



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:39 pm BST

PDB ID : 3PIO  
Title : Crystal structure of the synergistic antibiotic pair lankamycin and lankacidin in complex with the large ribosomal subunit  
Authors : Belousoff, M.J.; Shapira, T.; Bashan, A.; Zimmerman, E.; Arakawa, K.; Kinashi, H.; Rozenberg, H.; Yonath, A.  
Deposited on : 2010-11-07  
Resolution : 3.25 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

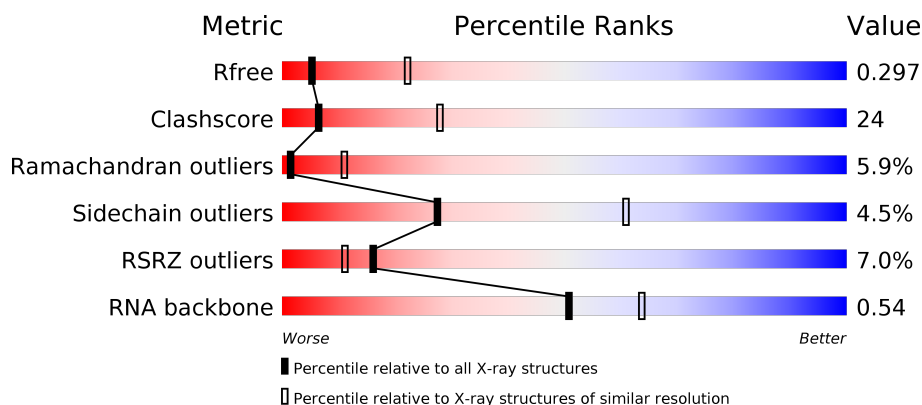
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)
RNA backbone	3102	1034 (3.58-2.90)

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	2880	<div> <div>3%</div> <div>32% 40% 18% 8%</div> </div>
2	Y	123	<div> <div>2%</div> <div>48% 41% 8%</div> </div>
3	A	274	<div> <div>5%</div> <div>42% 45% 5% 8%</div> </div>
4	B	211	<div> <div>%</div> <div>48% 43% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	<div> <div>95%</div> <div>62%38%</div> </div>

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
34	K	X	3074	-	-	-	X

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 84383 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 RIBOSOMAL 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2657	Total	C	N	O	P	0	0	0
			57035	25441	10530	18408	2656			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	253	Total	C	N	O	S	0	0	0
			1920	1196	382	340	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	63	Total	C	N	O	S	0	0	0
			451	280	82	86	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	134	Total	C	N	O	S	0	0	0
			1011	619	206	186				

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	126	Total	C	N	O	S	0	0	0
			1004	633	197	172	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O		0	0	0
			552	341	116	95				

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

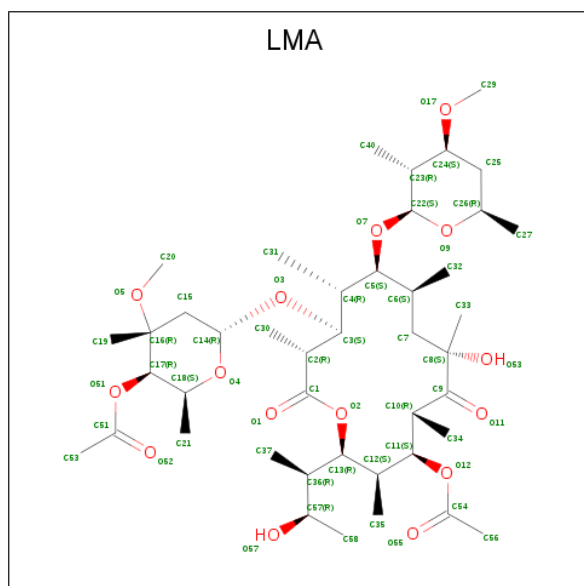
- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	37	Total	C	N	O	S	0	0	0
			297	179	66	47	5			

- Molecule 31 is Lankamycin (three-letter code: LMA) (formula:  $C_{43}H_{74}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	X	1	Total	C	O	0	0
			58	43	15		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	151	Total	Mg	0	0
			151	151		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	I	1	Total 1	Mg 1	0	0
32	Y	1	Total 1	Mg 1	0	0
32	C	1	Total 1	Mg 1	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	37	Total 37	Na 37	0	0
33	A	1	Total 1	Na 1	0	0
33	Z	1	Total 1	Na 1	0	0
33	Y	2	Total 2	Na 2	0	0
33	K	1	Total 1	Na 1	0	0

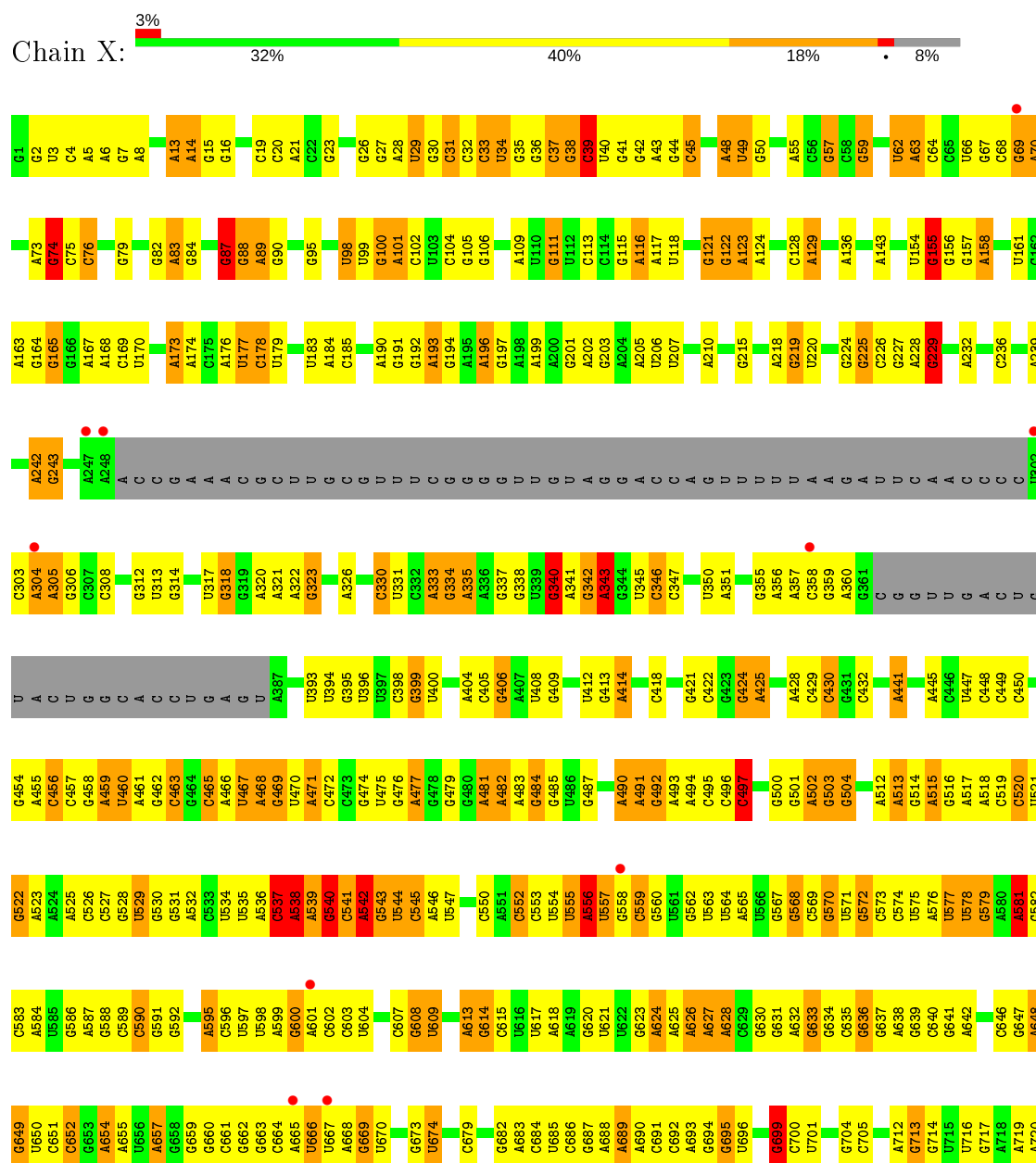
- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	X	14	Total 14	K 14	0	0
34	M	1	Total 1	K 1	0	0

### 3 Residue-property plots

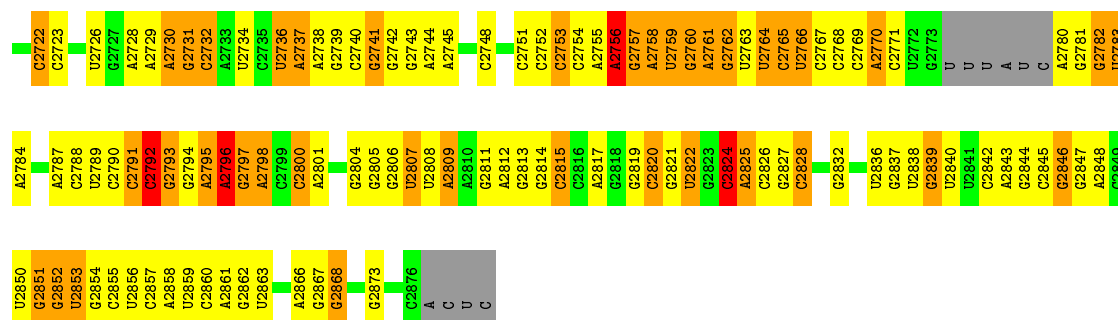
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: RIBOSOMAL 23S RNA

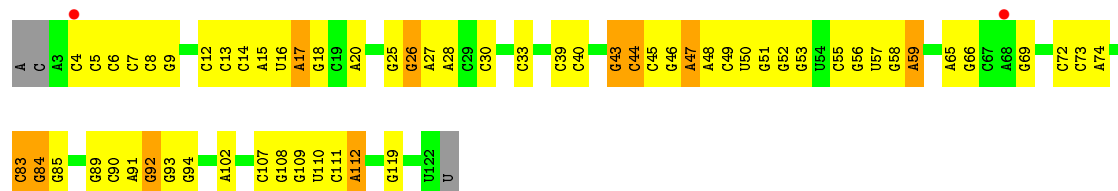


U1656	G1573	A1493	C1422	G1346	C1283	G1211	G1131	G1062	G989	A923	C853	A787	C721
A1657	A1574	G1494	A1423	C1347	G1284	U1212	C1132	G1067	A994	C924	G854	G788	C725
G1660	G1575	G1495	G1428	C1348	A1285	U1213	G1133	A1068	A994	G925	G855	G789	G726
G1662	G1576	G1496	G1429	G1351	U1286	C1214	C1134	A1069	A999	C926	U859	A790	U
G1663	G1577	G1497	G1430	G1352	A1287	A1215	C1135	G1069	A999	G927	U860	G791	G
G1664	G1578	A1498	G1431	G1353	U1288	G1216	G1136	G1070	G1000	G928	G861	U792	C
A1665	G1579	A1499	U1431	A1353	A1289	U1217	U1141	U1071	A1001	G929	G862	A	
A1666	A1584	U1500	A1432	A1354	A1290	C1218	G1142	U1072	C1002	G931	G867	A795	
A1667	A1585	U1505	A1433	A1355	A1291	G1219	G1143	G1073	C1003	G932	U868	A796	
G1668	U1592	C1506	G1435	G1357	A1293	C1220	C1145	C1075	U1005	G933	C869	A797	
A1669	U1593	A1507	G1436	C1358	G1294	G1223	G1146	U1076	C1006	A935	C870	G798	
G1670	C1593	A1508	A1437	G1359	U1295	A1224	G1147	U1077	A1007	C936	U871	C737	
A1671	A1594	A1509	G1438	G1360	G1296	G1225	G1148	A1078	G1008	U800	G872	U800	
A1671	A1595	A1510	G1439	G1361	A1297	A1226	G1149	G1079	C1009	G938	U873	G739	
A1672	A1511	A1511	G1440	A1362	U1298	C1229	C1150	A1080	U1010	C939	A874	A740	
C1673	U1601	A1512	A1441	C1363	A1299	G1230	U1151	A1081	A1011	G940	G875	A802	
C1674	G1602	U1513	C1442	C1364	A1300	C1230	C1152	G1082	A1011	U941	A876	C804	
C1675	C1514	C1514	G1443	U1370	U1301	C1234	A1153	C1083	U1015	U942	G877	G805	
C1676		G1522	C1444	G1371	C1302	C1235	C1160	C1084	C1016	U943	C878	A806	
U1677	U1607	A	U1447	A1372	U1303	G1236	C1160	G1085	C1017	U944	A807	A747	
U1678	U1608	C	U1447	G1373	C1305	A1242	C1164	C1086	G1018	G945	C808	A748	
U1679	G1609	A	G1450	G1374	U1306	G1245	G1165	C1087	U1019	U946	C809	A749	
U1680	A1610	U1526		G1382	U1307	G1251	C1171	A1095	A1020	C947	U810	C749	
A1681	U1611	G1527	A1453	A1378	G1309	C1252	G1172	A1096	A1021	C948	G811	C750	
A1682	U1612	C1528	U1454	A1379	C1310	C1253	U1173	A1097	U1022	G949	U812	G751	
G1683	G1613	C1528	A1455	G1380	G1311	G1254	G1174	G1098	G1024	G950	A813	G752	
G1684	C1614		C1456	G1381	C1312	A1259	U1170	C1094	A1025	G951	G814	G753	
A1685	C1615	C1531	A1457	G1382	U1313	G1251	A1171	A1095	U1026	A952	A815	G754	
A1686			A1457	G1382	U1314	G1252	U1172	A1096	C1027	G953	U816	C755	
C1687	A1619	U1537	A1458	A1386	A1314	C1253	U1173	A1097	U1027	U954	G	G756	
U1688	U1538	A1538	U1459	G1387	A1315	C1254	G1173	A1098	C1031	G955	G	A817	
U1689	G1622	U1539	G1460	G1387	G1316	G1255	G1174	G1099	A1032	A956	C819	G758	
U1690	C1623	C1540	C1461	A1391	G1317	G1256	A1175	A1099	U1034	G957	U820	G759	
A1691	A1624	G1541	A1462	A1392	A1321	C1257	U1176	G1100	U1034	G958	A821	U760	
C1692	A1625	G1542	A1463	G1393	G1322	U1257	A1179	G1104	G1035	C959	G822	G761	
A1693	G1626	U1543	A1464	G1393	G1323	G1258	C1182	U1105	G1036	U960	U823	A762	
A1694	C1627	A1544	G1465	A1397	G1324	A1259	C1183	A1106	U1037	C961	C	C765	
U1695	C1628	U1545	C1466	A1398	U1325	G1261	G1184	U1107	G1042	G965	C	A766	
C1696	G1629	U1551	U1467	G1399	U1326	G1262	C	A1109	A1043	A966	C	U826	
U1697	A1630	U1551	A1468	A1400	G1327	U1263	G1184	U1109	U1044	C967	C827	G767	
C1698	C1631	C1552	U1469	A1401	C1328	C1264	G	A1114	A1044	C967	C830	U768	
A1699	A1632	G1553	G1470	A1402	U1329	G1265	A	C1115	G1045	U967	C830	C769	
C1700	C1633	G1554	G1471	A1403	G1330	A1267	A	U1046	U1046	C968	U770	U770	
C1701	A1634	A1555	A1472	A1404	G1331	U1268	G	G1116	A970	U969	C771	A832	
C1702	G1635	A1556	U1473	A1405	U1332	G1269	C	G1117	U1048	A	U	G772	
G1703			A1474	G1407	G1332	C1270	G1191	G1118	C1049	A971	C	G836	
U1704	C1641	U1560	U1475	A1408	G1333	C1271	G1191	U1119	U1050	C972	C	U837	
	G1642	A1561	G1476	U1409	A1334	C1271	A1192	U1119	G1050	U973	A911	A838	
U1710	A1643	G1562	U1477	U1410	U1335	G1272	G1193	C1120	U1051	U974	A912	U775	
G1711	G1644	U1563	U1478	C1411	G1336	G1273	G1193	G1121	C1052	U974	A913	G776	
U1712	U1645	U1564	G1479	C1412	G1337	C1274	G1196	A1122	G1053	G977	C914	A777	
G1713	G1712	G1565	G1480	U1413	G1338	G1275	G1196	G1123	C1054	U977	C915	U778	
A1714	C1648	G1566	U1481	G1414	U1339	U1276	G1200	U1124	A1055	C982	U916	U779	
A1715		U1567	U1482	C1415	C1340	G1277	G1201	G1125	U1056	G983	U917	U780	
G1716	U1651	A1568	G1483		G1341	C1277	U1201	A1126	A1057	G983	C917	G781	
A1717	G1652	A1569	U1484	C1418	U1342	A1278	U1202	G1126	U1057	A984	A918	U782	
A1718	C1653	C1570	U1490	G1419	U1343	G1279	A1203	G1127	G1058	G985	U919	G783	
G1719	A1654	G1571	G1491	G1419	C1344	U1280	G1204	G1128	A1059	A986	G920	U784	
G1720		C1572	U1421	A1420	G1345	A1281	G1205	A1129	C1060	G987	U921	U785	
						C1282	G1205	A1129	A1061	C989	A922	C786	

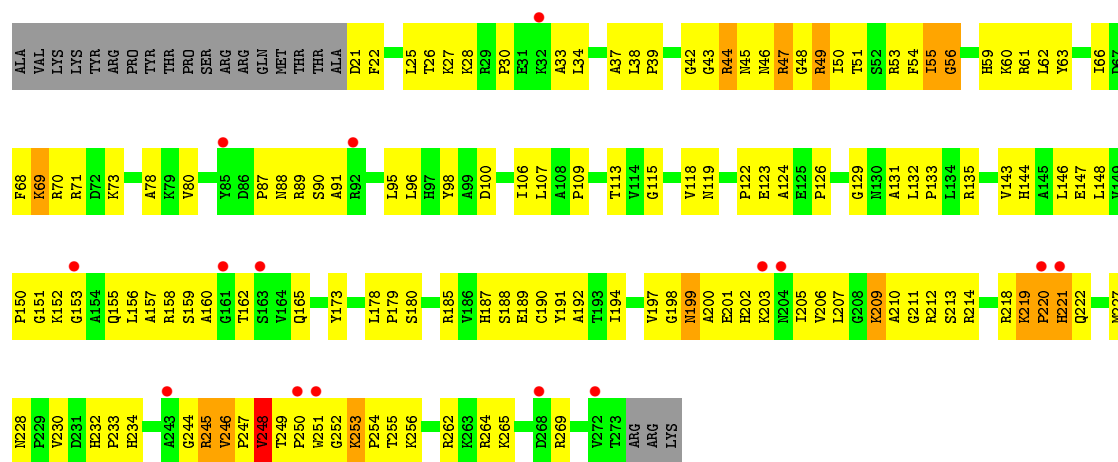
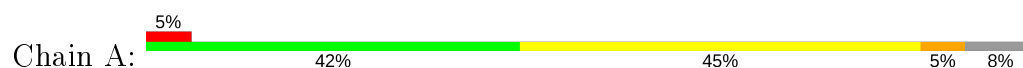
A2658	A2659	U2584	U2516	G2433	A2371	A2290	U2211	U	A2073	G2007	A1943	G1878	A1793	G1721
C2660	C2661	G2588	C2517	U2436	A2372	U2291	G2217	G	U2074	C2008	C1944	G1879	A1796	G1722
G2662	G2663	U2590	C2519	G2437	C2373	C2292	G2218	A	U2075	U2009	C1945	U1881	G	U1723
C2664	C2665	G2591	A2520	U2441	G2375	G2293	U2219	G	C2082	G2010	A1800	A1884	A1799	C1724
U2666	U2667	U2592	G2521	U2442	U2376	U2298	A2220	G	G2083	A2012	G1948	C1885	A1801	G1730
C2668	C2669	U2593	G2522	C2443	U2377	A2299	G2221	C	G2084	A2013	A1949	C1886	C1801	U1733
U2669	U2670	G2594	G2523	C2444	G2378	G2300	U2222	A	G2085	A2014	G1951	G1887	A1802	C1734
C2671	C2672	U2595	G2527	C2445	U2380	A2301	U2223	A	U2087	A2016	A1952	C1888	U1804	U1733
G2673	G2674	G2596	U2528	C2446	C2382	G2302	U2224	C	U	U2017	A1953	G	G1805	U1737
C2675	C2676	U2597	G2529	G2447	C2383	A2306	C2227	G	C	C2018	A1954	C	G1806	G1741
U2677	U2678	C2670	U2530	U2448	G2384	G2310	U2228	U	C	C2019	G1955	C	A1807	G1742
C2679	C2680	A2600	G2532	U2452	U2385	U2311	G2229	G	U	C2023	A1960	C	C1808	U1747
U2681	U2682	U2534	U2533	C2453	U2386	A2312	C2233	A	C	U2024	G	G	G1809	G1748
C2683	C2684	U2540	G2541	C2454	U2387	G2313	G2234	A	C	A2025	U1963	A	A1811	C1743
A2684	A2685	U2542	U2543	U2455	U2388	A2314	G2235	U	C	C2026	A1964	A	U1812	G1744
G2686	G2687	C2605	A2544	C2456	G2389	A2315	U2236	A	U	C2027	U1965	C	A1813	A1746
U2676	U2677	A2608	U2545	U2457	A2390	C2321	C2237	C	U	G2028	U1966	U	G1814	G1747
C2678	C2679	G2609	U2546	U2458	U2391	U2322	C2238	C	G	U2029	G1967	A	G1815	U1748
U2680	U2681	U2610	A2547	C2459	G2392	U2323	C2239	A	C	A2030	U1968	U	U1816	G1749
C2682	C2683	A2611	A2548	G2468	G2393	G2324	U2241	C	U	A2031	G1969	A	U1817	A1751
U2684	U2685	G2612	A2549	G2469	G2394	A2325	C2242	C	A	C2032	G1970	C	A1821	U1752
C2686	C2687	A2613	G2547	U2470	G2395	C2326	C2243	U	G	G2033	C1971	G	G1822	A1753
A2688	A2689	U2614	U2548	U2471	G2396	U2327	A2245	G	U	A2034	G1972	G	C1825	G1754
G2689	G2690	G2615	G2549	C2475	U2397	G2328	A2246	A	C	G2035	C1973	U	U1826	C1757
U2691	U2692	U2616	C2550	U2476	U2398	G2329	A2247	G	C	A2037	G1974	C	G1827	G1758
C2693	C2694	G2617	G2551	C2477	A2401	G2330	U2251	A	G	C2038	U1975	C	C1830	G1761
U2695	U2696	A2618	U2552	C2478	U2402	A2331	A2252	G	G	G2039	C1977	A	G1831	C1762
G2697	G2698	U2622	G2553	C2479	C2403	G2336	A2253	G	C	A2040	U1978	U	C1834	G1763
U2700	U2701	A2623	C2554	U2480	A2404	A2337	C2254	C	C	G2041	U1979	A	G1835	A1764
C2702	C2703	G2624	A2555	G2481	C2405	G2338	G2255	C	U	A2042	C1979	U	C1836	G1765
U2704	U2705	U2625	G2556	A2482	C2406	A2339	G2256	C	U	G2043	A1981	C	G1837	U1766
G2706	G2707	U2626	G2557	U2483	G2407	G2340	A2257	C	C	A2044	C1982	U	G1838	U1767
U2708	U2709	U2627	U2558	G2484	G2408	C2341	G2258	G	G	C2046	A1983	U	A1839	U1768
C2710	C2711	U2628	G2559	U2485	U2409	U2342	G2259	A	A	C2047	A1984	U	A1840	U1769
U2712	U2713	U2629	U2560	C2486	U2410	U2343	C2260	G	C	C2048	G1987	U	G1841	U1770
G2714	G2715	G2630	G2561	U2487	A2413	A2348	G2261	A	A	A1921	A1988	U	G1842	A1771
U2716	U2717	U2634	U2562	U2490	G2414	G2349	G2262	C	C	G2050	C1989	U	C1843	C1772
C2718	C2719	A2635	U2563	C2491	G2415	G2350	C2263	U	U	U2051	U1990	U	G1844	C1773
U2720	U2721	U2636	G2564	U2492	U2416	G2351	C2264	C	C	G2052	C1991	U	G1845	A1774
G2722	G2723	G2637	A2565	U2493	U2417	G2352	A2265	G	G	G2053	G1992	U	A1851	A1775
U2724	U2725	A2638	G2566	C2494	A2418	A2353	A2266	C	C	A2054	G1993	U	G1852	A1776
U2726	U2727	G2639	A2567	G2495	C2419	A2354	G2267	U	U	C2056	U1994	U	G1853	G1779
C2728	C2729	U2640	U2568	C2496	C2420	A2355	A2268	U	U	G2057	A1996	U	G1854	A1780
U2730	U2731	G2641	G2569	A2497	C2421	G2356	A2269	C	C	U2058	A1997	U	G1855	C1781
G2732	G2733	U2642	U2570	U2498	C2422	U2357	C2270	U	U	G2059	A1998	U	A1782	A1782
U2734	U2735	U2643	U2571	C2499	G2423	G2360	C2271	C	C	A2060	G1999	U	G1864	U1787
C2736	C2737	G2644	G2572	U2500	G2424	G2361	G2272	U	U	C2061	U2000	U	A1867	C1788
U2738	U2739	U2645	U2573	U2501	G2425	G2362	G2273	C	C	G2062	G2001	U	A1868	U1789
G2740	G2741	U2646	G2574	G2502	G2426	G2363	G2274	G	G	A2063	G2002	U	G1871	G1790
U2742	U2743	C2647	U2575	C2503	A2427	G2364	A2204	C	C	U2064	A2003	U	C1941	C1792
C2744	C2745	U2648	G2576	G2504	U2428	U2365	C2205	U	U	A2065	G2004	U	G1871	G1792
U2746	U2747	U2649	U2577	U2505	U2429	A2367	G2286	C	C	U2066	U2005	U	G1871	G1792
G2748	G2749	A2650	G2578	U2506	A2430	G2368	G2287	C	C	G2067	G2006	U	G1871	G1792
U2750	U2751	U2651	A2581	U2507	A2431	U2369	A2288	C	C	U2067	G2006	U	G1871	G1792
C2752	C2753	U2652	G2582	U2508	A2432	G2370	A2289	C	C	U2067	G2006	U	G1871	G1792
U2754	U2755	U2653	U2583	A2509	A2433									



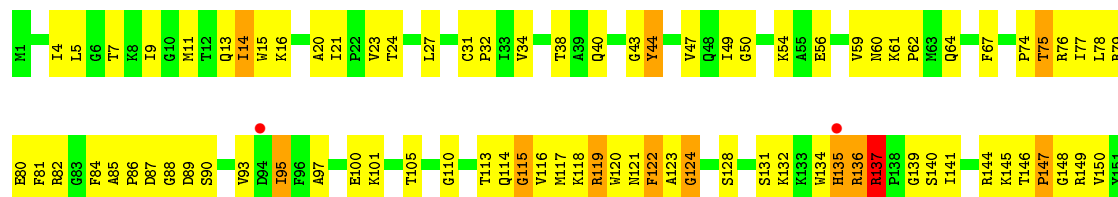
### • Molecule 2: 5S ribosomal RNA



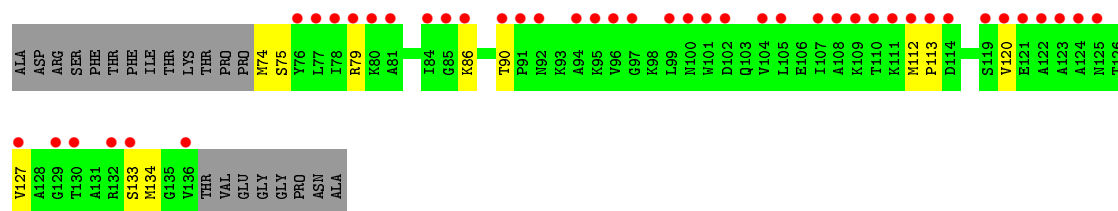
### • Molecule 3: 50S ribosomal protein L2



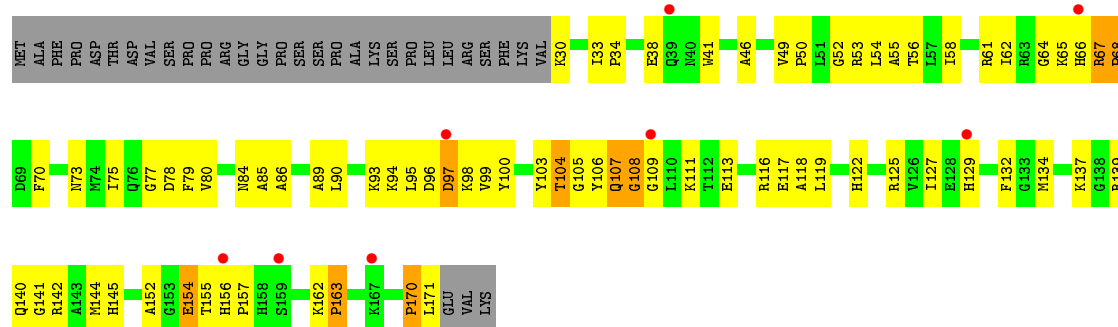
### • Molecule 4: 50S ribosomal protein L3



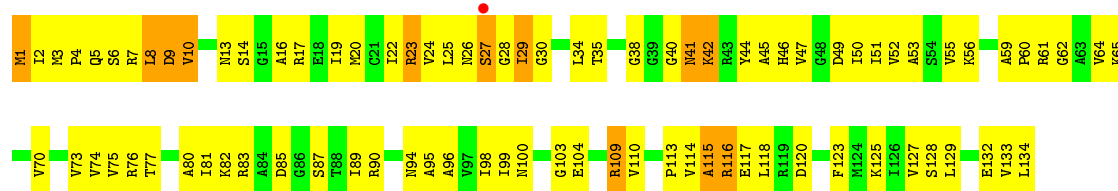




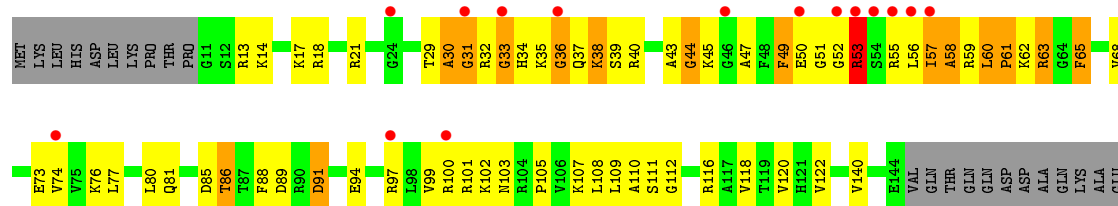
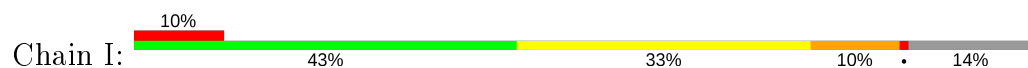
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14



• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16

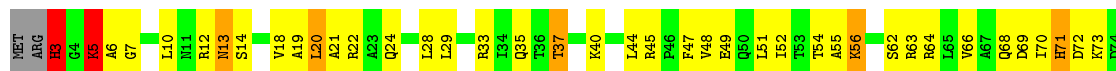






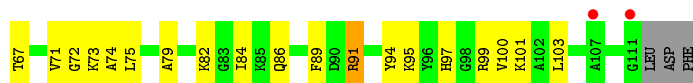
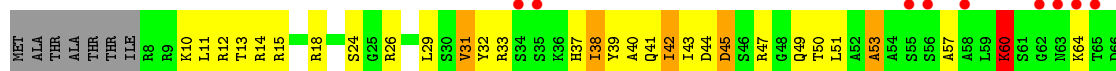
- Molecule 13: 50S ribosomal protein L17

Chain K: 38% 50% 8% . .



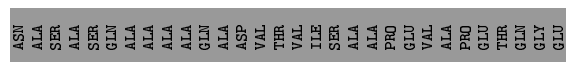
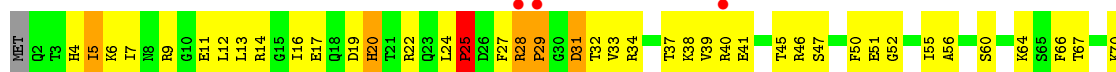
- Molecule 14: 50S ribosomal protein L18

Chain L: 10% 48% 37% 5% . 9%



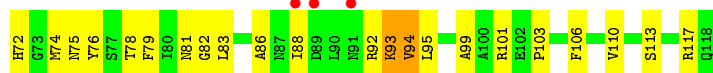
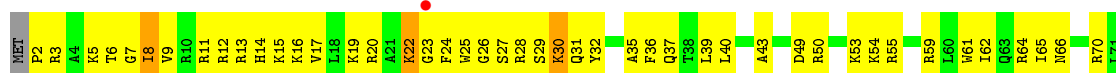
- Molecule 15: 50S ribosomal protein L19

Chain M: 2% 26% 34% 5% . 35%

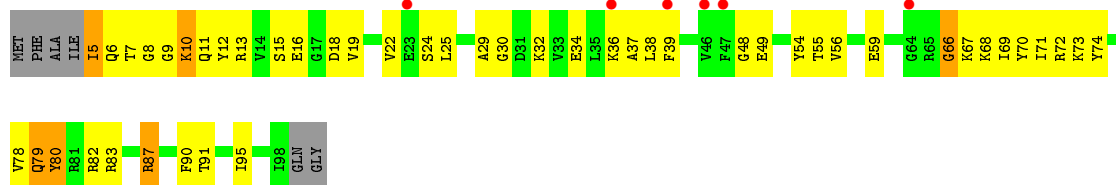


- Molecule 16: 50S ribosomal protein L20

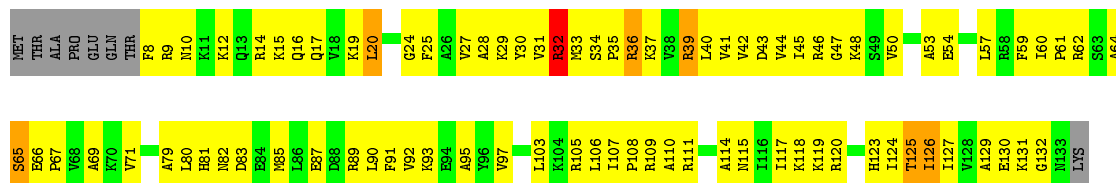
Chain N: 3% 42% 53% . .



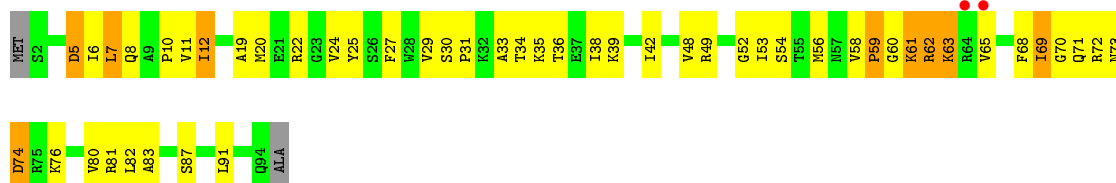
- Molecule 17: 50S ribosomal protein L21



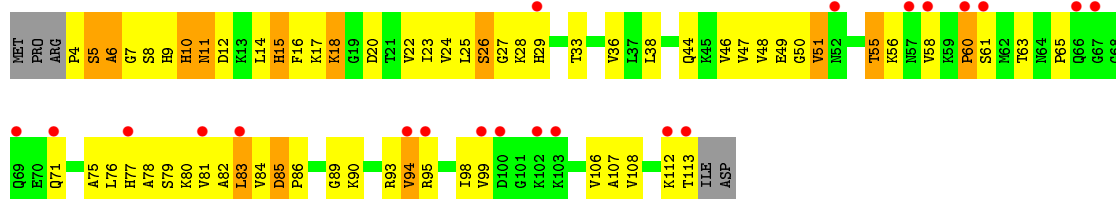
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23

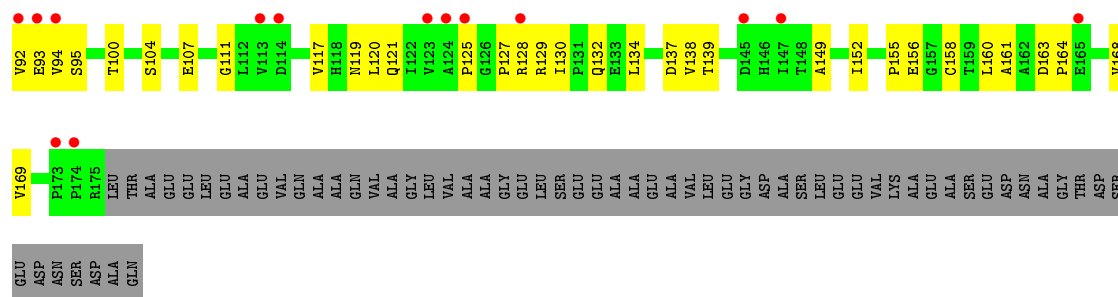


- Molecule 20: 50S ribosomal protein L24

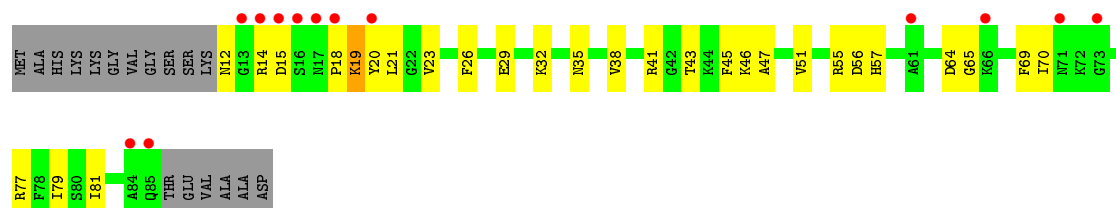


- Molecule 21: 50S ribosomal protein L25

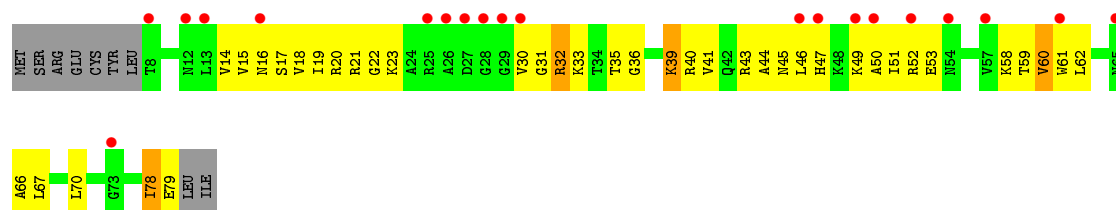
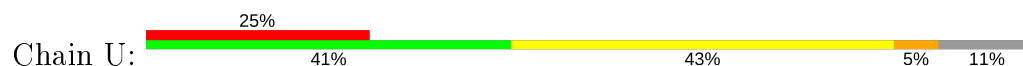




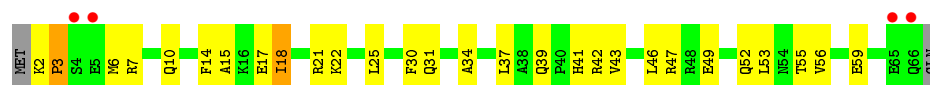
- Molecule 22: 50S ribosomal protein L27



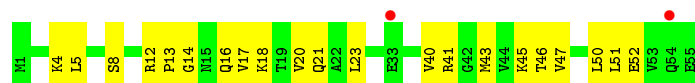
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30

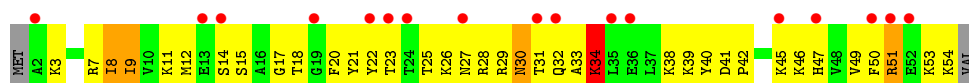


- Molecule 26: 50S ribosomal protein L32

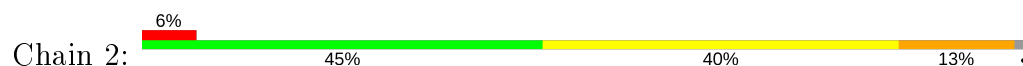




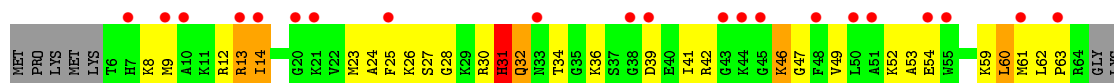
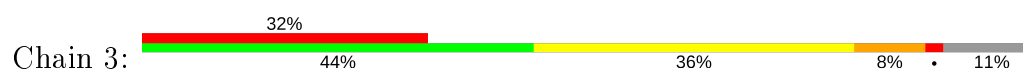
- Molecule 27: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.59 Å   410.20 Å   695.08 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 3.25 34.75 – 3.25	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-3.25) 93.3 (34.75-3.25)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.25 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.252   ,   0.294 0.258   ,   0.297	Depositor DCC
$R_{free}$ test set	3585 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.8	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	84383	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: NA, K, MG, LMA

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	0.69	12/63867 (0.0%)	1.28	804/99618 (0.8%)
2	Y	0.46	0/2863	0.86	5/4461 (0.1%)
3	A	0.49	1/1958 (0.1%)	0.65	2/2638 (0.1%)
4	B	0.55	0/1567	0.79	0/2105
5	C	0.52	0/1504	0.67	0/2036
6	D	0.31	0/1419	0.45	0/1903
7	E	0.33	0/1308	0.48	0/1771
8	F	0.22	0/455	0.37	0/611
9	G	0.57	0/1138	0.70	0/1539
10	H	0.63	0/1007	0.84	0/1352
11	I	0.54	0/1022	0.64	0/1366
12	J	0.48	0/1113	0.63	0/1486
13	K	0.81	1/886 (0.1%)	1.06	6/1188 (0.5%)
14	L	0.40	0/785	0.56	0/1048
15	M	0.67	0/884	0.88	1/1186 (0.1%)
16	N	0.55	0/994	0.71	0/1323
17	O	0.44	0/750	0.62	0/1000
18	P	0.58	0/1017	0.79	1/1362 (0.1%)
19	Q	0.47	0/737	0.63	0/988
20	R	0.45	0/835	0.59	0/1121
21	S	0.33	0/1370	0.48	0/1862
22	T	0.43	0/563	0.56	0/747
23	U	0.40	0/556	0.58	0/741
24	V	0.31	0/529	0.47	0/704
25	W	0.39	0/426	0.65	0/568
26	Z	0.56	0/464	0.79	0/622
27	1	0.48	0/438	0.56	0/583
28	2	0.56	0/387	0.71	0/509
29	3	0.59	0/468	0.65	0/614
30	4	0.22	0/298	0.37	0/390
All	All	0.63	14/91608 (0.0%)	1.15	819/137442 (0.6%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1977	C	P-O5'	-7.09	1.52	1.59
1	X	774	A	N7-C5	7.06	1.43	1.39
1	X	1333	G	O3'-P	-6.43	1.53	1.61
1	X	1202	U	O3'-P	-6.42	1.53	1.61
1	X	774	A	N9-C8	6.38	1.42	1.37
1	X	1975	G	C6-N1	-6.25	1.35	1.39
1	X	1688	U	C2-N3	6.11	1.42	1.37
1	X	774	A	N3-C4	6.01	1.38	1.34
1	X	2857	C	N1-C6	-6.01	1.33	1.37
1	X	577	U	C4-O4	5.82	1.28	1.23
13	K	3	HIS	CA-C	5.60	1.67	1.52
1	X	2398	U	C2-N3	-5.53	1.33	1.37
3	A	248	VAL	CB-CG2	-5.21	1.42	1.52
1	X	1467	U	N1-C2	5.12	1.43	1.38

