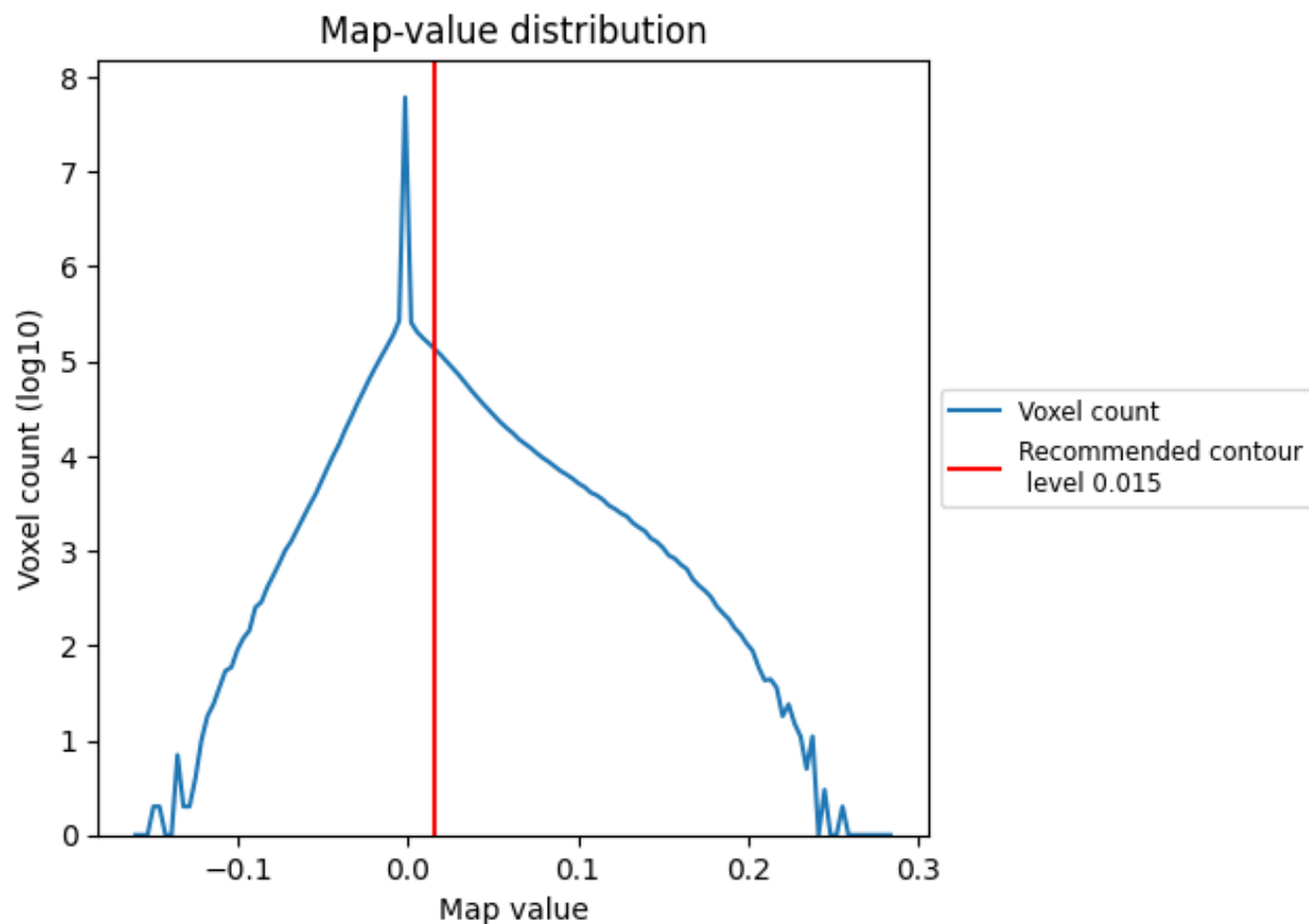
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

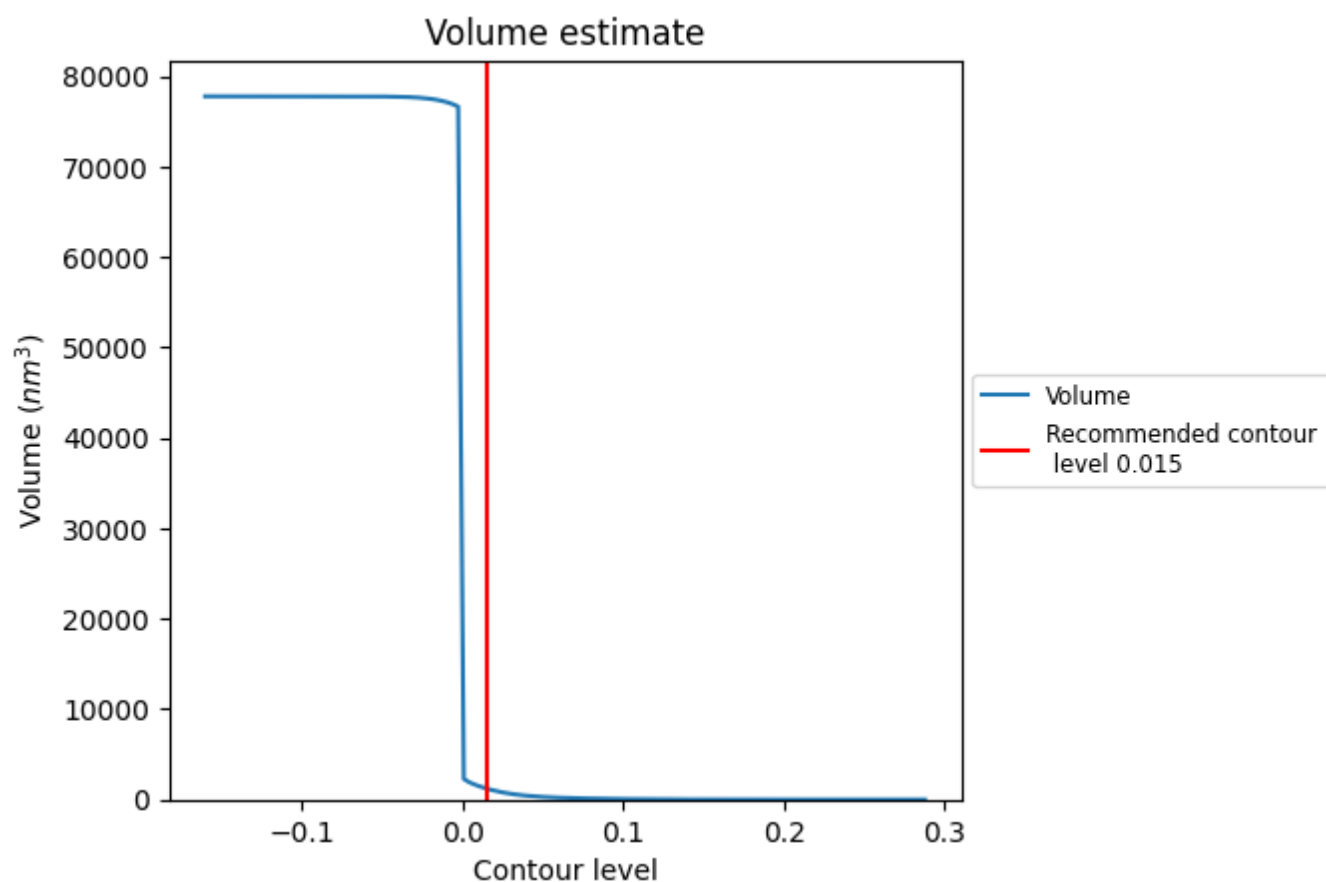
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

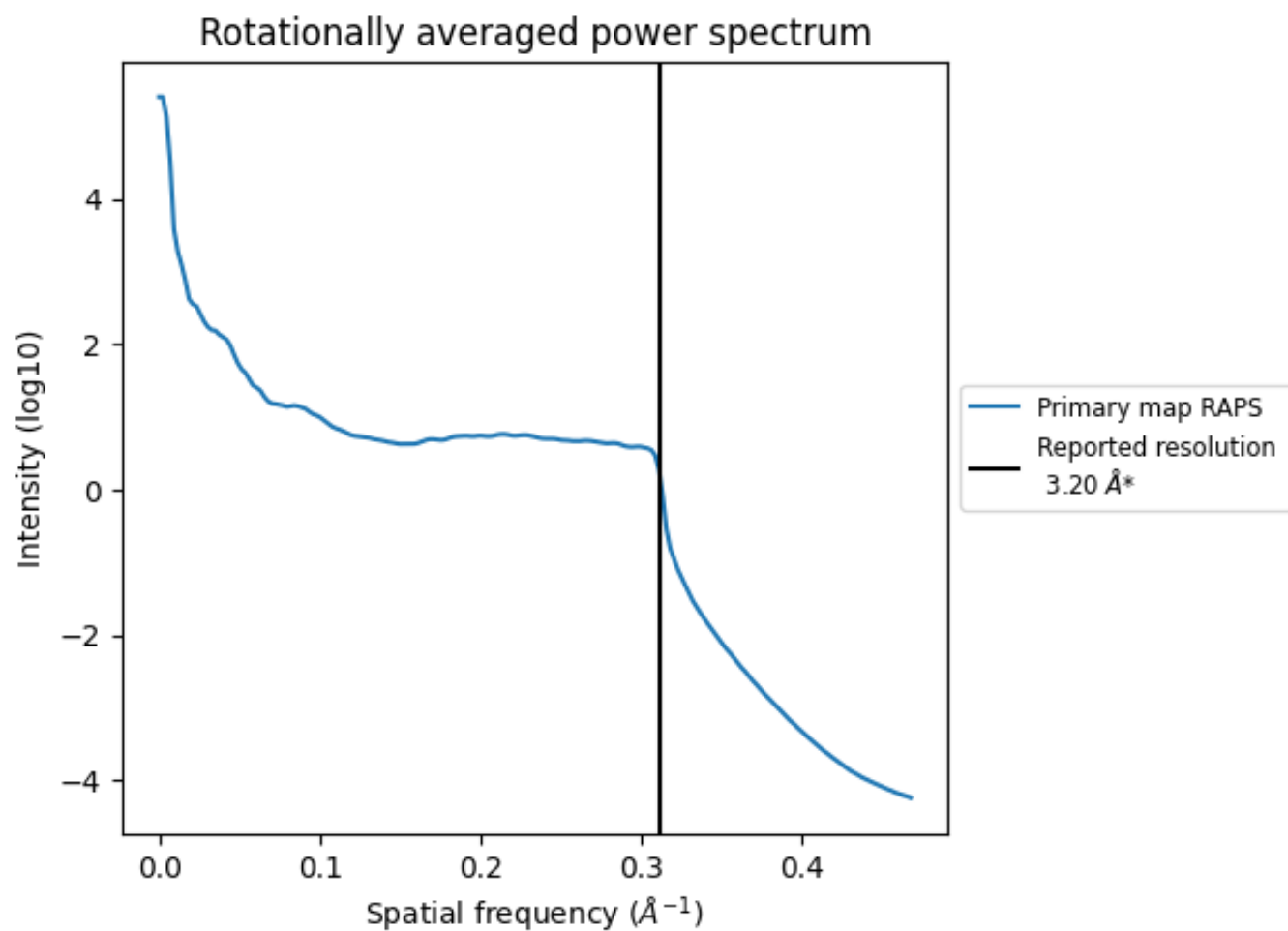
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1203 nm^3 ; this corresponds