



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:45 pm BST

PDB ID : 5NRG  
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with RB02  
Authors : Yonath, A.; Matzov, D.; Eyal, Z.; Ben Hamou, R.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Fridman, M.  
Deposited on : 2017-04-23  
Resolution : 3.44 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

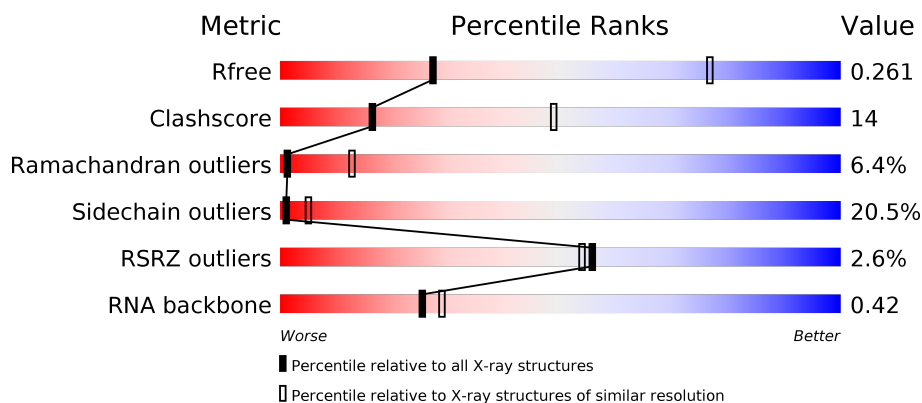
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.44 Å.

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








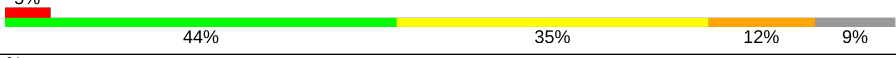





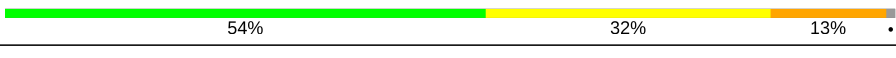



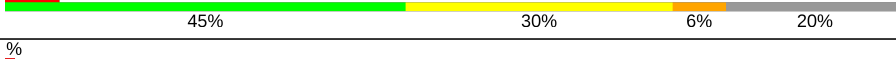

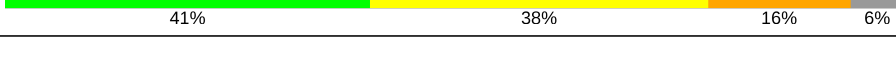

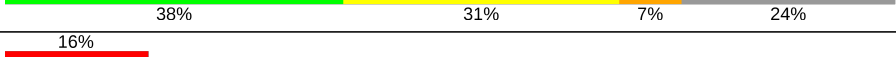
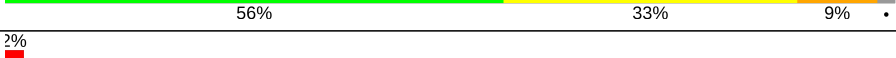
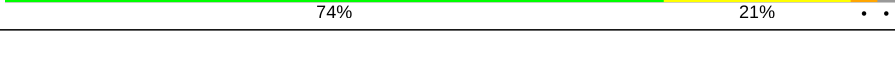
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)
RNA backbone	3102	1024 (3.92-2.96)

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

Mol	Chain	Length	Quality of chain
1	X	2923	<div> <div> <div>1%</div> <div>34%</div> <div>38%</div> <div>18%</div> <div>7%</div> </div> </div>
2	Y	114	<div> <div>2%</div> <div>42%</div> <div>39%</div> <div>18%</div> <div>•</div> </div>
3	A	277	<div> <div>4%</div> <div>51%</div> <div>33%</div> <div>10%</div> <div>6%</div> </div>
4	B	220	<div> <div>57%</div> <div>34%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	140	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	V	69	
23	W	59	
24	Z	58	
25	2	45	
26	3	66	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MN	X	3062	-	-	-	X
29	MN	X	3075	-	-	-	X
30	MG	3	104	-	-	-	X
30	MG	J	201	-	-	-	X
30	MG	X	3202	-	-	-	X
30	MG	X	3242	-	-	-	X
30	MG	X	3260	-	-	-	X
30	MG	X	3264	-	-	-	X
30	MG	X	3266	-	-	-	X
30	MG	X	3271	-	-	-	X
30	MG	X	3274	-	-	-	X
30	MG	X	3279	-	-	-	X
30	MG	X	3280	-	-	-	X
30	MG	X	3283	-	-	-	X

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 80800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2710	Total	C	N	O	P	0	1	0
			58141	25956	10658	18816	2711			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	114	Total	C	N	O	P	0	0	0
			2430	1086	436	794	114			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	260	Total	C	N	O	S	0	0	0
			1641	1008	314	315	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1534	961	287	281	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	198	Total	C	N	O	S	0	0	0
			1365	852	256	255	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	137	Total	C	N	O	S	0	0	0
			926	580	165	177	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	E	147	Total	C	N	O	0	0	0
			793	481	154	158			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1062	664	194	201	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			902	561	173	166	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	127	Total	C	N	O	0	0	0
			780	467	162	151			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1011	651	184	172	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			883	539	176	167	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	110	Total	C	N	O	0	0	0
			672	410	126	136			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	111	Total	C	N	O	0	0	0
			779	492	147	140			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S	0	0	0
			937	590	186	157	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	101	Total	C	N	O	0	0	0
			700	445	128	127			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S	0	0	0
			852	532	161	156	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	90	Total	C	N	O	S	0	0	0
			656	411	111	132	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	102	Total	C	N	O	0	0	0
			596	365	111	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	174	Total	C	N	O	S	0	0	0
			1145	722	204	217	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	76	Total	C	N	O	0	0	0
			561	349	107	105			

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	0	0	0
			519	319	96	104			

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	W	57	Total	C	N	O	0	0	0
			437	272	83	82			

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Z	44	Total	C	N	O	S	0	0	0
			337	205	75	54	3			

- Molecule 25 is a protein called 50S ribosomal protein L34.

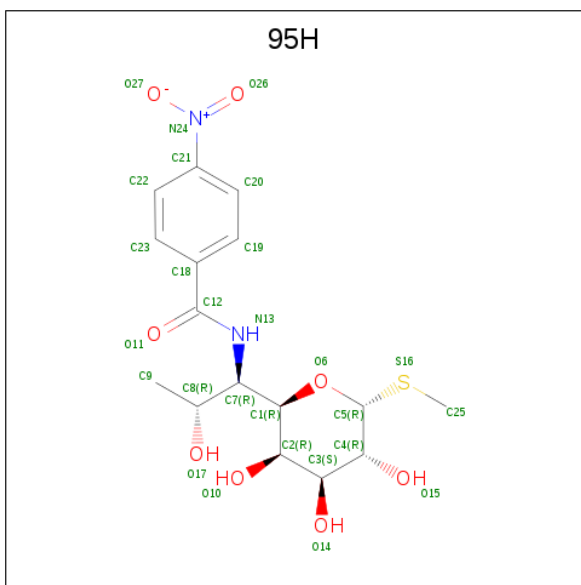
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	44	Total	C	N	O	S	0	0	0
			360	219	87	53	1			

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	65	Total	C	N	O	S	0	0	0
			419	257	83	78	1			

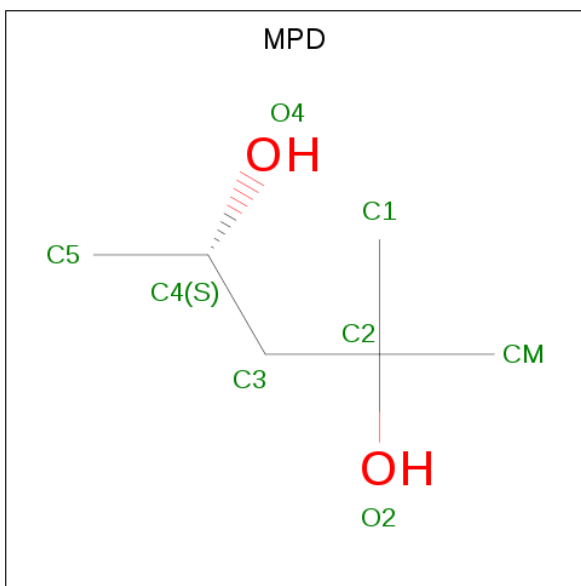
- Molecule 27 is {N}-[(1 {R},2 {R})-1-[(2 {R},3 {R},4 {S},5 {R},6 {R})-6-methylsulfanyl-3,4,5-tris(oxidanyl)oxan-2-yl]-2-oxidanyl-propyl]-4-nitro-benzamide (three-letter code: 95H) (formula: C<sub>16</sub>H<sub>22</sub>N<sub>2</sub>O<sub>8</sub>S).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	X	1	Total	C	N	O	S	1	0
			27	16	2	8	1		

- Molecule 28 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	X	1	Total	C	O	0	0
			8	6	2		
28	X	1	Total	C	O	0	0
			8	6	2		

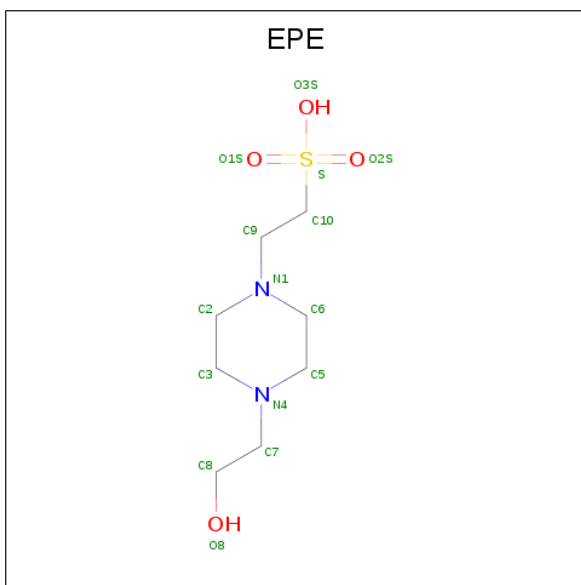
- Molecule 29 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	E	1	Total 1	Mn 1	0	0
29	I	1	Total 1	Mn 1	0	0
29	Z	1	Total 1	Mn 1	0	0
29	X	203	Total 203	Mn 203	0	0
29	Y	1	Total 1	Mn 1	0	0
29	3	3	Total 3	Mn 3	0	0

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

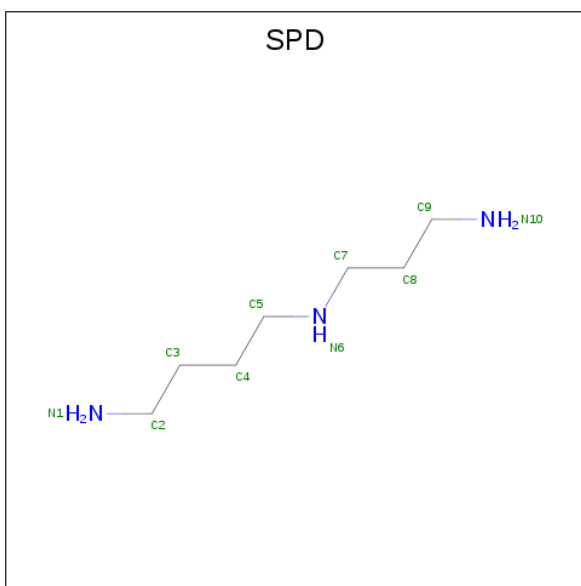
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	G	1	Total 1	Mg 1	0	0
30	J	1	Total 1	Mg 1	0	0
30	C	1	Total 1	Mg 1	0	0
30	X	78	Total 78	Mg 78	0	0
30	Y	2	Total 2	Mg 2	0	0
30	3	1	Total 1	Mg 1	0	0

- Molecule 31 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 32 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).

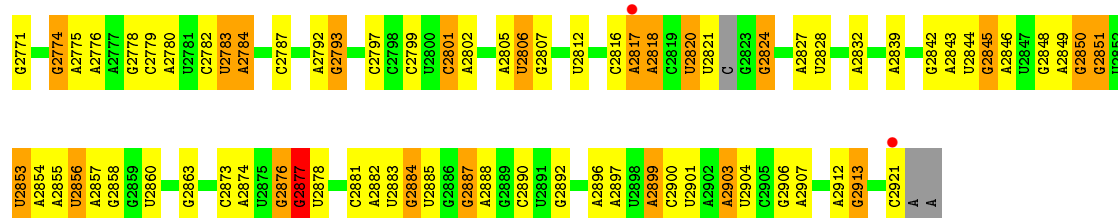


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	N	0	0
			10	7	3		



G1695	G1696	G1697	G1698	G1699	G1700	G1701	G1702	G1703	G1704	G1705	G1706	G1707	G1708	G1709	G1710	G1711	G1712	G1713	G1714	G1715	G1716	G1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1726	G1727	G1728	G1729	G1730	G1731	G1732	G1733	G1734	G1735	G1736	G1737	G1738	G1739	G1740	G1741	G1742	G1743	G1744	G1745	G1746	G1747	G1748	G1749	G1750	G1751	G1752	G1753	G1754	G1755	G1756	G1757	G1758	G1759	G1760																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569	G1570	G1571	G1572	G1573	G1574	G1575	G1576	G1577	G1578	G1579	G1580	G1581	G1582	G1583	G1584	G1585	G1586	G1587	G1588	G1589	G1590	G1591	G1592	G1593	G1594	G1595	G1596	G1597	G1598	G1599	G1600	G1601	G1602	G1603	G1604	G1605	G1606	G1607	G1608	G1609																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
A1422	C1423	A1424	G1425	G1426	G1427	G1428	G1429	A1430	C1431	A1432	A1433	A1434	C1435	A1436	G1437	A1438	A1439	C1440	C1441	A1442	A1443	C1444	A1445	C1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
A1353	G1354	A1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	A1390	A1391	A1392	A1393	A1394	G1395	A1396	G1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
U1212	G1213	G1214	G1215	U1216	G1217	G1218	G1219	A1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	A1231	G1232	A1233	G1234	U1235	U1236	U1237	U1238	A1239	A1240	A1241	A1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253	G1254	G1255	G1256	G1257	G1258	G1259	G1260	G1261	U1262	U1263	G1264	G1265	A1266	U1267	G1268	G1269	U1270	G1271	U1272	G1273	A1274	G1275	G1276	G1277	G1278	G1279	U1280	U1281	A1282																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G1005	G1006	G1007	G1008	G1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	A1017	A1018	A1019	G1020	G1021	G1022	A1023	A1024	A1025	A1026	G1027	G1028	G1029	G1030	G1031	A1032	U1033	U1034	U1035	U1036	U1037	G1038	G1039	A1040	G1041	G1042	U1043	A1044	A1045	A1046	A1047	U1048	U1049	G1050	G1051	A1052	A1053	A1054	A1055	U1056	A1057	U1058	U1059	U1060	U1061	U1062	U1063	A1064	A1065	U1066	U1067	G1068	U1069	U1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	G1201	G1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1575	A1576	A1577	A1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1598	A1599	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607	A1608	A1609	A1610	A1611	A1612	A1613	A1614	A1615	A1616	A1617	A1618	A1619	A1620	A1621	A1622	A1623	A1624	A1625	A1626	A1627	A1628	A1629	A1630	A1631	A1632	A1633	A1634	A1635	A1636	A1637	A1638	A1639	A1640	A1641	A1642	A1643	A1644	A1645	A1646	A1647	A1648	A1649	A1650	A1651	A1652	A1653	A1654	A1655	A1656	A1657	A1658	A1659	A1660	A1661	A1662	A1663	A1664	A1665	A1666	A1667	A1668	A1669	A1670	A1671	A1672	A1673	A1674	A1675	A1676	A1677	A1678	A1679	A1680	A1681	A1682	A1683	A1684	A1685	A1686	A1687	A1688	A1689	A1690	A1691	A1692	A1693	A1694	A1695	A1696	A1697	A1698	A1699	A1700	A1701	A1702	A1703	A1704	A1705	A1706	A1707	A1708	A1709	A1710	A1711	A1712	A1713	A1714	A1715	A1716	A1717	A1718	A1719	A1720	A1721	A1722	A1723	A1724	A1725	A1726	A1727	A1728	A1729	A1730	A1731	A1732	A1733	A1734	A1735	A1736	A1737	A1738	A1739	A1740	A1741	A1742	A1743	A1744	A1745	A1746	A1747	A1748	A1749	A1750	A1751	A1752	A1753	A1754	A1755	A1756	A1757	A1758	A1759	A1760
U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								

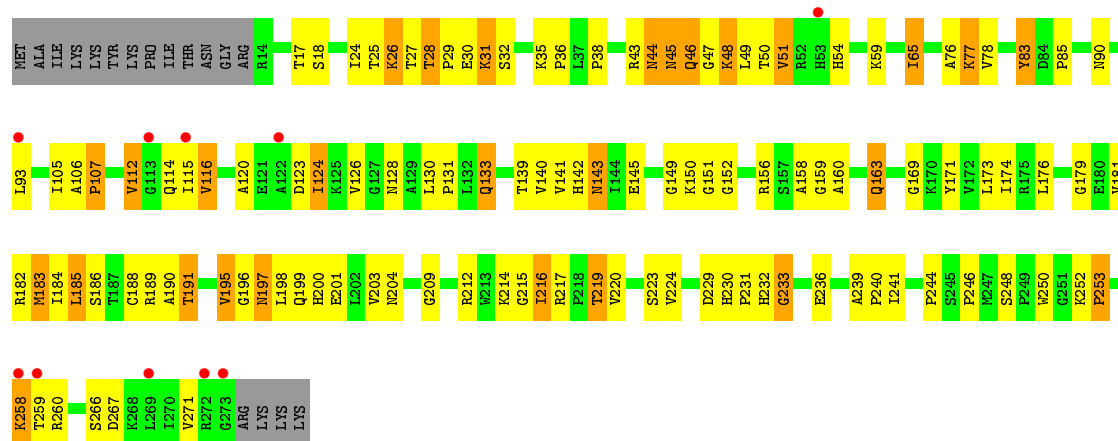
[illegible]



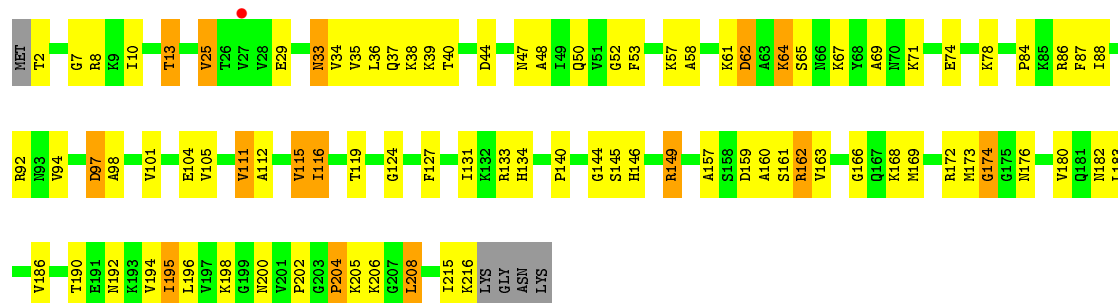
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

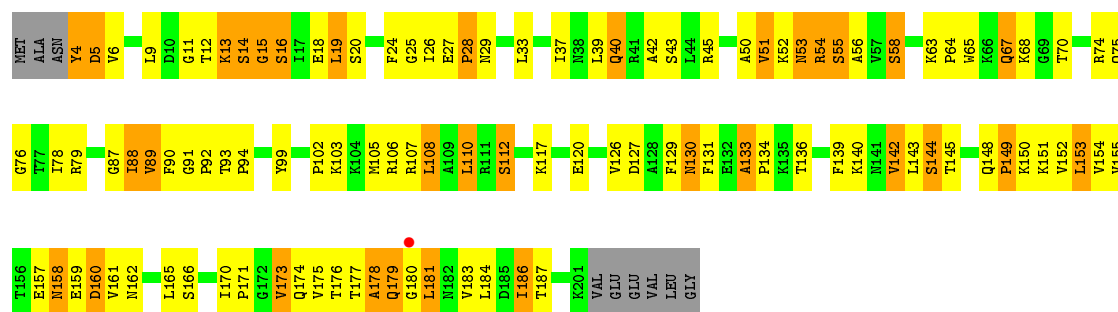


• Molecule 4: 50S ribosomal protein L3



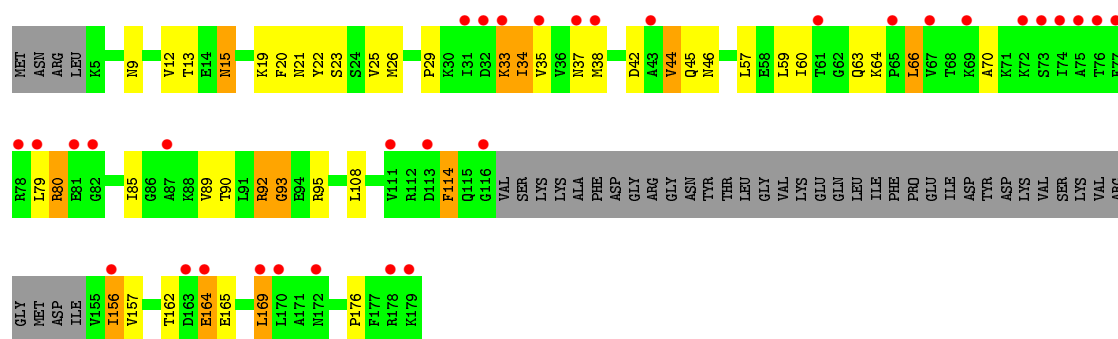
• Molecule 5: 50S ribosomal protein L4

Chain C: 



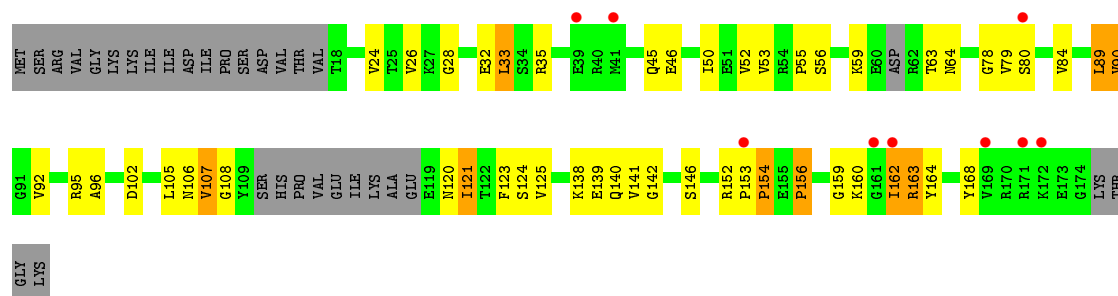
• Molecule 6: 50S ribosomal protein L5

Chain D: 



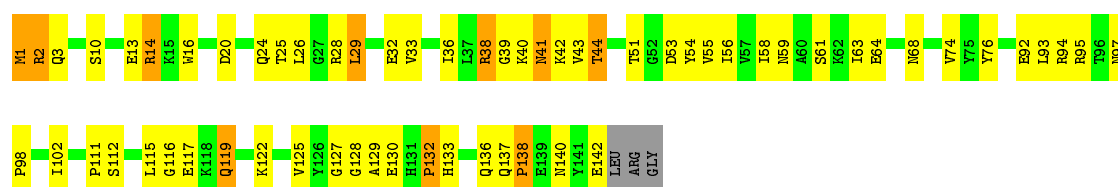
• Molecule 7: 50S ribosomal protein L6

Chain E: 



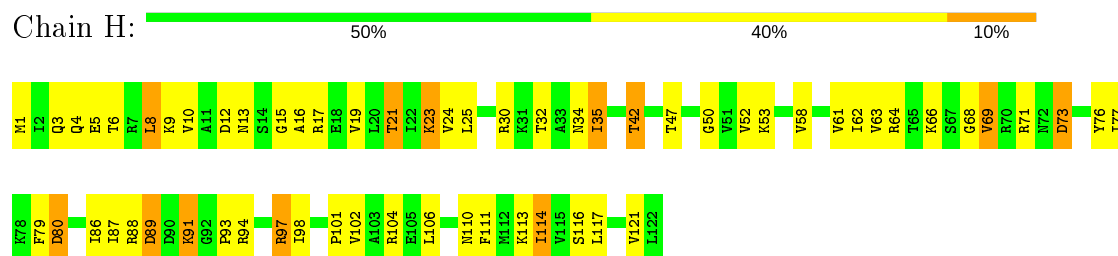
• Molecule 8: 50S ribosomal protein L13

Chain G: 

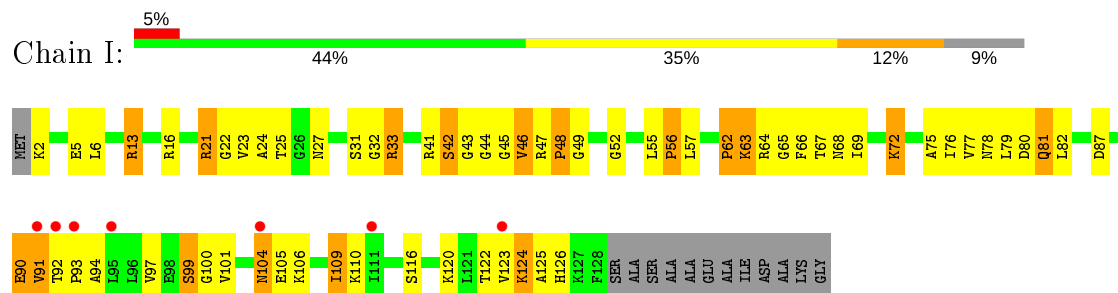




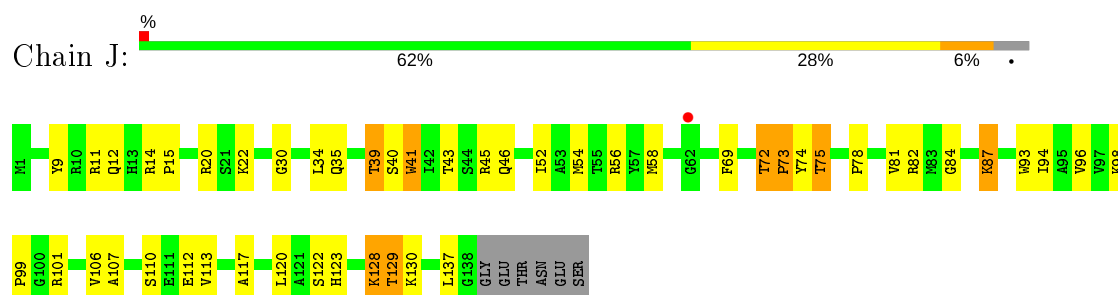
- Molecule 9: 50S ribosomal protein L14



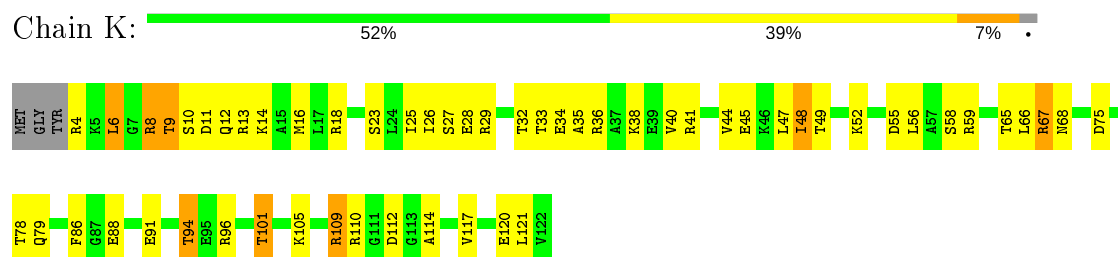
- Molecule 10: 50S ribosomal protein L15



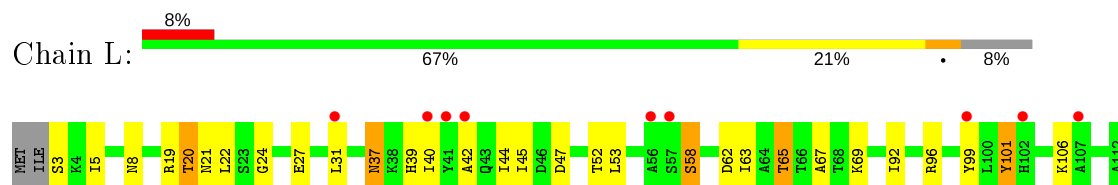
- Molecule 11: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L17



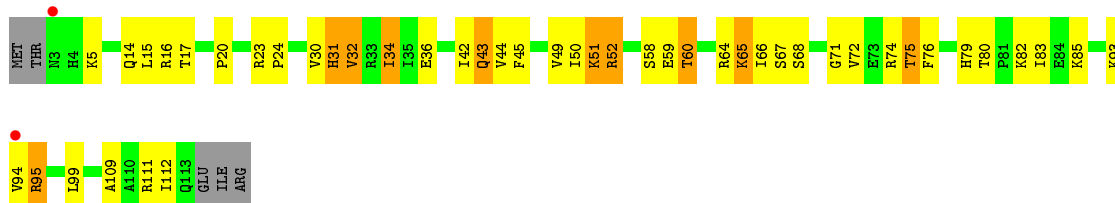
- Molecule 13: 50S ribosomal protein L18



ARG  
GLU  
SER  
GLY  
LEU  
GLU  
PHE

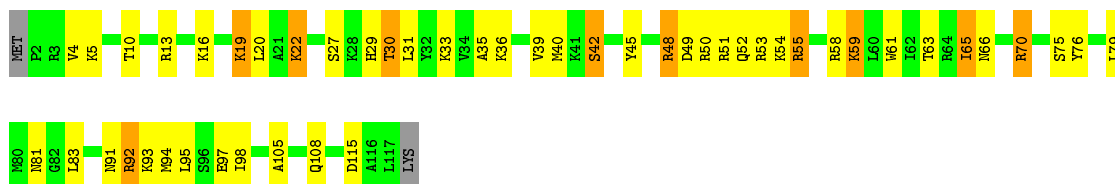
• Molecule 14: 50S ribosomal protein L19

Chain M:  2% 56% 31% 9%



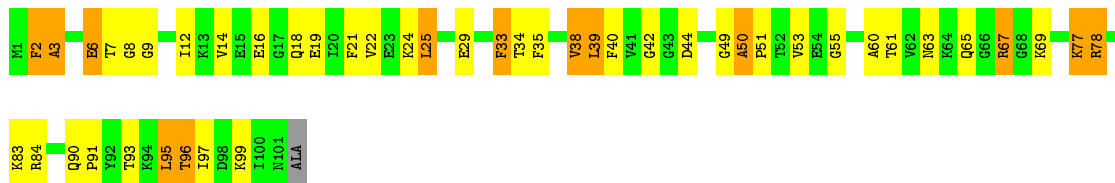
• Molecule 15: 50S ribosomal protein L20

Chain N:  57% 33% 8%



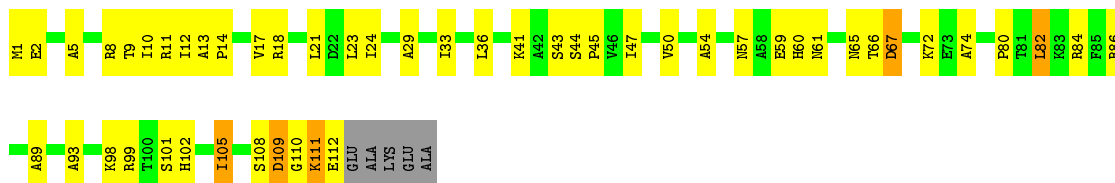
• Molecule 16: 50S ribosomal protein L21

Chain O:  54% 32% 13%



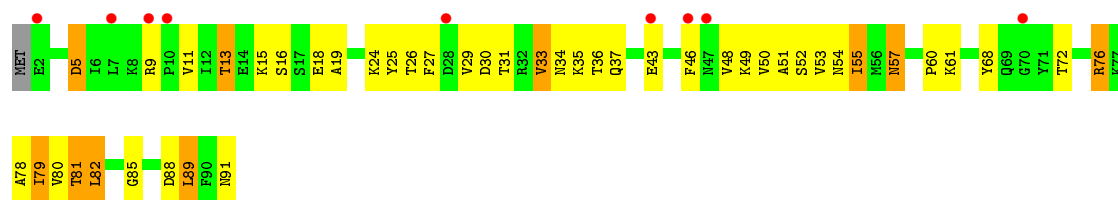
• Molecule 17: 50S ribosomal protein L22

Chain P:  53% 38% 9%

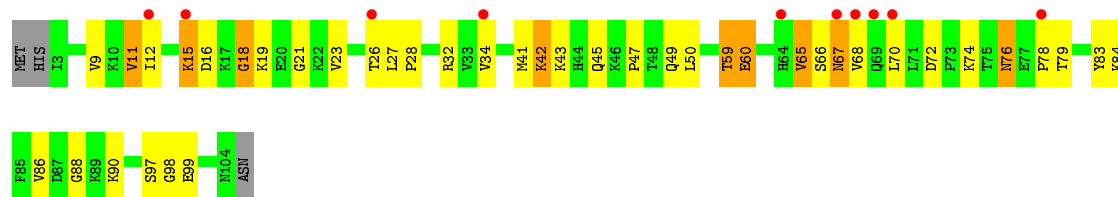


• Molecule 18: 50S ribosomal protein L23

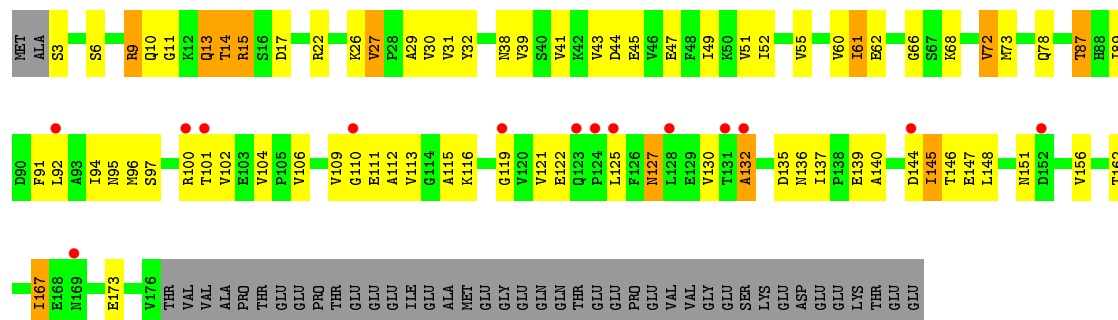
Chain Q:  10% 49% 38% 11%



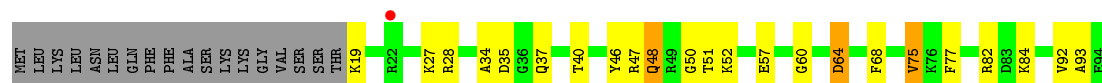
- Molecule 19: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L29

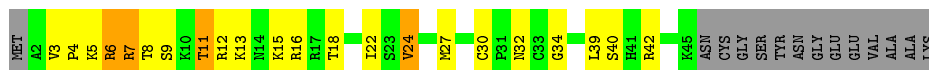


- Molecule 23: 50S ribosomal protein L30

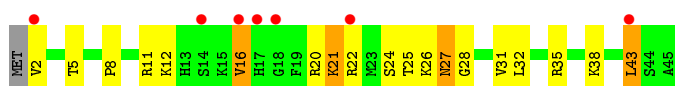




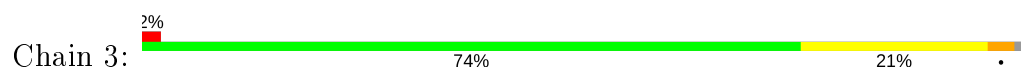
- Molecule 24: 50S ribosomal protein L32



- Molecule 25: 50S ribosomal protein L34



- Molecule 26: 50S ribosomal protein L35



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	279.80 Å   279.80 Å   873.27 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	49.37 – 3.44 49.77 – 3.44	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.37-3.44) 96.1 (49.77-3.44)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 3.48 Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.219   ,   0.261 0.219   ,   0.261	Depositor DCC
$R_{free}$ test set	12721 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.6	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23   ,   72.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	80800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, MPD, 95H, EPE, SPD

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	X	0.86	66/65104 (0.1%)	1.53	1119/101503 (1.1%)
2	Y	0.76	1/2717 (0.0%)	1.41	46/4232 (1.1%)
3	A	0.49	0/1665	0.73	0/2275
4	B	0.58	0/1557	0.71	0/2102
5	C	0.60	0/1386	0.82	1/1890 (0.1%)
6	D	0.45	1/934 (0.1%)	0.53	0/1273
7	E	0.29	0/798	0.58	0/1102
8	G	0.47	0/1083	0.67	0/1466
9	H	0.49	0/908	0.71	0/1221
10	I	0.45	0/789	0.77	0/1073
11	J	0.57	1/1034 (0.1%)	0.65	1/1401 (0.1%)
12	K	0.40	0/885	0.62	0/1185
13	L	0.35	0/678	0.58	0/934
14	M	0.53	0/790	0.80	0/1071
15	N	0.62	0/949	0.79	0/1258
16	O	0.62	1/710 (0.1%)	0.84	1/962 (0.1%)
17	P	0.64	0/860	0.73	0/1159
18	Q	0.46	0/662	0.62	0/898
19	R	0.44	0/601	0.67	0/830
20	S	0.43	0/1158	0.58	0/1588
21	T	0.49	0/567	0.70	0/756
22	V	0.43	0/520	0.61	0/694
23	W	0.56	0/439	0.67	0/592
24	Z	0.59	0/342	0.73	0/456
25	2	0.66	0/363	0.73	0/475
26	3	0.41	0/424	0.70	0/578
All	All	0.79	70/87923 (0.1%)	1.39	1168/132974 (0.9%)

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
3	A	0	3
4	B	0	5
5	C	0	5
7	E	0	1
8	G	0	5
9	H	0	1
10	I	0	4
11	J	0	1
14	M	0	1
16	O	0	2
18	Q	0	1
19	R	0	2
All	All	0	31

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2088	G	C8-N7	15.26	1.40	1.30
1	X	2474	G	C8-N7	15.10	1.40	1.30
1	X	2059	G	C5-C4	12.16	1.46	1.38
1	X	1000	G	C5-C4	-11.92	1.30	1.38
1	X	1931	G	N3-C4	10.72	1.43	1.35
1	X	1715	U	C5-C6	10.55	1.43	1.34
1	X	2845	G	N9-C4	-10.19	1.29	1.38
1	X	1186	A	N9-C4	-10.07	1.31	1.37
1	X	828	A	N9-C4	-9.88	1.31	1.37
11	J	69	PHE	C-N	-9.63	1.16	1.34
1	X	2089[A]	A	N3-C4	9.41	1.40	1.34
1	X	2089[B]	A	N3-C4	9.41	1.40	1.34
1	X	1289	A	N9-C4	-9.22	1.32	1.37
1	X	2474	G	N9-C8	9.10	1.44	1.37
1	X	1931	G	N9-C4	8.76	1.45	1.38
1	X	2088	G	N7-C5	8.66	1.44	1.39
6	D	108	LEU	C-N	8.62	1.50	1.34
1	X	1715	U	N1-C6	7.62	1.44	1.38
1	X	1000	G	N7-C5	7.32	1.43	1.39
1	X	630	G	N9-C4	-7.18	1.32	1.38
1	X	2845	G	C2-N3	-6.86	1.27	1.32
16	O	77	LYS	CA-CB	6.69	1.68	1.53
1	X	2088	G	N9-C8	6.68	1.42	1.37
1	X	373	A	C6-N6	6.62	1.39	1.33
1	X	2740	A	N9-C4	-6.59	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1303	A	N9-C4	-6.57	1.33	1.37
1	X	550	A	P-O5'	6.54	1.66	1.59
1	X	992	A	N9-C4	-6.44	1.33	1.37
1	X	2797	C	C4-N4	6.39	1.39	1.33
1	X	1065	A	N9-C4	-6.38	1.34	1.37
1	X	1289	A	C5-C4	6.25	1.43	1.38
1	X	2059	G	C8-N7	6.24	1.34	1.30
1	X	1000	G	N9-C8	-5.94	1.33	1.37
2	Y	92	G	N9-C4	-5.93	1.33	1.38
1	X	1278	G	N9-C4	-5.84	1.33	1.38
1	X	428	G	N9-C4	5.80	1.42	1.38
1	X	2446	U	C5-C6	5.77	1.39	1.34
1	X	373	A	C5-C4	5.76	1.42	1.38
1	X	1178	C	N1-C6	5.74	1.40	1.37
1	X	2707	C	N1-C6	-5.74	1.33	1.37
1	X	350	G	N9-C4	5.70	1.42	1.38
1	X	1186	A	N3-C4	-5.66	1.31	1.34
1	X	1758	A	N9-C4	5.66	1.41	1.37
1	X	1303	A	C5-C6	-5.64	1.35	1.41
1	X	1751	G	N9-C8	5.64	1.41	1.37
1	X	428	G	N3-C4	5.60	1.39	1.35
1	X	518	A	N9-C4	-5.56	1.34	1.37
1	X	515	G	N9-C8	5.55	1.41	1.37
1	X	2059	G	C5-C6	5.52	1.47	1.42
1	X	2402	G	N7-C5	5.51	1.42	1.39
1	X	1289	A	N3-C4	-5.44	1.31	1.34
1	X	2545	A	N9-C4	5.44	1.41	1.37
1	X	1289	A	N9-C8	5.43	1.42	1.37
1	X	859	C	N1-C6	-5.39	1.33	1.37
1	X	1360	G	N9-C4	-5.36	1.33	1.38
1	X	955	A	N3-C4	5.34	1.38	1.34
1	X	2059	G	N9-C8	5.33	1.41	1.37
1	X	1065	A	N3-C4	-5.27	1.31	1.34
1	X	553	A	C5-C6	5.25	1.45	1.41
1	X	2661	A	C5-C4	-5.24	1.35	1.38
1	X	575	G	N9-C8	5.24	1.41	1.37
1	X	54	G	C8-N7	5.24	1.34	1.30
1	X	503	A	C5-C6	-5.23	1.36	1.41
1	X	1489	A	N9-C4	5.20	1.41	1.37
1	X	602	G	N9-C4	-5.18	1.33	1.38
1	X	1003	A	N9-C4	-5.13	1.34	1.37
1	X	2740	A	N3-C4	-5.10	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2845	G	N3-C4	-5.07	1.31	1.35
1	X	1285	A	N9-C4	-5.04	1.34	1.37
1	X	515	G	C5-C4	5.02	1.41	1.38