All (819) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1975	G	N1-C6-O6	-19.89	107.97	119.90
1	X	774	A	C5-N7-C8	-17.57	95.12	103.90
1	X	774	A	C4-C5-C6	-17.47	108.26	117.00
1	X	1670	G	C8-N9-C4	15.74	112.69	106.40
1	X	774	A	C4-C5-N7	14.89	118.15	110.70
1	X	1679	U	C5-C6-N1	-14.87	115.27	122.70
1	X	1683	G	N1-C6-O6	-14.47	111.22	119.90
1	X	1467	U	N3-C2-O2	-14.36	112.15	122.20
1	X	2480	C	N3-C2-O2	13.37	131.26	121.90
1	X	1305	C	C6-N1-C2	12.91	125.46	120.30
1	X	1683	G	C5-C6-O6	12.88	136.33	128.60
1	X	774	A	N1-C2-N3	-12.52	123.04	129.30
1	X	1670	G	N7-C8-N9	-12.50	106.85	113.10
1	X	2548	G	N1-C6-O6	-12.12	112.63	119.90
1	X	2480	C	N1-C2-O2	-11.88	111.77	118.90
1	X	774	A	N7-C8-N9	11.32	119.46	113.80
1	X	1266	G	C5-N7-C8	11.31	109.95	104.30
1	X	968	C	N1-C2-O2	11.09	125.56	118.90
1	X	989	G	C8-N9-C4	11.06	110.82	106.40
1	X	1663	C	N1-C2-O2	10.96	125.48	118.90
1	X	1975	G	C5-C6-N1	10.95	116.97	111.50
1	X	2703	C	C6-N1-C2	10.84	124.64	120.30
1	X	2634	G	C8-N9-C4	10.81	110.72	106.40
1	X	1975	G	C5-C6-O6	10.74	135.04	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1266	G	C4-C5-N7	-10.72	106.51	110.80
1	X	1982	C	C5-C6-N1	-10.67	115.67	121.00
1	X	2666	U	C5-C6-N1	-10.63	117.39	122.70
1	X	1674	C	C5-C6-N1	-10.58	115.71	121.00
1	X	1288	A	C5-C6-N1	-10.57	112.42	117.70
1	X	1467	U	N1-C2-O2	10.44	130.11	122.80
1	X	1288	A	C2-N3-C4	-10.44	105.38	110.60
1	X	527	C	N1-C2-O2	10.41	125.14	118.90
1	X	2805	G	N1-C6-O6	-10.28	113.73	119.90
1	X	1674	C	C6-N1-C2	10.24	124.40	120.30
1	X	1291	G	C8-N9-C4	10.18	110.47	106.40
1	X	559	C	C5-C6-N1	10.15	126.07	121.00
1	X	2590	U	C4-C5-C6	10.12	125.77	119.70
1	X	522	G	N1-C6-O6	10.07	125.94	119.90
1	X	2590	U	N1-C2-N3	9.93	120.86	114.90
1	X	577	U	N3-C4-C5	-9.82	108.71	114.60
1	X	2398	U	N3-C4-C5	9.73	120.44	114.60
1	X	774	A	C5-C6-N1	9.68	122.54	117.70
1	X	2590	U	N1-C2-O2	-9.54	116.12	122.80
1	X	1679	U	C2-N3-C4	-9.46	121.33	127.00
1	X	1266	G	N7-C8-N9	-9.40	108.40	113.10
1	X	1212	U	C5-C6-N1	-9.39	118.00	122.70
1	X	2618	A	N1-C2-N3	9.38	133.99	129.30
1	X	1981	A	N7-C8-N9	-9.28	109.16	113.80
1	X	1676	U	C5-C6-N1	-9.23	118.08	122.70
1	X	503	G	C8-N9-C4	9.13	110.05	106.40
1	X	1981	A	C5-N7-C8	9.13	108.46	103.90
1	X	2815	C	C6-N1-C2	9.12	123.95	120.30
1	X	789	G	N1-C6-O6	9.11	125.37	119.90
1	X	1309	G	C8-N9-C4	9.09	110.04	106.40
1	X	1211	G	C8-N9-C4	9.07	110.03	106.40
1	X	2815	C	C5-C6-N1	-9.07	116.46	121.00
1	X	796	A	N1-C6-N6	9.06	124.03	118.60
1	X	538	A	C2-N3-C4	8.99	115.09	110.60
1	X	2846	G	C8-N9-C4	8.97	109.99	106.40
1	X	1770	U	C5-C6-N1	-8.96	118.22	122.70
1	X	2665	G	N7-C8-N9	-8.95	108.63	113.10
1	X	2665	G	C8-N9-C4	8.89	109.96	106.40
1	X	2807	U	C5-C6-N1	-8.88	118.26	122.70
1	X	2553	G	C8-N9-C4	-8.88	102.85	106.40
1	X	774	A	N9-C4-C5	-8.85	102.26	105.80
1	X	2038	C	N1-C2-O2	8.83	124.20	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2548	G	C5-C6-O6	8.76	133.85	128.60
1	X	2705	A	C8-N9-C4	8.76	109.30	105.80
1	X	1702	C	C6-N1-C2	8.73	123.79	120.30
1	X	1660	G	N1-C6-O6	-8.71	114.68	119.90
1	X	559	C	C2-N3-C4	8.65	124.23	119.90
1	X	1743	C	C5-C6-N1	-8.65	116.68	121.00
1	X	1982	C	C4-C5-C6	8.63	121.72	117.40
1	X	1937	G	C8-N9-C4	8.62	109.85	106.40
3	A	248	VAL	CG1-CB-CG2	-8.59	97.16	110.90
1	X	989	G	N7-C8-N9	-8.57	108.82	113.10
1	X	2712	G	N1-C6-O6	-8.56	114.77	119.90
1	X	1279	G	N7-C8-N9	-8.53	108.83	113.10
1	X	1968	G	C8-N9-C4	8.48	109.79	106.40
1	X	2496	C	N3-C4-C5	8.46	125.28	121.90
1	X	1678	G	N1-C6-O6	-8.45	114.83	119.90
1	X	2597	G	C5-C6-O6	8.38	133.63	128.60
1	X	1662	G	N1-C6-O6	-8.37	114.88	119.90
1	X	1670	G	C5-N7-C8	8.30	108.45	104.30
1	X	2689	C	C6-N1-C2	8.23	123.59	120.30
1	X	1688	U	N3-C4-O4	8.14	125.10	119.40
1	X	1993	G	C2-N3-C4	-8.12	107.84	111.90
1	X	2792	C	C5-C6-N1	-8.08	116.96	121.00
1	X	1966	C	C5-C6-N1	-8.07	116.96	121.00
1	X	2033	C	N3-C2-O2	-8.07	116.25	121.90
1	X	1981	A	C8-N9-C4	8.05	109.02	105.80
1	X	1278	A	C8-N9-C4	-8.04	102.59	105.80
1	X	961	G	C5-C6-O6	8.03	133.42	128.60
1	X	1305	C	C5-C6-N1	-8.03	116.99	121.00
1	X	1653	C	C6-N1-C2	8.03	123.51	120.30
1	X	787	A	C2-N3-C4	-8.02	106.59	110.60
1	X	2713	A	C8-N9-C4	8.01	109.00	105.80
1	X	1978	U	N1-C2-O2	-8.01	117.19	122.80
1	X	1279	G	C5-N7-C8	7.99	108.30	104.30
1	X	538	A	C5-C6-N1	7.94	121.67	117.70
1	X	2809	A	C5-C6-N6	-7.94	117.35	123.70
1	X	1700	C	C6-N1-C2	7.92	123.47	120.30
1	X	1291	G	N7-C8-N9	-7.92	109.14	113.10
1	X	2478	C	C6-N1-C2	-7.92	117.13	120.30
1	X	741	G	N7-C8-N9	-7.91	109.15	113.10
1	X	1702	C	C5-C6-N1	-7.86	117.07	121.00
1	X	559	C	C6-N1-C2	-7.83	117.17	120.30
1	X	1680	U	C5-C6-N1	-7.83	118.78	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	689	A	C5-N7-C8	-7.83	99.99	103.90
1	X	2681	A	N1-C6-N6	7.82	123.29	118.60
1	X	741	G	C8-N9-C4	7.80	109.52	106.40
1	X	1984	A	N1-C6-N6	-7.79	113.93	118.60
1	X	2665	G	C5-N7-C8	7.78	108.19	104.30
1	X	1679	U	C6-N1-C2	7.76	125.66	121.00
1	X	1991	C	C5-C6-N1	-7.76	117.12	121.00
1	X	1984	A	N1-C2-N3	7.76	133.18	129.30
1	X	1975	G	C6-N1-C2	-7.69	120.49	125.10
1	X	2703	C	C5-C6-N1	-7.68	117.16	121.00
1	X	2590	U	C5-C6-N1	-7.67	118.86	122.70
1	X	1655	C	C5-C6-N1	-7.67	117.17	121.00
1	X	2855	C	N3-C2-O2	7.67	127.27	121.90
1	X	968	C	C2-N1-C1'	7.63	127.19	118.80
1	X	2655	C	C6-N1-C2	7.63	123.35	120.30
1	X	2247	A	N1-C6-N6	7.61	123.17	118.60
1	X	520	C	N1-C2-O2	-7.58	114.35	118.90
1	X	1642	G	C2-N3-C4	-7.57	108.11	111.90
1	X	1278	A	N7-C8-N9	7.55	117.57	113.80
1	X	1980	A	C5-N7-C8	7.54	107.67	103.90
1	X	1212	U	C5-C4-O4	7.53	130.42	125.90
1	X	2493	U	C5-C6-N1	-7.53	118.93	122.70
1	X	2023	C	C6-N1-C2	7.51	123.31	120.30
1	X	1982	C	C2-N3-C4	-7.50	116.15	119.90
1	X	1211	G	N9-C4-C5	-7.48	102.41	105.40
1	X	2701	A	N1-C2-N3	7.46	133.03	129.30
1	X	1304	U	C5-C6-N1	-7.46	118.97	122.70
1	X	1995	G	C8-N9-C4	7.46	109.38	106.40
1	X	2705	A	N9-C4-C5	-7.45	102.82	105.80
1	X	542	A	N1-C6-N6	7.44	123.07	118.60
1	X	1305	C	N3-C2-O2	7.42	127.09	121.90
1	X	2430	A	N1-C6-N6	-7.41	114.16	118.60
1	X	968	C	C6-N1-C1'	-7.40	111.92	120.80
1	X	1674	C	N3-C4-C5	7.37	124.85	121.90
1	X	1270	C	N3-C4-C5	-7.35	118.96	121.90
1	X	1674	C	C2-N3-C4	-7.34	116.23	119.90
1	X	1700	C	C5-C6-N1	-7.34	117.33	121.00
1	X	1993	G	N1-C6-O6	7.33	124.30	119.90
1	X	825	C	C6-N1-C2	7.32	123.23	120.30
1	X	1674	C	N3-C4-N4	-7.32	112.88	118.00
18	P	32	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	X	1211	G	N3-C2-N2	7.30	125.01	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2805	G	C5-C6-O6	7.28	132.97	128.60
1	X	538	A	N1-C2-N3	-7.28	125.66	129.30
1	X	1683	G	C6-C5-N7	7.27	134.76	130.40
1	X	1275	A	N1-C6-N6	7.27	122.96	118.60
1	X	2766	U	C5-C6-N1	-7.26	119.07	122.70
1	X	1928	G	N1-C6-O6	-7.26	115.55	119.90
1	X	1622	G	N1-C6-O6	-7.25	115.55	119.90
1	X	787	A	C5-C6-N1	-7.25	114.08	117.70
1	X	1748	U	N3-C2-O2	7.24	127.27	122.20
1	X	1142	G	N3-C2-N2	7.23	124.96	119.90
1	X	1467	U	C4-C5-C6	7.22	124.03	119.70
1	X	1743	C	C6-N1-C2	7.22	123.19	120.30
1	X	1775	A	C8-N9-C4	7.22	108.69	105.80
1	X	527	C	C6-N1-C2	-7.21	117.42	120.30
1	X	2748	C	C6-N1-C2	7.20	123.18	120.30
1	X	1989	C	N3-C2-O2	7.17	126.92	121.90
1	X	542	A	N7-C8-N9	7.16	117.38	113.80
1	X	2671	C	C6-N1-C2	-7.14	117.44	120.30
1	X	1937	G	N7-C8-N9	-7.14	109.53	113.10
1	X	2717	G	C5-C6-N1	7.13	115.07	111.50
1	X	966	A	N1-C6-N6	7.13	122.88	118.60
1	X	1341	G	C8-N9-C4	7.12	109.25	106.40
1	X	2398	U	N3-C4-O4	-7.12	114.42	119.40
1	X	1278	A	N1-C6-N6	7.10	122.86	118.60
1	X	2611	A	C8-N9-C4	7.10	108.64	105.80
1	X	961	G	N1-C6-O6	-7.10	115.64	119.90
1	X	2040	A	C8-N9-C4	7.10	108.64	105.80
1	X	825	C	N1-C2-O2	-7.10	114.64	118.90
1	X	1305	C	N1-C2-O2	-7.08	114.65	118.90
1	X	2809	A	C5-C6-N1	7.06	121.23	117.70
1	X	1279	G	C8-N9-C4	7.06	109.22	106.40
1	X	2820	C	N3-C4-N4	-7.06	113.06	118.00
1	X	1245	G	N1-C6-O6	-7.05	115.67	119.90
1	X	545	C	C5-C6-N1	-7.04	117.48	121.00
1	X	2423	G	N1-C6-O6	-7.03	115.68	119.90
1	X	2765	C	C5-C6-N1	-7.03	117.48	121.00
1	X	1972	G	C8-N9-C4	-7.03	103.59	106.40
1	X	1289	A	N9-C4-C5	-7.02	102.99	105.80
1	X	1471	G	C5-C6-N1	7.01	115.01	111.50
1	X	2569	A	C8-N9-C4	7.01	108.60	105.80
1	X	1321	A	C8-N9-C4	7.01	108.60	105.80
1	X	883	A	C8-N9-C4	7.00	108.60	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1286	U	N1-C2-O2	-7.00	117.90	122.80
1	X	1679	U	C4-C5-C6	7.00	123.90	119.70
1	X	1663	C	N1-C2-N3	-6.99	114.31	119.20
1	X	789	G	C5-C6-O6	-6.99	124.41	128.60
1	X	799	C	C6-N1-C2	6.98	123.09	120.30
1	X	1989	C	C4-C5-C6	-6.97	113.91	117.40
1	X	2702	G	N1-C6-O6	-6.96	115.72	119.90
1	X	2551	A	C8-N9-C4	6.95	108.58	105.80
13	K	99	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	X	2741	G	C8-N9-C4	6.92	109.17	106.40
1	X	2793	G	C8-N9-C4	6.91	109.16	106.40
1	X	527	C	N3-C2-O2	-6.91	117.06	121.90
1	X	1720	G	C8-N9-C4	6.91	109.16	106.40
1	X	1766	U	C5-C6-N1	-6.90	119.25	122.70
1	X	2600	A	N1-C6-N6	-6.90	114.46	118.60
1	X	2520	A	N1-C6-N6	-6.89	114.47	118.60
1	X	741	G	C5-N7-C8	6.88	107.74	104.30
1	X	2634	G	N7-C8-N9	-6.88	109.66	113.10
1	X	746	G	N1-C6-O6	-6.87	115.78	119.90
1	X	757	U	C5-C6-N1	-6.87	119.26	122.70
1	X	2807	U	C6-N1-C2	6.87	125.12	121.00
1	X	840	U	C5-C6-N1	-6.87	119.27	122.70
1	X	1633	C	C6-N1-C2	6.87	123.05	120.30
1	X	802	A	N1-C6-N6	6.86	122.72	118.60
1	X	1682	A	C2-N3-C4	6.86	114.03	110.60
1	X	542	A	C5-N7-C8	-6.86	100.47	103.90
1	X	1324	G	N1-C6-O6	6.85	124.01	119.90
1	X	545	C	C6-N1-C2	6.85	123.04	120.30
1	X	1670	G	N3-C4-C5	6.85	132.02	128.60
1	X	2559	U	N3-C4-O4	6.84	124.19	119.40
1	X	1773	C	N1-C2-O2	6.83	123.00	118.90
1	X	1471	G	N3-C4-N9	6.83	130.10	126.00
1	X	841	G	C4-C5-N7	6.82	113.53	110.80
1	X	841	G	C5-N7-C8	-6.79	100.90	104.30
1	X	1676	U	C6-N1-C2	6.77	125.06	121.00
1	X	1920	A	C8-N9-C4	6.76	108.50	105.80
1	X	1655	C	C6-N1-C2	6.76	123.00	120.30
1	X	2655	C	C5-C6-N1	-6.75	117.63	121.00
1	X	527	C	C5-C6-N1	6.73	124.36	121.00
1	X	2467	A	N1-C6-N6	-6.73	114.56	118.60
1	X	1920	A	N7-C8-N9	-6.73	110.44	113.80
1	X	2852	G	C8-N9-C4	6.71	109.08	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1966	C	C6-N1-C2	6.70	122.98	120.30
1	X	1968	G	N7-C8-N9	-6.70	109.75	113.10
1	X	577	U	C4-C5-C6	6.69	123.72	119.70
1	X	1576	G	C8-N9-C4	-6.69	103.72	106.40
1	X	1285	A	C5-C6-N1	-6.68	114.36	117.70
1	X	1339	U	N3-C2-O2	-6.67	117.53	122.20
1	X	559	C	N3-C4-C5	-6.66	119.24	121.90
1	X	1748	U	C6-N1-C2	6.66	124.99	121.00
1	X	544	U	N3-C2-O2	-6.65	117.54	122.20
1	X	1931	G	C8-N9-C4	-6.63	103.75	106.40
1	X	2007	G	C4-C5-N7	-6.63	108.15	110.80
1	X	2495	G	N1-C6-O6	-6.62	115.93	119.90
1	X	2398	U	C2-N3-C4	-6.61	123.03	127.00
1	X	1653	C	C5-C6-N1	-6.61	117.70	121.00
1	X	477	A	C8-N9-C4	6.60	108.44	105.80
1	X	1988	A	C8-N9-C4	6.60	108.44	105.80
1	X	196	A	N1-C6-N6	-6.60	114.64	118.60
1	X	1770	U	C5-C4-O4	6.60	129.86	125.90
1	X	951	G	N1-C6-O6	-6.59	115.95	119.90
1	X	936	A	N1-C6-N6	-6.59	114.65	118.60
1	X	1975	G	N1-C2-N2	-6.57	110.28	116.20
1	X	841	G	N3-C4-C5	6.57	131.88	128.60
1	X	2418	A	C8-N9-C4	-6.57	103.17	105.80
1	X	699	G	N3-C4-C5	6.57	131.88	128.60
1	X	1822	C	C5-C6-N1	-6.56	117.72	121.00
1	X	465	C	C5-C6-N1	-6.56	117.72	121.00
1	X	825	C	N3-C2-O2	6.56	126.49	121.90
1	X	747	A	C8-N9-C4	6.55	108.42	105.80
1	X	2815	C	N3-C4-N4	-6.55	113.42	118.00
1	X	2623	A	C8-N9-C4	6.54	108.42	105.80
1	X	1309	G	N7-C8-N9	-6.54	109.83	113.10
1	X	1682	A	C5-C6-N6	-6.53	118.48	123.70
1	X	2406	C	N1-C2-O2	-6.51	114.99	118.90
1	X	2792	C	C2-N3-C4	-6.50	116.65	119.90
1	X	1259	A	C8-N9-C4	6.50	108.40	105.80
1	X	1991	C	C4-C5-C6	6.48	120.64	117.40
1	X	695	G	C8-N9-C4	6.48	108.99	106.40
1	X	460	U	C5-C6-N1	6.47	125.94	122.70
1	X	1006	C	N1-C2-O2	6.47	122.78	118.90
1	X	2686	C	C4-C5-C6	6.47	120.63	117.40
1	X	340	G	C8-N9-C4	6.47	108.99	106.40
1	X	1270	C	C4-C5-C6	6.46	120.63	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	550	C	C5-C6-N1	-6.45	117.77	121.00
1	X	2559	U	C5-C4-O4	-6.45	122.03	125.90
1	X	2431	C	N1-C2-O2	6.45	122.77	118.90
1	X	520	C	C6-N1-C2	-6.45	117.72	120.30
1	X	513	A	N1-C2-N3	6.44	132.52	129.30
1	X	2701	A	C2-N3-C4	-6.44	107.38	110.60
1	X	586	G	C8-N9-C4	6.44	108.97	106.40
1	X	581	A	N1-C6-N6	6.41	122.45	118.60
1	X	832	A	N9-C4-C5	-6.40	103.24	105.80
1	X	2760	G	C8-N9-C4	6.39	108.96	106.40
1	X	1571	G	C8-N9-C4	-6.39	103.84	106.40
1	X	691	C	C6-N1-C2	6.39	122.86	120.30
1	X	853	C	C6-N1-C2	6.38	122.85	120.30
1	X	1816	G	C8-N9-C4	6.38	108.95	106.40
1	X	2711	G	C8-N9-C4	6.38	108.95	106.40
1	X	2666	U	C2-N3-C4	-6.37	123.18	127.00
1	X	806	A	N1-C6-N6	-6.37	114.78	118.60
1	X	575	U	C5-C4-O4	6.37	129.72	125.90
1	X	1324	G	C5-C6-O6	-6.36	124.79	128.60
1	X	2718	A	C5-C6-N1	6.35	120.88	117.70
1	X	2704	U	C5-C6-N1	-6.35	119.53	122.70
1	X	2492	G	N3-C4-C5	-6.34	125.43	128.60
1	X	2331	A	N1-C6-N6	-6.34	114.80	118.60
1	X	1816	G	N7-C8-N9	-6.33	109.93	113.10
1	X	1623	C	N1-C2-O2	6.33	122.70	118.90
1	X	2854	G	N1-C6-O6	6.33	123.69	119.90
1	X	1205	G	C8-N9-C4	6.32	108.93	106.40
1	X	1699	A	C2-N3-C4	-6.32	107.44	110.60
1	X	1035	G	C8-N9-C4	-6.31	103.87	106.40
1	X	822	G	N3-C4-C5	-6.31	125.44	128.60
1	X	527	C	C2-N3-C4	6.31	123.05	119.90
1	X	528	G	N1-C6-O6	-6.30	116.12	119.90
1	X	2495	G	N3-C2-N2	6.30	124.31	119.90
1	X	2314	A	C5-C6-N1	6.29	120.85	117.70
1	X	2634	G	N9-C4-C5	-6.29	102.88	105.40
1	X	1974	U	N1-C2-O2	6.29	127.20	122.80
1	X	2553	G	N7-C8-N9	6.28	116.24	113.10
1	X	542	A	C2-N3-C4	-6.28	107.46	110.60
1	X	1540	C	C6-N1-C2	-6.28	117.79	120.30
1	X	1292	A	N1-C2-N3	6.28	132.44	129.30
1	X	1289	A	N1-C6-N6	6.27	122.36	118.60
1	X	2240	C	N3-C2-O2	-6.27	117.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1975	G	C8-N9-C1'	-6.26	118.86	127.00
1	X	2846	G	N7-C8-N9	-6.26	109.97	113.10
1	X	1980	A	N1-C6-N6	-6.26	114.84	118.60
1	X	590	C	N3-C4-N4	-6.24	113.63	118.00
1	X	1274	C	C6-N1-C2	6.24	122.80	120.30
1	X	1277	G	C8-N9-C4	6.24	108.90	106.40
1	X	122	G	C2-N3-C4	-6.24	108.78	111.90
1	X	689	A	C4-C5-N7	6.24	113.82	110.70
1	X	1312	G	N1-C6-O6	6.24	123.64	119.90
1	X	808	C	C6-N1-C2	6.23	122.79	120.30
1	X	1981	A	C4-C5-N7	-6.23	107.58	110.70
1	X	537	C	C5-C6-N1	-6.23	117.89	121.00
1	X	2033	C	N1-C2-O2	6.23	122.64	118.90
1	X	2711	G	N7-C8-N9	-6.23	109.99	113.10
1	X	754	G	C8-N9-C4	6.22	108.89	106.40
1	X	2686	C	N3-C2-O2	-6.22	117.54	121.90
1	X	542	A	C8-N9-C4	-6.22	103.31	105.80
1	X	608	G	N7-C8-N9	-6.22	109.99	113.10
1	X	774	A	N3-C4-C5	6.21	131.15	126.80
1	X	774	A	C2-N3-C4	6.21	113.70	110.60
1	X	1996	A	N7-C8-N9	6.19	116.90	113.80
1	X	1682	A	N3-C4-C5	-6.19	122.47	126.80
1	X	1292	A	C8-N9-C4	6.18	108.27	105.80
1	X	1713	G	N1-C6-O6	-6.17	116.19	119.90
1	X	1288	A	C4-C5-C6	6.16	120.08	117.00
1	X	1285	A	C2-N3-C4	-6.15	107.52	110.60
1	X	1291	G	C6-N1-C2	-6.15	121.41	125.10
1	X	1223	G	C2-N3-C4	-6.14	108.83	111.90
1	X	689	A	N7-C8-N9	6.13	116.87	113.80
1	X	2038	C	N3-C2-O2	-6.11	117.62	121.90
1	X	1378	A	C8-N9-C4	6.11	108.24	105.80
1	X	1993	G	C5-C6-N1	-6.11	108.45	111.50
1	X	771	C	N3-C2-O2	-6.10	117.63	121.90
1	X	1288	A	N1-C2-N3	6.10	132.35	129.30
1	X	1622	G	C8-N9-C4	6.09	108.84	106.40
1	X	534	U	C5-C6-N1	-6.09	119.66	122.70
1	X	799	C	C5-C6-N1	-6.09	117.96	121.00
1	X	1266	G	C4-C5-C6	6.08	122.45	118.80
1	X	2314	A	C2-N3-C4	6.08	113.64	110.60
1	X	1663	C	C2-N3-C4	6.08	122.94	119.90
1	X	822	G	C4-C5-N7	-6.07	108.37	110.80
1	X	1622	G	C5-C6-O6	6.07	132.24	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2227	C	N1-C2-O2	-6.07	115.26	118.90
1	X	1278	A	C6-C5-N7	-6.07	128.05	132.30
1	X	1687	C	C4-C5-C6	6.07	120.43	117.40
1	X	1467	U	C5-C6-N1	-6.06	119.67	122.70
1	X	600	G	N1-C6-O6	6.06	123.54	119.90
1	X	808	C	C5-C6-N1	-6.06	117.97	121.00
1	X	522	G	C4-C5-N7	6.06	113.22	110.80
1	X	608	G	C5-N7-C8	6.06	107.33	104.30
1	X	2551	A	N7-C8-N9	-6.06	110.77	113.80
1	X	2597	G	N1-C6-O6	-6.06	116.27	119.90
1	X	522	G	C5-C6-O6	-6.06	124.97	128.60
1	X	2677	U	C5-C6-N1	-6.05	119.67	122.70
1	X	1694	A	C8-N9-C4	6.05	108.22	105.80
1	X	1260	A	C8-N9-C4	6.05	108.22	105.80
1	X	1212	U	N3-C4-O4	-6.04	115.17	119.40
1	X	1015	U	C6-N1-C2	-6.04	117.38	121.00
1	X	497	C	N1-C2-O2	-6.03	115.28	118.90
1	X	1471	G	C5-C6-O6	-6.03	124.98	128.60
1	X	2626	U	N3-C2-O2	-6.02	117.99	122.20
1	X	1676	U	C2-N3-C4	-6.02	123.39	127.00
1	X	1678	G	N7-C8-N9	-6.02	110.09	113.10
1	X	1672	A	N1-C6-N6	6.01	122.21	118.60
1	X	2707	G	N1-C2-N2	6.01	121.61	116.20
1	X	1960	A	C8-N9-C4	6.01	108.20	105.80
1	X	577	U	C2-N3-C4	6.00	130.60	127.00
1	X	957	G	N1-C6-O6	-6.00	116.30	119.90
1	X	832	A	N1-C6-N6	5.99	122.19	118.60
1	X	2629	U	C5-C6-N1	-5.99	119.71	122.70
1	X	155	G	C8-N9-C4	-5.99	104.01	106.40
1	X	974	U	C5-C6-N1	-5.98	119.71	122.70
1	X	966	A	N9-C4-C5	-5.98	103.41	105.80
1	X	713	G	N7-C8-N9	-5.98	110.11	113.10
1	X	1956	G	C8-N9-C4	5.98	108.79	106.40
1	X	2495	G	N3-C4-C5	-5.97	125.61	128.60
1	X	2001	G	C2-N3-C4	-5.97	108.92	111.90
1	X	2688	G	C8-N9-C4	5.96	108.78	106.40
1	X	2854	G	C4-C5-N7	5.96	113.18	110.80
1	X	1652	G	C2-N3-C4	-5.96	108.92	111.90
1	X	552	C	C6-N1-C2	5.96	122.68	120.30
1	X	540	G	C6-N1-C2	5.95	128.67	125.10
1	X	2666	U	C4-C5-C6	5.95	123.27	119.70
1	X	2852	G	C2-N3-C4	-5.95	108.93	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1917	C	N1-C2-O2	5.94	122.46	118.90
1	X	608	G	C8-N9-C4	5.92	108.77	106.40
1	X	1969	G	C5-C6-O6	-5.92	125.05	128.60
1	X	430	C	C6-N1-C2	-5.91	117.94	120.30
1	X	1216	G	N1-C6-O6	-5.91	116.35	119.90
1	X	713	G	C8-N9-C4	5.91	108.76	106.40
1	X	479	G	C8-N9-C4	5.91	108.76	106.40
1	X	1767	G	N1-C6-O6	5.90	123.44	119.90
1	X	1278	A	C5-N7-C8	-5.90	100.95	103.90
1	X	1981	A	C6-N1-C2	-5.90	115.06	118.60
1	X	2822	U	N3-C2-O2	5.90	126.33	122.20
1	X	2258	G	C8-N9-C4	5.90	108.76	106.40
1	X	1699	A	C5-C6-N1	-5.89	114.75	117.70
1	X	1306	U	C2-N3-C4	-5.89	123.47	127.00
1	X	2712	G	C5-C6-O6	5.89	132.13	128.60
1	X	522	G	N3-C4-C5	5.88	131.54	128.60
1	X	544	U	C5-C6-N1	-5.88	119.76	122.70
1	X	1569	A	C6-N1-C2	-5.88	115.07	118.60
1	X	1770	U	N3-C4-O4	-5.88	115.29	119.40
1	X	2791	C	C5-C6-N1	-5.88	118.06	121.00
1	X	1211	G	N1-C2-N2	-5.87	110.92	116.20
1	X	2822	U	C5-C4-O4	-5.87	122.38	125.90
13	K	96	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	X	766	A	N1-C6-N6	-5.86	115.08	118.60
1	X	1680	U	C6-N1-C2	5.86	124.51	121.00
1	X	854	G	N1-C6-O6	5.86	123.41	119.90
1	X	465	C	C4-C5-C6	5.85	120.33	117.40
1	X	716	U	C5-C6-N1	-5.85	119.78	122.70
1	X	883	A	N7-C8-N9	-5.84	110.88	113.80
1	X	2656	G	C8-N9-C4	5.84	108.74	106.40
1	X	1225	G	N1-C6-O6	-5.84	116.40	119.90
1	X	2791	C	C2-N3-C4	-5.84	116.98	119.90
1	X	1272	G	C8-N9-C4	5.84	108.73	106.40
1	X	590	C	C5-C4-N4	5.84	124.28	120.20
1	X	1468	A	N7-C8-N9	-5.83	110.89	113.80
1	X	1678	G	C5-C6-N1	5.82	114.41	111.50
1	X	2370	G	C8-N9-C4	5.82	108.73	106.40
1	X	2710	C	C4-C5-C6	5.82	120.31	117.40
1	X	1578	U	C5-C6-N1	-5.82	119.79	122.70
1	X	1678	G	C5-N7-C8	5.82	107.21	104.30
1	X	748	A	C8-N9-C4	5.81	108.12	105.80
1	X	122	G	N3-C4-C5	5.81	131.50	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	497	C	N3-C2-O2	5.80	125.96	121.90
1	X	2792	C	C4-C5-C6	5.79	120.30	117.40
1	X	1766	U	C6-N1-C2	5.79	124.48	121.00
1	X	2853	U	N3-C4-O4	-5.79	115.34	119.40
1	X	1689	U	C5-C6-N1	-5.78	119.81	122.70
1	X	1974	U	N3-C2-O2	-5.78	118.15	122.20
1	X	1317	G	N1-C6-O6	5.78	123.37	119.90
1	X	1004	A	C8-N9-C4	-5.77	103.49	105.80
1	X	2686	C	C5-C6-N1	-5.76	118.12	121.00
1	X	1998	A	N1-C6-N6	-5.76	115.14	118.60
1	X	1991	C	C5-C4-N4	5.76	124.23	120.20
1	X	1683	G	C4-C5-C6	-5.76	115.35	118.80
1	X	2484	G	C8-N9-C4	-5.76	104.10	106.40
1	X	1996	A	C8-N9-C4	-5.75	103.50	105.80
1	X	609	U	C5-C6-N1	-5.75	119.83	122.70
1	X	1816	G	C5-N7-C8	5.75	107.17	104.30
1	X	2828	C	C5-C4-N4	-5.75	116.18	120.20
13	K	3	HIS	N-CA-C	5.75	126.52	111.00
1	X	814	G	C5-C6-O6	-5.74	125.16	128.60
1	X	789	G	C4-C5-N7	5.74	113.09	110.80
1	X	540	G	N3-C4-C5	5.74	131.47	128.60
1	X	2791	C	C6-N1-C2	5.74	122.59	120.30
1	X	2480	C	C6-N1-C2	5.73	122.59	120.30
1	X	2856	U	C5-C6-N1	5.73	125.57	122.70
1	X	2306	A	N1-C6-N6	5.73	122.04	118.60
1	X	1989	C	N1-C2-O2	-5.72	115.47	118.90
1	X	2703	C	C2-N1-C1'	-5.72	112.51	118.80
1	X	609	U	C6-N1-C2	5.71	124.43	121.00
1	X	2003	A	N1-C6-N6	-5.71	115.18	118.60
1	X	1315	A	N1-C6-N6	-5.70	115.18	118.60
1	X	2637	C	C6-N1-C2	5.70	122.58	120.30
1	X	661	C	C6-N1-C2	-5.70	118.02	120.30
1	X	1291	G	N1-C2-N3	5.70	127.32	123.90
1	X	2495	G	C5-C6-N1	5.70	114.35	111.50
1	X	2655	C	C2-N3-C4	-5.70	117.05	119.90
1	X	974	U	C4-C5-C6	5.70	123.12	119.70
1	X	1270	C	C6-N1-C2	-5.70	118.02	120.30
1	X	2590	U	N3-C4-C5	-5.70	111.18	114.60
1	X	579	G	C4-C5-N7	-5.69	108.52	110.80
1	X	57	G	C8-N9-C4	-5.69	104.12	106.40
1	X	490	A	C5-C6-N1	5.69	120.55	117.70
1	X	1669	A	C8-N9-C4	5.69	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2700	U	C5-C6-N1	-5.69	119.86	122.70
1	X	1642	G	C5-C6-N1	-5.69	108.66	111.50
1	X	1290	A	C8-N9-C4	5.68	108.07	105.80
1	X	1622	G	N7-C8-N9	-5.67	110.26	113.10
1	X	1277	G	N3-C2-N2	5.67	123.87	119.90
1	X	2371	A	C8-N9-C4	-5.67	103.53	105.80
1	X	1625	A	C2-N3-C4	-5.67	107.77	110.60
1	X	2430	A	C5-C6-N6	5.67	128.23	123.70
1	X	985	G	N3-C4-C5	-5.66	125.77	128.60
1	X	590	C	N3-C2-O2	-5.66	117.94	121.90
1	X	2710	C	C5-C6-N1	-5.66	118.17	121.00
1	X	691	C	C5-C6-N1	-5.66	118.17	121.00
1	X	1288	A	N1-C6-N6	5.66	122.00	118.60
1	X	1682	A	C6-N1-C2	-5.66	115.20	118.60
1	X	2403	C	C4-C5-C6	5.66	120.23	117.40
1	X	1006	C	N3-C2-O2	-5.66	117.94	121.90
1	X	502	A	C8-N9-C4	5.65	108.06	105.80
1	X	1344	C	N3-C4-C5	5.65	124.16	121.90
1	X	2681	A	C5-C6-N6	-5.65	119.18	123.70
1	X	2592	U	C5-C6-N1	-5.64	119.88	122.70
1	X	229	G	N3-C4-C5	5.64	131.42	128.60
1	X	2756	A	C6-N1-C2	-5.64	115.22	118.60
1	X	1932	G	C4-C5-N7	-5.63	108.55	110.80
1	X	1344	C	N1-C2-O2	5.63	122.28	118.90
1	X	1665	C	N3-C4-N4	-5.63	114.06	118.00
1	X	2060	A	C2-N3-C4	5.62	113.41	110.60
1	X	1750	A	C6-N1-C2	-5.62	115.23	118.60
1	X	2223	U	C5-C6-N1	-5.62	119.89	122.70
1	X	2705	A	N1-C6-N6	5.61	121.97	118.60
1	X	1664	G	N3-C4-C5	5.60	131.40	128.60
1	X	1988	A	N7-C8-N9	-5.60	111.00	113.80
2	Y	92	G	C8-N9-C4	5.60	108.64	106.40
1	X	472	C	N1-C2-O2	-5.60	115.54	118.90
1	X	2739	G	C2-N3-C4	5.60	114.70	111.90
1	X	1256	C	C5-C6-N1	-5.60	118.20	121.00
1	X	2681	A	C4-C5-N7	5.60	113.50	110.70
1	X	2669	C	N3-C4-C5	-5.60	119.66	121.90
1	X	556	A	N1-C6-N6	5.59	121.96	118.60
1	X	1991	C	N3-C4-N4	-5.59	114.08	118.00
1	X	985	G	C8-N9-C4	-5.59	104.16	106.40
1	X	1289	A	C8-N9-C4	5.58	108.03	105.80
1	X	1745	C	N1-C2-O2	-5.58	115.55	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1672	A	C5-C6-N6	-5.58	119.24	123.70
1	X	2549	G	N7-C8-N9	-5.58	110.31	113.10
1	X	2003	A	C2-N3-C4	5.58	113.39	110.60
1	X	822	G	C5-N7-C8	5.57	107.09	104.30
1	X	503	G	N7-C8-N9	-5.57	110.31	113.10
1	X	674	U	N1-C2-O2	-5.57	118.90	122.80
1	X	2713	A	N7-C8-N9	-5.57	111.02	113.80
1	X	1688	U	N3-C4-C5	-5.56	111.26	114.60
1	X	577	U	C5-C4-O4	5.56	129.24	125.90
1	X	961	G	C4-C5-N7	-5.56	108.58	110.80
1	X	236	C	C6-N1-C2	-5.55	118.08	120.30
1	X	39	C	C6-N1-C2	-5.55	118.08	120.30
1	X	1573	G	N1-C6-O6	-5.55	116.57	119.90
1	X	766	A	C6-N1-C2	-5.55	115.27	118.60
1	X	1292	A	C2-N3-C4	-5.55	107.83	110.60
1	X	1625	A	C5-C6-N1	-5.54	114.93	117.70
1	X	1204	G	N3-C4-C5	-5.54	125.83	128.60
1	X	550	C	C2-N3-C4	-5.54	117.13	119.90
1	X	2671	C	C5-C6-N1	5.54	123.77	121.00
1	X	827	C	C6-N1-C2	5.54	122.52	120.30
1	X	1769	U	C5-C6-N1	-5.53	119.93	122.70
1	X	1142	G	N9-C4-C5	-5.53	103.19	105.40
1	X	1670	G	N9-C4-C5	-5.53	103.19	105.40
1	X	2753	C	N1-C2-O2	-5.53	115.58	118.90
1	X	460	U	C6-N1-C2	-5.53	117.68	121.00
1	X	1685	A	C5-C6-N1	5.53	120.46	117.70
1	X	343	A	C8-N9-C4	-5.52	103.59	105.80
1	X	809	C	C5-C6-N1	-5.52	118.24	121.00
1	X	2342	U	C5-C6-N1	-5.52	119.94	122.70
1	X	804	C	C5-C6-N1	-5.51	118.24	121.00
1	X	1341	G	N9-C4-C5	-5.51	103.19	105.40
1	X	1265	G	C5-N7-C8	5.51	107.06	104.30
1	X	1468	A	N1-C6-N6	-5.51	115.29	118.60
1	X	802	A	C2-N3-C4	-5.51	107.84	110.60
1	X	608	G	C4-C5-N7	-5.51	108.60	110.80
1	X	1412	C	N3-C2-O2	5.51	125.75	121.90
1	X	2475	C	C6-N1-C2	-5.51	118.10	120.30
1	X	2765	C	N3-C4-N4	-5.51	114.14	118.00
1	X	1980	A	N7-C8-N9	-5.50	111.05	113.80
1	X	577	U	C6-N1-C2	-5.49	117.70	121.00
13	K	99	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	X	165	G	C8-N9-C4	5.49	108.60	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2707	G	N1-C6-O6	5.49	123.19	119.90
1	X	37	C	C6-N1-C2	-5.49	118.11	120.30
1	X	1176	U	C5-C6-N1	-5.49	119.96	122.70
1	X	1633	C	C5-C6-N1	-5.49	118.26	121.00
1	X	2716	G	C4-C5-N7	-5.48	108.61	110.80
1	X	2432	A	N7-C8-N9	5.48	116.54	113.80
1	X	2854	G	C5-C6-O6	-5.48	125.31	128.60
1	X	814	G	N1-C6-O6	5.47	123.18	119.90
1	X	2240	C	N1-C2-O2	5.47	122.18	118.90
1	X	2685	A	C2-N3-C4	-5.47	107.87	110.60
1	X	2686	C	C2-N3-C4	-5.47	117.17	119.90
1	X	2486	C	C6-N1-C2	-5.46	118.11	120.30
1	X	1025	A	N1-C6-N6	-5.46	115.32	118.60
2	Y	83	C	N3-C4-C5	-5.46	119.72	121.90
1	X	1999	U	C6-N1-C2	5.46	124.28	121.00
1	X	741	G	C4-C5-N7	-5.46	108.62	110.80
1	X	1977	C	N3-C4-N4	5.46	121.82	118.00
1	X	1966	C	C2-N3-C4	-5.46	117.17	119.90
1	X	1226	A	C2-N3-C4	-5.45	107.88	110.60
1	X	2496	C	C6-N1-C2	5.44	122.48	120.30
1	X	1472	C	C6-N1-C2	5.43	122.47	120.30
1	X	559	C	N3-C4-N4	5.43	121.80	118.00
1	X	2793	G	N7-C8-N9	-5.43	110.39	113.10
1	X	229	G	C8-N9-C4	5.43	108.57	106.40
1	X	2663	U	C5-C4-O4	5.43	129.16	125.90
1	X	1293	A	C8-N9-C4	5.41	107.97	105.80
1	X	2787	A	N1-C2-N3	5.41	132.01	129.30
1	X	789	G	C6-C5-N7	-5.41	127.15	130.40
1	X	2331	A	C5-C6-N6	5.41	128.03	123.70
1	X	2852	G	N1-C2-N3	5.41	127.15	123.90
1	X	2851	G	C8-N9-C4	5.41	108.56	106.40
1	X	1975	G	N3-C4-N9	5.40	129.24	126.00
1	X	699	G	C5-N7-C8	-5.40	101.60	104.30
1	X	1260	A	N1-C6-N6	-5.40	115.36	118.60
1	X	1344	C	C6-N1-C2	5.39	122.46	120.30
1	X	1995	G	N7-C8-N9	-5.39	110.40	113.10
1	X	989	G	C5-N7-C8	5.39	107.00	104.30
1	X	471	A	C8-N9-C4	5.39	107.95	105.80
1	X	2716	G	C5-N7-C8	5.39	106.99	104.30
1	X	788	G	C5-C6-N1	5.38	114.19	111.50
1	X	406	G	N1-C6-O6	-5.38	116.67	119.90
1	X	1969	G	N3-C4-N9	5.37	129.22	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2567	G	C8-N9-C4	-5.37	104.25	106.40
1	X	31	C	C6-N1-C2	-5.37	118.15	120.30
1	X	1779	C	N1-C2-O2	-5.37	115.68	118.90
1	X	2800	C	C6-N1-C2	-5.37	118.15	120.30
1	X	2034	A	C2-N3-C4	5.37	113.28	110.60
1	X	762	A	N1-C6-N6	5.36	121.82	118.60
1	X	1801	C	C5-C6-N1	-5.36	118.32	121.00
1	X	1984	A	C6-N1-C2	-5.36	115.38	118.60
1	X	2699	G	C6-N1-C2	5.36	128.31	125.10
1	X	1339	U	N1-C2-O2	5.35	126.55	122.80
1	X	2591	C	N1-C2-O2	-5.35	115.69	118.90
1	X	2832	G	C5-N7-C8	-5.35	101.62	104.30
1	X	1275	A	C5-N7-C8	-5.35	101.23	103.90
1	X	1266	G	N1-C2-N3	5.34	127.11	123.90
1	X	1670	G	C2-N3-C4	-5.34	109.23	111.90
1	X	1298	G	C5-C6-O6	5.34	131.81	128.60
1	X	1312	G	N3-C2-N2	5.34	123.64	119.90
1	X	2656	G	N7-C8-N9	-5.34	110.43	113.10
1	X	832	A	C4-C5-N7	5.33	113.37	110.70
1	X	23	G	C5-C6-O6	5.33	131.80	128.60
1	X	2712	G	C8-N9-C4	5.33	108.53	106.40
1	X	527	C	C2-N1-C1'	5.33	124.66	118.80
1	X	570	G	N3-C2-N2	-5.32	116.17	119.90
1	X	1274	C	N1-C2-N3	-5.32	115.47	119.20
1	X	1442	C	N3-C4-C5	5.32	124.03	121.90
1	X	2478	C	N3-C4-N4	5.32	121.72	118.00
1	X	1246	G	N1-C6-O6	-5.32	116.71	119.90
1	X	1980	A	C4-C5-N7	-5.31	108.04	110.70
1	X	1652	G	N3-C4-C5	5.30	131.25	128.60
1	X	2519	C	N3-C4-C5	-5.30	119.78	121.90
1	X	346	C	C4-C5-C6	5.30	120.05	117.40
1	X	1685	A	N1-C6-N6	-5.30	115.42	118.60
1	X	1266	G	C5-C6-N1	-5.30	108.85	111.50
1	X	1321	A	N7-C8-N9	-5.30	111.15	113.80
1	X	754	G	N7-C8-N9	-5.30	110.45	113.10
1	X	465	C	C6-N1-C2	5.29	122.42	120.30
1	X	2478	C	C5-C6-N1	5.29	123.65	121.00
1	X	497	C	C6-N1-C2	5.29	122.42	120.30
1	X	2432	A	C8-N9-C4	-5.29	103.69	105.80
1	X	544	U	N1-C2-O2	5.28	126.50	122.80
1	X	949	G	C8-N9-C4	5.28	108.51	106.40
1	X	1939	U	N1-C2-O2	-5.28	119.11	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1763	G	N3-C2-N2	5.27	123.59	119.90
1	X	826	U	C5-C4-O4	5.27	129.06	125.90
1	X	699	G	C6-N1-C2	5.26	128.26	125.10
1	X	1742	G	C8-N9-C4	5.26	108.51	106.40
1	X	1665	C	N3-C4-C5	5.26	124.00	121.90
1	X	714	G	N1-C6-O6	-5.26	116.75	119.90
1	X	1211	G	N7-C8-N9	-5.26	110.47	113.10
1	X	796	A	C5-N7-C8	-5.25	101.27	103.90
1	X	714	G	C4-C5-N7	-5.25	108.70	110.80
13	K	10	LEU	CB-CG-CD2	5.25	119.93	111.00
1	X	2233	C	C5-C6-N1	-5.25	118.38	121.00
1	X	2809	A	C2-N3-C4	5.25	113.22	110.60
1	X	1468	A	C5-N7-C8	5.25	106.52	103.90
1	X	2717	G	N1-C6-O6	-5.25	116.75	119.90
1	X	772	G	C5-C6-N1	5.25	114.12	111.50
1	X	550	C	N1-C2-O2	-5.24	115.75	118.90
1	X	2616	U	C5-C4-O4	-5.24	122.75	125.90
1	X	1667	A	C8-N9-C4	5.24	107.90	105.80
1	X	568	G	C4-C5-N7	-5.24	108.71	110.80
1	X	2700	U	C5-C4-O4	5.24	129.04	125.90
1	X	2665	G	C4-C5-N7	-5.23	108.71	110.80
1	X	757	U	N3-C2-O2	-5.23	118.54	122.20
1	X	1662	G	C4-C5-N7	-5.23	108.71	110.80
1	X	2618	A	N9-C4-C5	5.23	107.89	105.80
1	X	2007	G	C5-N7-C8	5.23	106.91	104.30
13	K	5	LYS	CD-CE-NZ	5.23	123.72	111.70
1	X	2555	G	C8-N9-C4	5.22	108.49	106.40
1	X	1312	G	C6-C5-N7	-5.22	127.27	130.40
1	X	1931	G	N7-C8-N9	5.22	115.71	113.10
1	X	2667	C	N3-C2-O2	5.22	125.55	121.90
1	X	2807	U	N3-C4-O4	-5.22	115.75	119.40
1	X	537	C	C2-N3-C4	-5.21	117.29	119.90
1	X	1223	G	N1-C6-O6	5.21	123.03	119.90
1	X	1995	G	N1-C6-O6	-5.21	116.77	119.90
1	X	607	C	N3-C2-O2	-5.21	118.25	121.90
1	X	704	G	C5-C6-O6	5.21	131.72	128.60
1	X	2853	U	N1-C2-O2	5.21	126.45	122.80
1	X	1290	A	N1-C6-N6	5.21	121.72	118.60
1	X	2371	A	N9-C4-C5	5.20	107.88	105.80
1	X	2791	C	N3-C4-C5	5.20	123.98	121.90
1	X	121	G	C4-C5-N7	-5.20	108.72	110.80
1	X	1459	U	N3-C2-O2	5.19	125.83	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2748	C	N3-C2-O2	5.19	125.53	121.90
1	X	1662	G	C5-C6-O6	5.18	131.71	128.60
1	X	2815	C	N3-C4-C5	5.17	123.97	121.90
1	X	538	A	C5-C6-N6	-5.17	119.56	123.70
1	X	2766	U	N3-C4-O4	-5.16	115.79	119.40
1	X	2618	A	C6-N1-C2	-5.16	115.50	118.60
1	X	87	G	C8-N9-C4	-5.16	104.34	106.40
1	X	1743	C	C4-C5-C6	5.16	119.98	117.40
1	X	2683	C	C6-N1-C2	5.16	122.36	120.30
3	A	21	ASP	CB-CG-OD2	5.16	122.94	118.30
1	X	1665	C	C6-N1-C2	5.16	122.36	120.30
1	X	2796	A	C4-C5-C6	5.16	119.58	117.00
1	X	504	G	C2-N3-C4	-5.15	109.32	111.90
1	X	1278	A	C4-C5-C6	5.15	119.58	117.00
1	X	2824	C	C6-N1-C2	5.15	122.36	120.30
2	Y	84	G	C8-N9-C4	5.15	108.46	106.40
1	X	529	U	C6-N1-C2	-5.15	117.91	121.00
1	X	1694	A	C2-N3-C4	-5.15	108.03	110.60
1	X	1716	G	N1-C6-O6	-5.15	116.81	119.90
1	X	2848	A	C2-N3-C4	5.15	113.18	110.60
1	X	522	G	C5-N7-C8	-5.15	101.72	104.30
1	X	1992	G	C8-N9-C4	5.15	108.46	106.40
1	X	481	A	N1-C6-N6	5.15	121.69	118.60
1	X	1282	A	C2-N3-C4	-5.15	108.03	110.60
1	X	1764	A	N1-C2-N3	5.15	131.87	129.30
1	X	1993	G	N3-C4-C5	5.15	131.17	128.60
1	X	537	C	N3-C2-O2	-5.14	118.30	121.90
1	X	2592	U	C4-C5-C6	5.14	122.79	119.70
1	X	1260	A	N7-C8-N9	-5.14	111.23	113.80
1	X	544	U	N3-C4-O4	-5.14	115.80	119.40
1	X	1748	U	N1-C2-O2	-5.14	119.20	122.80
1	X	2594	U	C5-C6-N1	5.14	125.27	122.70
1	X	1632	A	C8-N9-C4	-5.14	103.75	105.80
1	X	1721	G	C8-N9-C4	5.14	108.45	106.40
1	X	1032	A	C8-N9-C4	-5.13	103.75	105.80
1	X	2224	U	C5-C4-O4	5.13	128.98	125.90
1	X	1467	U	C2-N1-C1'	5.13	123.85	117.70
1	X	2565	C	C6-N1-C2	-5.12	118.25	120.30
1	X	2611	A	N7-C8-N9	-5.12	111.24	113.80
1	X	2329	C	N3-C2-O2	5.12	125.48	121.90
1	X	1357	U	C5-C6-N1	-5.12	120.14	122.70
1	X	1998	A	N7-C8-N9	-5.11	111.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1678	G	C8-N9-C4	5.11	108.44	106.40
1	X	1770	U	N1-C2-N3	5.11	117.97	114.90
1	X	1822	C	C2-N3-C4	-5.11	117.35	119.90
1	X	2007	G	C5-C6-O6	5.10	131.66	128.60
1	X	459	A	P-O3'-C3'	5.10	125.82	119.70
1	X	1276	U	C5-C6-N1	-5.10	120.15	122.70
1	X	1305	C	C2-N3-C4	-5.10	117.35	119.90
1	X	1816	G	C4-C5-N7	-5.10	108.76	110.80
1	X	2520	A	C5-C6-N6	5.10	127.78	123.70
1	X	2815	C	C2-N3-C4	-5.10	117.35	119.90
1	X	2839	G	C8-N9-C4	5.10	108.44	106.40
1	X	2681	A	N9-C4-C5	-5.10	103.76	105.80
1	X	1281	A	N1-C2-N3	5.09	131.85	129.30
1	X	1302	C	C2-N1-C1'	-5.09	113.20	118.80
1	X	74	G	C8-N9-C4	5.09	108.44	106.40
1	X	345	U	N1-C2-O2	-5.09	119.24	122.80
1	X	2797	G	N3-C4-C5	-5.09	126.06	128.60
1	X	2590	U	C2-N3-C4	-5.09	123.95	127.00
1	X	1328	C	N3-C2-O2	-5.09	118.34	121.90
1	X	2623	A	N7-C8-N9	-5.08	111.26	113.80
1	X	2666	U	N1-C2-N3	5.08	117.95	114.90
1	X	2033	C	C6-N1-C2	-5.08	118.27	120.30
1	X	2680	U	N3-C2-O2	5.08	125.75	122.20
1	X	2764	U	C5-C6-N1	-5.08	120.16	122.70
1	X	29	U	C5-C6-N1	5.07	125.24	122.70
1	X	2008	C	N3-C4-C5	-5.07	119.87	121.90
1	X	330	C	C6-N1-C2	-5.07	118.27	120.30
1	X	695	G	N7-C8-N9	-5.07	110.57	113.10
1	X	1294	G	N1-C2-N3	5.07	126.94	123.90
1	X	2483	U	C6-N1-C2	-5.07	117.96	121.00
1	X	2556	A	N9-C4-C5	5.07	107.83	105.80
1	X	2748	C	N1-C2-O2	-5.07	115.86	118.90
1	X	190	A	C8-N9-C4	5.06	107.83	105.80
1	X	550	C	C6-N1-C2	5.06	122.33	120.30
1	X	1145	C	N1-C2-O2	-5.06	115.86	118.90
1	X	1999	U	N3-C2-O2	5.06	125.74	122.20
1	X	2408	G	C8-N9-C4	-5.06	104.38	106.40
1	X	2398	U	N3-C2-O2	-5.05	118.66	122.20
1	X	2658	A	C8-N9-C4	5.05	107.82	105.80
1	X	2760	G	N7-C8-N9	-5.05	110.57	113.10
1	X	1391	A	C8-N9-C4	5.05	107.82	105.80
2	Y	85	G	C2-N3-C4	-5.05	109.38	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1631	C	C5-C6-N1	-5.05	118.48	121.00
1	X	2804	G	C8-N9-C4	5.05	108.42	106.40
1	X	69	G	C8-N9-C4	5.05	108.42	106.40
15	M	71	ILE	CG1-CB-CG2	-5.05	100.30	111.40
1	X	2722	C	C6-N1-C2	5.04	122.32	120.30
1	X	196	A	C4-C5-N7	-5.04	108.18	110.70
1	X	1687	C	N3-C4-C5	-5.04	119.88	121.90
1	X	2260	C	N3-C4-C5	5.04	123.91	121.90
1	X	2556	A	C8-N9-C4	-5.04	103.79	105.80
1	X	340	G	N7-C8-N9	-5.03	110.58	113.10
1	X	1344	C	C5-C6-N1	-5.03	118.48	121.00
1	X	1614	C	N1-C2-O2	-5.03	115.88	118.90
1	X	2437	G	C5-C6-O6	-5.03	125.58	128.60
1	X	2005	U	C5-C6-N1	-5.03	120.19	122.70
1	X	122	G	C5-C6-N1	-5.03	108.99	111.50
1	X	542	A	C6-C5-N7	-5.03	128.78	132.30
1	X	1750	A	N1-C2-N3	5.03	131.81	129.30
1	X	1775	A	N7-C8-N9	-5.03	111.29	113.80
1	X	1979	C	N1-C2-O2	-5.03	115.88	118.90
1	X	1235	C	C6-N1-C2	5.02	122.31	120.30
1	X	2569	A	N7-C8-N9	-5.02	111.29	113.80
1	X	748	A	N1-C6-N6	5.02	121.61	118.60
1	X	966	A	C8-N9-C4	5.02	107.81	105.80
1	X	2375	G	C8-N9-C4	5.02	108.41	106.40
1	X	2545	A	N1-C6-N6	5.02	121.61	118.60
1	X	1652	G	N1-C6-O6	5.01	122.91	119.90
1	X	1660	G	C5-C6-O6	5.01	131.61	128.60
1	X	2542	U	C6-N1-C2	5.01	124.01	121.00
2	Y	20	A	C8-N9-C4	5.01	107.81	105.80
1	X	1274	C	C5-C4-N4	-5.01	116.69	120.20
1	X	2578	G	N3-C4-N9	5.01	129.01	126.00
1	X	2695	C	C6-N1-C2	-5.01	118.30	120.30
1	X	2762	G	N1-C6-O6	5.01	122.91	119.90
1	X	1339	U	C2-N1-C1'	5.01	123.71	117.70
1	X	490	A	N1-C6-N6	-5.01	115.60	118.60
1	X	1652	G	N9-C4-C5	-5.01	103.40	105.40
1	X	1687	C	C5-C6-N1	-5.01	118.50	121.00
1	X	1767	G	C5-C6-O6	-5.00	125.60	128.60
1	X	2798	A	C4-C5-N7	5.00	113.20	110.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57035	0	28741	1817	0
2	Y	2561	0	1306	48	0
3	A	1920	0	1974	176	0
4	B	1539	0	1600	147	0
5	C	1481	0	1504	120	0
6	D	1400	0	1481	61	0
7	E	1286	0	1336	44	0
8	F	451	0	474	7	0
9	G	1114	0	1144	100	0
10	H	997	0	1046	98	0
11	I	1011	0	1047	98	0
12	J	1090	0	1125	78	0
13	K	878	0	930	80	0
14	L	779	0	820	72	0
15	M	871	0	894	99	0
16	N	978	0	1020	82	0
17	O	741	0	756	45	0
18	P	1004	0	1083	88	0
19	Q	726	0	753	50	0
20	R	825	0	881	69	0
21	S	1345	0	1372	43	0
22	T	556	0	579	38	0
23	U	552	0	604	48	0
24	V	525	0	546	29	0
25	W	424	0	470	17	0
26	Z	452	0	457	53	0
27	1	431	0	456	58	0
28	2	383	0	414	52	0
29	3	462	0	506	63	0
30	4	297	0	330	23	0
31	X	58	0	69	13	0
32	C	1	0	0	0	0
32	I	1	0	0	0	0
32	X	151	0	0	0	0
32	Y	1	0	0	0	0
33	A	1	0	0	0	0
33	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	X	37	0	0	0	0
33	Y	2	0	0	0	0
33	Z	1	0	0	0	0
34	M	1	0	0	0	0
34	X	14	0	0	0	0
All	All	84383	0	55718	3336	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 24.