to an approximate mass of 1087 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

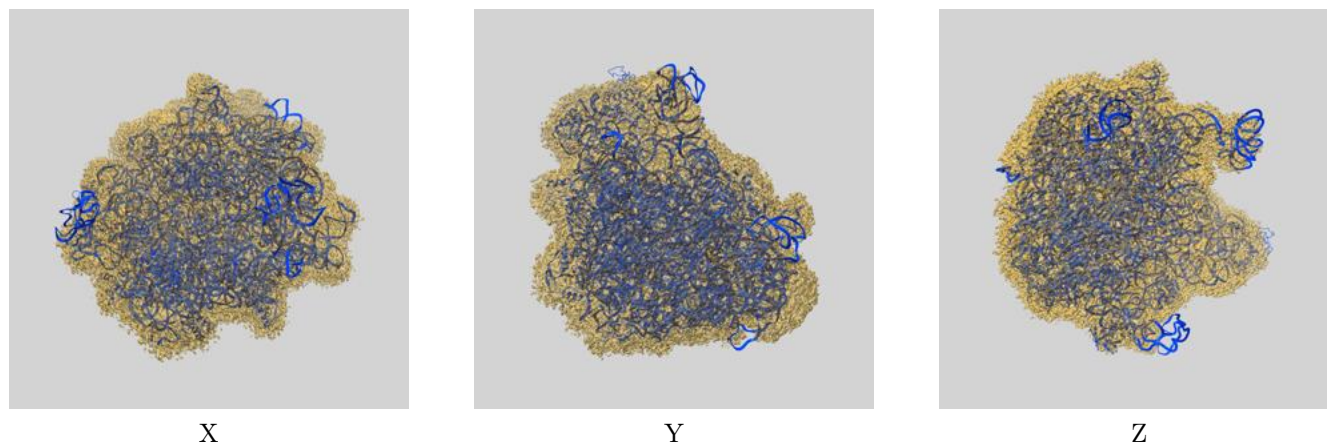
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

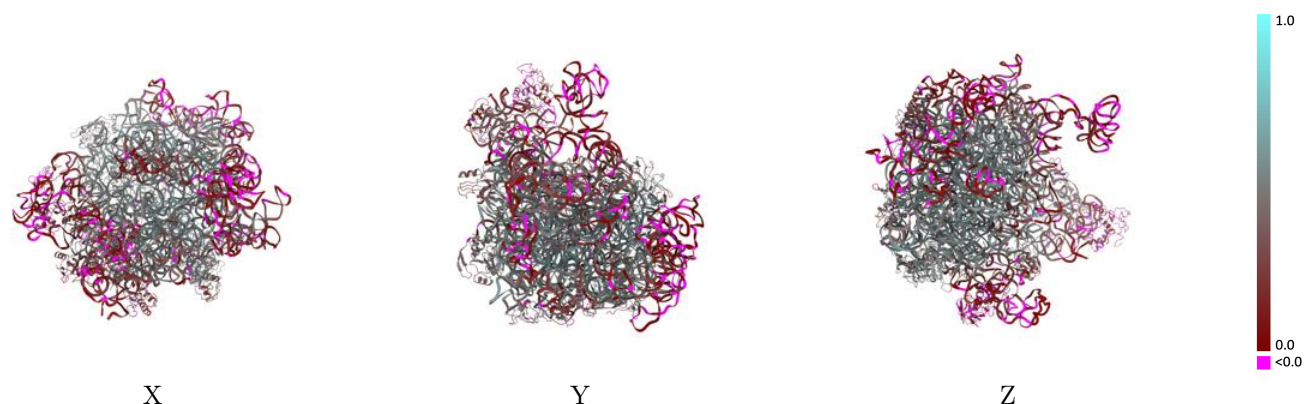
This section contains information regarding the fit between EMDB map EMD-10078 and PDB model 6S12. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



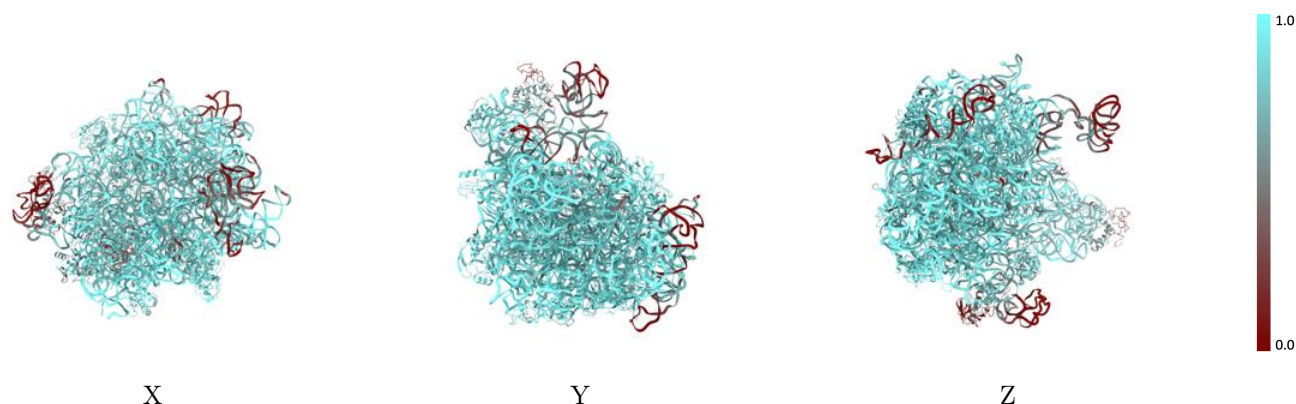
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



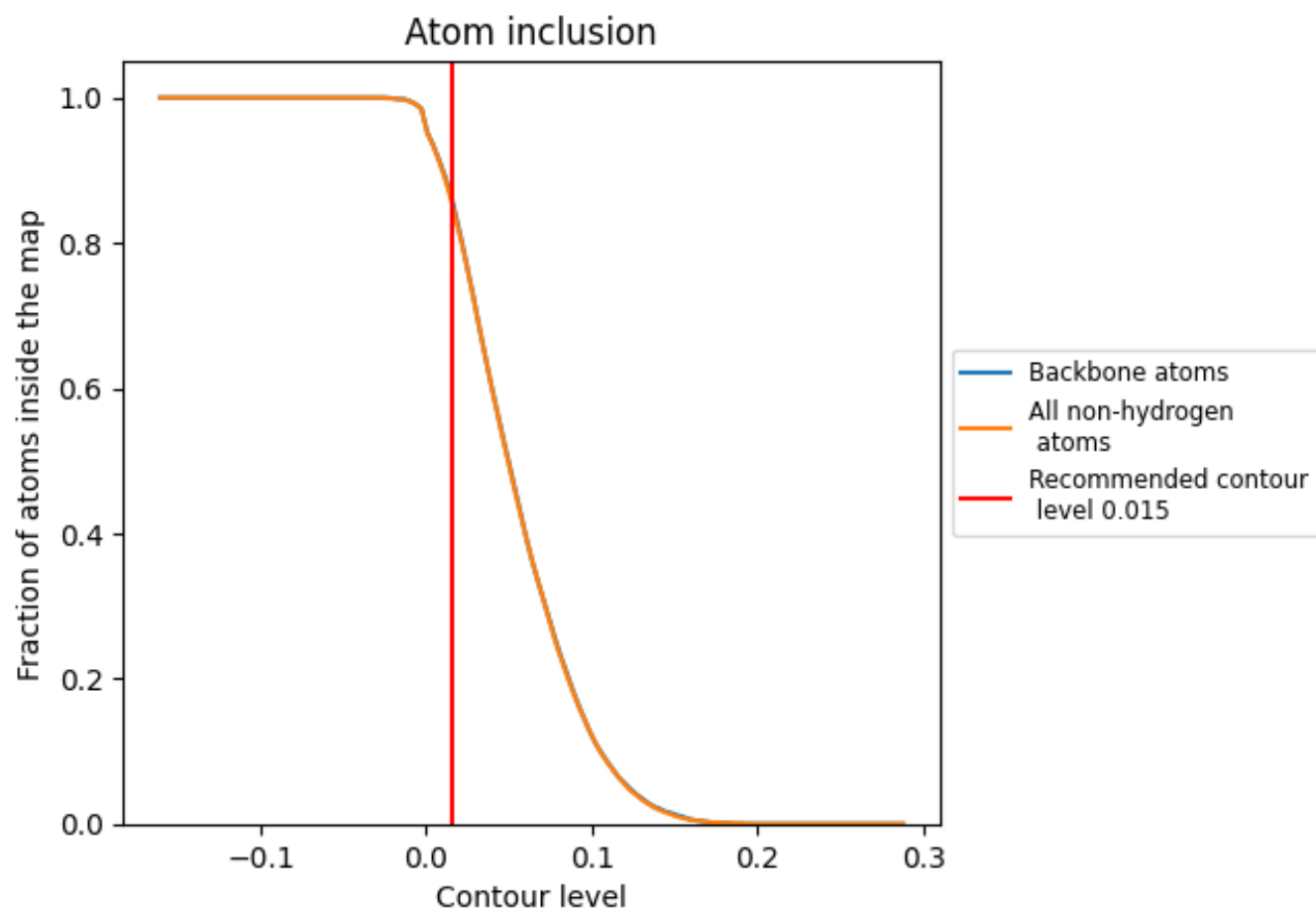
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).































































9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8590	 0.3640
1	 0.5010	 0.1650
2	 0.9020	 0.4630
3	 0.8980	 0.4510
4	 0.5050	 0.0530
A	 0.8760	 0.3690
B	 0.9060	 0.2130
C	 0.8870	 0.4390
D	 0.9270	 0.4850
E	 0.9040	 0.4640
F	 0.6080	 0.0970
G	 0.3130	 0.0670
H	 0.9140	 0.4760
I	 0.8750	 0.4380
J	 0.9000	 0.4190
K	 0.8670	 0.3600
L	 0.8990	 0.4580
M	 0.8390	 0.2650
N	 0.9220	 0.4640
O	 0.9090	 0.4850
P	 0.9140	 0.4630
Q	 0.8700	 0.4230
R	 0.8860	 0.3960
S	 0.8390	 0.3390
T	 0.7120	 0.2510
U	 0.8890	 0.4270
V	 0.7740	 0.3170
W	 0.8440	 0.2920
X	 0.9090	 0.4770
Y	 0.2120	 0.0390
Z	 0.8470	 0.3190