All (1168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2474	G	C5-N7-C8	-23.23	92.68	104.30
1	X	2088	G	C5-N7-C8	-21.74	93.43	104.30
1	X	2059	G	C6-C5-N7	20.68	142.81	130.40
1	X	2059	G	C4-C5-C6	-20.37	106.58	118.80
1	X	2845	G	N3-C4-C5	18.55	137.88	128.60
1	X	2088	G	N7-C8-N9	18.50	122.35	113.10
1	X	2059	G	N3-C4-N9	-18.40	114.96	126.00
1	X	2474	G	N7-C8-N9	18.30	122.25	113.10
1	X	1303	A	C2-N3-C4	-17.05	102.07	110.60
1	X	2845	G	N3-C4-N9	-16.89	115.87	126.00
1	X	2474	G	C8-N9-C4	-16.52	99.79	106.40
1	X	2088	G	C8-N9-C4	-16.52	99.79	106.40
1	X	2474	G	C4-C5-N7	16.41	117.36	110.80
1	X	1186	A	C2-N3-C4	-16.05	102.58	110.60
1	X	1560	A	N1-C6-N6	-15.97	109.02	118.60
1	X	1065	A	C2-N3-C4	-15.77	102.71	110.60
1	X	2059	G	N3-C4-C5	14.91	136.06	128.60
1	X	1931	G	N3-C4-N9	13.53	134.12	126.00
1	X	1289	A	C2-N3-C4	-13.50	103.85	110.60
1	X	1000	G	C5-C6-O6	13.43	136.66	128.60
1	X	2059	G	C8-N9-C4	-12.99	101.20	106.40
1	X	630	G	N3-C4-C5	12.92	135.06	128.60
1	X	2845	G	C2-N3-C4	-12.92	105.44	111.90
1	X	2059	G	N7-C8-N9	12.89	119.55	113.10
1	X	2797	C	N3-C4-C5	-12.73	116.81	121.90
1	X	1715	U	C5-C6-N1	12.63	129.01	122.70
1	X	2079	G	C5-C6-O6	-12.50	121.10	128.60
1	X	2797	C	C5-C4-N4	12.47	128.93	120.20
1	X	721	A	C2-N3-C4	-12.43	104.39	110.60
1	X	373	A	C5-C6-N1	-12.16	111.62	117.70
2	Y	93	C	N3-C2-O2	-12.10	113.43	121.90
1	X	1278	G	N3-C4-N9	-12.08	118.75	126.00
1	X	1000	G	N1-C6-O6	-11.98	112.71	119.90
1	X	1843	U	C5-C6-N1	11.78	128.59	122.70
1	X	2845	G	N3-C2-N2	-11.65	111.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2716	U	C5-C4-O4	11.61	132.87	125.90
1	X	515	G	C4-C5-N7	11.56	115.42	110.80
1	X	1186	A	C5-C6-N1	-11.46	111.97	117.70
1	X	2845	G	C5-N7-C8	-11.44	98.58	104.30
1	X	1244	G	N9-C4-C5	11.32	109.93	105.40
1	X	575	G	C5-N7-C8	-11.30	98.65	104.30
1	X	515	G	N7-C8-N9	11.30	118.75	113.10
1	X	1229	G	O5'-P-OP2	-11.27	95.56	105.70
1	X	1702	C	OP1-P-OP2	11.22	136.42	119.60
1	X	630	G	N3-C4-N9	-11.18	119.29	126.00
1	X	630	G	C2-N3-C4	-10.88	106.46	111.90
1	X	1278	G	N3-C4-C5	10.80	134.00	128.60
1	X	1520	A	C2-N3-C4	-10.80	105.20	110.60
1	X	797	A	N1-C6-N6	10.79	125.08	118.60
1	X	2433	C	N1-C2-O2	10.79	125.37	118.90
1	X	515	G	C5-N7-C8	-10.72	98.94	104.30
1	X	1289	A	C5-N7-C8	-10.72	98.54	103.90
1	X	2059	G	N1-C6-O6	-10.70	113.48	119.90
1	X	1715	U	C6-N1-C1'	10.64	136.09	121.20
1	X	350	G	N3-C4-C5	-10.63	123.28	128.60
2	Y	92	G	N3-C4-C5	10.63	133.92	128.60
1	X	2474	G	C6-C5-N7	-10.57	124.06	130.40
1	X	1065	A	N1-C2-N3	10.38	134.49	129.30
1	X	1702	C	O5'-P-OP2	-10.37	96.37	105.70
1	X	1000	G	N9-C4-C5	10.34	109.54	105.40
1	X	1560	A	C5-C6-N1	10.25	122.83	117.70
1	X	2088	G	N9-C4-C5	10.20	109.48	105.40
1	X	955	A	N9-C4-C5	-10.17	101.73	105.80
1	X	350	G	N3-C4-N9	10.12	132.07	126.00
1	X	2845	G	N1-C6-O6	10.10	125.96	119.90
2	Y	93	C	N1-C2-O2	10.10	124.96	118.90
1	X	695	C	N3-C4-C5	-10.07	117.87	121.90
1	X	2088	G	C4-C5-N7	10.05	114.82	110.80
1	X	828	A	C2-N3-C4	-10.02	105.59	110.60
1	X	858	U	O5'-P-OP2	-10.00	96.70	105.70
1	X	1065	A	C5-C6-N1	-9.99	112.70	117.70
1	X	323	C	C6-N1-C2	-9.99	116.31	120.30
1	X	1931	G	N9-C4-C5	-9.97	101.41	105.40
1	X	2081	A	N1-C2-N3	9.91	134.25	129.30
2	Y	88	U	C2-N1-C1'	9.91	129.59	117.70
1	X	2411	A	O4'-C1'-N9	9.90	116.12	108.20
1	X	1715	U	C4-C5-C6	-9.88	113.77	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	503	A	C5-N7-C8	-9.87	98.97	103.90
1	X	2716	U	N3-C4-O4	-9.87	112.49	119.40
1	X	1303	A	N3-C4-C5	9.81	133.67	126.80
1	X	2474	G	N1-C6-O6	9.79	125.77	119.90
1	X	2474	G	C8-N9-C1'	9.71	139.62	127.00
1	X	1957	G	C6-C5-N7	9.66	136.19	130.40
1	X	1024	A	N1-C6-N6	9.63	124.38	118.60
1	X	1065	A	N1-C6-N6	9.62	124.37	118.60
1	X	2740	A	C5-C6-N1	-9.55	112.92	117.70
1	X	2088	G	C8-N9-C1'	9.54	139.40	127.00
1	X	1165	C	C6-N1-C2	-9.53	116.49	120.30
1	X	2089[A]	A	C6-C5-N7	-9.50	125.65	132.30
1	X	2089[B]	A	C6-C5-N7	-9.50	125.65	132.30
1	X	515	G	C8-N9-C4	-9.48	102.61	106.40
1	X	2059	G	C5-C6-N1	9.41	116.21	111.50
1	X	575	G	N7-C8-N9	9.41	117.80	113.10
1	X	575	G	C4-C5-N7	9.37	114.55	110.80
1	X	515	G	C6-C5-N7	-9.36	124.78	130.40
1	X	2740	A	C2-N3-C4	-9.35	105.92	110.60
1	X	828	A	C5-N7-C8	-9.35	99.22	103.90
1	X	797	A	C6-C5-N7	-9.32	125.78	132.30
1	X	373	A	N1-C2-N3	9.30	133.95	129.30
1	X	373	A	C2-N3-C4	-9.30	105.95	110.60
1	X	1179	C	N1-C2-O2	9.27	124.46	118.90
1	X	1065	A	C5-N7-C8	-9.19	99.30	103.90
1	X	2740	A	N1-C6-N6	9.16	124.10	118.60
1	X	2720	A	C5-C6-N1	9.16	122.28	117.70
1	X	1257	G	C8-N9-C4	-9.15	102.74	106.40
1	X	2088	G	N3-C4-N9	-9.14	120.52	126.00
1	X	2079	G	N1-C6-O6	9.13	125.38	119.90
1	X	797	A	C5-N7-C8	-9.06	99.37	103.90
1	X	2081	A	C2-N3-C4	-9.06	106.07	110.60
1	X	1179	C	N3-C2-O2	-9.06	115.56	121.90
1	X	1303	A	C5-C6-N1	-9.05	113.18	117.70
1	X	630	G	C5-N7-C8	-9.02	99.79	104.30
1	X	955	A	N1-C6-N6	9.01	124.00	118.60
1	X	791	U	N3-C4-C5	-8.96	109.23	114.60
1	X	1360	G	N1-C6-O6	8.96	125.27	119.90
1	X	2844	U	N1-C2-N3	8.92	120.25	114.90
1	X	2526	C	N1-C2-O2	8.90	124.24	118.90
1	X	721	A	C5-C6-N1	-8.89	113.25	117.70
1	X	1963	A	C2-N3-C4	-8.89	106.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	88	U	N1-C2-O2	8.89	129.02	122.80
2	Y	88	U	N3-C2-O2	-8.88	115.99	122.20
1	X	1186	A	N1-C6-N6	8.86	123.92	118.60
1	X	1715	U	C6-N1-C2	-8.84	115.70	121.00
1	X	2059	G	N9-C4-C5	8.82	108.93	105.40
1	X	350	G	C5-C6-N1	8.82	115.91	111.50
1	X	1303	A	C5-N7-C8	-8.79	99.50	103.90
1	X	2877	G	N3-C4-C5	-8.75	124.22	128.60
1	X	1828	U	C2-N1-C1'	8.72	128.16	117.70
1	X	268	A	O4'-C1'-N9	8.69	115.15	108.20
1	X	791	U	C6-N1-C2	-8.67	115.80	121.00
1	X	1806	U	C5-C6-N1	-8.67	118.37	122.70
1	X	2047	A	N1-C6-N6	-8.67	113.40	118.60
1	X	2021	C	C6-N1-C2	-8.66	116.83	120.30
1	X	2079	G	N9-C4-C5	-8.63	101.95	105.40
1	X	2089[A]	A	C8-N9-C1'	-8.61	112.21	127.70
1	X	2089[B]	A	C8-N9-C1'	-8.61	112.21	127.70
1	X	1065	A	N7-C8-N9	8.60	118.10	113.80
1	X	2066	G	N1-C6-O6	8.59	125.05	119.90
1	X	1516	C	C6-N1-C2	-8.58	116.87	120.30
1	X	828	A	N3-C4-C5	8.54	132.78	126.80
1	X	198	A	N1-C6-N6	8.53	123.72	118.60
1	X	2261	A	N1-C6-N6	8.50	123.70	118.60
1	X	2079	G	C4-C5-N7	8.50	114.20	110.80
1	X	2391	C	C6-N1-C2	8.50	123.70	120.30
1	X	877	G	O5'-P-OP2	8.49	120.89	110.70
1	X	1303	A	C4-C5-N7	8.47	114.94	110.70
1	X	373	A	C4-C5-C6	8.46	121.23	117.00
1	X	1560	A	C6-N1-C2	-8.45	113.53	118.60
1	X	428	G	C2-N3-C4	8.44	116.12	111.90
2	Y	86	C	N3-C2-O2	-8.43	116.00	121.90
1	X	1931	G	N3-C4-C5	-8.43	124.39	128.60
1	X	1244	G	C8-N9-C4	-8.41	103.04	106.40
1	X	568	C	C6-N1-C2	8.38	123.65	120.30
1	X	323	C	C2-N1-C1'	8.37	128.01	118.80
1	X	1957	G	N3-C4-N9	-8.37	120.98	126.00
1	X	428	G	N3-C4-C5	-8.36	124.42	128.60
1	X	2059	G	C5-N7-C8	-8.35	100.12	104.30
1	X	2712	G	N1-C6-O6	8.35	124.91	119.90
1	X	2740	A	C6-C5-N7	-8.32	126.47	132.30
1	X	1957	G	C4-C5-C6	-8.32	113.81	118.80
1	X	588	G	C8-N9-C4	8.31	109.73	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2877	G	C2-N3-C4	8.31	116.06	111.90
1	X	1953	U	O4'-C1'-N1	8.30	114.84	108.20
2	Y	92	G	N3-C4-N9	-8.27	121.04	126.00
1	X	2845	G	N1-C2-N2	8.26	123.63	116.20
1	X	362	C	C6-N1-C2	-8.25	117.00	120.30
1	X	1050	C	C6-N1-C2	8.25	123.60	120.30
1	X	1520	A	C8-N9-C4	8.24	109.10	105.80
1	X	323	C	C5-C6-N1	8.23	125.12	121.00
1	X	828	A	N1-C6-N6	8.23	123.54	118.60
1	X	1000	G	N3-C4-N9	-8.21	121.07	126.00
1	X	797	A	N7-C8-N9	8.20	117.90	113.80
1	X	2080	G	C5-C6-O6	-8.19	123.69	128.60
1	X	797	A	C4-C5-N7	8.18	114.79	110.70
2	Y	93	C	C6-N1-C2	-8.16	117.03	120.30
1	X	503	A	C2-N3-C4	-8.15	106.53	110.60
1	X	1065	A	C6-C5-N7	-8.15	126.60	132.30
1	X	1186	A	N3-C4-C5	8.12	132.48	126.80
1	X	2599	A	N1-C6-N6	8.12	123.47	118.60
1	X	2565	C	C6-N1-C2	8.11	123.55	120.30
1	X	2529	G	N1-C6-O6	8.11	124.76	119.90
1	X	1289	A	N7-C8-N9	8.09	117.85	113.80
1	X	428	G	N3-C4-N9	8.08	130.85	126.00
1	X	1230	G	C8-N9-C4	8.08	109.63	106.40
1	X	1990	C	C5-C6-N1	8.08	125.04	121.00
1	X	1178	C	C6-N1-C2	-8.07	117.07	120.30
1	X	834	A	C8-N9-C4	-8.06	102.57	105.80
1	X	2529	G	C6-C5-N7	-8.02	125.59	130.40
1	X	2716	U	C2-N1-C1'	-8.01	108.08	117.70
1	X	503	A	N7-C8-N9	8.01	117.80	113.80
1	X	996	G	C6-C5-N7	-8.00	125.60	130.40
1	X	2591	A	C8-N9-C4	-8.00	102.60	105.80
1	X	1520	A	N1-C2-N3	7.99	133.29	129.30
1	X	503	A	C4-C5-N7	7.97	114.68	110.70
1	X	2089[A]	A	C4-N9-C1'	7.96	140.63	126.30
1	X	2089[B]	A	C4-N9-C1'	7.96	140.63	126.30
1	X	1715	U	C2-N1-C1'	-7.94	108.17	117.70
1	X	350	G	C2-N3-C4	7.94	115.87	111.90
1	X	996	G	N1-C6-O6	7.94	124.66	119.90
1	X	2748	A	N1-C6-N6	7.94	123.36	118.60
1	X	12	U	N3-C2-O2	-7.93	116.65	122.20
1	X	1244	G	C4-C5-N7	-7.92	107.63	110.80
1	X	721	A	N1-C6-N6	7.91	123.35	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2021	C	N3-C4-C5	-7.91	118.74	121.90
1	X	834	A	N9-C4-C5	7.91	108.96	105.80
1	X	955	A	C8-N9-C4	7.91	108.96	105.80
1	X	1715	U	C2-N3-C4	7.91	131.74	127.00
1	X	2472	G	C2-N3-C4	7.89	115.85	111.90
1	X	2474	G	C5-C6-O6	-7.88	123.87	128.60
1	X	575	G	N3-C4-C5	7.87	132.54	128.60
1	X	617	A	C8-N9-C4	7.87	108.95	105.80
1	X	853	G	C4-C5-N7	-7.87	107.65	110.80
1	X	2446	U	C5-C6-N1	7.86	126.63	122.70
1	X	828	A	C4-C5-N7	7.86	114.63	110.70
1	X	1499	U	N3-C2-O2	-7.83	116.72	122.20
2	Y	99	U	N3-C2-O2	-7.83	116.72	122.20
1	X	2845	G	C4-C5-N7	7.82	113.93	110.80
1	X	955	A	N1-C2-N3	-7.82	125.39	129.30
1	X	1229	G	C5-C6-O6	-7.81	123.92	128.60
2	Y	86	C	N1-C2-O2	7.78	123.57	118.90
1	X	2797	C	C6-N1-C2	-7.77	117.19	120.30
1	X	122	G	N1-C6-O6	-7.75	115.25	119.90
1	X	1065	A	C8-N9-C4	-7.74	102.70	105.80
1	X	2238	U	C2-N1-C1'	7.70	126.94	117.70
1	X	2670	G	N1-C6-O6	-7.70	115.28	119.90
1	X	2845	G	C5-C6-N1	-7.69	107.66	111.50
1	X	1289	A	N3-C4-C5	7.68	132.18	126.80
2	Y	86	C	C2-N1-C1'	7.65	127.21	118.80
1	X	1021	G	C8-N9-C4	7.65	109.46	106.40
1	X	2440	G	N1-C6-O6	7.65	124.49	119.90
1	X	1360	G	C2-N3-C4	-7.63	108.09	111.90
1	X	1186	A	N1-C2-N3	7.62	133.11	129.30
1	X	2640	U	C5-C6-N1	-7.62	118.89	122.70
1	X	955	A	C5-C6-N6	-7.60	117.62	123.70
1	X	1272	U	N3-C4-C5	-7.60	110.04	114.60
1	X	1978	U	C6-N1-C2	-7.60	116.44	121.00
1	X	2391	C	C5-C6-N1	-7.59	117.20	121.00
1	X	1732	U	N1-C2-N3	7.57	119.44	114.90
1	X	695	C	C2-N3-C4	7.53	123.67	119.90
1	X	588	G	N9-C4-C5	-7.53	102.39	105.40
1	X	2541	U	C5-C6-N1	-7.53	118.94	122.70
1	X	1843	U	C4-C5-C6	-7.51	115.19	119.70
1	X	2709	U	C5-C6-N1	-7.51	118.95	122.70
1	X	2797	C	C6-N1-C1'	7.50	129.80	120.80
2	Y	99	U	N1-C2-O2	7.50	128.05	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2446	U	C6-N1-C1'	7.49	131.69	121.20
1	X	2474	G	N3-C4-N9	-7.48	121.51	126.00
2	Y	79	C	C2-N1-C1'	7.47	127.02	118.80
1	X	2716	U	C5-C6-N1	-7.47	118.97	122.70
1	X	2006	C	C6-N1-C2	-7.47	117.31	120.30
1	X	661	U	N3-C4-O4	7.44	124.61	119.40
1	X	2845	G	C8-N9-C1'	7.44	136.67	127.00
1	X	2066	G	C5-C6-N1	-7.43	107.79	111.50
1	X	1289	A	N3-C4-N9	-7.42	121.46	127.40
1	X	2887	G	N3-C4-N9	7.42	130.45	126.00
1	X	2044	C	C4-C5-C6	7.42	121.11	117.40
1	X	695	C	N3-C4-N4	7.38	123.16	118.00
1	X	1230	G	N7-C8-N9	-7.38	109.41	113.10
1	X	1544	G	C2-N3-C4	7.36	115.58	111.90
1	X	1308	C	C2-N3-C4	-7.34	116.23	119.90
1	X	1226	G	N1-C6-O6	7.34	124.30	119.90
1	X	2064	A	C8-N9-C4	-7.34	102.86	105.80
1	X	557	G	O4'-C1'-N9	7.33	114.07	108.20
1	X	2541	U	C6-N1-C2	7.32	125.39	121.00
1	X	2717	A	C2-N3-C4	7.31	114.25	110.60
1	X	1229	G	N1-C6-O6	7.30	124.28	119.90
1	X	892	U	C5-C6-N1	-7.29	119.05	122.70
2	Y	79	C	C6-N1-C1'	-7.29	112.05	120.80
1	X	2302	C	N3-C4-C5	-7.28	118.99	121.90
1	X	635	G	C8-N9-C4	-7.27	103.49	106.40
1	X	1543	G	N3-C4-N9	7.26	130.35	126.00
1	X	2576	G	N3-C4-C5	-7.25	124.97	128.60
1	X	1064	A	C8-N9-C4	7.22	108.69	105.80
1	X	2576	G	N3-C4-N9	7.22	130.33	126.00
1	X	2576	G	C4-N9-C1'	7.21	135.88	126.50
1	X	2608	G	C5-C6-O6	7.21	132.93	128.60
1	X	2851	G	C8-N9-C4	-7.20	103.52	106.40
1	X	1968	C	C6-N1-C2	-7.19	117.42	120.30
1	X	2799	C	N1-C2-O2	-7.19	114.59	118.90
1	X	321	U	O4'-C1'-N1	7.18	113.94	108.20
1	X	797	A	O4'-C1'-N9	7.17	113.94	108.20
1	X	211	C	C6-N1-C2	7.17	123.17	120.30
1	X	2608	G	N1-C6-O6	-7.16	115.60	119.90
1	X	491	C	C6-N1-C2	-7.14	117.44	120.30
1	X	496	G	C8-N9-C4	-7.14	103.54	106.40
1	X	1257	G	N7-C8-N9	7.13	116.66	113.10
1	X	54	G	C5-N7-C8	-7.12	100.74	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	795	A	C5-C6-N6	-7.12	118.00	123.70
1	X	15	G	C8-N9-C4	7.12	109.25	106.40
1	X	2877	G	N3-C4-N9	7.11	130.27	126.00
1	X	1175	G	C6-N1-C2	-7.11	120.83	125.10
1	X	666	A	N1-C6-N6	7.10	122.86	118.60
1	X	698	U	N1-C2-O2	7.09	127.77	122.80
1	X	2045	A	N1-C2-N3	7.08	132.84	129.30
1	X	503	A	N1-C6-N6	7.06	122.83	118.60
1	X	1367	C	C2-N1-C1'	7.04	126.55	118.80
1	X	122	G	C6-C5-N7	7.04	134.62	130.40
1	X	1303	A	N1-C6-N6	7.02	122.81	118.60
1	X	1765	A	O4'-C1'-N9	7.01	113.81	108.20
1	X	1520	A	N9-C4-C5	-7.00	103.00	105.80
1	X	625	G	N3-C4-N9	6.99	130.20	126.00
1	X	890	G	P-O3'-C3'	6.99	128.09	119.70
1	X	2877	G	C5-C6-N1	6.99	114.99	111.50
1	X	2044	C	N1-C2-N3	6.99	124.09	119.20
1	X	184	C	C5-C6-N1	6.97	124.49	121.00
1	X	728	U	N3-C4-O4	6.97	124.28	119.40
1	X	1289	A	N1-C2-N3	6.96	132.78	129.30
1	X	721	A	C5-N7-C8	-6.96	100.42	103.90
1	X	1229	G	C4-C5-N7	6.96	113.58	110.80
1	X	373	A	C8-N9-C4	-6.95	103.02	105.80
1	X	728	U	C6-N1-C2	-6.95	116.83	121.00
1	X	996	G	C5-C6-O6	-6.93	124.44	128.60
1	X	54	G	C8-N9-C4	-6.92	103.63	106.40
1	X	1658	A	N1-C6-N6	6.91	122.75	118.60
1	X	2602	C	C6-N1-C2	-6.91	117.54	120.30
1	X	1244	G	N3-C4-N9	-6.90	121.86	126.00
1	X	496	G	N7-C8-N9	6.90	116.55	113.10
1	X	373	A	N7-C8-N9	6.90	117.25	113.80
1	X	2740	A	C4-C5-C6	6.90	120.45	117.00
1	X	2512	G	N1-C6-O6	6.90	124.04	119.90
1	X	1560	A	N9-C4-C5	6.89	108.56	105.80
1	X	2756	G	C5-C6-O6	6.88	132.73	128.60
1	X	852	U	C4-C5-C6	6.87	123.82	119.70
1	X	721	A	C6-C5-N7	-6.86	127.50	132.30
1	X	1828	U	C5-C6-N1	6.85	126.13	122.70
1	X	666	A	N7-C8-N9	6.85	117.22	113.80
1	X	2644	C	C6-N1-C2	6.84	123.04	120.30
1	X	428	G	C4-N9-C1'	6.84	135.39	126.50
1	X	2433	C	N3-C2-O2	-6.83	117.12	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2740	A	C5-N7-C8	-6.83	100.49	103.90
1	X	1015	C	C6-N1-C2	-6.81	117.58	120.30
1	X	1453	G	N3-C4-C5	-6.81	125.20	128.60
1	X	1028	G	C5-C6-N1	6.80	114.90	111.50
1	X	2565	C	N3-C4-C5	6.80	124.62	121.90
1	X	637	U	N3-C2-O2	-6.79	117.44	122.20
1	X	992	A	C5-C6-N1	-6.79	114.30	117.70
1	X	350	G	O4'-C1'-N9	6.79	113.63	108.20
1	X	54	G	N7-C8-N9	6.79	116.49	113.10
1	X	698	U	N3-C2-O2	-6.79	117.45	122.20
1	X	992	A	C2-N3-C4	-6.78	107.21	110.60
1	X	661	U	C5-C6-N1	6.78	126.09	122.70
1	X	2606	C	N3-C4-C5	-6.77	119.19	121.90
1	X	210	A	C8-N9-C4	6.77	108.51	105.80
1	X	2844	U	N1-C2-O2	-6.76	118.06	122.80
1	X	2876	G	C8-N9-C4	-6.76	103.69	106.40
1	X	1026	C	N3-C4-C5	6.76	124.60	121.90
1	X	849	A	N1-C6-N6	6.76	122.65	118.60
1	X	2398	G	C5-C6-N1	-6.75	108.12	111.50
1	X	575	G	C2-N3-C4	-6.75	108.53	111.90
1	X	2512	G	N3-C4-C5	6.75	131.97	128.60
1	X	367	A	N1-C6-N6	-6.71	114.57	118.60
1	X	2089[A]	A	C4-C5-C6	6.71	120.36	117.00
1	X	2089[B]	A	C4-C5-C6	6.71	120.36	117.00
1	X	1241	A	C8-N9-C4	6.70	108.48	105.80
1	X	2682	G	OP2-P-O3'	6.69	119.92	105.20
2	Y	82	C	N3-C2-O2	-6.68	117.22	121.90
2	Y	15	C	C5-C4-N4	-6.67	115.53	120.20
1	X	2064	A	N7-C8-N9	6.66	117.13	113.80
1	X	630	G	C4-C5-N7	6.66	113.46	110.80
1	X	985	A	C2-N3-C4	-6.66	107.27	110.60
2	Y	88	U	C6-N1-C1'	-6.66	111.88	121.20
1	X	2298	G	N1-C2-N2	-6.65	110.22	116.20
1	X	376	A	C8-N9-C4	-6.64	103.14	105.80
1	X	1229	G	N9-C4-C5	-6.64	102.74	105.40
1	X	1732	U	O4'-C1'-N1	6.64	113.51	108.20
1	X	2774	G	C6-C5-N7	-6.64	126.42	130.40
1	X	983	G	C8-N9-C4	-6.63	103.75	106.40
2	Y	92	G	N1-C6-O6	6.63	123.88	119.90
1	X	2657	G	N7-C8-N9	6.62	116.41	113.10
1	X	1293	U	N1-C2-N3	6.62	118.87	114.90
1	X	1732	U	C6-N1-C1'	6.62	130.46	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2529	G	C4-C5-N7	6.62	113.45	110.80
1	X	2657	G	C5-N7-C8	-6.61	100.99	104.30
1	X	124	A	C8-N9-C4	6.61	108.44	105.80
1	X	2576	G	C8-N9-C1'	-6.61	118.41	127.00
1	X	1866	G	C8-N9-C4	-6.60	103.76	106.40
1	X	152	C	N3-C2-O2	-6.58	117.30	121.90
1	X	644	C	C5-C6-N1	6.57	124.28	121.00
1	X	852	U	N1-C2-N3	6.57	118.84	114.90
1	X	2845	G	C4-N9-C1'	-6.56	117.97	126.50
2	Y	91	C	C6-N1-C2	-6.56	117.67	120.30
1	X	389	A	C8-N9-C4	-6.56	103.18	105.80
1	X	2517	G	C8-N9-C4	6.56	109.02	106.40
1	X	1560	A	C8-N9-C4	-6.55	103.18	105.80
1	X	728	U	N3-C4-C5	-6.54	110.68	114.60
1	X	2591	A	N7-C8-N9	6.54	117.07	113.80
1	X	377	U	O5'-P-OP2	-6.54	99.81	105.70
1	X	528	C	C6-N1-C2	-6.53	117.69	120.30
1	X	1751	G	N1-C6-O6	6.53	123.82	119.90
1	X	2044	C	C6-N1-C2	-6.53	117.69	120.30
1	X	680	C	C6-N1-C2	-6.53	117.69	120.30
1	X	369	G	C8-N9-C4	-6.52	103.79	106.40
1	X	666	A	C5-N7-C8	-6.52	100.64	103.90
1	X	711	G	C8-N9-C4	6.51	109.00	106.40
1	X	2603	G	N9-C4-C5	-6.50	102.80	105.40
1	X	350	G	C4-N9-C1'	6.50	134.95	126.50
1	X	853	G	N3-C2-N2	-6.49	115.36	119.90
2	Y	79	C	N3-C4-N4	6.47	122.53	118.00
1	X	743	C	C6-N1-C2	6.46	122.89	120.30
1	X	2063	C	C5-C6-N1	6.46	124.23	121.00
1	X	660	A	O4'-C1'-N9	6.46	113.36	108.20
2	Y	105	G	N9-C4-C5	-6.45	102.82	105.40
1	X	2078	A	N1-C2-N3	6.45	132.52	129.30
1	X	12	U	C2-N1-C1'	6.45	125.44	117.70
1	X	662	G	N3-C4-N9	6.45	129.87	126.00
1	X	2709	U	C2-N3-C4	-6.44	123.14	127.00
1	X	1715	U	O4'-C1'-N1	6.43	113.35	108.20
1	X	2066	G	C6-C5-N7	-6.43	126.54	130.40
1	X	2039	G	N1-C6-O6	6.42	123.75	119.90
1	X	2546	U	C5-C6-N1	-6.42	119.49	122.70
1	X	1953	U	C2-N1-C1'	-6.41	110.01	117.70
1	X	1931	G	C8-N9-C1'	-6.41	118.67	127.00
2	Y	105	G	C8-N9-C4	6.40	108.96	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	122	G	C4-N9-C1'	-6.40	118.18	126.50
1	X	2532	G	O5'-P-OP2	-6.40	99.94	105.70
1	X	1275	A	O4'-C1'-N9	6.40	113.32	108.20
1	X	64	A	C8-N9-C4	-6.39	103.24	105.80
1	X	2522	G	N1-C6-O6	6.39	123.74	119.90
1	X	2724	G	C2-N3-C4	-6.39	108.71	111.90
1	X	1652	A	N1-C6-N6	-6.38	114.77	118.60
1	X	1091	G	P-O3'-C3'	6.37	127.35	119.70
2	Y	91	C	N3-C4-C5	-6.37	119.35	121.90
1	X	1931	G	C6-C5-N7	-6.37	126.58	130.40
1	X	1560	A	C2-N3-C4	6.37	113.78	110.60
1	X	505	U	O5'-P-OP2	-6.36	99.97	105.70
1	X	853	G	C5-C6-N1	-6.36	108.32	111.50
1	X	1168	C	N1-C2-O2	6.35	122.71	118.90
2	Y	78	C	N3-C2-O2	-6.35	117.46	121.90
1	X	2711	U	O5'-P-OP2	6.35	118.32	110.70
1	X	2595	C	C6-N1-C2	6.34	122.84	120.30
1	X	2556	G	N3-C4-N9	-6.34	122.20	126.00
1	X	2657	G	N1-C6-O6	6.33	123.70	119.90
1	X	1017	A	C8-N9-C4	-6.33	103.27	105.80
1	X	12	U	N1-C2-O2	6.33	127.23	122.80
1	X	2446	U	O4'-C1'-N1	6.32	113.26	108.20
1	X	2709	U	N3-C2-O2	-6.32	117.77	122.20
1	X	1179	C	O5'-P-OP2	-6.32	100.01	105.70
1	X	1279	C	C5-C4-N4	-6.32	115.78	120.20
1	X	834	A	N1-C2-N3	6.31	132.46	129.30
1	X	828	A	C5-C6-N1	-6.31	114.55	117.70
1	X	2858	G	C8-N9-C4	6.31	108.92	106.40
2	Y	95	A	N1-C6-N6	6.30	122.38	118.60
1	X	1977	G	C5-C6-N1	-6.30	108.35	111.50
1	X	721	A	N1-C2-N3	6.29	132.44	129.30
1	X	1028	G	C5-C6-O6	-6.29	124.83	128.60
1	X	1978	U	C5-C6-N1	6.28	125.84	122.70
2	Y	95	A	C8-N9-C4	6.28	108.31	105.80
1	X	515	G	O4'-C1'-N9	6.28	113.22	108.20
1	X	611	U	N1-C2-N3	6.28	118.67	114.90
1	X	2079	G	N3-C4-N9	6.27	129.76	126.00
1	X	1543	G	N3-C4-C5	-6.27	125.46	128.60
1	X	2381	A	C5-C6-N1	6.27	120.83	117.70
1	X	1791	G	N3-C4-N9	-6.27	122.24	126.00
1	X	1758	A	C2-N3-C4	6.26	113.73	110.60
1	X	378	C	C6-N1-C2	-6.25	117.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2334	G	N3-C4-N9	-6.25	122.25	126.00
1	X	1811	A	C4-C5-C6	6.25	120.13	117.00
1	X	251	G	C5-C6-O6	-6.25	124.85	128.60
1	X	2076	A	N1-C2-N3	6.25	132.43	129.30
1	X	603	C	N3-C2-O2	-6.25	117.53	121.90
1	X	2720	A	N1-C6-N6	-6.25	114.85	118.60
1	X	1303	A	C6-N1-C2	6.25	122.35	118.60
1	X	1955	A	C2-N3-C4	6.25	113.72	110.60
2	Y	79	C	C5-C4-N4	-6.24	115.83	120.20
1	X	683	G	N9-C4-C5	6.24	107.90	105.40
1	X	1957	G	N3-C4-C5	6.24	131.72	128.60
1	X	608	C	C6-N1-C2	-6.22	117.81	120.30
1	X	1050	C	N3-C4-C5	6.21	124.38	121.90
1	X	1303	A	C6-C5-N7	-6.20	127.96	132.30
1	X	2556	G	C5-C6-N1	-6.20	108.40	111.50
1	X	834	A	N1-C6-N6	-6.19	114.89	118.60
1	X	2649	U	O4'-C1'-N1	6.19	113.16	108.20
1	X	2720	A	C2-N3-C4	6.19	113.70	110.60
1	X	2797	C	C2-N3-C4	6.19	123.00	119.90
1	X	2712	G	C2-N3-C4	-6.19	108.81	111.90
1	X	2642	U	C5-C4-O4	-6.19	122.19	125.90
1	X	2322	C	C6-N1-C2	-6.18	117.83	120.30
1	X	1707	U	N1-C2-N3	6.18	118.61	114.90
1	X	575	G	C8-N9-C4	-6.17	103.93	106.40
1	X	2583	C	C2-N1-C1'	6.17	125.58	118.80
1	X	2718	C	C6-N1-C2	-6.17	117.83	120.30
1	X	617	A	C2-N3-C4	-6.17	107.52	110.60
1	X	2080	G	C5-C6-N1	6.16	114.58	111.50
1	X	302	A	C8-N9-C4	6.16	108.26	105.80
1	X	1435	C	C5-C6-N1	6.16	124.08	121.00
1	X	1024	A	N9-C4-C5	-6.15	103.34	105.80
1	X	1175	G	N3-C4-C5	-6.15	125.53	128.60
2	Y	93	C	C2-N1-C1'	6.15	125.57	118.80
1	X	1990	C	C2-N3-C4	6.15	122.97	119.90
1	X	2361	U	C5-C6-N1	6.14	125.77	122.70
1	X	9	U	C2-N1-C1'	6.14	125.07	117.70
1	X	1360	G	C6-C5-N7	-6.14	126.72	130.40
1	X	1855	G	C8-N9-C4	-6.13	103.95	106.40
1	X	2089[A]	A	C4-C5-N7	6.13	113.77	110.70
1	X	2089[B]	A	C4-C5-N7	6.13	113.77	110.70
1	X	548	A	O4'-C1'-N9	6.13	113.10	108.20
1	X	2712	G	C5-C6-N1	-6.11	108.44	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2238	U	C6-N1-C1'	-6.11	112.64	121.20
1	X	1806	U	C2-N1-C1'	-6.11	110.37	117.70
1	X	1182	G	N1-C6-O6	6.11	123.56	119.90
1	X	488	G	N3-C4-C5	-6.10	125.55	128.60
1	X	1865	C	O4'-C1'-N1	6.09	113.08	108.20
1	X	503	A	C6-C5-N7	-6.09	128.04	132.30
1	X	1042	C	C4-C5-C6	6.08	120.44	117.40
1	X	1360	G	N3-C4-C5	6.08	131.64	128.60
1	X	683	G	C8-N9-C4	-6.08	103.97	106.40
1	X	985	A	N1-C2-N3	6.08	132.34	129.30
1	X	102	A	C2-N3-C4	-6.08	107.56	110.60
1	X	376	A	N7-C8-N9	6.08	116.84	113.80
1	X	2583	C	C6-N1-C2	-6.08	117.87	120.30
1	X	854	G	N3-C4-C5	-6.07	125.56	128.60
1	X	2446	U	C6-N1-C2	-6.06	117.36	121.00
1	X	2888	A	N1-C6-N6	-6.06	114.96	118.60
1	X	630	G	C8-N9-C1'	6.06	134.87	127.00
1	X	2546	U	C2-N3-C4	-6.05	123.37	127.00
1	X	612	U	N3-C4-C5	-6.05	110.97	114.60
1	X	660	A	C8-N9-C4	-6.05	103.38	105.80
1	X	1278	G	C8-N9-C4	-6.05	103.98	106.40
1	X	2337	A	C2-N3-C4	6.04	113.62	110.60
1	X	588	G	C5-C6-O6	-6.04	124.98	128.60
1	X	1499	U	N1-C2-O2	6.04	127.03	122.80
1	X	797	A	C2-N3-C4	-6.04	107.58	110.60
1	X	2637	C	C6-N1-C2	6.04	122.71	120.30
1	X	2006	C	N3-C4-C5	-6.03	119.49	121.90
2	Y	85	A	C8-N9-C4	6.02	108.21	105.80
1	X	656	G	C8-N9-C4	-6.02	103.99	106.40
1	X	2076	A	C6-N1-C2	-6.02	114.99	118.60
1	X	2419	A	N7-C8-N9	6.01	116.81	113.80
1	X	2682	G	N3-C4-N9	-6.01	122.39	126.00
1	X	2391	C	N3-C4-C5	6.01	124.30	121.90
2	Y	92	G	C6-N1-C2	6.01	128.71	125.10
1	X	675	G	N1-C6-O6	6.01	123.50	119.90
1	X	428	G	O4'-C1'-N9	6.01	113.00	108.20
1	X	1065	A	C4-C5-N7	6.01	113.70	110.70
1	X	2469	C	C6-N1-C2	6.01	122.70	120.30
1	X	2716	U	C6-N1-C1'	6.01	129.61	121.20
1	X	575	G	N3-C4-N9	-6.00	122.40	126.00
1	X	1320	G	C8-N9-C4	-6.00	104.00	106.40
1	X	2062	G	O4'-C1'-N9	6.00	113.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1453	G	N3-C4-N9	5.99	129.60	126.00
1	X	2640	U	C2-N3-C4	-5.99	123.40	127.00
5	C	181	LEU	CA-CB-CG	-5.99	101.51	115.30
11	J	84	GLY	N-CA-C	5.99	128.08	113.10
1	X	1559	G	N1-C2-N3	-5.99	120.31	123.90
1	X	2545	A	C2-N3-C4	5.99	113.59	110.60
1	X	2743	U	C5-C6-N1	-5.99	119.71	122.70
1	X	51	G	N3-C4-N9	5.98	129.59	126.00
1	X	1931	G	C4-N9-C1'	5.98	134.28	126.50
1	X	985	A	C5-C6-N1	-5.98	114.71	117.70
1	X	2017	C	N1-C2-O2	-5.98	115.31	118.90
1	X	2095	U	C5-C4-O4	-5.98	122.31	125.90
1	X	2877	G	N1-C6-O6	-5.98	116.31	119.90
1	X	1186	A	N3-C4-N9	-5.97	122.62	127.40
1	X	2472	G	C8-N9-C4	-5.97	104.01	106.40
1	X	2583	C	N1-C2-O2	5.97	122.48	118.90
1	X	2812	U	N1-C2-N3	5.97	118.48	114.90
1	X	122	G	C8-N9-C1'	5.96	134.75	127.00
1	X	2682	G	N3-C4-C5	5.96	131.58	128.60
1	X	2757	U	N1-C2-N3	5.96	118.48	114.90
1	X	2672	G	C5-C6-N1	-5.96	108.52	111.50
1	X	2887	G	C8-N9-C1'	-5.96	119.25	127.00
1	X	1709	A	N1-C6-N6	5.96	122.17	118.60
1	X	2657	G	C4-C5-N7	5.96	113.18	110.80
1	X	1028	G	C4-C5-N7	5.95	113.18	110.80
1	X	1229	G	C8-N9-C4	5.95	108.78	106.40
1	X	198	A	N9-C4-C5	-5.95	103.42	105.80
1	X	1308	C	N3-C4-C5	5.95	124.28	121.90
1	X	1245	G	C8-N9-C4	-5.94	104.02	106.40
1	X	1229	G	O5'-P-OP1	5.94	117.83	110.70
1	X	659	A	OP1-P-O3'	5.94	118.26	105.20
1	X	34	U	C5-C6-N1	5.93	125.67	122.70
1	X	1466	G	C4-N9-C1'	5.92	134.20	126.50
1	X	2419	A	C6-C5-N7	-5.92	128.15	132.30
1	X	1714	C	N3-C4-N4	5.91	122.14	118.00
1	X	834	A	C6-N1-C2	-5.91	115.05	118.60
1	X	198	A	C8-N9-C4	5.91	108.16	105.80
1	X	2609	G	C4-C5-N7	5.91	113.16	110.80
2	Y	65	G	N1-C6-O6	-5.91	116.36	119.90
1	X	555	C	O5'-P-OP2	-5.91	100.38	105.70
1	X	2474	G	N9-C4-C5	5.90	107.76	105.40
1	X	1466	G	C8-N9-C4	-5.90	104.04	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2703	C	C5-C6-N1	-5.90	118.05	121.00
1	X	20	C	C5-C6-N1	5.89	123.95	121.00
1	X	73	A	C8-N9-C4	-5.89	103.44	105.80
1	X	389	A	N7-C8-N9	5.89	116.75	113.80
1	X	835	U	C5-C6-N1	5.89	125.65	122.70
1	X	2881	C	C6-N1-C2	-5.89	117.94	120.30
1	X	533	C	N1-C2-O2	-5.89	115.37	118.90
1	X	1659	C	N3-C4-N4	5.88	122.12	118.00
1	X	2419	A	C5-C6-N1	-5.88	114.76	117.70
2	Y	77	G	C8-N9-C4	-5.88	104.05	106.40
1	X	1038	C	C6-N1-C2	-5.87	117.95	120.30
1	X	1186	A	C6-C5-N7	-5.87	128.19	132.30
1	X	2626	G	N1-C6-O6	-5.87	116.38	119.90
1	X	1186	A	C5-N7-C8	-5.87	100.97	103.90
1	X	835	U	C5-C4-O4	-5.87	122.38	125.90
1	X	1273	G	N9-C4-C5	5.87	107.75	105.40
1	X	36	G	N3-C4-C5	-5.86	125.67	128.60
1	X	1439	U	C6-N1-C2	-5.86	117.49	121.00
1	X	1648	C	C6-N1-C2	-5.86	117.96	120.30
1	X	1360	G	C4-C5-N7	5.86	113.14	110.80
1	X	51	G	N3-C4-C5	-5.85	125.67	128.60
1	X	1180	G	N1-C6-O6	5.85	123.41	119.90
1	X	695	C	C5-C6-N1	5.85	123.93	121.00
1	X	1866	G	C4-N9-C1'	5.85	134.10	126.50
1	X	1953	U	N1-C1'-C2'	5.85	121.60	114.00
1	X	2039	G	N3-C2-N2	-5.85	115.81	119.90
1	X	78	U	C2-N1-C1'	5.85	124.72	117.70
1	X	870	C	C6-N1-C2	-5.84	117.96	120.30
1	X	1746	G	N3-C4-N9	-5.84	122.49	126.00
1	X	1716	C	C5-C6-N1	5.84	123.92	121.00
1	X	263	G	C8-N9-C4	-5.83	104.07	106.40
1	X	666	A	C8-N9-C4	-5.83	103.47	105.80
1	X	1288	G	C5-C6-N1	5.83	114.42	111.50
1	X	2073	G	C8-N9-C4	-5.83	104.07	106.40
1	X	214	G	N1-C6-O6	5.83	123.40	119.90
1	X	662	G	N3-C4-C5	-5.83	125.69	128.60
1	X	2740	A	N7-C8-N9	5.83	116.72	113.80
1	X	728	U	C5-C6-N1	5.83	125.61	122.70
1	X	1024	A	C6-C5-N7	-5.83	128.22	132.30
1	X	2657	G	C5-C6-O6	-5.83	125.10	128.60
1	X	70	G	N3-C4-C5	-5.83	125.69	128.60
1	X	251	G	N1-C6-O6	5.82	123.39	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	509	G	C6-C5-N7	-5.82	126.91	130.40
1	X	788	A	C2-N3-C4	-5.82	107.69	110.60
1	X	1244	G	N3-C2-N2	-5.82	115.83	119.90
1	X	2080	G	C6-N1-C2	-5.82	121.61	125.10
1	X	1065	A	N3-C4-C5	5.82	130.87	126.80
1	X	1701	U	N1-C2-N3	5.81	118.39	114.90
1	X	1716	C	C2-N1-C1'	5.81	125.19	118.80
1	X	2419	A	C2-N3-C4	-5.81	107.69	110.60
1	X	2525	C	N3-C2-O2	5.81	125.97	121.90
1	X	577	A	N1-C6-N6	-5.81	115.11	118.60
1	X	1303	A	N3-C4-N9	-5.81	122.75	127.40
1	X	1026	C	C5-C4-N4	-5.80	116.14	120.20
1	X	514	G	N3-C4-C5	-5.80	125.70	128.60
1	X	695	C	C6-N1-C2	-5.80	117.98	120.30
1	X	1663	G	C4-C5-N7	5.79	113.12	110.80
1	X	853	G	N9-C4-C5	5.79	107.72	105.40
1	X	1716	C	N1-C2-O2	5.79	122.37	118.90
1	X	1978	U	C6-N1-C1'	5.78	129.29	121.20
1	X	1751	G	C5-C6-N1	-5.78	108.61	111.50
1	X	1811	A	N1-C6-N6	5.78	122.07	118.60
1	X	862	C	C6-N1-C2	5.78	122.61	120.30
1	X	2261	A	C5-N7-C8	-5.78	101.01	103.90
1	X	2521	G	N1-C6-O6	5.78	123.37	119.90
1	X	102	A	N1-C2-N3	5.77	132.19	129.30
1	X	2038	U	OP1-P-O3'	5.77	117.90	105.20
1	X	1016	G	N1-C6-O6	-5.77	116.44	119.90
1	X	1301	U	N1-C2-N3	5.77	118.36	114.90
1	X	1278	G	C5-N7-C8	-5.77	101.42	104.30
1	X	35	G	C2-N3-C4	-5.76	109.02	111.90
1	X	1257	G	N3-C4-C5	-5.76	125.72	128.60
1	X	660	A	OP1-P-OP2	-5.76	110.96	119.60
1	X	1828	U	C6-N1-C1'	-5.76	113.13	121.20
1	X	2726	C	N1-C2-O2	-5.76	115.44	118.90
1	X	985	A	N7-C8-N9	5.75	116.68	113.80
1	X	1855	G	C5-C6-O6	5.75	132.05	128.60
1	X	2457	A	C2-N3-C4	-5.75	107.72	110.60
2	Y	92	G	C5-C6-N1	-5.75	108.62	111.50
1	X	1243	G	N1-C6-O6	5.75	123.35	119.90
1	X	1687	G	N1-C6-O6	5.75	123.35	119.90
1	X	1968	C	C2-N1-C1'	5.75	125.12	118.80
1	X	2062	G	O5'-P-OP2	-5.75	100.53	105.70
1	X	102	A	C5-C6-N1	-5.75	114.83	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	440	C	N1-C2-O2	5.75	122.35	118.90
1	X	902	A	N9-C4-C5	5.75	108.10	105.80
1	X	78	U	N3-C2-O2	-5.74	118.18	122.20
1	X	605	U	C5-C4-O4	5.74	129.35	125.90
1	X	2419	A	C8-N9-C4	-5.74	103.50	105.80
1	X	2063	C	C6-N1-C2	-5.74	118.00	120.30
1	X	778	G	C5-C6-O6	-5.74	125.16	128.60
1	X	855	U	C2-N3-C4	-5.74	123.56	127.00
1	X	1228	A	C2-N3-C4	-5.74	107.73	110.60
1	X	554	C	C5-C6-N1	5.74	123.87	121.00
1	X	2844	U	C2-N3-C4	-5.74	123.56	127.00
1	X	2084	G	N3-C4-C5	-5.73	125.73	128.60
1	X	2599	A	C8-N9-C4	5.73	108.09	105.80
1	X	20	C	N3-C4-N4	5.73	122.01	118.00
1	X	2051	C	OP2-P-O3'	5.73	117.81	105.20
1	X	1351	C	N1-C2-O2	5.73	122.34	118.90
1	X	1175	G	N3-C4-N9	5.72	129.44	126.00
1	X	2757	U	C6-N1-C2	-5.72	117.57	121.00
1	X	2622	G	C5-C6-O6	-5.72	125.17	128.60
1	X	2845	G	N7-C8-N9	5.72	115.96	113.10
1	X	1466	G	N7-C8-N9	5.71	115.96	113.10
1	X	1977	G	O5'-P-OP1	-5.71	100.56	105.70
1	X	989	A	C5-C6-N6	-5.71	119.13	123.70
1	X	2887	G	N9-C4-C5	-5.71	103.12	105.40
1	X	1300	G	N1-C2-N3	5.71	127.33	123.90
1	X	506	A	N1-C6-N6	5.71	122.02	118.60
1	X	642	U	N3-C4-O4	-5.71	115.41	119.40
1	X	876	G	N3-C4-C5	-5.71	125.75	128.60
1	X	2576	G	C6-C5-N7	-5.70	126.98	130.40
1	X	1646	U	N3-C4-O4	5.70	123.39	119.40
1	X	1794	C	C6-N1-C2	-5.70	118.02	120.30
1	X	1686	G	N1-C6-O6	5.70	123.32	119.90
1	X	2545	A	C8-N9-C4	-5.70	103.52	105.80
1	X	214	G	C5-C6-N1	-5.69	108.65	111.50
1	X	428	G	C8-N9-C1'	-5.69	119.60	127.00
1	X	1180	G	C2-N3-C4	-5.69	109.05	111.90
1	X	1915	G	C2-N3-C4	5.69	114.75	111.90
1	X	622	A	OP1-P-O3'	5.69	117.71	105.20
1	X	1244	G	C5-C6-O6	5.69	132.01	128.60
1	X	428	G	C5-C6-N1	5.68	114.34	111.50
1	X	608	C	N3-C4-N4	5.68	121.98	118.00
1	X	1876	G	C8-N9-C4	-5.68	104.13	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	791	U	N1-C2-N3	5.68	118.31	114.90
1	X	2548	C	C6-N1-C2	-5.68	118.03	120.30
2	Y	86	C	C6-N1-C1'	-5.68	113.98	120.80
1	X	2089[A]	A	N3-C4-N9	5.68	131.94	127.40
1	X	2089[B]	A	N3-C4-N9	5.68	131.94	127.40
1	X	2797	C	C4-C5-C6	5.68	120.24	117.40
1	X	1171	A	N1-C6-N6	-5.67	115.19	118.60
1	X	1791	G	N3-C4-C5	5.67	131.44	128.60
1	X	625	G	N9-C4-C5	-5.67	103.13	105.40
1	X	2469	C	O5'-P-OP2	-5.67	100.59	105.70
1	X	70	G	C2-N3-C4	5.67	114.73	111.90
1	X	1806	U	N1-C2-O2	-5.67	118.83	122.80
1	X	1953	U	C6-N1-C1'	5.67	129.13	121.20
1	X	2361	U	C2-N1-C1'	5.66	124.50	117.70
1	X	985	A	C8-N9-C4	-5.66	103.53	105.80
1	X	2756	G	C2-N3-C4	-5.65	109.07	111.90
1	X	1186	A	O4'-C1'-N9	-5.65	103.68	108.20
1	X	2650	G	N1-C6-O6	5.65	123.29	119.90
1	X	532	C	N1-C2-O2	-5.65	115.51	118.90
1	X	1399	C	C6-N1-C2	-5.65	118.04	120.30
1	X	2062	G	OP1-P-OP2	5.65	128.07	119.60
2	Y	58	G	N3-C4-C5	5.65	131.42	128.60
2	Y	79	C	N1-C2-O2	5.65	122.29	118.90
1	X	1289	A	C5-C6-N1	-5.64	114.88	117.70
1	X	2078	A	C4-C5-C6	5.64	119.82	117.00
1	X	877	G	C2-N3-C4	5.64	114.72	111.90
1	X	2754	G	N1-C6-O6	-5.64	116.52	119.90
1	X	707	G	N1-C6-O6	5.63	123.28	119.90
1	X	2043	U	OP1-P-O3'	5.63	117.58	105.20
1	X	2446	U	C2-N1-C1'	-5.63	110.95	117.70
1	X	2710	C	O5'-P-OP2	-5.63	100.63	105.70
1	X	1047	G	N1-C6-O6	5.63	123.28	119.90
1	X	365	A	C8-N9-C4	-5.62	103.55	105.80
1	X	1732	U	C6-N1-C2	-5.62	117.63	121.00
1	X	1565	U	C6-N1-C2	-5.62	117.63	121.00
1	X	2703	C	C2-N3-C4	-5.62	117.09	119.90
1	X	980	U	O5'-P-OP2	-5.62	100.65	105.70
1	X	1367	C	C6-N1-C1'	-5.61	114.07	120.80
1	X	1237	U	C5-C4-O4	5.61	129.26	125.90
1	X	1401	G	C4-N9-C1'	5.61	133.79	126.50
1	X	993	C	C6-N1-C2	5.61	122.54	120.30
1	X	2495	A	O4'-C1'-N9	5.61	112.69	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	341	G	C5-C6-O6	-5.60	125.24	128.60
1	X	2853	U	C6-N1-C2	5.60	124.36	121.00
1	X	797	A	C4-N9-C1'	5.60	136.38	126.30
1	X	532	C	N3-C4-C5	-5.60	119.66	121.90
1	X	2731	C	N1-C2-O2	5.59	122.25	118.90
1	X	1001	A	C8-N9-C4	5.59	108.03	105.80
1	X	2059	G	O5'-P-OP2	-5.59	100.67	105.70
1	X	1599	G	N3-C4-C5	5.58	131.39	128.60
1	X	2743	U	C2-N3-C4	-5.58	123.65	127.00
1	X	1516	C	N3-C2-O2	-5.58	117.99	121.90
1	X	1599	G	N3-C4-N9	-5.58	122.65	126.00
1	X	1544	G	C5-C6-N1	5.58	114.29	111.50
1	X	2801	C	N3-C4-C5	5.58	124.13	121.90
1	X	706	U	N3-C2-O2	-5.58	118.30	122.20
1	X	2552	G	C5-C6-O6	-5.58	125.25	128.60
1	X	1308	C	C5-C6-N1	-5.57	118.21	121.00
1	X	2411	A	N1-C2-N3	5.57	132.09	129.30
1	X	1175	G	C5-C6-N1	5.57	114.28	111.50
1	X	1303	A	N9-C4-C5	-5.57	103.57	105.80
1	X	2603	G	C4-C5-N7	5.57	113.03	110.80
1	X	2018	U	N3-C2-O2	-5.57	118.30	122.20
1	X	2050	A	O5'-P-OP1	-5.57	100.69	105.70
1	X	795	A	C5-C6-N1	5.57	120.48	117.70
1	X	1806	U	C2-N3-C4	-5.57	123.66	127.00
1	X	2066	G	C4-C5-C6	5.57	122.14	118.80
1	X	639	U	N1-C2-O2	5.56	126.69	122.80
1	X	119	U	OP1-P-OP2	-5.56	111.26	119.60
1	X	1703	U	N3-C4-O4	-5.56	115.51	119.40
1	X	1065	A	N3-C4-N9	-5.56	122.95	127.40
1	X	528	C	N3-C4-C5	-5.56	119.68	121.90
1	X	1570	G	N3-C4-C5	-5.56	125.82	128.60
1	X	656	G	N7-C8-N9	5.55	115.88	113.10
1	X	2797	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	955	A	N3-C4-N9	5.55	131.84	127.40
1	X	1990	C	C6-N1-C2	-5.55	118.08	120.30
1	X	2077	C	N3-C2-O2	-5.55	118.01	121.90
1	X	2673	C	N3-C4-N4	5.55	121.88	118.00
1	X	1560	A	C5-C6-N6	5.55	128.14	123.70
1	X	902	A	N1-C6-N6	-5.55	115.27	118.60
1	X	1360	G	C5-N7-C8	-5.55	101.53	104.30
1	X	2358	G	C5-C6-N1	-5.55	108.73	111.50
1	X	35	G	N1-C2-N3	5.54	127.22	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1672	G	N1-C6-O6	5.54	123.22	119.90
1	X	511	G	C8-N9-C4	-5.53	104.19	106.40
1	X	963	A	C2-N3-C4	-5.53	107.83	110.60
1	X	610	U	N1-C2-N3	5.53	118.22	114.90
1	X	721	A	N3-C4-C5	5.53	130.67	126.80
1	X	21	A	C2-N3-C4	-5.53	107.84	110.60
1	X	1972	G	N1-C2-N3	-5.53	120.58	123.90
1	X	2044	C	N3-C4-C5	-5.52	119.69	121.90
1	X	1356	G	N1-C6-O6	5.52	123.21	119.90
1	X	2748	A	C5-C6-N6	-5.52	119.28	123.70
1	X	721	A	C4-C5-N7	5.52	113.46	110.70
1	X	2512	G	C2-N3-C4	-5.52	109.14	111.90
1	X	511	G	N3-C4-C5	-5.52	125.84	128.60
1	X	793	G	O4'-C1'-N9	5.52	112.61	108.20
1	X	1184	C	C6-N1-C2	5.52	122.51	120.30
1	X	1303	A	N7-C8-N9	5.52	116.56	113.80
1	X	1691	G	N3-C4-N9	-5.51	122.69	126.00
1	X	1609	U	N3-C4-O4	5.51	123.26	119.40
2	Y	77	G	N7-C8-N9	5.51	115.86	113.10
1	X	511	G	C5-C6-O6	5.51	131.91	128.60
1	X	1506	C	N1-C2-O2	5.51	122.20	118.90
1	X	1452	C	C6-N1-C2	-5.50	118.10	120.30
1	X	1703	U	C5-C6-N1	-5.50	119.95	122.70
1	X	2632	U	C6-N1-C2	-5.50	117.70	121.00
1	X	2842	G	C2-N3-C4	-5.49	109.15	111.90
1	X	2390	U	C5-C6-N1	-5.49	119.96	122.70
1	X	1332	C	C6-N1-C2	-5.49	118.11	120.30
1	X	2474	G	C2-N3-C4	-5.48	109.16	111.90
1	X	2887	G	C4-N9-C1'	5.48	133.63	126.50
1	X	1420	U	C6-N1-C2	-5.48	117.71	121.00
1	X	2298	G	C4-C5-N7	5.47	112.99	110.80
1	X	503	A	C8-N9-C4	-5.47	103.61	105.80
1	X	617	A	N7-C8-N9	-5.47	111.06	113.80
1	X	2429	U	C5-C6-N1	5.47	125.44	122.70
1	X	717	C	C6-N1-C2	-5.47	118.11	120.30
1	X	1591	G	C4-N9-C1'	5.47	133.61	126.50
1	X	1225	G	C8-N9-C4	-5.47	104.21	106.40
1	X	2378	G	N1-C6-O6	-5.47	116.62	119.90
1	X	996	G	C4-C5-N7	5.46	112.99	110.80
1	X	2074	C	N1-C2-O2	-5.46	115.62	118.90
1	X	835	U	C2-N1-C1'	5.46	124.25	117.70
1	X	1029	C	O5'-P-OP2	-5.46	100.79	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1976	G	C4-N9-C1'	5.46	133.59	126.50
1	X	715	A	O4'-C1'-N9	-5.45	103.84	108.20
1	X	824	A	C8-N9-C4	-5.45	103.62	105.80
1	X	2056	G	N3-C4-C5	5.45	131.32	128.60
1	X	2278	G	N3-C4-N9	5.44	129.27	126.00
1	X	1707	U	C6-N1-C2	-5.44	117.74	121.00
1	X	2394	G	C8-N9-C4	-5.44	104.22	106.40
1	X	1781	C	O5'-P-OP2	-5.44	100.81	105.70
1	X	2419	A	N1-C6-N6	5.43	121.86	118.60
1	X	610	U	C5-C6-N1	-5.43	119.98	122.70
1	X	611	U	N3-C2-O2	-5.43	118.40	122.20
1	X	727	G	C6-C5-N7	-5.43	127.14	130.40
1	X	2567	C	C5-C6-N1	-5.43	118.28	121.00
1	X	2079	G	C8-N9-C4	5.43	108.57	106.40
2	Y	105	G	C8-N9-C1'	-5.42	119.95	127.00
1	X	523	A	C4-C5-C6	5.42	119.71	117.00
1	X	1602	U	O4'-C1'-N1	5.42	112.53	108.20
1	X	2474	G	N9-C1'-C2'	5.42	121.04	114.00
1	X	70	G	P-O3'-C3'	5.41	126.19	119.70
1	X	501	C	C6-N1-C2	5.41	122.47	120.30
1	X	440	C	N3-C2-O2	-5.41	118.11	121.90
1	X	607	C	C2-N3-C4	-5.41	117.19	119.90
1	X	1042	C	C5-C6-N1	-5.41	118.29	121.00
1	X	1931	G	C4-C5-N7	5.41	112.96	110.80
1	X	2640	U	OP1-P-OP2	5.41	127.71	119.60
1	X	721	A	N7-C8-N9	5.41	116.50	113.80
1	X	1065	A	C4-C5-C6	5.40	119.70	117.00
1	X	378	C	C5-C6-N1	5.40	123.70	121.00
1	X	1705	G	C2-N3-C4	-5.40	109.20	111.90
1	X	2552	G	C5-C6-N1	5.39	114.20	111.50
1	X	791	U	C6-N1-C1'	5.39	128.74	121.20
1	X	2018	U	C2-N3-C4	-5.38	123.77	127.00
1	X	2045	A	C6-N1-C2	-5.38	115.37	118.60
1	X	511	G	N1-C6-O6	-5.38	116.67	119.90
1	X	1746	G	N1-C6-O6	5.38	123.13	119.90
1	X	78	U	N1-C2-O2	5.38	126.57	122.80
1	X	21	A	C4-C5-C6	5.38	119.69	117.00
1	X	457	G	C8-N9-C4	-5.38	104.25	106.40
1	X	1278	G	N7-C8-N9	5.37	115.78	113.10
1	X	1320	G	N3-C4-C5	-5.37	125.92	128.60
1	X	2603	G	C8-N9-C4	5.37	108.55	106.40
1	X	1660	A	C4-C5-C6	5.37	119.68	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2433	C	C2-N1-C1'	5.37	124.70	118.80
1	X	242	U	C4-C5-C6	5.36	122.92	119.70
1	X	1294	G	N3-C4-C5	-5.36	125.92	128.60
1	X	817	G	N3-C4-C5	-5.36	125.92	128.60
1	X	2278	G	C4-N9-C1'	5.36	133.46	126.50
1	X	1591	G	C8-N9-C4	-5.36	104.26	106.40
1	X	1702	C	C6-N1-C2	5.36	122.44	120.30
1	X	2483	C	C6-N1-C2	5.36	122.44	120.30
1	X	1232	G	N3-C4-N9	-5.35	122.79	126.00
1	X	1312	A	OP1-P-O3'	5.35	116.97	105.20
1	X	595	G	N1-C2-N3	5.35	127.11	123.90
1	X	2524	A	N1-C6-N6	-5.35	115.39	118.60
1	X	2599	A	N9-C4-C5	-5.35	103.66	105.80
1	X	532	C	N3-C4-N4	5.35	121.74	118.00
1	X	698	U	C2-N1-C1'	5.35	124.12	117.70
1	X	1300	G	C2-N3-C4	-5.35	109.23	111.90
1	X	791	U	C4-C5-C6	5.34	122.91	119.70
1	X	1768	C	C6-N1-C2	-5.34	118.16	120.30
1	X	2752	A	C8-N9-C4	-5.34	103.66	105.80
1	X	2797	C	N3-C4-N4	-5.34	114.26	118.00
1	X	2551	G	C5-N7-C8	-5.34	101.63	104.30
1	X	588	G	N3-C4-N9	5.33	129.20	126.00
1	X	661	U	C6-N1-C2	-5.33	117.80	121.00
1	X	43	A	O4'-C1'-N9	5.33	112.47	108.20
1	X	374	U	N3-C2-O2	-5.33	118.47	122.20
1	X	2302	C	C4-C5-C6	5.33	120.07	117.40
1	X	2476	U	C6-N1-C2	5.33	124.20	121.00
1	X	1570	G	N3-C4-N9	5.33	129.20	126.00
1	X	1658	A	C5-N7-C8	-5.33	101.24	103.90
1	X	2657	G	C6-C5-N7	-5.33	127.20	130.40
1	X	1838	G	C6-C5-N7	-5.32	127.21	130.40
1	X	526	A	N1-C6-N6	5.32	121.79	118.60
1	X	365	A	N9-C4-C5	5.31	107.93	105.80
1	X	1232	G	N3-C4-C5	5.31	131.25	128.60
1	X	509	G	N1-C6-O6	5.31	123.09	119.90
1	X	828	A	N3-C4-N9	-5.31	123.15	127.40
1	X	198	A	C5-C6-N6	-5.30	119.46	123.70
1	X	1021	G	N7-C8-N9	-5.30	110.45	113.10
1	X	1368	C	C6-N1-C2	5.30	122.42	120.30
1	X	1294	G	C6-N1-C2	-5.30	121.92	125.10
1	X	1689	G	C4-C5-N7	-5.30	108.68	110.80
1	X	2047	A	C6-N1-C2	-5.30	115.42	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1479	G	N3-C4-N9	-5.30	122.82	126.00
1	X	2089[A]	A	N3-C4-C5	-5.30	123.09	126.80
1	X	2089[B]	A	N3-C4-C5	-5.30	123.09	126.80
1	X	696	G	C2-N3-C4	5.29	114.55	111.90
1	X	1566	G	C8-N9-C4	-5.29	104.28	106.40
1	X	2381	A	C6-N1-C2	-5.29	115.43	118.60
1	X	1395	G	N1-C6-O6	5.29	123.07	119.90
1	X	34	U	C2-N1-C1'	5.29	124.04	117.70
1	X	630	G	N7-C8-N9	5.29	115.74	113.10
1	X	797	A	C5-C6-N6	-5.29	119.47	123.70
2	Y	92	G	N1-C2-N2	5.29	120.96	116.20
1	X	373	A	C5-C6-N6	5.28	127.93	123.70
1	X	1278	G	C6-N1-C2	5.28	128.27	125.10
1	X	549	U	P-O3'-C3'	5.28	126.04	119.70
1	X	262	G	C5-C6-O6	5.28	131.77	128.60
1	X	637	U	C5-C4-O4	5.28	129.07	125.90
1	X	1686	G	C5-N7-C8	-5.28	101.66	104.30
1	X	1981	G	N1-C2-N3	5.28	127.06	123.90
1	X	122	G	C4-C5-C6	-5.27	115.64	118.80
1	X	1659	C	N1-C2-O2	-5.27	115.74	118.90
1	X	2797	C	C2-N1-C1'	-5.27	113.00	118.80
1	X	1758	A	N3-C4-C5	-5.27	123.11	126.80
1	X	2082	C	C6-N1-C2	5.27	122.41	120.30
1	X	197	G	C2-N3-C4	-5.27	109.27	111.90
1	X	553	A	N1-C6-N6	-5.27	115.44	118.60
1	X	2068	U	C6-N1-C2	-5.27	117.84	121.00
1	X	1054	A	N1-C6-N6	-5.26	115.44	118.60
2	Y	78	C	C5-C4-N4	5.26	123.89	120.20
1	X	374	U	N1-C2-O2	5.26	126.48	122.80
1	X	1963	A	N1-C2-N3	5.26	131.93	129.30
1	X	1005	G	O5'-P-OP2	-5.26	100.97	105.70
1	X	2060	A	N1-C6-N6	-5.26	115.44	118.60
1	X	376	A	C4-N9-C1'	5.26	135.76	126.30
1	X	82	G	C5-C6-N1	-5.26	108.87	111.50
1	X	515	G	N3-C2-N2	5.26	123.58	119.90
1	X	73	A	C2-N3-C4	5.25	113.23	110.60
1	X	1278	G	C5-C6-N1	-5.25	108.87	111.50
1	X	2073	G	C6-C5-N7	-5.25	127.25	130.40
1	X	2529	G	C5-C6-O6	-5.25	125.45	128.60
1	X	2876	G	N9-C4-C5	5.25	107.50	105.40
1	X	1360	G	C5-C6-O6	-5.25	125.45	128.60
1	X	1004	A	C4-C5-C6	-5.25	114.38	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1289	A	C4-C5-N7	5.25	113.32	110.70
1	X	1343	U	C5-C6-N1	5.25	125.32	122.70
1	X	1602	U	C5-C4-O4	5.25	129.05	125.90
1	X	2661	A	N7-C8-N9	-5.25	111.18	113.80
1	X	1180	G	C4-C5-N7	5.25	112.90	110.80
1	X	1479	G	C5-C6-N1	-5.25	108.88	111.50
1	X	2641	A	C6-N1-C2	-5.25	115.45	118.60
1	X	102	A	C4-C5-C6	5.24	119.62	117.00
1	X	2094	G	N3-C4-N9	5.24	129.15	126.00
1	X	350	G	C8-N9-C1'	-5.24	120.19	127.00
1	X	605	U	N1-C2-N3	5.24	118.04	114.90
1	X	599	A	C6-N1-C2	-5.24	115.46	118.60
1	X	2052	C	OP1-P-OP2	-5.24	111.75	119.60
1	X	2565	C	C5-C6-N1	-5.24	118.38	121.00
1	X	350	G	C6-N1-C2	-5.23	121.96	125.10
1	X	1807	A	N1-C6-N6	5.23	121.74	118.60
1	X	2472	G	N9-C4-C5	5.23	107.49	105.40
2	Y	80	A	N1-C6-N6	5.23	121.74	118.60
1	X	1843	U	C5-C4-O4	-5.23	122.76	125.90
1	X	2682	G	C4-N9-C1'	-5.23	119.70	126.50
1	X	28	A	OP2-P-O3'	5.22	116.69	105.20
1	X	1511	C	C6-N1-C2	-5.22	118.21	120.30
1	X	2597	G	N1-C6-O6	-5.22	116.77	119.90
1	X	1291	A	OP1-P-OP2	5.22	127.43	119.60
1	X	465	C	C5-C6-N1	-5.22	118.39	121.00
1	X	586	C	C2-N1-C1'	-5.22	113.06	118.80
1	X	1245	G	C4-C5-C6	5.22	121.93	118.80
1	X	1291	A	O5'-P-OP2	-5.22	101.00	105.70
1	X	1691	G	N3-C4-C5	5.21	131.21	128.60
1	X	1056	U	O4'-C1'-N1	5.21	112.37	108.20
1	X	1180	G	C6-C5-N7	-5.21	127.27	130.40
1	X	1703	U	C5-C4-O4	5.21	129.03	125.90
1	X	2619	G	N3-C4-N9	5.21	129.13	126.00
1	X	494	U	N1-C2-O2	-5.21	119.15	122.80
1	X	1006	G	C5-C6-N1	-5.21	108.89	111.50
1	X	2278	G	C8-N9-C1'	-5.21	120.23	127.00
1	X	2609	G	C6-C5-N7	-5.21	127.28	130.40
16	O	25	LEU	CA-CB-CG	-5.21	103.32	115.30
2	Y	88	U	C5-C6-N1	5.21	125.30	122.70
1	X	1017	A	N7-C8-N9	5.21	116.40	113.80
1	X	2534	C	N3-C2-O2	-5.21	118.26	121.90
1	X	1636	U	P-O3'-C3'	5.20	125.94	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	648	G	C4-C5-N7	-5.20	108.72	110.80
1	X	2261	A	C6-C5-N7	-5.20	128.66	132.30
1	X	297	G	N3-C4-N9	-5.20	122.88	126.00
1	X	630	G	C4-N9-C1'	-5.20	119.74	126.50
1	X	2620	U	C5-C6-N1	5.20	125.30	122.70
1	X	635	G	N7-C8-N9	5.20	115.70	113.10
1	X	1050	C	C5-C6-N1	-5.20	118.40	121.00
1	X	2043	U	N1-C2-N3	5.19	118.02	114.90
1	X	2044	C	OP2-P-O3'	5.19	116.62	105.20
1	X	885	C	C4-C5-C6	5.19	119.99	117.40
1	X	1955	A	C5-C6-N1	5.18	120.29	117.70
1	X	1978	U	O4'-C1'-N1	5.18	112.35	108.20
1	X	559	A	C8-N9-C4	5.18	107.87	105.80
1	X	1047	G	C6-C5-N7	-5.18	127.29	130.40
1	X	2654	G	C8-N9-C4	-5.18	104.33	106.40
1	X	2793	G	C8-N9-C4	-5.18	104.33	106.40
1	X	2064	A	C5-N7-C8	-5.18	101.31	103.90
1	X	2727	G	C8-N9-C4	5.18	108.47	106.40
1	X	778	G	N1-C6-O6	5.17	123.00	119.90
1	X	1712	A	OP2-P-O3'	5.17	116.58	105.20
1	X	2740	A	N1-C2-N3	5.17	131.89	129.30
1	X	1291	A	C8-N9-C4	5.17	107.87	105.80
1	X	34	U	N1-C2-O2	5.17	126.42	122.80
1	X	1295	C	OP1-P-OP2	5.17	127.35	119.60
1	X	1732	U	C5-C4-O4	5.17	129.00	125.90
1	X	2576	G	C4-C5-C6	5.17	121.90	118.80
1	X	1721	A	C8-N9-C4	-5.16	103.73	105.80
1	X	2724	G	N1-C6-O6	5.16	123.00	119.90
1	X	1968	C	N1-C2-O2	5.16	122.00	118.90
1	X	1686	G	C4-C5-N7	5.16	112.86	110.80
1	X	263	G	C6-C5-N7	-5.16	127.31	130.40
1	X	568	C	C5-C6-N1	-5.16	118.42	121.00
1	X	1953	U	C3'-C2'-C1'	-5.16	97.38	101.50
1	X	70	G	O4'-C1'-N9	5.16	112.33	108.20
1	X	2066	G	C8-N9-C4	-5.16	104.34	106.40
1	X	2839	A	C2-N3-C4	5.16	113.18	110.60
1	X	1160	C	C6-N1-C2	5.15	122.36	120.30
1	X	12	U	C6-N1-C2	-5.15	117.91	121.00
1	X	2504	C	C5-C6-N1	5.15	123.57	121.00
1	X	1245	G	N3-C4-C5	-5.15	126.03	128.60
1	X	152	C	N1-C2-O2	5.14	121.99	118.90
1	X	1153	C	N1-C2-O2	5.14	121.99	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1232	G	C2-N3-C4	-5.14	109.33	111.90
1	X	1412	G	C2-N3-C4	5.14	114.47	111.90
1	X	892	U	C2-N1-C1'	-5.14	111.53	117.70
1	X	985	A	O5'-P-OP1	-5.14	101.07	105.70
1	X	1356	G	C5-C6-O6	-5.14	125.52	128.60
1	X	2433	C	P-O3'-C3'	5.14	125.87	119.70
1	X	1023	A	C2-N3-C4	-5.14	108.03	110.60
1	X	381	G	C6-C5-N7	-5.14	127.32	130.40
1	X	1566	G	N3-C4-C5	-5.14	126.03	128.60
1	X	2446	U	C4-C5-C6	-5.14	116.62	119.70
1	X	569	U	N3-C2-O2	5.13	125.79	122.20
1	X	1168	C	N3-C2-O2	-5.13	118.31	121.90
1	X	1182	G	C5-C6-O6	-5.13	125.52	128.60
1	X	1244	G	C6-C5-N7	5.13	133.48	130.40
1	X	2393	A	C8-N9-C4	5.13	107.85	105.80
1	X	2724	G	N3-C4-C5	5.13	131.16	128.60
1	X	2851	G	N7-C8-N9	5.13	115.66	113.10
1	X	1080	G	N1-C6-O6	5.13	122.97	119.90
1	X	1746	G	C8-N9-C4	-5.13	104.35	106.40
1	X	536	A	C2-N3-C4	-5.12	108.04	110.60
1	X	2063	C	C4-C5-C6	-5.12	114.84	117.40
2	Y	73	G	C4-C5-N7	-5.12	108.75	110.80
1	X	577	A	C2-N3-C4	5.12	113.16	110.60
2	Y	95	A	N9-C4-C5	-5.12	103.75	105.80
1	X	169	G	O4'-C1'-N9	5.12	112.29	108.20
1	X	2583	C	C5-C6-N1	5.12	123.56	121.00
1	X	435	A	C8-N9-C4	5.12	107.85	105.80
1	X	613	G	OP2-P-O3'	5.11	116.45	105.20
1	X	1244	G	C8-N9-C1'	5.11	133.64	127.00
1	X	1855	G	N3-C4-C5	-5.11	126.05	128.60
1	X	1262	U	C6-N1-C2	5.11	124.06	121.00
1	X	2269	G	N1-C6-O6	5.10	122.96	119.90
1	X	2383	C	C6-N1-C2	-5.10	118.26	120.30
1	X	590	U	C5-C4-O4	5.10	128.96	125.90
1	X	1963	A	C5-C6-N1	-5.10	115.15	117.70
1	X	1802	U	C5-C6-N1	-5.10	120.15	122.70
1	X	601	G	N1-C6-O6	-5.10	116.84	119.90
1	X	1867	G	C4-N9-C1'	5.10	133.13	126.50
1	X	2567	C	C6-N1-C2	5.10	122.34	120.30
1	X	323	C	C2-N3-C4	5.10	122.45	119.90
1	X	675	G	C6-C5-N7	-5.10	127.34	130.40
1	X	852	U	C6-N1-C2	-5.10	117.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1200	A	C8-N9-C4	-5.10	103.76	105.80
1	X	1273	G	C8-N9-C4	-5.10	104.36	106.40
1	X	1784	U	N3-C4-O4	5.10	122.97	119.40
1	X	1838	G	C8-N9-C4	-5.10	104.36	106.40
1	X	2023	C	OP1-P-O3'	5.09	116.41	105.20
1	X	1711	G	O5'-P-OP1	-5.09	101.12	105.70
1	X	2406	G	N1-C6-O6	5.09	122.95	119.90
1	X	1712	A	N1-C6-N6	5.09	121.65	118.60
1	X	2334	G	N3-C4-C5	5.09	131.14	128.60
1	X	558	A	OP2-P-O3'	5.09	116.39	105.20
1	X	1022	G	C5-C6-O6	-5.08	125.55	128.60
1	X	36	G	N3-C4-N9	5.08	129.05	126.00
1	X	797	A	C8-N9-C4	-5.08	103.77	105.80
1	X	2615	G	N1-C6-O6	-5.08	116.85	119.90
2	Y	109	C	N1-C2-O2	5.08	121.95	118.90
1	X	1020	G	N1-C6-O6	-5.08	116.85	119.90
1	X	2700	G	N1-C6-O6	5.08	122.95	119.90
1	X	14	A	C5-C6-N1	-5.08	115.16	117.70
1	X	2706	A	N3-C4-C5	5.07	130.35	126.80
1	X	556	U	C6-N1-C2	5.07	124.04	121.00
1	X	1293	U	C4-C5-C6	5.07	122.74	119.70
1	X	263	G	N1-C6-O6	5.07	122.94	119.90
1	X	1041	G	C8-N9-C4	5.07	108.43	106.40
1	X	1169	G	N9-C4-C5	5.07	107.43	105.40
1	X	1393	C	C5-C6-N1	5.07	123.53	121.00
1	X	1972	G	C4-C5-N7	5.07	112.83	110.80
1	X	21	A	N1-C2-N3	5.07	131.83	129.30
1	X	1458	A	O4'-C1'-N9	5.06	112.25	108.20
1	X	2885	U	N3-C4-O4	5.06	122.94	119.40
1	X	1686	G	C5-C6-O6	-5.06	125.56	128.60
1	X	381	G	C4-N9-C1'	5.06	133.08	126.50
1	X	988	C	OP1-P-OP2	-5.06	112.02	119.60
1	X	2529	G	C5-N7-C8	-5.06	101.77	104.30
1	X	367	A	C5-C6-N1	5.06	120.23	117.70
1	X	1972	G	C5-C6-O6	-5.06	125.57	128.60
1	X	2670	G	N9-C4-C5	5.06	107.42	105.40
1	X	69	C	N3-C2-O2	-5.05	118.36	121.90
1	X	666	A	C2-N3-C4	-5.05	108.07	110.60
1	X	1972	G	C2-N3-C4	5.05	114.43	111.90
1	X	2602	C	C5-C6-N1	5.05	123.53	121.00
1	X	363	A	N1-C6-N6	5.05	121.63	118.60
1	X	705	U	C5-C6-N1	-5.05	120.17	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2601	G	C8-N9-C4	-5.05	104.38	106.40
1	X	2619	G	C6-C5-N7	-5.05	127.37	130.40
1	X	514	G	N1-C2-N2	-5.05	111.66	116.20
1	X	1431	U	C5-C6-N1	5.05	125.22	122.70
1	X	1460	U	C6-N1-C2	-5.04	117.97	121.00
1	X	2627	A	C2-N3-C4	-5.04	108.08	110.60
1	X	1009	C	O5'-P-OP2	-5.04	101.16	105.70
1	X	20	C	C5-C4-N4	-5.04	116.67	120.20
1	X	795	A	C4-C5-N7	5.04	113.22	110.70
1	X	2599	A	C4-C5-C6	5.04	119.52	117.00
1	X	2682	G	O4'-C1'-N9	5.04	112.23	108.20
1	X	2839	A	C5-C6-N1	5.04	120.22	117.70
1	X	2887	G	C4-C5-N7	5.04	112.81	110.80
1	X	516	A	C4-C5-C6	5.04	119.52	117.00
1	X	1279	C	C2-N1-C1'	5.04	124.34	118.80
1	X	1968	C	N3-C2-O2	-5.03	118.38	121.90
1	X	542	A	C8-N9-C4	5.03	107.81	105.80
1	X	1066	G	O5'-P-OP2	-5.03	101.17	105.70
1	X	1226	G	C5-C6-N1	-5.03	108.99	111.50
1	X	349	U	O5'-P-OP2	-5.03	101.18	105.70
1	X	1901	C	P-O3'-C3'	5.03	125.73	119.70
1	X	2601	G	N1-C6-O6	-5.03	116.88	119.90
1	X	1310	A	C8-N9-C4	5.02	107.81	105.80
1	X	2648	G	C8-N9-C4	-5.02	104.39	106.40
1	X	2793	G	N7-C8-N9	5.02	115.61	113.10
1	X	2735	G	C5-C6-N1	-5.02	108.99	111.50
1	X	70	G	C5-C6-N1	5.02	114.01	111.50
1	X	297	G	N9-C4-C5	5.02	107.41	105.40
1	X	631	U	N1-C2-N3	5.02	117.91	114.90
1	X	1704	C	O5'-P-OP1	5.02	116.72	110.70
1	X	1782	A	C2-N3-C4	-5.01	108.09	110.60
1	X	1183	G	N1-C6-O6	-5.01	116.89	119.90
1	X	74	U	C6-N1-C2	-5.01	117.99	121.00
1	X	102	A	C6-C5-N7	-5.01	128.79	132.30
1	X	607	C	OP1-P-O3'	5.01	116.22	105.20
1	X	883	C	N3-C2-O2	5.01	125.41	121.90
1	X	2446	U	C2-N3-C4	5.01	130.01	127.00
1	X	2715	G	C5-C6-N1	-5.01	108.99	111.50
1	X	2021	C	C2-N3-C4	5.00	122.40	119.90
1	X	1915	G	N3-C4-C5	-5.00	126.10	128.60
1	X	2382	C	N3-C4-C5	5.00	123.90	121.90