All (3336) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2044:G:OP1	5:C:62:LYS:HG3	1.36	1.18
15:M:28:ARG:HB2	15:M:29:PRO:HD3	1.29	1.14
9:G:103:TYR:HB3	9:G:107:GLN:HE21	1.14	1.12
4:B:9:ILE:HD11	4:B:27:LEU:HB2	1.32	1.10
4:B:116:VAL:HG22	4:B:136:ARG:NE	1.69	1.05
9:G:67:ARG:HB3	9:G:70:PHE:HA	1.39	1.05
28:2:10:ARG:H	28:2:10:ARG:HD2	1.19	1.05
10:H:83:ARG:HD2	10:H:89:ILE:HD11	1.38	1.05
9:G:100:TYR:HB2	9:G:116:ARG:HH11	1.20	1.04
4:B:116:VAL:HG22	4:B:136:ARG:HE	1.21	1.03
23:U:17:SER:HB2	23:U:44:ALA:HA	1.36	1.03
5:C:176:ASN:HD21	5:C:178:TYR:HB3	1.22	1.03
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.71	1.02
1:X:591:G:H2'	1:X:592:G:C8	1.94	1.02
3:A:96:LEU:HD12	3:A:106:ILE:HD12	1.43	1.00
1:X:552:C:H2'	1:X:553:C:H5''	1.41	1.00
3:A:244:GLY:H	3:A:245:ARG:NH1	1.60	1.00
16:N:50:ARG:HA	16:N:53:LYS:HE2	1.43	1.00
6:D:38:GLU:HB3	6:D:87:ILE:HB	1.42	0.99
2:Y:17:A:H1'	2:Y:112:A:C8	1.97	0.99
9:G:106:TYR:CE2	9:G:108:GLY:HA3	1.99	0.98
1:X:2797:G:OP2	13:K:3:HIS:CE1	2.16	0.97
14:L:31:VAL:HG23	14:L:38:ILE:HD13	1.46	0.97
3:A:49:ARG:HD2	3:A:49:ARG:H	1.29	0.97
29:3:13:ARG:HH11	29:3:25:PHE:HB2	1.30	0.96
1:X:1466:C:H2'	1:X:1467:U:O4'	1.67	0.95
4:B:14:ILE:HG12	15:M:20:HIS:CD2	2.02	0.95
9:G:132:PHE:HD2	9:G:145:HIS:CD2	1.84	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:20:ARG:HD3	23:U:43:ARG:HH22	1.30	0.94
1:X:2592:U:H2'	26:Z:5:PRO:HG2	1.48	0.93
5:C:176:ASN:HD22	5:C:179:ASP:H	1.10	0.93
1:X:2736:U:H3	1:X:2738:A:H62	1.05	0.93
1:X:540:G:H2'	1:X:542:A:H2	1.31	0.93
1:X:760:U:C6	26:Z:3:LYS:HE2	2.04	0.92
1:X:2170:C:H3'	1:X:2171:U:H5''	1.49	0.92
9:G:132:PHE:CD2	9:G:145:HIS:CD2	2.57	0.91
1:X:2757:G:H5''	1:X:2758:A:H5'	1.49	0.91
4:B:14:ILE:HA	15:M:20:HIS:HD2	1.34	0.91
3:A:44:ARG:HD2	3:A:44:ARG:N	1.83	0.91
4:B:110:GLY:HA2	4:B:161:GLY:HA3	1.52	0.91
1:X:2044:G:OP1	5:C:62:LYS:CG	2.18	0.91
22:T:12:ASN:HB3	22:T:14:ARG:HG2	1.51	0.91
1:X:225:G:C2	1:X:2410:U:H4'	2.05	0.91
31:X:2881:LMA:H37B	31:X:2881:LMA:H35	1.52	0.91
13:K:45:ARG:HG3	13:K:95:THR:HG21	1.54	0.90
23:U:49:LYS:HB3	23:U:61:TRP:CE3	2.05	0.90
5:C:26:VAL:HG22	11:I:18:ARG:HH12	1.35	0.90
1:X:2426:G:H3'	1:X:2479:U:OP2	1.72	0.90
1:X:2447:G:HO2'	1:X:2448:A:H8	0.91	0.90
15:M:11:GLU:HG3	15:M:14:ARG:HH11	1.36	0.90
1:X:635:C:H2'	1:X:636:G:H5''	1.50	0.90
9:G:103:TYR:HB3	9:G:107:GLN:NE2	1.86	0.89
20:R:15:HIS:HD1	20:R:16:PHE:HD2	1.19	0.89
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.53	0.89
20:R:18:LYS:HD3	20:R:18:LYS:H	1.36	0.89
20:R:22:VAL:HG11	20:R:80:LYS:HE3	1.54	0.89
2:Y:119:G:H4'	14:L:57:ALA:HB3	1.55	0.89
18:P:66:GLU:HB3	18:P:67:PRO:HD3	1.53	0.88
1:X:347:C:H4'	20:R:15:HIS:CD2	2.08	0.88
1:X:870:C:H1'	22:T:26:PHE:HE2	1.39	0.88
15:M:33:VAL:HG22	15:M:51:GLU:HB2	1.53	0.88
27:I:34:LYS:HA	27:I:34:LYS:HE3	1.56	0.88
1:X:1296:G:H22	1:X:1299:A:H5''	1.39	0.87
1:X:2204:A:H4'	1:X:2205:C:O5'	1.71	0.87
7:E:103:LEU:HD21	7:E:131:ILE:HD13	1.55	0.87
12:J:15:ARG:HD3	12:J:73:LYS:HG3	1.56	0.87
13:K:84:ALA:HB3	13:K:85:PRO:HD3	1.55	0.87
3:A:44:ARG:HD2	3:A:44:ARG:H	1.34	0.87
2:Y:59:A:H1'	6:D:27:ALA:HB2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1816:G:OP1	3:A:53:ARG:HD3	1.75	0.86
7:E:105:MET:HB2	7:E:113:VAL:HB	1.57	0.86
13:K:100:VAL:HG12	13:K:101:GLY:N	1.90	0.86
1:X:2811:G:H2'	1:X:2812:A:C8	2.11	0.86
1:X:870:C:H4'	22:T:23:VAL:HG21	1.56	0.86
1:X:1086:C:H3'	1:X:1087:C:H5''	1.57	0.86
2:Y:33:C:H42	2:Y:53:G:H1	1.22	0.86
9:G:106:TYR:CE2	9:G:108:GLY:CA	2.59	0.85
10:H:25:LEU:HD11	10:H:52:VAL:HG23	1.55	0.85
1:X:1790:G:H4'	1:X:1791:C:O5'	1.77	0.85
1:X:1067:G:H21	1:X:1114:A:H62	1.21	0.85
1:X:313:U:H2'	1:X:314:G:H8	1.39	0.85
4:B:76:ARG:NH1	15:M:4:HIS:HB2	1.91	0.85
5:C:163:ASN:HD21	5:C:167:VAL:H	1.21	0.85
28:2:37:LYS:O	28:2:40:HIS:HE1	1.59	0.85
1:X:2598:C:O2'	1:X:2599:U:H5'	1.77	0.85
12:J:42:TRP:HB3	12:J:95:VAL:HG11	1.55	0.84
31:X:2881:LMA:H32	31:X:2881:LMA:O53	1.76	0.84
11:I:31:GLY:O	11:I:32:ARG:HG3	1.77	0.84
1:X:347:C:H4'	20:R:15:HIS:HD2	1.38	0.84
20:R:15:HIS:ND1	20:R:16:PHE:HD2	1.75	0.84
25:W:46:THR:HG22	25:W:47:VAL:HG13	1.60	0.84
1:X:918:A:H2'	1:X:919:U:H5''	1.60	0.84
3:A:173:TYR:HA	3:A:187:HIS:HA	1.60	0.84
3:A:43:GLY:C	3:A:44:ARG:HH11	1.81	0.83
1:X:1811:A:H4'	1:X:1812:U:O5'	1.78	0.83
9:G:162:LYS:H	9:G:163:PRO:HD2	1.43	0.83
1:X:504:G:H4'	18:P:27:VAL:HG13	1.60	0.83
1:X:1469:U:H5'	1:X:1470:G:OP2	1.77	0.83
13:K:49:GLU:OE1	13:K:95:THR:HG22	1.77	0.83
16:N:66:ASN:HB2	16:N:70:ARG:HH12	1.43	0.83
10:H:2:ILE:HB	10:H:45:ALA:HB3	1.60	0.83
4:B:131:SER:HB2	4:B:134:TRP:CD1	2.12	0.83
18:P:85:MET:HE3	18:P:130:GLU:HG3	1.61	0.82
13:K:98:LEU:HD23	26:Z:45:ILE:HD11	1.59	0.82
1:X:165:G:H1	1:X:185:C:H42	1.27	0.82
1:X:2266:A:O2'	1:X:2267:A:H2'	1.78	0.82
1:X:1147:G:H2'	1:X:1148:G:H8	1.45	0.82
4:B:146:THR:HB	4:B:147:PRO:HD2	1.59	0.82
1:X:1631:C:H1'	18:P:108:PRO:HG2	1.59	0.82
20:R:22:VAL:HG13	20:R:81:VAL:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2194:A:H3'	1:X:2195:C:H5''	1.60	0.82
1:X:595:A:H5'	5:C:83:ALA:HB3	1.62	0.81
1:X:2796:A:P	13:K:3:HIS:HE2	2.03	0.81
18:P:95:ALA:HB2	18:P:126:ILE:HD13	1.61	0.81
26:Z:42:SER:O	26:Z:44:HIS:HD2	1.63	0.81
1:X:2200:G:H2'	1:X:2201:G:C8	2.15	0.81
1:X:2289:A:H2	6:D:79:LEU:HD11	1.44	0.81
23:U:20:ARG:HD3	23:U:43:ARG:NH2	1.94	0.81
3:A:80:VAL:HB	3:A:115:GLY:H	1.46	0.81
27:1:9:ILE:HA	27:1:28:ARG:HA	1.62	0.80
3:A:25:LEU:CB	3:A:206:VAL:HG22	2.12	0.80
14:L:37:HIS:CE1	14:L:57:ALA:HB2	2.16	0.80
1:X:938:G:O2'	1:X:939:C:H5'	1.82	0.80
1:X:540:G:H2'	1:X:542:A:C2	2.16	0.80
1:X:2797:G:OP2	13:K:3:HIS:HE1	1.60	0.80
18:P:103:LEU:HB2	18:P:119:LYS:HB2	1.62	0.80
20:R:90:LYS:HB2	20:R:108:VAL:HG21	1.64	0.80
1:X:408:U:H2'	1:X:409:G:C8	2.16	0.80
1:X:1053:G:H4'	1:X:1054:C:OP1	1.80	0.80
28:2:43:THR:O	28:2:43:THR:HG22	1.78	0.79
15:M:99:VAL:HG21	15:M:104:LEU:HD21	1.62	0.79
1:X:1016:C:O2'	9:G:56:THR:HG21	1.81	0.79
4:B:174:GLU:HB3	4:B:183:LEU:HD12	1.64	0.79
1:X:37:C:H1'	5:C:44:SER:OG	1.83	0.79
10:H:13:ASN:HD21	10:H:109:ARG:HG2	1.48	0.79
10:H:116:ARG:HD2	15:M:38:LYS:NZ	1.98	0.79
1:X:2861:A:O2'	26:Z:31:THR:HG23	1.83	0.79
1:X:666:U:H2'	1:X:667:U:H5''	1.64	0.79
27:1:39:LYS:NZ	27:1:47:HIS:HA	1.98	0.79
1:X:1630:A:N1	18:P:114:ALA:HB2	1.98	0.79
13:K:49:GLU:O	13:K:52:ILE:HG12	1.83	0.79
18:P:41:VAL:O	18:P:44:VAL:HG22	1.82	0.79
22:T:43:THR:O	22:T:43:THR:HG22	1.82	0.79
5:C:154:ASP:O	5:C:157:THR:HG22	1.83	0.78
1:X:1142:G:N3	9:G:103:TYR:HD2	1.80	0.78
3:A:69:LYS:HD3	3:A:69:LYS:H	1.48	0.78
16:N:66:ASN:HB2	16:N:70:ARG:NH1	1.98	0.78
1:X:824:U:C2'	11:I:30:ALA:HB2	2.14	0.78
1:X:2672:U:H2'	1:X:2673:G:H8	1.49	0.78
10:H:27:SER:HA	10:H:50:ILE:HD12	1.64	0.78
1:X:1404:C:H5'	1:X:1405:A:OP2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:168:A:H2'	1:X:169:C:C6	2.19	0.78
1:X:469:G:H5'	28:2:39:ARG:HB2	1.66	0.77
27:1:14:SER:HB2	27:1:22:TYR:HA	1.67	0.77
28:2:37:LYS:O	28:2:40:HIS:CE1	2.37	0.77
1:X:2796:A:OP2	13:K:3:HIS:NE2	2.16	0.77
1:X:1976:U:H4'	4:B:128:SER:OG	1.83	0.77
1:X:317:U:H2'	1:X:318:G:H5'	1.65	0.77
10:H:76:ARG:O	10:H:94:ASN:HA	1.84	0.77
1:X:2659:C:H5'	4:B:189:PRO:HA	1.65	0.77
3:A:61:ARG:HD3	3:A:88:ASN:OD1	1.85	0.77
18:P:87:GLU:HA	18:P:90:LEU:HG	1.67	0.77
1:X:313:U:H2'	1:X:314:G:C8	2.20	0.77
5:C:5:ASN:HA	5:C:118:VAL:HG23	1.67	0.77
14:L:89:PHE:HB3	14:L:91:ARG:NH2	1.99	0.77
1:X:1584:G:H5'	3:A:62:LEU:HG	1.67	0.77
27:1:39:LYS:CE	27:1:47:HIS:HA	2.15	0.76
16:N:6:THR:O	16:N:9:VAL:HG23	1.84	0.76
1:X:492:G:H22	1:X:519:C:H42	1.32	0.76
4:B:78:LEU:O	4:B:79:ARG:HD3	1.86	0.76
10:H:10:VAL:HG23	10:H:17:ARG:O	1.84	0.76
11:I:74:VAL:HG13	11:I:109:LEU:HD12	1.68	0.76
15:M:28:ARG:CB	15:M:29:PRO:HD3	2.11	0.76
5:C:162:ARG:HD2	5:C:162:ARG:C	2.05	0.76
1:X:2495:G:O2'	1:X:2496:C:H5'	1.85	0.76
27:1:29:ARG:HA	27:1:33:ALA:CB	2.16	0.76
13:K:98:LEU:HD21	26:Z:56:GLN:HG2	1.67	0.76
19:Q:53:ILE:HD13	19:Q:80:VAL:HG12	1.65	0.76
2:Y:51:G:H2'	2:Y:52:G:C8	2.21	0.76
3:A:143:VAL:HG12	3:A:194:ILE:HA	1.67	0.76
27:1:8:ILE:H	27:1:8:ILE:HD13	1.49	0.75
1:X:824:U:H2'	11:I:30:ALA:HB2	1.66	0.75
1:X:2590:U:C5	26:Z:4:HIS:NE2	2.53	0.75
1:X:1314:A:O2'	1:X:1315:A:H3'	1.86	0.75
27:1:14:SER:CB	27:1:23:THR:H	1.99	0.75
10:H:99:ILE:HD12	10:H:103:GLY:HA2	1.67	0.75
1:X:542:A:H2'	16:N:28:ARG:NE	2.01	0.75
1:X:1441:A:H4'	1:X:1442:C:O5'	1.84	0.75
3:A:71:ARG:HG2	3:A:191:TYR:CE1	2.22	0.75
5:C:162:ARG:O	5:C:162:ARG:HD2	1.86	0.75
1:X:1016:C:HO2'	1:X:1023:U:H5	1.34	0.75
11:I:43:ALA:O	11:I:45:LYS:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1048:U:H3	1:X:1129:A:H61	1.33	0.75
1:X:2811:G:H2'	1:X:2812:A:H8	1.49	0.75
27:1:29:ARG:HA	27:1:33:ALA:HB2	1.67	0.75
14:L:38:ILE:HD12	14:L:39:TYR:H	1.51	0.75
18:P:59:PHE:HD1	26:Z:30:LEU:HD11	1.52	0.75
21:S:51:LEU:H	21:S:51:LEU:HD23	1.51	0.75
1:X:128:C:H2'	1:X:129:A:H5''	1.68	0.75
12:J:99:LYS:HE3	12:J:100:PRO:HD2	1.69	0.74
1:X:1673:C:H2'	1:X:1674:C:H6	1.52	0.74
2:Y:51:G:H2'	2:Y:52:G:H8	1.51	0.74
4:B:11:MET:HG2	4:B:24:THR:OG1	1.87	0.74
1:X:2484:G:O2'	1:X:2485:U:H5''	1.87	0.74
3:A:209:LYS:HE3	3:A:209:LYS:HA	1.68	0.74
21:S:100:THR:HG23	21:S:138:VAL:HG11	1.69	0.74
1:X:1444:C:H42	1:X:1579:G:H1	1.33	0.74
4:B:14:ILE:HD12	4:B:23:VAL:HG21	1.70	0.74
13:K:28:LEU:C	13:K:28:LEU:HD23	2.08	0.74
1:X:1173:G:H4'	17:O:22:VAL:HG22	1.70	0.74
19:Q:62:ARG:O	19:Q:63:LYS:HB3	1.88	0.74
1:X:754:G:H2'	1:X:755:C:H6	1.52	0.74
29:3:30:ARG:HH21	29:3:31:HIS:CE1	2.06	0.74
29:3:60:LEU:HD12	29:3:63:PRO:HG2	1.69	0.74
1:X:2245:A:H4'	1:X:2246:A:N3	2.02	0.74
1:X:161:U:H4'	1:X:194:G:H21	1.51	0.73
1:X:2590:U:C5	26:Z:4:HIS:CE1	2.76	0.73
15:M:32:THR:O	15:M:51:GLU:HA	1.89	0.73
1:X:2660:C:H42	1:X:2707:G:H1	1.37	0.73
1:X:552:C:C2'	1:X:553:C:H5''	2.17	0.73
15:M:104:LEU:HA	15:M:106:TYR:CE2	2.24	0.73
26:Z:6:VAL:HG13	26:Z:7:PRO:HD2	1.70	0.73
29:3:13:ARG:NH1	29:3:25:PHE:HB2	2.03	0.73
3:A:245:ARG:C	3:A:253:LYS:HE2	2.09	0.73
3:A:54:PHE:O	3:A:55:ILE:HB	1.87	0.73
6:D:60:ILE:HG13	6:D:61:THR:HG23	1.71	0.73
13:K:87:TYR:HE1	13:K:94:TYR:HD1	1.36	0.73
1:X:590:C:H2'	1:X:591:G:H8	1.54	0.73
26:Z:52:TYR:O	26:Z:53:ASP:HB2	1.89	0.73
1:X:1336:G:H2'	1:X:1337:G:H5'	1.69	0.73
1:X:1542:G:H22	1:X:1562:G:H1	1.37	0.73
18:P:37:LYS:HE2	18:P:64:ALA:HB2	1.71	0.72
1:X:73:A:H5''	1:X:74:G:O4'	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:13:ARG:HD2	29:3:25:PHE:N	2.04	0.72
23:U:51:ILE:HG23	23:U:59:THR:HG22	1.71	0.72
18:P:25:PHE:HD1	18:P:127:ILE:HD11	1.54	0.72
14:L:38:ILE:HD11	14:L:40:ALA:H	1.53	0.72
1:X:177:U:H3'	23:U:40:ARG:HH21	1.53	0.72
1:X:2734:U:H4'	30:4:26:ILE:HD13	1.70	0.72
11:I:58:ALA:HA	29:3:12:ARG:HH21	1.54	0.72
20:R:29:HIS:CD2	20:R:51:VAL:HG22	2.24	0.72
1:X:1278:A:H2	1:X:1997:A:H62	1.37	0.72
1:X:394:U:OP1	23:U:19:ILE:HD11	1.89	0.72
1:X:1277:G:OP1	26:Z:19:ARG:NH2	2.22	0.72
1:X:540:G:C2'	1:X:542:A:H2	2.02	0.72
1:X:2825:A:H2'	1:X:2825:A:N3	2.04	0.72
1:X:797:A:C5	3:A:230:VAL:HG21	2.24	0.72
1:X:1656:U:C2'	1:X:1657:A:H5''	2.20	0.72
1:X:2218:G:H5'	3:A:250:PRO:HD3	1.70	0.72
1:X:654:A:N3	1:X:654:A:H3'	2.04	0.72
1:X:73:A:H3'	1:X:74:G:H5'	1.72	0.72
26:Z:58:LEU:H	26:Z:58:LEU:HD12	1.54	0.72
9:G:103:TYR:CB	9:G:107:GLN:HE21	1.99	0.72
11:I:49:PHE:HD1	11:I:50:GLU:H	1.38	0.72
24:V:42:ARG:O	24:V:46:LEU:HG	1.90	0.72
1:X:2260:C:O2'	1:X:2261:G:H5'	1.89	0.72
1:X:1884:A:O2'	3:A:245:ARG:HG2	1.90	0.71
1:X:2284:U:H4'	6:D:133:LYS:HG2	1.70	0.71
1:X:2736:U:H5''	30:4:19:ARG:HG2	1.72	0.71
1:X:1714:A:H5''	1:X:1715:A:H2'	1.71	0.71
1:X:635:C:C2'	1:X:636:G:H5''	2.20	0.71
3:A:253:LYS:H	3:A:254:PRO:HD2	1.55	0.71
6:D:4:LEU:HG	6:D:5:LYS:H	1.54	0.71
1:X:1688:U:HO2'	1:X:1690:U:H5	1.38	0.71
1:X:841:G:H2'	1:X:842:A:C8	2.26	0.71
16:N:99:ALA:HB2	16:N:106:PHE:CD1	2.26	0.71
1:X:2291:U:O2'	6:D:86:GLY:HA3	1.91	0.71
28:2:43:THR:O	28:2:43:THR:CG2	2.38	0.71
13:K:45:ARG:HG3	13:K:95:THR:CG2	2.21	0.71
1:X:1745:C:H2'	1:X:1746:A:O4'	1.91	0.71
3:A:45:ASN:HB3	3:A:50:ILE:HA	1.71	0.71
4:B:144:ARG:HG2	4:B:145:LYS:H	1.55	0.71
1:X:2704:U:H2'	1:X:2705:A:C2	2.26	0.71
13:K:28:LEU:O	13:K:28:LEU:HD23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:504:G:H4'	18:P:27:VAL:CG1	2.21	0.71
1:X:870:C:H1'	22:T:26:PHE:CE2	2.23	0.70
1:X:839:U:H5''	1:X:2408:G:OP2	1.91	0.70
9:G:132:PHE:HB2	9:G:145:HIS:CD2	2.26	0.70
10:H:23:ARG:HB3	10:H:23:ARG:NH2	2.06	0.70
1:X:1147:G:H2'	1:X:1148:G:C8	2.26	0.70
9:G:106:TYR:HE2	9:G:108:GLY:HA3	1.54	0.70
25:W:4:LYS:HG3	25:W:52:GLU:HB3	1.73	0.70
1:X:2048:C:H1'	1:X:2428:U:H3	1.56	0.70
1:X:2051:U:H3	1:X:2409:A:H62	1.38	0.70
1:X:2781:G:H2'	1:X:2782:G:H5''	1.72	0.70
1:X:557:U:H4'	1:X:558:G:O4'	1.92	0.70
15:M:34:ARG:HH21	15:M:91:VAL:HG21	1.55	0.70
15:M:104:LEU:HD23	15:M:106:TYR:HE2	1.57	0.70
16:N:17:VAL:HG21	16:N:32:TYR:HE1	1.55	0.70
1:X:590:C:H2'	1:X:591:G:C8	2.27	0.70
19:Q:12:ILE:H	19:Q:12:ILE:HD13	1.55	0.70
1:X:2194:A:C3'	1:X:2195:C:H5''	2.21	0.70
1:X:242:A:O2'	1:X:243:G:H4'	1.90	0.70
1:X:2592:U:H2'	26:Z:5:PRO:CG	2.21	0.70
14:L:38:ILE:CD1	14:L:40:ALA:H	2.05	0.70
1:X:1174:G:N2	1:X:1175:A:C4	2.60	0.70
4:B:116:VAL:HG13	4:B:136:ARG:HH21	1.57	0.70
10:H:41:ASN:O	10:H:42:LYS:O	2.10	0.70
20:R:23:ILE:HG22	20:R:33:THR:HB	1.73	0.69
1:X:2756:A:H4'	1:X:2757:G:O5'	1.91	0.69
1:X:595:A:H5'	5:C:83:ALA:CB	2.22	0.69
2:Y:39:C:H5'	2:Y:40:C:OP2	1.92	0.69
15:M:34:ARG:CZ	15:M:88:VAL:HG11	2.22	0.69
10:H:110:VAL:HG23	10:H:129:LEU:HB2	1.74	0.69
19:Q:63:LYS:HD3	19:Q:69:ILE:HA	1.73	0.69
1:X:1043:A:H5'	30:4:7:VAL:O	1.92	0.69
1:X:183:U:H6	1:X:183:U:O5'	1.76	0.69
1:X:539:A:C5	1:X:2025:A:C2	2.80	0.69
1:X:564:U:H2'	1:X:565:A:C8	2.27	0.69
1:X:2324:G:N3	1:X:2360:C:H2'	2.07	0.69
3:A:44:ARG:HH11	3:A:44:ARG:N	1.91	0.69
5:C:153:ASP:O	5:C:154:ASP:HB3	1.91	0.69
1:X:45:C:OP2	1:X:192:G:H2'	1.93	0.69
1:X:1148:G:H5''	1:X:1149:G:OP2	1.93	0.69
1:X:2240:C:O2'	1:X:2241:U:H5'	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:543:G:H5'	16:N:24:PHE:CE1	2.28	0.69
1:X:591:G:H2'	1:X:592:G:H8	1.57	0.69
16:N:101:ARG:O	16:N:103:PRO:HD3	1.93	0.69
24:V:18:ILE:HG22	24:V:22:LYS:HE2	1.74	0.69
1:X:1656:U:H2'	1:X:1657:A:H5''	1.75	0.69
10:H:116:ARG:CZ	15:M:38:LYS:HE3	2.23	0.69
9:G:70:PHE:HB3	16:N:64:ARG:HG2	1.74	0.69
1:X:2660:C:N4	1:X:2707:G:H1	1.91	0.69
1:X:538:A:C4'	1:X:539:A:OP1	2.41	0.69
1:X:538:A:N3	1:X:538:A:H2'	2.06	0.69
3:A:71:ARG:HH22	3:A:150:PRO:HA	1.57	0.69
1:X:2293:G:H5''	6:D:35:VAL:HG21	1.75	0.69
1:X:971:A:H61	12:J:83:ARG:HH22	1.40	0.69
4:B:60:ASN:HB3	4:B:62:PRO:HD2	1.74	0.69
14:L:89:PHE:HZ	14:L:103:LEU:HD22	1.58	0.69
1:X:2670:C:H4'	1:X:2846:G:O2'	1.93	0.69
1:X:317:U:C2'	1:X:318:G:H5'	2.22	0.69
4:B:131:SER:HB2	4:B:134:TRP:NE1	2.08	0.68
10:H:47:VAL:HA	10:H:74:VAL:HG12	1.75	0.68
15:M:39:VAL:HG12	15:M:45:THR:HG23	1.75	0.68
1:X:1442:C:O2'	1:X:1585:A:OP2	2.08	0.68
1:X:239:A:H5''	1:X:621:U:H5'	1.75	0.68
1:X:2293:G:H5'	6:D:35:VAL:HG11	1.76	0.68
1:X:1166:A:H5''	16:N:55:ARG:HD3	1.74	0.68
1:X:491:A:H4'	20:R:55:THR:HB	1.74	0.68
3:A:218:ARG:HG2	3:A:219:LYS:H	1.58	0.68
1:X:342:G:H4'	1:X:343:A:OP2	1.92	0.68
4:B:155:ARG:HG3	4:B:155:ARG:HH11	1.57	0.68
12:J:12:LYS:O	12:J:13:GLN:HB2	1.93	0.68
1:X:1096:A:H4'	1:X:1097:A:OP1	1.93	0.68
10:H:75:VAL:HG12	10:H:118:LEU:HD21	1.76	0.68
28:2:42:LEU:HD12	28:2:42:LEU:N	2.09	0.68
16:N:72:HIS:HD2	16:N:110:VAL:HG21	1.58	0.68
1:X:1493:A:H2'	1:X:1494:G:O4'	1.94	0.68
1:X:919:U:H2'	1:X:920:G:H8	1.59	0.68
1:X:337:G:HO2'	20:R:9:HIS:HD1	1.42	0.68
30:4:19:ARG:HD2	30:4:24:LEU:HD22	1.75	0.67
16:N:49:ASP:O	16:N:53:LYS:HG2	1.94	0.67
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.74	0.67
13:K:51:LEU:HD21	13:K:70:ILE:HD11	1.74	0.67
1:X:2447:G:O2'	1:X:2448:A:H8	1.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:597:U:H2'	1:X:598:U:C6	2.29	0.67
1:X:1976:U:H4'	4:B:128:SER:CB	2.24	0.67
1:X:1988:A:H5''	1:X:1989:C:OP2	1.94	0.67
1:X:408:U:H2'	1:X:409:G:H8	1.59	0.67
1:X:854:G:H1	1:X:948:C:H42	1.41	0.67
9:G:84:ASN:O	9:G:152:ALA:HA	1.94	0.67
11:I:61:PRO:HD3	29:3:27:SER:HB3	1.75	0.67
4:B:183:LEU:HD21	15:M:16:ILE:HG21	1.76	0.67
5:C:176:ASN:ND2	5:C:178:TYR:HB3	2.03	0.67
13:K:87:TYR:HE1	13:K:94:TYR:CD1	2.12	0.67
1:X:2551:A:N7	4:B:145:LYS:HB2	2.08	0.67
12:J:64:LYS:NZ	12:J:110:VAL:HG13	2.10	0.67
12:J:66:TYR:HB2	12:J:106:GLU:HG2	1.75	0.67
17:O:34:GLU:HB2	17:O:56:VAL:CG2	2.24	0.67
1:X:494:A:C8	20:R:56:LYS:HD2	2.30	0.67
1:X:1357:U:H4'	1:X:1397:A:C6	2.30	0.67
15:M:39:VAL:HG12	15:M:45:THR:OG1	1.93	0.67
23:U:23:LYS:HB2	23:U:35:THR:HG23	1.76	0.67
1:X:923:A:H5''	1:X:924:C:H5''	1.74	0.67
7:E:146:ALA:O	7:E:150:LYS:HG3	1.95	0.67
23:U:22:GLY:HA3	23:U:39:LYS:HG3	1.77	0.67
1:X:1991:C:H2'	1:X:1992:G:H8	1.60	0.67
1:X:652:C:H42	1:X:657:A:H61	1.41	0.67
3:A:78:ALA:HB2	3:A:98:TYR:HD1	1.59	0.66
1:X:1141:U:C4	4:B:147:PRO:HG3	2.29	0.66
1:X:1978:U:C2	1:X:1979:C:C5	2.83	0.66
1:X:2200:G:H2'	1:X:2201:G:H8	1.58	0.66
1:X:38:G:H4'	1:X:39:C:OP1	1.95	0.66
1:X:538:A:H3'	9:G:142:ARG:HH12	1.57	0.66
4:B:120:TRP:CD2	4:B:155:ARG:HD2	2.30	0.66
12:J:40:PRO:HB3	12:J:99:LYS:HZ2	1.60	0.66
19:Q:27:PHE:CZ	19:Q:42:ILE:HD13	2.30	0.66
20:R:75:ALA:O	20:R:76:LEU:HD23	1.95	0.66
5:C:151:VAL:HG12	5:C:173:ALA:HA	1.76	0.66
6:D:65:PRO:HB3	6:D:89:VAL:HG22	1.77	0.66
9:G:162:LYS:N	9:G:163:PRO:HD2	2.09	0.66
10:H:1:MET:HB3	10:H:44:TYR:HB3	1.75	0.66
19:Q:10:PRO:HD3	24:V:30:PHE:CD2	2.30	0.66
1:X:1563:U:H2'	1:X:1564:U:C6	2.31	0.66
3:A:246:VAL:HG12	3:A:252:GLY:N	2.11	0.66
18:P:67:PRO:O	18:P:71:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2043:A:H62	5:C:68:ARG:NH1	1.93	0.66
1:X:2675:U:H2'	1:X:2676:G:C8	2.31	0.66
29:3:13:ARG:HD2	29:3:25:PHE:H	1.60	0.66
29:3:46:LYS:HE3	29:3:46:LYS:HA	1.77	0.66
1:X:1107:A:H3'	1:X:1108:U:H5''	1.78	0.66
1:X:1941:C:O2'	1:X:1942:G:H5'	1.96	0.66
5:C:163:ASN:HD21	5:C:167:VAL:N	1.93	0.66
15:M:66:PHE:HD2	15:M:83:PHE:CE1	2.14	0.66
16:N:61:TRP:O	16:N:65:ILE:HG13	1.96	0.66
1:X:2409:A:H4'	1:X:2410:U:OP1	1.96	0.66
1:X:2543:A:C2	1:X:2626:U:H4'	2.30	0.66
1:X:826:U:H2'	1:X:827:C:C6	2.29	0.66
1:X:984:A:C2	1:X:1201:G:N2	2.64	0.66
1:X:1469:U:H5	13:K:64:ARG:HH21	1.42	0.66
1:X:1343:C:O2'	1:X:1344:C:H5'	1.96	0.66
1:X:1683:G:O2'	1:X:1684:G:H5'	1.95	0.66
3:A:244:GLY:N	3:A:245:ARG:NH1	2.41	0.66
4:B:76:ARG:HH12	15:M:4:HIS:HB2	1.61	0.66
1:X:1968:G:H2'	1:X:1969:G:H8	1.59	0.66
29:3:9:MET:HG3	29:3:60:LEU:HD22	1.77	0.66
1:X:1300:A:H5'	13:K:103:ARG:HD2	1.78	0.66
22:T:23:VAL:HG13	22:T:38:VAL:HG22	1.77	0.66
22:T:21:LEU:HD21	22:T:41:ARG:HE	1.59	0.66
1:X:1468:A:OP2	1:X:1468:A:C8	2.49	0.66
27:1:39:LYS:HE2	27:1:47:HIS:HA	1.75	0.66
1:X:477:A:OP1	28:2:34:ARG:NH2	2.29	0.66
4:B:13:GLN:O	4:B:14:ILE:HG13	1.96	0.66
1:X:879:A:H2'	1:X:879:A:N3	2.10	0.66
9:G:132:PHE:CD2	9:G:145:HIS:CG	2.84	0.65
12:J:116:LYS:O	12:J:120:ARG:HB2	1.95	0.65
15:M:37:THR:CG2	15:M:39:VAL:HG13	2.26	0.65
28:2:37:LYS:C	28:2:40:HIS:HE1	2.00	0.65
3:A:219:LYS:HD2	3:A:219:LYS:C	2.17	0.65
5:C:46:ARG:HB3	5:C:51:VAL:HG23	1.79	0.65
1:X:1053:G:C4'	1:X:1054:C:OP1	2.43	0.65
1:X:1128:G:H2'	1:X:1129:A:H5''	1.78	0.65
1:X:1938:U:H1'	1:X:1939:U:OP1	1.97	0.65
1:X:2705:A:N3	1:X:2705:A:O4'	2.28	0.65
9:G:107:GLN:O	9:G:109:GLY:N	2.29	0.65
10:H:2:ILE:O	10:H:44:TYR:HA	1.96	0.65
10:H:42:LYS:HE3	10:H:44:TYR:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:76:THR:HB	12:J:88:LYS:O	1.96	0.65
13:K:33:ARG:HG3	13:K:114:GLU:HB3	1.77	0.65
1:X:1299:A:O2'	1:X:1301:U:OP2	2.14	0.65
1:X:2372:A:H5''	11:I:61:PRO:HA	1.79	0.65
12:J:42:TRP:HB3	12:J:95:VAL:CG1	2.26	0.65
21:S:69:VAL:HG13	21:S:81:VAL:HG22	1.79	0.65
1:X:591:G:C2'	1:X:592:G:C8	2.78	0.65
24:V:2:LYS:HA	24:V:6:MET:HE1	1.78	0.65
1:X:626:A:C8	5:C:174:GLY:HA3	2.31	0.65
18:P:59:PHE:CD1	26:Z:30:LEU:HD11	2.31	0.65
3:A:87:PRO:O	3:A:88:ASN:HB2	1.97	0.65
1:X:1673:C:H5''	4:B:136:ARG:HB3	1.79	0.65
5:C:95:LEU:HD21	5:C:99:VAL:HB	1.77	0.65
10:H:42:LYS:NZ	10:H:46:HIS:HD2	1.95	0.65
1:X:227:G:OP2	29:3:8:LYS:HE3	1.95	0.65
1:X:1270:C:H4'	5:C:77:PHE:CE2	2.32	0.65
19:Q:22:ARG:NH1	19:Q:24:VAL:HG21	2.12	0.65
1:X:448:C:H5	1:X:449:C:C4	2.14	0.65
4:B:141:ILE:HG22	4:B:150:VAL:HB	1.79	0.65
5:C:27:LEU:O	5:C:31:VAL:HG22	1.96	0.65
15:M:104:LEU:HD23	15:M:106:TYR:CE2	2.31	0.65
1:X:603:C:H5'	29:3:62:LEU:HD22	1.79	0.65
12:J:77:LYS:O	12:J:79:PRO:HD3	1.97	0.65
14:L:33:ARG:HG2	14:L:38:ILE:HB	1.78	0.65
1:X:2788:C:H2'	1:X:2789:U:H6	1.61	0.65
1:X:617:U:H5	1:X:632:A:N1	1.95	0.65
5:C:176:ASN:HD22	5:C:179:ASP:N	1.89	0.65
1:X:177:U:O4	1:X:225:G:C2	2.50	0.65
1:X:2441:U:H2'	1:X:2442:C:C6	2.32	0.65
15:M:103:LYS:O	15:M:104:LEU:HB2	1.95	0.64
1:X:48:A:H4'	1:X:49:U:O5'	1.97	0.64
1:X:754:G:H2'	1:X:755:C:C6	2.31	0.64
7:E:43:VAL:HG23	7:E:52:VAL:HG22	1.79	0.64
1:X:38:G:C4'	1:X:39:C:OP1	2.44	0.64
1:X:2328:G:OP2	29:3:42:ARG:HG3	1.97	0.64
16:N:30:LYS:HB3	16:N:30:LYS:NZ	2.13	0.64
1:X:1153:A:OP1	1:X:1153:A:H4'	1.97	0.64
13:K:75:VAL:O	13:K:79:VAL:HG12	1.97	0.64
14:L:31:VAL:HG23	14:L:38:ILE:CD1	2.24	0.64
24:V:37:LEU:HD23	24:V:39:GLN:H	1.62	0.64
1:X:2426:G:C3'	1:X:2479:U:OP2	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2262:C:OP1	27:1:3:LYS:HE2	1.96	0.64
4:B:49:ILE:HG22	4:B:79:ARG:O	1.97	0.64
6:D:132:ILE:HG13	6:D:154:ILE:HD13	1.79	0.64
17:O:73:LYS:HB2	17:O:82:ARG:HB2	1.78	0.64
18:P:85:MET:CE	18:P:130:GLU:HG3	2.28	0.64
21:S:13:LYS:HB2	21:S:13:LYS:NZ	2.13	0.64
1:X:2426:G:H4'	1:X:2427:A:O5'	1.97	0.64
1:X:2265:A:OP1	27:1:28:ARG:HD2	1.97	0.64
18:P:41:VAL:HG21	18:P:64:ALA:HB3	1.79	0.64
1:X:2598:C:C4'	4:B:150:VAL:HG22	2.27	0.64
1:X:163:A:H2'	1:X:164:G:C8	2.33	0.64
1:X:26:G:C6	1:X:27:G:N1	2.66	0.64
1:X:2660:C:N3	1:X:2707:G:N2	2.46	0.64
1:X:346:C:H2'	1:X:347:C:H6	1.61	0.64
4:B:116:VAL:CG2	4:B:136:ARG:HE	2.05	0.64
11:I:18:ARG:HB2	11:I:21:ARG:HB2	1.80	0.64
19:Q:7:LEU:HD22	19:Q:8:GLN:N	2.12	0.64
1:X:459:A:C2	1:X:466:A:C8	2.86	0.64
1:X:790:A:N7	1:X:806:A:H2	1.95	0.64
1:X:840:U:H4'	1:X:841:G:C2	2.33	0.64
26:Z:51:TYR:HA	26:Z:55:ARG:HA	1.78	0.64
3:A:219:LYS:O	3:A:219:LYS:HD2	1.97	0.64
12:J:40:PRO:HB3	12:J:99:LYS:HD2	1.79	0.64
14:L:89:PHE:CZ	14:L:103:LEU:HD22	2.32	0.64
15:M:34:ARG:NH1	15:M:88:VAL:HG21	2.12	0.64
1:X:2640:G:H2'	1:X:2641:A:C8	2.33	0.64
1:X:82:G:N2	1:X:83:A:H62	1.96	0.64
12:J:28:VAL:HG21	12:J:135:ARG:HA	1.80	0.64
16:N:99:ALA:HB2	16:N:106:PHE:CE1	2.33	0.64
20:R:85:ASP:HB3	20:R:86:PRO:HD3	1.80	0.64
1:X:1182:U:H3	1:X:1193:G:H22	1.45	0.64
28:2:14:LYS:HE3	28:2:14:LYS:HA	1.80	0.63
4:B:49:ILE:HG21	4:B:81:PHE:HE2	1.62	0.63
5:C:95:LEU:CD2	5:C:99:VAL:HB	2.28	0.63
2:Y:30:C:OP1	14:L:37:HIS:HB3	1.97	0.63
15:M:55:ILE:HB	15:M:103:LYS:O	1.99	0.63
1:X:1007:A:H1'	17:O:6:GLN:HG2	1.79	0.63
1:X:2533:U:C4	1:X:2534:U:O4	2.51	0.63
2:Y:51:G:OP1	14:L:97:HIS:HD2	1.81	0.63
19:Q:7:LEU:HD22	19:Q:7:LEU:C	2.18	0.63
1:X:1329:U:H2'	1:X:1330:G:H8	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1685:A:O4'	1:X:1686:A:C2	2.51	0.63
1:X:1979:C:H4'	1:X:1980:A:OP1	1.97	0.63
1:X:2043:A:O4'	1:X:2481:G:O4'	2.16	0.63
1:X:859:U:O2'	1:X:860:U:C2	2.50	0.63
4:B:176:ARG:HE	15:M:16:ILE:HG12	1.63	0.63
9:G:132:PHE:HD2	9:G:145:HIS:CG	2.16	0.63
3:A:245:ARG:O	3:A:253:LYS:HE2	1.99	0.63
18:P:126:ILE:HD12	18:P:127:ILE:H	1.63	0.63
18:P:35:PRO:O	18:P:39:ARG:HD3	1.98	0.63
1:X:1332:G:C6	1:X:1333:G:O6	2.51	0.63
1:X:1775:A:H4'	1:X:1776:A:O5'	1.98	0.63
1:X:822:G:C2'	1:X:823:U:H5'	2.29	0.63
21:S:3:LEU:HD23	21:S:56:VAL:HG22	1.81	0.63
23:U:22:GLY:HA3	23:U:39:LYS:HE3	1.81	0.63
1:X:16:G:C2	1:X:535:U:O2	2.51	0.63
1:X:2240:C:C2'	1:X:2241:U:H5'	2.28	0.63
1:X:484:G:N1	1:X:485:G:C6	2.66	0.63
1:X:617:U:H5	1:X:632:A:C2	2.16	0.63
9:G:154:GLU:O	9:G:157:PRO:HD2	1.98	0.63
12:J:128:ILE:O	12:J:128:ILE:HD12	1.99	0.63
14:L:38:ILE:HD12	14:L:39:TYR:N	2.14	0.63
1:X:1392:U:OP1	1:X:1392:U:H6	1.82	0.63
1:X:1469:U:OP1	1:X:1470:G:OP2	2.17	0.63
1:X:1715:A:C8	1:X:1717:A:O4'	2.52	0.63
1:X:2516:U:H2'	1:X:2517:C:C6	2.34	0.63
4:B:136:ARG:HG2	4:B:137:ARG:N	2.14	0.63
1:X:458:G:H4'	1:X:459:A:H5'	1.80	0.63
1:X:789:G:O2'	1:X:790:A:OP2	2.11	0.63
9:G:85:ALA:HB1	9:G:127:ILE:HD13	1.81	0.63
2:Y:17:A:H1'	2:Y:112:A:N9	2.13	0.63
5:C:176:ASN:ND2	5:C:179:ASP:H	1.91	0.62
7:E:127:GLU:HG3	7:E:128:PRO:HD2	1.79	0.62
13:K:73:LYS:O	13:K:76:VAL:HG12	1.98	0.62
21:S:168:VAL:HG12	21:S:169:VAL:HG13	1.80	0.62
1:X:2424:G:O2'	1:X:2425:G:H5'	1.99	0.62
1:X:787:A:H5''	3:A:49:ARG:HH22	1.63	0.62
1:X:968:C:N4	1:X:970:A:C6	2.67	0.62
28:2:25:LYS:N	28:2:25:LYS:HE2	2.14	0.62
10:H:47:VAL:HA	10:H:74:VAL:CG1	2.29	0.62
13:K:81:ASP:O	13:K:85:PRO:HG2	1.98	0.62
15:M:37:THR:HG22	15:M:39:VAL:HG13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1166:A:H5''	16:N:55:ARG:HH11	1.63	0.62
1:X:1827:G:H1'	1:X:1914:U:C2	2.34	0.62
1:X:1856:U:OP1	1:X:2389:G:O2'	2.17	0.62
27:1:34:LYS:HE2	27:1:53:LYS:NZ	2.14	0.62
10:H:109:ARG:HA	10:H:129:LEU:HD13	1.79	0.62
1:X:1432:G:O6	1:X:1594:U:H5''	2.00	0.62
1:X:2039:G:H2'	1:X:2039:G:N3	2.14	0.62
1:X:2378:G:H1	1:X:2396:C:H42	1.45	0.62
3:A:68:PHE:HE2	3:A:107:LEU:HD11	1.63	0.62
10:H:125:LYS:O	10:H:128:SER:HB2	1.98	0.62
17:O:67:LYS:HD2	17:O:68:LYS:H	1.65	0.62
1:X:1837:G:H2'	1:X:1838:G:C8	2.35	0.62
1:X:1919:A:N7	1:X:1928:G:C6	2.67	0.62
1:X:2336:G:N2	1:X:2339:A:OP2	2.32	0.62
1:X:2642:G:H2'	1:X:2643:G:O4'	1.99	0.62
1:X:931:G:H4'	2:Y:83:C:H4'	1.80	0.62
3:A:211:GLY:HA2	3:A:214:ARG:HG2	1.80	0.62
1:X:1223:G:H5'	1:X:1224:A:H3'	1.81	0.62
1:X:1420:A:C2	1:X:1612:U:O2	2.52	0.62
1:X:1779:C:H2'	1:X:1780:A:C8	2.34	0.62
13:K:62:SER:O	13:K:66:VAL:HG23	2.00	0.62
16:N:32:TYR:O	16:N:35:ALA:HB3	1.99	0.62
22:T:23:VAL:HA	22:T:38:VAL:HG13	1.82	0.62
1:X:2379:G:H1	1:X:2395:C:H42	1.46	0.62
1:X:2705:A:N7	1:X:2707:G:C4	2.68	0.62
1:X:685:U:C2	1:X:822:G:N2	2.68	0.62
7:E:124:ALA:HB3	7:E:132:ASP:HB3	1.82	0.62
1:X:2011:U:H2'	1:X:2012:A:H8	1.65	0.62
1:X:2518:C:H4'	30:4:3:VAL:HG21	1.82	0.62
1:X:2824:C:H4'	1:X:2825:A:O5'	2.00	0.62
1:X:919:U:H2'	1:X:920:G:C8	2.34	0.62
4:B:144:ARG:HG2	4:B:145:LYS:N	2.15	0.62
1:X:1837:G:H2'	1:X:1838:G:H8	1.64	0.62
1:X:572:G:H5'	1:X:581:A:H4'	1.81	0.62
12:J:40:PRO:HB3	12:J:99:LYS:CD	2.30	0.62
1:X:100:G:H4'	1:X:101:A:OP1	2.00	0.62
1:X:1978:U:H2'	1:X:1979:C:C6	2.35	0.62
1:X:467:U:O2'	1:X:468:A:O5'	2.17	0.62
4:B:147:PRO:O	4:B:149:ARG:N	2.33	0.62
13:K:72:ASP:CG	13:K:75:VAL:HG23	2.20	0.62
20:R:15:HIS:ND1	20:R:16:PHE:CD2	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:16:PHE:HZ	20:R:46:VAL:HG22	1.65	0.62
1:X:75:C:O2	1:X:109:A:H2	1.83	0.62
1:X:1811:A:H1'	1:X:1812:U:OP2	2.00	0.62
5:C:128:ALA:O	5:C:130:THR:N	2.31	0.61
10:H:42:LYS:HZ2	10:H:46:HIS:HD2	1.47	0.61
12:J:92:GLU:HG3	12:J:93:TYR:HD2	1.65	0.61
15:M:104:LEU:HA	15:M:106:TYR:HE2	1.64	0.61
1:X:2426:G:C4	1:X:2479:U:H5	2.18	0.61
1:X:334:G:H4'	1:X:335:A:O5'	1.98	0.61
1:X:757:U:O2'	1:X:758:G:H5'	2.00	0.61
9:G:104:THR:OG1	9:G:105:GLY:N	2.32	0.61
10:H:116:ARG:HD2	15:M:38:LYS:HZ1	1.65	0.61
18:P:14:ARG:HA	18:P:17:GLN:HG2	1.82	0.61
1:X:663:G:H3'	1:X:664:C:H5''	1.81	0.61
29:3:34:THR:OG1	29:3:41:ILE:HD11	1.99	0.61
11:I:56:LEU:HD22	29:3:52:LYS:HZ2	1.65	0.61
1:X:2011:U:H2'	1:X:2012:A:C8	2.34	0.61
1:X:2598:C:O4'	4:B:150:VAL:HG22	1.99	0.61
1:X:334:G:C2'	5:C:162:ARG:HD3	2.29	0.61
14:L:89:PHE:HB3	14:L:91:ARG:HH21	1.64	0.61
19:Q:12:ILE:O	19:Q:12:ILE:HG12	1.99	0.61
1:X:2026:C:N4	1:X:2757:G:C2	2.69	0.61
28:2:10:ARG:H	28:2:10:ARG:CD	1.97	0.61
11:I:56:LEU:HB3	29:3:52:LYS:HE3	1.82	0.61
8:F:112:MET:HB2	8:F:113:PRO:HD3	1.80	0.61
1:X:1164:C:H2'	1:X:1165:G:O4'	2.01	0.61
1:X:1479:G:H2'	1:X:1480:G:C8	2.35	0.61
1:X:218:A:C8	1:X:220:U:C2	2.88	0.61
5:C:102:LEU:O	5:C:102:LEU:HD23	2.00	0.61
15:M:28:ARG:HB2	15:M:29:PRO:CD	2.19	0.61
1:X:1225:G:H2'	1:X:1249:G:H22	1.65	0.61
1:X:2409:A:C4'	1:X:2410:U:OP1	2.48	0.61
1:X:2604:G:H2'	1:X:2605:C:C6	2.36	0.61
27:1:28:ARG:HB2	27:1:30:ASN:OD1	2.01	0.61
21:S:127:PRO:O	21:S:128:ARG:HG2	2.00	0.61
1:X:2064:U:H5''	23:U:43:ARG:HH11	1.66	0.61
1:X:2690:A:OP1	1:X:2692:A:P	2.58	0.61
1:X:736:G:H2'	1:X:737:C:O4'	2.01	0.61
14:L:33:ARG:HE	14:L:38:ILE:HB	1.66	0.61
18:P:92:VAL:HG13	18:P:126:ILE:CD1	2.29	0.61
19:Q:35:LYS:HD3	19:Q:53:ILE:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:25:LEU:HD13	24:V:46:LEU:HD12	1.82	0.61
1:X:1096:A:C4'	1:X:1097:A:OP1	2.47	0.61
1:X:1964:A:H5''	1:X:1965:U:OP2	1.99	0.61
9:G:55:ALA:C	9:G:134:MET:HE1	2.20	0.61
11:I:51:GLY:O	11:I:55:ARG:NH1	2.31	0.61
25:W:23:LEU:HD21	25:W:43:MET:HB3	1.82	0.61
1:X:163:A:H2'	1:X:164:G:H8	1.66	0.61
1:X:2064:U:H5''	23:U:43:ARG:NH1	2.16	0.61
1:X:38:G:H1'	1:X:39:C:O5'	2.01	0.61
1:X:971:A:N6	12:J:83:ARG:HH22	1.99	0.61
9:G:89:ALA:C	9:G:90:LEU:HD12	2.22	0.61
11:I:107:LYS:HG2	11:I:109:LEU:HD21	1.83	0.61
11:I:62:LYS:HG2	11:I:63:ARG:H	1.66	0.61
1:X:2310:G:H4'	22:T:43:THR:H	1.66	0.61
1:X:529:U:H2'	1:X:530:G:H8	1.66	0.61
21:S:49:THR:OG1	21:S:132:GLN:HA	2.00	0.60
1:X:1438:G:C2'	1:X:1439:G:H5'	2.31	0.60
1:X:2222:U:H2'	1:X:2223:U:C6	2.36	0.60
1:X:688:A:H62	1:X:816:U:H3	1.49	0.60
2:Y:9:G:H5''	14:L:32:TYR:CD1	2.36	0.60
27:1:34:LYS:HE2	27:1:53:LYS:HZ2	1.66	0.60
1:X:2201:G:H5'	3:A:189:GLU:OE1	2.00	0.60
12:J:64:LYS:HZ3	12:J:110:VAL:HG13	1.66	0.60
13:K:24:GLN:HB3	13:K:44:LEU:HD22	1.83	0.60
15:M:39:VAL:HG12	15:M:45:THR:CG2	2.31	0.60
1:X:538:A:O2'	1:X:539:A:H5''	2.01	0.60
1:X:638:A:C8	11:I:74:VAL:HG11	2.36	0.60
1:X:613:A:C6	1:X:668:A:H1'	2.37	0.60
1:X:692:C:H42	1:X:811:G:H1	1.49	0.60
3:A:71:ARG:HH12	3:A:150:PRO:HB3	1.66	0.60
11:I:29:THR:O	11:I:30:ALA:HB3	2.01	0.60
15:M:5:ILE:HD13	15:M:7:ILE:HG22	1.81	0.60
16:N:22:LYS:HG3	16:N:23:GLY:H	1.66	0.60
1:X:178:C:O5'	23:U:40:ARG:NH2	2.33	0.60
1:X:1288:A:H2	1:X:1662:G:H21	1.47	0.60
1:X:2662:C:O2	10:H:82:LYS:NZ	2.33	0.60
1:X:2859:U:N3	26:Z:52:TYR:CE1	2.69	0.60
28:2:17:GLY:O	28:2:20:ALA:HB3	2.01	0.60
3:A:49:ARG:HD2	3:A:49:ARG:N	2.10	0.60
5:C:15:ILE:HD11	5:C:195:ILE:H	1.67	0.60
11:I:91:ASP:HA	11:I:94:GLU:OE2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:935:C:H1'	22:T:29:GLU:HG2	1.81	0.60
1:X:1357:U:O2'	1:X:1358:C:P	2.59	0.60
1:X:192:G:H4'	1:X:193:A:H4'	1.83	0.60
1:X:2016:A:O2'	1:X:2018:G:OP2	2.18	0.60
1:X:2048:C:H1'	1:X:2428:U:N3	2.17	0.60
1:X:753:U:H2'	1:X:754:G:C8	2.37	0.60
1:X:999:A:H5''	25:W:8:SER:HB2	1.82	0.60
2:Y:33:C:N4	2:Y:53:G:H1	1.97	0.60
29:3:31:HIS:O	29:3:32:GLN:C	2.39	0.60
4:B:134:TRP:O	4:B:135:HIS:C	2.40	0.60
4:B:155:ARG:NH1	4:B:155:ARG:HG3	2.15	0.60
7:E:87:LEU:HB2	7:E:131:ILE:HB	1.82	0.60
7:E:154:PRO:HA	7:E:160:LYS:O	2.01	0.60
15:M:34:ARG:NH1	15:M:81:PHE:HB3	2.15	0.60
1:X:1744:G:N2	1:X:1747:G:OP2	2.31	0.60
31:X:2881:LMA:O55	31:X:2881:LMA:H12	2.00	0.60
28:2:15:THR:O	28:2:16:HIS:HB2	2.02	0.60
5:C:151:VAL:CG1	5:C:173:ALA:HA	2.31	0.60
12:J:29:ALA:HB3	12:J:68:ARG:HH21	1.65	0.60
1:X:1226:A:C8	1:X:1250:A:H2	2.18	0.60
1:X:2311:U:H4'	1:X:2315:A:N6	2.16	0.60
1:X:455:A:H2	1:X:1258:G:N3	1.99	0.60
1:X:521:U:H5''	1:X:522:G:OP2	2.01	0.60
1:X:817:A:H5''	1:X:818:G:OP1	2.01	0.60
13:K:73:LYS:HA	13:K:76:VAL:HG12	1.83	0.60
16:N:62:ILE:HG23	16:N:76:TYR:CE1	2.37	0.60
17:O:36:LYS:NZ	17:O:54:TYR:HB3	2.15	0.60
1:X:1666:G:H1	1:X:1991:C:H42	1.47	0.60
1:X:2229:G:H5'	12:J:84:MET:HG2	1.83	0.60
1:X:2782:G:H2'	1:X:2783:U:O5'	2.01	0.60
1:X:2796:A:H2'	1:X:2797:G:H8	1.66	0.60
1:X:695:G:H5''	28:2:26:SER:HB2	1.83	0.60
1:X:1479:G:H2'	1:X:1480:G:H8	1.67	0.60
1:X:1693:A:N3	1:X:1976:U:H5'	2.16	0.60
1:X:1770:U:H5	1:X:1775:A:N7	2.00	0.60
1:X:1977:C:O2	1:X:1977:C:H2'	2.02	0.60
1:X:2616:U:H5''	4:B:82:ARG:NH2	2.16	0.60
1:X:28:A:H1'	1:X:523:A:C2	2.37	0.60
1:X:48:A:H4'	1:X:49:U:C5'	2.32	0.60
6:D:5:LYS:O	6:D:8:TYR:HB3	2.01	0.60
6:D:60:ILE:HG22	6:D:140:GLU:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:94:PHE:HE2	7:E:160:LYS:HB3	1.66	0.60
10:H:16:ALA:HB3	10:H:98:ILE:HD11	1.82	0.60
16:N:25:TRP:CE3	16:N:26:GLY:CA	2.85	0.60
21:S:155:PRO:HG2	21:S:158:CYS:SG	2.42	0.60
22:T:47:ALA:HB1	22:T:51:VAL:O	2.02	0.60
1:X:1886:G:O2'	1:X:1887:G:H5'	2.02	0.60
1:X:2074:U:H3'	1:X:2075:U:H5''	1.83	0.60
1:X:2700:U:H2'	1:X:2700:U:O2	2.02	0.60
19:Q:68:PHE:O	19:Q:69:ILE:HD12	2.01	0.59
1:X:1016:C:O2'	1:X:1023:U:C5	2.54	0.59
1:X:1050:G:H1	1:X:1127:C:H42	1.49	0.59
1:X:1399:C:H2'	1:X:1400:A:H8	1.66	0.59
1:X:1468:A:H8	1:X:1468:A:OP2	1.85	0.59
1:X:760:U:C5	26:Z:3:LYS:HG3	2.37	0.59
26:Z:10:LYS:HG2	26:Z:11:THR:N	2.15	0.59
1:X:122:G:H2'	28:2:19:ARG:HH21	1.67	0.59
5:C:176:ASN:HB3	5:C:179:ASP:OD2	2.02	0.59
16:N:79:PHE:HE2	16:N:95:LEU:HD21	1.66	0.59
19:Q:31:PRO:HA	19:Q:76:LYS:HD2	1.82	0.59
1:X:1329:U:O2'	1:X:1330:G:H5'	2.02	0.59
1:X:1337:G:C2	1:X:1341:G:N1	2.70	0.59
1:X:1505:U:H2'	1:X:1506:C:H5''	1.85	0.59
1:X:1751:A:H2'	1:X:1752:U:C6	2.37	0.59
1:X:2736:U:H5''	30:4:19:ARG:CG	2.32	0.59
1:X:699:G:C6	28:2:12:ARG:HA	2.37	0.59
5:C:27:LEU:HD23	5:C:181:LEU:HD22	1.84	0.59
9:G:61:ARG:HG2	9:G:65:LYS:HD2	1.82	0.59
18:P:106:LEU:HD23	18:P:106:LEU:C	2.23	0.59
18:P:92:VAL:HG13	18:P:126:ILE:HD11	1.83	0.59
18:P:39:ARG:HD2	18:P:97:VAL:HB	1.84	0.59
1:X:1925:C:H2'	1:X:1926:U:C5	2.37	0.59
1:X:314:G:N1	1:X:326:A:C2	2.71	0.59
1:X:538:A:H4'	1:X:539:A:OP1	2.02	0.59
28:2:34:ARG:HH11	28:2:42:LEU:HG	1.67	0.59
10:H:29:ILE:HG21	10:H:123:PHE:CE1	2.37	0.59
17:O:19:VAL:HG13	17:O:90:PHE:CD1	2.37	0.59
20:R:38:LEU:HB2	20:R:47:VAL:CG2	2.33	0.59
1:X:1433:A:H62	1:X:1435:G:H1'	1.67	0.59
1:X:1314:A:H2	1:X:1642:G:H21	1.50	0.59
1:X:761:G:OP2	18:P:110:ALA:CB	2.50	0.59
1:X:2350:G:O2'	27:1:46:LYS:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:163:ASN:ND2	5:C:167:VAL:H	1.97	0.59
6:D:13:ARG:HB3	6:D:14:PRO:HD3	1.84	0.59
10:H:13:ASN:ND2	10:H:109:ARG:HG2	2.16	0.59
1:X:824:U:O2'	11:I:30:ALA:HB2	2.02	0.59
1:X:1182:U:C4'	1:X:1183:C:OP1	2.50	0.59
1:X:1623:C:H4'	1:X:1624:A:O5'	2.02	0.59
6:D:117:ILE:HD12	6:D:175:LEU:HD11	1.83	0.59
13:K:13:ASN:OD1	13:K:14:SER:N	2.35	0.59
14:L:60:LYS:HZ2	14:L:64:LYS:HE2	1.68	0.59
17:O:15:SER:HA	17:O:95:ILE:O	2.03	0.59
1:X:1173:G:H2'	1:X:1174:G:H8	1.68	0.59
1:X:1361:G:H1	1:X:1614:C:N4	2.01	0.59
1:X:2245:A:H4'	1:X:2246:A:C2	2.37	0.59
17:O:11:GLN:HE22	17:O:38:LEU:HD12	1.68	0.59
1:X:338:G:H1'	20:R:10:HIS:HE1	1.67	0.59
20:R:81:VAL:HG11	20:R:89:GLY:CA	2.32	0.59
1:X:1310:C:H2'	1:X:1311:C:H6	1.66	0.59
1:X:13:A:N3	1:X:15:G:C6	2.71	0.59
1:X:1909:U:H5	1:X:1910:A:H62	1.49	0.59
1:X:2010:G:O6	1:X:2016:A:C8	2.55	0.59
1:X:2845:C:H6	1:X:2845:C:H3'	1.67	0.59
1:X:597:U:H2'	1:X:598:U:H6	1.67	0.59
1:X:1976:U:H5''	4:B:128:SER:HB3	1.83	0.59
4:B:14:ILE:HA	15:M:20:HIS:CD2	2.26	0.59
12:J:44:LYS:HD3	12:J:47:GLN:NE2	2.17	0.59
1:X:29:U:H6	1:X:29:U:O5'	1.85	0.59
10:H:133:VAL:HG12	10:H:133:VAL:O	2.01	0.59
1:X:762:A:H2	1:X:766:A:HO2'	1.48	0.59
3:A:25:LEU:CB	3:A:206:VAL:H	2.15	0.59
7:E:7:GLN:O	7:E:9:ILE:HG13	2.02	0.59
1:X:1996:A:C2	18:P:109:ARG:NH2	2.71	0.59
20:R:38:LEU:HB2	20:R:47:VAL:HG23	1.83	0.59
24:V:43:VAL:O	24:V:47:ARG:HG2	2.03	0.59
1:X:1234:C:O2	1:X:1242:A:C2	2.56	0.59
1:X:1665:C:H2'	1:X:1666:G:O4'	2.03	0.59
1:X:2209:G:H5''	23:U:46:LEU:HB2	1.83	0.59
31:X:2881:LMA:H34B	31:X:2881:LMA:C54	2.33	0.59
1:X:321:A:C2	1:X:323:G:H1'	2.38	0.59
1:X:40:U:H2'	1:X:41:G:O4'	2.02	0.59
1:X:57:G:C4	1:X:69:G:N2	2.71	0.59
10:H:28:GLY:O	10:H:35:THR:OG1	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1430:G:H2'	1:X:1431:U:C6	2.38	0.58
1:X:1684:G:C2	1:X:1974:U:C5	2.91	0.58
1:X:712:A:H2'	1:X:713:G:O4'	2.03	0.58
4:B:116:VAL:HG22	4:B:136:ARG:CD	2.32	0.58
5:C:26:VAL:HG22	11:I:18:ARG:NH1	2.13	0.58
12:J:40:PRO:CB	12:J:99:LYS:HZ2	2.15	0.58
12:J:92:GLU:HG3	12:J:93:TYR:CD2	2.38	0.58
1:X:1466:C:C2'	1:X:1467:U:O4'	2.47	0.58
1:X:2781:G:C2'	1:X:2782:G:H5''	2.32	0.58
20:R:29:HIS:HD2	20:R:51:VAL:HG22	1.67	0.58
21:S:120:LEU:HD23	21:S:121:GLN:N	2.18	0.58
1:X:1270:C:O2	5:C:78:VAL:HG23	2.02	0.58
1:X:177:U:H3'	23:U:40:ARG:NH2	2.18	0.58
1:X:2674:C:O2'	1:X:2675:U:H5'	2.03	0.58
9:G:62:ILE:O	9:G:77:GLY:HA3	2.03	0.58
16:N:24:PHE:HB2	16:N:29:SER:HB3	1.86	0.58
1:X:1468:A:H8	1:X:1468:A:P	2.26	0.58
1:X:1628:C:H5'	28:2:7:PRO:HG2	1.85	0.58
1:X:2256:G:OP2	12:J:86:LYS:HD2	2.04	0.58
16:N:40:LEU:HB3	17:O:74:TYR:CE2	2.38	0.58
1:X:1699:A:H61	1:X:1723:U:H3	1.52	0.58
1:X:2625:U:O5'	1:X:2625:U:H6	1.84	0.58
1:X:555:U:H3'	1:X:556:A:H8	1.67	0.58
1:X:757:U:C2'	1:X:758:G:H5'	2.33	0.58
1:X:334:G:H2'	5:C:162:ARG:HD3	1.86	0.58
1:X:547:U:H1'	9:G:73:ASN:HD21	1.68	0.58
1:X:1433:A:C4	1:X:1595:A:H2	2.21	0.58
1:X:306:G:N2	1:X:355:G:H1'	2.19	0.58
1:X:540:G:C2'	1:X:542:A:C2	2.84	0.58
29:3:8:LYS:HG3	29:3:12:ARG:NH1	2.17	0.58
4:B:59:VAL:HG21	4:B:74:PRO:HB3	1.85	0.58
7:E:90:ARG:HH21	7:E:163:ARG:NH1	2.01	0.58
1:X:1304:U:O2'	1:X:1305:C:H5'	2.04	0.58
1:X:2323:U:O2'	27:1:38:LYS:HB3	2.04	0.58
1:X:2796:A:H2'	1:X:2797:G:C8	2.39	0.58
1:X:923:A:C5	12:J:12:LYS:HE2	2.39	0.58
3:A:131:ALA:HA	3:A:192:ALA:O	2.03	0.58
19:Q:35:LYS:HA	19:Q:38:ILE:CG2	2.32	0.58
1:X:2695:C:H2'	1:X:2696:A:H8	1.69	0.58
27:1:14:SER:HB2	27:1:23:THR:H	1.67	0.58
4:B:118:LYS:HG2	4:B:160:MET:SD	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1919:A:H1'	1:X:1923:U:N3	2.18	0.58
1:X:2237:C:H3'	1:X:2238:G:H5'	1.86	0.58
1:X:721:C:H42	1:X:736:G:H1	1.52	0.58
1:X:836:G:H2'	1:X:837:U:H6	1.68	0.58
1:X:2339:A:OP1	29:3:49:VAL:HG22	2.04	0.58
5:C:62:LYS:HD3	5:C:63:GLY:N	2.19	0.58
19:Q:61:LYS:HB2	19:Q:72:ARG:HD3	1.86	0.58
22:T:12:ASN:CB	22:T:14:ARG:HG2	2.29	0.58
23:U:78:ILE:HD13	23:U:79:GLU:N	2.19	0.58
1:X:839:U:H5''	1:X:2408:G:P	2.44	0.58
1:X:797:A:N7	3:A:230:VAL:HG21	2.18	0.58
26:Z:51:TYR:CD2	26:Z:55:ARG:HB2	2.39	0.58
17:O:5:ILE:HD11	17:O:9:GLY:HA2	1.84	0.57
1:X:1496:G:C4'	1:X:1497:C:OP1	2.52	0.57
27:1:40:TYR:HB2	27:1:50:PHE:CD2	2.38	0.57
28:2:42:LEU:N	28:2:42:LEU:CD1	2.66	0.57
3:A:207:LEU:HA	3:A:212:ARG:HH11	1.69	0.57
17:O:68:LYS:HD2	17:O:69:ILE:N	2.19	0.57
1:X:1469:U:C5'	1:X:1470:G:OP2	2.51	0.57
1:X:2522:G:C6	1:X:2523:G:C6	2.92	0.57
1:X:820:U:OP1	11:I:40:ARG:NH2	2.37	0.57
3:A:109:PRO:HA	3:A:197:VAL:HA	1.86	0.57
4:B:100:GLU:O	4:B:172:VAL:HG23	2.03	0.57
7:E:16:THR:HB	7:E:27:LYS:HB2	1.85	0.57
18:P:37:LYS:O	18:P:40:LEU:HB2	2.04	0.57
1:X:1674:C:H2'	1:X:1675:C:C6	2.40	0.57
1:X:2447:G:O2'	1:X:2448:A:C8	2.51	0.57
1:X:2663:U:C4	1:X:2664:G:N7	2.72	0.57
1:X:318:G:H21	1:X:341:A:H62	1.53	0.57
1:X:761:G:OP2	18:P:110:ALA:HB2	2.04	0.57
27:1:8:ILE:O	27:1:9:ILE:HG12	2.04	0.57
1:X:1142:G:N3	9:G:103:TYR:CD2	2.68	0.57
1:X:1182:U:H4'	1:X:1183:C:OP1	2.04	0.57
1:X:577:U:H2'	1:X:579:G:OP2	2.03	0.57
1:X:760:U:C6	26:Z:3:LYS:CE	2.81	0.57
3:A:244:GLY:H	3:A:245:ARG:HH11	1.45	0.57
3:A:43:GLY:C	3:A:44:ARG:NH1	2.55	0.57
15:M:67:THR:OG1	15:M:80:VAL:HG22	2.04	0.57
1:X:1224:A:H5'	18:P:10:ASN:ND2	2.19	0.57
1:X:1850:G:H21	1:X:1867:A:H8	1.50	0.57
1:X:684:C:H5	11:I:43:ALA:HA	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:13:ARG:HG3	6:D:28:VAL:HG21	1.86	0.57
10:H:1:MET:N	10:H:1:MET:HE2	2.20	0.57
1:X:637:G:H1	11:I:101:ARG:HD3	1.70	0.57
20:R:20:ASP:O	20:R:36:VAL:HG23	2.05	0.57
1:X:2617:G:HO2'	1:X:2618:A:H8	1.51	0.57
1:X:555:U:H3'	1:X:556:A:C8	2.39	0.57
1:X:759:C:C2'	1:X:760:U:OP2	2.52	0.57
1:X:923:A:H5''	1:X:924:C:C5'	2.34	0.57
4:B:136:ARG:CG	4:B:137:ARG:H	2.18	0.57
12:J:22:ALA:HB2	12:J:100:PRO:O	2.05	0.57
9:G:70:PHE:HB2	16:N:64:ARG:NE	2.19	0.57
22:T:43:THR:HG23	22:T:46:LYS:HG2	1.86	0.57
1:X:1441:A:O4'	1:X:1442:C:C6	2.58	0.57
1:X:2571:G:C6	1:X:2572:U:C2	2.92	0.57
1:X:487:G:H4'	1:X:512:A:N1	2.20	0.57
5:C:148:VAL:HG22	5:C:185:ARG:HB2	1.86	0.57
7:E:117:PRO:HD3	7:E:123:PHE:HE1	1.70	0.57
9:G:61:ARG:HE	9:G:65:LYS:CD	2.17	0.57
15:M:50:PHE:CZ	15:M:70:LYS:HB3	2.39	0.57
23:U:17:SER:CB	23:U:44:ALA:HA	2.25	0.57
1:X:567:G:H5'	9:G:140:GLN:OE1	2.04	0.57
1:X:750:C:C4	1:X:751:G:N7	2.73	0.57
11:I:56:LEU:HB3	29:3:52:LYS:CE	2.34	0.57
4:B:136:ARG:HG2	4:B:137:ARG:H	1.68	0.57
9:G:75:ILE:HG13	9:G:75:ILE:O	2.04	0.57
10:H:85:ASP:OD2	10:H:87:SER:N	2.37	0.57
13:K:18:VAL:HG12	13:K:19:ALA:N	2.20	0.57
13:K:51:LEU:CD2	13:K:70:ILE:HD11	2.34	0.57
1:X:1223:G:H4'	1:X:1224:A:O5'	2.05	0.57
1:X:173:A:H2'	1:X:173:A:N3	2.18	0.57
1:X:1773:C:O2'	1:X:2588:U:H5''	2.05	0.57
1:X:1918:G:C4	1:X:1945:C:N4	2.73	0.57
1:X:1967:U:H2'	1:X:1968:G:H8	1.68	0.57
1:X:538:A:N6	1:X:2026:C:O5'	2.37	0.57
1:X:2262:C:H5'	27:1:7:ARG:HH22	1.70	0.57
1:X:2490:U:H2'	1:X:2491:C:O4'	2.05	0.57
1:X:623:G:H21	1:X:626:A:H2	1.53	0.57
19:Q:62:ARG:NH1	19:Q:73:ASN:ND2	2.52	0.57
1:X:2494:C:O2'	1:X:2495:G:H5'	2.04	0.57
1:X:2545:A:H61	10:H:40:GLY:HA3	1.69	0.57
1:X:2671:C:O2'	1:X:2672:U:H5'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:836:G:H2'	1:X:837:U:C6	2.39	0.57
1:X:88:G:C8	1:X:89:A:C8	2.92	0.57
7:E:15:VAL:HG11	7:E:76:VAL:HG13	1.87	0.56
15:M:34:ARG:HD3	15:M:88:VAL:HG22	1.87	0.56
1:X:494:A:H5'	20:R:58:VAL:HG22	1.87	0.56
1:X:1135:C:H2'	1:X:1136:G:O4'	2.03	0.56
1:X:1322:G:H4'	28:2:7:PRO:HB2	1.87	0.56
1:X:1696:C:C5	1:X:1697:U:C5	2.93	0.56
1:X:2728:A:O2'	7:E:63:ALA:HA	2.04	0.56
31:X:2881:LMA:C32	31:X:2881:LMA:O53	2.50	0.56
11:I:89:ASP:OD2	11:I:120:VAL:HA	2.05	0.56
1:X:1644:G:O2'	1:X:1645:U:H5'	2.05	0.56
1:X:2426:G:H1'	1:X:2427:A:OP2	2.05	0.56
1:X:2757:G:C5'	1:X:2758:A:H5'	2.31	0.56
1:X:617:U:C5	1:X:632:A:N1	2.74	0.56
4:B:34:VAL:HG21	4:B:78:LEU:HD22	1.88	0.56
1:X:2728:A:C2	1:X:2737:A:C5	2.93	0.56
1:X:503:G:H2'	1:X:504:G:O4'	2.05	0.56
2:Y:25:G:H2'	2:Y:26:G:C5	2.40	0.56
26:Z:58:LEU:HD12	26:Z:58:LEU:N	2.20	0.56
28:2:34:ARG:HH11	28:2:42:LEU:HA	1.70	0.56
6:D:108:LEU:HB2	6:D:109:PRO:HD3	1.87	0.56
9:G:141:GLY:O	9:G:144:MET:N	2.37	0.56
1:X:2372:A:H5''	11:I:61:PRO:CA	2.35	0.56
23:U:52:ARG:HG3	23:U:62:LEU:HD22	1.85	0.56
1:X:1033:G:H2'	9:G:97:ASP:OD1	2.04	0.56
1:X:1687:C:H4'	1:X:1977:C:O2'	2.06	0.56
1:X:1769:U:C5	1:X:1775:A:C2	2.94	0.56
1:X:686:C:C2'	1:X:687:G:H5'	2.35	0.56
1:X:825:C:H5'	11:I:30:ALA:HB1	1.86	0.56
5:C:102:LEU:HD21	5:C:106:MET:CE	2.35	0.56
13:K:90:ARG:O	13:K:90:ARG:HG3	2.05	0.56
24:V:25:LEU:HD13	24:V:46:LEU:HB2	1.87	0.56
1:X:1016:C:O2'	1:X:1023:U:H5	1.86	0.56
1:X:1949:A:N6	1:X:2581:A:H62	2.03	0.56
1:X:2634:G:O2'	1:X:2635:U:C5	2.59	0.56
1:X:2845:C:C6	1:X:2845:C:H3'	2.40	0.56
1:X:459:A:H4'	1:X:461:A:C8	2.40	0.56
1:X:48:A:N6	1:X:154:U:H5	2.04	0.56
1:X:540:G:H5''	1:X:541:C:OP2	2.05	0.56
7:E:57:ASP:HB3	7:E:62:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:39:VAL:CG1	15:M:45:THR:HG23	2.35	0.56
19:Q:11:VAL:HG23	19:Q:27:PHE:HA	1.87	0.56
22:T:51:VAL:HG21	22:T:79:ILE:O	2.06	0.56
1:X:1006:C:OP2	16:N:54:LYS:NZ	2.23	0.56
1:X:1073:G:H21	8:F:133:SER:HB3	1.69	0.56
1:X:219:G:H2'	1:X:220:U:OP2	2.05	0.56
2:Y:107:C:H2'	2:Y:108:G:O4'	2.06	0.56
4:B:7:THR:CG2	4:B:193:GLY:HA2	2.35	0.56
13:K:76:VAL:O	13:K:80:MET:HB2	2.05	0.56
10:H:132:GLU:HB2	15:M:73:PHE:HE1	1.71	0.56
17:O:78:VAL:O	17:O:79:GLN:HB2	2.06	0.56
1:X:1016:C:H1'	1:X:1023:U:C5	2.41	0.56
1:X:1129:A:C6	1:X:1130:U:N3	2.74	0.56
1:X:1218:C:H4'	11:I:13:ARG:HH11	1.69	0.56
1:X:2262:C:H2'	1:X:2263:C:O4'	2.05	0.56
1:X:2383:C:H2'	1:X:2384:G:O4'	2.05	0.56
1:X:88:G:H3'	1:X:89:A:H5''	1.88	0.56
4:B:56:GLU:HG2	4:B:74:PRO:HG2	1.87	0.56
5:C:187:VAL:O	5:C:187:VAL:HG12	2.05	0.56
11:I:85:ASP:HA	11:I:116:ARG:HH12	1.71	0.56
20:R:25:LEU:HD23	20:R:26:SER:HB3	1.87	0.56
24:V:25:LEU:CD1	24:V:46:LEU:HD12	2.36	0.56
1:X:1478:U:H2'	1:X:1479:G:H8	1.70	0.56
1:X:1712:G:H2'	1:X:1713:G:H5'	1.88	0.56
1:X:2016:A:C5	1:X:2019:C:C4	2.94	0.56
1:X:1834:G:N2	1:X:1884:A:C6	2.73	0.56
1:X:1967:U:H2'	1:X:1968:G:C8	2.40	0.56
1:X:2170:C:H3'	1:X:2171:U:C5'	2.32	0.56