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	156	ARG	Peptide
3	A	195	VAL	Peptide
3	A	50	THR	Peptide
4	B	159	ASP	Peptide
4	B	166	GLY	Peptide
4	B	204	PRO	Peptide
4	B	58	ALA	Peptide
4	B	97	ASP	Peptide
5	C	133	ALA	Peptide
5	C	142	VAL	Peptide
5	C	165	LEU	Peptide
5	C	28	PRO	Peptide
5	C	53	ASN	Peptide
7	E	152	ARG	Peptide
8	G	132	PRO	Peptide
8	G	136	GLN	Peptide
8	G	137	GLN	Peptide
8	G	138	PRO	Peptide
8	G	68	ASN	Peptide
9	H	110	ASN	Peptide
10	I	23	VAL	Peptide
10	I	24	ALA	Peptide
10	I	49	GLY	Peptide
10	I	81	GLN	Peptide
11	J	99	PRO	Peptide
14	M	45	PHE	Peptide
16	O	55	GLY	Peptide
16	O	77	LYS	Peptide
18	Q	55	ILE	Peptide
19	R	74	LYS	Peptide
19	R	83	TYR	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	58141	0	29232	1120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	2430	0	1229	57	0
3	A	1641	0	1415	71	0
4	B	1534	0	1495	52	0
5	C	1365	0	1258	88	0
6	D	926	0	824	33	0
7	E	793	0	475	17	0
8	G	1062	0	1000	34	0
9	H	902	0	956	39	0
10	I	780	0	621	38	0
11	J	1011	0	988	30	0
12	K	883	0	890	41	0
13	L	672	0	515	13	0
14	M	779	0	726	28	0
15	N	937	0	1003	47	0
16	O	700	0	629	32	0
17	P	852	0	905	32	0
18	Q	656	0	615	33	0
19	R	596	0	450	23	0
20	S	1145	0	991	40	0
21	T	561	0	555	16	0
22	V	519	0	530	24	0
23	W	437	0	474	18	0
24	Z	337	0	343	19	0
25	2	360	0	402	16	0
26	3	419	0	323	10	0
27	X	27	0	0	2	0
28	X	16	0	28	2	0
29	3	3	0	0	0	0
29	E	1	0	0	0	0
29	I	1	0	0	0	0
29	X	203	0	0	0	0
29	Y	1	0	0	0	0
29	Z	1	0	0	0	0
30	3	1	0	0	0	0
30	C	1	0	0	0	0
30	G	1	0	0	0	0
30	J	1	0	0	0	0
30	X	78	0	0	0	0
30	Y	2	0	0	0	0
31	X	15	0	17	0	0
32	X	10	0	19	3	0
All	All	80800	0	48908	1794	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 14.