1:X:2073:A:H61	1:X:2208:U:H3	1.52	0.56
1:X:2844:G:C2	1:X:2845:C:O2	2.58	0.56
1:X:760:U:HO2'	1:X:761:G:P	2.28	0.56
1:X:877:G:H1	1:X:924:C:H42	1.54	0.56
26:Z:31:THR:HG22	26:Z:32:GLU:N	2.21	0.56
1:X:2323:U:H3'	27:1:39:LYS:O	2.05	0.56
1:X:2734:U:H4'	30:4:26:ILE:CD1	2.35	0.56
7:E:7:GLN:HB2	7:E:8:PRO:HD3	1.88	0.56
10:H:75:VAL:HG12	10:H:118:LEU:CD2	2.36	0.56
12:J:42:TRP:CB	12:J:95:VAL:HG11	2.31	0.56
14:L:37:HIS:NE2	14:L:39:TYR:CZ	2.74	0.56
1:X:101:A:H2'	1:X:102:C:O4'	2.06	0.56
1:X:1068:A:H2'	1:X:1069:G:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1310:C:H2'	1:X:1311:C:C6	2.41	0.56
1:X:1423:A:C2	1:X:1609:G:C2	2.94	0.56
1:X:1407:G:H4'	1:X:1619:A:H4'	1.87	0.56
1:X:305:A:C2	1:X:356:A:C2	2.94	0.56
2:Y:90:C:H2'	2:Y:91:A:O4'	2.06	0.56
1:X:1810:U:OP2	3:A:158:ARG:HD3	2.06	0.56
4:B:85:ALA:N	4:B:86:PRO:HD3	2.21	0.56
1:X:1310:C:C2	1:X:1311:C:C5	2.94	0.56
1:X:2499:C:C2'	1:X:2500:C:H5'	2.35	0.56
1:X:2666:U:O2'	1:X:2667:C:H5'	2.06	0.56
27:1:14:SER:HB3	27:1:50:PHE:CZ	2.41	0.55
3:A:159:SER:O	3:A:197:VAL:HG21	2.06	0.55
6:D:118:ASN:HB3	6:D:122:PHE:HZ	1.69	0.55
12:J:32:ASP:H	12:J:108:ALA:HB2	1.70	0.55
17:O:13:ARG:HD2	17:O:95:ILE:HG13	1.88	0.55
19:Q:20:MET:HA	19:Q:24:VAL:O	2.06	0.55
1:X:177:U:C4'	23:U:40:ARG:HE	2.19	0.55
25:W:4:LYS:CG	25:W:52:GLU:HB3	2.36	0.55
1:X:2397:A:H2'	1:X:2398:U:O4'	2.06	0.55
26:Z:14:SER:O	26:Z:18:MET:HG3	2.06	0.55
1:X:538:A:H5''	9:G:142:ARG:HH12	1.72	0.55
14:L:38:ILE:HD11	14:L:40:ALA:N	2.21	0.55
21:S:51:LEU:CD2	21:S:51:LEU:H	2.18	0.55
1:X:393:U:H1'	23:U:18:VAL:HG21	1.88	0.55
1:X:1329:U:H2'	1:X:1330:G:C8	2.41	0.55
1:X:2672:U:H2'	1:X:2673:G:C8	2.38	0.55
1:X:516:G:H4'	1:X:519:C:O2	2.07	0.55
2:Y:58:G:H4'	2:Y:59:A:H8	1.70	0.55
10:H:80:ALA:HB2	10:H:90:ARG:HD3	1.87	0.55
16:N:93:LYS:O	16:N:94:VAL:HB	2.06	0.55
1:X:1333:G:C2	1:X:1342:U:H5'	2.41	0.55
1:X:1466:C:C5	1:X:1467:U:O2	2.59	0.55
1:X:1643:A:H61	1:X:1656:U:H3	1.54	0.55
1:X:521:U:O4	1:X:522:G:N2	2.40	0.55
1:X:967:G:O6	12:J:17:ARG:NH2	2.38	0.55
26:Z:31:THR:O	26:Z:39:LYS:HA	2.06	0.55
5:C:26:VAL:O	5:C:30:VAL:HG23	2.06	0.55
1:X:969:U:O4	12:J:18:MET:HA	2.06	0.55
15:M:102:ALA:O	15:M:103:LYS:HD2	2.06	0.55
1:X:2426:G:C4	1:X:2479:U:C5	2.94	0.55
1:X:496:C:C2'	1:X:497:C:H5'	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:807:A:H2'	1:X:808:C:H6	1.71	0.55
1:X:760:U:C5	26:Z:3:LYS:HE2	2.41	0.55
3:A:218:ARG:HG2	3:A:219:LYS:N	2.21	0.55
3:A:44:ARG:HE	3:A:56:GLY:HA2	1.71	0.55
6:D:38:GLU:HG2	6:D:57:LEU:HD11	1.88	0.55
14:L:43:ILE:HG23	14:L:49:GLN:O	2.06	0.55
21:S:100:THR:CG2	21:S:138:VAL:HG11	2.36	0.55
1:X:70:A:OP2	1:X:111:G:H4'	2.06	0.55
1:X:1299:A:HO2'	1:X:1301:U:P	2.29	0.55
1:X:1474:A:H2'	1:X:1474:A:N3	2.22	0.55
1:X:1684:G:N3	1:X:1974:U:C5	2.75	0.55
1:X:2251:U:H5''	1:X:2252:A:OP1	2.06	0.55
1:X:2274:C:OP2	14:L:11:LEU:HD21	2.06	0.55
29:3:8:LYS:HG3	29:3:12:ARG:HH12	1.71	0.55
13:K:79:VAL:HG13	13:K:80:MET:N	2.21	0.55
13:K:84:ALA:HB3	13:K:85:PRO:CD	2.32	0.55
20:R:48:VAL:HG12	20:R:50:GLY:H	1.72	0.55
21:S:120:LEU:C	21:S:120:LEU:HD23	2.27	0.55
21:S:95:SER:HB3	21:S:119:ASN:HD21	1.72	0.55
1:X:1974:U:H2'	1:X:1975:G:H5'	1.87	0.55
1:X:794:A:H5'	3:A:219:LYS:NZ	2.22	0.55
1:X:822:G:O2'	1:X:823:U:H5'	2.07	0.55
2:Y:50:U:H2'	2:Y:51:G:C8	2.41	0.55
28:2:34:ARG:NH1	28:2:42:LEU:HG	2.21	0.55
11:I:31:GLY:HA3	11:I:34:HIS:ND1	2.22	0.55
1:X:1031:C:H1'	1:X:1032:A:OP2	2.06	0.55
1:X:1655:C:H4'	1:X:2689:C:O2	2.06	0.55
1:X:1699:A:H2'	1:X:1700:C:C6	2.41	0.55
1:X:218:A:C8	1:X:220:U:O2	2.60	0.55
1:X:2728:A:C2	1:X:2737:A:C6	2.95	0.55
3:A:252:GLY:HA3	3:A:256:LYS:NZ	2.21	0.55
9:G:103:TYR:CE1	9:G:111:LYS:HB2	2.41	0.55
10:H:29:ILE:HG12	10:H:30:GLY:N	2.19	0.55
15:M:66:PHE:CD2	15:M:83:PHE:CE1	2.94	0.55
22:T:65:GLY:HA3	22:T:81:ILE:HG22	1.88	0.55
1:X:115:G:C6	1:X:117:A:N6	2.75	0.55
1:X:1744:G:H2'	1:X:1746:A:OP2	2.07	0.55
1:X:174:A:H2	1:X:2413:A:N6	2.05	0.55
1:X:1673:C:H42	1:X:1987:G:H1	1.54	0.55
1:X:2013:A:H4'	1:X:2014:A:C8	2.41	0.55
1:X:2013:A:H4'	1:X:2014:A:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2453:C:H5'	1:X:2454:C:OP2	2.07	0.55
1:X:2705:A:C8	1:X:2707:G:C5	2.95	0.55
1:X:839:U:OP1	1:X:2408:G:OP1	2.24	0.55
14:L:42:ILE:HD13	14:L:43:ILE:N	2.22	0.55
20:R:15:HIS:CE1	20:R:16:PHE:CD2	2.94	0.55
1:X:1141:U:H3	1:X:2008:C:H5''	1.72	0.55
1:X:1507:A:O4'	3:A:100:ASP:HB3	2.06	0.55
1:X:2375:G:H2'	1:X:2376:G:H8	1.72	0.55
1:X:2404:A:C4'	1:X:2405:A:OP2	2.55	0.55
1:X:2821:G:C6	1:X:2846:G:N2	2.75	0.55
1:X:807:A:H2'	1:X:808:C:C6	2.42	0.55
2:Y:8:C:H1'	14:L:39:TYR:OH	2.07	0.55
17:O:6:GLN:O	17:O:7:THR:OG1	2.19	0.55
1:X:2235:G:N2	1:X:2254:C:N4	2.55	0.55
3:A:26:THR:HG22	3:A:27:LYS:N	2.21	0.54
4:B:93:VAL:C	4:B:95:ILE:H	2.10	0.54
10:H:127:VAL:HG13	10:H:133:VAL:HG21	1.88	0.54
1:X:1182:U:O2'	1:X:1183:C:H5''	2.07	0.54
1:X:1272:G:H2'	1:X:1273:G:C8	2.42	0.54
1:X:1447:U:H1'	1:X:1577:G:N2	2.22	0.54
1:X:1769:U:H5	1:X:1775:A:C2	2.25	0.54
1:X:2477:C:OP2	1:X:2478:C:OP2	2.26	0.54
1:X:2557:G:N7	4:B:140:SER:HB3	2.22	0.54
1:X:2751:C:H2'	1:X:2752:C:C6	2.42	0.54
1:X:958:G:H2'	1:X:959:C:C6	2.42	0.54
9:G:103:TYR:CZ	9:G:111:LYS:HB2	2.42	0.54
9:G:94:LYS:HG2	9:G:117:GLU:HB2	1.89	0.54
12:J:16:GLY:O	12:J:17:ARG:HB3	2.06	0.54
19:Q:29:VAL:HG11	19:Q:38:ILE:HD11	1.89	0.54
19:Q:62:ARG:O	19:Q:70:GLY:HA3	2.07	0.54
23:U:32:ARG:NE	23:U:32:ARG:H	2.05	0.54
1:X:1062:G:H4'	1:X:2732:C:O2'	2.07	0.54
1:X:2355:A:H2'	1:X:2356:A:O4'	2.07	0.54
1:X:2031:A:C2	1:X:2600:A:C2	2.94	0.54
10:H:16:ALA:CB	10:H:98:ILE:HD11	2.36	0.54
1:X:883:A:H5'	12:J:10:PHE:O	2.06	0.54
25:W:13:PRO:O	25:W:17:VAL:HG23	2.07	0.54
1:X:1813:A:H2'	1:X:1814:G:C8	2.43	0.54
1:X:1922:U:O4'	1:X:1922:U:O2	2.25	0.54
1:X:2542:U:H2'	1:X:2544:A:OP2	2.07	0.54
1:X:2674:C:H2'	1:X:2675:U:H6	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1981:A:O3'	1:X:2704:U:H4'	2.07	0.54
1:X:2660:C:C2	1:X:2704:U:O4	2.60	0.54
1:X:962:C:H42	1:X:977:G:H1	1.56	0.54
3:A:245:ARG:HA	3:A:253:LYS:HZ1	1.71	0.54
14:L:51:LEU:N	14:L:51:LEU:HD12	2.23	0.54
17:O:10:LYS:HD2	17:O:37:ALA:HB3	1.90	0.54
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.89	0.54
19:Q:48:VAL:CG2	19:Q:82:LEU:HD22	2.38	0.54
20:R:106:VAL:O	20:R:107:ALA:HB2	2.06	0.54
1:X:1974:U:H2'	1:X:1975:G:C5'	2.38	0.54
1:X:1978:U:H2'	1:X:1979:C:C5	2.42	0.54
1:X:2201:G:H2'	1:X:2202:G:H8	1.72	0.54
1:X:2570:C:H2'	1:X:2571:G:C8	2.43	0.54
1:X:2791:C:O2'	1:X:2792:C:H5'	2.07	0.54
27:1:51:ARG:C	27:1:51:ARG:HD2	2.28	0.54
6:D:112:ARG:H	6:D:112:ARG:HD2	1.73	0.54
4:B:9:ILE:HG22	15:M:13:LEU:HD11	1.90	0.54
16:N:17:VAL:HG21	16:N:32:TYR:CE1	2.40	0.54
18:P:37:LYS:HE2	18:P:64:ALA:CB	2.36	0.54
1:X:1478:U:H2'	1:X:1479:G:C8	2.43	0.54
1:X:742:G:C4	1:X:1766:U:O2	2.61	0.54
1:X:2044:G:N7	1:X:2482:A:O4'	2.40	0.54
1:X:536:A:N6	1:X:2605:C:H4'	2.22	0.54
1:X:2836:U:C2	1:X:2837:G:C8	2.95	0.54
1:X:494:A:N7	20:R:56:LYS:NZ	2.50	0.54
2:Y:56:G:H2'	2:Y:57:U:O4'	2.08	0.54
9:G:117:GLU:C	9:G:119:LEU:H	2.11	0.54
10:H:46:HIS:HB2	10:H:49:ASP:OD2	2.08	0.54
14:L:43:ILE:HD12	14:L:43:ILE:N	2.21	0.54
21:S:100:THR:HG23	21:S:138:VAL:CG1	2.38	0.54
1:X:1076:U:OP1	8:F:86:LYS:HD3	2.07	0.54
1:X:1212:U:H2'	1:X:1213:U:C6	2.43	0.54
1:X:1356:G:N2	1:X:1418:C:C2	2.76	0.54
1:X:1607:A:H1'	1:X:1608:U:O5'	2.08	0.54
1:X:2074:U:H3'	1:X:2075:U:C5'	2.37	0.54
1:X:225:G:N7	1:X:227:G:N3	2.55	0.54
27:1:14:SER:HB3	27:1:50:PHE:HZ	1.72	0.54
27:1:9:ILE:HG22	27:1:28:ARG:HB2	1.89	0.54
29:3:13:ARG:CD	29:3:25:PHE:H	2.20	0.54
1:X:2616:U:H5'	4:B:44:TYR:CE1	2.43	0.54
1:X:2292:C:H5'	6:D:37:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:137:LYS:O	9:G:137:LYS:HG2	2.07	0.54
9:G:61:ARG:HA	9:G:65:LYS:HB2	1.88	0.54
11:I:57:ILE:O	11:I:58:ALA:O	2.25	0.54
13:K:103:ARG:CG	13:K:104:ARG:N	2.70	0.54
14:L:33:ARG:HE	14:L:38:ILE:CB	2.21	0.54
20:R:17:LYS:O	20:R:36:VAL:HG11	2.07	0.54
23:U:17:SER:OG	23:U:45:ASN:N	2.40	0.54
1:X:1283:C:H5'	1:X:1284:G:O5'	2.08	0.54
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.41	0.54
1:X:1644:G:H2'	1:X:1645:U:C6	2.43	0.54
1:X:2262:C:H5'	27:1:7:ARG:NH2	2.22	0.54
1:X:456:C:OP2	16:N:2:PRO:HD3	2.08	0.54
10:H:117:GLU:HA	10:H:120:ASP:OD2	2.08	0.54
10:H:29:ILE:HB	10:H:34:LEU:CD2	2.37	0.54
10:H:17:ARG:HE	10:H:59:ALA:HB2	1.73	0.54
14:L:89:PHE:O	14:L:91:ARG:NH2	2.41	0.54
16:N:25:TRP:CE3	16:N:26:GLY:N	2.75	0.54
1:X:1074:G:H1	1:X:1086:C:N4	2.05	0.54
1:X:1179:A:C2	1:X:1196:G:C2	2.95	0.54
1:X:1336:G:O6	1:X:1337:G:C6	2.61	0.54
1:X:2507:U:OP1	30:4:31:LYS:HE3	2.08	0.54
1:X:2696:A:H2'	1:X:2697:G:H8	1.72	0.54
1:X:623:G:N2	1:X:626:A:H2	2.05	0.54
1:X:754:G:C4	1:X:755:C:C5	2.96	0.54
1:X:999:A:OP2	25:W:8:SER:HB3	2.08	0.54
27:1:41:ASP:HB3	27:1:47:HIS:H	1.72	0.54
16:N:8:ILE:O	16:N:12:ARG:HG3	2.08	0.54
1:X:2043:A:N6	5:C:68:ARG:NH1	2.56	0.54
1:X:2837:G:H2'	1:X:2838:U:H6	1.72	0.54
1:X:537:C:H1'	1:X:538:A:C6	2.43	0.54
1:X:666:U:C2'	1:X:667:U:H5''	2.35	0.54
11:I:62:LYS:HD2	29:3:25:PHE:CE1	2.43	0.54
4:B:116:VAL:HG22	4:B:136:ARG:CG	2.38	0.54
9:G:41:TRP:CZ3	9:G:79:PHE:CG	2.96	0.54
10:H:24:VAL:HG12	10:H:42:LYS:HG2	1.88	0.54
20:R:15:HIS:CE1	20:R:16:PHE:HD2	2.26	0.54
1:X:1337:G:C4	1:X:1341:G:O6	2.61	0.54
1:X:26:G:C6	1:X:27:G:C6	2.96	0.54
1:X:471:A:C2	1:X:481:A:C4	2.96	0.54
1:X:699:G:O6	28:2:12:ARG:HA	2.08	0.54
11:I:62:LYS:HD2	29:3:25:PHE:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2218:G:OP1	3:A:250:PRO:HB3	2.09	0.53
3:A:44:ARG:CD	3:A:44:ARG:N	2.64	0.53
4:B:154:LYS:HG3	4:B:155:ARG:N	2.21	0.53
5:C:43:ALA:HB1	5:C:86:PRO:O	2.08	0.53
18:P:32:ARG:NH2	18:P:120:ARG:O	2.41	0.53
1:X:1607:A:C4'	1:X:1608:U:OP1	2.55	0.53
1:X:623:G:H3'	1:X:624:A:H5''	1.89	0.53
1:X:954:U:OP2	11:I:38:LYS:NZ	2.38	0.53
29:3:24:ALA:O	29:3:47:GLY:N	2.42	0.53
1:X:1810:U:C5	3:A:158:ARG:HD2	2.43	0.53
1:X:2554:C:O2'	4:B:140:SER:HB3	2.08	0.53
4:B:4:ILE:HG12	4:B:31:CYS:SG	2.48	0.53
7:E:107:ILE:HD11	7:E:151:VAL:HG11	1.90	0.53
12:J:15:ARG:CD	12:J:73:LYS:HG3	2.32	0.53
18:P:8:PHE:O	18:P:9:ARG:HB2	2.09	0.53
23:U:21:ARG:C	23:U:39:LYS:HD2	2.28	0.53
24:V:37:LEU:C	24:V:37:LEU:HD23	2.29	0.53
1:X:1265:G:H22	16:N:37:GLN:NE2	2.06	0.53
1:X:1337:G:C5	1:X:1341:G:O6	2.61	0.53
1:X:1923:U:H1'	1:X:1924:C:OP2	2.08	0.53
1:X:2045:A:O2'	1:X:2046:C:C5'	2.56	0.53
1:X:2218:G:H5'	3:A:250:PRO:CD	2.38	0.53
1:X:1773:C:H2'	1:X:2587:G:O2'	2.07	0.53
1:X:2593:A:H5'	26:Z:5:PRO:HB3	1.90	0.53
1:X:544:U:H2'	1:X:545:C:C6	2.43	0.53
1:X:637:G:N1	11:I:101:ARG:HD3	2.22	0.53
3:A:37:ALA:HB1	3:A:63:TYR:O	2.07	0.53
1:X:334:G:N2	5:C:162:ARG:NH2	2.55	0.53
1:X:1392:U:C6	1:X:1392:U:OP1	2.61	0.53
1:X:1420:A:H2	1:X:1612:U:O2	1.90	0.53
1:X:1944:C:H2'	1:X:1945:C:O4'	2.07	0.53
1:X:2292:C:H5'	6:D:37:ASN:HD22	1.73	0.53
1:X:2598:C:C2'	1:X:2599:U:H5'	2.37	0.53
1:X:2026:C:C4	1:X:2757:G:C2	2.97	0.53
3:A:109:PRO:HB3	3:A:144:HIS:CE1	2.44	0.53
3:A:246:VAL:C	3:A:253:LYS:HD3	2.29	0.53
4:B:121:ASN:O	4:B:122:PHE:C	2.47	0.53
1:X:38:G:N2	5:C:42:THR:HG22	2.23	0.53
10:H:65:LYS:HD2	10:H:65:LYS:N	2.24	0.53
1:X:1744:G:OP1	15:M:100:ARG:CD	2.57	0.53
15:M:27:PHE:HB3	15:M:93:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:34:ARG:HE	15:M:91:VAL:HG22	1.72	0.53
18:P:106:LEU:O	18:P:106:LEU:HD23	2.08	0.53
20:R:44:GLN:O	20:R:77:HIS:HA	2.08	0.53
21:S:130:ILE:HD12	21:S:130:ILE:N	2.23	0.53
24:V:31:GLN:HA	24:V:34:ALA:HB3	1.90	0.53
1:X:1173:G:H4'	17:O:22:VAL:CG2	2.36	0.53
1:X:1182:U:H1'	1:X:1183:C:O5'	2.08	0.53
1:X:1407:G:H3'	1:X:1407:G:N3	2.24	0.53
1:X:2041:A:N1	31:X:2881:LMA:H40A	2.24	0.53
1:X:2282:G:O2'	6:D:129:ASN:HB2	2.08	0.53
1:X:652:C:N4	1:X:657:A:H61	2.06	0.53
27:1:11:LYS:N	27:1:11:LYS:HD2	2.24	0.53
27:1:9:ILE:HG22	27:1:28:ARG:CB	2.37	0.53
6:D:104:ILE:HD13	6:D:174:GLY:HA3	1.91	0.53
9:G:96:ASP:O	9:G:98:LYS:N	2.41	0.53
12:J:40:PRO:HB3	12:J:99:LYS:NZ	2.23	0.53
1:X:99:U:H3'	1:X:100:G:H5''	1.90	0.53
1:X:1257:U:H2'	1:X:1258:G:C8	2.44	0.53
1:X:1677:C:H42	1:X:1983:G:H1	1.56	0.53
1:X:224:G:C2	1:X:229:G:C6	2.96	0.53
1:X:559:C:H2'	1:X:560:G:O4'	2.08	0.53
1:X:867:G:C2	1:X:936:A:C2	2.96	0.53
13:K:87:TYR:OH	13:K:115:LEU:HB3	2.08	0.53
13:K:28:LEU:HD21	13:K:115:LEU:HD21	1.90	0.53
13:K:55:ALA:HB2	13:K:66:VAL:HG21	1.91	0.53
14:L:37:HIS:CG	14:L:37:HIS:O	2.61	0.53
14:L:42:ILE:O	14:L:50:THR:HG23	2.08	0.53
1:X:57:G:OP1	19:Q:74:ASP:HB2	2.09	0.53
1:X:2366:U:H1'	22:T:41:ARG:NH1	2.24	0.53
1:X:2217:G:H2'	1:X:2217:G:N3	2.23	0.53
1:X:2392:G:H2'	1:X:2393:G:H8	1.74	0.53
1:X:2664:G:C6	1:X:2705:A:N6	2.76	0.53
1:X:589:C:H4'	16:N:31:GLN:NE2	2.24	0.53
1:X:673:G:H2'	1:X:674:U:C6	2.43	0.53
28:2:42:LEU:H	28:2:42:LEU:CD1	2.22	0.53
29:3:41:ILE:HG22	29:3:42:ARG:HD3	1.91	0.53
10:H:19:ILE:O	10:H:19:ILE:HG13	2.08	0.53
17:O:68:LYS:HD2	17:O:69:ILE:H	1.74	0.53
17:O:70:TYR:CD2	17:O:83:ARG:NH1	2.73	0.53
1:X:1002:C:H6	1:X:1002:C:O5'	1.92	0.53
1:X:1544:A:C2	1:X:1560:A:C2	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1810:U:C6	3:A:158:ARG:HD2	2.44	0.53
1:X:668:A:H2'	1:X:669:G:O4'	2.09	0.53
1:X:999:A:H5''	25:W:8:SER:CB	2.38	0.53
4:B:31:CYS:HB3	4:B:49:ILE:CG1	2.39	0.53
11:I:49:PHE:CD1	11:I:50:GLU:N	2.76	0.53
12:J:99:LYS:CE	12:J:100:PRO:HD2	2.38	0.53
1:X:1357:U:C2'	1:X:1358:C:OP1	2.56	0.53
1:X:2039:G:C8	1:X:2556:A:C6	2.97	0.53
1:X:2598:C:H4'	4:B:150:VAL:HG22	1.91	0.53
4:B:134:TRP:CD1	4:B:134:TRP:N	2.74	0.53
7:E:137:ASP:HB3	7:E:140:LEU:HD12	1.91	0.53
10:H:51:ILE:HD12	10:H:52:VAL:O	2.08	0.53
21:S:149:ALA:O	21:S:160:LEU:HD11	2.08	0.53
1:X:591:G:H1	1:X:1271:C:H42	1.57	0.53
1:X:1433:A:H62	1:X:1435:G:C1'	2.22	0.53
1:X:1888:C:H2'	1:X:1913:G:N7	2.23	0.53
1:X:1938:U:H4'	1:X:1939:U:OP2	2.08	0.53
1:X:2486:C:C2	1:X:2562:G:C2	2.96	0.53
1:X:1949:A:H61	1:X:2581:A:H62	1.56	0.53
1:X:304:A:C6	1:X:359:G:N2	2.77	0.53
1:X:500:G:H2'	1:X:501:G:O4'	2.09	0.53
1:X:760:U:O2'	1:X:761:G:P	2.66	0.53
1:X:746:G:O6	1:X:774:A:C8	2.62	0.53
3:A:66:ILE:HD11	3:A:107:LEU:HD12	1.89	0.53
3:A:73:LYS:HE2	3:A:98:TYR:CD2	2.44	0.53
5:C:74:VAL:HG23	5:C:76:THR:H	1.74	0.53
9:G:100:TYR:CB	9:G:116:ARG:HH11	2.08	0.53
13:K:103:ARG:CG	13:K:104:ARG:H	2.22	0.53
18:P:25:PHE:CD1	18:P:127:ILE:HD11	2.40	0.53
1:X:518:A:N6	18:P:30:TYR:CD1	2.77	0.53
1:X:455:A:H1'	1:X:1215:A:O4'	2.09	0.53
1:X:1257:U:H2'	1:X:1258:G:H8	1.73	0.53
1:X:1370:U:H2'	1:X:1371:G:O4'	2.08	0.53
1:X:1399:C:O2'	1:X:1400:A:H5'	2.09	0.53
1:X:1688:U:O2'	1:X:1690:U:H5	1.90	0.53
1:X:2311:U:C4'	1:X:2315:A:N6	2.71	0.53
1:X:474:G:N2	1:X:477:A:OP2	2.38	0.53
1:X:746:G:C5	1:X:774:A:C5	2.97	0.53
13:K:90:ARG:HD2	13:K:94:TYR:HB2	1.92	0.52
1:X:1174:G:C2	1:X:1175:A:C5	2.96	0.52
3:A:28:LYS:NZ	3:A:30:PRO:HG3	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:116:VAL:H	4:B:136:ARG:CD	2.22	0.52
10:H:2:ILE:CB	10:H:45:ALA:HB3	2.37	0.52
1:X:1218:C:H4'	11:I:13:ARG:NH1	2.23	0.52
12:J:43:ILE:HG13	12:J:98:VAL:HG21	1.91	0.52
24:V:17:GLU:HB3	24:V:21:ARG:NH1	2.24	0.52
1:X:1053:G:H1'	1:X:1054:C:O5'	2.08	0.52
1:X:75:C:N3	1:X:109:A:C2	2.77	0.52
1:X:1145:C:C6	1:X:1147:G:OP2	2.62	0.52
1:X:2528:G:C2	1:X:2529:G:N7	2.77	0.52
28:2:25:LYS:NZ	28:2:28:ARG:HG3	2.24	0.52
30:4:15:LYS:HB2	30:4:26:ILE:HG13	1.90	0.52
9:G:61:ARG:NE	9:G:65:LYS:HD2	2.24	0.52
10:H:26:ASN:HB3	10:H:38:GLY:H	1.73	0.52
11:I:43:ALA:O	11:I:45:LYS:CB	2.57	0.52
2:Y:9:G:H5''	14:L:32:TYR:CE1	2.44	0.52
1:X:1429:A:H1'	1:X:1603:A:C6	2.43	0.52
1:X:463:C:C2	1:X:465:C:C5	2.97	0.52
1:X:762:A:H2	1:X:766:A:O2'	1.91	0.52
1:X:810:U:H2'	1:X:811:G:O4'	2.09	0.52
3:A:247:PRO:C	3:A:249:THR:H	2.12	0.52
3:A:38:LEU:HB3	3:A:39:PRO:HD2	1.92	0.52
12:J:69:ILE:HD13	12:J:104:MET:HB3	1.90	0.52
12:J:64:LYS:HD3	12:J:108:ALA:O	2.09	0.52
18:P:80:LEU:HD11	18:P:87:GLU:HB3	1.91	0.52
1:X:1010:U:O2'	1:X:1011:A:H5'	2.09	0.52
1:X:1746:A:C2	1:X:2696:A:H1'	2.44	0.52
1:X:1811:A:H2'	3:A:179:PRO:HG2	1.91	0.52
1:X:2468:G:O2'	1:X:2469:G:H5'	2.09	0.52
1:X:2664:G:N2	1:X:2665:G:H1'	2.23	0.52
1:X:758:G:C2'	1:X:759:C:OP1	2.57	0.52
6:D:40:LEU:HD11	6:D:50:ILE:HA	1.91	0.52
16:N:24:PHE:CB	16:N:29:SER:HB3	2.40	0.52
17:O:13:ARG:HD3	17:O:16:GLU:HB2	1.90	0.52
18:P:110:ALA:O	18:P:111:ARG:HB2	2.08	0.52
21:S:47:SER:OG	21:S:48:THR:N	2.42	0.52
1:X:1433:A:C4	1:X:1595:A:C2	2.98	0.52
1:X:1976:U:C5	1:X:1977:C:C5	2.97	0.52
1:X:2340:C:OP1	29:3:27:SER:N	2.36	0.52
1:X:2815:C:H42	1:X:2852:G:H1	1.57	0.52
1:X:513:A:C6	1:X:516:G:C6	2.97	0.52
28:2:19:ARG:NH1	28:2:19:ARG:HB2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:78:ALA:HB2	3:A:98:TYR:CD1	2.43	0.52
1:X:2289:A:C2	6:D:79:LEU:HD11	2.34	0.52
1:X:538:A:H3'	9:G:142:ARG:HH22	1.74	0.52
10:H:9:ASP:HB2	10:H:95:ALA:HB2	1.90	0.52
16:N:16:LYS:O	16:N:19:LYS:HG2	2.09	0.52
1:X:793:G:H21	1:X:796:A:H62	1.57	0.52
1:X:795:A:H5'	1:X:796:A:C2	2.44	0.52
1:X:968:C:N4	1:X:970:A:C5	2.78	0.52
1:X:659:G:H1'	29:3:46:LYS:HG3	1.92	0.52
1:X:1976:U:C5'	4:B:128:SER:HB3	2.39	0.52
9:G:162:LYS:N	9:G:163:PRO:CD	2.72	0.52
13:K:85:PRO:O	13:K:88:ALA:HB2	2.10	0.52
16:N:11:ARG:HB3	16:N:15:LYS:HZ1	1.75	0.52
16:N:7:GLY:O	16:N:9:VAL:HG23	2.10	0.52
1:X:1867:A:O2'	1:X:1868:A:C8	2.63	0.52
1:X:983:G:H3'	1:X:984:A:C5'	2.39	0.52
1:X:15:G:H4'	26:Z:21:SER:HB2	1.91	0.52
3:A:148:LEU:CD2	3:A:156:LEU:HD11	2.40	0.52
4:B:115:GLY:HA3	4:B:136:ARG:HD2	1.92	0.52
19:Q:29:VAL:HG11	19:Q:38:ILE:CD1	2.40	0.52
22:T:45:PHE:HA	22:T:77:ARG:HB2	1.92	0.52
1:X:1355:A:HO2'	1:X:1357:U:P	2.32	0.52
1:X:1920:A:H5''	1:X:1921:A:OP2	2.09	0.52
1:X:1963:G:O2'	1:X:1965:U:OP2	2.28	0.52
1:X:2234:G:H2'	1:X:2235:G:O4'	2.09	0.52
1:X:2422:C:O2'	1:X:2423:G:H5'	2.10	0.52
1:X:2736:U:H3	1:X:2738:A:N6	1.89	0.52
1:X:399:G:H4'	23:U:21:ARG:HH12	1.75	0.52
1:X:2736:U:C5'	30:4:19:ARG:HG2	2.40	0.52
1:X:2722:C:OP1	30:4:35:ARG:HD2	2.10	0.52
4:B:131:SER:HB2	4:B:134:TRP:HE1	1.74	0.52
18:P:45:ILE:O	18:P:48:LYS:HG2	2.10	0.52
21:S:128:ARG:HG3	21:S:129:ARG:HG3	1.91	0.52
1:X:1224:A:H4'	1:X:1225:G:OP2	2.10	0.52
1:X:13:A:N3	1:X:15:G:O6	2.43	0.52
1:X:203:G:H1'	1:X:205:A:H61	1.75	0.52
1:X:2264:C:OP2	27:1:28:ARG:HD3	2.10	0.52
1:X:689:A:H1'	1:X:2422:C:O4'	2.10	0.52
1:X:2706:U:OP1	1:X:2706:U:C6	2.63	0.52
1:X:537:C:O2'	1:X:538:A:C4	2.61	0.52
1:X:215:G:H21	1:X:632:A:H8	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:57:G:N3	1:X:69:G:N2	2.58	0.52
1:X:941:U:H2'	1:X:942:U:O4'	2.09	0.52
27:1:51:ARG:HD2	27:1:51:ARG:O	2.10	0.52
28:2:19:ARG:HB2	28:2:19:ARG:CZ	2.40	0.52
1:X:603:C:H5''	29:3:62:LEU:HD13	1.92	0.52
6:D:36:VAL:HB	6:D:89:VAL:HB	1.90	0.52
6:D:4:LEU:CG	6:D:5:LYS:H	2.23	0.52
2:Y:9:G:H21	14:L:41:GLN:HE22	1.58	0.52
21:S:134:LEU:HD21	21:S:152:ILE:HG21	1.91	0.52
1:X:1255:A:H2'	1:X:1256:C:C6	2.44	0.52
1:X:1290:A:H5''	13:K:40:LYS:HZ3	1.75	0.52
1:X:1467:U:H6	1:X:1467:U:H3'	1.74	0.52
1:X:1505:U:O2	1:X:1506:C:H5	1.92	0.52
1:X:2180:U:H5	1:X:2203:G:C5	2.28	0.52
1:X:659:G:O2'	1:X:660:G:H5'	2.09	0.52
2:Y:44:C:H42	6:D:88:LYS:NZ	2.07	0.52
1:X:787:A:H5''	3:A:49:ARG:NH2	2.26	0.51
1:X:178:C:OP2	23:U:40:ARG:CZ	2.58	0.51
1:X:1351:G:O2'	1:X:1352:G:H5'	2.10	0.51
1:X:2839:G:H2'	1:X:2840:U:C6	2.46	0.51
1:X:882:C:H42	1:X:920:G:H1	1.59	0.51
27:1:11:LYS:H	27:1:11:LYS:HD2	1.75	0.51
16:N:79:PHE:O	16:N:83:LEU:HD13	2.11	0.51
17:O:66:GLY:O	17:O:87:ARG:NH2	2.43	0.51
20:R:93:ARG:O	20:R:94:VAL:C	2.48	0.51
24:V:2:LYS:CG	24:V:3:PRO:HD3	2.40	0.51
1:X:540:G:C6	1:X:2005:U:H5''	2.45	0.51
1:X:2033:C:N4	1:X:2034:A:C6	2.78	0.51
1:X:2338:C:H2'	1:X:2339:A:O4'	2.09	0.51
1:X:2382:C:N4	1:X:2393:G:H1	2.08	0.51
1:X:2457:A:N7	1:X:2458:U:C5	2.78	0.51
1:X:2674:C:H2'	1:X:2675:U:C6	2.46	0.51
1:X:2782:G:C2'	1:X:2783:U:O5'	2.57	0.51
1:X:652:C:H42	1:X:657:A:N6	2.06	0.51
1:X:613:A:O4'	1:X:668:A:H2	1.92	0.51
9:G:95:LEU:HD21	9:G:117:GLU:OE1	2.10	0.51
11:I:32:ARG:HH22	17:O:82:ARG:HE	1.58	0.51
1:X:1644:G:H2'	1:X:1645:U:H6	1.75	0.51
1:X:1724:C:N3	1:X:1747:G:C6	2.78	0.51
1:X:2368:G:H5''	1:X:2369:U:O4'	2.10	0.51
1:X:618:A:C2	1:X:632:A:C5	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:753:U:H2'	1:X:754:G:H8	1.76	0.51
3:A:22:PHE:O	3:A:209:LYS:HG3	2.11	0.51
4:B:188:ILE:CG2	4:B:189:PRO:CD	2.88	0.51
20:R:16:PHE:CZ	20:R:46:VAL:HG22	2.44	0.51
24:V:6:MET:CE	24:V:56:VAL:HG21	2.41	0.51
1:X:1923:U:OP2	1:X:2582:G:N2	2.35	0.51
1:X:2314:A:O2'	1:X:2315:A:C8	2.64	0.51
1:X:2424:G:C2'	1:X:2425:G:H5'	2.40	0.51
1:X:356:A:H2'	1:X:357:A:C8	2.46	0.51
1:X:542:A:H2'	16:N:28:ARG:HE	1.73	0.51
28:2:25:LYS:HZ2	28:2:28:ARG:HG3	1.75	0.51
6:D:80:ARG:H	6:D:80:ARG:HD2	1.75	0.51
9:G:58:ILE:HG23	9:G:80:VAL:HG11	1.92	0.51
12:J:96:SER:O	12:J:98:VAL:HG23	2.11	0.51
1:X:1332:G:O6	1:X:1333:G:O6	2.28	0.51
1:X:1685:A:H4'	1:X:1686:A:O5'	2.11	0.51
1:X:1941:C:C2'	1:X:1942:G:H5'	2.41	0.51
1:X:2046:C:O2	1:X:2430:A:C2	2.64	0.51
1:X:219:G:C2'	1:X:220:U:OP2	2.59	0.51
1:X:2238:G:C2	1:X:2261:G:C6	2.98	0.51
1:X:2426:G:C5	1:X:2479:U:C5	2.99	0.51
1:X:2623:A:C2'	1:X:2624:G:H5'	2.41	0.51
1:X:469:G:H3'	28:2:39:ARG:O	2.10	0.51
1:X:525:A:C2'	1:X:526:C:H5'	2.40	0.51
1:X:778:G:H2'	1:X:779:U:H6	1.75	0.51
27:1:8:ILE:H	27:1:8:ILE:CD1	2.23	0.51
7:E:90:ARG:NH2	7:E:163:ARG:HH12	2.08	0.51
11:I:57:ILE:HG22	11:I:58:ALA:N	2.25	0.51
16:N:81:ASN:ND2	16:N:117:ARG:NH2	2.58	0.51
1:X:1781:C:C6	1:X:1781:C:H5'	2.46	0.51
1:X:2629:U:H2'	1:X:2630:C:H6	1.76	0.51
1:X:2653:A:O3'	10:H:42:LYS:HA	2.11	0.51
28:2:19:ARG:O	28:2:23:LYS:HG3	2.09	0.51
5:C:45:THR:HG21	5:C:86:PRO:HD2	1.93	0.51
11:I:85:ASP:HA	11:I:116:ARG:NH1	2.25	0.51
14:L:29:LEU:HD23	14:L:89:PHE:CE1	2.45	0.51
14:L:79:ALA:HB1	14:L:84:ILE:HB	1.92	0.51
24:V:49:GLU:O	24:V:53:LEU:HG	2.11	0.51
1:X:121:G:H2'	1:X:122:G:O4'	2.10	0.51
1:X:1496:G:O2'	1:X:1497:C:H5''	2.10	0.51
1:X:1787:U:H2'	1:X:1788:C:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2014:A:C6	1:X:2477:C:H1'	2.45	0.51