All (1794) 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)
5:C:40:GLN:HE22	5:C:178:ALA:HB2	1.24	1.00
1:X:1835:U:H2'	1:X:1836:A:H5''	1.45	0.98
1:X:1515:G:H1	1:X:1564:G:H1	1.11	0.96
1:X:2850:G:OP2	4:B:86:ARG:NH2	2.00	0.93
1:X:630:G:OP2	10:I:21:ARG:NH2	2.03	0.92
1:X:922:G:O6	1:X:943:C:N4	2.03	0.92
1:X:1352:C:H42	1:X:1374:G:H1	1.17	0.92
8:G:94:ARG:HA	8:G:98:PRO:HB3	1.50	0.92
1:X:152:C:H41	1:X:177:G:H1	1.10	0.92
1:X:273:A:OP2	1:X:297:G:N2	2.02	0.92
18:Q:61:LYS:H	18:Q:72:THR:HG22	1.33	0.91
1:X:83:G:H21	1:X:102:A:H2	1.18	0.91
1:X:1487:G:N2	1:X:1597:U:O2	2.03	0.90
1:X:1815:C:H5''	3:A:224:VAL:HG11	1.49	0.90
1:X:2707:C:H5'	4:B:202:PRO:HA	1.53	0.90
1:X:1303:A:H2	1:X:2041:A:H62	1.17	0.90
2:Y:21:G:H1	2:Y:58:G:H1	1.17	0.89
18:Q:82:LEU:HD12	18:Q:85:GLY:HA3	1.52	0.88
1:X:1683:U:H2'	1:X:1684:A:H5''	1.56	0.88
5:C:54:ARG:O	5:C:56:ALA:N	2.06	0.88
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.56	0.87
2:Y:48:A:OP1	13:L:67:ALA:N	2.06	0.87
23:W:40:ASN:HB3	23:W:43:ILE:H	1.39	0.86
1:X:124:A:H5'	25:2:20:ARG:HD3	1.55	0.86
1:X:1247:G:O2'	1:X:1275:A:N6	2.09	0.86
1:X:2088:G:OP1	5:C:68:LYS:NZ	2.08	0.85
22:V:7:ARG:O	22:V:60:ARG:NH2	2.09	0.85
1:X:1542:C:H3'	1:X:1543:G:H5''	1.56	0.85
1:X:198:A:N6	1:X:201:C:OP2	2.10	0.85
5:C:25:GLY:O	5:C:27:GLU:N	2.10	0.84
1:X:2496:A:O2'	11:J:56:ARG:NH1	2.09	0.84
1:X:131:G:N1	1:X:148:U:O2	2.12	0.83
1:X:1501:G:H22	1:X:2729:G:H22	1.26	0.83
1:X:2649:U:O2'	1:X:2845:G:N2	2.12	0.82
4:B:8:ARG:NH1	4:B:206:LYS:O	2.13	0.82
9:H:76:TYR:HB2	14:M:75:THR:HG23	1.59	0.82
1:X:658:A:H3'	1:X:659:A:H5''	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:33:LEU:HD11	5:C:181:LEU:HD11	1.62	0.81
17:P:2:GLU:HG3	17:P:109:ASP:H	1.45	0.81
7:E:78:GLY:O	7:E:80:SER:N	2.13	0.81
1:X:503:A:H2	1:X:517:A:H62	1.26	0.81
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.14	0.80
3:A:46:GLN:OE1	3:A:48:LYS:N	2.15	0.80
20:S:49:ILE:HA	20:S:52:ILE:HG22	1.63	0.80
2:Y:15:C:H42	2:Y:105:G:H21	1.27	0.80
9:H:93:PRO:HD3	9:H:114:ILE:HG22	1.63	0.79
1:X:1832:C:H1'	3:A:51:VAL:HG21	1.64	0.79
13:L:19:ARG:NH1	13:L:47:ASP:OD2	2.16	0.79
1:X:151:U:H2'	1:X:152:C:O2	1.83	0.79
9:H:88:ARG:HB3	9:H:94:ARG:HD3	1.64	0.78
1:X:498:G:H21	1:X:503:A:H8	1.28	0.78
1:X:778:G:O6	1:X:806:A:C8	2.36	0.78
3:A:212:ARG:HG2	3:A:216:ILE:HA	1.65	0.78
25:2:16:VAL:H	25:2:21:LYS:HG3	1.49	0.78
1:X:1472:C:N4	1:X:1617:A:OP2	2.15	0.78
1:X:504:G:C8	25:2:38:LYS:HG2	2.19	0.77
12:K:105:LYS:HB2	24:Z:42:ARG:HG2	1.66	0.77
20:S:113:VAL:HB	20:S:147:GLU:HA	1.65	0.77
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.17	0.77
1:X:1065:A:H62	1:X:1185:U:H3	1.33	0.77
1:X:1465:G:H2'	1:X:1466:G:C8	2.19	0.77
24:Z:15:LYS:O	24:Z:18:THR:HG23	1.85	0.77
5:C:108:LEU:O	5:C:112:SER:OG	2.02	0.77
1:X:1512:U:H2'	1:X:1513:A:C8	2.20	0.77
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.67	0.77
1:X:778:G:O6	1:X:806:A:N7	2.18	0.77
3:A:107:PRO:HA	3:A:195:VAL:HA	1.66	0.76
5:C:176:THR:OG1	5:C:179:GLN:OE1	2.02	0.76
1:X:787:U:H2'	1:X:788:A:C8	2.20	0.76
1:X:243:U:O2	1:X:260:A:N6	2.17	0.76
20:S:109:VAL:HG11	20:S:145:ILE:H	1.50	0.76
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.67	0.76
10:I:106:LYS:H	10:I:125:ALA:HB1	1.51	0.76
5:C:177:THR:O	5:C:181:LEU:HD12	1.86	0.75
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.20	0.75
1:X:1514:A:H3'	1:X:1515:G:H8	1.50	0.75
1:X:1212:U:H3	1:X:1220:A:H61	1.32	0.75
1:X:1866:G:C6	1:X:1954:A:H5''	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:14:SER:OG	5:C:14:SER:O	2.03	0.75
1:X:721:A:H8	1:X:2096:G:H21	1.33	0.75
1:X:2717:A:OP1	12:K:4:ARG:NH2	2.18	0.75
18:Q:34:ASN:ND2	18:Q:37:GLN:OE1	2.19	0.74
3:A:179:GLY:H	3:A:271:VAL:HG13	1.50	0.74
20:S:109:VAL:HB	20:S:144:ASP:HA	1.69	0.74
1:X:1886:A:N6	1:X:1910:G:O2'	2.20	0.74
3:A:131:PRO:HA	3:A:189:ARG:HA	1.69	0.74
18:Q:26:THR:HB	18:Q:79:ILE:HG22	1.68	0.74
1:X:788:A:O2'	1:X:1703:U:OP1	2.06	0.74
3:A:45:ASN:OD1	3:A:45:ASN:N	2.21	0.73
18:Q:5:ASP:OD1	18:Q:5:ASP:N	2.21	0.73
1:X:1593:G:H5'	1:X:1593:G:H8	1.54	0.73
1:X:2883:U:H2'	1:X:2884:G:H8	1.52	0.73
2:Y:15:C:N4	2:Y:105:G:H21	1.86	0.73
21:T:48:GLN:NE2	21:T:50:GLY:O	2.21	0.73
1:X:1492:G:N7	1:X:1493:U:H5	1.87	0.73
1:X:719:G:H1'	5:C:74:ARG:HE	1.54	0.73
1:X:319:G:H22	1:X:326:A:H61	1.37	0.72
14:M:16:ARG:H	14:M:79:HIS:HD2	1.36	0.72
1:X:460:C:O2	1:X:1891:U:O2'	2.06	0.72
5:C:103:LYS:HA	5:C:106:ARG:HD2	1.71	0.72
1:X:2232:A:N6	1:X:2246:U:O4	2.17	0.72
1:X:323:C:H5'	1:X:324:A:C8	2.24	0.72
16:O:25:LEU:HD22	16:O:33:PHE:HE2	1.55	0.72
1:X:422:G:H1	1:X:444:C:H42	1.38	0.72
5:C:117:LYS:NZ	5:C:183:VAL:O	2.18	0.72
1:X:1323:A:O2'	1:X:1325:U:OP2	2.07	0.72
1:X:717:C:H5''	5:C:89:VAL:HG11	1.71	0.72
1:X:2883:U:H2'	1:X:2884:G:C8	2.24	0.72
5:C:40:GLN:NE2	5:C:178:ALA:HB2	2.01	0.72
4:B:38:LYS:NZ	4:B:97:ASP:HA	2.05	0.71
1:X:2358:G:O2'	1:X:2363:A:N1	2.23	0.71
15:N:91:ASN:O	15:N:93:LYS:N	2.23	0.71
16:O:63:ASN:H	16:O:95:LEU:HA	1.54	0.71
1:X:1440:A:O2'	1:X:1514:A:O2'	2.08	0.71
1:X:715:A:H4'	1:X:716:C:H5''	1.72	0.71
21:T:35:ASP:HA	21:T:75:VAL:HG12	1.73	0.71
1:X:1415:A:O2'	1:X:1417:G:N7	2.21	0.71
1:X:755:C:H42	1:X:766:G:H1	1.39	0.70
3:A:142:HIS:N	3:A:191:THR:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:162:THR:HG22	6:D:164:GLU:H	1.55	0.70
1:X:1383:G:N2	1:X:1644:C:O2	2.25	0.70
1:X:682:A:H4'	1:X:683:G:H5'	1.74	0.70
4:B:192:ASN:HB3	4:B:194:VAL:HG23	1.74	0.70
1:X:1563:U:H2'	1:X:1564:G:H8	1.57	0.70
10:I:120:LYS:HA	10:I:124:LYS:HA	1.74	0.70
1:X:2351:U:H3	1:X:2358:G:H1	1.37	0.70
1:X:2712:G:OP2	14:M:51:LYS:NZ	2.19	0.70
6:D:38:MET:HG2	6:D:57:LEU:HD22	1.73	0.69
18:Q:91:ASN:ND2	22:V:36:GLN:OE1	2.25	0.69
12:K:8:ARG:HD2	12:K:16:MET:HE2	1.73	0.69
1:X:1302:G:OP1	24:Z:16:ARG:NH2	2.25	0.69
14:M:52:ARG:HG3	14:M:52:ARG:HH11	1.55	0.69
1:X:1063:U:H3	1:X:1186:A:H62	1.41	0.69
4:B:97:ASP:OD1	4:B:98:ALA:N	2.25	0.69
1:X:83:G:H1	1:X:101:G:HO2'	1.39	0.69
1:X:2355:A:H2'	1:X:2356:A:C8	2.27	0.69
5:C:78:ILE:HD12	5:C:79:ARG:HG2	1.74	0.69
22:V:59:GLU:O	22:V:63:GLU:N	2.23	0.69
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.29	0.68
10:I:78:ASN:ND2	10:I:105:GLU:O	2.26	0.68
18:Q:50:VAL:HA	18:Q:82:LEU:HA	1.74	0.68
1:X:1563:U:H2'	1:X:1564:G:C8	2.28	0.68
1:X:2126:C:O4'	1:X:2218:G:N2	2.26	0.68
1:X:659:A:O2'	1:X:660:A:O5'	2.12	0.68
9:H:79:PHE:HD1	14:M:72:VAL:HG22	1.59	0.68
1:X:735:C:O2'	1:X:825:G:OP1	2.12	0.68
1:X:1289:A:OP1	15:N:13:ARG:NH1	2.27	0.67
3:A:54:HIS:HB2	3:A:215:GLY:HA2	1.77	0.67
1:X:2311:U:H3	1:X:2411:A:N6	1.92	0.67
1:X:1174:U:O2	4:B:162:ARG:NH2	2.27	0.67
1:X:1934:G:O2'	1:X:1935:C:O4'	2.11	0.67
1:X:841:C:H2'	1:X:842:U:C6	2.28	0.67
1:X:539:G:OP1	17:P:8:ARG:NH1	2.28	0.67
12:K:6:LEU:HB3	12:K:13:ARG:NH1	2.10	0.67
18:Q:16:SER:HB2	18:Q:26:THR:HG21	1.76	0.67
21:T:92:VAL:HG22	21:T:93:ALA:H	1.60	0.67
1:X:2843:A:OP1	4:B:127:PHE:HB2	1.95	0.67
1:X:2419:A:H2	1:X:2451:C:H42	1.41	0.66
2:Y:15:C:H42	2:Y:105:G:N2	1.92	0.66
1:X:498:G:OP1	5:C:58:SER:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:579:U:H5'	15:N:42:SER:OG	1.95	0.66
2:Y:79:C:H42	2:Y:92:G:H1	1.42	0.66
10:I:80:ASP:O	10:I:82:LEU:N	2.27	0.66
15:N:59:LYS:O	15:N:63:THR:HG23	1.96	0.66
1:X:2101:U:H2'	1:X:2102:U:C6	2.31	0.66
1:X:2571:G:OP1	32:X:3286:SPD:N1	2.29	0.66
2:Y:18:G:H1	2:Y:61:U:H3	1.42	0.66
1:X:658:A:H3'	1:X:659:A:C5'	2.26	0.66
4:B:87:PHE:CD2	4:B:208:LEU:HD13	2.31	0.66
18:Q:25:TYR:HD2	18:Q:82:LEU:HD21	1.60	0.66
1:X:132:C:N3	1:X:147:G:N2	2.42	0.66
1:X:235:G:N2	1:X:466:C:OP1	2.28	0.66
16:O:19:GLU:HA	16:O:96:THR:HA	1.77	0.66
1:X:2329:U:H2'	1:X:2330:G:H8	1.59	0.66
1:X:793:G:H5''	17:P:89:ALA:HB2	1.78	0.66
3:A:24:ILE:HG22	3:A:25:THR:H	1.59	0.66
6:D:22:TYR:OH	6:D:165:GLU:OE2	2.14	0.66
23:W:40:ASN:HB2	23:W:43:ILE:HB	1.78	0.66
1:X:457:G:OP1	1:X:2434:A:P	2.53	0.66
1:X:1275:A:OP1	1:X:1275:A:H4'	1.94	0.66
1:X:1449:A:H61	1:X:1459:A:H5'	1.61	0.66
5:C:37:ILE:HD11	5:C:181:LEU:HD13	1.76	0.66
21:T:46:TYR:HD2	21:T:48:GLN:HG2	1.61	0.66
1:X:1405:G:H2'	1:X:1406:G:H8	1.60	0.66
1:X:1244:G:H1	1:X:1278:G:H1	1.44	0.65
1:X:1663:G:HO2'	25:2:2:VAL:N	1.94	0.65
1:X:1756:U:H2'	1:X:1757:U:H5'	1.77	0.65
1:X:1465:G:H2'	1:X:1466:G:H8	1.60	0.65
1:X:1846:A:H4'	1:X:1847:U:H5''	1.78	0.65
1:X:1872:G:H1	1:X:1922:C:H42	1.43	0.65
1:X:299:U:O2'	1:X:300:G:N7	2.29	0.65
1:X:1092:A:N6	1:X:1156:G:O2'	2.30	0.65
1:X:415:U:H3	1:X:450:C:N4	1.94	0.65
28:X:3002:MPD:O4	28:X:3002:MPD:O2	2.14	0.65
15:N:45:TYR:O	15:N:48:ARG:HG3	1.97	0.65
1:X:162:A:H3'	1:X:163:U:H2'	1.77	0.65
1:X:258:A:H1'	1:X:430:A:C8	2.32	0.65
1:X:650:U:H3	1:X:666:A:H2	1.42	0.65
16:O:7:THR:OG1	16:O:8:GLY:N	2.28	0.65
1:X:1092:A:H61	1:X:1156:G:H1'	1.60	0.65
1:X:1933:G:N2	1:X:1934:G:O4'	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:862:C:H42	1:X:1229:G:H1	1.44	0.65
1:X:1422:A:O2'	1:X:1423:C:O4'	2.13	0.65
1:X:1823:U:H2'	1:X:1824:C:C6	2.32	0.65
6:D:12:VAL:O	6:D:15:ASN:ND2	2.26	0.65
15:N:52:GLN:O	15:N:55:ARG:HG3	1.96	0.64
1:X:1461:C:N4	1:X:1462:G:N7	2.45	0.64
1:X:1550:G:HO2'	1:X:1554:A:H2	1.43	0.64
1:X:1560:A:H3'	1:X:1561:G:H8	1.62	0.64
2:Y:74:G:H21	20:S:78:GLN:HE22	1.44	0.64
5:C:12:THR:HG22	5:C:13:LYS:H	1.62	0.64
1:X:2339:U:O2	6:D:37:ASN:ND2	2.30	0.64
3:A:244:PRO:HA	3:A:250:TRP:HA	1.77	0.64
11:J:43:THR:N	11:J:46:GLN:OE1	2.27	0.64
1:X:1540:U:O2	1:X:1625:U:O2'	2.16	0.64
1:X:2007:G:O2'	1:X:2009:U:OP2	2.14	0.64
1:X:2876:G:H2'	1:X:2877:G:O4'	1.97	0.64
1:X:1261:G:OP1	16:O:67:ARG:NH1	2.30	0.64
1:X:683:G:C6	1:X:696:G:C6	2.86	0.64
2:Y:39:G:C8	6:D:66:LEU:HD21	2.32	0.64
11:J:30:GLY:HA2	11:J:107:ALA:HB2	1.79	0.64
2:Y:39:G:H8	6:D:66:LEU:HD21	1.63	0.64
10:I:90:GLU:HG3	10:I:91:VAL:HG23	1.79	0.64
1:X:118:A:O2'	1:X:119:U:O2	2.15	0.64
7:E:156:PRO:HG2	7:E:159:GLY:O	1.98	0.64
1:X:152:C:N4	1:X:177:G:H1	1.90	0.64
1:X:361:U:H2'	1:X:362:C:H6	1.63	0.64
3:A:160:ALA:CB	3:A:195:VAL:H	2.10	0.64
1:X:1063:U:H3	1:X:1186:A:N6	1.96	0.64
1:X:1528:G:H22	1:X:1545:U:H3	1.46	0.64
5:C:64:PRO:HD3	5:C:76:GLY:O	1.98	0.63
13:L:37:ASN:OD1	13:L:37:ASN:N	2.29	0.63
1:X:2314:A:O2'	1:X:2315:A:O5'	2.16	0.63
2:Y:113:G:C2	2:Y:114:C:H1'	2.33	0.63
21:T:48:GLN:HE22	21:T:51:THR:HA	1.63	0.63
1:X:1815:C:C5'	3:A:224:VAL:HG11	2.25	0.63
5:C:158:ASN:ND2	5:C:158:ASN:O	2.30	0.63
5:C:180:GLY:H	5:C:183:VAL:CG2	2.12	0.63
16:O:25:LEU:HD22	16:O:33:PHE:CE2	2.34	0.63
20:S:109:VAL:HG13	20:S:110:GLY:H	1.62	0.63
7:E:24:VAL:HA	7:E:28:GLY:HA3	1.79	0.63
1:X:321:U:O2'	1:X:322:A:OP2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:78:U:H2'	1:X:79:U:C6	2.33	0.63
1:X:828:A:H2'	1:X:829:U:H4'	1.79	0.63
1:X:1953:U:N3	1:X:1954:A:N7	2.43	0.63
1:X:810:A:H2'	1:X:811:C:C6	2.34	0.63
23:W:30:LYS:O	23:W:33:SER:OG	2.15	0.63
2:Y:74:G:H21	20:S:78:GLN:NE2	1.97	0.63
17:P:2:GLU:OE1	17:P:109:ASP:HB2	1.99	0.63
1:X:858:U:H2'	1:X:859:C:C6	2.34	0.63
1:X:878:C:H2'	1:X:879:U:C6	2.34	0.63
5:C:4:TYR:HD2	5:C:20:SER:H	1.45	0.63
1:X:1217:U:H3'	1:X:1218:G:C8	2.34	0.62
1:X:1377:U:OP1	18:Q:15:LYS:NZ	2.26	0.62
1:X:2370:U:O2'	1:X:2400:U:O2'	2.16	0.62
16:O:16:GLU:OE2	16:O:99:LYS:HA	1.99	0.62
22:V:25:LEU:HA	22:V:28:LEU:HD12	1.80	0.62
1:X:1963:A:H2	1:X:1970:U:H3	1.48	0.62
1:X:1592:A:O2'	1:X:1593:G:OP2	2.16	0.62
1:X:514:G:H2'	1:X:515:G:H5'	1.81	0.62
1:X:942:C:H2'	1:X:943:C:C5	2.33	0.62
2:Y:92:G:OP1	20:S:14:THR:OG1	2.14	0.62
1:X:2856:U:H2'	1:X:2857:A:C8	2.34	0.62
1:X:684:U:H2'	1:X:685:C:C6	2.34	0.62
23:W:18:THR:HB	23:W:49:LYS:HZ3	1.64	0.62
1:X:1479:G:N2	1:X:1605:A:N1	2.46	0.62
22:V:61:GLU:O	22:V:65:SER:OG	2.18	0.62
23:W:18:THR:HB	23:W:49:LYS:NZ	2.14	0.62
22:V:4:LYS:NZ	22:V:5:GLU:O	2.23	0.62
1:X:1756:U:C2'	1:X:1757:U:H5'	2.30	0.62
1:X:2618:C:H2'	1:X:2619:G:H8	1.64	0.62
1:X:706:U:O2'	10:I:13:ARG:HA	2.00	0.62
1:X:1091:G:O2'	1:X:1092:A:OP2	2.15	0.62
1:X:2532:G:OP1	27:X:3001:95H:O14	2.18	0.62
1:X:353:A:O2'	1:X:354:A:OP2	2.17	0.62
8:G:58:ILE:HD11	8:G:129:ALA:HA	1.82	0.62
19:R:97:SER:O	19:R:99:GLU:HG2	1.99	0.62
1:X:218:G:H4'	1:X:219:A:H4'	1.81	0.62
1:X:2333:U:OP2	1:X:2334:G:N2	2.33	0.62
22:V:60:ARG:HA	22:V:63:GLU:HB3	1.81	0.61
1:X:2492:C:N4	1:X:2512:G:O6	2.17	0.61
20:S:11:GLY:O	20:S:13:GLN:NE2	2.33	0.61
1:X:363:A:OP2	5:C:134:PRO:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1708:A:H61	1:X:2023:C:H42	1.48	0.61
1:X:460:C:H2'	1:X:461:A:C8	2.35	0.61
1:X:679:G:H2'	1:X:680:C:C6	2.34	0.61
1:X:921:C:H42	1:X:944:G:H1	1.49	0.61
2:Y:3:U:H3	2:Y:112:G:H22	1.46	0.61
1:X:2329:U:H2'	1:X:2330:G:C8	2.35	0.61
21:T:46:TYR:CD2	21:T:48:GLN:HG2	2.36	0.61
1:X:2051:C:H2'	1:X:2052:C:H6	1.65	0.61
5:C:133:ALA:HB1	5:C:136:THR:OG1	2.01	0.61
1:X:1488:A:O2'	1:X:1489:A:OP1	2.18	0.61
1:X:162:A:OP1	1:X:166:A:N6	2.33	0.61
1:X:2060:A:O2'	1:X:2062:G:OP2	2.18	0.61
1:X:319:G:N3	1:X:319:G:H2'	2.16	0.61
1:X:2116:U:H2'	1:X:2117:A:C8	2.35	0.61
10:I:43:GLY:O	10:I:45:GLY:N	2.33	0.61
1:X:1039:C:C5	8:G:1:MET:HG2	2.36	0.61
1:X:75:G:N2	1:X:111:U:O2	2.33	0.61
1:X:119:U:O2'	1:X:120:G:O5'	2.12	0.61
1:X:1819:G:O2'	1:X:1857:C:OP1	2.17	0.61
1:X:2101:U:HO2'	1:X:2624:G:HO2'	1.46	0.61
1:X:613:G:H2'	1:X:2057:A:N7	2.14	0.61
1:X:1097:U:O4	1:X:1151:G:N1	2.34	0.61
1:X:1593:G:C8	1:X:1593:G:H5'	2.36	0.61
1:X:1596:G:H2'	1:X:1597:U:H6	1.64	0.61
1:X:2618:C:H2'	1:X:2619:G:C8	2.35	0.61
1:X:498:G:N2	1:X:503:A:H8	1.98	0.61
3:A:18:SER:O	3:A:18:SER:OG	2.17	0.61
2:Y:40:C:C2'	6:D:63:GLN:HE21	2.14	0.61
5:C:129:PHE:CD1	5:C:157:GLU:HG3	2.36	0.60
6:D:162:THR:HB	6:D:165:GLU:HB3	1.83	0.60
1:X:378:C:H2'	1:X:379:C:H6	1.66	0.60
1:X:459:C:O2'	1:X:1907:U:O2'	2.09	0.60
1:X:460:C:H2'	1:X:461:A:H8	1.66	0.60
4:B:48:ALA:HB2	4:B:92:ARG:HB3	1.82	0.60
1:X:1847:U:O2	3:A:201:GLU:N	2.27	0.60
1:X:365:A:OP1	5:C:161:VAL:CG2	2.50	0.60
2:Y:38:U:O2'	2:Y:43:A:N6	2.33	0.60
1:X:1152:U:H2'	1:X:1153:C:H6	1.67	0.60
1:X:1487:G:H2'	1:X:1488:A:C8	2.36	0.60
1:X:811:C:N4	1:X:812:U:O4	2.34	0.60
1:X:527:G:OP2	19:R:45:GLN:NE2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:90:A:O2'	1:X:91:A:H8	1.83	0.60
1:X:1498:U:HO2'	1:X:1499:U:H5	1.50	0.60
1:X:152:C:OP1	1:X:1396:A:O2'	2.18	0.60
1:X:1522:G:N2	1:X:1558:U:O2	2.21	0.60
1:X:921:C:H41	1:X:942:C:N4	1.99	0.60
1:X:2382:C:H1'	21:T:47:ARG:NH1	2.16	0.60
1:X:2445:A:H2'	1:X:2446:U:O4'	2.00	0.60
1:X:634:C:HO2'	26:3:2:PRO:N	1.99	0.60
16:O:39:LEU:O	16:O:49:GLY:HA3	2.01	0.60
20:S:109:VAL:HG11	20:S:145:ILE:N	2.16	0.60
1:X:2500:U:OP1	1:X:2502:C:N4	2.34	0.60
1:X:268:A:N6	1:X:473:U:O2'	2.34	0.60
1:X:606:G:OP2	16:O:78:ARG:NH2	2.35	0.60
4:B:10:ILE:HD11	4:B:29:GLU:HB2	1.84	0.60
12:K:59:ARG:HA	12:K:86:PHE:CZ	2.37	0.60
5:C:148:GLN:H	5:C:166:SER:HA	1.67	0.60
5:C:179:GLN:H	5:C:179:GLN:CD	2.05	0.59
5:C:53:ASN:C	5:C:55:SER:H	2.05	0.59
5:C:6:VAL:HG13	5:C:15:GLY:HA2	1.84	0.59
23:W:8:LEU:HB2	23:W:28:LEU:HD22	1.83	0.59
1:X:450:C:H4'	1:X:451:U:H5'	1.83	0.59
26:3:24:ARG:CB	26:3:47:ALA:HB1	2.33	0.59
1:X:2077:C:H1'	4:B:169:MET:HE1	1.82	0.59
10:I:106:LYS:N	10:I:125:ALA:HB1	2.17	0.59
19:R:28:PRO:HD2	19:R:34:VAL:HA	1.82	0.59
1:X:1614:A:O4'	1:X:1615:G:N2	2.35	0.59
22:V:25:LEU:HB2	22:V:46:VAL:HG11	1.85	0.59
3:A:160:ALA:HB3	3:A:195:VAL:H	1.66	0.59
1:X:629:A:H62	1:X:1289:A:H2	1.50	0.59
1:X:591:A:H4'	1:X:592:A:H5'	1.84	0.59
9:H:80:ASP:OD2	14:M:64:ARG:NH2	2.36	0.59
14:M:16:ARG:N	14:M:79:HIS:HD2	2.01	0.59
18:Q:60:PRO:HB3	18:Q:72:THR:O	2.02	0.59
19:R:11:VAL:HA	19:R:21:GLY:HA2	1.83	0.59
1:X:2357:G:O3'	21:T:52:LYS:HE2	2.03	0.59
7:E:123:PHE:O	7:E:125:VAL:N	2.32	0.59
1:X:342:A:N1	1:X:365:A:O2'	2.30	0.59
3:A:145:GLU:HA	3:A:152:GLY:HA2	1.84	0.59
11:J:75:THR:HG21	11:J:87:LYS:HB2	1.84	0.59
14:M:16:ARG:H	14:M:79:HIS:CD2	2.20	0.59
18:Q:89:LEU:HB2	22:V:30:PHE:HE1	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1597:U:O3'	1:X:1767:G:N2	2.36	0.59
2:Y:78:C:H42	20:S:15:ARG:HH22	1.51	0.59
3:A:46:GLN:HE22	3:A:48:LYS:NZ	2.01	0.59
9:H:73:ASP:OD1	9:H:73:ASP:N	2.32	0.59
1:X:1300:G:P	17:P:99:ARG:HH22	2.26	0.59
1:X:1280:U:H2'	1:X:1281:U:C6	2.37	0.59
1:X:1281:U:H2'	1:X:1282:A:C8	2.38	0.59
1:X:1636:U:O2'	1:X:1637:A:OP1	2.19	0.59
1:X:1866:G:H2'	1:X:1954:A:N3	2.18	0.59
1:X:2216:U:H2'	1:X:2217:G:N1	2.17	0.59
1:X:630:G:P	10:I:21:ARG:HH22	2.26	0.58
1:X:1359:A:OP1	17:P:11:ARG:HD3	2.02	0.58
1:X:1091:G:O2'	1:X:1154:G:N1	2.36	0.58
1:X:2687:A:OP1	1:X:2687:A:H8	1.85	0.58
1:X:90:A:O2'	1:X:91:A:O5'	2.21	0.58
10:I:99:SER:O	10:I:101:VAL:N	2.36	0.58
1:X:1353:A:H2'	1:X:1354:G:C8	2.38	0.58
1:X:1365:G:H2'	1:X:1367:C:C5	2.38	0.58
6:D:93:GLY:O	6:D:95:ARG:N	2.37	0.58
12:K:36:ARG:O	12:K:40:VAL:HG12	2.03	0.58
1:X:1013:U:O3'	23:W:14:GLY:HA2	2.03	0.58
1:X:1269:A:H2'	1:X:1270:U:H6	1.67	0.58
1:X:2370:U:H2'	1:X:2371:U:C6	2.38	0.58
10:I:63:LYS:HG3	10:I:91:VAL:HB	1.85	0.58
20:S:51:VAL:HG11	20:S:61:ILE:HD12	1.85	0.58
23:W:5:GLN:HB2	23:W:36:VAL:HG12	1.86	0.58
1:X:1018:A:O5'	1:X:1225:G:N2	2.36	0.58
1:X:2383:C:H4'	21:T:28:ARG:HD3	1.85	0.58
1:X:188:C:H42	1:X:214:G:H1	1.51	0.58
1:X:2092:C:H1'	1:X:2476:U:H3	1.68	0.58
1:X:339:A:H2'	1:X:340:C:H6	1.69	0.58
1:X:168:A:H3'	1:X:169:G:H5'	1.85	0.58
8:G:39:GLY:HA3	8:G:51:THR:HG23	1.85	0.58
8:G:20:ASP:HA	8:G:58:ILE:HG22	1.85	0.58
14:M:32:VAL:HA	14:M:42:ILE:HD13	1.86	0.58
19:R:59:THR:OG1	19:R:60:GLU:N	2.37	0.58
1:X:126:A:H5''	1:X:127:C:O4'	2.04	0.58
1:X:132:C:N4	1:X:134:U:O4	2.37	0.58
1:X:1514:A:N6	1:X:1565:U:H3	2.01	0.58
12:K:27:SER:O	12:K:29:ARG:N	2.35	0.58
1:X:2322:C:H1'	1:X:2365:G:N2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:515:G:H22	25:2:38:LYS:HD2	1.69	0.58
1:X:2431:C:H2'	1:X:2432:G:O4'	2.04	0.58
3:A:149:GLY:O	3:A:151:GLY:N	2.33	0.58
9:H:6:THR:O	9:H:21:THR:HG22	2.03	0.58
1:X:365:A:OP1	5:C:161:VAL:HG21	2.04	0.57
20:S:44:ASP:OD2	20:S:47:GLU:HG3	2.04	0.57
1:X:1442:C:H2'	1:X:1443:A:C8	2.39	0.57
1:X:1887:G:H22	1:X:1910:G:H1'	1.69	0.57
1:X:2314:A:HO2'	1:X:2315:A:P	2.26	0.57
1:X:234:C:O2'	1:X:235:G:O4'	2.22	0.57
1:X:2360:A:H5'	1:X:2362:A:H1'	1.86	0.57
1:X:695:C:N3	1:X:696:G:C5	2.72	0.57
1:X:1206:G:N2	16:O:90:GLN:OE1	2.27	0.57
3:A:163:GLN:O	3:A:174:ILE:HG23	2.04	0.57
5:C:5:ASP:OD1	5:C:5:ASP:N	2.37	0.57
1:X:2446:U:H2'	1:X:2447:C:C6	2.38	0.57
25:2:16:VAL:N	25:2:21:LYS:HG3	2.17	0.57
8:G:2:ARG:HA	8:G:2:ARG:HH11	1.70	0.57
9:H:23:LYS:HA	9:H:23:LYS:HE3	1.86	0.57
1:X:1410:A:H2'	1:X:1411:G:O4'	2.04	0.57
1:X:1957:G:O2'	1:X:1995:G:O6	2.17	0.57
1:X:2906:G:H2'	1:X:2907:A:C8	2.40	0.57
18:Q:89:LEU:HB2	22:V:30:PHE:CE1	2.38	0.57
11:J:78:PRO:HB2	11:J:81:VAL:HG21	1.86	0.57
1:X:140:A:N3	1:X:1445:C:O2'	2.30	0.57
1:X:1488:A:H3'	1:X:1489:A:C2	2.39	0.57
1:X:1758:A:N7	1:X:1772:G:N1	2.51	0.57
2:Y:37:A:O2'	2:Y:44:A:N1	2.37	0.57
1:X:1373:U:H2'	1:X:1374:G:C8	2.40	0.57
1:X:1452:C:HO2'	1:X:1631:G:N2	2.02	0.57
1:X:1828:U:H4'	1:X:1828:U:OP2	2.02	0.57
1:X:259:A:H2'	1:X:260:A:C8	2.39	0.57
5:C:11:GLY:HA2	5:C:142:VAL:HG12	1.87	0.57
15:N:66:ASN:OD1	15:N:70:ARG:NH1	2.31	0.57
10:I:32:GLY:O	10:I:33:ARG:HD3	2.04	0.57
11:J:39:THR:HG23	11:J:98:LYS:HA	1.87	0.57
1:X:1238:U:H1'	15:N:4:VAL:HG22	1.86	0.57
3:A:209:GLY:HA2	3:A:212:ARG:HB2	1.87	0.57
15:N:29:HIS:CD2	15:N:30:THR:HG22	2.40	0.57
20:S:112:ALA:H	20:S:116:LYS:HE3	1.70	0.57
20:S:31:VAL:HG12	20:S:91:PHE:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1314:A:H5''	12:K:36:ARG:NH1	2.20	0.57
1:X:187:C:H2'	1:X:188:C:H6	1.69	0.57
1:X:271:C:H5'	1:X:324:A:O2'	2.05	0.57
1:X:2906:G:H2'	1:X:2907:A:H8	1.70	0.57
1:X:328:G:N2	1:X:329:A:N7	2.53	0.57
1:X:1625:U:O4	1:X:1626:A:N6	2.38	0.56
17:P:23:LEU:HD23	24:Z:24:VAL:HG13	1.87	0.56
20:S:106:VAL:HG23	20:S:127:ASN:HA	1.86	0.56
1:X:1244:G:H22	1:X:1278:G:N2	2.03	0.56
1:X:1558:U:N3	1:X:1559:G:N7	2.53	0.56
1:X:169:G:HO2'	1:X:170:C:H6	1.52	0.56
1:X:1864:C:H1'	1:X:1955:A:N3	2.20	0.56
1:X:661:U:H2'	1:X:662:G:H8	1.69	0.56
1:X:90:A:H4'	1:X:91:A:H5'	1.86	0.56
16:O:33:PHE:HD1	16:O:34:THR:N	2.02	0.56
19:R:97:SER:O	19:R:99:GLU:N	2.38	0.56
1:X:1197:C:H2'	1:X:1198:G:O4'	2.05	0.56
1:X:683:G:H2'	1:X:684:U:H6	1.70	0.56
1:X:1514:A:H61	1:X:1565:U:H3	1.52	0.56
1:X:2370:U:H2'	1:X:2371:U:H6	1.70	0.56
1:X:501:C:H3'	1:X:502:C:H5''	1.87	0.56
1:X:554:C:H5'	1:X:555:C:OP2	2.06	0.56
17:P:111:LYS:HE2	17:P:112:GLU:N	2.20	0.56
1:X:1542:C:H3'	1:X:1543:G:C5'	2.33	0.56
1:X:1523:G:H1'	1:X:1556:G:H1	1.71	0.56
1:X:2334:G:O3'	1:X:2337:A:N6	2.39	0.56
8:G:2:ARG:HA	8:G:2:ARG:NH1	2.21	0.56
15:N:76:TYR:OH	15:N:92:ARG:NH1	2.39	0.56
20:S:61:ILE:HG23	20:S:72:VAL:HG12	1.87	0.56
1:X:1382:C:N4	1:X:1383:G:O6	2.39	0.56
1:X:2354:A:H2'	1:X:2355:A:C8	2.40	0.56
1:X:2687:A:H2'	1:X:2688:G:C8	2.41	0.56
1:X:681:G:O2'	1:X:683:G:H4'	2.05	0.56
1:X:785:C:H5'	1:X:1811:A:H3'	1.88	0.56
11:J:34:LEU:HD11	11:J:129:THR:HB	1.88	0.56
1:X:532:C:H4'	17:P:60:HIS:CD2	2.41	0.56
1:X:1963:A:H2	1:X:1970:U:N3	2.03	0.56
21:T:60:GLY:HA3	21:T:68:PHE:CZ	2.40	0.56
1:X:2333:U:OP1	1:X:2334:G:N1	2.39	0.56
1:X:2411:A:HO2'	1:X:2412:C:P	2.29	0.56
1:X:946:A:H2'	1:X:947:U:H5'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:44:ASN:N	3:A:44:ASN:OD1	2.38	0.56
1:X:2860:U:H5''	12:K:49:THR:HG21	1.87	0.56
1:X:678:A:N3	1:X:2430:C:H4'	2.21	0.56
9:H:15:GLY:HA3	9:H:50:GLY:HA3	1.86	0.55
1:X:139:U:O2'	1:X:140:A:O5'	2.25	0.55
1:X:1481:A:H61	1:X:1603:U:H3	1.53	0.55
1:X:1835:U:H2'	1:X:1836:A:C5'	2.27	0.55
1:X:606:G:H22	1:X:621:A:H2	1.52	0.55
8:G:26:LEU:HA	8:G:63:ILE:HD11	1.88	0.55
1:X:268:A:O2'	1:X:269:G:H4'	2.06	0.55
1:X:157:U:H2'	1:X:158:G:H8	1.70	0.55
1:X:797:A:H62	1:X:2636:U:H3	1.55	0.55
6:D:57:LEU:HD12	6:D:60:ILE:HD12	1.87	0.55
1:X:1096:C:N4	1:X:1152:U:O4	2.39	0.55
9:H:114:ILE:HA	9:H:117:LEU:HD13	1.87	0.55
12:K:67:ARG:O	12:K:68:ASN:HB2	2.07	0.55
1:X:1449:A:N6	1:X:1459:A:H5'	2.22	0.55
1:X:1515:G:N2	1:X:1564:G:N2	2.55	0.55
1:X:1658:A:H8	1:X:1658:A:P	2.30	0.55
1:X:1953:U:H1'	1:X:1954:A:H5'	1.88	0.55
1:X:1870:C:O2'	3:A:253:PRO:HB2	2.06	0.55
5:C:51:VAL:HG11	5:C:91:GLY:HA3	1.89	0.55
7:E:154:PRO:HA	7:E:162:ILE:HG22	1.88	0.55
12:K:23:SER:HA	12:K:26:ILE:HD12	1.89	0.55
12:K:40:VAL:O	12:K:44:VAL:HG12	2.07	0.55
1:X:1505:G:H8	1:X:1506:C:C5	2.25	0.55
1:X:1523:G:H1'	1:X:1556:G:N1	2.22	0.55
17:P:9:THR:HG22	17:P:80:PRO:HD2	1.89	0.55
1:X:1065:A:H3'	1:X:1065:A:C8	2.42	0.55
1:X:1510:U:H2'	1:X:1511:C:O4'	2.06	0.55
1:X:2324:C:H42	1:X:2348:G:H1	1.53	0.55
1:X:293:U:H2'	1:X:294:G:C8	2.42	0.55
8:G:44:THR:OG1	8:G:44:THR:O	2.24	0.55
12:K:55:ASP:OD1	12:K:55:ASP:N	2.40	0.55
13:L:39:HIS:HB2	13:L:58:SER:OG	2.07	0.55
19:R:76:ASN:N	19:R:76:ASN:OD1	2.35	0.55
1:X:1933:G:N3	1:X:1934:G:H5'	2.22	0.55
2:Y:78:C:H2'	2:Y:79:C:C5	2.42	0.55
10:I:106:LYS:H	10:I:125:ALA:CB	2.18	0.55
14:M:30:VAL:HB	14:M:85:LYS:HG2	1.88	0.55
1:X:1476:G:H2'	1:X:1477:U:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1918:G:O2'	1:X:2262:G:O2'	2.19	0.55
1:X:280:C:H2'	1:X:281:A:C8	2.42	0.55
2:Y:91:C:H2'	2:Y:92:G:C8	2.42	0.55
5:C:154:VAL:HG12	5:C:155:VAL:H	1.72	0.55
5:C:4:TYR:HB2	5:C:19:LEU:HA	1.88	0.55
1:X:140:A:H61	1:X:1639:G:HO2'	1.54	0.55
1:X:1493:U:H1'	1:X:1494:G:H5'	1.89	0.55
10:I:62:PRO:O	10:I:90:GLU:HG2	2.07	0.54
1:X:1683:U:C2'	1:X:1684:A:H5''	2.34	0.54
1:X:319:G:H22	1:X:326:A:N6	2.03	0.54
1:X:877:G:H2'	1:X:878:C:C6	2.41	0.54
3:A:182:ARG:HA	3:A:266:SER:HA	1.89	0.54
13:L:20:THR:HG23	13:L:21:ASN:H	1.71	0.54
18:Q:46:PHE:HB2	18:Q:48:VAL:HG22	1.89	0.54
1:X:17:G:OP1	24:Z:11:THR:HB	2.06	0.54
6:D:9:ASN:O	6:D:13:THR:OG1	2.16	0.54
16:O:60:ALA:HB1	16:O:96:THR:O	2.07	0.54
1:X:1766:C:H2'	1:X:1767:G:H5'	1.89	0.54
3:A:45:ASN:HB3	3:A:49:LEU:O	2.07	0.54
1:X:1810:A:H5'	1:X:2635:G:H4'	1.89	0.54
2:Y:40:C:H2'	6:D:63:GLN:HE21	1.72	0.54
4:B:162:ARG:HG2	4:B:163:VAL:N	2.22	0.54
1:X:1695:G:OP1	12:K:33:THR:HG21	2.06	0.54
19:R:72:ASP:CB	19:R:99:GLU:HG3	2.37	0.54
1:X:1177:A:H4'	1:X:1178:C:H5'	1.88	0.54
2:Y:77:G:H1	2:Y:94:U:H3	1.56	0.54
5:C:136:THR:O	5:C:140:LYS:N	2.33	0.54
5:C:139:PHE:O	5:C:142:VAL:HG13	2.07	0.54
5:C:160:ASP:OD1	5:C:160:ASP:N	2.38	0.54
8:G:54:TYR:CD2	8:G:122:LYS:HB3	2.43	0.54
1:X:1400:C:H42	1:X:1405:G:H1	1.55	0.54
1:X:1527:A:H61	1:X:1546:A:H62	1.56	0.54
1:X:2010:U:H4'	1:X:2633:C:H4'	1.89	0.54
7:E:160:LYS:CB	7:E:163:ARG:HE	2.21	0.54
19:R:42:LYS:HG2	19:R:43:LYS:N	2.23	0.54
1:X:1038:C:OP2	15:N:54:LYS:NZ	2.39	0.54
3:A:83:TYR:CD2	3:A:85:PRO:HD2	2.43	0.54
4:B:215:ILE:O	4:B:216:LYS:HG2	2.08	0.54
1:X:179:A:OP2	1:X:179:A:H8	1.91	0.54
1:X:1847:U:C5	3:A:159:GLY:HA3	2.42	0.54
1:X:2335:G:P	1:X:2337:A:H62	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:907:G:H2'	1:X:908:A:O4'	2.08	0.54
2:Y:79:C:N3	2:Y:92:G:N2	2.52	0.54
1:X:1492:G:N2	1:X:1508:C:N3	2.52	0.54
1:X:687:G:N2	1:X:690:U:OP2	2.41	0.54
5:C:107:ARG:HA	5:C:110:LEU:HD12	1.90	0.54
1:X:1876:G:H2'	1:X:1877:G:C8	2.43	0.54
1:X:2470:C:H2'	1:X:2471:G:C8	2.42	0.54
1:X:633:A:H2'	1:X:634:C:O4'	2.08	0.54
1:X:739:U:OP1	3:A:59:LYS:NZ	2.35	0.54
5:C:13:LYS:O	5:C:15:GLY:N	2.40	0.53
9:H:35:ILE:HA	9:H:62:ILE:HG22	1.90	0.53
1:X:660:A:O2'	1:X:661:U:O5'	2.25	0.53
1:X:1700:C:H2'	1:X:1701:U:C6	2.44	0.53
1:X:1973:U:H2'	1:X:1974:C:C6	2.43	0.53
1:X:676:A:N3	1:X:2442:G:O2'	2.39	0.53
1:X:778:G:C6	1:X:806:A:N7	2.76	0.53
4:B:33:ASN:HB3	4:B:105:VAL:HG12	1.91	0.53
21:T:35:ASP:HB2	21:T:77:PHE:HD1	1.74	0.53
1:X:100:U:H3'	1:X:101:G:H5'	1.91	0.53
1:X:2410:G:C5	1:X:2411:A:H2	2.25	0.53
1:X:2625:A:OP1	3:A:233:GLY:HA3	2.09	0.53
20:S:112:ALA:HB1	20:S:115:ALA:HB3	1.89	0.53
1:X:967:C:O2'	21:T:34:ALA:HB2	2.08	0.53
1:X:1395:G:C8	1:X:1408:G:O6	2.61	0.53
1:X:292:U:H2'	1:X:293:U:C6	2.43	0.53
1:X:641:A:H62	28:X:3003:MPD:H52	1.72	0.53
1:X:661:U:O2'	1:X:662:G:H5'	2.08	0.53
1:X:665:G:H4'	1:X:666:A:H5''	1.90	0.53
5:C:33:LEU:HD21	5:C:181:LEU:HD21	1.91	0.53
17:P:29:ALA:O	17:P:33:ILE:HG12	2.08	0.53
1:X:2642:U:H1'	24:Z:4:PRO:HB3	1.91	0.53
5:C:53:ASN:C	5:C:55:SER:N	2.63	0.53
1:X:1767:G:HO2'	1:X:1768:C:H6	1.55	0.53
1:X:189:G:H2'	1:X:190:G:H8	1.73	0.53
1:X:343:A:H1'	1:X:362:C:H1'	1.90	0.53
1:X:1352:C:H2'	1:X:1353:A:H8	1.74	0.53
1:X:2391:C:H2'	1:X:2392:G:O4'	2.08	0.53
1:X:340:C:H2'	1:X:341:G:O4'	2.09	0.53
18:Q:54:ASN:HB2	18:Q:79:ILE:HG12	1.91	0.53
1:X:1373:U:H2'	1:X:1374:G:H8	1.73	0.53
1:X:328:G:HO2'	1:X:329:A:H8	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:28:GLY:O	25:2:32:LEU:HG	2.09	0.53
1:X:2625:A:OP1	3:A:239:ALA:HB1	2.09	0.53
14:M:66:ILE:HA	14:M:71:GLY:HA2	1.90	0.53
16:O:38:VAL:O	16:O:53:VAL:HG12	2.09	0.53
1:X:1526:G:N1	1:X:1548:U:O4	2.37	0.53
1:X:153:G:O2'	1:X:154:A:P	2.67	0.53
1:X:1680:U:H2'	1:X:1681:U:H6	1.73	0.53
1:X:1866:G:H2'	1:X:1954:A:C2	2.44	0.53
1:X:259:A:H2'	1:X:260:A:H8	1.74	0.53
1:X:311:U:H2'	1:X:312:A:H8	1.74	0.53
12:K:109:ARG:HD3	12:K:112:ASP:OD1	2.08	0.52
12:K:14:LYS:O	12:K:18:ARG:HG3	2.08	0.52
12:K:32:THR:HG22	12:K:33:THR:N	2.23	0.52
12:K:91:GLU:N	12:K:91:GLU:OE2	2.41	0.52
18:Q:15:LYS:HA	18:Q:18:GLU:HG2	1.91	0.52
1:X:1281:U:H2'	1:X:1282:A:H8	1.73	0.52
1:X:1469:G:O2'	1:X:1470:G:C8	2.62	0.52
1:X:1482:U:H2'	1:X:1483:A:H8	1.74	0.52
1:X:1746:G:H2'	1:X:1747:G:H8	1.74	0.52
1:X:2650:G:O5'	1:X:2845:G:N2	2.42	0.52
1:X:683:G:H2'	1:X:684:U:C6	2.44	0.52
1:X:864:A:OP2	1:X:1226:G:N2	2.27	0.52
17:P:5:ALA:HB3	17:P:54:ALA:HB2	1.90	0.52
1:X:2089[B]:A:O2'	1:X:2090:C:H6	1.91	0.52
3:A:196:GLY:O	3:A:198:LEU:N	2.43	0.52
18:Q:51:ALA:N	18:Q:81:THR:O	2.37	0.52
1:X:1241:A:H2'	1:X:1242:A:C8	2.44	0.52
1:X:1478:A:H2'	1:X:1479:G:O4'	2.10	0.52
1:X:1494:G:O2'	1:X:1495:C:H5'	2.09	0.52
9:H:61:VAL:HB	9:H:87:ILE:HD11	1.91	0.52
1:X:178:A:OP2	1:X:178:A:H8	1.93	0.52
1:X:1836:A:O2'	1:X:1837:A:O5'	2.28	0.52
1:X:645:A:O2'	1:X:647:G:O2'	2.24	0.52
1:X:665:G:H4'	1:X:666:A:C5'	2.39	0.52
14:M:93:LYS:H	14:M:111:ARG:CB	2.23	0.52
1:X:1244:G:N2	1:X:1278:G:N2	2.58	0.52
1:X:1520:A:H2	1:X:1560:A:C6	2.26	0.52
1:X:1074:G:OP2	11:J:128:LYS:NZ	2.40	0.52
1:X:661:U:H2'	1:X:662:G:C8	2.45	0.52
1:X:695:C:H6	1:X:695:C:O5'	1.93	0.52
15:N:27:SER:HA	15:N:30:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:6:GLU:HB2	16:O:39:LEU:HD23	1.91	0.52
11:J:81:VAL:HG12	11:J:82:ARG:O	2.10	0.52
1:X:1322:G:N2	1:X:1365:G:H5''	2.25	0.52
1:X:1573:A:N1	1:X:1591:G:O2'	2.42	0.52
5:C:42:ALA:O	5:C:45:ARG:HG2	2.09	0.52
3:A:105:ILE:O	3:A:107:PRO:HD3	2.10	0.52
19:R:27:LEU:HA	19:R:34:VAL:HG22	1.92	0.52
1:X:1492:G:N2	1:X:1508:C:C4	2.78	0.52
1:X:2250:A:H2'	1:X:2251:G:O4'	2.10	0.52
2:Y:4:G:H1	2:Y:111:A:H62	1.57	0.52
1:X:1469:G:OP2	1:X:1469:G:H8	1.93	0.51
1:X:1627:G:H2'	1:X:1628:A:H5''	1.91	0.51
1:X:1760:G:N1	1:X:1761:G:O6	2.42	0.51
1:X:214:G:OP1	25:2:26:LYS:NZ	2.42	0.51
1:X:387:G:N2	1:X:388:A:N7	2.57	0.51
1:X:572:C:N4	1:X:2806:U:OP2	2.43	0.51
1:X:580:C:O3'	15:N:53:ARG:NH1	2.42	0.51
1:X:956:A:H2'	11:J:9:TYR:OH	2.10	0.51
12:K:8:ARG:O	12:K:13:ARG:NH1	2.43	0.51
1:X:1053:A:O4'	15:N:59:LYS:HG2	2.10	0.51
16:O:2:PHE:HB3	16:O:42:GLY:H	1.76	0.51
17:P:57:ASN:O	17:P:61:ASN:HB2	2.11	0.51
1:X:1269:A:H2'	1:X:1270:U:C6	2.46	0.51
1:X:1636:U:H2'	1:X:1637:A:C8	2.45	0.51
1:X:1400:C:O2'	1:X:1836:A:H1'	2.09	0.51
1:X:1848:A:H2'	1:X:1849:G:C8	2.44	0.51
1:X:2446:U:H2'	1:X:2447:C:H6	1.74	0.51
1:X:339:A:H2'	1:X:340:C:C6	2.44	0.51
1:X:1916:A:H1'	1:X:2114:G:H5'	1.92	0.51
1:X:321:U:H1'	1:X:322:A:H5''	1.93	0.51
1:X:785:C:H42	1:X:802:G:H1	1.57	0.51
3:A:169:GLY:C	3:A:171:TYR:H	2.13	0.51
12:K:27:SER:C	12:K:29:ARG:H	2.14	0.51
1:X:169:G:O2'	1:X:170:C:H6	1.93	0.51
1:X:2774:G:O6	1:X:2782:C:H5''	2.11	0.51
1:X:344:U:O2'	1:X:345:C:H5''	2.10	0.51
1:X:577:A:N3	1:X:577:A:H2'	2.25	0.51
1:X:921:C:N4	1:X:922:G:N7	2.58	0.51
8:G:59:ASN:H	8:G:128:GLY:H	1.59	0.51
20:S:60:VAL:HG23	20:S:94:ILE:HD11	1.91	0.51
1:X:1391:A:C8	1:X:1392:G:C8	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2465:U:O2'	1:X:2466:A:H5''	2.10	0.51
1:X:2620:U:H2'	1:X:2621:C:C6	2.45	0.51
1:X:659:A:O2'	1:X:660:A:P	2.68	0.51
8:G:116:GLY:HA2	8:G:119:GLN:HG3	1.90	0.51
10:I:104:ASN:OD1	10:I:104:ASN:N	2.43	0.51
20:S:132:ALA:HB3	20:S:137:ILE:CB	2.40	0.51
1:X:111:U:H5'	1:X:112:U:OP2	2.10	0.51
1:X:1933:G:N3	1:X:1933:G:H2'	2.25	0.51
1:X:2668:A:H2'	1:X:2669:G:C8	2.46	0.51
1:X:2903:A:H5'	1:X:2904:U:H5'	1.91	0.51
1:X:540:G:N3	17:P:61:ASN:ND2	2.52	0.51
10:I:64:ARG:O	10:I:93:PRO:HD2	2.11	0.51
11:J:73:PRO:HB3	11:J:93:TRP:CZ3	2.45	0.51
1:X:83:G:N2	1:X:102:A:H2	1.97	0.51
1:X:1063:U:O2'	1:X:1065:A:H2	1.93	0.51
1:X:1482:U:H2'	1:X:1483:A:C8	2.45	0.51
1:X:2892:G:H21	12:K:4:ARG:HH12	1.59	0.51
2:Y:78:C:H2'	2:Y:79:C:H5	1.75	0.51
22:V:46:VAL:O	22:V:50:ILE:HG13	2.10	0.51
1:X:82:G:N1	1:X:102:A:OP2	2.35	0.51
1:X:1313:G:OP2	1:X:1689:G:O2'	2.20	0.51
1:X:665:G:H4'	1:X:666:A:O5'	2.10	0.51
23:W:40:ASN:CB	23:W:43:ILE:H	2.18	0.51
1:X:1096:C:H42	1:X:1151:G:N2	2.09	0.51
1:X:148:U:H2'	1:X:149:U:C6	2.46	0.51
1:X:514:G:C2'	1:X:515:G:H5'	2.40	0.51
1:X:90:A:O2'	1:X:91:A:P	2.68	0.51
24:Z:30:CYS:HB3	24:Z:34:GLY:HA3	1.93	0.51
5:C:171:PRO:HB2	5:C:173:VAL:HG12	1.92	0.51
1:X:2470:C:H2'	1:X:2471:G:H8	1.77	0.51
1:X:87:U:H5''	1:X:88:G:H5'	1.93	0.51
5:C:6:VAL:HG13	5:C:15:GLY:CA	2.41	0.50
23:W:11:SER:OG	23:W:13:ILE:HG13	2.09	0.50
1:X:1843:U:H3'	1:X:1843:U:H6	1.76	0.50
1:X:1909:C:H2'	1:X:1910:G:O4'	2.11	0.50
1:X:2051:C:H2'	1:X:2052:C:C6	2.45	0.50
1:X:2253:C:H2'	1:X:2254:A:O4'	2.11	0.50
1:X:296:G:H5'	1:X:297:G:OP2	2.10	0.50
1:X:304:G:N2	1:X:414:C:C2	2.79	0.50
1:X:43:A:H2'	1:X:44:A:O4'	2.11	0.50
8:G:24:GLN:O	8:G:63:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:117:LEU:H	9:H:117:LEU:HD12	1.75	0.50
1:X:183:A:H5'	1:X:481:C:H1'	1.94	0.50
3:A:107:PRO:CA	3:A:195:VAL:HA	2.40	0.50
3:A:77:LYS:HA	3:A:93:LEU:HA	1.94	0.50
10:I:125:ALA:O	10:I:126:HIS:ND1	2.44	0.50
11:J:110:SER:HB3	11:J:113:VAL:HG23	1.94	0.50
17:P:9:THR:HG23	17:P:102:HIS:HE1	1.77	0.50
18:Q:43:GLU:OE2	18:Q:49:LYS:HA	2.11	0.50
1:X:1303:A:H2	1:X:2041:A:N6	1.99	0.50
1:X:1830:A:H3'	1:X:1831:A:H8	1.76	0.50
1:X:2511:G:OP1	11:J:45:ARG:HD3	2.12	0.50
4:B:33:ASN:HB3	4:B:105:VAL:CG1	2.41	0.50
7:E:120:ASN:OD1	7:E:121:ILE:N	2.42	0.50
17:P:1:MET:HG2	17:P:2:GLU:OE2	2.11	0.50
1:X:1356:G:C5	1:X:1357:G:C6	2.99	0.50
1:X:1463:A:H3'	1:X:1464:U:H5''	1.92	0.50
1:X:1508:C:O2'	1:X:1509:G:O5'	2.29	0.50
1:X:1770:C:H1'	1:X:1771:A:H5'	1.92	0.50
1:X:1708:A:H61	1:X:2023:C:N4	2.09	0.50
1:X:281:A:H2'	1:X:282:A:O4'	2.10	0.50
1:X:731:U:O5'	25:2:12:LYS:NZ	2.45	0.50
4:B:140:PRO:HG2	4:B:145:SER:HB2	1.92	0.50
1:X:322:A:H2'	1:X:323:C:O4'	2.12	0.50
1:X:793:G:H2'	1:X:795:A:N7	2.26	0.50
24:Z:39:LEU:HB2	24:Z:42:ARG:HD2	1.92	0.50
5:C:64:PRO:HG3	5:C:78:ILE:HG23	1.93	0.50
12:K:55:ASP:OD1	12:K:58:SER:OG	2.22	0.50
15:N:61:TRP:O	15:N:65:ILE:HG12	2.10	0.50
1:X:1245:G:C2	1:X:1278:G:C2	3.00	0.50
1:X:1550:G:O2'	1:X:1554:A:H2	1.92	0.50
1:X:2338:A:H3'	1:X:2339:U:C6	2.47	0.50
1:X:563:G:H2'	1:X:564:U:C6	2.46	0.50
1:X:813:G:H2'	1:X:814:A:C8	2.47	0.50
13:L:39:HIS:CD2	13:L:58:SER:HB2	2.47	0.50
1:X:1144:C:H5''	1:X:1145:U:OP2	2.12	0.50
1:X:1346:G:H4'	25:2:8:PRO:HG2	1.93	0.50
1:X:2244:G:C2	1:X:2245:G:C8	3.00	0.50
3:A:212:ARG:HH11	3:A:216:ILE:HB	1.77	0.50
4:B:39:LYS:O	4:B:47:ASN:HA	2.11	0.50
15:N:19:LYS:HE3	15:N:19:LYS:HA	1.94	0.50
1:X:623:C:O3'	15:N:31:LEU:HD13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:24:LYS:HA	16:O:93:THR:OG1	2.11	0.50
1:X:1049:C:H1'	1:X:1056:U:C4	2.46	0.50
1:X:1513:A:H2'	1:X:1514:A:O4'	2.12	0.50
1:X:1761:G:H21	1:X:1762:U:H1'	1.76	0.50
1:X:2341:A:H2'	1:X:2342:U:C6	2.47	0.50
6:D:35:VAL:HG22	6:D:90:THR:HG23	1.94	0.50
6:D:44:VAL:HB	6:D:46:ASN:H	1.76	0.50
9:H:71:ARG:NH2	9:H:104:ARG:HG3	2.26	0.50
20:S:73:MET:HG3	20:S:94:ILE:HD13	1.94	0.50
1:X:1244:G:N2	1:X:1278:G:H22	2.10	0.50
1:X:1543:G:N7	1:X:1544:G:C2	2.80	0.50
1:X:2220:U:H2'	1:X:2221:U:C6	2.47	0.50
1:X:344:U:HO2'	1:X:345:C:H6	1.59	0.50
6:D:114:PHE:CB	6:D:176:PRO:HB2	2.41	0.49
17:P:67:ASP:N	17:P:67:ASP:OD1	2.45	0.49
20:S:45:GLU:HG2	20:S:49:ILE:HD11	1.94	0.49
1:X:345:C:H2'	1:X:346:A:C8	2.46	0.49
3:A:239:ALA:N	3:A:240:PRO:HD3	2.27	0.49
19:R:70:LEU:HA	19:R:76:ASN:HA	1.94	0.49
1:X:1275:A:H2'	1:X:1276:G:O4'	2.11	0.49
1:X:2817:A:O2'	1:X:2818:A:OP2	2.28	0.49
15:N:27:SER:HB2	15:N:31:LEU:HG	1.94	0.49
19:R:12:ILE:CG2	19:R:18:GLY:HA2	2.42	0.49
23:W:40:ASN:O	23:W:44:ARG:HB2	2.13	0.49
1:X:1250:G:O2'	1:X:1274:G:N2	2.35	0.49
1:X:1732:U:H2'	1:X:1742:A:N6	2.27	0.49
1:X:989:A:C4	1:X:2475:A:C2	3.00	0.49
1:X:2642:U:C2	24:Z:4:PRO:HA	2.47	0.49
1:X:305:A:H61	1:X:411:A:H62	1.60	0.49
1:X:389:A:H2'	1:X:390:A:O4'	2.12	0.49
1:X:646:A:C8	1:X:700:A:C6	3.00	0.49
4:B:115:VAL:HG23	4:B:182:ASN:HA	1.93	0.49
1:X:1491:C:O2	1:X:1492:G:N2	2.45	0.49
1:X:153:G:O2'	1:X:154:A:OP2	2.28	0.49
1:X:1303:A:N6	1:X:2040:A:H5''	2.26	0.49
1:X:2352:G:H8	1:X:2352:G:O5'	1.95	0.49
1:X:338:G:H1	1:X:386:C:H42	1.60	0.49
1:X:811:C:H2'	1:X:812:U:H5'	1.94	0.49
2:Y:55:A:H5'	6:D:23:SER:OG	2.12	0.49
5:C:158:ASN:C	5:C:160:ASP:H	2.14	0.49
8:G:115:LEU:O	8:G:119:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:88:ARG:O	9:H:89:ASP:HB2	2.13	0.49
10:I:116:SER:HB2	10:I:126:HIS:NE2	2.28	0.49
15:N:36:LYS:HG2	15:N:40:MET:HE2	1.95	0.49
1:X:1306:A:H2'	1:X:1307:G:O4'	2.13	0.49
1:X:1700:C:H2'	1:X:1701:U:H6	1.77	0.49
1:X:1762:U:H5'	1:X:1763:U:OP2	2.12	0.49
1:X:2299:U:H5''	1:X:2300:A:OP1	2.13	0.49
1:X:2342:U:O3'	13:L:3:SER:N	2.46	0.49
1:X:955:A:N7	1:X:956:A:C6	2.81	0.49
20:S:27:VAL:HG13	20:S:43:VAL:HG23	1.93	0.49
1:X:1072:A:H1'	1:X:2514:G:H5'	1.94	0.49
1:X:119:U:HO2'	1:X:120:G:P	2.35	0.49
1:X:1423:C:O2'	1:X:1512:U:H1'	2.13	0.49
1:X:1505:G:C8	1:X:1506:C:C5	3.00	0.49
1:X:1680:U:H2'	1:X:1681:U:C6	2.48	0.49
1:X:170:C:H2'	1:X:171:A:C8	2.47	0.49
1:X:591:A:H4'	1:X:592:A:C5'	2.43	0.49
1:X:786:U:H2'	1:X:787:U:O4'	2.13	0.49
3:A:223:SER:HA	3:A:232:HIS:HB2	1.95	0.49
4:B:104:GLU:H	4:B:104:GLU:CD	2.16	0.49
1:X:1424:A:H2'	1:X:1425:G:C8	2.47	0.49
1:X:189:G:H2'	1:X:190:G:C8	2.48	0.49
1:X:2848:G:C2	1:X:2849:A:N7	2.81	0.49
1:X:506:A:H5'	1:X:507:C:H5	1.77	0.49
12:K:29:ARG:HB3	12:K:120:GLU:HB3	1.94	0.49
20:S:135:ASP:O	20:S:137:ILE:N	2.46	0.49
23:W:44:ARG:HA	23:W:47:ILE:HD12	1.93	0.49
1:X:1151:G:H2'	1:X:1151:G:N3	2.27	0.49
1:X:1543:G:N7	1:X:1544:G:N1	2.61	0.49
1:X:2314:A:O2'	1:X:2315:A:H3'	2.12	0.49
1:X:372:A:H62	19:R:15:LYS:HG2	1.77	0.49
1:X:753:U:H3	1:X:768:A:H61	1.60	0.49
4:B:38:LYS:HZ1	4:B:97:ASP:HA	1.76	0.49
6:D:162:THR:HB	6:D:165:GLU:H	1.78	0.49
1:X:1245:G:C2	1:X:1246:C:C5	3.00	0.49
1:X:2241:C:H2'	1:X:2242:G:O4'	2.12	0.49
1:X:463:C:H2'	1:X:464:U:C6	2.48	0.49
1:X:876:G:H22	10:I:46:VAL:HG11	1.76	0.49
5:C:53:ASN:CB	5:C:87:GLY:HA2	2.43	0.49
5:C:93:THR:HB	5:C:94:PRO:HD2	1.95	0.49
15:N:94:MET:HE3	16:O:12:ILE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1781:C:H2'	1:X:1782:A:C8	2.47	0.49
1:X:2912:A:H4'	1:X:2913:G:O4'	2.13	0.49
22:V:44:ARG:O	22:V:48:LYS:HG3	2.12	0.48
1:X:2231:C:O2'	1:X:2232:A:H8	1.96	0.48
1:X:323:C:O2	1:X:323:C:H2'	2.13	0.48
1:X:631:U:H2'	1:X:632:U:C6	2.48	0.48
1:X:685:C:H2'	1:X:686:U:C6	2.48	0.48
2:Y:14:G:C6	2:Y:67:G:C2	3.01	0.48
1:X:1352:C:H2'	1:X:1353:A:C8	2.48	0.48
1:X:1746:G:C2'	1:X:1747:G:H8	2.27	0.48
1:X:2232:A:H5'	1:X:2233:C:P	2.53	0.48
1:X:683:G:N2	1:X:697:U:C6	2.77	0.48
3:A:123:ASP:OD2	3:A:124:ILE:HG13	2.13	0.48
3:A:26:LYS:HE3	3:A:26:LYS:HB2	1.60	0.48
9:H:68:GLY:O	9:H:69:VAL:HG23	2.12	0.48
1:X:2901:U:O2'	12:K:101:THR:O	2.29	0.48
15:N:48:ARG:HD2	15:N:49:ASP:OD1	2.12	0.48
22:V:49:THR:O	22:V:53:LEU:HG	2.13	0.48
6:D:29:PRO:HB2	6:D:169:LEU:HD12	1.95	0.48
20:S:6:SER:HB3	20:S:43:VAL:HG12	1.95	0.48
1:X:1452:C:N4	1:X:1458:A:OP1	2.44	0.48
1:X:1887:G:H2'	1:X:1888:U:C6	2.48	0.48
1:X:2581:U:H2'	1:X:2582:U:C6	2.48	0.48
1:X:1754:C:HO2'	1:X:2878:U:H3	1.60	0.48
1:X:896:U:H4'	23:W:46:GLN:HA	1.95	0.48
5:C:12:THR:O	5:C:13:LYS:HD2	2.12	0.48
1:X:1039:C:C6	8:G:1:MET:HG2	2.48	0.48
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.95	0.48
18:Q:25:TYR:CE2	18:Q:82:LEU:HD11	2.48	0.48
1:X:1015:C:H2'	1:X:1016:G:O4'	2.13	0.48
1:X:1016:G:H3'	1:X:1017:A:H5''	1.95	0.48
1:X:1494:G:N7	1:X:1495:C:H5	2.11	0.48
1:X:280:C:H2'	1:X:281:A:H8	1.77	0.48
1:X:1498:U:O2'	1:X:1499:U:H5	1.95	0.48
1:X:1805:U:H2'	1:X:1811:A:N6	2.27	0.48
1:X:2731:C:H2'	1:X:2732:A:O4'	2.13	0.48
11:J:35:GLN:HB3	11:J:130:LYS:HB3	1.96	0.48
17:P:21:LEU:HD22	17:P:74:ALA:HB1	1.96	0.48
1:X:1337:A:H4'	1:X:1338:U:H5''	1.95	0.48
1:X:1955:A:C8	1:X:1956:G:H1'	2.49	0.48
1:X:525:A:N3	1:X:527:G:H5''	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:27:ASN:O	25:2:31:VAL:N	2.44	0.48
5:C:9:LEU:CB	5:C:12:THR:HB	2.44	0.48
10:I:41:ARG:O	10:I:42:SER:OG	2.30	0.48
1:X:1023:A:H2'	1:X:1026:C:H42	1.79	0.48
1:X:2268:A:H2'	1:X:2269:G:C8	2.49	0.48
1:X:235:G:H4'	1:X:236:A:OP1	2.12	0.48
1:X:502:C:O2'	1:X:503:A:O5'	2.30	0.48
1:X:810:A:H2'	1:X:811:C:H6	1.78	0.48
1:X:923:A:N6	1:X:946:A:N7	2.61	0.48
1:X:888:G:N2	1:X:980:U:C2	2.82	0.48
2:Y:3:U:H3	2:Y:112:G:H1	1.60	0.48
4:B:133:ARG:HA	4:B:173:MET:SD	2.53	0.48
18:Q:31:THR:C	18:Q:33:VAL:H	2.17	0.48
1:X:1151:G:N2	1:X:1152:U:O4	2.47	0.48
1:X:2308:C:O2'	1:X:2309:G:H5'	2.13	0.48
1:X:2331:G:N2	1:X:2339:U:H3	2.12	0.48
1:X:2391:C:H5'	21:T:64:ASP:HB2	1.94	0.48
1:X:323:C:H5'	1:X:324:A:N7	2.28	0.48
1:X:3:U:H2'	1:X:4:U:C6	2.48	0.48
3:A:46:GLN:OE1	3:A:47:GLY:N	2.47	0.48
11:J:15:PRO:HG3	11:J:72:THR:HG21	1.95	0.48
17:P:50:VAL:HB	17:P:105:ILE:HD11	1.96	0.48
20:S:156:VAL:N	20:S:173:GLU:O	2.47	0.48
1:X:1070:A:H1'	1:X:1178:C:H41	1.79	0.48
1:X:1289:A:H5''	15:N:13:ARG:HH12	1.79	0.48
1:X:1313:G:H2'	1:X:1314:A:H8	1.79	0.48
1:X:1436:C:O2'	1:X:1437:U:P	2.72	0.48
1:X:187:C:H2'	1:X:188:C:C6	2.49	0.48
1:X:1978:U:H2'	1:X:1980:A:OP2	2.14	0.48
1:X:2331:G:H22	1:X:2339:U:H3	1.62	0.48
1:X:2342:U:H2'	1:X:2343:U:C6	2.49	0.48
1:X:2801:C:H2'	1:X:2802:A:O4'	2.14	0.48
1:X:323:C:H5'	1:X:324:A:H8	1.77	0.48
7:E:90:VAL:O	7:E:92:VAL:N	2.46	0.47
9:H:25:LEU:HA	9:H:25:LEU:HD23	1.76	0.47
14:M:65:LYS:HD2	14:M:66:ILE:H	1.79	0.47
14:M:74:ARG:HG2	14:M:76:PHE:CE2	2.48	0.47
15:N:16:LYS:O	15:N:20:LEU:HG	2.14	0.47
18:Q:57:ASN:HB3	18:Q:76:ARG:HD3	1.96	0.47
1:X:118:A:H4'	1:X:119:U:H5'	1.95	0.47
1:X:1504:U:O2	1:X:1505:G:N2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2320:C:H2'	1:X:2321:C:O4'	2.13	0.47
1:X:945:A:H2'	1:X:946:A:H5'	1.96	0.47
9:H:63:VAL:HG13	9:H:102:VAL:HG13	1.95	0.47
1:X:1055:A:OP1	15:N:75:SER:HB2	2.13	0.47
1:X:1270:U:H2'	1:X:1271:G:C8	2.49	0.47
1:X:1511:C:H5'	1:X:1512:U:OP1	2.15	0.47
1:X:2820:U:H1'	1:X:2824:G:N2	2.29	0.47
1:X:483:C:H2'	1:X:484:U:C6	2.49	0.47
1:X:525:A:H4'	1:X:526:A:OP1	2.14	0.47
1:X:889:U:C2'	1:X:890:G:H5'	2.44	0.47
1:X:938:G:H5'	1:X:939:U:OP2	2.13	0.47
24:Z:30:CYS:CB	24:Z:34:GLY:HA3	2.44	0.47
6:D:33:LYS:HE2	6:D:92:ARG:HH12	1.79	0.47
14:M:52:ARG:HA	14:M:60:THR:O	2.14	0.47
19:R:9:VAL:HG22	19:R:23:VAL:HG22	1.95	0.47
20:S:111:GLU:O	20:S:146:THR:HA	2.15	0.47
1:X:1323:A:HO2'	1:X:1325:U:P	2.31	0.47
1:X:1466:G:C6	1:X:1467:G:C8	3.02	0.47
1:X:1508:C:H1'	1:X:1593:G:H22	1.79	0.47
1:X:1775:G:H2'	1:X:1776:A:C8	2.49	0.47
1:X:2873:C:H42	1:X:2884:G:H1	1.63	0.47
5:C:184:LEU:HA	5:C:184:LEU:HD23	1.81	0.47
6:D:33:LYS:HG3	6:D:157:VAL:HG21	1.96	0.47
15:N:19:LYS:HE3	15:N:22:LYS:HE3	1.96	0.47
1:X:1353:A:H2'	1:X:1354:G:H8	1.79	0.47
1:X:1990:C:H4'	1:X:1991:G:OP1	2.13	0.47
1:X:2736:G:H2'	1:X:2737:C:C6	2.49	0.47
1:X:378:C:H2'	1:X:379:C:C6	2.45	0.47
1:X:381:G:N2	1:X:382:U:H1'	2.29	0.47
1:X:499:A:N3	1:X:503:A:O2'	2.42	0.47
1:X:725:A:H2'	1:X:726:G:C8	2.49	0.47
1:X:77:U:H2'	1:X:78:U:C6	2.49	0.47
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.95	0.47
10:I:66:PHE:O	10:I:94:ALA:HA	2.15	0.47
22:V:58:ARG:HA	22:V:61:GLU:HB3	1.96	0.47
1:X:1490:G:O2'	1:X:1491:C:O4'	2.24	0.47
1:X:1554:A:H2'	1:X:1555:G:C5	2.50	0.47
1:X:1874:A:O2'	1:X:1875:A:N7	2.47	0.47
1:X:2221:U:H2'	1:X:2222:U:O4'	2.14	0.47
1:X:2672:G:O6	32:X:3286:SPD:H32	2.14	0.47
1:X:770:G:C6	1:X:771:G:N1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:12:U:OP2	2:Y:68:A:O2'	2.21	0.47
8:G:25:THR:HB	8:G:28:ARG:HG3	1.95	0.47
14:M:94:VAL:HG21	14:M:99:LEU:HD21	1.96	0.47
1:X:1562:C:H2'	1:X:1563:U:C6	2.50	0.47
1:X:619:U:H2'	1:X:620:G:C8	2.50	0.47
4:B:134:HIS:ND1	4:B:168:LYS:HB3	2.30	0.47
5:C:150:LYS:HA	5:C:187:THR:O	2.14	0.47
1:X:2732:A:H2'	1:X:2733:A:O4'	2.13	0.47
1:X:2874:A:O5'	1:X:2874:A:H8	1.98	0.47
1:X:124:A:C5'	25:2:20:ARG:HD3	2.37	0.47
16:O:50:ALA:HB1	16:O:51:PRO:HD2	1.97	0.47
22:V:22:LYS:HE2	22:V:22:LYS:HB3	1.60	0.47
1:X:1398:G:N3	1:X:1398:G:H2'	2.30	0.47
1:X:329:A:N3	1:X:329:A:H2'	2.29	0.47
1:X:778:G:C6	1:X:806:A:C5	3.03	0.47
4:B:62:ASP:OD1	4:B:62:ASP:N	2.48	0.47
1:X:1186:A:C4	1:X:1188:A:C8	3.03	0.47
1:X:1379:A:C6	1:X:1382:C:N3	2.82	0.47
1:X:1514:A:H3'	1:X:1515:G:C8	2.39	0.47
1:X:24:G:H2'	1:X:25:U:C6	2.50	0.47
2:Y:53:U:O2'	6:D:26:MET:HG2	2.14	0.47
1:X:1381:U:O2'	1:X:1421:A:H2'	2.14	0.47
1:X:1760:G:C2	1:X:1761:G:N7	2.83	0.47
1:X:2775:A:H2'	1:X:2776:A:C8	2.50	0.47
1:X:33:U:O2'	1:X:34:U:H5''	2.15	0.47
5:C:11:GLY:HA2	5:C:142:VAL:CG1	2.45	0.47
12:K:45:GLU:O	12:K:49:THR:HG23	2.15	0.47
15:N:50:ARG:HG2	15:N:53:ARG:NH2	2.30	0.47
1:X:1145:U:O2'	1:X:1146:C:H5''	2.15	0.47
1:X:1286:G:N2	5:C:88:ILE:HG21	2.30	0.47
1:X:1528:G:H1	1:X:1545:U:H3	1.62	0.47
1:X:168:A:C3'	1:X:169:G:H5'	2.45	0.47
1:X:1740:G:C6	1:X:1741:G:C4	3.03	0.47
1:X:2021:C:H2'	1:X:2021:C:O2	2.14	0.47
1:X:2347:A:N3	1:X:2347:A:H2'	2.29	0.47
1:X:2367:A:H2'	1:X:2368:G:H8	1.80	0.47
1:X:250:G:H4'	1:X:432:G:C5	2.50	0.47
1:X:2603:G:H5''	1:X:2604:A:OP1	2.15	0.47
1:X:2671:A:H62	32:X:3286:SPD:H52	1.80	0.47
1:X:1385:G:C2	1:X:1643:C:C2	3.03	0.46
1:X:1392:G:H2'	1:X:1393:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2623:U:H2'	1:X:2624:G:O4'	2.15	0.46
1:X:364:A:H5''	5:C:159:GLU:HB3	1.98	0.46
1:X:365:A:H5'	1:X:383:A:H1'	1.95	0.46
1:X:384:G:C6	1:X:385:U:C4	3.02	0.46
1:X:474:A:OP2	1:X:474:A:H8	1.98	0.46
1:X:506:A:H5'	1:X:507:C:C5	2.50	0.46
14:M:24:PRO:HA	14:M:49:VAL:HB	1.96	0.46
16:O:33:PHE:CD1	16:O:34:THR:N	2.83	0.46
18:Q:89:LEU:HB3	18:Q:91:ASN:H	1.79	0.46
1:X:119:U:O2'	1:X:120:G:P	2.74	0.46
1:X:1528:G:N2	1:X:1545:U:H3	2.11	0.46
1:X:562:C:O2'	17:P:18:ARG:NH2	2.47	0.46
1:X:757:G:N3	1:X:757:G:H2'	2.29	0.46
3:A:90:ASN:HA	3:A:106:ALA:H	1.81	0.46
1:X:1699:A:H1'	4:B:127:PHE:CE1	2.50	0.46
5:C:149:PRO:HD2	5:C:186:ILE:HA	1.97	0.46
10:I:91:VAL:HG12	10:I:92:THR:H	1.79	0.46
14:M:31:HIS:HB3	14:M:83:ILE:HD12	1.95	0.46
1:X:1040:A:H4'	15:N:91:ASN:ND2	2.31	0.46
16:O:67:ARG:HA	16:O:91:PRO:HA	1.96	0.46
17:P:36:LEU:HA	17:P:36:LEU:HD23	1.66	0.46
1:X:2229:C:H5'	1:X:2230:G:OP1	2.15	0.46
1:X:2349:A:H2'	1:X:2350:G:O4'	2.16	0.46
1:X:247:A:H5''	1:X:248:G:OP2	2.15	0.46
1:X:2591:A:C6	1:X:2592:A:N1	2.83	0.46
1:X:666:A:H3'	1:X:667:G:H8	1.80	0.46
4:B:194:VAL:HG12	4:B:195:ILE:N	2.31	0.46
15:N:58:ARG:HA	15:N:61:TRP:CE3	2.50	0.46
16:O:3:ALA:HA	16:O:40:PHE:O	2.16	0.46
1:X:164:A:H1'	1:X:165:C:H5'	1.97	0.46
1:X:177:G:O2'	1:X:178:A:H5'	2.15	0.46
1:X:1501:G:N2	1:X:2729:G:H22	2.03	0.46
1:X:506:A:H3'	1:X:507:C:H6	1.81	0.46
1:X:1658:A:C2	17:P:93:ALA:HB2	2.51	0.46
1:X:1084:U:H2'	1:X:1085:U:O4'	2.15	0.46
1:X:1159:A:H2'	1:X:1160:C:O4'	2.15	0.46
1:X:1318:G:N2	1:X:1327:C:C2	2.84	0.46
1:X:1333:A:H2'	1:X:1334:C:C6	2.50	0.46
1:X:1364:C:H2'	1:X:1365:G:O4'	2.15	0.46
1:X:1423:C:H2'	1:X:1424:A:H8	1.80	0.46
1:X:437:A:O2'	1:X:456:G:OP1	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:922:G:N2	1:X:924:G:H5''	2.31	0.46
5:C:4:TYR:HD2	5:C:19:LEU:HA	1.79	0.46
7:E:89:LEU:HD13	7:E:89:LEU:HA	1.77	0.46
1:X:909:G:OP2	11:J:22:LYS:HE2	2.15	0.46
13:L:31:LEU:HA	13:L:44:ILE:HD13	1.96	0.46
22:V:6:ILE:O	22:V:9:LEU:HD22	2.15	0.46
1:X:1072:A:N3	1:X:2513:G:O2'	2.42	0.46
1:X:1092:A:O2'	1:X:1093:C:O4'	2.33	0.46
1:X:1400:C:HO2'	1:X:1836:A:H1'	1.79	0.46
2:Y:22:G:O5'	2:Y:22:G:H8	1.99	0.46
2:Y:58:G:O5'	2:Y:58:G:H8	1.99	0.46
17:P:36:LEU:HD11	17:P:47:ILE:HG22	1.98	0.46
1:X:1484:G:C2	1:X:1599:G:N2	2.84	0.46
1:X:1563:U:C2'	1:X:1564:G:H8	2.28	0.46
1:X:1697:G:C6	12:K:6:LEU:HD12	2.51	0.46
1:X:2005:A:H2'	1:X:2006:C:O4'	2.15	0.46
1:X:2124:U:H3	1:X:2219:C:H42	1.64	0.46
1:X:2314:A:O2'	1:X:2315:A:P	2.73	0.46
1:X:568:C:O2	1:X:597:U:O2'	2.30	0.46
3:A:116:VAL:HA	3:A:128:ASN:HA	1.98	0.46
3:A:174:ILE:O	3:A:181:VAL:HG13	2.16	0.46
4:B:116:ILE:HG12	4:B:183:LEU:O	2.15	0.46
5:C:171:PRO:O	5:C:173:VAL:N	2.45	0.46
12:K:38:LYS:HB3	12:K:41:ARG:HH21	1.81	0.46
15:N:94:MET:O	15:N:98:ILE:HG13	2.16	0.46
1:X:1044:A:H2'	1:X:1045:A:C8	2.51	0.46
1:X:1233:A:H2'	1:X:1234:G:O4'	2.16	0.46
1:X:1644:C:N4	1:X:1645:G:O6	2.49	0.46
1:X:1847:U:C4	3:A:159:GLY:HA3	2.50	0.46
1:X:2072:C:H5''	24:Z:15:LYS:HD2	1.97	0.46
1:X:2776:A:H1'	7:E:64:ASN:CB	2.45	0.46
1:X:592:A:O2'	1:X:593:U:O5'	2.34	0.46
3:A:31:LYS:NZ	3:A:32:SER:HA	2.31	0.46
5:C:12:THR:HG22	5:C:13:LYS:N	2.30	0.46
1:X:631:U:H1'	5:C:90:PHE:CD1	2.51	0.46
6:D:33:LYS:NZ	6:D:92:ARG:HH22	2.14	0.46
12:K:52:LYS:HE3	12:K:94:THR:HA	1.97	0.46
1:X:139:U:O2'	1:X:140:A:H8	1.98	0.46
1:X:1508:C:N3	1:X:1509:G:N1	2.63	0.46
1:X:15:G:O2'	24:Z:18:THR:HG21	2.15	0.46
1:X:2876:G:N1	1:X:2877:G:C8	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:695:C:N3	1:X:696:G:C6	2.83	0.46
1:X:921:C:H5	1:X:942:C:H41	1.63	0.46
3:A:76:ALA:HB1	3:A:112:VAL:O	2.16	0.46
5:C:39:LEU:HD11	5:C:99:TYR:O	2.15	0.46
2:Y:40:C:H6	6:D:66:LEU:HD12	1.81	0.46
17:P:24:ILE:HD12	17:P:24:ILE:HA	1.80	0.46
1:X:1400:C:N4	1:X:1405:G:H1	2.14	0.46
1:X:1644:C:P	18:Q:76:ARG:HH12	2.39	0.46
1:X:2377:C:H2'	1:X:2378:G:O4'	2.16	0.46
1:X:2725:U:H2'	1:X:2726:C:C6	2.51	0.46
2:Y:21:G:H2'	2:Y:22:G:C8	2.51	0.46
8:G:56:ILE:HG21	8:G:130:GLU:HG2	1.98	0.45
14:M:65:LYS:CD	14:M:66:ILE:H	2.28	0.45
15:N:22:LYS:CE	15:N:22:LYS:HA	2.46	0.45
22:V:10:THR:OG1	22:V:13:GLU:HG3	2.16	0.45
1:X:1708:A:N6	1:X:2023:C:H42	2.13	0.45
1:X:1884:G:O2'	1:X:1912:A:N6	2.50	0.45
1:X:1994:C:H2'	1:X:1995:G:H5'	1.97	0.45
1:X:242:U:H2'	1:X:243:U:C6	2.51	0.45
1:X:769:U:H2'	1:X:770:G:O4'	2.16	0.45
3:A:65:ILE:HA	3:A:65:ILE:HD12	1.71	0.45
5:C:129:PHE:CG	5:C:130:ASN:N	2.84	0.45
11:J:41:TRP:CE3	11:J:94:ILE:HG21	2.50	0.45
19:R:41:MET:HA	19:R:60:GLU:HB2	1.98	0.45
1:X:1515:G:HO2'	1:X:1516:C:P	2.39	0.45
1:X:1612:C:C4	1:X:1614:A:C2	3.04	0.45
1:X:460:C:H5''	1:X:1906:C:O2'	2.15	0.45
1:X:1008:C:O2'	1:X:2300:A:N3	2.42	0.45
1:X:2507:C:H2'	1:X:2508:G:H5'	1.98	0.45
1:X:489:A:OP1	5:C:45:ARG:HB2	2.16	0.45
1:X:755:C:N4	1:X:766:G:H1	2.11	0.45
1:X:948:U:H2'	1:X:949:C:C6	2.50	0.45
9:H:16:ALA:HB3	9:H:86:ILE:HD11	1.99	0.45
12:K:48:ILE:O	12:K:52:LYS:HG3	2.16	0.45
16:O:14:VAL:HG13	16:O:97:ILE:HG13	1.99	0.45
1:X:1643:C:P	18:Q:35:LYS:HG3	2.56	0.45
1:X:1488:A:N1	1:X:1596:G:C2	2.84	0.45
1:X:2082:C:H2'	1:X:2531:U:H4'	1.99	0.45
1:X:300:G:N2	1:X:302:A:N6	2.65	0.45
1:X:519:G:O2'	1:X:520:G:H5'	2.17	0.45
1:X:554:C:H5''	1:X:554:C:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:797:A:N6	1:X:2636:U:H3	2.14	0.45
4:B:131:ILE:HD11	4:B:149:ARG:NH2	2.31	0.45
13:L:19:ARG:CZ	13:L:45:ILE:HD11	2.46	0.45
1:X:1452:C:O2'	1:X:1631:G:N2	2.49	0.45
1:X:1876:G:H2'	1:X:1877:G:H8	1.81	0.45
1:X:619:U:H4'	1:X:2529:G:C8	2.52	0.45
1:X:657:U:C4	1:X:659:A:N6	2.84	0.45
1:X:650:U:N3	1:X:666:A:C2	2.79	0.45
1:X:720:A:O2'	1:X:721:A:H5'	2.17	0.45
3:A:141:VAL:HG13	3:A:190:ALA:HB1	1.99	0.45
1:X:106:A:H2'	1:X:107:G:H8	1.82	0.45
1:X:1378:U:OP2	1:X:1431:U:O2'	2.32	0.45
1:X:1494:G:N2	1:X:1505:G:C8	2.82	0.45
1:X:1838:G:O5'	1:X:1838:G:H8	1.98	0.45
1:X:1933:G:C2	1:X:1952:C:C4	3.05	0.45
1:X:1983:U:H1'	1:X:2579:U:OP1	2.16	0.45
1:X:305:A:C2	1:X:413:C:C2	3.04	0.45
1:X:683:G:C2	1:X:696:G:C4	3.05	0.45
1:X:805:G:H2'	1:X:806:A:O4'	2.15	0.45
1:X:946:A:C2'	1:X:947:U:H5'	2.46	0.45
2:Y:40:C:C6	6:D:66:LEU:HD12	2.52	0.45
9:H:50:GLY:O	9:H:53:LYS:NZ	2.37	0.45
1:X:1449:A:H4'	1:X:1450:A:OP1	2.15	0.45
1:X:1998:A:O2'	1:X:1999:G:OP1	2.33	0.45
1:X:2048:G:N3	1:X:2048:G:H2'	2.32	0.45
1:X:2319:U:H2'	1:X:2320:C:C6	2.52	0.45
1:X:2367:A:H2'	1:X:2368:G:C8	2.51	0.45
1:X:267:G:H2'	1:X:268:A:H5''	1.99	0.45
1:X:361:U:H2'	1:X:362:C:C6	2.47	0.45
1:X:937:G:C2	1:X:938:G:H4'	2.52	0.45
2:Y:94:U:C5	2:Y:95:A:C5	3.05	0.45
25:2:22:ARG:O	25:2:28:GLY:HA3	2.17	0.45
8:G:142:GLU:N	8:G:142:GLU:OE1	2.50	0.45
1:X:2385:A:H61	10:I:47:ARG:NH2	2.15	0.45
14:M:31:HIS:ND1	14:M:43:GLN:O	2.49	0.45
1:X:1290:G:N3	15:N:33:LYS:HG2	2.32	0.45
19:R:15:LYS:HG2	19:R:16:ASP:H	1.82	0.45
20:S:101:THR:HA	20:S:130:VAL:O	2.17	0.45
1:X:1272:U:H2'	1:X:1273:G:O4'	2.17	0.45
1:X:139:U:O2'	1:X:140:A:C8	2.68	0.45
1:X:2231:C:O2'	1:X:2232:A:O4'	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:442:G:O5'	1:X:442:G:H8	1.99	0.45
5:C:117:LYS:HE2	5:C:180:GLY:O	2.17	0.45
9:H:64:ARG:NH1	9:H:101:PRO:O	2.47	0.45
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.99	0.45
23:W:40:ASN:HB3	23:W:43:ILE:N	2.20	0.45
1:X:1176:U:H3'	1:X:1176:U:OP2	2.17	0.45
1:X:2003:U:H2'	1:X:2004:A:N7	2.32	0.45
1:X:2701:G:H5''	9:H:30:ARG:HE	1.81	0.45
1:X:295:G:H2'	1:X:296:G:O4'	2.17	0.45
1:X:309:U:O2'	1:X:310:C:OP2	2.31	0.45
1:X:749:G:HO2'	1:X:750:A:P	2.38	0.45
24:Z:9:SER:OG	24:Z:12:ARG:N	2.42	0.45
26:3:60:GLN:OE1	26:3:60:GLN:HA	2.17	0.45
7:E:156:PRO:CD	7:E:160:LYS:HA	2.47	0.45
12:K:109:ARG:HD2	12:K:114:ALA:HB3	1.98	0.45
17:P:10:ILE:O	17:P:12:ILE:N	2.50	0.45
19:R:84:LYS:HA	19:R:90:LYS:HA	1.99	0.45
1:X:1516:C:H2'	1:X:1517:A:H8	1.82	0.45
1:X:251:G:N7	1:X:253:G:H1'	2.32	0.45
12:K:29:ARG:HB3	12:K:120:GLU:CB	2.47	0.45
12:K:38:LYS:O	12:K:41:ARG:HB3	2.16	0.45
14:M:31:HIS:HD1	14:M:31:HIS:H	1.64	0.45
18:Q:57:ASN:ND2	18:Q:57:ASN:H	2.14	0.45
18:Q:61:LYS:N	18:Q:72:THR:HG22	2.16	0.45
23:W:47:ILE:HG23	23:W:54:VAL:HG11	1.98	0.45
1:X:2845:G:C5	1:X:2846:A:C8	3.05	0.45
1:X:2896:A:H2'	1:X:2897:A:C8	2.51	0.45
1:X:397:U:HO2'	1:X:398:C:H6	1.65	0.45
1:X:986:G:O5'	1:X:986:G:H8	2.00	0.45
2:Y:90:C:H2'	2:Y:91:C:C6	2.52	0.45
1:X:123:G:N7	25:2:20:ARG:NH2	2.65	0.44
4:B:134:HIS:CD2	4:B:168:LYS:HE2	2.51	0.44
10:I:63:LYS:HG3	10:I:91:VAL:CB	2.47	0.44
22:V:37:LEU:HD22	22:V:39:GLU:H	1.80	0.44
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.44	0.44
1:X:1356:G:O2'	1:X:1357:G:H5'	2.16	0.44
1:X:1474:C:H2'	1:X:1475:A:C8	2.52	0.44
1:X:1793:C:H2'	1:X:1794:C:H6	1.82	0.44
1:X:49:A:C5	1:X:179:A:C6	3.05	0.44
1:X:2418:G:C6	1:X:2454:C:H1'	2.53	0.44
1:X:498:G:C6	1:X:499:A:C6	3.04	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:141:VAL:CG1	3:A:190:ALA:HB1	2.47	0.44
1:X:1438:G:H2'	1:X:1439:U:O4'	2.17	0.44
1:X:1612:C:O2'	1:X:1613:G:H5''	2.18	0.44
1:X:2218:G:H2'	1:X:2219:C:C6	2.52	0.44
1:X:2234:C:H42	1:X:2244:G:H22	1.64	0.44
1:X:24:G:H2'	1:X:25:U:H6	1.82	0.44
1:X:360:A:C6	1:X:361:U:C4	3.05	0.44
1:X:338:G:H1	1:X:386:C:N4	2.15	0.44
1:X:411:A:C2'	1:X:412:U:H5'	2.47	0.44
1:X:813:G:H2'	1:X:814:A:H8	1.81	0.44
1:X:1265:G:N7	15:N:16:LYS:HE3	2.33	0.44
20:S:29:ALA:N	20:S:41:VAL:O	2.49	0.44
1:X:968:A:H4'	21:T:37:GLN:HG3	2.00	0.44
1:X:1806:U:C5	1:X:1811:A:N7	2.86	0.44
1:X:1839:G:H2'	1:X:1840:U:H6	1.83	0.44
1:X:236:A:O5'	1:X:236:A:C8	2.71	0.44
1:X:237:U:H2'	1:X:238:U:O4'	2.16	0.44
1:X:2422:C:H2'	1:X:2423:G:C8	2.53	0.44
1:X:2775:A:H2'	1:X:2776:A:H8	1.81	0.44
1:X:448:A:H8	1:X:448:A:OP2	2.00	0.44
4:B:13:THR:O	4:B:25:VAL:HG12	2.18	0.44
4:B:38:LYS:HZ3	4:B:97:ASP:HA	1.78	0.44
5:C:54:ARG:C	5:C:56:ALA:N	2.71	0.44
8:G:59:ASN:HA	8:G:127:GLY:HA2	2.00	0.44
9:H:98:ILE:HG12	9:H:117:LEU:HB2	2.00	0.44
1:X:1442:C:H2'	1:X:1443:A:H8	1.80	0.44
1:X:1507:A:H2'	1:X:1508:C:H5'	1.99	0.44
1:X:1612:C:H5''	3:A:26:LYS:HD3	1.99	0.44
1:X:1842:A:H4'	1:X:1843:U:OP1	2.17	0.44
1:X:2249:G:C6	1:X:2250:A:C6	3.06	0.44
2:Y:86:C:C5	2:Y:88:U:C2	3.05	0.44
9:H:61:VAL:O	9:H:63:VAL:HG23	2.17	0.44
1:X:2305:A:OP1	11:J:11:ARG:HG3	2.18	0.44
19:R:41:MET:HA	19:R:60:GLU:CB	2.48	0.44
20:S:95:ASN:O	20:S:96:MET:HB2	2.17	0.44
1:X:1872:G:H1	1:X:1922:C:N4	2.13	0.44
1:X:321:U:HO2'	1:X:322:A:P	2.36	0.44
1:X:937:G:N3	1:X:937:G:H2'	2.32	0.44
1:X:1302:G:H5'	24:Z:8:THR:OG1	2.18	0.44
5:C:4:TYR:CD2	5:C:19:LEU:HA	2.53	0.44
8:G:13:GLU:O	8:G:42:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:7:G:H4'	8:G:16:TRP:CH2	2.52	0.44
9:H:17:ARG:NH2	9:H:47:THR:HA	2.32	0.44
1:X:1259:U:H2'	1:X:1260:C:C6	2.53	0.44
1:X:1314:A:H2'	1:X:1315:C:C6	2.52	0.44
1:X:2496:A:H2'	1:X:2497:G:O4'	2.17	0.44
1:X:2607:U:OP1	4:B:146:HIS:ND1	2.50	0.44
1:X:2632:U:H2'	1:X:2633:C:C6	2.53	0.44
1:X:356:A:H2'	1:X:357:U:O4'	2.18	0.44
1:X:889:U:H2'	1:X:890:G:H5'	1.99	0.44
1:X:995:U:OP1	2:Y:85:A:N1	2.50	0.44
9:H:12:ASP:HA	9:H:97:ARG:O	2.18	0.44
2:Y:75:U:P	20:S:22:ARG:HH22	2.40	0.44
1:X:1245:G:C2	1:X:1246:C:C6	3.06	0.44
1:X:120:G:H4'	1:X:150:A:H5'	2.00	0.44
1:X:1542:C:H1'	1:X:1624:C:O2'	2.17	0.44
1:X:1761:G:O2'	1:X:1762:U:O5'	2.35	0.44
1:X:1848:A:H2'	1:X:1849:G:H8	1.83	0.44
1:X:1882:G:H2'	1:X:1883:A:O4'	2.18	0.44
1:X:2293:A:C2	1:X:2299:U:C5	3.06	0.44
1:X:463:C:H2'	1:X:464:U:H6	1.83	0.44
1:X:502:C:HO2'	1:X:503:A:P	2.41	0.44
1:X:730:A:C8	1:X:819:A:C6	3.06	0.44
25:2:21:LYS:O	25:2:24:SER:OG	2.36	0.44
26:3:54:ASP:O	26:3:57:ARG:N	2.49	0.44
1:X:1332:C:H4'	12:K:67:ARG:NH1	2.33	0.44
19:R:32:ARG:O	19:R:65:VAL:HG23	2.18	0.44
1:X:1153:C:N3	1:X:1154:G:N2	2.65	0.44
1:X:2620:U:H2'	1:X:2621:C:H6	1.82	0.44
24:Z:39:LEU:HA	24:Z:39:LEU:HD23	1.80	0.44
4:B:53:PHE:HB3	4:B:87:PHE:HB2	2.00	0.44
10:I:62:PRO:HD2	10:I:90:GLU:OE2	2.18	0.44
14:M:52:ARG:HG3	14:M:52:ARG:NH1	2.25	0.44
18:Q:19:ALA:HB1	18:Q:24:LYS:HB2	2.00	0.44
22:V:7:ARG:C	22:V:9:LEU:H	2.21	0.44
1:X:1065:A:C3'	1:X:1065:A:C8	3.00	0.44
1:X:143:U:O2'	18:Q:36:THR:OG1	2.28	0.44
1:X:1880:A:C6	1:X:1916:A:C6	3.06	0.44
1:X:265:A:C2	1:X:476:A:N3	2.86	0.44
1:X:2671:A:N6	1:X:2672:G:C6	2.85	0.44
1:X:2752:A:H1'	1:X:2753:U:H2'	2.00	0.44
2:Y:111:A:H2'	2:Y:112:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:105:LEU:O	7:E:107:VAL:N	2.51	0.43
8:G:38:ARG:HH11	8:G:111:PRO:HG3	1.83	0.43
1:X:1515:G:N2	1:X:1516:C:C2	2.86	0.43
1:X:1773:A:H2'	1:X:1774:A:H8	1.83	0.43
1:X:622:A:O2'	1:X:2046:U:OP1	2.35	0.43
1:X:2411:A:O2'	1:X:2412:C:OP1	2.34	0.43
1:X:2479:C:N4	1:X:2480:A:N6	2.66	0.43
1:X:2587:C:H2'	1:X:2588:A:O4'	2.18	0.43
1:X:2668:A:H2'	1:X:2669:G:H8	1.82	0.43
1:X:817:G:H2'	1:X:818:U:C6	2.53	0.43
3:A:171:TYR:HA	3:A:185:LEU:HA	2.01	0.43
3:A:258:LYS:HD2	3:A:260:ARG:HG2	2.00	0.43
8:G:40:LYS:O	8:G:41:ASN:HB2	2.18	0.43
18:Q:11:VAL:HG12	18:Q:13:THR:HG23	1.99	0.43
1:X:1342:C:H2'	1:X:1343:U:O4'	2.17	0.43
1:X:172:U:H3'	1:X:173:A:H8	1.84	0.43
1:X:1771:A:O2'	1:X:1772:G:O5'	2.32	0.43
1:X:249:C:H2'	1:X:250:G:O4'	2.17	0.43
1:X:411:A:H2'	1:X:412:U:H5'	1.98	0.43
1:X:441:C:H2'	1:X:442:G:C8	2.52	0.43
1:X:712:U:H2'	1:X:713:A:O4'	2.17	0.43
26:3:49:LEU:N	26:3:49:LEU:HD23	2.33	0.43
3:A:158:ALA:HB1	3:A:197:ASN:C	2.38	0.43
5:C:143:LEU:HD23	5:C:143:LEU:HA	1.72	0.43
5:C:9:LEU:CB	5:C:14:SER:HB3	2.47	0.43
10:I:109:ILE:HD12	10:I:109:ILE:H	1.82	0.43
1:X:1150:A:H8	1:X:1151:G:H8	1.66	0.43
1:X:1501:G:H1	1:X:2729:G:H1	1.66	0.43
1:X:1726:A:C2	1:X:1727:C:C2	3.07	0.43
1:X:1843:U:H3'	1:X:1843:U:C6	2.53	0.43
1:X:2319:U:H4'	1:X:2402:G:H4'	2.00	0.43
1:X:2605:G:OP2	1:X:2605:G:H4'	2.17	0.43
1:X:305:A:N6	1:X:411:A:H62	2.16	0.43
1:X:321:U:C4	1:X:326:A:C6	3.05	0.43
1:X:329:A:N6	1:X:398:C:N4	2.66	0.43
1:X:871:U:O2'	10:I:46:VAL:HG12	2.17	0.43
1:X:923:A:C6	1:X:945:A:N6	2.87	0.43
2:Y:11:A:H4'	2:Y:13:A:C8	2.53	0.43
4:B:64:LYS:HG2	4:B:64:LYS:H	1.52	0.43
5:C:170:ILE:HD12	5:C:174:GLN:O	2.18	0.43
10:I:45:GLY:C	10:I:46:VAL:HG23	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:870:C:H1'	10:I:47:ARG:HH21	1.82	0.43
1:X:2036:G:OP1	17:P:41:LYS:HE2	2.18	0.43
17:P:82:LEU:O	17:P:84:ARG:HG2	2.19	0.43
23:W:39:ASP:OD1	23:W:44:ARG:NH2	2.52	0.43
1:X:1013:U:H2'	1:X:1014:U:C6	2.53	0.43
1:X:1382:C:H42	1:X:1645:G:H1	1.66	0.43
1:X:1516:C:C4	1:X:1517:A:N7	2.87	0.43
1:X:1760:G:C6	1:X:1761:G:N7	2.87	0.43
1:X:1840:U:H2'	1:X:1841:G:O4'	2.19	0.43
1:X:2224:U:O2'	1:X:2225:A:H5''	2.18	0.43
1:X:2255:G:H2'	1:X:2256:U:O4'	2.17	0.43
1:X:2348:G:H5''	1:X:2349:A:OP2	2.17	0.43
1:X:666:A:H2'	1:X:667:G:H5'	2.00	0.43
3:A:258:LYS:HZ1	3:A:260:ARG:HB3	1.82	0.43
5:C:102:PRO:HD2	5:C:105:MET:HE3	2.00	0.43
12:K:9:THR:HG22	12:K:12:GLN:H	1.83	0.43
14:M:52:ARG:CG	14:M:52:ARG:HH11	2.26	0.43
15:N:105:ALA:HB1	16:O:40:PHE:HZ	1.82	0.43
20:S:32:TYR:O	20:S:92:LEU:HD12	2.18	0.43
1:X:1312:A:H4'	1:X:1313:G:OP1	2.19	0.43
1:X:2018:U:O2'	1:X:2019:G:H5'	2.18	0.43
1:X:2126:C:N3	1:X:2217:G:N1	2.66	0.43
1:X:2362:A:C8	1:X:2364:G:C6	3.06	0.43
1:X:2719:C:H4'	1:X:2890:C:O2	2.18	0.43
1:X:2783:U:H4'	1:X:2784:A:OP1	2.18	0.43
2:Y:11:A:H4'	2:Y:13:A:N7	2.33	0.43
3:A:143:ASN:OD1	3:A:152:GLY:HA3	2.17	0.43
10:I:65:GLY:HA2	10:I:93:PRO:HG2	2.00	0.43
1:X:1155:A:H1'	1:X:1156:G:O4'	2.18	0.43
1:X:1773:A:H2'	1:X:1774:A:C8	2.54	0.43
1:X:1836:A:H2'	1:X:1837:A:C8	2.53	0.43
1:X:1953:U:N3	1:X:1955:A:N1	2.66	0.43
1:X:1963:A:H1'	1:X:1967:U:C2	2.53	0.43
1:X:2229:C:H42	1:X:2248:G:H1	1.65	0.43
1:X:2324:C:N4	1:X:2348:G:H1	2.15	0.43
1:X:338:G:H2'	1:X:339:A:H8	1.84	0.43
4:B:182:ASN:C	4:B:183:LEU:HD12	2.39	0.43
4:B:34:VAL:HG12	4:B:35:VAL:O	2.19	0.43
9:H:91:LYS:HB3	9:H:111:PHE:CB	2.49	0.43
10:I:105:GLU:HA	10:I:125:ALA:HB2	2.00	0.43
12:K:67:ARG:HD3	12:K:67:ARG:HA	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1286:G:C6	5:C:51:VAL:HG23	2.53	0.43
1:X:147:G:H2'	1:X:148:U:O4'	2.19	0.43
1:X:1512:U:H2'	1:X:1513:A:H8	1.81	0.43
1:X:1560:A:H5'	1:X:1561:G:OP2	2.19	0.43
1:X:1788:U:C3'	1:X:1789:A:H5''	2.48	0.43
1:X:2419:A:H2	1:X:2451:C:N4	2.14	0.43
1:X:2587:C:C2	1:X:2588:A:C8	3.06	0.43
1:X:266:A:H2'	1:X:267:G:O4'	2.17	0.43
1:X:909:G:C6	1:X:910:C:N4	2.87	0.43
2:Y:13:A:N3	2:Y:106:U:N3	2.66	0.43
2:Y:108:G:O2'	2:Y:109:C:H5'	2.19	0.43
2:Y:80:A:C6	2:Y:92:G:N1	2.86	0.43
3:A:173:LEU:HG	3:A:183:MET:HB2	1.99	0.43
1:X:2646:U:H4'	4:B:163:VAL:HG12	2.01	0.43
8:G:33:VAL:HG13	8:G:55:VAL:HG11	2.01	0.43
9:H:87:ILE:HG22	9:H:88:ARG:N	2.33	0.43
1:X:1423:C:H2'	1:X:1424:A:C8	2.54	0.43
1:X:1841:G:H3'	1:X:1842:A:H2'	2.00	0.43
1:X:538:G:H2'	1:X:539:G:O4'	2.18	0.43
1:X:548:A:H4'	1:X:549:U:H5''	2.00	0.43
1:X:683:G:C8	1:X:684:U:C5	3.07	0.43
1:X:792:U:C4	1:X:2640:U:C5	3.07	0.43
3:A:25:THR:HG22	3:A:203:VAL:HA	2.00	0.43
8:G:40:LYS:O	8:G:41:ASN:CB	2.67	0.43
8:G:97:ASN:OD1	8:G:97:ASN:N	2.51	0.43
10:I:91:VAL:O	10:I:92:THR:OG1	2.32	0.43
1:X:1511:C:H2'	1:X:1567:A:N6	2.34	0.43
1:X:1753:U:C2	1:X:1777:G:N2	2.87	0.43
1:X:1885:G:O2'	1:X:1886:A:P	2.77	0.43
1:X:2448:G:H5''	1:X:2449:C:OP2	2.18	0.43
1:X:401:U:H2'	1:X:402:C:O4'	2.18	0.43
1:X:629:A:H5'	5:C:89:VAL:CG2	2.49	0.43
1:X:773:G:O2'	1:X:774:G:H5'	2.18	0.43
3:A:231:PRO:HD3	3:A:246:PRO:HA	1.99	0.43
3:A:28:THR:HA	3:A:29:PRO:HD3	1.86	0.43
8:G:95:ARG:HB3	8:G:95:ARG:HE	1.63	0.43
11:J:113:VAL:O	11:J:117:ALA:N	2.37	0.43
16:O:39:LEU:HA	16:O:39:LEU:HD13	1.72	0.43
1:X:1595:C:H2'	1:X:1596:G:O4'	2.19	0.43
1:X:1725:G:H21	1:X:1789:A:H3'	1.84	0.43
1:X:1730:C:H2'	1:X:1731:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2433:C:O2	1:X:2433:C:H2'	2.18	0.43
5:C:14:SER:O	5:C:16:SER:N	2.49	0.42
1:X:1195:A:H4'	15:N:81:ASN:CG	2.39	0.42
20:S:29:ALA:HB2	20:S:89:ILE:HB	2.01	0.42
1:X:1162:C:H2'	1:X:1163:U:O4'	2.19	0.42
1:X:1270:U:H2'	1:X:1271:G:H8	1.83	0.42
1:X:1363:U:HO2'	1:X:2037:G:HO2'	1.63	0.42
1:X:1395:G:N2	1:X:1409:U:OP2	2.45	0.42
1:X:1511:C:H2'	1:X:1567:A:H61	1.84	0.42
1:X:162:A:H2'	1:X:162:A:N3	2.34	0.42
1:X:2314:A:H2	1:X:2373:A:H62	1.66	0.42
1:X:2719:C:H2'	1:X:2720:A:O4'	2.19	0.42
1:X:2649:U:C2'	1:X:2845:G:H22	2.31	0.42
1:X:327:G:H2'	1:X:327:G:N3	2.34	0.42
1:X:328:G:O2'	1:X:329:A:H8	2.02	0.42
1:X:673:G:C5	1:X:681:G:N2	2.87	0.42
1:X:691:A:H5'	1:X:692:G:OP2	2.19	0.42
25:2:35:ARG:HD3	25:2:43:LEU:O	2.18	0.42
5:C:178:ALA:O	5:C:181:LEU:HB2	2.19	0.42
11:J:35:GLN:O	11:J:129:THR:HA	2.18	0.42
1:X:1066:G:N2	1:X:1186:A:C2	2.88	0.42
1:X:1323:A:O2'	1:X:1324:A:H5''	2.19	0.42
1:X:1312:A:N6	1:X:1333:A:H4'	2.34	0.42
1:X:2089[B]:A:H61	27:X:3001:95H:C8	2.32	0.42
1:X:302:A:N1	1:X:450:C:C4	2.87	0.42
1:X:341:G:H5''	1:X:342:A:OP1	2.19	0.42
1:X:7:G:H4'	8:G:16:TRP:HH2	1.83	0.42
26:3:23:LYS:O	26:3:49:LEU:HA	2.19	0.42
5:C:4:TYR:CB	5:C:19:LEU:HA	2.49	0.42
20:S:167:ILE:HD12	20:S:167:ILE:H	1.85	0.42
22:V:28:LEU:HD21	22:V:42:ARG:HD2	2.00	0.42
1:X:83:G:N1	1:X:101:G:O2'	2.41	0.42
1:X:1429:G:C2	1:X:1430:A:C6	3.08	0.42
1:X:1349:U:C2	1:X:1647:A:C2	3.07	0.42
1:X:2358:G:H4'	21:T:51:THR:H	1.85	0.42
1:X:2682:G:O2'	1:X:2683:U:P	2.77	0.42
1:X:2760:A:N1	4:B:216:LYS:HB2	2.34	0.42
1:X:2877:G:H5'	1:X:2878:U:OP2	2.20	0.42
1:X:460:C:H1'	1:X:1891:U:O2'	2.19	0.42
1:X:843:G:H2'	1:X:844:G:C8	2.54	0.42
1:X:994:A:H2'	1:X:995:U:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:106:LEU:H	9:H:106:LEU:HD12	1.83	0.42
11:J:40:SER:OG	11:J:41:TRP:N	2.52	0.42
16:O:67:ARG:HG3	16:O:67:ARG:H	1.40	0.42
18:Q:26:THR:CB	18:Q:79:ILE:HG22	2.42	0.42
1:X:1053:A:H5''	15:N:63:THR:HG22	2.02	0.42
1:X:1280:U:H2'	1:X:1281:U:H6	1.82	0.42
1:X:190:G:H2'	1:X:191:A:O4'	2.20	0.42
1:X:201:C:H2'	1:X:202:A:H5''	2.02	0.42
1:X:290:U:H1'	1:X:291:G:N7	2.34	0.42
1:X:332:A:H61	1:X:394:U:H3	1.68	0.42
2:Y:16:A:C2	2:Y:17:A:C5	3.08	0.42
2:Y:79:C:N4	2:Y:92:G:H1	2.12	0.42
24:Z:7:ARG:HD3	24:Z:7:ARG:HH11	1.73	0.42
22:V:63:GLU:HA	22:V:66:LYS:HG3	2.01	0.42
1:X:1330:U:H2'	1:X:1331:C:O4'	2.19	0.42
1:X:1458:A:H5''	1:X:1630:A:C2	2.55	0.42
1:X:1518:G:N2	1:X:1519:U:C2	2.88	0.42
1:X:2693:C:H5''	1:X:2694:C:OP2	2.20	0.42
1:X:683:G:N1	1:X:696:G:C5	2.88	0.42
1:X:767:A:H2'	1:X:768:A:C8	2.54	0.42
3:A:173:LEU:HA	3:A:183:MET:HA	2.02	0.42
3:A:212:ARG:NH1	3:A:216:ILE:HB	2.34	0.42
3:A:258:LYS:HZ2	3:A:260:ARG:HA	1.85	0.42
4:B:36:LEU:HD12	4:B:52:GLY:HA3	2.02	0.42
9:H:19:VAL:HG23	9:H:42:THR:O	2.20	0.42
20:S:22:ARG:NE	20:S:87:THR:HG22	2.35	0.42
1:X:1065:A:H3'	1:X:1065:A:H8	1.82	0.42
1:X:1275:A:C8	1:X:1276:G:H1'	2.54	0.42
1:X:1637:A:N3	1:X:1637:A:H2'	2.35	0.42
1:X:1953:U:N3	1:X:1954:A:C8	2.86	0.42
1:X:245:G:H5''	26:3:64:TYR:CE2	2.55	0.42
1:X:323:C:O5'	1:X:324:A:OP2	2.37	0.42
1:X:49:A:H5''	1:X:51:G:O4'	2.20	0.42
1:X:868:A:H2'	1:X:869:G:C8	2.54	0.42
1:X:956:A:H2	1:X:2304:G:N3	2.17	0.42
2:Y:105:G:H8	2:Y:105:G:H2'	1.59	0.42
3:A:145:GLU:OE1	3:A:188:CYS:HA	2.19	0.42
5:C:179:GLN:OE1	5:C:179:GLN:N	2.43	0.42
13:L:19:ARG:NH2	13:L:45:ILE:HD11	2.34	0.42
16:O:7:THR:O	16:O:9:GLY:N	2.49	0.42
20:S:14:THR:HG23	20:S:17:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1602:U:O2'	1:X:1603:U:OP1	2.28	0.42
1:X:1701:U:H2'	1:X:1702:C:C6	2.55	0.42
1:X:2217:G:C8	1:X:2218:G:C6	3.07	0.42
1:X:2290:C:H4'	1:X:2356:A:H4'	2.01	0.42
1:X:2854:A:H2'	1:X:2899:A:H61	1.84	0.42
1:X:665:G:N3	1:X:665:G:H2'	2.34	0.42
1:X:2417:U:H5'	26:3:35:ASN:HB3	2.01	0.42
1:X:2850:G:H5'	4:B:67:LYS:HB2	2.01	0.42
2:Y:93:C:H41	20:S:15:ARG:NH2	2.18	0.42
1:X:177:G:H8	1:X:177:G:O5'	2.03	0.42
1:X:1817:C:OP1	3:A:219:THR:HG23	2.19	0.42
1:X:1858:G:H2'	1:X:1859:C:C6	2.55	0.42
1:X:1865:C:N4	1:X:1926:A:C4	2.87	0.42
1:X:2222:U:C2	1:X:2223:C:H5	2.38	0.42
1:X:349:U:C5	1:X:350:G:C5	3.07	0.42
1:X:352:A:H1'	1:X:372:A:N3	2.35	0.42
1:X:720:A:C8	1:X:849:A:C6	3.07	0.42
3:A:133:GLN:N	3:A:186:SER:O	2.52	0.42
1:X:2707:C:H1'	4:B:200:ASN:OD1	2.20	0.42
8:G:29:LEU:O	8:G:33:VAL:HG23	2.20	0.42
8:G:42:LYS:HD2	8:G:51:THR:O	2.20	0.42
11:J:78:PRO:HB2	11:J:81:VAL:CG2	2.50	0.42
15:N:35:ALA:O	15:N:39:VAL:HG23	2.20	0.42
1:X:1092:A:H2	1:X:1156:G:H21	1.62	0.42
1:X:1542:C:C5	1:X:1543:G:C8	3.08	0.42
1:X:2338:A:H5''	1:X:2339:U:OP2	2.19	0.42
1:X:367:A:H2'	1:X:368:A:O4'	2.19	0.42
1:X:368:A:H8	1:X:368:A:O5'	2.03	0.42
1:X:523:A:H2'	1:X:524:A:O4'	2.20	0.42
1:X:847:A:C6	1:X:848:U:N3	2.87	0.42
1:X:2760:A:C2	4:B:216:LYS:HB2	2.55	0.42
5:C:153:LEU:O	5:C:153:LEU:HD22	2.20	0.42
9:H:117:LEU:N	9:H:117:LEU:HD12	2.35	0.42
10:I:6:LEU:HD23	10:I:6:LEU:HA	1.84	0.42
1:X:1042:C:P	15:N:92:ARG:HH21	2.43	0.42
17:P:72:LYS:HD3	17:P:108:SER:HB2	2.02	0.42
20:S:9:ARG:HD2	20:S:13:GLN:OE1	2.19	0.42
1:X:1185:U:H4'	1:X:1186:A:O4'	2.19	0.42
1:X:1759:G:N2	1:X:1760:G:C2	2.88	0.42
1:X:190:G:C2	1:X:213:C:O2	2.72	0.42
1:X:812:U:H2'	1:X:812:U:H6	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:826:A:H8	1:X:826:A:O5'	2.03	0.42
1:X:90:A:C8	1:X:90:A:OP1	2.72	0.42
1:X:923:A:N6	1:X:945:A:N7	2.68	0.42
1:X:926:G:H22	1:X:939:U:C2'	2.32	0.42
3:A:120:ALA:HA	3:A:130:LEU:HD21	2.01	0.41
4:B:111:VAL:HG23	4:B:112:ALA:O	2.20	0.41
6:D:35:VAL:HA	6:D:89:VAL:O	2.20	0.41
11:J:73:PRO:HB3	11:J:93:TRP:CE3	2.54	0.41
11:J:74:TYR:CE1	11:J:94:ILE:HD11	2.54	0.41
22:V:44:ARG:O	22:V:47:ARG:HG3	2.20	0.41
1:X:1508:C:N3	1:X:1509:G:C2	2.87	0.41
1:X:1885:G:H1'	1:X:1911:A:H62	1.84	0.41
1:X:2388:A:OP1	26:3:26:ARG:HG2	2.20	0.41
1:X:2851:G:C8	4:B:64:LYS:HG3	2.55	0.41
1:X:79:U:C4	1:X:80:G:N7	2.88	0.41
3:A:46:GLN:HE22	3:A:48:LYS:HZ2	1.67	0.41
5:C:63:LYS:NZ	5:C:75:GLN:O	2.53	0.41
7:E:89:LEU:HD12	7:E:90:VAL:H	1.85	0.41
9:H:13:ASN:OD1	9:H:13:ASN:N	2.52	0.41
16:O:35:PHE:HZ	16:O:95:LEU:HD11	1.85	0.41
17:P:111:LYS:HD2	17:P:111:LYS:HA	1.66	0.41
1:X:1092:A:H61	1:X:1156:G:C1'	2.29	0.41
1:X:1364:C:O3'	12:K:110:ARG:NH2	2.54	0.41
1:X:1562:C:C2	1:X:1563:U:C5	3.08	0.41
1:X:1847:U:O2	3:A:200:HIS:HB3	2.20	0.41
1:X:1854:U:H2'	1:X:1855:G:O4'	2.20	0.41
1:X:1903:A:H2'	1:X:1904:A:O4'	2.20	0.41
1:X:2028:A:H2'	1:X:2029:G:O4'	2.20	0.41
1:X:2245:G:C6	1:X:2246:U:N3	2.88	0.41
1:X:2555:U:O3'	1:X:2556:G:H8	2.02	0.41
1:X:2580:G:C2	1:X:2610:G:H1'	2.56	0.41
1:X:455:A:H8	1:X:455:A:O5'	2.03	0.41
1:X:77:U:H2'	1:X:78:U:H6	1.85	0.41
1:X:660:A:H5''	5:C:43:SER:HB2	2.02	0.41
6:D:64:LYS:HD3	6:D:64:LYS:HA	1.91	0.41
7:E:140:GLN:C	7:E:142:GLY:H	2.24	0.41
1:X:1244:G:N2	1:X:1279:C:C2	2.88	0.41
1:X:2591:A:C2	1:X:2674:U:H4'	2.55	0.41
5:C:51:VAL:HB	5:C:92:PRO:HD2	2.02	0.41
6:D:60:ILE:HG13	6:D:60:ILE:H	1.63	0.41
9:H:102:VAL:O	9:H:121:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:55:LEU:HA	10:I:56:PRO:HD3	1.73	0.41
15:N:4:VAL:HG12	15:N:5:LYS:O	2.20	0.41
19:R:42:LYS:HD2	19:R:59:THR:HG23	2.02	0.41
1:X:1522:G:N2	1:X:1558:U:H1'	2.36	0.41
1:X:2049:U:OP2	24:Z:12:ARG:NH2	2.47	0.41
1:X:244:A:H61	1:X:258:A:H5''	1.85	0.41
1:X:2286:G:C8	1:X:2454:C:C4	3.08	0.41
1:X:325:A:C2	1:X:326:A:C4	3.08	0.41
1:X:797:A:C2	1:X:1808:U:C2	3.08	0.41
1:X:706:U:H1'	10:I:13:ARG:H	1.86	0.41
12:K:47:LEU:HD13	12:K:66:LEU:CD1	2.50	0.41
15:N:91:ASN:O	15:N:91:ASN:CG	2.58	0.41
18:Q:11:VAL:HG23	18:Q:27:PHE:HA	2.03	0.41
20:S:31:VAL:HG22	20:S:39:VAL:O	2.21	0.41
22:V:43:ILE:H	22:V:43:ILE:HG13	1.39	0.41
22:V:63:GLU:HA	22:V:66:LYS:NZ	2.35	0.41
1:X:1245:G:N2	1:X:1246:C:C2	2.88	0.41
1:X:1378:U:H2'	1:X:1434:U:O2	2.20	0.41
1:X:1480:G:H2'	1:X:1481:A:O4'	2.21	0.41
1:X:1491:C:C2	1:X:1492:G:N2	2.88	0.41
1:X:1933:G:C2	1:X:1934:G:H5'	2.55	0.41
1:X:218:G:C4'	1:X:219:A:H4'	2.50	0.41
1:X:2239:A:H62	1:X:2241:C:H42	1.68	0.41
1:X:2249:G:C2	1:X:2250:A:C4	3.08	0.41
1:X:2294:A:H5''	1:X:2295:A:H5'	2.02	0.41
1:X:2309:G:H4'	1:X:2416:G:O2'	2.20	0.41
1:X:2310:C:H2'	1:X:2311:U:O4'	2.21	0.41
1:X:2570:G:H2'	1:X:2571:G:C8	2.55	0.41
1:X:778:G:H8	1:X:778:G:O5'	2.03	0.41
6:D:157:VAL:O	6:D:157:VAL:HG12	2.20	0.41
7:E:153:PRO:HA	7:E:154:PRO:HD3	1.52	0.41
11:J:87:LYS:HE2	11:J:87:LYS:HB2	1.70	0.41
16:O:21:PHE:CD1	16:O:21:PHE:N	2.89	0.41
1:X:1281:U:C2	1:X:1282:A:C8	3.09	0.41
1:X:1492:G:C8	1:X:1493:U:H5	2.38	0.41
1:X:153:G:C2	1:X:177:G:C2	3.09	0.41
1:X:157:U:C2	1:X:158:G:C8	3.08	0.41
1:X:1963:A:H2	1:X:1970:U:C4	2.37	0.41
1:X:2088:G:C8	1:X:2528:C:H1'	2.55	0.41
1:X:2234:C:N4	1:X:2244:G:H22	2.19	0.41
1:X:2398:G:C6	1:X:2399:G:N7	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2474:G:C8	1:X:2528:C:O4'	2.74	0.41
1:X:2512:G:H5''	11:J:46:GLN:HE21	1.84	0.41
1:X:2530:A:H4'	1:X:2531:U:OP1	2.20	0.41
1:X:2599:A:O2'	1:X:2602:C:OP1	2.38	0.41
1:X:383:A:N6	1:X:384:G:C2	2.89	0.41
1:X:390:A:H2'	1:X:391:A:C8	2.55	0.41
1:X:820:G:C4	1:X:839:A:C8	3.09	0.41
4:B:37:GLN:OE1	4:B:39:LYS:HE3	2.20	0.41
5:C:4:TYR:HB3	5:C:5:ASP:H	1.50	0.41
6:D:57:LEU:HA	6:D:57:LEU:HD12	1.93	0.41
9:H:24:VAL:HG11	9:H:30:ARG:HG2	2.03	0.41
9:H:17:ARG:NH2	9:H:47:THR:HG22	2.35	0.41
16:O:25:LEU:HD23	16:O:25:LEU:HA	1.72	0.41
16:O:65:GLN:HG3	16:O:93:THR:HG23	2.01	0.41
23:W:17:GLU:O	23:W:21:LYS:HG3	2.21	0.41
1:X:1379:A:O2'	1:X:1381:U:OP2	2.31	0.41
1:X:1526:G:H22	1:X:1547:C:N4	2.18	0.41
1:X:1872:G:H2'	1:X:1873:G:O4'	2.21	0.41
1:X:2239:A:H62	1:X:2241:C:N4	2.18	0.41
1:X:2634:G:H2'	1:X:2635:G:O4'	2.20	0.41
1:X:2704:A:H2'	1:X:2705:U:C6	2.55	0.41
1:X:2876:G:C4	1:X:2882:A:C2	3.08	0.41
2:Y:18:G:H2'	2:Y:19:G:H8	1.86	0.41
2:Y:81:A:H61	2:Y:90:C:H42	1.69	0.41
1:X:788:A:OP1	4:B:144:GLY:HA2	2.21	0.41
4:B:69:ALA:HB2	4:B:84:PRO:HB3	2.01	0.41
5:C:151:LYS:HA	5:C:170:ILE:O	2.20	0.41
8:G:32:GLU:O	8:G:36:ILE:HG12	2.20	0.41
11:J:54:MET:HE1	11:J:106:VAL:HG11	2.03	0.41
1:X:1695:G:H5''	12:K:35:ALA:CB	2.51	0.41
13:L:40:ILE:HD11	13:L:101:TYR:CZ	2.55	0.41
15:N:65:ILE:CD1	15:N:95:LEU:HB3	2.50	0.41
15:N:93:LYS:O	15:N:97:GLU:HB2	2.21	0.41
17:P:14:PRO:O	17:P:18:ARG:HG3	2.21	0.41
1:X:862:C:N4	1:X:1229:G:H1	2.16	0.41
1:X:1850:G:H2'	1:X:1851:G:O4'	2.20	0.41
1:X:1903:A:H2'	1:X:1904:A:C8	2.56	0.41
1:X:1928:A:H2'	1:X:1929:C:H6	1.86	0.41
1:X:870:C:H4'	1:X:2455:G:C5	2.56	0.41
1:X:400:C:H2'	1:X:401:U:O4'	2.21	0.41
1:X:422:G:H1	1:X:444:C:N4	2.12	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:454:G:H1	1:X:465:C:H42	1.68	0.41
1:X:726:G:H5''	1:X:727:G:OP2	2.21	0.41
1:X:987:U:C2'	1:X:988:C:H5'	2.51	0.41
6:D:34:ILE:HD11	6:D:156:ILE:HA	2.03	0.41
8:G:102:ILE:HB	8:G:125:VAL:HG11	2.03	0.41
14:M:15:LEU:HA	14:M:79:HIS:CD2	2.55	0.41
14:M:34:ILE:HG13	14:M:82:LYS:HE3	2.02	0.41
1:X:125:A:H8	1:X:126:A:C5	2.39	0.41
1:X:1301:U:OP1	24:Z:13:LYS:NZ	2.29	0.41
1:X:1746:G:HO2'	1:X:1747:G:H8	1.69	0.41
1:X:1770:C:O2'	1:X:1771:A:H5'	2.20	0.41
1:X:1788:U:H3	1:X:1789:A:N6	2.19	0.41
1:X:1825:U:O2'	1:X:1829:A:N3	2.48	0.41
1:X:187:C:H4'	1:X:220:A:C2	2.56	0.41
1:X:1953:U:N3	1:X:1955:A:C6	2.89	0.41
1:X:2269:G:H2'	1:X:2270:U:O4'	2.21	0.41
1:X:49:A:C6	1:X:179:A:C5	3.09	0.41
1:X:864:A:C4	1:X:1228:A:C2	3.08	0.41
1:X:947:U:H2'	1:X:948:U:C6	2.56	0.41
9:H:8:LEU:HD12	9:H:8:LEU:N	2.36	0.41
1:X:1045:A:H2'	1:X:1046:G:O4'	2.21	0.41
1:X:1352:C:N3	1:X:1374:G:N2	2.48	0.41
1:X:1780:G:OP1	14:M:95:ARG:HD2	2.21	0.41
1:X:2563:G:C6	1:X:2564:U:C4	3.08	0.41
1:X:272:C:H5'	1:X:297:G:C6	2.56	0.41
1:X:2876:G:C6	1:X:2877:G:C5	3.09	0.41
1:X:608:C:H2'	1:X:609:U:O4'	2.21	0.41
1:X:241:C:O2'	1:X:651:A:N3	2.48	0.41
26:3:33:PHE:C	26:3:35:ASN:H	2.24	0.41
3:A:139:THR:HG22	3:A:140:VAL:O	2.21	0.41
8:G:74:VAL:HB	8:G:76:TYR:CE1	2.56	0.41
15:N:105:ALA:HB1	16:O:40:PHE:CZ	2.56	0.41
19:R:15:LYS:HB3	19:R:18:GLY:H	1.86	0.41
1:X:992:A:H1'	1:X:1028:G:C8	2.56	0.41
1:X:1212:U:H2'	1:X:1213:C:O4'	2.21	0.41
1:X:1490:G:H2'	1:X:1491:C:C6	2.56	0.41
1:X:1832:C:H2'	1:X:1833:C:H6	1.86	0.41
1:X:439:U:H2'	1:X:440:C:H6	1.85	0.41
1:X:503:A:N1	1:X:517:A:N7	2.69	0.41
1:X:660:A:N7	5:C:176:THR:HG22	2.36	0.41
1:X:716:C:H2'	1:X:717:C:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:775:A:O2'	1:X:776:C:H5'	2.21	0.41
1:X:857:C:H5'	10:I:22:GLY:HA3	2.01	0.41
1:X:886:A:C2	1:X:982:G:C2	3.09	0.41
10:I:63:LYS:HA	10:I:91:VAL:HG23	2.03	0.40
14:M:49:VAL:O	14:M:50:ILE:HD13	2.21	0.40
16:O:2:PHE:HB3	16:O:42:GLY:N	2.36	0.40
20:S:95:ASN:C	20:S:97:SER:H	2.24	0.40
1:X:1155:A:H1'	1:X:1156:G:C4'	2.50	0.40
1:X:1652:A:H1'	1:X:1654:A:OP2	2.20	0.40
1:X:2223:C:H2'	1:X:2224:U:C6	2.57	0.40
1:X:2231:C:HO2'	1:X:2232:A:H8	1.69	0.40
1:X:2248:G:C2	1:X:2249:G:C8	3.09	0.40
1:X:284:C:H2'	1:X:286:U:OP1	2.21	0.40
1:X:317:G:H3'	1:X:317:G:N3	2.35	0.40
1:X:327:G:C2	1:X:328:G:N7	2.89	0.40
1:X:505:U:H2'	1:X:506:A:H5''	2.02	0.40
1:X:58:G:N2	1:X:70:G:C4	2.89	0.40
1:X:811:C:N4	1:X:812:U:C4	2.89	0.40
24:Z:5:LYS:O	24:Z:6:ARG:HG2	2.21	0.40
11:J:43:THR:HG22	11:J:45:ARG:H	1.85	0.40
11:J:52:ILE:CG2	11:J:56:ARG:HH21	2.34	0.40
18:Q:57:ASN:OD1	18:Q:76:ARG:NH1	2.54	0.40
21:T:52:LYS:HE3	21:T:52:LYS:HB2	1.78	0.40
1:X:133:A:C8	1:X:134:U:C6	3.09	0.40
1:X:1760:G:N1	1:X:1761:G:N7	2.69	0.40
1:X:1904:A:H2'	1:X:1905:G:O4'	2.21	0.40
1:X:2000:G:C5	1:X:2001:C:C5	3.09	0.40
1:X:2638:C:H2'	1:X:2639:C:C6	2.55	0.40
1:X:457:G:OP1	1:X:2434:A:OP1	2.39	0.40
1:X:652:A:H2'	1:X:653:G:H5'	2.01	0.40
1:X:662:G:H2'	1:X:663:U:O4'	2.21	0.40
2:Y:21:G:H22	2:Y:58:G:N2	2.19	0.40
8:G:14:ARG:HB2	8:G:53:ASP:HA	2.03	0.40
9:H:1:MET:HB3	9:H:1:MET:HE2	1.39	0.40
12:K:52:LYS:NZ	12:K:96:ARG:O	2.52	0.40
15:N:83:LEU:HD23	15:N:83:LEU:HA	1.71	0.40
17:P:13:ALA:O	17:P:17:VAL:HG23	2.20	0.40
18:Q:55:ILE:CD1	18:Q:78:ALA:HB2	2.52	0.40
23:W:22:THR:O	23:W:26:LEU:HD12	2.21	0.40
1:X:1701:U:H2'	1:X:1702:C:H6	1.87	0.40
1:X:2410:G:C6	1:X:2411:A:C2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2494:C:H4'	11:J:123:HIS:CE1	2.57	0.40
1:X:2504:C:H5''	1:X:2506:U:O4	2.21	0.40
1:X:2646:U:H5'	4:B:163:VAL:O	2.21	0.40
1:X:2549:U:O2'	1:X:2674:U:OP1	2.22	0.40
2:Y:21:G:N2	2:Y:58:G:N2	2.69	0.40
2:Y:39:G:H5'	2:Y:40:C:H5''	2.02	0.40
4:B:36:LEU:N	4:B:50:GLN:O	2.48	0.40
2:Y:41:C:O4'	6:D:63:GLN:NE2	2.55	0.40
1:X:2694:C:O2	7:E:108:GLY:HA2	2.21	0.40
7:E:33:LEU:C	7:E:35:ARG:H	2.24	0.40
17:P:44:SER:N	17:P:45:PRO:HD2	2.36	0.40
1:X:1379:A:N1	1:X:1382:C:N3	2.70	0.40
1:X:1449:A:O2'	1:X:1451:U:O4	2.19	0.40
1:X:2126:C:N3	1:X:2217:G:C6	2.89	0.40
1:X:350:G:H2'	1:X:352:A:OP2	2.22	0.40
1:X:410:G:OP2	1:X:410:G:H8	2.05	0.40
4:B:182:ASN:O	4:B:183:LEU:HD12	2.22	0.40
5:C:64:PRO:HB2	5:C:65:TRP:CE3	2.56	0.40
6:D:70:ALA:HB2	6:D:85:ILE:HD12	2.03	0.40
13:L:39:HIS:C	13:L:40:ILE:HD12	2.42	0.40
13:L:65:THR:O	13:L:69:LYS:N	2.49	0.40
19:R:66:SER:N	19:R:67:ASN:OD1	2.55	0.40
19:R:86:VAL:O	19:R:88:GLY:N	2.55	0.40
1:X:1524:C:H42	1:X:1550:G:H1	1.69	0.40
1:X:1594:U:H3'	1:X:1595:C:H5'	2.03	0.40
1:X:1933:G:H2'	1:X:1934:G:C5'	2.52	0.40
1:X:2236:C:H5''	1:X:2237:U:O5'	2.21	0.40
1:X:268:A:H2'	1:X:269:G:O4'	2.21	0.40
1:X:2779:C:H2'	1:X:2780:A:O4'	2.21	0.40
1:X:2848:G:H2'	1:X:2849:A:H8	1.86	0.40
1:X:286:U:H5''	1:X:287:G:OP1	2.22	0.40
1:X:502:C:O2'	1:X:503:A:P	2.80	0.40
1:X:660:A:C8	5:C:176:THR:HG22	2.56	0.40
1:X:922:G:N1	1:X:924:G:N7	2.69	0.40
2:Y:8:A:C2	2:Y:108:G:H8	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	258/277 (93%)	189 (73%)	47 (18%)	22 (8%)	1	8
4	B	213/220 (97%)	180 (84%)	22 (10%)	11 (5%)	2	17
5	C	196/207 (95%)	147 (75%)	30 (15%)	19 (10%)	0	6
6	D	133/179 (74%)	115 (86%)	14 (10%)	4 (3%)	4	29
7	E	141/178 (79%)	79 (56%)	35 (25%)	27 (19%)	0	1
8	G	140/145 (97%)	127 (91%)	9 (6%)	4 (3%)	4	30
9	H	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	9	41
10	I	125/140 (89%)	65 (52%)	34 (27%)	26 (21%)	0	1
11	J	136/144 (94%)	121 (89%)	11 (8%)	4 (3%)	4	30
12	K	117/122 (96%)	105 (90%)	7 (6%)	5 (4%)	2	21
13	L	108/119 (91%)	83 (77%)	15 (14%)	10 (9%)	0	7
14	M	109/116 (94%)	88 (81%)	14 (13%)	7 (6%)	1	13
15	N	114/118 (97%)	111 (97%)	2 (2%)	1 (1%)	17	54
16	O	99/102 (97%)	81 (82%)	14 (14%)	4 (4%)	3	23
17	P	110/117 (94%)	103 (94%)	6 (6%)	1 (1%)	17	54
18	Q	88/91 (97%)	75 (85%)	12 (14%)	1 (1%)	14	50
19	R	100/105 (95%)	71 (71%)	19 (19%)	10 (10%)	0	6
20	S	172/217 (79%)	133 (77%)	25 (14%)	14 (8%)	1	9
21	T	74/94 (79%)	61 (82%)	11 (15%)	2 (3%)	5	32
22	V	63/69 (91%)	59 (94%)	3 (5%)	1 (2%)	9	42
23	W	55/59 (93%)	52 (94%)	3 (6%)	0	100	100
24	Z	42/58 (72%)	37 (88%)	4 (10%)	1 (2%)	6	34
25	2	42/45 (93%)	39 (93%)	2 (5%)	1 (2%)	6	34
26	3	63/66 (96%)	49 (78%)	11 (18%)	3 (5%)	2	19
All	All	2818/3110 (91%)	2280 (81%)	358 (13%)	180 (6%)	1	13