1:X:48:A:H8	1:X:50:G:H21	1.57	0.51
1:X:603:C:C5'	29:3:62:LEU:HD22	2.40	0.51
1:X:626:A:O2'	5:C:176:ASN:HB2	2.10	0.51
11:I:49:PHE:CZ	29:3:59:LYS:HE3	2.46	0.51
5:C:137:ALA:HB1	5:C:142:LEU:CB	2.41	0.51
10:H:14:SER:OG	10:H:98:ILE:HD12	2.11	0.51
13:K:103:ARG:HG3	13:K:104:ARG:H	1.76	0.51
18:P:126:ILE:HD12	18:P:127:ILE:N	2.25	0.51
1:X:2033:C:C4	1:X:2034:A:C6	2.99	0.51
1:X:303:C:N3	1:X:360:A:H2	2.08	0.51
1:X:746:G:C8	1:X:774:A:N6	2.79	0.51
1:X:75:C:C2	1:X:109:A:H2	2.28	0.51
6:D:34:ILE:HD12	6:D:156:ILE:HG12	1.92	0.51
10:H:3:MET:O	10:H:6:SER:HB2	2.11	0.51
11:I:57:ILE:HG22	29:3:12:ARG:NH2	2.25	0.51
15:M:75:GLU:O	15:M:77:VAL:HG23	2.10	0.51
20:R:18:LYS:HD3	20:R:18:LYS:N	2.13	0.51
1:X:1607:A:H4'	1:X:1608:U:OP1	2.11	0.51
1:X:2617:G:O2'	1:X:2618:A:H8	1.93	0.51
1:X:2806:G:O4'	1:X:2858:A:C2	2.63	0.51
1:X:350:U:O5'	1:X:350:U:H6	1.94	0.51
1:X:62:U:H4'	1:X:63:A:OP1	2.10	0.51
1:X:746:G:N7	1:X:774:A:N7	2.58	0.51
3:A:247:PRO:O	3:A:249:THR:N	2.44	0.51
4:B:84:PHE:CE2	4:B:86:PRO:CD	2.94	0.51
5:C:117:LEU:HD23	5:C:118:VAL:N	2.26	0.51
13:K:69:ASP:O	13:K:71:HIS:ND1	2.44	0.51
21:S:94:VAL:HG23	21:S:125:PRO:HG3	1.93	0.51
1:X:2310:G:H4'	22:T:43:THR:N	2.25	0.51
1:X:2329:C:N4	1:X:2330:G:C6	2.79	0.51
1:X:2364:C:H2'	1:X:2365:U:C6	2.46	0.51
1:X:330:C:H2'	1:X:331:U:O4'	2.11	0.51
1:X:459:A:H1'	1:X:461:A:N6	2.26	0.51
1:X:482:A:C6	1:X:483:A:C2	2.99	0.51
26:Z:3:LYS:HB3	26:Z:5:PRO:HD2	1.93	0.51
4:B:78:LEU:O	4:B:79:ARG:CD	2.59	0.50
5:C:111:ARG:O	5:C:116:LYS:HB3	2.11	0.50
5:C:130:THR:O	5:C:133:PHE:HB3	2.10	0.50
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.93	0.50
1:X:2475:C:OP1	12:J:83:ARG:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1744:G:OP1	15:M:100:ARG:HD2	2.10	0.50
4:B:181:LEU:HD13	15:M:16:ILE:HD11	1.93	0.50
17:O:80:TYR:HE2	17:O:82:ARG:CZ	2.24	0.50
1:X:1069:G:H3'	1:X:1070:G:H5''	1.92	0.50
1:X:1223:G:C5'	1:X:1224:A:H3'	2.41	0.50
1:X:1300:A:C5'	13:K:103:ARG:HD2	2.41	0.50
1:X:1631:C:H5	1:X:1633:C:C2	2.29	0.50
1:X:2238:G:N1	1:X:2261:G:C6	2.79	0.50
1:X:838:A:H4'	1:X:2407:G:C5	2.47	0.50
1:X:2705:A:C4'	1:X:2706:U:OP1	2.59	0.50
1:X:558:G:N3	1:X:558:G:H3'	2.26	0.50
1:X:751:G:O2'	1:X:752:G:O5'	2.29	0.50
1:X:2265:A:P	27:1:28:ARG:HD2	2.51	0.50
3:A:71:ARG:NH2	3:A:150:PRO:HA	2.25	0.50
7:E:96:ALA:HB2	7:E:105:MET:HE1	1.92	0.50
15:M:104:LEU:C	15:M:106:TYR:H	2.13	0.50
16:N:61:TRP:CZ3	16:N:94:VAL:N	2.75	0.50
18:P:41:VAL:O	18:P:44:VAL:CG2	2.58	0.50
1:X:2210:C:OP1	23:U:45:ASN:HA	2.11	0.50
1:X:1404:C:H41	1:X:1407:G:P	2.34	0.50
1:X:2016:A:C5	1:X:2019:C:N4	2.80	0.50
1:X:2329:C:H6	1:X:2329:C:H3'	1.76	0.50
1:X:2373:C:C5	1:X:2374:C:C5	2.99	0.50
1:X:2375:G:H4'	23:U:32:ARG:O	2.11	0.50
1:X:2634:G:H2'	1:X:2643:G:O6	2.11	0.50
1:X:538:A:C2	1:X:2025:A:C5	3.00	0.50
1:X:877:G:C6	1:X:878:C:N4	2.79	0.50
1:X:2262:C:OP1	27:1:3:LYS:HB3	2.10	0.50
1:X:2659:C:C5'	4:B:189:PRO:HA	2.37	0.50
4:B:20:ALA:HB2	10:H:85:ASP:O	2.11	0.50
11:I:58:ALA:C	11:I:60:LEU:H	2.14	0.50
1:X:2372:A:OP1	11:I:61:PRO:HB3	2.12	0.50
18:P:66:GLU:HB3	18:P:67:PRO:CD	2.32	0.50
21:S:121:GLN:O	21:S:161:ALA:HB3	2.10	0.50
1:X:95:G:H4'	24:V:41:HIS:CG	2.46	0.50
1:X:1692:C:C5	1:X:1693:A:C5	2.98	0.50
1:X:2180:U:O4	1:X:2203:G:H2'	2.11	0.50
1:X:2379:G:N2	1:X:2380:U:O2	2.44	0.50
1:X:789:G:C2	1:X:2220:A:OP1	2.64	0.50
1:X:2796:A:O3'	4:B:162:MET:HE1	2.12	0.50
4:B:61:LYS:N	4:B:62:PRO:CD	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:61:PRO:HG3	29:3:27:SER:HA	1.93	0.50
15:M:25:PRO:O	15:M:27:PHE:CD2	2.64	0.50
16:N:25:TRP:CE3	16:N:26:GLY:HA3	2.47	0.50
1:X:1020:A:H4'	16:N:59:ARG:HG3	1.92	0.50
1:X:1324:G:HO2'	1:X:1325:U:H5	1.60	0.50
1:X:765:C:C5	1:X:1772:C:C2	2.99	0.50
1:X:1787:U:H4'	3:A:255:THR:H	1.76	0.50
1:X:1945:C:O2'	1:X:1946:U:C5	2.65	0.50
1:X:2598:C:H5'	4:B:150:VAL:O	2.11	0.50
1:X:573:C:H2'	1:X:574:C:H6	1.77	0.50
1:X:633:G:H2'	1:X:634:G:C8	2.46	0.50
3:A:95:LEU:O	3:A:95:LEU:HG	2.11	0.50
25:W:40:VAL:HA	25:W:43:MET:CG	2.41	0.50
1:X:1050:G:H2'	1:X:1051:U:H5'	1.93	0.50
1:X:1145:C:C5	1:X:1147:G:P	3.05	0.50
1:X:1987:G:C6	1:X:1988:A:C5	3.00	0.50
1:X:2562:G:C6	1:X:2563:U:N3	2.79	0.50
31:X:2881:LMA:C37	31:X:2881:LMA:H35	2.30	0.50
1:X:465:C:O2	1:X:467:U:C6	2.65	0.50
1:X:958:G:H2'	1:X:959:C:H6	1.76	0.50
1:X:966:A:N6	1:X:967:G:C6	2.80	0.50
4:B:188:ILE:CG2	4:B:189:PRO:HD2	2.41	0.50
15:M:11:GLU:HG3	15:M:14:ARG:NH1	2.18	0.50
18:P:95:ALA:HB2	18:P:126:ILE:CD1	2.37	0.50
20:R:23:ILE:HD12	20:R:23:ILE:O	2.11	0.50
1:X:1007:A:N6	1:X:1171:A:C6	2.79	0.50
1:X:1354:A:O3'	19:Q:54:SER:HB2	2.12	0.50
1:X:2729:A:C6	1:X:2730:A:N6	2.80	0.50
31:X:2881:LMA:H57	31:X:2881:LMA:O55	2.11	0.50
1:X:562:G:H2'	1:X:563:U:O4'	2.11	0.50
27:1:39:LYS:HZ3	27:1:41:ASP:HB3	1.76	0.50
5:C:48:ARG:O	5:C:51:VAL:HG22	2.11	0.50
6:D:134:GLU:HG2	6:D:136:LEU:H	1.76	0.50
18:P:87:GLU:HA	18:P:90:LEU:CG	2.39	0.50
21:S:88:TYR:C	21:S:127:PRO:HG2	2.31	0.50
1:X:1629:G:C6	1:X:1633:C:C5	2.99	0.50
1:X:2016:A:C6	1:X:2019:C:C4	2.99	0.50
1:X:459:A:N6	1:X:484:G:H1'	2.27	0.50
6:D:106:ILE:HG21	6:D:139:PRO:HB3	1.94	0.50
7:E:94:PHE:CG	7:E:107:ILE:HG22	2.46	0.50
14:L:14:ARG:O	14:L:18:ARG:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:66:ALA:O	23:U:70:LEU:HB2	2.12	0.50
1:X:1457:A:C2	1:X:1565:G:C2	2.99	0.50
1:X:158:A:H2	1:X:447:U:O2'	1.95	0.50
1:X:2409:A:O2'	1:X:2410:U:C5	2.65	0.50
1:X:2722:C:H2'	1:X:2723:C:H6	1.76	0.50
1:X:841:G:H4'	1:X:844:G:N1	2.27	0.50
1:X:986:A:C2	1:X:1001:A:C8	2.99	0.50
26:Z:52:TYR:O	26:Z:53:ASP:CB	2.58	0.50
1:X:795:A:C2	3:A:227:MET:HE2	2.47	0.50
1:X:2551:A:H62	4:B:145:LYS:HD2	1.77	0.50
12:J:35:LEU:HD12	12:J:131:LYS:O	2.11	0.50
13:K:63:ARG:HA	13:K:80:MET:HE1	1.94	0.50
4:B:14:ILE:CA	15:M:20:HIS:HD2	2.14	0.50
1:X:2571:G:C6	1:X:2572:U:N3	2.79	0.50
1:X:2757:G:OP2	1:X:2761:A:O2'	2.26	0.50
1:X:320:A:N3	1:X:340:G:O2'	2.42	0.50
1:X:588:G:N2	1:X:1275:A:C4	2.80	0.50
1:X:642:A:O2'	11:I:65:PHE:HB3	2.12	0.50
3:A:43:GLY:H	3:A:44:ARG:NH1	2.10	0.49
7:E:103:LEU:HD21	7:E:105:MET:HE3	1.94	0.49
13:K:68:GLN:O	13:K:71:HIS:CE1	2.65	0.49
16:N:40:LEU:O	16:N:43:ALA:HB3	2.12	0.49
1:X:1255:A:H2'	1:X:1256:C:H6	1.76	0.49
1:X:1469:U:H5''	1:X:1470:G:N7	2.27	0.49
1:X:1747:G:H5'	1:X:1748:U:OP1	2.12	0.49
1:X:1774:A:H5'	1:X:2587:G:H4'	1.93	0.49
1:X:2282:G:C2	1:X:2293:G:C2	3.00	0.49
1:X:754:G:C6	1:X:755:C:N4	2.80	0.49
1:X:79:G:H1	1:X:104:C:H42	1.58	0.49
4:B:147:PRO:O	4:B:149:ARG:HG3	2.12	0.49
9:G:99:VAL:HG12	9:G:99:VAL:O	2.11	0.49
11:I:80:LEU:HD13	11:I:120:VAL:HG22	1.94	0.49
11:I:94:GLU:HB2	11:I:97:ARG:HH11	1.76	0.49
15:M:104:LEU:O	15:M:106:TYR:N	2.44	0.49
18:P:34:SER:HA	18:P:120:ARG:HB2	1.94	0.49
1:X:409:G:O3'	23:U:47:HIS:HE1	1.95	0.49
23:U:49:LYS:HB3	23:U:61:TRP:CZ3	2.47	0.49
1:X:1056:U:H1'	1:X:1058:G:C2	2.47	0.49
1:X:1336:G:C2'	1:X:1337:G:H5'	2.39	0.49
1:X:1351:G:C2	1:X:1352:G:C4	3.01	0.49
1:X:1926:U:O4'	1:X:1928:G:H5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2016:A:O4'	1:X:2016:A:OP2	2.30	0.49
1:X:2338:C:H42	1:X:2407:G:H1	1.60	0.49
1:X:26:G:C5	1:X:27:G:C6	3.00	0.49
1:X:490:A:C4	1:X:492:G:O4'	2.65	0.49
1:X:537:C:H1'	1:X:538:A:N1	2.27	0.49
1:X:969:U:H4'	1:X:970:A:OP2	2.13	0.49
3:A:89:ARG:HG2	3:A:91:ALA:HB3	1.94	0.49
4:B:114:GLN:OE1	4:B:114:GLN:HA	2.11	0.49
5:C:148:VAL:HB	5:C:167:VAL:HG12	1.94	0.49
5:C:14:THR:O	5:C:15:ILE:HB	2.11	0.49
1:X:334:G:C3'	5:C:162:ARG:HD3	2.42	0.49
19:Q:5:ASP:O	19:Q:6:ILE:HB	2.12	0.49
1:X:1145:C:C6	1:X:1147:G:P	3.06	0.49
1:X:2045:A:O2'	1:X:2046:C:O4'	2.30	0.49
1:X:2053:G:N2	1:X:2054:A:N3	2.61	0.49
1:X:2369:U:H5'	29:3:36:LYS:NZ	2.27	0.49
1:X:33:C:H4'	1:X:34:U:OP1	2.10	0.49
1:X:471:A:C2	1:X:481:A:C5	3.00	0.49
1:X:595:A:OP1	5:C:83:ALA:HB3	2.12	0.49
1:X:124:A:OP2	28:2:44:VAL:CG1	2.60	0.49
5:C:14:THR:HG22	5:C:15:ILE:H	1.75	0.49
14:L:37:HIS:CD2	14:L:39:TYR:CZ	3.01	0.49
14:L:91:ARG:H	14:L:91:ARG:NE	2.11	0.49
16:N:66:ASN:CB	16:N:76:TYR:HB2	2.36	0.49
16:N:61:TRP:HZ3	16:N:94:VAL:H	1.54	0.49
18:P:19:LYS:O	18:P:20:LEU:HB3	2.12	0.49
20:R:98:ILE:HG22	20:R:99:VAL:HG13	1.94	0.49
24:V:52:GLN:O	24:V:56:VAL:HG23	2.12	0.49
1:X:105:G:C2'	1:X:106:G:H5'	2.42	0.49
1:X:116:A:OP2	1:X:117:A:H2'	2.12	0.49
1:X:1976:U:OP2	1:X:1976:U:H3'	2.13	0.49
1:X:20:C:O2'	1:X:21:A:H5'	2.12	0.49
1:X:2490:U:O2	4:B:139:GLY:HA3	2.12	0.49
1:X:2499:C:H2'	1:X:2500:C:H5'	1.93	0.49
1:X:2569:A:H2'	1:X:2570:C:C6	2.47	0.49
1:X:2730:A:H5''	1:X:2731:G:OP1	2.12	0.49
1:X:346:C:H2'	1:X:347:C:C6	2.44	0.49
1:X:2262:C:P	27:1:7:ARG:HH22	2.36	0.49
29:3:14:ILE:O	29:3:14:ILE:HG12	2.13	0.49
5:C:28:HIS:ND1	11:I:17:LYS:HA	2.27	0.49
9:G:38:GLU:HG3	9:G:68:PRO:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:56:LEU:HD22	29:3:52:LYS:NZ	2.26	0.49
1:X:1202:U:H5'	17:O:78:VAL:HG22	1.93	0.49
18:P:64:ALA:O	18:P:67:PRO:HD2	2.12	0.49
21:S:13:LYS:HG3	21:S:18:MET:HB2	1.94	0.49
1:X:2045:A:O2'	1:X:2046:C:O5'	2.30	0.49
1:X:2836:U:O2'	1:X:2837:G:H5'	2.12	0.49
1:X:668:A:O2'	1:X:669:G:O4'	2.31	0.49
1:X:173:A:O2'	1:X:818:G:O6	2.30	0.49
11:I:58:ALA:CA	29:3:12:ARG:HH21	2.23	0.49
4:B:188:ILE:HG23	4:B:189:PRO:HD2	1.94	0.49
1:X:334:G:H3'	5:C:162:ARG:HD3	1.93	0.49
6:D:4:LEU:HD22	6:D:101:GLU:HB2	1.94	0.49
7:E:127:GLU:CG	7:E:128:PRO:HD2	2.43	0.49
12:J:95:VAL:HG12	12:J:96:SER:N	2.27	0.49
1:X:1693:A:C2	1:X:1976:U:H5'	2.47	0.49
1:X:1997:A:H5'	18:P:115:ASN:ND2	2.27	0.49
1:X:1142:G:C8	1:X:2008:C:H4'	2.48	0.49
1:X:2015:G:O4'	1:X:2015:G:OP1	2.30	0.49
1:X:525:A:C8	1:X:526:C:C6	3.01	0.49
1:X:717:G:H1'	1:X:739:G:N2	2.27	0.49
1:X:759:C:O2'	1:X:760:U:OP2	2.30	0.49
29:3:30:ARG:HH21	29:3:31:HIS:HE1	1.60	0.49
5:C:172:VAL:O	5:C:173:ALA:C	2.50	0.49
6:D:51:ASP:O	6:D:55:LYS:HG2	2.12	0.49
10:H:1:MET:H3	10:H:1:MET:HE2	1.76	0.49
13:K:28:LEU:CD2	13:K:28:LEU:C	2.77	0.49
25:W:16:GLN:O	25:W:20:VAL:HG23	2.13	0.49
1:X:2044:G:N7	1:X:2480:C:H4'	2.27	0.49
1:X:2657:G:H2'	1:X:2658:A:O4'	2.12	0.49
1:X:2845:C:C6	1:X:2845:C:C3'	2.95	0.49
1:X:484:G:C2	1:X:485:G:C5	3.01	0.49
1:X:67:G:N2	1:X:73:A:C4	2.81	0.49
1:X:705:C:H4'	3:A:42:GLY:O	2.13	0.49
6:D:123:ASP:OD2	6:D:127:ASN:HB2	2.13	0.49
10:H:64:VAL:C	10:H:65:LYS:HD2	2.33	0.49
13:K:106:ASP:OD1	13:K:108:VAL:HG23	2.12	0.49
17:O:34:GLU:HB2	17:O:56:VAL:HG23	1.93	0.49
19:Q:35:LYS:HG2	19:Q:35:LYS:O	2.13	0.49
1:X:2404:A:H4'	1:X:2405:A:OP2	2.11	0.49
1:X:2553:G:C2	1:X:2554:C:O2	2.66	0.49
1:X:2583:U:O2'	1:X:2584:U:H5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2797:G:H2'	1:X:2798:A:H5''	1.93	0.49
1:X:502:A:H2'	1:X:503:G:O4'	2.12	0.49
1:X:725:C:H2'	1:X:726:G:C8	2.47	0.49
1:X:693:A:C4	1:X:811:G:N2	2.81	0.49
1:X:945:G:H2'	1:X:946:U:H6	1.76	0.49
2:Y:73:C:H2'	2:Y:74:A:O4'	2.12	0.49
29:3:13:ARG:CD	29:3:25:PHE:HD1	2.25	0.49
29:3:62:LEU:HB3	29:3:63:PRO:HD3	1.95	0.49
4:B:4:ILE:HG12	4:B:5:LEU:H	1.78	0.49
1:X:2291:U:P	6:D:71:LYS:HD2	2.53	0.49
17:O:67:LYS:HD2	17:O:68:LYS:N	2.27	0.49
1:X:1096:A:H1'	1:X:1097:A:O5'	2.13	0.49
1:X:1770:U:C5	1:X:1775:A:N7	2.81	0.49
1:X:2407:G:H21	11:I:59:ARG:HH22	1.61	0.49
1:X:485:G:C6	1:X:520:C:N4	2.81	0.49
3:A:222:GLN:OE1	3:A:222:GLN:HA	2.13	0.49
4:B:188:ILE:HG23	4:B:189:PRO:CD	2.43	0.49
4:B:183:LEU:HD21	15:M:16:ILE:HD13	1.95	0.49
15:M:16:ILE:HG22	15:M:16:ILE:O	2.13	0.49
18:P:24:GLY:O	18:P:127:ILE:HA	2.13	0.49
1:X:1398:G:H4'	1:X:1398:G:OP1	2.13	0.49
1:X:1811:A:H4'	1:X:1812:U:C5'	2.42	0.49
1:X:36:G:N2	1:X:457:C:C2	2.81	0.49
1:X:648:A:H4'	1:X:649:G:H5'	1.94	0.49
1:X:596:C:H5'	5:C:84:PHE:HE1	1.78	0.48
11:I:73:GLU:OE1	11:I:73:GLU:N	2.46	0.48
1:X:1052:C:H42	1:X:1125:G:H1	1.58	0.48
1:X:1226:A:C8	1:X:1250:A:C2	3.01	0.48
1:X:1429:A:O2'	1:X:1430:G:H4'	2.13	0.48
1:X:1836:C:H42	1:X:1879:G:H1	1.61	0.48
1:X:2629:U:H2'	1:X:2630:C:C6	2.48	0.48
1:X:346:C:C6	1:X:347:C:H5	2.30	0.48
4:B:116:VAL:H	4:B:136:ARG:NE	2.12	0.48
5:C:102:LEU:HD21	5:C:106:MET:HE3	1.95	0.48
5:C:2:ALA:N	5:C:12:GLY:O	2.46	0.48
1:X:2654:A:H5'	10:H:41:ASN:HB2	1.95	0.48
10:H:19:ILE:HG22	10:H:55:VAL:HA	1.95	0.48
12:J:110:VAL:HB	12:J:114:GLN:HB2	1.94	0.48
19:Q:38:ILE:O	19:Q:42:ILE:HG22	2.13	0.48
19:Q:68:PHE:O	19:Q:69:ILE:C	2.51	0.48
24:V:2:LYS:HG3	24:V:3:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:5:LEU:HA	25:W:51:LEU:HD23	1.94	0.48
1:X:1003:C:O3'	17:O:71:ILE:HD13	2.13	0.48
1:X:1032:A:C2	1:X:1034:U:C2	3.01	0.48
1:X:1054:C:H42	1:X:1123:G:H1	1.61	0.48
1:X:1629:G:C6	1:X:1633:C:C6	3.01	0.48
1:X:1685:A:C5	1:X:1691:G:C5	3.01	0.48
1:X:178:C:H2'	1:X:179:U:H6	1.78	0.48
1:X:1911:A:H2'	1:X:1912:G:O4'	2.12	0.48
1:X:224:G:H4'	1:X:399:G:C4	2.48	0.48
1:X:2387:U:H2'	1:X:2388:G:H8	1.78	0.48
1:X:2622:G:H2'	1:X:2623:A:O4'	2.13	0.48
1:X:2665:G:C5	1:X:2666:U:C4	3.01	0.48
1:X:2796:A:C2	1:X:2797:G:C4	3.01	0.48
1:X:781:G:H2'	1:X:782:U:C6	2.48	0.48
1:X:874:A:H2'	1:X:875:G:O4'	2.13	0.48
27:1:38:LYS:HD3	27:1:40:TYR:HE1	1.78	0.48
4:B:115:GLY:O	4:B:119:ARG:HB2	2.12	0.48
4:B:49:ILE:HG21	4:B:81:PHE:CE2	2.45	0.48
4:B:88:GLY:O	4:B:89:ASP:OD1	2.31	0.48
5:C:47:THR:HG23	5:C:85:GLY:H	1.78	0.48
1:X:1992:G:H1'	13:K:106:ASP:O	2.12	0.48
16:N:20:ARG:HH12	17:O:83:ARG:NH2	2.11	0.48
20:R:11:ASN:ND2	20:R:11:ASN:O	2.36	0.48
1:X:1128:G:C2'	1:X:1129:A:H5''	2.42	0.48
1:X:1656:U:O2'	1:X:1657:A:H5''	2.12	0.48
1:X:1851:A:H2'	1:X:1852:G:O4'	2.12	0.48
1:X:2695:C:O2'	1:X:2696:A:H5'	2.13	0.48
1:X:73:A:H3'	1:X:74:G:C5'	2.42	0.48
1:X:692:C:N4	1:X:811:G:H1	2.10	0.48
1:X:860:U:C2'	1:X:860:U:O2	2.61	0.48
1:X:1796:A:H1'	3:A:51:THR:HG23	1.94	0.48
11:I:86:THR:OG1	11:I:118:VAL:HG12	2.12	0.48
14:L:31:VAL:CG2	14:L:33:ARG:HG3	2.44	0.48
10:H:113:PRO:HD3	15:M:73:PHE:HB2	1.95	0.48
18:P:25:PHE:CD2	18:P:25:PHE:C	2.87	0.48
18:P:91:PHE:CD1	18:P:129:ALA:O	2.66	0.48
19:Q:62:ARG:O	19:Q:70:GLY:CA	2.61	0.48
1:X:1008:G:C2	1:X:1170:U:O2	2.66	0.48
1:X:1118:G:C2'	1:X:1119:U:H5'	2.44	0.48
1:X:1631:C:H5	1:X:1633:C:C6	2.31	0.48
1:X:2299:A:H4'	1:X:2300:G:C2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2237:C:C4	1:X:2405:A:H5'	2.48	0.48
1:X:465:C:O2	1:X:467:U:H6	1.96	0.48
1:X:795:A:C2	3:A:227:MET:HG2	2.49	0.48
3:A:109:PRO:HB3	3:A:144:HIS:HE1	1.78	0.48
3:A:244:GLY:C	3:A:245:ARG:NE	2.67	0.48
4:B:116:VAL:N	4:B:136:ARG:HE	2.11	0.48
4:B:44:TYR:HB2	4:B:82:ARG:HH12	1.79	0.48
19:Q:63:LYS:HD3	19:Q:69:ILE:CA	2.43	0.48
1:X:1968:G:H2'	1:X:1969:G:C8	2.45	0.48
1:X:1980:A:C2	1:X:1981:A:C5	3.01	0.48
1:X:2064:U:H5'	23:U:41:VAL:HG21	1.96	0.48
1:X:2527:G:C6	1:X:2540:A:N1	2.82	0.48
1:X:2757:G:H5''	1:X:2758:A:C5'	2.33	0.48
1:X:2762:G:N2	1:X:2763:U:C2	2.82	0.48
1:X:2800:C:C5	1:X:2801:A:C8	3.01	0.48
31:X:2881:LMA:C54	31:X:2881:LMA:C34	2.91	0.48
1:X:573:C:H2'	1:X:574:C:C6	2.49	0.48
1:X:746:G:H3'	1:X:774:A:H61	1.78	0.48
1:X:76:C:O4'	24:V:55:THR:HG21	2.13	0.48
1:X:819:C:H2'	1:X:820:U:H6	1.77	0.48
3:A:201:GLU:HG3	3:A:203:LYS:H	1.78	0.48
4:B:105:THR:CG2	4:B:197:VAL:HB	2.44	0.48
1:X:334:G:H2'	5:C:162:ARG:CD	2.44	0.48
11:I:31:GLY:C	11:I:32:ARG:HG3	2.33	0.48
23:U:32:ARG:CZ	23:U:32:ARG:H	2.27	0.48
1:X:1033:G:C6	1:X:1151:U:C5	3.01	0.48
1:X:1357:U:H4'	1:X:1397:A:N6	2.27	0.48
1:X:1674:C:H2'	1:X:1674:C:O2	2.14	0.48
1:X:304:A:H62	1:X:356:A:N6	2.11	0.48
1:X:538:A:N6	1:X:2025:A:H2'	2.28	0.48
1:X:75:C:H2'	1:X:76:C:H5'	1.94	0.48
1:X:778:G:H2'	1:X:779:U:C6	2.48	0.48
26:Z:58:LEU:H	26:Z:58:LEU:CD1	2.24	0.48
27:1:34:LYS:HE3	27:1:34:LYS:CA	2.37	0.48
27:1:39:LYS:HD3	27:1:39:LYS:C	2.33	0.48
27:1:9:ILE:HD12	27:1:26:LYS:HD2	1.94	0.48
1:X:2796:A:H5''	4:B:162:MET:HE1	1.95	0.48
9:G:49:VAL:HG21	9:G:170:PRO:HG2	1.95	0.48
12:J:39:GLU:HB3	12:J:128:ILE:CG2	2.43	0.48
1:X:1560:A:C2'	1:X:1561:A:H5'	2.44	0.48
1:X:1762:C:C2	1:X:1763:G:C8	3.00	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1782:A:O3'	3:A:206:VAL:O	2.31	0.48
1:X:1813:A:OP1	3:A:160:ALA:HB3	2.14	0.48
1:X:1871:G:N3	1:X:1871:G:H3'	2.28	0.48
1:X:2426:G:C8	1:X:2479:U:C6	3.02	0.48
1:X:2812:A:H2'	1:X:2813:G:C8	2.49	0.48
1:X:476:G:H4'	28:2:16:HIS:CG	2.48	0.48
2:Y:65:A:H2'	2:Y:66:G:C8	2.48	0.48
28:2:40:HIS:O	28:2:41:GLN:CD	2.52	0.48
6:D:103:LEU:HD12	6:D:107:GLY:HA3	1.95	0.48
6:D:79:LEU:HD12	6:D:79:LEU:N	2.29	0.48
7:E:117:PRO:HD3	7:E:123:PHE:CE1	2.49	0.48
17:O:36:LYS:HZ1	17:O:54:TYR:HB3	1.78	0.48
19:Q:19:ALA:O	19:Q:24:VAL:HB	2.13	0.48
1:X:1283:C:H5'	1:X:1284:G:C5'	2.44	0.48
1:X:1469:U:H5	13:K:64:ARG:NH2	2.10	0.48
1:X:1836:C:C2	1:X:1880:G:N2	2.82	0.48
1:X:1774:A:N1	1:X:2566:A:H2'	2.29	0.48
1:X:321:A:O2'	1:X:322:A:H2'	2.14	0.48
28:2:40:HIS:O	28:2:41:GLN:OE1	2.31	0.48
4:B:60:ASN:O	4:B:64:GLN:HG3	2.13	0.48
9:G:56:THR:N	9:G:134:MET:HE1	2.28	0.48
13:K:84:ALA:N	13:K:85:PRO:HD2	2.29	0.48
15:M:60:SER:HA	15:M:64:LYS:HB2	1.95	0.48
18:P:60:ILE:HA	18:P:61:PRO:HD3	1.63	0.48
20:R:22:VAL:HG12	20:R:23:ILE:N	2.28	0.48
20:R:23:ILE:HD12	20:R:23:ILE:C	2.34	0.48
1:X:1482:U:H2'	1:X:1483:G:H8	1.78	0.48
1:X:2329:C:H2'	1:X:2330:G:O4'	2.14	0.48
1:X:2690:A:OP1	1:X:2692:A:OP2	2.31	0.48
1:X:2795:A:H1'	13:K:5:LYS:NZ	2.29	0.48
1:X:412:U:H2'	1:X:413:G:O4'	2.13	0.48
1:X:477:A:H4'	28:2:30:ILE:HD13	1.95	0.48
1:X:596:C:H5'	5:C:84:PHE:CE1	2.49	0.48
1:X:2265:A:H61	27:1:25:THR:HG21	1.79	0.48
27:1:41:ASP:HB2	27:1:46:LYS:HA	1.96	0.48
1:X:814:G:OP1	5:C:50:GLN:OE1	2.32	0.48
7:E:107:ILE:HD11	7:E:151:VAL:CG1	2.44	0.48
14:L:33:ARG:HH21	14:L:38:ILE:HG21	1.78	0.48
15:M:103:LYS:HG3	15:M:105:TYR:CZ	2.48	0.48
1:X:34:U:H1'	20:R:4:PRO:HA	1.96	0.48
21:S:104:SER:HA	21:S:139:THR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:23:LYS:HA	23:U:36:GLY:O	2.14	0.48
1:X:1175:A:C2	1:X:1176:U:C2	3.02	0.48
1:X:1229:C:H2'	1:X:1230:C:H6	1.79	0.48
1:X:1779:C:H2'	1:X:1780:A:H8	1.79	0.48
1:X:2192:U:C4	1:X:2193:C:C4	3.02	0.48
1:X:2552:C:H5''	1:X:2553:G:H5''	1.96	0.48
2:Y:50:U:H2'	2:Y:51:G:H8	1.78	0.48
27:1:40:TYR:H	27:1:50:PHE:HB3	1.79	0.47
27:1:45:LYS:O	27:1:46:LYS:HB2	2.13	0.47
1:X:1810:U:O4	3:A:155:GLN:HG2	2.14	0.47
3:A:44:ARG:HH21	3:A:56:GLY:HA2	1.79	0.47
4:B:136:ARG:CG	4:B:137:ARG:N	2.75	0.47
5:C:158:ARG:O	5:C:160:ALA:N	2.47	0.47
5:C:107:ALA:HB1	5:C:180:ILE:HD13	1.96	0.47
7:E:139:GLN:O	7:E:143:GLN:HG3	2.14	0.47
1:X:538:A:H5''	9:G:142:ARG:NH1	2.29	0.47
11:I:32:ARG:HD2	11:I:32:ARG:O	2.14	0.47
15:M:19:ASP:C	15:M:20:HIS:ND1	2.68	0.47
16:N:7:GLY:O	16:N:8:ILE:HG12	2.14	0.47
16:N:88:ILE:HA	17:O:49:GLU:HG3	1.96	0.47
1:X:1223:G:C6	1:X:1250:A:N7	2.82	0.47
1:X:1441:A:H1'	1:X:1442:C:OP2	2.14	0.47
1:X:2273:C:H2'	1:X:2274:C:C6	2.49	0.47
1:X:2821:G:H2'	1:X:2822:U:C6	2.48	0.47
1:X:224:G:H4'	1:X:399:G:C5	2.49	0.47
1:X:815:A:C6	1:X:816:U:C4	3.01	0.47
1:X:1142:G:C2	9:G:103:TYR:HD2	2.31	0.47
22:T:65:GLY:HA3	22:T:81:ILE:CG2	2.44	0.47
1:X:161:U:H4'	1:X:194:G:N2	2.26	0.47
1:X:2285:U:C2	6:D:150:ARG:NH2	2.82	0.47
1:X:2401:A:N3	1:X:2403:C:C4	2.82	0.47
1:X:2639:A:H2'	1:X:2640:G:O4'	2.13	0.47
1:X:2860:C:H2'	1:X:2861:A:O4'	2.14	0.47
1:X:308:C:H4'	20:R:95:ARG:CZ	2.44	0.47
1:X:640:C:H4'	1:X:660:G:N3	2.29	0.47
2:Y:16:U:H4'	2:Y:72:C:O2	2.14	0.47
1:X:1781:C:H1'	3:A:210:ALA:HB2	1.95	0.47
5:C:102:LEU:HD21	5:C:106:MET:HE1	1.96	0.47
7:E:137:ASP:OD2	7:E:140:LEU:HG	2.13	0.47
9:G:132:PHE:CE2	9:G:145:HIS:HB2	2.48	0.47
12:J:133:VAL:HG12	21:S:76:ARG:HE	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:30:GLY:O	17:O:32:LYS:HG2	2.15	0.47
20:R:106:VAL:HG23	20:R:113:THR:HG21	1.96	0.47
22:T:43:THR:HG22	22:T:46:LYS:HE2	1.96	0.47
1:X:1025:A:H2	1:X:1160:C:C2	2.32	0.47
1:X:1326:U:H4'	1:X:1345:G:H4'	1.97	0.47
1:X:1979:C:O2	1:X:1980:A:H1'	2.15	0.47
1:X:2324:G:C2	1:X:2360:C:H2'	2.48	0.47
1:X:983:G:O2'	1:X:984:A:OP1	2.32	0.47
10:H:115:ALA:HB3	10:H:118:LEU:HD13	1.96	0.47
10:H:62:GLY:O	10:H:65:LYS:NZ	2.43	0.47
15:M:34:ARG:HH11	15:M:88:VAL:HG21	1.77	0.47
18:P:107:ILE:HG21	18:P:117:ILE:HG12	1.96	0.47
1:X:1074:G:H4'	8:F:134:MET:HG3	1.97	0.47
1:X:1755:G:C6	1:X:1972:G:C2	3.01	0.47
1:X:2053:G:C2	1:X:2054:A:C4	3.01	0.47
1:X:2237:C:O2'	1:X:2406:C:OP2	2.18	0.47
1:X:2825:A:N7	1:X:2843:A:O2'	2.32	0.47
1:X:521:U:C5	1:X:522:G:C2	3.03	0.47
10:H:41:ASN:HB2	10:H:42:LYS:H	1.53	0.47
23:U:22:GLY:HA3	23:U:39:LYS:CG	2.44	0.47
1:X:1482:U:H2'	1:X:1483:G:C8	2.49	0.47
1:X:977:G:O4'	1:X:2246:A:N6	2.48	0.47
1:X:467:U:HO2'	1:X:468:A:P	2.37	0.47
1:X:888:G:N2	1:X:915:C:C2	2.82	0.47
1:X:1780:A:H5''	3:A:222:GLN:OE1	2.15	0.47
3:A:45:ASN:CB	3:A:50:ILE:HA	2.39	0.47
4:B:97:ALA:HB3	4:B:100:GLU:HG3	1.96	0.47
10:H:115:ALA:HB3	10:H:118:LEU:CD1	2.45	0.47
1:X:2541:U:O2'	10:H:23:ARG:NH1	2.47	0.47
13:K:21:ALA:HB1	13:K:47:PHE:CD2	2.50	0.47
13:K:56:LYS:HG2	13:K:56:LYS:O	2.15	0.47
17:O:36:LYS:HE3	17:O:55:THR:CA	2.44	0.47
17:O:10:LYS:HD2	17:O:37:ALA:CB	2.45	0.47
20:R:23:ILE:HD11	20:R:81:VAL:HB	1.97	0.47
1:X:1802:A:H2'	1:X:1803:G:O4'	2.15	0.47
1:X:1813:A:H2'	1:X:1814:G:H8	1.78	0.47
1:X:1830:C:H42	1:X:1881:U:H3'	1.78	0.47
1:X:193:A:C4	1:X:445:A:C2	3.03	0.47
1:X:2673:G:C4	1:X:2674:C:C5	3.03	0.47
1:X:525:A:H2'	1:X:526:C:H5'	1.96	0.47
1:X:55:A:C2	1:X:113:C:O2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:694:G:H2'	1:X:695:G:O4'	2.15	0.47
1:X:1791:C:OP1	3:A:264:ARG:HG3	2.14	0.47
9:G:122:HIS:HB3	9:G:125:ARG:HG2	1.96	0.47
14:L:26:ARG:HD3	14:L:86:GLN:HB3	1.96	0.47
14:L:31:VAL:HG11	14:L:89:PHE:HE2	1.80	0.47
1:X:1087:C:OP1	8:F:90:THR:HG22	2.14	0.47
1:X:2171:U:H4'	1:X:2171:U:OP1	2.13	0.47
1:X:2199:C:H2'	1:X:2200:G:H5'	1.96	0.47
1:X:2237:C:C3'	1:X:2238:G:H5'	2.44	0.47
1:X:2264:C:H42	1:X:2362:G:H1	1.63	0.47
1:X:2769:C:H2'	1:X:2770:A:C8	2.49	0.47
1:X:305:A:N1	1:X:356:A:C2	2.83	0.47
1:X:573:C:H2'	1:X:574:C:O4'	2.14	0.47
1:X:819:C:C2	1:X:820:U:C5	3.01	0.47
26:Z:16:ARG:NH1	26:Z:17:ASP:OD1	2.47	0.47
3:A:162:THR:OG1	3:A:197:VAL:HG22	2.15	0.47
3:A:247:PRO:C	3:A:249:THR:N	2.68	0.47
7:E:98:LEU:HD12	7:E:102:ALA:O	2.15	0.47