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	35	LYS
3	A	36	PRO
3	A	38	PRO
3	A	51	VAL
3	A	77	LYS
3	A	78	VAL
3	A	124	ILE
3	A	248	SER
3	A	253	PRO
4	B	61	LYS
4	B	101	VAL
4	B	176	ASN
5	C	29	ASN
5	C	52	LYS
5	C	55	SER
5	C	67	GLN
5	C	127	ASP
6	D	19	LYS
7	E	33	LEU
7	E	52	VAL
7	E	53	VAL
7	E	79	VAL
7	E	90	VAL
7	E	106	ASN
7	E	107	VAL
7	E	141	VAL
7	E	156	PRO
8	G	10	SER
8	G	138	PRO
9	H	89	ASP
9	H	113	LYS
10	I	27	ASN
10	I	44	GLY
10	I	46	VAL
10	I	48	PRO
10	I	56	PRO
10	I	57	LEU
10	I	62	PRO
10	I	76	ILE
10	I	99	SER
14	M	34	ILE
14	M	109	ALA

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Mol	Chain	Res	Type
16	O	50	ALA
19	R	47	PRO
19	R	67	ASN
20	S	140	ALA
3	A	126	VAL
3	A	197	ASN
3	A	233	GLY
4	B	94	VAL
4	B	160	ALA
4	B	204	PRO
5	C	24	PHE
5	C	26	ILE
5	C	28	PRO
5	C	126	VAL
5	C	173	VAL
7	E	50	ILE
7	E	55	PRO
7	E	56	SER
7	E	59	LYS
7	E	95	ARG
7	E	124	SER
7	E	154	PRO
8	G	41	ASN
10	I	25	THR
10	I	63	LYS
10	I	81	GLN
10	I	100	GLY
10	I	123	VAL
11	J	20	ARG
13	L	5	ILE
13	L	20	THR
13	L	22	LEU
14	M	36	GLU
15	N	92	ARG
16	O	3	ALA
16	O	69	LYS
19	R	18	GLY
19	R	19	LYS
19	R	98	GLY
20	S	38	ASN
20	S	55	VAL
20	S	66	GLY