11:I:29:THR:O	11:I:30:ALA:CB	2.63	0.47
12:J:137:VAL:CG1	12:J:139:ASP:OD2	2.63	0.47
18:P:29:LYS:HB3	18:P:30:TYR:CD2	2.50	0.47
20:R:10:HIS:ND1	20:R:10:HIS:N	2.63	0.47
1:X:1919:A:H2	1:X:1925:C:H42	1.62	0.47
1:X:1974:U:O2'	1:X:1975:G:H5''	2.14	0.47
1:X:19:C:O2	1:X:532:A:C2	2.68	0.47
1:X:2327:U:O4	1:X:2361:G:N2	2.47	0.47
1:X:2387:U:H2'	1:X:2388:G:C8	2.48	0.47
1:X:2675:U:H2'	1:X:2676:G:H8	1.79	0.47
1:X:668:A:C2'	1:X:669:G:O4'	2.62	0.47
3:A:150:PRO:HD3	3:A:187:HIS:NE2	2.29	0.47
4:B:84:PHE:CD2	4:B:86:PRO:HD3	2.50	0.47
12:J:44:LYS:HB2	12:J:47:GLN:HG3	1.96	0.47
13:K:20:LEU:O	13:K:22:ARG:N	2.48	0.47
14:L:100:VAL:HG13	14:L:101:LYS:N	2.29	0.47
14:L:91:ARG:HB2	14:L:94:TYR:HD1	1.79	0.47
16:N:14:HIS:HD2	16:N:32:TYR:CE1	2.33	0.47
18:P:66:GLU:O	18:P:69:ALA:HB3	2.15	0.47
20:R:81:VAL:HG11	20:R:89:GLY:HA2	1.97	0.47
21:S:1:MET:H1	21:S:52:PHE:HE2	1.63	0.47
2:Y:94:G:H5''	21:S:74:ARG:HH12	1.78	0.47
1:X:537:C:C5	1:X:2759:U:H2'	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:555:U:O2'	1:X:1234:C:H5'	2.14	0.47
2:Y:58:G:C4'	2:Y:59:A:H8	2.28	0.47
2:Y:7:C:H2'	2:Y:8:C:H6	1.80	0.47
18:P:59:PHE:CD1	26:Z:30:LEU:CD1	2.97	0.47
4:B:67:PHE:CE1	4:B:75:THR:HG22	2.50	0.47
5:C:22:VAL:HG21	5:C:110:SER:HA	1.97	0.47
7:E:103:LEU:HD12	7:E:104:GLU:N	2.30	0.47
10:H:70:VAL:HG13	10:H:70:VAL:O	2.15	0.47
11:I:14:LYS:O	11:I:14:LYS:HG3	2.15	0.47
11:I:55:ARG:O	11:I:56:LEU:HB2	2.15	0.47
1:X:2407:G:H21	11:I:59:ARG:HH12	1.61	0.47
12:J:76:THR:HA	12:J:89:GLY:O	2.15	0.47
14:L:31:VAL:HG11	14:L:89:PHE:CE2	2.50	0.47
15:M:34:ARG:HH21	15:M:91:VAL:CG2	2.23	0.47
16:N:22:LYS:C	16:N:24:PHE:H	2.19	0.47
1:X:1025:A:C2	1:X:1160:C:C2	3.03	0.47
1:X:1438:G:H2'	1:X:1439:G:H5'	1.97	0.47
1:X:1496:G:H1'	1:X:1497:C:O5'	2.14	0.47
1:X:1725:C:C2	1:X:1742:G:N2	2.83	0.47
1:X:1978:U:H3'	1:X:1979:C:H5''	1.97	0.47
1:X:2705:A:H62	1:X:2707:G:N2	2.13	0.47
1:X:2793:G:O2'	1:X:2794:G:H5'	2.14	0.47
1:X:591:G:C2'	1:X:592:G:H8	2.21	0.47
1:X:647:G:O2'	1:X:649:G:H4'	2.14	0.47
1:X:2505:G:H1'	30:4:1:MET:HB3	1.97	0.47
3:A:118:VAL:HG13	3:A:129:GLY:O	2.15	0.47
7:E:149:ARG:HA	7:E:162:VAL:HB	1.97	0.47
9:G:132:PHE:HB2	9:G:145:HIS:NE2	2.30	0.47
16:N:7:GLY:O	16:N:8:ILE:CG1	2.63	0.47
17:O:19:VAL:CG1	17:O:90:PHE:CD1	2.98	0.47
21:S:71:MET:SD	21:S:71:MET:N	2.88	0.47
1:X:393:U:O2'	23:U:18:VAL:HB	2.15	0.47
1:X:115:G:C6	1:X:117:A:C6	3.03	0.47
1:X:1811:A:C4'	1:X:1812:U:O5'	2.58	0.47
1:X:1950:C:N4	1:X:1951:G:C6	2.83	0.47
1:X:2026:C:N3	1:X:2757:G:N2	2.63	0.47
1:X:2055:G:O2'	1:X:2056:C:H5'	2.15	0.47
1:X:2494:C:O2	1:X:2549:G:C2	2.68	0.47
1:X:2560:G:N2	1:X:2560:G:OP2	2.47	0.47
1:X:31:C:O2'	1:X:32:C:H5'	2.15	0.47
1:X:461:A:C5	1:X:462:G:C5	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:492:G:O2'	1:X:516:G:N2	2.48	0.47
1:X:695:G:H5''	28:2:26:SER:CB	2.44	0.46
1:X:2256:G:P	12:J:86:LYS:HD2	2.55	0.46
16:N:86:ALA:C	16:N:88:ILE:N	2.69	0.46
1:X:165:G:H1	1:X:185:C:N4	2.04	0.46
1:X:1950:C:C4	1:X:1951:G:C5	3.03	0.46
1:X:2659:C:H2'	1:X:2660:C:C6	2.50	0.46
1:X:306:G:H22	1:X:355:G:H1'	1.78	0.46
1:X:514:G:H2'	1:X:514:G:N3	2.30	0.46
1:X:538:A:O4'	1:X:539:A:OP1	2.33	0.46
1:X:618:A:C2	1:X:632:A:N7	2.82	0.46
1:X:638:A:N7	11:I:74:VAL:HG11	2.31	0.46
1:X:760:U:C4	26:Z:3:LYS:HG3	2.50	0.46
13:K:98:LEU:CD2	26:Z:56:GLN:HG2	2.41	0.46
29:3:31:HIS:O	29:3:32:GLN:O	2.33	0.46
1:X:1790:G:C5	3:A:178:LEU:HD13	2.50	0.46
5:C:163:ASN:HD22	5:C:164:VAL:N	2.13	0.46
9:G:104:THR:H	9:G:107:GLN:HG3	1.79	0.46
10:H:100:ASN:OD1	10:H:100:ASN:C	2.54	0.46
13:K:84:ALA:N	13:K:85:PRO:CD	2.78	0.46
19:Q:25:TYR:HE2	19:Q:82:LEU:HD12	1.80	0.46
20:R:84:VAL:HA	20:R:90:LYS:HE2	1.97	0.46
1:X:1730:G:C2	1:X:1737:G:C2	3.02	0.46
1:X:2282:G:C2	1:X:2293:G:N2	2.82	0.46
1:X:654:A:N6	1:X:2348:A:O2'	2.48	0.46
1:X:2379:G:C2	1:X:2380:U:O2	2.68	0.46
1:X:2447:G:C8	1:X:2455:A:C2	3.03	0.46
31:X:2881:LMA:O55	31:X:2881:LMA:C34	2.64	0.46
1:X:797:A:H5''	3:A:228:ASN:OD1	2.15	0.46
4:B:84:PHE:CZ	4:B:86:PRO:HG2	2.51	0.46
5:C:179:ASP:O	5:C:182:ARG:HB3	2.16	0.46
10:H:7:ARG:C	10:H:8:LEU:HD23	2.36	0.46
11:I:102:LYS:O	11:I:103:ASN:HB3	2.15	0.46
12:J:40:PRO:HB3	12:J:99:LYS:CE	2.46	0.46
15:M:60:SER:CA	15:M:64:LYS:HB2	2.45	0.46
16:N:81:ASN:HD22	16:N:117:ARG:NH2	2.14	0.46
22:T:43:THR:CG2	22:T:46:LYS:HG2	2.45	0.46
1:X:1312:G:H5''	1:X:1313:U:OP1	2.15	0.46
1:X:48:A:N6	1:X:154:U:C5	2.81	0.46
1:X:2240:C:C4	1:X:2259:G:N1	2.84	0.46
1:X:45:C:N4	1:X:191:G:OP2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:491:A:H3'	1:X:492:G:H5''	1.97	0.46
1:X:591:G:H1	1:X:1271:C:N4	2.13	0.46
2:Y:89:G:C6	2:Y:93:G:C6	3.03	0.46
7:E:157:TYR:O	7:E:171:LEU:HD23	2.15	0.46
9:G:141:GLY:O	9:G:144:MET:HB2	2.15	0.46
10:H:22:ILE:HB	10:H:52:VAL:HG12	1.97	0.46
10:H:47:VAL:HG22	10:H:77:THR:HG23	1.97	0.46
11:I:51:GLY:HA3	29:3:59:LYS:NZ	2.30	0.46
1:X:2371:A:O2'	11:I:59:ARG:O	2.23	0.46
13:K:79:VAL:HA	13:K:83:VAL:CG2	2.45	0.46
16:N:13:ARG:O	16:N:17:VAL:HG23	2.16	0.46
17:O:22:VAL:HA	17:O:91:THR:HG22	1.96	0.46
25:W:12:ARG:HG2	25:W:12:ARG:HH11	1.81	0.46
1:X:1514:C:H4'	1:X:1592:U:O2'	2.15	0.46
1:X:42:G:H2'	1:X:43:A:O4'	2.16	0.46
1:X:476:G:H4'	28:2:16:HIS:ND1	2.31	0.46
1:X:633:G:H2'	1:X:634:G:H8	1.79	0.46
1:X:170:U:H5''	1:X:816:U:H1'	1.97	0.46
28:2:15:THR:O	28:2:16:HIS:CB	2.61	0.46
3:A:135:ARG:HB3	3:A:188:SER:HB2	1.97	0.46
3:A:246:VAL:HG12	3:A:251:TRP:H	1.80	0.46
5:C:45:THR:HB	5:C:86:PRO:HG2	1.98	0.46
9:G:61:ARG:HE	9:G:65:LYS:HD2	1.78	0.46
1:X:1835:C:H5'	3:A:256:LYS:HE2	1.98	0.46
1:X:1840:A:H2'	1:X:1841:G:O4'	2.15	0.46
1:X:1981:A:H4'	1:X:2704:U:O2'	2.15	0.46
1:X:2522:G:H2'	1:X:2523:G:C8	2.50	0.46
1:X:2664:G:N2	1:X:2665:G:C1'	2.78	0.46
1:X:2819:G:H2'	1:X:2820:C:H6	1.79	0.46
1:X:303:C:H2'	1:X:304:A:H5''	1.98	0.46
1:X:317:U:C3'	1:X:318:G:H5'	2.46	0.46
1:X:518:A:C6	18:P:30:TYR:CE1	3.04	0.46
1:X:518:A:N6	18:P:30:TYR:CE1	2.83	0.46
1:X:742:G:N7	3:A:210:ALA:O	2.49	0.46
1:X:832:A:C4	1:X:1203:A:C2	3.04	0.46
1:X:82:G:N2	1:X:83:A:N6	2.60	0.46
3:A:80:VAL:HB	3:A:115:GLY:N	2.21	0.46
4:B:120:TRP:O	4:B:121:ASN:HB2	2.15	0.46
4:B:61:LYS:HB3	4:B:62:PRO:HD3	1.97	0.46
4:B:44:TYR:HD1	4:B:82:ARG:NH1	2.14	0.46
7:E:103:LEU:HD12	7:E:104:GLU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:132:PHE:CD2	9:G:145:HIS:HB2	2.51	0.46
15:M:55:ILE:HG22	15:M:104:LEU:HB2	1.98	0.46
1:X:2726:U:O5'	1:X:2726:U:H6	1.98	0.46
3:A:33:ALA:O	3:A:34:LEU:HB3	2.15	0.46
1:X:1672:A:O4'	4:B:113:THR:HG22	2.16	0.46
4:B:31:CYS:HB3	4:B:49:ILE:HG12	1.97	0.46
5:C:58:MET:HG2	5:C:59:TYR:N	2.31	0.46
10:H:2:ILE:HD12	10:H:2:ILE:HG23	1.69	0.46
10:H:7:ARG:O	10:H:8:LEU:HD23	2.16	0.46
15:M:24:LEU:HD11	15:M:34:ARG:HH22	1.81	0.46
15:M:6:LYS:HD2	15:M:6:LYS:N	2.31	0.46
15:M:82:PRO:O	15:M:84:ALA:N	2.48	0.46
18:P:37:LYS:HE2	18:P:64:ALA:H	1.80	0.46
1:X:1050:G:C2'	1:X:1051:U:H5'	2.45	0.46
1:X:1347:C:O2'	1:X:1348:C:H5'	2.16	0.46
1:X:1467:U:C3'	1:X:1467:U:C6	2.99	0.46
1:X:1469:U:H5'	1:X:1470:G:P	2.55	0.46
1:X:1496:G:H4'	1:X:1497:C:OP1	2.15	0.46
1:X:178:C:H2'	1:X:179:U:C6	2.50	0.46
1:X:2327:U:H5'	27:1:21:TYR:CE1	2.50	0.46
1:X:2445:C:H2'	1:X:2446:C:C6	2.51	0.46
1:X:2677:U:H2'	1:X:2678:C:C6	2.51	0.46
1:X:2704:U:C2'	1:X:2705:A:C2	2.98	0.46
1:X:2026:C:C4	1:X:2757:G:N3	2.83	0.46
1:X:568:G:H2'	1:X:569:C:O4'	2.15	0.46
1:X:640:C:H4'	1:X:660:G:H21	1.81	0.46
27:1:28:ARG:NH1	27:1:28:ARG:HB3	2.30	0.46
3:A:147:GLU:HB2	3:A:190:CYS:HB3	1.97	0.46
4:B:4:ILE:HD11	4:B:90:SER:O	2.16	0.46
1:X:1270:C:H4'	5:C:77:PHE:CD2	2.51	0.46
12:J:86:LYS:O	12:J:88:LYS:HG3	2.16	0.46
13:K:20:LEU:HA	13:K:20:LEU:HD12	1.70	0.46
14:L:82:LYS:HB2	14:L:84:ILE:CD1	2.45	0.46
1:X:1141:U:N3	1:X:2008:C:H5''	2.30	0.46
1:X:1326:U:H3'	1:X:1326:U:O2	2.16	0.46
1:X:1469:U:H5''	1:X:1470:G:C8	2.51	0.46
1:X:1444:C:N4	1:X:1579:G:H1	2.08	0.46
1:X:1628:C:H5'	28:2:7:PRO:CG	2.46	0.46
1:X:1641:C:H2'	1:X:1642:G:O4'	2.16	0.46
1:X:1712:G:C2'	1:X:1713:G:H5'	2.45	0.46
1:X:1790:G:C6	1:X:1811:A:N7	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1841:G:C2'	1:X:1842:G:H5'	2.46	0.46
1:X:1854:G:H1'	1:X:1864:G:N2	2.31	0.46
1:X:2082:C:H2'	1:X:2083:G:H5'	1.96	0.46
1:X:2442:C:H2'	1:X:2443:C:C6	2.51	0.46
1:X:2484:G:O2'	1:X:2485:U:C5'	2.61	0.46
1:X:2837:G:H2'	1:X:2838:U:C6	2.50	0.46
1:X:513:A:C5	1:X:516:G:C6	3.04	0.46
1:X:699:G:H4'	1:X:700:C:OP2	2.15	0.46
1:X:820:U:H2'	1:X:821:A:C8	2.51	0.46
3:A:118:VAL:HG22	3:A:129:GLY:HA3	1.97	0.46
4:B:16:LYS:HB3	4:B:21:ILE:HD11	1.97	0.46
9:G:84:ASN:O	9:G:85:ALA:HB3	2.16	0.46
10:H:116:ARG:CG	10:H:116:ARG:O	2.64	0.46
13:K:82:GLU:O	13:K:86:LYS:HG3	2.16	0.46
16:N:70:ARG:HH11	16:N:70:ARG:HG3	1.80	0.46
16:N:94:VAL:O	16:N:94:VAL:HG12	2.15	0.46
19:Q:34:THR:O	19:Q:38:ILE:HG22	2.16	0.46
19:Q:39:LYS:HA	19:Q:42:ILE:HG22	1.98	0.46
19:Q:58:VAL:HA	19:Q:59:PRO:HD2	1.61	0.46
1:X:1790:G:N2	3:A:156:LEU:HD23	2.31	0.46
1:X:1837:G:C2	1:X:1879:G:C2	3.04	0.46
1:X:1922:U:H3'	1:X:1923:U:H5''	1.98	0.46
1:X:2324:G:HO2'	1:X:2360:C:HO2'	1.46	0.46
1:X:2581:A:N3	1:X:2581:A:H5''	2.31	0.46
1:X:1061:A:C2	1:X:2731:G:N1	2.84	0.46
1:X:2736:U:OP2	30:4:17:VAL:HG11	2.16	0.46
1:X:531:G:H2'	1:X:532:A:C8	2.50	0.46
1:X:579:G:OP1	1:X:983:G:O3'	2.34	0.46
29:3:13:ARG:NH1	29:3:26:LYS:N	2.64	0.46
4:B:9:ILE:HD13	15:M:12:LEU:HD13	1.98	0.46
9:G:125:ARG:HD2	9:G:129:HIS:CE1	2.50	0.46
11:I:73:GLU:OE1	11:I:105:PRO:O	2.34	0.46
13:K:87:TYR:CE1	13:K:94:TYR:HB3	2.51	0.46
1:X:168:A:H2'	1:X:169:C:H6	1.73	0.46
1:X:1790:G:C6	3:A:178:LEU:HD13	2.50	0.46
1:X:1941:C:H2'	1:X:1942:G:H8	1.81	0.46
1:X:1947:G:O2'	1:X:1950:C:OP2	2.31	0.46
1:X:2014:A:C5	1:X:2477:C:H1'	2.51	0.46
1:X:219:G:N2	1:X:232:A:OP2	2.45	0.46
1:X:2495:G:C2'	1:X:2496:C:H5'	2.45	0.46
1:X:2707:G:C8	1:X:2708:U:C5	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2862:G:H1'	26:Z:29:ASN:HD21	1.81	0.46
1:X:321:A:P	20:R:27:GLY:H	2.40	0.46
1:X:314:G:C2	1:X:326:A:C2	3.04	0.46
1:X:242:A:N7	1:X:441:A:C6	2.84	0.46
1:X:193:A:N3	1:X:445:A:C2	2.84	0.46
1:X:689:A:C2	1:X:690:A:C8	3.04	0.46
26:Z:51:TYR:CE2	26:Z:55:ARG:HB2	2.51	0.46
27:1:18:THR:O	27:1:20:PHE:CE1	2.68	0.45
1:X:1790:G:H21	3:A:156:LEU:HD23	1.82	0.45
12:J:99:LYS:CD	12:J:100:PRO:HD2	2.45	0.45
15:M:9:ARG:HA	15:M:12:LEU:HD12	1.98	0.45
21:S:117:VAL:HG22	21:S:168:VAL:HA	1.98	0.45
1:X:177:U:H4'	23:U:40:ARG:HE	1.81	0.45
25:W:40:VAL:HA	25:W:43:MET:HG3	1.98	0.45
1:X:1289:A:C2	1:X:1290:A:C8	3.04	0.45
1:X:1573:G:O6	1:X:1574:A:N6	2.49	0.45
1:X:2048:C:O2'	1:X:2049:C:H5'	2.16	0.45
1:X:2477:C:H6	1:X:2477:C:H5'	1.81	0.45
1:X:2722:C:H2'	1:X:2723:C:C6	2.51	0.45
1:X:812:G:H3'	1:X:813:A:H2'	1.97	0.45
1:X:825:C:H2'	1:X:826:U:H6	1.81	0.45
2:Y:72:C:H42	2:Y:109:G:H1	1.63	0.45
11:I:56:LEU:HD13	29:3:52:LYS:HE3	1.98	0.45
29:3:59:LYS:O	29:3:60:LEU:HB2	2.16	0.45
3:A:244:GLY:O	3:A:245:ARG:NE	2.49	0.45
5:C:39:ARG:HH21	5:C:91:TYR:CB	2.29	0.45
6:D:135:GLN:CD	6:D:150:ARG:H	2.19	0.45
10:H:28:GLY:O	10:H:35:THR:N	2.31	0.45
16:N:30:LYS:HB3	16:N:30:LYS:HZ2	1.81	0.45
1:X:1166:A:C5'	16:N:55:ARG:HH11	2.27	0.45
1:X:1022:A:OP1	16:N:75:ASN:ND2	2.50	0.45
1:X:321:A:OP1	20:R:26:SER:HA	2.15	0.45
1:X:1086:C:H3'	1:X:1087:C:C5'	2.36	0.45
1:X:1226:A:N1	1:X:1250:A:H1'	2.31	0.45
1:X:1438:G:O2'	1:X:1439:G:H5'	2.16	0.45
1:X:1505:U:O2	1:X:1506:C:C5	2.68	0.45
1:X:1791:C:N4	1:X:1810:U:O2'	2.49	0.45
1:X:2245:A:H4'	1:X:2246:A:C4	2.50	0.45
1:X:2444:C:O2'	1:X:2445:C:H5'	2.16	0.45
1:X:2685:A:C2	1:X:2686:C:H1'	2.51	0.45
1:X:333:A:C5	1:X:351:A:C2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:696:U:O5'	1:X:696:U:H6	1.99	0.45
1:X:883:A:H1'	12:J:11:ARG:HH21	1.80	0.45
1:X:15:G:O2'	26:Z:18:MET:HA	2.15	0.45
1:X:15:G:C4'	26:Z:21:SER:HB2	2.45	0.45
26:Z:6:VAL:HG13	26:Z:7:PRO:CD	2.43	0.45
3:A:90:SER:O	3:A:199:ASN:OD1	2.34	0.45
1:X:2218:G:O4'	3:A:250:PRO:HG3	2.15	0.45
4:B:116:VAL:H	4:B:136:ARG:HE	1.65	0.45
10:H:29:ILE:HB	10:H:34:LEU:HD23	1.97	0.45
11:I:35:LYS:O	11:I:36:GLY:O	2.34	0.45
12:J:26:ASP:HB3	12:J:27:TYR:H	1.61	0.45
13:K:35:GLN:HB3	13:K:112:LEU:HD23	1.98	0.45
14:L:37:HIS:CD2	14:L:39:TYR:CE1	3.05	0.45
14:L:42:ILE:HG22	14:L:53:ALA:N	2.31	0.45
9:G:70:PHE:CB	16:N:64:ARG:HG2	2.44	0.45
18:P:79:ALA:HA	18:P:83:ASP:HB2	1.99	0.45
24:V:14:PHE:O	24:V:18:ILE:HG13	2.16	0.45
25:W:18:LYS:O	25:W:21:GLN:HB3	2.16	0.45
1:X:1631:C:H5	1:X:1633:C:C4	2.34	0.45
1:X:1643:A:H1'	1:X:1657:A:C2	2.50	0.45
1:X:1978:U:H2'	1:X:1979:C:H6	1.80	0.45
1:X:484:G:N1	1:X:485:G:C5	2.83	0.45
1:X:493:A:OP2	1:X:517:A:N6	2.42	0.45
1:X:538:A:C2	1:X:2025:A:C6	3.04	0.45
1:X:2265:A:H3'	27:1:32:GLN:HB2	1.97	0.45
3:A:246:VAL:HG12	3:A:252:GLY:H	1.78	0.45
8:F:75:SER:O	8:F:79:ARG:HG3	2.16	0.45
9:G:117:GLU:C	9:G:119:LEU:N	2.69	0.45
9:G:84:ASN:C	9:G:86:ALA:H	2.20	0.45
11:I:56:LEU:HB3	29:3:52:LYS:HZ1	1.81	0.45
14:L:67:THR:O	14:L:71:VAL:HG12	2.16	0.45
15:M:22:ARG:NH1	15:M:24:LEU:HD21	2.31	0.45
16:N:50:ARG:O	16:N:54:LYS:HE2	2.16	0.45
19:Q:91:LEU:N	19:Q:91:LEU:HD22	2.31	0.45
24:V:7:ARG:HD2	24:V:7:ARG:C	2.37	0.45
1:X:1414:G:C6	1:X:1415:C:N3	2.85	0.45
1:X:1756:C:O2'	1:X:1757:C:H5'	2.16	0.45
1:X:2843:A:H2'	1:X:2844:G:O4'	2.15	0.45
1:X:635:C:O2'	1:X:670:U:OP1	2.30	0.45
4:B:116:VAL:CG1	4:B:136:ARG:HH21	2.29	0.45
1:X:883:A:C5'	12:J:10:PHE:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:61:LYS:HG2	19:Q:61:LYS:O	2.15	0.45
1:X:1200:G:H2'	1:X:1201:G:O4'	2.17	0.45
1:X:1514:C:O4'	1:X:1593:C:H4'	2.16	0.45
1:X:1834:G:N2	1:X:1884:A:C5	2.85	0.45
1:X:1941:C:H2'	1:X:1942:G:C8	2.51	0.45
1:X:2087:U:H3	1:X:2169:A:H2	1.65	0.45
1:X:2201:G:H2'	1:X:2202:G:C8	2.51	0.45
1:X:304:A:C5	1:X:359:G:N2	2.85	0.45
1:X:719:A:H2'	1:X:720:A:O4'	2.17	0.45
1:X:957:G:H2'	1:X:958:G:C8	2.51	0.45
1:X:2594:U:C6	26:Z:7:PRO:HA	2.52	0.45
1:X:1791:C:P	3:A:264:ARG:HG3	2.56	0.45
9:G:55:ALA:HB1	9:G:134:MET:CE	2.46	0.45
11:I:49:PHE:CE1	29:3:59:LYS:HE3	2.51	0.45
11:I:53:ARG:C	11:I:53:ARG:HD2	2.37	0.45
20:R:60:PRO:HB2	20:R:61:SER:H	1.61	0.45
21:S:71:MET:HA	21:S:78:PRO:HA	1.98	0.45
25:W:14:GLY:O	25:W:18:LYS:HG2	2.17	0.45
1:X:1174:G:C2	1:X:1175:A:C8	3.05	0.45
1:X:455:A:C2	1:X:1258:G:N3	2.83	0.45
1:X:1437:A:H2'	1:X:1438:G:C8	2.52	0.45
1:X:1752:U:O5'	1:X:1752:U:H6	2.00	0.45
1:X:1673:C:N4	1:X:1987:G:H1	2.15	0.45
1:X:1987:G:C5	1:X:1988:A:C8	3.04	0.45
1:X:2708:U:H2'	1:X:2709:C:C6	2.52	0.45
1:X:207:U:O4	1:X:432:C:H4'	2.16	0.45
1:X:495:C:H2'	1:X:496:C:C6	2.52	0.45
1:X:2002:A:H62	26:Z:9:LYS:NZ	2.14	0.45
30:4:22:ARG:HD2	30:4:37:GLY:HA3	1.99	0.45
30:4:9:LYS:HD2	30:4:9:LYS:N	2.32	0.45
5:C:72:ARG:HG3	5:C:77:PHE:CD2	2.51	0.45
6:D:61:THR:HG22	6:D:99:PHE:CD1	2.51	0.45
7:E:56:SER:H	7:E:61:HIS:CD2	2.35	0.45
11:I:107:LYS:HG3	11:I:108:LEU:N	2.32	0.45
11:I:45:LYS:HD3	11:I:45:LYS:C	2.37	0.45
12:J:71:PRO:HA	12:J:96:SER:HB2	1.99	0.45
14:L:11:LEU:HD23	14:L:14:ARG:NH1	2.31	0.45
18:P:71:VAL:HG12	18:P:126:ILE:CG2	2.47	0.45
21:S:73:LYS:O	21:S:74:ARG:HB2	2.16	0.45
1:X:1226:A:C5	1:X:1250:A:N3	2.85	0.45
1:X:1332:G:C6	1:X:1333:G:C6	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:167:A:C4	1:X:184:A:C2	3.04	0.45
1:X:1763:G:C2'	1:X:1764:A:H5'	2.46	0.45
1:X:1770:U:O2	1:X:1774:A:C6	2.70	0.45
1:X:1805:G:N3	3:A:51:THR:HG21	2.31	0.45
1:X:2066:G:C6	1:X:2067:U:N3	2.85	0.45
1:X:2299:A:H3'	1:X:2299:A:N3	2.31	0.45
1:X:537:C:H5	1:X:2759:U:H2'	1.82	0.45
1:X:27:G:N2	1:X:522:G:H1'	2.32	0.45
1:X:487:G:O4'	1:X:515:A:C2	2.70	0.45
1:X:686:C:O2'	1:X:687:G:H5'	2.17	0.45
1:X:854:G:H2'	1:X:855:G:C8	2.52	0.45
1:X:982:C:C4	1:X:983:G:N7	2.85	0.45
18:P:40:LEU:HD22	26:Z:25:LEU:CD1	2.46	0.45
1:X:1507:A:H5'	3:A:100:ASP:OD1	2.17	0.45
4:B:117:MET:HA	4:B:121:ASN:O	2.17	0.45
1:X:2551:A:C8	4:B:144:ARG:HD3	2.52	0.45
5:C:33:TRP:HD1	5:C:93:TYR:CE1	2.35	0.45
11:I:43:ALA:O	11:I:45:LYS:HB2	2.17	0.45
12:J:48:ILE:HD12	12:J:71:PRO:HG3	1.99	0.45
25:W:41:ARG:HB3	25:W:45:LYS:NZ	2.32	0.45
1:X:1710:U:H5'	1:X:1711:C:C5	2.51	0.45
1:X:771:C:O2	1:X:1964:A:H2	1.99	0.45
1:X:2321:C:O2'	1:X:2353:G:H5''	2.17	0.45
1:X:2409:A:O2'	1:X:2410:U:C6	2.70	0.45
1:X:2651:U:H2'	1:X:2652:G:O5'	2.17	0.45
1:X:2702:G:H4'	13:K:5:LYS:HE2	1.99	0.45
1:X:571:U:C4	1:X:2019:C:O4'	2.69	0.45
2:Y:17:A:C1'	2:Y:112:A:C8	2.86	0.45
3:A:122:PRO:HG2	3:A:123:GLU:CD	2.38	0.45
6:D:34:ILE:HD13	6:D:156:ILE:HA	1.99	0.45
1:X:609:U:H4'	11:I:18:ARG:CZ	2.47	0.45
12:J:39:GLU:HB3	12:J:128:ILE:HB	1.99	0.45
15:M:99:VAL:CG2	15:M:100:ARG:N	2.79	0.45
16:N:66:ASN:N	16:N:66:ASN:OD1	2.47	0.45
23:U:67:LEU:HD23	23:U:67:LEU:C	2.37	0.45
1:X:1017:C:H2'	1:X:1018:C:H6	1.82	0.45
1:X:1391:A:C4'	1:X:1392:U:OP1	2.64	0.45
1:X:1849:G:C6	1:X:1850:G:N1	2.85	0.45
1:X:2769:C:H1'	1:X:2866:A:H2	1.82	0.45
1:X:2780:A:O2'	1:X:2781:G:H5'	2.16	0.45
1:X:571:U:C2	1:X:581:A:C8	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:133:PRO:HD3	3:A:191:TYR:CE2	2.51	0.45
4:B:82:ARG:C	4:B:84:PHE:H	2.19	0.45
9:G:116:ARG:HD2	9:G:119:LEU:HD12	1.99	0.45
9:G:154:GLU:OE2	9:G:155:THR:HG22	2.16	0.45
9:G:61:ARG:HE	9:G:65:LYS:HD3	1.80	0.45
10:H:24:VAL:CG1	10:H:42:LYS:HG2	2.46	0.45
10:H:116:ARG:NE	15:M:38:LYS:HE3	2.32	0.45
16:N:106:PHE:O	16:N:110:VAL:HG23	2.17	0.45
19:Q:48:VAL:HG22	19:Q:49:ARG:O	2.16	0.45
20:R:25:LEU:HB2	20:R:81:VAL:HG23	1.98	0.45
1:X:1008:G:O2'	1:X:1009:C:H5'	2.16	0.45
1:X:124:A:OP2	28:2:44:VAL:HG11	2.17	0.45
1:X:1381:G:H2'	1:X:1382:G:H8	1.82	0.45
1:X:1631:C:H5	1:X:1633:C:C5	2.34	0.45
1:X:2260:C:C2'	1:X:2261:G:H5'	2.47	0.45
1:X:1678:G:H4'	1:X:2691:C:N4	2.31	0.45
1:X:2825:A:C2	1:X:2826:C:C2	3.05	0.45
1:X:757:U:H3	1:X:766:A:H61	1.65	0.45
1:X:832:A:N3	1:X:1203:A:C2	2.85	0.45
29:3:13:ARG:HD3	29:3:25:PHE:HD1	1.83	0.44
4:B:11:MET:HA	4:B:23:VAL:O	2.16	0.44
5:C:163:ASN:HD22	5:C:163:ASN:C	2.21	0.44
5:C:53:LYS:O	5:C:54:THR:OG1	2.30	0.44
1:X:648:A:H5''	11:I:110:ALA:O	2.17	0.44
12:J:29:ALA:HB3	12:J:68:ARG:NH2	2.30	0.44
12:J:36:ILE:CG2	12:J:37:ALA:N	2.80	0.44
18:P:118:LYS:HE3	18:P:118:LYS:HB2	1.80	0.44
1:X:1213:U:H2'	1:X:1214:C:C6	2.52	0.44
1:X:1283:C:H5''	1:X:1284:G:H5'	1.99	0.44
1:X:1405:A:N6	1:X:1406:A:N6	2.65	0.44
1:X:1710:U:H5'	1:X:1711:C:H5	1.82	0.44
1:X:1884:A:O2'	3:A:245:ARG:CG	2.64	0.44
1:X:2499:C:O2'	1:X:2500:C:H5'	2.17	0.44
1:X:2673:G:H2'	1:X:2674:C:H6	1.82	0.44
1:X:830:C:O2'	1:X:852:U:H5''	2.17	0.44
1:X:940:G:O6	1:X:941:U:O4	2.35	0.44
4:B:14:ILE:HD12	4:B:23:VAL:CG2	2.43	0.44
9:G:66:HIS:O	9:G:70:PHE:CE1	2.70	0.44
11:I:120:VAL:HB	11:I:140:VAL:HG22	1.98	0.44
15:M:31:ASP:HA	15:M:52:GLY:O	2.18	0.44
17:O:36:LYS:HE2	17:O:56:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:12:ASN:C	22:T:14:ARG:H	2.20	0.44
1:X:1656:U:H4'	1:X:2678:C:H4'	1.99	0.44
1:X:1674:C:C2'	1:X:1674:C:O2	2.64	0.44
1:X:2340:C:P	29:3:27:SER:OG	2.75	0.44
1:X:2494:C:H2'	1:X:2495:G:C8	2.52	0.44
1:X:2825:A:C6	1:X:2826:C:C4	3.05	0.44
1:X:430:C:H1'	1:X:2386:G:N2	2.32	0.44
1:X:627:A:H2'	1:X:628:A:C8	2.52	0.44
1:X:641:G:H4'	1:X:651:C:O2'	2.18	0.44
1:X:693:A:C5	1:X:811:G:N2	2.85	0.44
1:X:820:U:H2'	1:X:821:A:H8	1.81	0.44
1:X:867:G:H1	1:X:935:C:H42	1.65	0.44
1:X:918:A:C2'	1:X:919:U:H5''	2.40	0.44
1:X:2200:G:O2'	3:A:150:PRO:HG2	2.17	0.44
3:A:56:GLY:H	3:A:218:ARG:H	1.65	0.44
4:B:32:PRO:HD2	4:B:50:GLY:O	2.16	0.44
9:G:162:LYS:H	9:G:163:PRO:CD	2.20	0.44
13:K:71:HIS:HD1	13:K:71:HIS:N	2.15	0.44
15:M:104:LEU:HA	15:M:106:TYR:CD2	2.51	0.44
18:P:19:LYS:O	18:P:20:LEU:CB	2.66	0.44
20:R:51:VAL:HG12	20:R:51:VAL:O	2.17	0.44
20:R:6:ALA:C	20:R:8:SER:H	2.21	0.44
1:X:1567:A:H2'	1:X:1568:A:O4'	2.16	0.44
1:X:1923:U:H4'	1:X:1924:C:O5'	2.17	0.44
1:X:1924:C:C2	1:X:1948:C:C2	3.05	0.44
1:X:2173:G:H2'	1:X:2174:G:C8	2.52	0.44
1:X:43:A:C6	1:X:44:G:C6	3.05	0.44
1:X:459:A:N6	1:X:484:G:C4	2.85	0.44
1:X:538:A:H62	1:X:2026:C:C5'	2.30	0.44
1:X:546:A:H2'	1:X:547:U:C6	2.53	0.44
1:X:822:G:H2'	1:X:823:U:H5'	1.99	0.44
5:C:3:GLN:HB2	5:C:116:LYS:HD2	1.99	0.44
6:D:29:PRO:HB2	6:D:169:LEU:HD22	2.00	0.44
6:D:78:LYS:HG2	6:D:80:ARG:NH1	2.32	0.44
2:Y:47:A:C8	6:D:92:ARG:NH1	2.85	0.44
10:H:60:PRO:O	10:H:61:ARG:HB2	2.17	0.44
12:J:99:LYS:HG3	12:J:100:PRO:HD2	2.00	0.44
12:J:22:ALA:HA	12:J:99:LYS:HB3	2.00	0.44
22:T:45:PHE:CD2	22:T:77:ARG:HB3	2.52	0.44
1:X:1453:A:C2	1:X:1569:A:C6	3.06	0.44
1:X:1437:A:C2	1:X:1592:U:O2	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1722:G:C6	1:X:1723:U:N3	2.86	0.44
1:X:2754:C:H2'	1:X:2755:A:O4'	2.17	0.44
28:2:41:GLN:HA	28:2:41:GLN:OE1	2.17	0.44
3:A:47:ARG:HD3	3:A:47:ARG:C	2.38	0.44
3:A:69:LYS:CD	3:A:69:LYS:H	2.23	0.44
3:A:71:ARG:HH12	3:A:150:PRO:CB	2.30	0.44
9:G:132:PHE:CB	9:G:145:HIS:CD2	2.99	0.44
9:G:93:LYS:HB3	9:G:97:ASP:HB3	1.99	0.44
11:I:637:G:H1	11:I:101:ARG:CD	2.30	0.44
13:K:12:ARG:NH2	13:K:20:LEU:HD22	2.32	0.44
19:Q:53:ILE:CD1	19:Q:80:VAL:HG12	2.42	0.44
21:S:107:GLU:HA	21:S:111:GLY:O	2.17	0.44
1:X:1450:G:N3	1:X:1573:G:C2	2.85	0.44
1:X:2495:G:C6	1:X:2496:C:N4	2.86	0.44
1:X:2494:C:C2	1:X:2549:G:C2	3.06	0.44
1:X:2616:U:H5''	4:B:82:ARG:HH22	1.80	0.44
1:X:395:G:C2	1:X:406:G:C2	3.05	0.44
1:X:779:U:O4	1:X:780:U:O4	2.36	0.44
1:X:819:C:H2'	1:X:820:U:C6	2.53	0.44
3:A:151:GLY:O	3:A:153:GLY:N	2.51	0.44
5:C:191:ALA:HA	5:C:194:GLU:HB3	1.99	0.44
7:E:105:MET:CE	7:E:131:ILE:HD11	2.47	0.44
1:X:576:A:O3'	11:I:40:ARG:NH1	2.51	0.44
11:I:43:ALA:O	11:I:44:GLY:C	2.55	0.44
1:X:1817:U:H4'	3:A:253:LYS:HZ2	1.82	0.44
1:X:2235:G:N2	1:X:2254:C:C4	2.86	0.44
1:X:2670:C:O3'	1:X:2846:G:H4'	2.18	0.44
1:X:538:A:C2'	1:X:538:A:N3	2.79	0.44
1:X:843:G:O4'	1:X:2427:A:N1	2.51	0.44
1:X:861:G:N2	1:X:943:U:H1'	2.33	0.44
29:3:36:LYS:HE2	29:3:36:LYS:HB2	1.83	0.44
1:X:2554:C:O2'	4:B:140:SER:CB	2.66	0.44
4:B:14:ILE:HG12	15:M:20:HIS:HD2	1.76	0.44
11:I:107:LYS:HB2	11:I:107:LYS:HE2	1.84	0.44
14:L:37:HIS:HE1	14:L:57:ALA:HB2	1.76	0.44
1:X:935:C:C1'	22:T:29:GLU:HG2	2.46	0.44