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Mol	Chain	Res	Type
20	S	148	LEU
22	V	6	ILE
26	3	23	LYS
3	A	107	PRO
3	A	236	GLU
3	A	252	LYS
4	B	157	ALA
4	B	161	SER
4	B	205	LYS
5	C	54	ARG
5	C	144	SER
5	C	149	PRO
5	C	178	ALA
6	D	80	ARG
6	D	114	PHE
7	E	32	GLU
7	E	45	GLN
7	E	102	ASP
7	E	121	ILE
10	I	13	ARG
10	I	68	ASN
10	I	75	ALA
12	K	75	ASP
12	K	78	THR
12	K	79	GLN
13	L	42	ALA
13	L	99	TYR
14	M	59	GLU
19	R	49	GLN
19	R	50	LEU
20	S	10	GLN
20	S	68	LYS
20	S	104	VAL
20	S	139	GLU
21	T	82	ARG
21	T	84	LYS
26	3	15	LYS
3	A	44	ASN
5	C	120	GLU
5	C	130	ASN
7	E	46	GLU
7	E	96	ALA

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Mol	Chain	Res	Type
7	E	139	GLU
7	E	164	TYR
8	G	132	PRO
10	I	42	SER
10	I	72	LYS
10	I	124	LYS
11	J	14	ARG
11	J	73	PRO
11	J	101	ARG
13	L	92	ILE
16	O	44	ASP
18	Q	30	ASP
20	S	132	ALA
20	S	136	ASN
24	Z	32	ASN
3	A	191	THR
3	A	217	ARG
5	C	131	PHE
6	D	93	GLY
7	E	138	LYS
7	E	168	TYR
10	I	97	VAL
10	I	110	LYS
12	K	28	GLU
12	K	88	GLU
13	L	27	GLU
13	L	62	ASP
13	L	106	LYS
19	R	15	LYS
26	3	16	ARG
3	A	150	LYS
3	A	241	ILE
4	B	186	VAL
5	C	58	SER
10	I	91	VAL
13	L	24	GLY
14	M	23	ARG
14	M	112	ILE
17	P	110	GLY
20	S	119	GLY
20	S	151	ASN
4	B	174	GLY

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Mol	Chain	Res	Type
7	E	26	VAL
19	R	78	PRO
10	I	52	GLY
3	A	220	VAL
19	R	65	VAL
20	S	145	ILE
25	2	16	VAL
3	A	112	VAL
5	C	15	GLY
10	I	69	ILE
10	I	77	VAL
14	M	20	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	125/224 (56%)	93 (74%)	32 (26%)	0	2
4	B	146/177 (82%)	119 (82%)	27 (18%)	1	7
5	C	118/169 (70%)	92 (78%)	26 (22%)	1	4
6	D	78/158 (49%)	61 (78%)	17 (22%)	1	4
7	E	26/155 (17%)	20 (77%)	6 (23%)	1	3
8	G	103/123 (84%)	86 (84%)	17 (16%)	2	11
9	H	95/100 (95%)	74 (78%)	21 (22%)	1	4
10	I	51/108 (47%)	36 (71%)	15 (29%)	0	2
11	J	92/119 (77%)	78 (85%)	14 (15%)	3	15
12	K	84/102 (82%)	69 (82%)	15 (18%)	2	8
13	L	40/95 (42%)	31 (78%)	9 (22%)	1	3
14	M	68/102 (67%)	52 (76%)	16 (24%)	1	3
15	N	95/98 (97%)	81 (85%)	14 (15%)	3	16
16	O	56/86 (65%)	41 (73%)	15 (27%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	89/94 (95%)	77 (86%)	12 (14%)	4	19
18	Q	64/82 (78%)	48 (75%)	16 (25%)	0	3
19	R	36/90 (40%)	28 (78%)	8 (22%)	1	4
20	S	91/190 (48%)	71 (78%)	20 (22%)	1	4
21	T	53/75 (71%)	46 (87%)	7 (13%)	4	20
22	V	55/62 (89%)	38 (69%)	17 (31%)	0	2
23	W	50/53 (94%)	40 (80%)	10 (20%)	1	5
24	Z	35/51 (69%)	27 (77%)	8 (23%)	1	3
25	2	37/40 (92%)	31 (84%)	6 (16%)	2	12
26	3	26/57 (46%)	23 (88%)	3 (12%)	5	25
All	All	1713/2610 (66%)	1362 (80%)	351 (20%)	1	5

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	17	THR
3	A	26	LYS
3	A	27	THR
3	A	28	THR
3	A	30	GLU
3	A	31	LYS
3	A	43	ARG
3	A	45	ASN
3	A	46	GLN
3	A	48	LYS
3	A	65	ILE
3	A	83	TYR
3	A	114	GLN
3	A	115	ILE
3	A	116	VAL
3	A	133	GLN
3	A	143	ASN
3	A	163	GLN
3	A	176	LEU
3	A	183	MET
3	A	184	ILE
3	A	185	LEU
3	A	199	GLN

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Mol	Chain	Res	Type
3	A	204	ASN
3	A	214	LYS
3	A	216	ILE
3	A	219	THR
3	A	229	ASP
3	A	230	HIS
3	A	258	LYS
3	A	259	THR
3	A	267	ASP
4	B	2	THR
4	B	13	THR
4	B	25	VAL
4	B	33	ASN
4	B	40	THR
4	B	44	ASP
4	B	57	LYS
4	B	62	ASP
4	B	64	LYS
4	B	65	SER
4	B	71	LYS
4	B	74	GLU
4	B	78	LYS
4	B	88	ILE
4	B	111	VAL
4	B	115	VAL
4	B	116	ILE
4	B	119	THR
4	B	149	ARG
4	B	162	ARG
4	B	172	ARG
4	B	180	VAL
4	B	190	THR
4	B	195	ILE
4	B	196	LEU
4	B	198	LYS
4	B	208	LEU
5	C	4	TYR
5	C	5	ASP
5	C	13	LYS
5	C	14	SER
5	C	16	SER
5	C	18	GLU

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Mol	Chain	Res	Type
5	C	19	LEU
5	C	40	GLN
5	C	51	VAL
5	C	67	GLN
5	C	70	THR
5	C	88	ILE
5	C	89	VAL
5	C	108	LEU
5	C	110	LEU
5	C	112	SER
5	C	144	SER
5	C	145	THR
5	C	152	VAL
5	C	153	LEU
5	C	158	ASN
5	C	160	ASP
5	C	162	ASN
5	C	175	VAL
5	C	179	GLN
5	C	186	ILE
6	D	15	ASN
6	D	20	PHE
6	D	21	ASN
6	D	25	VAL
6	D	33	LYS
6	D	34	ILE
6	D	42	ASP
6	D	44	VAL
6	D	45	GLN
6	D	59	LEU
6	D	66	LEU
6	D	79	LEU
6	D	80	ARG
6	D	92	ARG
6	D	156	ILE
6	D	164	GLU
6	D	169	LEU
7	E	63	THR
7	E	84	VAL
7	E	89	LEU
7	E	146	SER
7	E	162	ILE

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Mol	Chain	Res	Type
7	E	163	ARG
8	G	1	MET
8	G	2	ARG
8	G	3	GLN
8	G	14	ARG
8	G	29	LEU
8	G	38	ARG
8	G	43	VAL
8	G	44	THR
8	G	61	SER
8	G	64	GLU
8	G	92	GLU
8	G	93	LEU
8	G	112	SER
8	G	117	GLU
8	G	119	GLN
8	G	133	HIS
8	G	140	ASN
9	H	3	GLN
9	H	8	LEU
9	H	9	LYS
9	H	10	VAL
9	H	21	THR
9	H	23	LYS
9	H	32	THR
9	H	34	ASN
9	H	35	ILE
9	H	42	THR
9	H	52	VAL
9	H	58	VAL
9	H	66	LYS
9	H	69	VAL
9	H	73	ASP
9	H	77	ILE
9	H	80	ASP
9	H	91	LYS
9	H	97	ARG
9	H	114	ILE
9	H	116	SER
10	I	2	LYS
10	I	5	GLU
10	I	16	ARG

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Mol	Chain	Res	Type
10	I	21	ARG
10	I	31	SER
10	I	33	ARG
10	I	48	PRO
10	I	67	THR
10	I	72	LYS
10	I	79	LEU
10	I	87	ASP
10	I	90	GLU
10	I	104	ASN
10	I	109	ILE
10	I	122	THR
11	J	12	GLN
11	J	39	THR
11	J	41	TRP
11	J	58	MET
11	J	72	THR
11	J	75	THR
11	J	87	LYS
11	J	96	VAL
11	J	112	GLU
11	J	120	LEU
11	J	122	SER
11	J	128	LYS
11	J	129	THR
11	J	137	LEU
12	K	6	LEU
12	K	8	ARG
12	K	9	THR
12	K	10	SER
12	K	11	ASP
12	K	25	ILE
12	K	34	GLU
12	K	48	ILE
12	K	56	LEU
12	K	65	THR
12	K	67	ARG
12	K	94	THR
12	K	101	THR
12	K	109	ARG
12	K	121	LEU
13	L	8	ASN

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Mol	Chain	Res	Type
13	L	37	ASN
13	L	52	THR
13	L	53	LEU
13	L	58	SER
13	L	63	ILE
13	L	65	THR
13	L	96	ARG
13	L	101	TYR
14	M	5	LYS
14	M	14	GLN
14	M	17	THR
14	M	31	HIS
14	M	32	VAL
14	M	43	GLN
14	M	44	VAL
14	M	51	LYS
14	M	52	ARG
14	M	58	SER
14	M	60	THR
14	M	65	LYS
14	M	67	SER
14	M	75	THR
14	M	80	THR
14	M	95	ARG
15	N	10	THR
15	N	19	LYS
15	N	22	LYS
15	N	30	THR
15	N	42	SER
15	N	48	ARG
15	N	51	ARG
15	N	55	ARG
15	N	59	LYS
15	N	65	ILE
15	N	70	ARG
15	N	79	LEU
15	N	108	GLN
15	N	115	ASP
16	O	2	PHE
16	O	6	GLU
16	O	18	GLN
16	O	22	VAL

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Mol	Chain	Res	Type
16	O	29	GLU
16	O	33	PHE
16	O	38	VAL
16	O	39	LEU
16	O	61	THR
16	O	67	ARG
16	O	78	ARG
16	O	83	LYS
16	O	84	ARG
16	O	95	LEU
16	O	96	THR
17	P	43	SER
17	P	59	GLU
17	P	65	ASN
17	P	66	THR
17	P	67	ASP
17	P	82	LEU
17	P	86	ARG
17	P	98	LYS
17	P	101	SER
17	P	105	ILE
17	P	109	ASP
17	P	111	LYS
18	Q	5	ASP
18	Q	9	ARG
18	Q	13	THR
18	Q	29	VAL
18	Q	33	VAL
18	Q	52	SER
18	Q	53	VAL
18	Q	57	ASN
18	Q	68	TYR
18	Q	76	ARG
18	Q	79	ILE
18	Q	80	VAL
18	Q	81	THR
18	Q	82	LEU
18	Q	88	ASP
18	Q	89	LEU
19	R	11	VAL
19	R	26	THR
19	R	42	LYS

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Mol	Chain	Res	Type
19	R	59	THR
19	R	60	GLU
19	R	68	VAL
19	R	76	ASN
19	R	79	THR
20	S	3	SER
20	S	9	ARG
20	S	13	GLN
20	S	14	THR
20	S	15	ARG
20	S	26	LYS
20	S	27	VAL
20	S	30	VAL
20	S	61	ILE
20	S	62	GLU
20	S	72	VAL
20	S	87	THR
20	S	100	ARG
20	S	102	VAL
20	S	121	VAL
20	S	122	GLU
20	S	125	LEU
20	S	127	ASN
20	S	162	THR
20	S	167	ILE
21	T	19	LYS
21	T	27	LYS
21	T	40	THR
21	T	48	GLN
21	T	57	GLU
21	T	64	ASP
21	T	75	VAL
22	V	4	LYS
22	V	7	ARG
22	V	9	LEU
22	V	16	GLU
22	V	25	LEU
22	V	26	PHE
22	V	32	LEU
22	V	37	LEU
22	V	38	GLU
22	V	43	ILE

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Mol	Chain	Res	Type
22	V	45	THR
22	V	47	ARG
22	V	49	THR
22	V	52	ARG
22	V	56	VAL
22	V	60	ARG
22	V	61	GLU
23	W	3	LYS
23	W	4	LEU
23	W	5	GLN
23	W	6	ILE
23	W	12	VAL
23	W	15	ARG
23	W	26	LEU
23	W	33	SER
23	W	40	ASN
23	W	51	LYS
24	Z	3	VAL
24	Z	6	ARG
24	Z	7	ARG
24	Z	11	THR
24	Z	22	ILE
24	Z	24	VAL
24	Z	27	MET
24	Z	40	SER
25	2	5	THR
25	2	11	ARG
25	2	21	LYS
25	2	25	THR
25	2	27	ASN
25	2	43	LEU
26	3	32	LEU
26	3	49	LEU
26	3	53	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
8	G	3	GLN
10	I	78	ASN
14	M	79	HIS
18	Q	91	ASN

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Mol	Chain	Res	Type
20	S	38	ASN
20	S	78	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2690/2923 (92%)	711 (26%)	31 (1%)
2	Y	113/114 (99%)	17 (15%)	0
All	All	2803/3037 (92%)	728 (25%)	31 (1%)

All (728) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	12	U
1	X	15	G
1	X	34	U
1	X	35	G
1	X	39	C
1	X	60	U
1	X	63	U
1	X	64	A
1	X	67	G
1	X	70	G
1	X	71	A
1	X	75	G
1	X	80	G
1	X	90	A
1	X	91	A
1	X	96	G
1	X	101	G
1	X	102	A
1	X	109	G
1	X	111	U
1	X	113	U
1	X	117	A
1	X	118	A
1	X	119	U
1	X	120	G
1	X	124	A
1	X	130	A
1	X	133	A

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Mol	Chain	Res	Type
1	X	134	U
1	X	136	A
1	X	139	U
1	X	140	A
1	X	144	C
1	X	152	C
1	X	154	A
1	X	157	U
1	X	163	U
1	X	164	A
1	X	165	C
1	X	166	A
1	X	167	U
1	X	168	A
1	X	169	G
1	X	170	C
1	X	172	U
1	X	173	A
1	X	175	C
1	X	176	A
1	X	178	A
1	X	179	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	184	C
1	X	199	A
1	X	202	A
1	X	207	A
1	X	217	G
1	X	219	A
1	X	225	A
1	X	229	A
1	X	230	A
1	X	232	U
1	X	233	U
1	X	235	G
1	X	247	A
1	X	248	G
1	X	251	G
1	X	255	G
1	X	268	A

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Mol	Chain	Res	Type
1	X	282	A
1	X	284	C
1	X	285	U
1	X	286	U
1	X	287	G
1	X	288	C
1	X	290	U
1	X	291	G
1	X	293	U
1	X	298	U
1	X	299	U
1	X	300	G
1	X	303	G
1	X	308	C
1	X	310	C
1	X	311	U
1	X	313	U
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	323	C
1	X	328	G
1	X	329	A
1	X	330	C
1	X	331	G
1	X	332	A
1	X	338	G
1	X	342	A
1	X	344	U
1	X	345	C
1	X	354	A
1	X	363	A
1	X	364	A
1	X	372	A
1	X	373	A
1	X	375	A
1	X	376	A
1	X	382	U
1	X	386	C
1	X	388	A
1	X	389	A

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Mol	Chain	Res	Type
1	X	390	A
1	X	392	U
1	X	394	U
1	X	395	U
1	X	399	U
1	X	401	U
1	X	403	U
1	X	404	U
1	X	405	G
1	X	406	A
1	X	412	U
1	X	413	C
1	X	416	G
1	X	417	A
1	X	418	G
1	X	426	G
1	X	432	G
1	X	440	C
1	X	444	C
1	X	447	A
1	X	448	A
1	X	449	U
1	X	450	C
1	X	451	U
1	X	452	G
1	X	457	G
1	X	466	C
1	X	470	G
1	X	474	A
1	X	497	U
1	X	503	A
1	X	504	G
1	X	506	A
1	X	523	A
1	X	525	A
1	X	526	A
1	X	527	G
1	X	539	G
1	X	543	G
1	X	549	U
1	X	550	A
1	X	553	A

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Mol	Chain	Res	Type
1	X	554	C
1	X	555	C
1	X	567	G
1	X	572	C
1	X	576	U
1	X	577	A
1	X	578	G
1	X	583	A
1	X	590	U
1	X	592	A
1	X	593	U
1	X	594	G
1	X	606	G
1	X	612	U
1	X	615	A
1	X	616	G
1	X	618	A
1	X	629	A
1	X	644	C
1	X	646	A
1	X	647	G
1	X	658	A
1	X	659	A
1	X	660	A
1	X	661	U
1	X	665	G
1	X	667	G
1	X	679	G
1	X	682	A
1	X	683	G
1	X	690	U
1	X	691	A
1	X	698	U
1	X	699	U
1	X	700	A
1	X	713	A
1	X	716	C
1	X	722	A
1	X	726	G
1	X	727	G
1	X	731	U
1	X	734	A

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Mol	Chain	Res	Type
1	X	738	U
1	X	740	G
1	X	744	A
1	X	749	G
1	X	755	C
1	X	757	G
1	X	765	U
1	X	766	G
1	X	767	A
1	X	768	A
1	X	772	A
1	X	773	G
1	X	774	G
1	X	775	A
1	X	776	C
1	X	783	G
1	X	784	A
1	X	785	C
1	X	792	U
1	X	793	G
1	X	802	G
1	X	807	U
1	X	809	A
1	X	813	G
1	X	814	A
1	X	820	G
1	X	822	G
1	X	827	A
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C
1	X	837	G
1	X	838	A
1	X	845	A
1	X	850	G
1	X	851	C
1	X	857	C
1	X	864	A
1	X	866	A
1	X	872	U
1	X	873	U

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Mol	Chain	Res	Type
1	X	875	G
1	X	890	G
1	X	891	A
1	X	921	C
1	X	922	G
1	X	923	A
1	X	924	G
1	X	925	G
1	X	926	G
1	X	938	G
1	X	940	U
1	X	942	C
1	X	943	C
1	X	947	U
1	X	955	A
1	X	959	C
1	X	969	A
1	X	970	U
1	X	971	U
1	X	977	A
1	X	985	A
1	X	986	G
1	X	987	U
1	X	988	C
1	X	989	A
1	X	990	G
1	X	1001	A
1	X	1005	G
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1029	C
1	X	1033	G
1	X	1034	A
1	X	1040	A
1	X	1043	U
1	X	1049	C
1	X	1052	A
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1064	A

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Mol	Chain	Res	Type
1	X	1066	G
1	X	1067	U
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1078	G
1	X	1085	U
1	X	1086	G
1	X	1087	C
1	X	1089	C
1	X	1090	A
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1098	A
1	X	1145	U
1	X	1146	C
1	X	1147	A
1	X	1150	A
1	X	1151	G
1	X	1152	U
1	X	1154	G
1	X	1155	A
1	X	1156	G
1	X	1172	A
1	X	1174	U
1	X	1176	U
1	X	1178	C
1	X	1185	U
1	X	1186	A
1	X	1187	A
1	X	1195	A
1	X	1200	A
1	X	1202	C
1	X	1213	C
1	X	1214	C
1	X	1215	U
1	X	1218	G
1	X	1220	A
1	X	1221	C
1	X	1248	U
1	X	1262	U

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Mol	Chain	Res	Type
1	X	1274	G
1	X	1275	A
1	X	1278	G
1	X	1285	A
1	X	1286	G
1	X	1291	A
1	X	1293	U
1	X	1294	G
1	X	1303	A
1	X	1309	G
1	X	1310	A
1	X	1313	G
1	X	1323	A
1	X	1324	A
1	X	1337	A
1	X	1338	U
1	X	1340	G
1	X	1349	U
1	X	1358	A
1	X	1365	G
1	X	1366	U
1	X	1379	A
1	X	1389	U
1	X	1395	G
1	X	1397	G
1	X	1398	G
1	X	1401	G
1	X	1402	A
1	X	1403	C
1	X	1405	G
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1424	A
1	X	1431	U
1	X	1432	A
1	X	1433	U
1	X	1435	C
1	X	1437	U
1	X	1440	A
1	X	1449	A

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Mol	Chain	Res	Type
1	X	1450	A
1	X	1451	U
1	X	1453	G
1	X	1454	U
1	X	1459	A
1	X	1460	U
1	X	1463	A
1	X	1464	U
1	X	1465	G
1	X	1466	G
1	X	1467	G
1	X	1468	G
1	X	1469	G
1	X	1470	G
1	X	1471	A
1	X	1472	C
1	X	1477	U
1	X	1480	G
1	X	1481	A
1	X	1487	G
1	X	1488	A
1	X	1489	A
1	X	1490	G
1	X	1491	C
1	X	1492	G
1	X	1493	U
1	X	1494	G
1	X	1495	C
1	X	1496	G
1	X	1499	U
1	X	1505	G
1	X	1508	C
1	X	1509	G
1	X	1510	U
1	X	1511	C
1	X	1515	G
1	X	1516	C
1	X	1519	U
1	X	1520	A
1	X	1521	A
1	X	1524	C
1	X	1525	U

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Mol	Chain	Res	Type
1	X	1526	G
1	X	1527	A
1	X	1529	U
1	X	1540	U
1	X	1541	C
1	X	1542	C
1	X	1543	G
1	X	1544	G
1	X	1546	A
1	X	1547	C
1	X	1548	U
1	X	1549	C
1	X	1550	G
1	X	1555	G
1	X	1556	G
1	X	1557	C
1	X	1560	A
1	X	1567	A
1	X	1570	G
1	X	1575	A
1	X	1592	A
1	X	1593	G
1	X	1594	U
1	X	1599	G
1	X	1602	U
1	X	1603	U
1	X	1605	A
1	X	1606	C
1	X	1613	G
1	X	1614	A
1	X	1616	A
1	X	1623	U
1	X	1625	U
1	X	1628	A
1	X	1630	A
1	X	1631	G
1	X	1636	U
1	X	1637	A
1	X	1638	G
1	X	1651	C
1	X	1652	A
1	X	1653	A

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Mol	Chain	Res	Type
1	X	1654	A
1	X	1657	G
1	X	1662	A
1	X	1663	G
1	X	1683	U
1	X	1684	A
1	X	1690	A
1	X	1691	G
1	X	1692	C
1	X	1709	A
1	X	1713	A
1	X	1718	G
1	X	1719	C
1	X	1737	U
1	X	1738	C
1	X	1740	G
1	X	1744	A
1	X	1745	A
1	X	1748	G
1	X	1756	U
1	X	1757	U
1	X	1760	G
1	X	1761	G
1	X	1762	U
1	X	1763	U
1	X	1765	A
1	X	1766	C
1	X	1767	G
1	X	1768	C
1	X	1770	C
1	X	1771	A
1	X	1772	G
1	X	1789	A
1	X	1790	G
1	X	1791	G
1	X	1800	A
1	X	1803	G
1	X	1808	U
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1835	U

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Mol	Chain	Res	Type
1	X	1836	A
1	X	1837	A
1	X	1843	U
1	X	1845	U
1	X	1846	A
1	X	1847	U
1	X	1848	A
1	X	1856	A
1	X	1860	C
1	X	1865	C
1	X	1866	G
1	X	1886	A
1	X	1901	C
1	X	1902	G
1	X	1903	A
1	X	1908	A
1	X	1909	C
1	X	1911	A
1	X	1912	A
1	X	1926	A
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1934	G
1	X	1935	C
1	X	1936	C
1	X	1954	A
1	X	1955	A
1	X	1956	G
1	X	1957	G
1	X	1964	A
1	X	1965	A
1	X	1982	U
1	X	1990	C
1	X	1991	G
1	X	1993	A
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2003	U
1	X	2009	U

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Mol	Chain	Res	Type
1	X	2019	G
1	X	2020	U
1	X	2024	A
1	X	2041	A
1	X	2045	A
1	X	2046	U
1	X	2050	A
1	X	2054	G
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2070	C
1	X	2077	C
1	X	2079	G
1	X	2082	C
1	X	2083	G
1	X	2087	A
1	X	2088	G
1	X	2094	G
1	X	2096	G
1	X	2107	G
1	X	2117	A
1	X	2119	U
1	X	2124	U
1	X	2125	U
1	X	2126	C
1	X	2217	G
1	X	2219	C
1	X	2221	U
1	X	2224	U
1	X	2225	A
1	X	2229	C
1	X	2230	G
1	X	2231	C
1	X	2232	A
1	X	2233	C
1	X	2236	C
1	X	2237	U
1	X	2238	U
1	X	2239	A
1	X	2240	U
1	X	2241	C

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Mol	Chain	Res	Type
1	X	2244	G
1	X	2246	U
1	X	2252	A
1	X	2262	G
1	X	2265	G
1	X	2266	G
1	X	2270	U
1	X	2295	A
1	X	2298	G
1	X	2306	G
1	X	2310	C
1	X	2315	A
1	X	2326	G
1	X	2332	U
1	X	2333	U
1	X	2334	G
1	X	2335	G
1	X	2336	A
1	X	2338	A
1	X	2347	A
1	X	2348	G
1	X	2352	G
1	X	2361	U
1	X	2362	A
1	X	2363	A
1	X	2372	G
1	X	2374	C
1	X	2377	C
1	X	2386	C
1	X	2393	A
1	X	2398	G
1	X	2399	G
1	X	2409	G
1	X	2410	G
1	X	2411	A
1	X	2412	C
1	X	2418	G
1	X	2429	U
1	X	2433	C
1	X	2434	A
1	X	2450	U
1	X	2452	A

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Mol	Chain	Res	Type
1	X	2456	G
1	X	2457	A
1	X	2459	A
1	X	2462	A
1	X	2468	C
1	X	2473	G
1	X	2475	A
1	X	2485	U
1	X	2486	A
1	X	2492	C
1	X	2495	A
1	X	2497	G
1	X	2500	U
1	X	2503	A
1	X	2504	C
1	X	2514	G
1	X	2529	G
1	X	2532	G
1	X	2533	U
1	X	2534	C
1	X	2540	A
1	X	2545	A
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2574	U
1	X	2576	G
1	X	2581	U
1	X	2590	U
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2603	G
1	X	2605	G
1	X	2609	G
1	X	2612	U
1	X	2628	C
1	X	2629	A
1	X	2636	U
1	X	2640	U

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Mol	Chain	Res	Type
1	X	2641	A
1	X	2642	U
1	X	2656	A
1	X	2657	G
1	X	2663	U
1	X	2664	U
1	X	2682	G
1	X	2683	U
1	X	2687	A
1	X	2696	G
1	X	2698	A
1	X	2709	U
1	X	2712	G
1	X	2715	G
1	X	2716	U
1	X	2717	A
1	X	2734	C
1	X	2740	A
1	X	2741	G
1	X	2751	U
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2771	G
1	X	2778	G
1	X	2784	A
1	X	2787	C
1	X	2792	A
1	X	2793	G
1	X	2805	A
1	X	2806	U
1	X	2807	G
1	X	2817	A
1	X	2818	A
1	X	2820	U
1	X	2821	U
1	X	2824	G
1	X	2827	A
1	X	2828	U
1	X	2832	A
1	X	2850	G
1	X	2853	U

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Mol	Chain	Res	Type
1	X	2855	A
1	X	2856	U
1	X	2863	G
1	X	2877	G
1	X	2884	G
1	X	2887	G
1	X	2899	A
1	X	2900	C
1	X	2903	A
1	X	2913	G
1	X	2921	C
2	Y	10	U
2	Y	23	U
2	Y	24	C
2	Y	34	C
2	Y	35	C
2	Y	39	G
2	Y	42	G
2	Y	43	A
2	Y	50	A
2	Y	54	U
2	Y	55	A
2	Y	74	G
2	Y	84	U
2	Y	87	G
2	Y	88	U
2	Y	106	U
2	Y	108	G

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	90	A
1	X	165	C
1	X	285	U
1	X	373	A
1	X	502	C
1	X	525	A
1	X	614	U
1	X	616	G
1	X	836	C
1	X	890	G

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Mol	Chain	Res	Type
1	X	1028	G
1	X	1091	G
1	X	1176	U
1	X	1310	A
1	X	1323	A
1	X	1488	A
1	X	1510	U
1	X	1520	A
1	X	1556	G
1	X	1636	U
1	X	1653	A
1	X	1885	G
1	X	1901	C
1	X	1963	A
1	X	2062	G
1	X	2087	A
1	X	2314	A
1	X	2433	C
1	X	2682	G
1	X	2783	U
1	X	2816	C

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 299 ligands modelled in this entry, 294 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	MPD	X	3002	-	7,7,7	0.34	0	9,10,10	0.15	0
27	95H	X	3001	-	25,28,28	1.86	5 (20%)	32,40,40	2.67	9 (28%)
28	MPD	X	3003	-	7,7,7	1.65	1 (14%)	9,10,10	0.68	0
32	SPD	X	3286	-	9,9,9	0.34	0	8,8,8	0.30	0
31	EPE	X	3285	-	15,15,15	0.54	0	18,20,20	0.74	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	MPD	X	3002	-	-	2/5/5/5	-
27	95H	X	3001	-	-	5/20/42/42	0/2/2/2
28	MPD	X	3003	-	-	1/5/5/5	-
32	SPD	X	3286	-	-	0/7/7/7	-
31	EPE	X	3285	-	-	5/9/19/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	3001	95H	C12-N13	6.46	1.48	1.34
28	X	3003	MPD	C3-C2	3.80	1.64	1.53
27	X	3001	95H	C18-C12	-3.27	1.43	1.50
27	X	3001	95H	C21-N24	2.94	1.52	1.45
27	X	3001	95H	O10-C2	-2.55	1.37	1.43
27	X	3001	95H	C20-C21	2.53	1.43	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	3001	95H	C22-C21-N24	-9.15	112.49	119.38
27	X	3001	95H	C20-C21-N24	7.11	124.73	119.38
27	X	3001	95H	C20-C19-C18	-4.25	115.83	120.78
27	X	3001	95H	C23-C18-C19	4.03	124.32	118.59
27	X	3001	95H	C18-C12-N13	-3.05	111.21	117.06
27	X	3001	95H	O10-C2-C1	2.74	117.21	109.94
27	X	3001	95H	C23-C18-C12	-2.71	111.85	120.62
31	X	3285	EPE	O2S-S-C10	2.35	109.75	106.92
27	X	3001	95H	O10-C2-C3	-2.21	105.23	110.35
27	X	3001	95H	C23-C22-C21	-2.18	117.05	120.08

There are no chirality outliers.

All (13) torsion outliers are listed below:

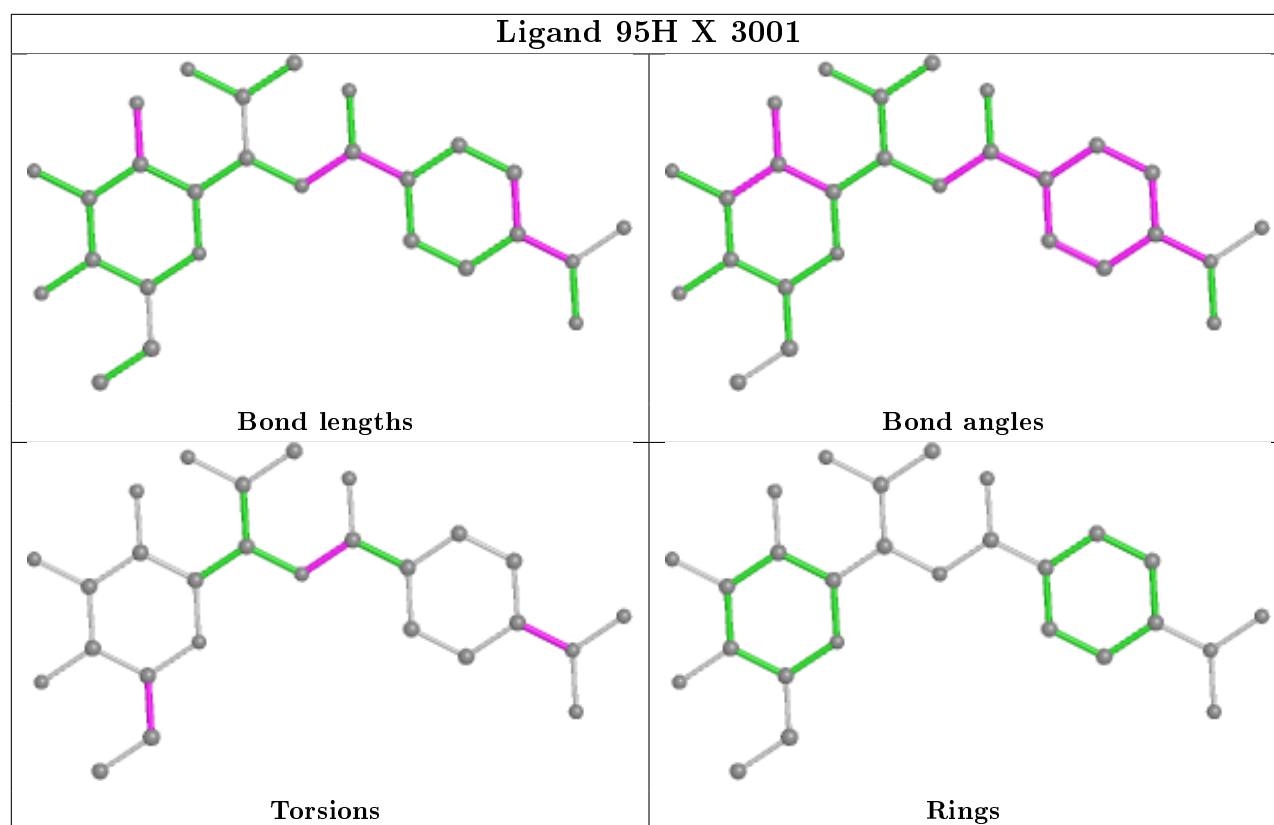
Mol	Chain	Res	Type	Atoms
31	X	3285	EPE	C10-C9-N1-C6
31	X	3285	EPE	C9-C10-S-O2S
27	X	3001	95H	O6-C5-S16-C25
27	X	3001	95H	C18-C12-N13-C7
27	X	3001	95H	O11-C12-N13-C7
31	X	3285	EPE	C9-C10-S-O3S
31	X	3285	EPE	C10-C9-N1-C2
27	X	3001	95H	C20-C21-N24-O26
27	X	3001	95H	C22-C21-N24-O26
28	X	3003	MPD	C2-C3-C4-C5
31	X	3285	EPE	C9-C10-S-O1S
28	X	3002	MPD	C1-C2-C3-C4
28	X	3002	MPD	C2-C3-C4-O4

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	X	3002	MPD	1	0
27	X	3001	95H	2	0
28	X	3003	MPD	1	0
32	X	3286	SPD	3	0

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



## 5.7 Other polymers [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
11	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	69:PHE	C	70:PRO	N	1.16

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	X	2710/2923 (92%)	-0.12	30 (1%) 80 77	46, 97, 197, 300	0
2	Y	114/114 (100%)	0.10	2 (1%) 68 66	68, 128, 188, 250	0
3	A	260/277 (93%)	0.18	10 (3%) 40 39	87, 134, 168, 183	0
4	B	215/220 (97%)	-0.22	1 (0%) 91 89	50, 74, 96, 119	0
5	C	198/207 (95%)	-0.15	1 (0%) 91 89	63, 92, 113, 140	0
6	D	137/179 (76%)	1.23	33 (24%) 0 1	162, 186, 212, 219	0
7	E	147/178 (82%)	0.00	9 (6%) 21 23	122, 156, 181, 185	0
8	G	142/145 (97%)	-0.22	0 100 100	58, 70, 87, 95	0
9	H	122/122 (100%)	-0.03	0 100 100	75, 93, 118, 125	0
10	I	127/140 (90%)	0.25	7 (5%) 25 26	49, 108, 135, 139	0
11	J	138/144 (95%)	-0.05	1 (0%) 87 85	69, 89, 116, 141	0
12	K	119/122 (97%)	-0.15	0 100 100	63, 81, 115, 135	0
13	L	110/119 (92%)	0.26	9 (8%) 11 14	106, 120, 143, 152	0
14	M	111/116 (95%)	-0.02	2 (1%) 68 66	77, 91, 127, 151	0
15	N	116/118 (98%)	-0.18	0 100 100	49, 65, 90, 102	0
16	O	101/102 (99%)	-0.40	0 100 100	47, 79, 98, 115	0
17	P	112/117 (95%)	-0.00	0 100 100	59, 70, 103, 129	0
18	Q	90/91 (98%)	0.44	9 (10%) 7 9	100, 123, 152, 170	0
19	R	102/105 (97%)	0.30	10 (9%) 7 10	95, 115, 171, 180	0
20	S	174/217 (80%)	0.17	14 (8%) 12 15	75, 102, 184, 192	0
21	T	76/94 (80%)	0.00	1 (1%) 77 74	76, 88, 113, 155	0
22	V	65/69 (94%)	0.04	1 (1%) 73 71	119, 136, 160, 164	0
23	W	57/59 (96%)	0.22	0 100 100	59, 71, 95, 103	0
24	Z	44/58 (75%)	0.02	0 100 100	55, 86, 144, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	2	44/45 (97%)	1.09	7 (15%) 1 3	80, 89, 96, 104	0
26	3	65/66 (98%)	-0.02	1 (1%) 73 71	70, 81, 95, 100	0
All	All	5696/6147 (92%)	-0.01	148 (2%) 56 54	46, 96, 186, 300	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	73	SER	12.7
6	D	74	ILE	11.5
6	D	75	ALA	9.1
6	D	179	LYS	7.7
6	D	32	ASP	5.6
6	D	77	PHE	5.5
13	L	42	ALA	5.2
13	L	40	ILE	5.2
3	A	269	LEU	4.9
25	2	17	HIS	4.8
6	D	72	LYS	4.6
6	D	76	THR	4.6
6	D	170	LEU	4.5
6	D	69	LYS	4.5
19	R	68	VAL	4.4
6	D	163	ASP	4.4
13	L	56	ALA	4.3
20	S	100	ARG	4.3
6	D	178	ARG	4.3
6	D	116	GLY	4.2
3	A	259	THR	4.1
1	X	1150	A	3.8
6	D	31	ILE	3.8
20	S	124	PRO	3.6
19	R	70	LEU	3.6
3	A	273	GLY	3.6
18	Q	2	GLU	3.6
20	S	123	GLN	3.6
6	D	113	ASP	3.5
14	M	3	ASN	3.5
18	Q	70	GLY	3.4
6	D	87	ALA	3.4
18	Q	43	GLU	3.4
19	R	34	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	X	2505	A	3.3
7	E	171	ARG	3.2
20	S	125	LEU	3.2
25	2	22	ARG	3.2
1	X	1906	C	3.1
3	A	272	ARG	3.1
13	L	41	TYR	3.1
10	I	104	ASN	3.1
18	Q	9	ARG	3.1
19	R	67	ASN	3.0
1	X	1931	G	3.0
6	D	81	GLU	2.9
6	D	43	ALA	2.9
6	D	38	MET	2.9
1	X	311	U	2.9
6	D	67	VAL	2.9
19	R	69	GLN	2.9
20	S	119	GLY	2.9
18	Q	46	PHE	2.8
10	I	92	THR	2.8
10	I	91	VAL	2.8
1	X	2921	C	2.8
1	X	306	C	2.8
6	D	33	LYS	2.7
1	X	1993	A	2.7
18	Q	10	PRO	2.7
1	X	2503	A	2.7
1	X	1932	C	2.7
2	Y	1	U	2.7
20	S	128	LEU	2.7
25	2	2	VAL	2.7
3	A	93	LEU	2.7
20	S	169	ASN	2.7
20	S	101	THR	2.7
1	X	1957	G	2.7
1	X	275	A	2.6
19	R	78	PRO	2.6
7	E	153	PRO	2.6
6	D	79	LEU	2.6
18	Q	7	LEU	2.6
6	D	164	GLU	2.6
1	X	2408	C	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
18	Q	28	ASP	2.6
20	S	144	ASP	2.6
25	2	18	GLY	2.6
1	X	1275	A	2.5
7	E	39	GLU	2.5
20	S	110	GLY	2.5
6	D	169	LEU	2.5
3	A	258	LYS	2.5
6	D	37	ASN	2.5
19	R	64	HIS	2.5
6	D	111	VAL	2.5
4	B	27	VAL	2.4
6	D	65	PRO	2.4
1	X	285	U	2.4
6	D	156	ILE	2.4
19	R	26	THR	2.4
19	R	15	LYS	2.4
7	E	80	SER	2.4
7	E	169	VAL	2.4
11	J	62	GLY	2.4
3	A	53	HIS	2.4
3	A	115	ILE	2.4
13	L	57	SER	2.4
25	2	14	SER	2.4
20	S	132	ALA	2.4
1	X	394	U	2.4
25	2	43	LEU	2.3
10	I	123	VAL	2.3
6	D	82	GLY	2.3
1	X	2501	U	2.3
3	A	113	GLY	2.3
2	Y	35	C	2.3
6	D	172	ASN	2.3
1	X	2502	C	2.3
10	I	95	LEU	2.3
7	E	162	ILE	2.3
13	L	107	ALA	2.3
1	X	2817	A	2.3
6	D	35	VAL	2.3
22	V	30	PHE	2.3
1	X	2335	G	2.2
21	T	22	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
10	I	93	PRO	2.2
10	I	111	ILE	2.2
1	X	2230	G	2.2
3	A	122	ALA	2.2
5	C	180	GLY	2.2
20	S	152	ASP	2.2
1	X	2498	A	2.2
1	X	453	G	2.2
20	S	131	THR	2.2
14	M	94	VAL	2.2
6	D	78	ARG	2.2
13	L	99	TYR	2.2
1	X	283	G	2.2
7	E	41	MET	2.1
25	2	16	VAL	2.1
13	L	31	LEU	2.1
1	X	2239	A	2.1
1	X	2409	G	2.1
1	X	454	G	2.1
13	L	102	HIS	2.1
7	E	161	GLY	2.1
6	D	61	THR	2.1
18	Q	47	ASN	2.1
1	X	310	C	2.1
1	X	284	C	2.1
19	R	12	ILE	2.0
7	E	172	LYS	2.0
20	S	92	LEU	2.0
26	3	2	PRO	2.0
1	X	406	A	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	MG	X	3255	1/1	-0.21	0.34	112,112,112,112	0
30	MG	J	201	1/1	0.17	2.12	107,107,107,107	0
30	MG	X	3268	1/1	0.21	0.31	134,134,134,134	0
30	MG	X	3240	1/1	0.28	0.30	87,87,87,87	0
29	MN	X	3145	1/1	0.37	0.32	144,144,144,144	0
30	MG	X	3224	1/1	0.38	0.28	97,97,97,97	0
30	MG	X	3271	1/1	0.42	0.67	90,90,90,90	0
30	MG	X	3246	1/1	0.43	0.27	131,131,131,131	0
30	MG	X	3261	1/1	0.46	0.36	163,163,163,163	0
30	MG	C	301	1/1	0.50	0.37	74,74,74,74	0
29	MN	X	3222	1/1	0.52	0.27	142,142,142,142	0
29	MN	X	3214	1/1	0.54	0.35	125,125,125,125	0
30	MG	X	3260	1/1	0.55	0.89	73,73,73,73	0
30	MG	X	3227	1/1	0.57	0.19	93,93,93,93	0
29	MN	X	3062	1/1	0.62	0.41	135,135,135,135	0
30	MG	X	3202	1/1	0.64	0.44	64,64,64,64	0
29	MN	X	3172	1/1	0.67	0.10	126,126,126,126	0
29	MN	X	3203	1/1	0.67	0.18	141,141,141,141	0
29	MN	X	3156	1/1	0.67	0.34	104,104,104,104	0
30	MG	X	3266	1/1	0.67	0.41	119,119,119,119	0
29	MN	X	3169	1/1	0.68	0.40	98,98,98,98	0
30	MG	X	3267	1/1	0.70	0.19	91,91,91,91	0
30	MG	X	3280	1/1	0.70	0.53	66,66,66,66	0
29	MN	X	3191	1/1	0.70	0.11	126,126,126,126	0
30	MG	X	3247	1/1	0.70	0.33	69,69,69,69	0
29	MN	X	3179	1/1	0.70	0.19	110,110,110,110	0
29	MN	X	3194	1/1	0.70	0.25	140,140,140,140	0
29	MN	X	3229	1/1	0.70	0.14	144,144,144,144	0
30	MG	3	104	1/1	0.70	0.47	56,56,56,56	0
29	MN	X	3234	1/1	0.71	0.22	137,137,137,137	0
29	MN	X	3075	1/1	0.73	0.45	102,102,102,102	0
30	MG	X	3283	1/1	0.73	0.42	59,59,59,59	0
29	MN	X	3142	1/1	0.73	0.11	111,111,111,111	0
30	MG	X	3242	1/1	0.74	0.41	60,60,60,60	0
29	MN	3	101	1/1	0.74	0.21	96,96,96,96	0
29	MN	X	3187	1/1	0.74	0.15	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MN	X	3141	1/1	0.74	0.29	104,104,104,104	0
29	MN	X	3231	1/1	0.75	0.17	125,125,125,125	0
29	MN	X	3205	1/1	0.75	0.13	143,143,143,143	0
30	MG	X	3265	1/1	0.75	0.24	73,73,73,73	0
30	MG	X	3274	1/1	0.76	0.86	69,69,69,69	0
30	MG	X	3181	1/1	0.76	0.36	89,89,89,89	0
30	MG	X	3257	1/1	0.77	0.04	156,156,156,156	0
30	MG	X	3279	1/1	0.77	0.54	66,66,66,66	0
29	MN	X	3131	1/1	0.77	0.35	114,114,114,114	0
30	MG	X	3264	1/1	0.78	0.47	102,102,102,102	0
30	MG	X	3228	1/1	0.78	0.24	65,65,65,65	0
30	MG	X	3112	1/1	0.78	0.38	84,84,84,84	0
29	MN	X	3198	1/1	0.80	0.34	100,100,100,100	0
29	MN	X	3171	1/1	0.80	0.18	117,117,117,117	0
30	MG	X	3204	1/1	0.81	0.28	67,67,67,67	0
29	MN	X	3189	1/1	0.81	0.14	123,123,123,123	0
30	MG	X	3196	1/1	0.81	0.50	78,78,78,78	0
30	MG	X	3276	1/1	0.81	0.82	67,67,67,67	0
29	MN	X	3051	1/1	0.81	0.22	100,100,100,100	0
29	MN	X	3096	1/1	0.81	0.46	98,98,98,98	0
29	MN	X	3092	1/1	0.81	0.24	87,87,87,87	0
29	MN	X	3150	1/1	0.81	0.22	98,98,98,98	0
29	MN	X	3192	1/1	0.82	0.10	106,106,106,106	0
30	MG	X	3182	1/1	0.82	0.81	53,53,53,53	0
29	MN	3	102	1/1	0.82	0.31	101,101,101,101	0
29	MN	X	3165	1/1	0.82	0.12	109,109,109,109	0
29	MN	X	3199	1/1	0.83	0.23	131,131,131,131	0
30	MG	X	3223	1/1	0.83	0.79	71,71,71,71	0
28	MPD	X	3003	8/8	0.83	0.30	80,80,80,80	0
30	MG	X	3217	1/1	0.83	0.66	64,64,64,64	0
29	MN	3	103	1/1	0.83	0.48	129,129,129,129	0
29	MN	X	3170	1/1	0.84	0.22	103,103,103,103	0
29	MN	X	3162	1/1	0.84	0.10	110,110,110,110	0
29	MN	X	3176	1/1	0.84	0.13	128,128,128,128	0
30	MG	X	3277	1/1	0.84	0.51	59,59,59,59	0
30	MG	X	3258	1/1	0.85	0.23	64,64,64,64	0
29	MN	X	3147	1/1	0.85	0.10	113,113,113,113	0
29	MN	X	3074	1/1	0.86	0.16	129,129,129,129	0
29	MN	Z	101	1/1	0.86	0.32	109,109,109,109	0
30	MG	X	3256	1/1	0.86	0.39	91,91,91,91	0
30	MG	X	3158	1/1	0.86	0.33	48,48,48,48	0
30	MG	X	3263	1/1	0.86	0.46	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MN	X	3212	1/1	0.87	0.19	117,117,117,117	0
29	MN	X	3235	1/1	0.87	0.10	118,118,118,118	0
29	MN	X	3157	1/1	0.87	0.18	87,87,87,87	0
30	MG	X	3251	1/1	0.87	0.16	65,65,65,65	0
30	MG	X	3168	1/1	0.87	0.18	73,73,73,73	0
29	MN	X	3225	1/1	0.87	0.23	101,101,101,101	0
29	MN	X	3006	1/1	0.87	0.14	49,49,49,49	0
29	MN	X	3178	1/1	0.88	0.27	108,108,108,108	0
29	MN	X	3164	1/1	0.88	0.24	110,110,110,110	0
29	MN	X	3185	1/1	0.88	0.14	100,100,100,100	0
29	MN	E	201	1/1	0.88	0.17	125,125,125,125	0
30	MG	X	3269	1/1	0.88	0.61	104,104,104,104	0
29	MN	X	3135	1/1	0.88	0.17	108,108,108,108	0
29	MN	X	3029	1/1	0.88	0.17	82,82,82,82	0
29	MN	X	3151	1/1	0.88	0.10	97,97,97,97	0
30	MG	X	3195	1/1	0.88	0.47	57,57,57,57	0
30	MG	X	3281	1/1	0.88	0.46	69,69,69,69	0
30	MG	X	3259	1/1	0.88	0.57	61,61,61,61	0
29	MN	X	3155	1/1	0.89	0.19	105,105,105,105	0
32	SPD	X	3286	10/10	0.89	0.25	65,65,65,65	0
30	MG	X	3239	1/1	0.89	0.33	46,46,46,46	0
30	MG	X	3253	1/1	0.89	0.27	90,90,90,90	0
29	MN	X	3037	1/1	0.89	0.20	78,78,78,78	0
29	MN	X	3018	1/1	0.89	0.30	86,86,86,86	0
29	MN	X	3123	1/1	0.89	0.19	109,109,109,109	0
29	MN	X	3016	1/1	0.89	0.17	87,87,87,87	0
30	MG	X	3197	1/1	0.89	0.35	54,54,54,54	0
29	MN	X	3215	1/1	0.90	0.18	119,119,119,119	0
29	MN	X	3073	1/1	0.90	0.17	120,120,120,120	0
29	MN	X	3190	1/1	0.90	0.21	117,117,117,117	0
30	MG	X	3218	1/1	0.90	0.29	74,74,74,74	0
30	MG	X	3232	1/1	0.90	0.10	67,67,67,67	0
30	MG	X	3238	1/1	0.90	0.76	58,58,58,58	0
30	MG	Y	203	1/1	0.90	0.07	122,122,122,122	0
29	MN	X	3163	1/1	0.90	0.14	99,99,99,99	0
29	MN	X	3206	1/1	0.90	0.21	127,127,127,127	0
29	MN	X	3154	1/1	0.90	0.25	114,114,114,114	0
29	MN	X	3052	1/1	0.90	0.14	121,121,121,121	0
29	MN	X	3082	1/1	0.91	0.19	59,59,59,59	0
30	MG	X	3152	1/1	0.91	0.33	57,57,57,57	0
29	MN	X	3184	1/1	0.91	0.09	126,126,126,126	0
29	MN	X	3208	1/1	0.91	0.15	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MN	X	3130	1/1	0.91	0.17	94,94,94,94	0
29	MN	X	3233	1/1	0.91	0.13	59,59,59,59	0
29	MN	X	3071	1/1	0.91	0.23	83,83,83,83	0
29	MN	X	3174	1/1	0.91	0.16	115,115,115,115	0
29	MN	X	3026	1/1	0.91	0.21	94,94,94,94	0
29	MN	X	3061	1/1	0.91	0.07	119,119,119,119	0
29	MN	X	3008	1/1	0.91	0.13	50,50,50,50	0
30	MG	X	3254	1/1	0.91	0.38	67,67,67,67	0
30	MG	X	3193	1/1	0.91	0.51	78,78,78,78	0
29	MN	X	3053	1/1	0.91	0.13	96,96,96,96	0
29	MN	X	3219	1/1	0.92	0.07	118,118,118,118	0
30	MG	X	3241	1/1	0.92	0.07	91,91,91,91	0
29	MN	X	3033	1/1	0.92	0.34	90,90,90,90	0
30	MG	X	3243	1/1	0.92	0.29	54,54,54,54	0
30	MG	X	3250	1/1	0.92	0.63	66,66,66,66	0
30	MG	X	3160	1/1	0.92	0.15	69,69,69,69	0
29	MN	X	3139	1/1	0.92	0.07	102,102,102,102	0
30	MG	X	3273	1/1	0.92	0.07	57,57,57,57	0
29	MN	X	3125	1/1	0.92	0.10	86,86,86,86	0
30	MG	X	3226	1/1	0.92	0.30	74,74,74,74	0
30	MG	X	3072	1/1	0.92	0.35	41,41,41,41	0
29	MN	X	3132	1/1	0.93	0.22	101,101,101,101	0
29	MN	X	3047	1/1	0.93	0.10	87,87,87,87	0
30	MG	X	3183	1/1	0.93	0.34	72,72,72,72	0
30	MG	X	3036	1/1	0.93	0.16	55,55,55,55	0
29	MN	X	3017	1/1	0.93	0.04	90,90,90,90	0
28	MPD	X	3002	8/8	0.93	0.32	96,96,96,96	0
29	MN	X	3013	1/1	0.93	0.41	67,67,67,67	0
30	MG	X	3252	1/1	0.93	0.39	60,60,60,60	0
29	MN	X	3031	1/1	0.93	0.18	80,80,80,80	0
29	MN	X	3188	1/1	0.93	0.29	117,117,117,117	0
29	MN	X	3067	1/1	0.93	0.18	103,103,103,103	0
29	MN	X	3109	1/1	0.93	0.21	87,87,87,87	0
30	MG	X	3126	1/1	0.93	0.44	58,58,58,58	0
30	MG	X	3201	1/1	0.93	0.38	66,66,66,66	0
29	MN	X	3167	1/1	0.94	0.08	110,110,110,110	0
29	MN	X	3055	1/1	0.94	0.11	129,129,129,129	0
29	MN	X	3076	1/1	0.94	0.14	93,93,93,93	0
29	MN	X	3221	1/1	0.94	0.07	141,141,141,141	0
29	MN	X	3209	1/1	0.94	0.13	105,105,105,105	0
29	MN	X	3144	1/1	0.94	0.13	80,80,80,80	0
30	MG	Y	202	1/1	0.94	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
29	MN	X	3161	1/1	0.94	0.07	130,130,130,130	0
30	MG	X	3270	1/1	0.94	0.26	68,68,68,68	0
29	MN	X	3120	1/1	0.94	0.14	72,72,72,72	0
29	MN	X	3186	1/1	0.94	0.17	104,104,104,104	0
29	MN	X	3133	1/1	0.94	0.18	85,85,85,85	0
29	MN	X	3081	1/1	0.94	0.17	57,57,57,57	0
29	MN	X	3159	1/1	0.94	0.18	104,104,104,104	0
30	MG	X	3058	1/1	0.94	0.49	63,63,63,63	0
27	95H	X	3001	27/27	0.94	0.24	52,52,52,52	19
29	MN	I	201	1/1	0.94	0.31	95,95,95,95	0
29	MN	X	3138	1/1	0.94	0.18	102,102,102,102	0
29	MN	X	3059	1/1	0.94	0.15	92,92,92,92	0
29	MN	X	3068	1/1	0.94	0.17	84,84,84,84	0
29	MN	X	3039	1/1	0.94	0.16	94,94,94,94	0
30	MG	X	3282	1/1	0.94	0.20	63,63,63,63	0
29	MN	X	3012	1/1	0.95	0.29	72,72,72,72	0
29	MN	X	3056	1/1	0.95	0.19	94,94,94,94	0
29	MN	X	3065	1/1	0.95	0.12	85,85,85,85	0
29	MN	X	3090	1/1	0.95	0.18	69,69,69,69	0
29	MN	X	3111	1/1	0.95	0.13	80,80,80,80	0
30	MG	X	3245	1/1	0.95	0.23	63,63,63,63	0
29	MN	X	3057	1/1	0.95	0.16	93,93,93,93	0
30	MG	X	3069	1/1	0.95	0.42	52,52,52,52	0
29	MN	X	3136	1/1	0.95	0.26	106,106,106,106	0
29	MN	X	3028	1/1	0.95	0.23	90,90,90,90	0
30	MG	G	201	1/1	0.95	0.24	25,25,25,25	0
30	MG	X	3249	1/1	0.95	0.16	89,89,89,89	0
29	MN	X	3088	1/1	0.95	0.22	68,68,68,68	0
29	MN	X	3207	1/1	0.95	0.09	92,92,92,92	0
29	MN	X	3005	1/1	0.95	0.30	53,53,53,53	0
29	MN	X	3045	1/1	0.95	0.13	88,88,88,88	0
30	MG	X	3248	1/1	0.95	0.42	66,66,66,66	0
31	EPE	X	3285	15/15	0.95	0.20	72,72,72,72	0
29	MN	X	3007	1/1	0.95	0.30	61,61,61,61	0
30	MG	X	3213	1/1	0.95	0.26	47,47,47,47	0
29	MN	X	3210	1/1	0.95	0.23	107,107,107,107	0
29	MN	X	3038	1/1	0.95	0.18	73,73,73,73	0
29	MN	X	3117	1/1	0.95	0.09	66,66,66,66	0
29	MN	X	3021	1/1	0.95	0.11	68,68,68,68	0
29	MN	X	3102	1/1	0.95	0.32	77,77,77,77	0
29	MN	X	3230	1/1	0.95	0.10	126,126,126,126	0
30	MG	X	3216	1/1	0.95	0.20	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MN	X	3048	1/1	0.96	0.07	117,117,117,117	0
30	MG	X	3237	1/1	0.96	0.17	93,93,93,93	0
30	MG	X	3032	1/1	0.96	0.59	31,31,31,31	0
29	MN	X	3175	1/1	0.96	0.11	103,103,103,103	0
29	MN	X	3106	1/1	0.96	0.21	99,99,99,99	0
29	MN	X	3119	1/1	0.96	0.08	77,77,77,77	0
29	MN	X	3140	1/1	0.96	0.07	100,100,100,100	0
29	MN	X	3173	1/1	0.96	0.44	112,112,112,112	0
29	MN	X	3091	1/1	0.96	0.13	61,61,61,61	0
29	MN	X	3105	1/1	0.96	0.17	71,71,71,71	0
29	MN	X	3098	1/1	0.96	0.41	70,70,70,70	0
29	MN	X	3066	1/1	0.96	0.12	91,91,91,91	0
29	MN	X	3127	1/1	0.96	0.15	79,79,79,79	0
29	MN	X	3046	1/1	0.96	0.12	94,94,94,94	0
29	MN	X	3054	1/1	0.96	0.34	82,82,82,82	0
29	MN	X	3103	1/1	0.96	0.47	81,81,81,81	0
29	MN	X	3023	1/1	0.96	0.21	70,70,70,70	0
29	MN	X	3134	1/1	0.96	0.11	84,84,84,84	0
29	MN	X	3084	1/1	0.96	0.28	71,71,71,71	0
29	MN	X	3100	1/1	0.96	0.18	59,59,59,59	0
29	MN	X	3064	1/1	0.96	0.37	124,124,124,124	0
29	MN	X	3035	1/1	0.96	0.43	104,104,104,104	0
29	MN	X	3107	1/1	0.96	0.24	68,68,68,68	0
29	MN	X	3060	1/1	0.97	0.10	84,84,84,84	0
29	MN	X	3015	1/1	0.97	0.38	63,63,63,63	0
29	MN	X	3094	1/1	0.97	0.12	83,83,83,83	0
30	MG	X	3244	1/1	0.97	0.23	57,57,57,57	0
29	MN	X	3116	1/1	0.97	0.31	78,78,78,78	0
29	MN	X	3166	1/1	0.97	0.11	95,95,95,95	0
29	MN	X	3236	1/1	0.97	0.06	104,104,104,104	0
29	MN	X	3063	1/1	0.97	0.17	140,140,140,140	0
29	MN	X	3200	1/1	0.97	0.11	136,136,136,136	0
29	MN	X	3114	1/1	0.97	0.20	65,65,65,65	0
29	MN	X	3110	1/1	0.97	0.20	65,65,65,65	0
30	MG	X	3275	1/1	0.97	0.25	57,57,57,57	0
29	MN	X	3220	1/1	0.97	0.06	112,112,112,112	0
29	MN	X	3113	1/1	0.97	0.09	75,75,75,75	0
30	MG	X	3262	1/1	0.97	0.28	82,82,82,82	0
29	MN	X	3093	1/1	0.97	0.14	61,61,61,61	0
29	MN	X	3148	1/1	0.97	0.39	91,91,91,91	0
29	MN	X	3278	1/1	0.97	0.14	99,99,99,99	0
29	MN	X	3146	1/1	0.97	0.09	101,101,101,101	0

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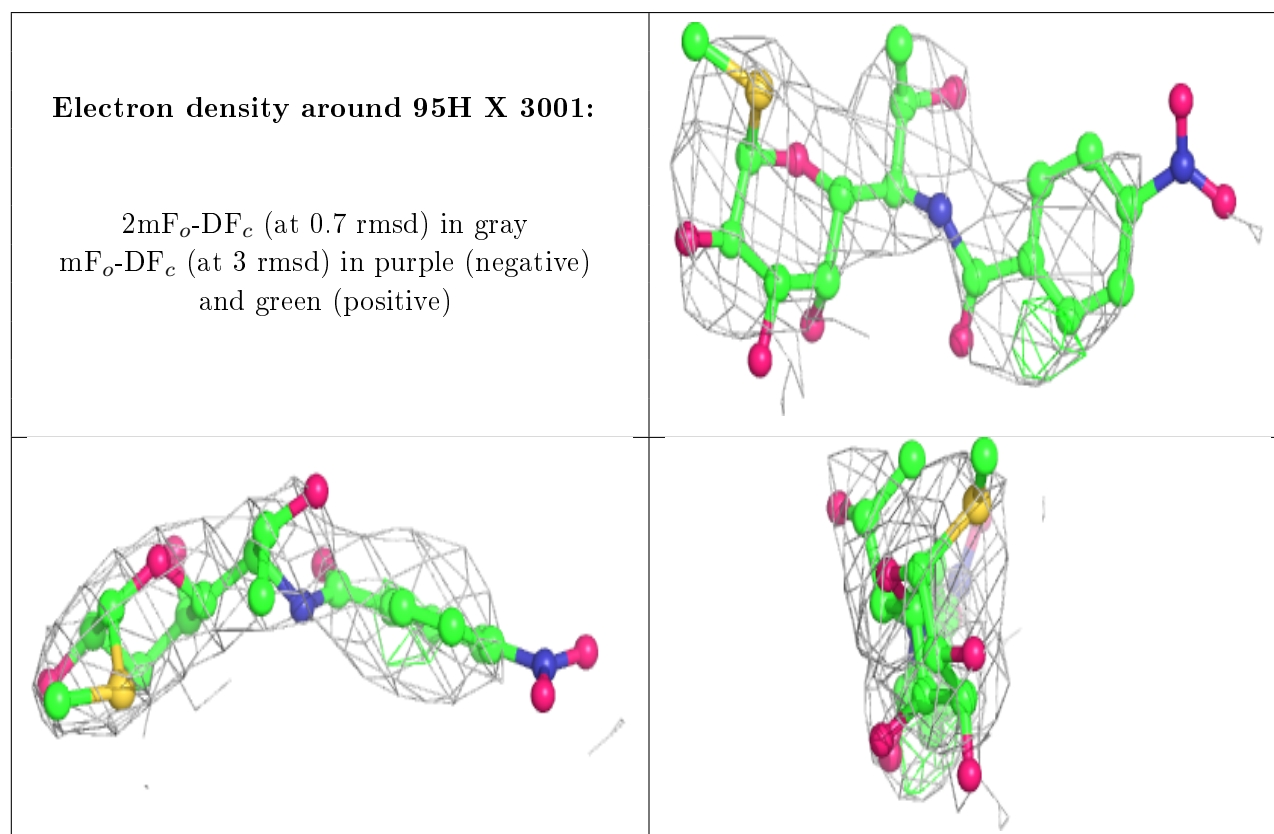
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MN	X	3020	1/1	0.97	0.15	78,78,78,78	0
29	MN	X	3087	1/1	0.97	0.18	63,63,63,63	0
29	MN	X	3027	1/1	0.97	0.15	89,89,89,89	0
29	MN	X	3137	1/1	0.97	0.18	72,72,72,72	0
29	MN	X	3097	1/1	0.97	0.15	79,79,79,79	0
29	MN	X	3089	1/1	0.97	0.14	69,69,69,69	0
29	MN	X	3177	1/1	0.98	0.43	110,110,110,110	0
29	MN	X	3024	1/1	0.98	0.23	74,74,74,74	0
29	MN	X	3034	1/1	0.98	0.11	94,94,94,94	0
29	MN	X	3050	1/1	0.98	0.19	98,98,98,98	0
29	MN	X	3083	1/1	0.98	0.19	56,56,56,56	0
29	MN	X	3049	1/1	0.98	0.23	81,81,81,81	0
29	MN	X	3041	1/1	0.98	0.09	75,75,75,75	0
29	MN	X	3143	1/1	0.98	0.22	44,44,44,44	0
29	MN	X	3030	1/1	0.98	0.06	89,89,89,89	0
29	MN	Y	201	1/1	0.98	0.07	95,95,95,95	0
29	MN	X	3044	1/1	0.98	0.18	93,93,93,93	0
29	MN	X	3070	1/1	0.98	0.27	97,97,97,97	0
29	MN	X	3025	1/1	0.98	0.12	79,79,79,79	0
29	MN	X	3101	1/1	0.98	0.19	60,60,60,60	0
29	MN	X	3108	1/1	0.98	0.21	70,70,70,70	0
29	MN	X	3080	1/1	0.98	0.21	59,59,59,59	0
29	MN	X	3040	1/1	0.98	0.16	79,79,79,79	0
29	MN	X	3115	1/1	0.98	0.19	63,63,63,63	0
29	MN	X	3095	1/1	0.98	0.12	69,69,69,69	0
29	MN	X	3079	1/1	0.98	0.12	70,70,70,70	0
29	MN	X	3043	1/1	0.99	0.18	79,79,79,79	0
29	MN	X	3122	1/1	0.99	0.19	82,82,82,82	0
29	MN	X	3211	1/1	0.99	0.12	100,100,100,100	0
29	MN	X	3004	1/1	0.99	0.29	60,60,60,60	0
29	MN	X	3128	1/1	0.99	0.14	62,62,62,62	0
29	MN	X	3153	1/1	0.99	0.17	99,99,99,99	0
29	MN	X	3014	1/1	0.99	0.19	56,56,56,56	0
29	MN	X	3099	1/1	0.99	0.19	73,73,73,73	0
29	MN	X	3010	1/1	0.99	0.31	59,59,59,59	0
29	MN	X	3022	1/1	0.99	0.14	74,74,74,74	0
29	MN	X	3011	1/1	0.99	0.28	40,40,40,40	0
29	MN	X	3124	1/1	0.99	0.22	76,76,76,76	0
29	MN	X	3042	1/1	0.99	0.14	80,80,80,80	0
29	MN	X	3009	1/1	0.99	0.28	59,59,59,59	0
29	MN	X	3104	1/1	0.99	0.26	86,86,86,86	0
29	MN	X	3085	1/1	0.99	0.25	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MN	X	3149	1/1	0.99	0.12	102,102,102,102	0
29	MN	X	3077	1/1	0.99	0.18	88,88,88,88	0
29	MN	X	3118	1/1	0.99	0.14	69,69,69,69	0
30	MG	X	3272	1/1	0.99	0.10	60,60,60,60	0
30	MG	X	3284	1/1	0.99	0.06	56,56,56,56	0
29	MN	X	3019	1/1	0.99	0.11	73,73,73,73	0
29	MN	X	3121	1/1	0.99	0.07	67,67,67,67	0
29	MN	X	3129	1/1	0.99	0.25	74,74,74,74	0
29	MN	X	3086	1/1	0.99	0.09	62,62,62,62	0
29	MN	X	3180	1/1	0.99	0.17	70,70,70,70	0
29	MN	X	3078	1/1	1.00	0.18	55,55,55,55	0

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.