23:U:59:THR:O	23:U:60:VAL:C	2.56	0.44
1:X:1001:A:H1'	1:X:1167:A:C2	2.53	0.44
1:X:13:A:C2	1:X:15:G:C6	3.06	0.44
1:X:1422:C:H2'	1:X:1423:A:C8	2.53	0.44
1:X:155:G:O2'	1:X:156:G:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1692:C:H2'	1:X:1693:A:O4'	2.18	0.44
1:X:2245:A:H5'	1:X:2246:A:C4	2.53	0.44
1:X:2329:C:C6	1:X:2329:C:H3'	2.53	0.44
1:X:2490:U:H2'	1:X:2491:C:C6	2.52	0.44
1:X:2780:A:H2'	1:X:2781:G:C8	2.53	0.44
1:X:459:A:C2	1:X:466:A:H2'	2.52	0.44
1:X:538:A:H4'	9:G:139:ARG:NE	2.33	0.44
1:X:541:C:N3	1:X:572:G:C8	2.86	0.44
4:B:67:PHE:CD2	4:B:74:PRO:HA	2.53	0.44
5:C:38:ARG:NH2	5:C:178:TYR:CE2	2.84	0.44
1:X:2289:A:N3	6:D:79:LEU:HD21	2.33	0.44
14:L:72:GLY:O	14:L:75:LEU:HB3	2.18	0.44
14:L:99:ARG:HG3	14:L:100:VAL:H	1.82	0.44
1:X:409:G:O3'	23:U:47:HIS:CE1	2.71	0.44
1:X:1070:G:H5'	1:X:1071:U:H2'	1.99	0.44
1:X:1007:A:C5	1:X:1171:A:C2	3.06	0.44
1:X:317:U:O2'	1:X:1224:A:N7	2.50	0.44
1:X:1255:A:C6	1:X:1256:C:C4	3.06	0.44
1:X:2026:C:H2'	1:X:2027:C:H6	1.82	0.44
1:X:2436:U:O2'	1:X:2437:G:H5'	2.18	0.44
1:X:2659:C:H2'	1:X:2660:C:H6	1.82	0.44
1:X:813:A:O4'	1:X:815:A:H5'	2.17	0.44
3:A:89:ARG:O	3:A:90:SER:C	2.55	0.44
5:C:102:LEU:C	5:C:102:LEU:HD23	2.37	0.44
6:D:51:ASP:HA	6:D:54:ALA:HB3	1.99	0.44
9:G:111:LYS:O	9:G:111:LYS:HG3	2.17	0.44
9:G:55:ALA:HB1	9:G:134:MET:HE1	1.98	0.44
10:H:114:VAL:O	10:H:115:ALA:O	2.36	0.44
20:R:16:PHE:HZ	20:R:46:VAL:CG2	2.31	0.44
21:S:127:PRO:C	21:S:129:ARG:H	2.21	0.44
22:T:18:PRO:O	22:T:19:LYS:HG2	2.17	0.44
1:X:1173:G:H2'	1:X:1174:G:C8	2.52	0.44
1:X:1313:U:H4'	1:X:1314:A:H5'	2.00	0.44
1:X:1335:A:C2	1:X:1346:C:O2'	2.69	0.44
1:X:1361:G:C6	1:X:1362:A:C6	3.06	0.44
1:X:1506:C:H2'	1:X:1507:A:H5'	1.99	0.44
1:X:1974:U:C2'	1:X:1975:G:C5'	2.96	0.44
1:X:2057:U:C2	1:X:2415:G:N2	2.86	0.44
1:X:2821:G:H2'	1:X:2822:U:O4'	2.18	0.44
1:X:313:U:O2'	1:X:314:G:H5'	2.18	0.44
1:X:555:U:HO2'	1:X:556:A:P	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:688:A:H5'	5:C:61:GLN:OE1	2.18	0.44
1:X:768:U:C4	1:X:769:C:C4	3.05	0.44
1:X:815:A:C6	1:X:816:U:N3	2.86	0.44
1:X:913:A:N7	1:X:914:C:C4	2.86	0.44
1:X:987:G:C2	1:X:988:G:C8	3.05	0.44
1:X:1812:U:O2	3:A:160:ALA:O	2.34	0.43
3:A:245:ARG:HD3	3:A:245:ARG:N	2.33	0.43
4:B:176:ARG:HH21	15:M:16:ILE:HA	1.83	0.43
5:C:111:ARG:HH12	5:C:181:LEU:HD12	1.82	0.43
5:C:54:THR:HB	5:C:73:SER:HB3	1.99	0.43
1:X:2285:U:O2	6:D:44:LYS:HD2	2.18	0.43
10:H:22:ILE:HG21	10:H:22:ILE:HD13	1.76	0.43
12:J:70:PHE:HA	12:J:71:PRO:HD3	1.66	0.43
13:K:20:LEU:O	13:K:21:ALA:C	2.55	0.43
2:Y:8:C:O2'	14:L:39:TYR:CE1	2.70	0.43
23:U:22:GLY:HA3	23:U:39:LYS:CE	2.46	0.43
1:X:1026:U:O2'	1:X:1027:C:H5'	2.18	0.43
1:X:122:G:H2'	28:2:19:ARG:NH2	2.33	0.43
1:X:1356:G:O5'	1:X:1356:G:H8	2.01	0.43
1:X:1686:A:OP2	1:X:1687:C:H5	2.01	0.43
1:X:1922:U:OP1	1:X:2583:U:O2'	2.32	0.43
1:X:538:A:N3	1:X:2025:A:C6	2.86	0.43
1:X:2210:C:C4	1:X:2211:U:C4	3.06	0.43
1:X:2668:U:O2	1:X:2693:U:O4'	2.36	0.43
1:X:2700:U:C2'	1:X:2700:U:O2	2.64	0.43
1:X:542:A:OP1	1:X:570:G:N2	2.49	0.43
1:X:599:A:H61	1:X:679:C:N4	2.16	0.43
3:A:207:LEU:C	3:A:212:ARG:HD3	2.38	0.43
3:A:69:LYS:N	3:A:69:LYS:HD3	2.25	0.43
10:H:82:LYS:HE3	10:H:82:LYS:HB2	1.78	0.43
1:X:1223:G:C5	1:X:1250:A:N6	2.86	0.43
1:X:1223:G:H4'	1:X:1224:A:C5'	2.48	0.43
1:X:1223:G:H5'	1:X:1225:G:O4'	2.18	0.43
1:X:1381:G:H2'	1:X:1382:G:C8	2.53	0.43
1:X:1405:A:C6	1:X:1406:A:C6	3.05	0.43
1:X:1511:A:N6	1:X:1512:A:N6	2.66	0.43
1:X:1631:C:C5	1:X:1633:C:C2	3.06	0.43
1:X:1724:C:C4	1:X:1747:G:C6	3.05	0.43
1:X:1835:C:C5'	3:A:256:LYS:HE2	2.48	0.43
1:X:1838:G:N2	1:X:1878:C:C2	2.86	0.43
1:X:1991:C:H2'	1:X:1992:G:C8	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2053:G:C2	1:X:2421:C:C2	3.05	0.43
1:X:2065:A:C2	1:X:2218:G:N3	2.86	0.43
1:X:2705:A:N7	1:X:2707:G:C5	2.85	0.43
1:X:2815:C:N4	1:X:2852:G:H1	2.16	0.43
1:X:620:G:N2	1:X:630:G:H1'	2.32	0.43
1:X:869:C:H4'	22:T:69:PHE:HB2	1.98	0.43
3:A:106:ILE:HG22	3:A:107:LEU:N	2.34	0.43
3:A:214:ARG:HA	3:A:214:ARG:HD2	1.84	0.43
4:B:54:LYS:HD2	4:B:59:VAL:HG22	1.99	0.43
7:E:105:MET:HE2	7:E:105:MET:HA	2.01	0.43
9:G:30:LYS:HE3	9:G:30:LYS:HB2	1.68	0.43
16:N:86:ALA:C	16:N:88:ILE:H	2.21	0.43
17:O:48:GLY:O	17:O:49:GLU:HB2	2.19	0.43
23:U:49:LYS:HB3	23:U:61:TRP:CD2	2.53	0.43
1:X:1336:G:C2	1:X:1346:C:H1'	2.53	0.43
1:X:1342:U:H3'	1:X:1343:C:H6	1.82	0.43
1:X:1346:C:O5'	1:X:1346:C:H6	2.02	0.43
1:X:2043:A:N6	5:C:68:ARG:HH12	2.16	0.43
1:X:2062:U:H2'	1:X:2063:A:C8	2.54	0.43
1:X:2664:G:N3	1:X:2664:G:H2'	2.32	0.43
1:X:799:C:O2'	1:X:800:U:H5'	2.19	0.43
1:X:475:U:C2	1:X:801:A:C6	3.06	0.43
2:Y:12:C:H2'	2:Y:13:C:O4'	2.18	0.43
26:Z:42:SER:O	26:Z:44:HIS:CD2	2.55	0.43
30:4:24:LEU:HD23	30:4:35:ARG:CZ	2.49	0.43
3:A:148:LEU:HD21	3:A:156:LEU:HD11	1.98	0.43
3:A:247:PRO:HD3	3:A:253:LYS:CG	2.49	0.43
3:A:27:LYS:HE2	3:A:205:ILE:HD13	2.01	0.43
7:E:56:SER:HB2	7:E:61:HIS:CE1	2.54	0.43
9:G:33:ILE:HB	9:G:34:PRO:HD2	2.01	0.43
17:O:29:ALA:HA	17:O:59:GLU:HB3	1.99	0.43
18:P:30:TYR:H	18:P:123:HIS:CE1	2.36	0.43
19:Q:35:LYS:HA	19:Q:38:ILE:HG22	1.98	0.43
22:T:32:LYS:H	22:T:35:ASN:HD22	1.65	0.43
24:V:6:MET:HE3	24:V:56:VAL:HG21	2.01	0.43
24:V:56:VAL:O	24:V:59:GLU:HB2	2.18	0.43
1:X:1252:C:H6	1:X:1252:C:H3'	1.83	0.43
1:X:1441:A:O4'	1:X:1442:C:C5	2.71	0.43
1:X:2445:C:C4	1:X:2446:C:N4	2.86	0.43
1:X:320:A:H1'	1:X:340:G:N3	2.34	0.43
1:X:470:U:OP1	28:2:40:HIS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:46:ASN:O	3:A:47:ARG:C	2.55	0.43
7:E:137:ASP:O	7:E:141:VAL:HG23	2.18	0.43
10:H:23:ARG:CZ	10:H:23:ARG:HB3	2.48	0.43
1:X:684:C:C5	11:I:43:ALA:HA	2.53	0.43
12:J:36:ILE:HG22	12:J:37:ALA:N	2.33	0.43
16:N:29:SER:C	16:N:30:LYS:HG2	2.38	0.43
19:Q:10:PRO:HD3	24:V:30:PHE:HD2	1.83	0.43
1:X:1002:C:O2	1:X:1175:A:C2	2.72	0.43
1:X:1220:G:N2	1:X:1253:C:C4	2.86	0.43
1:X:1467:U:H3'	1:X:1467:U:C6	2.53	0.43
1:X:1673:C:O2'	1:X:1674:C:H5'	2.18	0.43
1:X:2064:U:O2'	1:X:2065:A:H5'	2.18	0.43
1:X:2300:G:H3'	1:X:2300:G:N3	2.34	0.43
1:X:2370:G:H2'	1:X:2371:A:H2	1.83	0.43
1:X:2565:C:O2	1:X:2565:C:H2'	2.18	0.43
1:X:608:G:H2'	1:X:609:U:C6	2.53	0.43
1:X:797:A:O2'	1:X:798:G:H8	2.02	0.43
3:A:185:ARG:HH21	3:A:269:ARG:HH11	1.66	0.43
4:B:59:VAL:HG12	4:B:64:GLN:HG3	1.99	0.43
9:G:156:HIS:N	9:G:157:PRO:CD	2.82	0.43
12:J:21:ASP:C	12:J:99:LYS:HG2	2.38	0.43
18:P:14:ARG:HA	18:P:17:GLN:CG	2.48	0.43
24:V:17:GLU:O	24:V:21:ARG:HD3	2.18	0.43
1:X:1411:C:H2'	1:X:1412:C:H5'	2.00	0.43
1:X:1810:U:H5	3:A:158:ARG:NH1	2.16	0.43
1:X:1965:U:H2'	1:X:1966:C:H6	1.83	0.43
1:X:635:C:C3'	1:X:636:G:H5''	2.49	0.43
1:X:854:G:H1	1:X:948:C:N4	2.12	0.43
1:X:66:U:H1'	1:X:87:G:N2	2.33	0.43
1:X:916:U:C4	1:X:917:U:C4	3.07	0.43
1:X:957:G:H2'	1:X:958:G:H8	1.84	0.43
6:D:77:PHE:HB3	6:D:78:LYS:H	1.58	0.43
8:F:74:MET:SD	8:F:127:VAL:HG22	2.59	0.43
9:G:103:TYR:CE1	9:G:111:LYS:C	2.92	0.43
11:I:52:GLY:O	11:I:53:ARG:HB3	2.19	0.43
13:K:79:VAL:HG13	13:K:80:MET:H	1.83	0.43
14:L:33:ARG:NH2	14:L:103:LEU:HD12	2.34	0.43
4:B:14:ILE:CG1	15:M:20:HIS:CD2	2.88	0.43
16:N:20:ARG:HD2	16:N:39:LEU:HD13	2.01	0.43
19:Q:48:VAL:HG21	19:Q:82:LEU:HD22	2.00	0.43
1:X:1817:U:C4'	3:A:253:LYS:HD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:227:G:C6	1:X:228:A:C6	3.07	0.43
1:X:2426:G:C2'	1:X:2479:U:OP2	2.66	0.43
1:X:2742:G:O2'	1:X:2743:G:H5'	2.18	0.43
1:X:2766:U:O2'	1:X:2767:C:H5'	2.19	0.43
1:X:2791:C:C2	1:X:2806:G:N2	2.86	0.43
1:X:64:C:H3'	1:X:64:C:H6	1.82	0.43
29:3:13:ARG:C	29:3:23:MET:O	2.56	0.43
1:X:618:A:OP1	5:C:94:THR:HG21	2.19	0.43
9:G:156:HIS:HB2	9:G:157:PRO:HD3	2.01	0.43
10:H:104:GLU:HG2	10:H:125:LYS:NZ	2.33	0.43
15:M:103:LYS:O	15:M:104:LEU:CB	2.65	0.43
15:M:46:ARG:HG2	15:M:47:SER:N	2.34	0.43
18:P:107:ILE:O	18:P:107:ILE:HG23	2.18	0.43
1:X:1439:G:C2	1:X:1440:G:C2	3.07	0.43
1:X:2391:A:C8	1:X:2392:G:C8	3.07	0.43
1:X:2696:A:H2'	1:X:2697:G:C8	2.52	0.43
1:X:637:G:H1	11:I:101:ARG:CG	2.32	0.43
1:X:83:A:H1'	1:X:84:G:O4'	2.18	0.43
28:2:14:LYS:HD3	28:2:14:LYS:O	2.19	0.43
1:X:1673:C:H5'	4:B:136:ARG:HD3	2.01	0.43
5:C:163:ASN:ND2	5:C:163:ASN:C	2.72	0.43
9:G:61:ARG:HH22	9:G:78:ASP:HB2	1.84	0.43
10:H:116:ARG:NH1	15:M:38:LYS:HE3	2.33	0.43
20:R:77:HIS:C	20:R:79:SER:H	2.22	0.43
21:S:137:ASP:OD2	21:S:138:VAL:N	2.52	0.43
21:S:88:TYR:O	21:S:127:PRO:HG2	2.19	0.43
22:T:41:ARG:HD3	22:T:41:ARG:HA	1.76	0.43
23:U:32:ARG:HB2	23:U:33:LYS:H	1.63	0.43
1:X:1047:G:N2	1:X:1131:G:C4	2.87	0.43
1:X:1069:G:C3'	1:X:1070:G:H5''	2.49	0.43
1:X:1356:G:N2	1:X:1418:C:N3	2.67	0.43
1:X:239:A:H5'	1:X:620:G:O2'	2.18	0.43
1:X:321:A:OP1	20:R:27:GLY:N	2.47	0.43
1:X:482:A:N6	1:X:483:A:C2	2.87	0.43
1:X:538:A:H3'	9:G:142:ARG:NH1	2.30	0.43
1:X:872:G:OP2	1:X:872:G:C8	2.72	0.43
1:X:2323:U:O2'	27:1:40:TYR:CE1	2.71	0.43
3:A:262:ARG:O	3:A:265:LYS:HB3	2.19	0.43
6:D:12:VAL:O	6:D:16:LEU:HG	2.19	0.43
13:K:5:LYS:HB2	13:K:5:LYS:HE2	1.78	0.43
18:P:16:GLN:H	18:P:16:GLN:HG2	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1166:A:C2'	1:X:1167:A:H5''	2.49	0.43
1:X:1226:A:C4	1:X:1250:A:N3	2.87	0.43
1:X:1313:U:H4'	1:X:1314:A:O5'	2.18	0.43
1:X:1345:G:C5	1:X:1625:A:C5	3.07	0.43
1:X:1779:C:C5	1:X:1780:A:N7	2.87	0.43
1:X:2238:G:C5	1:X:2406:C:N4	2.87	0.43
1:X:2594:U:H2'	1:X:2595:C:H6	1.83	0.43
1:X:940:G:C6	1:X:941:U:C4	3.07	0.43
2:Y:5:C:H2'	2:Y:6:C:O4'	2.19	0.43
29:3:13:ARG:HD2	29:3:25:PHE:CD1	2.54	0.42
4:B:38:THR:HG22	4:B:40:GLN:H	1.84	0.42
5:C:148:VAL:HG12	5:C:149:LEU:N	2.34	0.42
10:H:116:ARG:HD2	15:M:38:LYS:CE	2.49	0.42
11:I:77:LEU:HB3	11:I:112:GLY:H	1.84	0.42
18:P:29:LYS:O	18:P:30:TYR:HB2	2.19	0.42
18:P:31:VAL:O	18:P:33:MET:N	2.43	0.42
23:U:22:GLY:HA3	23:U:39:LYS:CD	2.49	0.42
1:X:1166:A:H2'	1:X:1167:A:H5''	2.01	0.42
1:X:1453:A:C8	1:X:1454:U:C6	3.07	0.42
1:X:196:A:O2'	1:X:197:G:H5'	2.19	0.42
1:X:2301:A:H2'	1:X:2302:G:O4'	2.19	0.42
1:X:314:G:C6	1:X:326:A:C2	3.06	0.42
1:X:396:U:C4	1:X:398:C:C5	3.07	0.42
1:X:43:A:H2	1:X:448:C:H41	1.65	0.42
1:X:701:U:O5'	1:X:701:U:H6	2.01	0.42
1:X:840:U:C5	1:X:2409:A:C5	3.07	0.42
1:X:922:A:N7	1:X:923:A:C6	2.86	0.42
1:X:943:U:O2'	1:X:944:A:O4'	2.34	0.42
3:A:91:ALA:HA	3:A:199:ASN:OD1	2.19	0.42
5:C:172:VAL:O	5:C:172:VAL:HG12	2.19	0.42
1:X:2293:G:C5'	6:D:35:VAL:HG11	2.45	0.42
7:E:55:PRO:HB2	7:E:61:HIS:CD2	2.54	0.42
9:G:61:ARG:CD	9:G:65:LYS:HD2	2.49	0.42
2:Y:93:G:OP1	12:J:19:THR:HB	2.19	0.42
13:K:73:LYS:O	13:K:76:VAL:CG1	2.67	0.42
14:L:40:ALA:HB2	14:L:103:LEU:HD11	2.01	0.42
14:L:42:ILE:C	14:L:42:ILE:HD13	2.39	0.42
18:P:117:ILE:HD12	18:P:117:ILE:HG23	1.72	0.42
18:P:25:PHE:HD1	18:P:127:ILE:CD1	2.28	0.42
24:V:6:MET:HE2	24:V:56:VAL:HG21	2.02	0.42
1:X:1407:G:O6	1:X:1408:A:N6	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1462:C:H2'	1:X:1463:A:C8	2.54	0.42
1:X:1508:G:H5'	1:X:1509:A:H5''	2.00	0.42
1:X:1836:C:N3	1:X:1880:G:N2	2.67	0.42
1:X:2053:G:C2	1:X:2054:A:N3	2.88	0.42
1:X:2327:U:H6	1:X:2327:U:O5'	2.02	0.42
1:X:2363:G:OP1	22:T:55:ARG:HD2	2.19	0.42
1:X:2407:G:N2	11:I:59:ARG:HH22	2.18	0.42
1:X:2697:G:H2'	1:X:2698:G:O4'	2.20	0.42
1:X:2705:A:H4'	1:X:2706:U:OP1	2.18	0.42
1:X:334:G:N2	5:C:162:ARG:HH22	2.17	0.42
1:X:531:G:O2'	1:X:532:A:H5'	2.19	0.42
1:X:637:G:H8	1:X:637:G:O5'	2.02	0.42
1:X:7:G:H2'	1:X:8:A:O4'	2.19	0.42
28:2:34:ARG:HH11	28:2:42:LEU:CA	2.32	0.42
5:C:3:GLN:O	5:C:12:GLY:HA3	2.18	0.42
6:D:112:ARG:H	6:D:112:ARG:CD	2.30	0.42
10:H:27:SER:HB3	10:H:50:ILE:H	1.82	0.42
12:J:78:LYS:HE2	12:J:81:GLU:HA	2.01	0.42
13:K:100:VAL:HG12	13:K:101:GLY:H	1.75	0.42
10:H:116:ARG:HH22	15:M:41:GLU:HG2	1.83	0.42
18:P:47:GLY:HA2	18:P:92:VAL:O	2.19	0.42
1:X:1615:C:OP1	19:Q:35:LYS:HB2	2.20	0.42
1:X:1058:G:H2'	1:X:1121:G:O6	2.19	0.42
1:X:1685:A:C4	1:X:1691:G:N7	2.87	0.42
1:X:2045:A:C6	31:X:2881:LMA:H27	2.54	0.42
1:X:2497:A:H2'	1:X:2497:A:N3	2.34	0.42
1:X:331:U:H1'	5:C:162:ARG:HH21	1.84	0.42
1:X:68:C:H2'	1:X:69:G:O4'	2.19	0.42
1:X:700:C:O4'	28:2:4:THR:HA	2.18	0.42
1:X:971:A:H5''	1:X:972:C:OP2	2.19	0.42
1:X:2594:U:C2	26:Z:7:PRO:HA	2.54	0.42
9:G:140:GLN:O	9:G:144:MET:HG3	2.19	0.42
23:U:50:ALA:HB1	23:U:52:ARG:NH2	2.33	0.42
1:X:341:A:H2	1:X:1223:G:C8	2.37	0.42
1:X:1326:U:C2'	1:X:1326:U:O2	2.65	0.42
1:X:1363:C:O2'	1:X:1364:C:H5'	2.20	0.42
1:X:1672:A:O4'	4:B:113:THR:O	2.37	0.42
1:X:1710:U:H4'	1:X:1711:C:OP2	2.20	0.42
1:X:1279:G:O2'	1:X:1995:G:O6	2.23	0.42
1:X:2740:C:O2'	1:X:2741:G:H5'	2.19	0.42
1:X:318:G:N1	1:X:321:A:OP2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:404:A:C2	1:X:424:G:C2	3.08	0.42
1:X:487:G:H4'	1:X:512:A:H61	1.84	0.42
1:X:604:U:H5''	29:3:61:MET:SD	2.59	0.42
1:X:860:U:H2'	1:X:860:U:O2	2.17	0.42
30:4:19:ARG:HD2	30:4:24:LEU:HD13	2.01	0.42
3:A:119:ASN:HD22	3:A:124:ALA:HB2	1.85	0.42
3:A:251:TRP:O	3:A:256:LYS:NZ	2.41	0.42
3:A:252:GLY:HA3	3:A:256:LYS:CE	2.49	0.42
6:D:118:ASN:HB3	6:D:122:PHE:CZ	2.52	0.42
1:X:2291:U:HO2'	6:D:86:GLY:HA3	1.83	0.42
11:I:99:VAL:HG23	11:I:99:VAL:O	2.19	0.42
14:L:29:LEU:HD23	14:L:89:PHE:CD1	2.55	0.42
15:M:82:PRO:C	15:M:84:ALA:N	2.70	0.42
25:W:47:VAL:HB	25:W:50:LEU:HD12	2.01	0.42
1:X:1036:G:C4	1:X:1145:C:H1'	2.54	0.42
1:X:1203:A:OP1	11:I:33:GLY:O	2.38	0.42
1:X:1623:C:C4'	1:X:1624:A:O5'	2.67	0.42
1:X:805:G:C5	1:X:2419:C:C6	3.07	0.42
1:X:2852:G:O2'	1:X:2853:U:H5'	2.20	0.42
1:X:357:A:H2'	1:X:358:C:H5'	2.02	0.42
1:X:413:G:O2'	1:X:414:A:H5''	2.19	0.42
1:X:421:G:O2'	1:X:422:C:H5'	2.19	0.42
1:X:470:U:O4	1:X:481:A:C8	2.72	0.42
1:X:5:A:O2'	1:X:6:A:H5'	2.19	0.42
1:X:623:G:C3'	1:X:624:A:H5''	2.50	0.42
1:X:688:A:H4'	5:C:61:GLN:CG	2.49	0.42
1:X:781:G:H2'	1:X:782:U:O4'	2.19	0.42
30:4:19:ARG:HD2	30:4:24:LEU:CD2	2.46	0.42
5:C:48:ARG:H	5:C:48:ARG:HD2	1.84	0.42
7:E:171:LEU:N	7:E:171:LEU:HD12	2.35	0.42
9:G:106:TYR:O	9:G:106:TYR:CD2	2.73	0.42
9:G:61:ARG:NH2	9:G:61:ARG:HB3	2.35	0.42
13:K:94:TYR:CD2	13:K:115:LEU:O	2.72	0.42
14:L:47:ARG:C	14:L:49:GLN:H	2.23	0.42
16:N:14:HIS:CD2	16:N:32:TYR:CE2	3.07	0.42
18:P:93:LYS:HB2	18:P:129:ALA:HB3	2.01	0.42
18:P:28:ALA:HB2	18:P:71:VAL:HG22	2.02	0.42
19:Q:5:ASP:O	19:Q:7:LEU:HD12	2.20	0.42
23:U:51:ILE:O	23:U:52:ARG:HD3	2.18	0.42
1:X:1053:G:C6	1:X:1125:G:C2	3.08	0.42
1:X:1045:G:N2	1:X:1133:G:H1'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1174:G:C2	1:X:1175:A:C4	3.07	0.42
1:X:1499:A:C6	1:X:1500:U:N3	2.88	0.42
1:X:1970:G:O2'	1:X:1971:C:H5'	2.20	0.42
1:X:2629:U:OP1	10:H:35:THR:HG21	2.19	0.42
1:X:2790:C:H42	1:X:2806:G:H1	1.66	0.42
1:X:2825:A:N3	1:X:2825:A:C2'	2.80	0.42
1:X:396:U:C4	1:X:398:C:C6	3.07	0.42
1:X:454:G:C2	1:X:456:C:C2	3.07	0.42
1:X:806:A:OP2	1:X:2055:G:H5'	2.19	0.42
1:X:933:G:H2'	1:X:934:G:C8	2.55	0.42
26:Z:16:ARG:HD2	26:Z:16:ARG:C	2.40	0.42
1:X:659:G:C1'	29:3:46:LYS:HG3	2.49	0.42
29:3:60:LEU:HA	29:3:63:PRO:HG2	2.00	0.42
3:A:248:VAL:H	3:A:248:VAL:HG13	1.40	0.42
9:G:170:PRO:HB2	9:G:171:LEU:H	1.64	0.42
9:G:52:GLY:O	9:G:53:ARG:C	2.55	0.42
14:L:44:ASP:HB3	14:L:47:ARG:O	2.20	0.42
15:M:56:ALA:HB3	15:M:67:THR:H	1.84	0.42
15:M:82:PRO:O	15:M:83:PHE:C	2.58	0.42
15:M:99:VAL:HG22	15:M:100:ARG:N	2.34	0.42
1:X:456:C:P	16:N:2:PRO:HD3	2.60	0.42
17:O:11:GLN:HA	17:O:38:LEU:O	2.20	0.42
23:U:53:GLU:HA	23:U:58:LYS:HB2	2.02	0.42
1:X:1129:A:N6	1:X:1130:U:H3	2.18	0.42
1:X:128:C:C2'	1:X:129:A:H5''	2.46	0.42
1:X:1631:C:C5	1:X:1633:C:C6	3.07	0.42
1:X:224:G:N2	1:X:229:G:C6	2.87	0.42
1:X:2426:G:H4'	1:X:2427:A:C5'	2.49	0.42
1:X:2508:G:H5''	1:X:2509:A:H5''	2.01	0.42
1:X:2685:A:N1	1:X:2686:C:C2	2.87	0.42
1:X:2768:C:O2	1:X:2784:A:H2	2.02	0.42
1:X:424:G:H4'	1:X:425:A:OP1	2.19	0.42
1:X:843:G:O4'	1:X:2427:A:C2	2.73	0.42
1:X:98:U:N3	1:X:100:G:N2	2.67	0.42
1:X:334:G:H2'	5:C:162:ARG:NH1	2.35	0.42
11:I:76:LYS:HG3	11:I:111:SER:HB2	2.02	0.42
14:L:38:ILE:CD1	14:L:39:TYR:N	2.82	0.42
15:M:104:LEU:C	15:M:106:TYR:N	2.73	0.42
16:N:27:SER:HB2	16:N:31:GLN:HG3	2.02	0.42
17:O:38:LEU:HD13	17:O:39:PHE:N	2.35	0.42
18:P:107:ILE:CG2	18:P:117:ILE:HG12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:26:LYS:HE3	21:S:26:LYS:HB2	1.80	0.42
22:T:20:TYR:O	22:T:21:LEU:HB2	2.20	0.42
22:T:23:VAL:HA	22:T:38:VAL:HG22	2.02	0.42
1:X:1099:A:O3'	1:X:1100:G:H8	2.03	0.42
1:X:1386:A:H2'	1:X:1387:G:O4'	2.19	0.42
1:X:1357:U:C4'	1:X:1397:A:C6	3.01	0.42
1:X:1928:G:C6	1:X:1929:U:C4	3.07	0.42
1:X:2036:G:OP1	4:B:144:ARG:HG3	2.20	0.42
1:X:177:U:O4	1:X:225:G:N1	2.53	0.42
1:X:2788:C:O2'	1:X:2789:U:H5'	2.19	0.42
1:X:816:U:C4	1:X:817:A:N7	2.88	0.42
1:X:2004:U:P	26:Z:12:SER:HG	2.42	0.42
3:A:252:GLY:HA3	3:A:256:LYS:HZ1	1.84	0.42
4:B:167:VAL:HG11	4:B:170:LEU:HD21	2.02	0.42
5:C:62:LYS:HD3	5:C:62:LYS:C	2.39	0.42
9:G:106:TYR:CZ	9:G:108:GLY:CA	3.03	0.42
10:H:104:GLU:OE2	10:H:125:LYS:NZ	2.53	0.42
10:H:9:ASP:O	10:H:95:ALA:HB1	2.19	0.42
1:X:589:C:H4'	16:N:31:GLN:CD	2.40	0.42
18:P:27:VAL:HG23	18:P:125:THR:HG22	2.01	0.42
19:Q:30:SER:O	19:Q:33:ALA:HB3	2.19	0.42
20:R:38:LEU:H	20:R:47:VAL:HB	1.84	0.42
1:X:1081:A:H62	1:X:1108:U:H4'	1.84	0.42
1:X:1492:A:N6	1:X:1531:C:C4	2.87	0.42
1:X:1666:G:H1	1:X:1991:C:N4	2.14	0.42
1:X:1703:C:H2'	1:X:1704:G:O4'	2.19	0.42
1:X:1969:G:N2	1:X:1970:G:C4	2.88	0.42
1:X:1988:A:C5'	1:X:1989:C:OP2	2.64	0.42
1:X:448:C:H5	1:X:449:C:C5	2.37	0.42
1:X:42:G:N2	1:X:450:C:C2	2.88	0.42
1:X:759:C:H1'	1:X:761:G:N2	2.35	0.42
1:X:817:A:C5'	1:X:818:G:OP1	2.68	0.42
2:Y:43:G:H5'	2:Y:44:C:H5'	2.01	0.42
2:Y:48:A:N6	2:Y:49:C:C4	2.88	0.42
2:Y:58:G:H5''	2:Y:59:A:OP1	2.19	0.42
1:X:2722:C:P	30:4:35:ARG:HH11	2.43	0.42
3:A:198:GLY:O	3:A:200:ALA:N	2.53	0.42
3:A:245:ARG:HA	3:A:253:LYS:NZ	2.35	0.42
3:A:71:ARG:HH22	3:A:150:PRO:CA	2.30	0.42
5:C:14:THR:HG22	5:C:15:ILE:N	2.33	0.42
5:C:149:LEU:HD11	5:C:170:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:43:ALA:C	11:I:45:LYS:N	2.72	0.42
16:N:39:LEU:HD23	16:N:39:LEU:HA	1.83	0.42
17:O:72:ARG:HA	17:O:82:ARG:O	2.20	0.42
19:Q:61:LYS:HA	19:Q:71:GLN:O	2.20	0.42
20:R:10:HIS:C	20:R:12:ASP:H	2.22	0.42
1:X:1255:A:C5	1:X:1256:C:C5	3.08	0.42
1:X:1299:A:N6	1:X:1342:U:C2	2.88	0.42
1:X:1379:A:H2'	1:X:1380:C:O4'	2.20	0.42
1:X:1744:G:N2	1:X:1746:A:H3'	2.35	0.42
1:X:1886:G:H2'	1:X:1887:G:C8	2.55	0.42
1:X:1947:G:HO2'	1:X:1950:C:P	2.42	0.42
1:X:2329:C:C3'	1:X:2329:C:C6	3.03	0.42
1:X:971:A:H61	12:J:83:ARG:NH2	2.13	0.42
10:H:10:VAL:HG23	10:H:17:ARG:C	2.39	0.41
10:H:116:ARG:NH1	15:M:38:LYS:CE	2.83	0.41
14:L:43:ILE:HG22	14:L:44:ASP:N	2.34	0.41
15:M:39:VAL:HG12	15:M:45:THR:CB	2.50	0.41
17:O:12:TYR:HB2	17:O:39:PHE:HB2	2.02	0.41
18:P:89:ARG:HG2	18:P:131:LYS:H	1.84	0.41
1:X:1455:C:H4'	1:X:1644:G:OP1	2.20	0.41
1:X:1674:C:H2'	1:X:1675:C:H6	1.84	0.41
1:X:2273:C:OP2	14:L:15:ARG:NH2	2.53	0.41
1:X:2312:A:H4'	1:X:2313:G:O5'	2.19	0.41
1:X:2417:U:O2'	1:X:2418:A:H5''	2.20	0.41
1:X:591:G:C3'	1:X:592:G:H8	2.33	0.41
1:X:758:G:H2'	1:X:759:C:OP1	2.20	0.41
1:X:791:G:H5'	3:A:49:ARG:NH2	2.35	0.41
26:Z:4:HIS:CD2	26:Z:4:HIS:H	2.38	0.41
1:X:2263:C:OP2	27:1:9:ILE:HD13	2.20	0.41
28:2:25:LYS:HE2	28:2:25:LYS:CA	2.51	0.41
29:3:13:ARG:NE	29:3:25:PHE:H	2.17	0.41
29:3:53:ALA:O	29:3:54:GLU:C	2.58	0.41
3:A:147:GLU:HG2	3:A:153:GLY:O	2.19	0.41
3:A:198:GLY:O	3:A:199:ASN:C	2.58	0.41
4:B:47:VAL:O	4:B:80:GLU:HA	2.20	0.41
5:C:17:LEU:HA	5:C:18:PRO:HD3	1.81	0.41
14:L:91:ARG:CD	14:L:91:ARG:H	2.33	0.41
15:M:85:SER:HA	15:M:86:PRO:HD3	1.89	0.41
16:N:24:PHE:O	16:N:29:SER:HB3	2.21	0.41
16:N:36:PHE:O	16:N:39:LEU:HB2	2.20	0.41
16:N:82:GLY:HA3	16:N:113:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:12:LYS:O	18:P:15:LYS:HB2	2.20	0.41
18:P:50:VAL:O	18:P:53:ALA:HB3	2.20	0.41
18:P:81:HIS:HD2	18:P:82:ASN:ND2	2.18	0.41
19:Q:52:GLY:HA3	19:Q:81:ARG:HB3	2.02	0.41
20:R:18:LYS:H	20:R:18:LYS:CD	2.21	0.41
21:S:120:LEU:CD2	21:S:120:LEU:C	2.88	0.41
21:S:51:LEU:N	21:S:51:LEU:HD23	2.28	0.41
1:X:1175:A:C2	1:X:1176:U:N3	2.88	0.41
1:X:1509:A:N7	1:X:1510:A:C5	2.88	0.41
1:X:1830:C:N3	1:X:1881:U:C5	2.88	0.41
1:X:192:G:C4'	1:X:193:A:H4'	2.49	0.41
1:X:1922:U:H5	1:X:1950:C:HO2'	1.66	0.41
1:X:1826:U:H4'	1:X:1952:A:C5	2.55	0.41
1:X:2324:G:OP2	27:1:40:TYR:CD2	2.73	0.41
1:X:1750:A:H4'	1:X:2695:C:O4'	2.20	0.41
1:X:2737:A:OP1	1:X:2737:A:H8	2.02	0.41
1:X:428:A:H2'	1:X:429:C:C6	2.55	0.41
1:X:448:C:C5	1:X:449:C:C5	3.07	0.41
1:X:615:C:H41	11:I:100:ARG:NH1	2.18	0.41
1:X:664:C:C6	1:X:666:U:H5	2.38	0.41
1:X:751:G:O2'	1:X:752:G:P	2.78	0.41
1:X:803:C:H4'	1:X:804:C:OP2	2.19	0.41
1:X:861:G:C2	1:X:943:U:H1'	2.55	0.41
2:Y:7:C:H2'	2:Y:8:C:C6	2.56	0.41
4:B:116:VAL:HG13	4:B:136:ARG:HE	1.85	0.41
5:C:108:ILE:HG23	5:C:112:GLN:HE21	1.85	0.41
6:D:4:LEU:O	6:D:5:LYS:HB3	2.21	0.41
10:H:116:ARG:HH21	15:M:40:ARG:HB2	1.85	0.41
10:H:29:ILE:HG21	10:H:123:PHE:HE1	1.84	0.41
13:K:18:VAL:O	13:K:19:ALA:C	2.56	0.41
14:L:60:LYS:HG3	14:L:64:LYS:HZ3	1.85	0.41
18:P:50:VAL:O	18:P:54:GLU:HG3	2.21	0.41
1:X:1769:U:C5	1:X:1775:A:C4	3.08	0.41
1:X:1834:G:C2	1:X:1884:A:C6	3.08	0.41
1:X:2340:C:O3'	29:3:28:GLY:HA2	2.20	0.41
1:X:2695:C:H2'	1:X:2696:A:C8	2.52	0.41
1:X:2665:G:C2	1:X:2704:U:O2	2.73	0.41
1:X:2660:C:C2	1:X:2707:G:N2	2.88	0.41
1:X:2617:G:C5	1:X:2755:A:C6	3.07	0.41
2:Y:91:A:H2'	2:Y:92:G:C8	2.55	0.41
27:1:17:GLY:O	27:1:18:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:476:G:O4'	28:2:16:HIS:CE1	2.73	0.41
3:A:232:HIS:CG	3:A:233:PRO:HD2	2.55	0.41
3:A:59:HIS:O	3:A:60:LYS:C	2.58	0.41
5:C:150:LEU:HD13	5:C:167:VAL:HB	2.03	0.41
1:X:825:C:C5'	11:I:30:ALA:HB1	2.49	0.41
13:K:76:VAL:O	13:K:79:VAL:HG13	2.20	0.41
16:N:74:MET:HE3	16:N:78:THR:HG22	2.02	0.41
1:X:1354:A:H4'	19:Q:56:MET:HG2	2.02	0.41
21:S:92:VAL:HG22	21:S:93:GLU:N	2.36	0.41
22:T:56:ASP:O	22:T:57:HIS:HB2	2.21	0.41
1:X:1277:G:H8	1:X:1277:G:O5'	2.02	0.41
1:X:1356:G:H5'	1:X:1614:C:OP2	2.20	0.41
1:X:169:C:H2'	1:X:170:U:H5'	2.03	0.41
1:X:1744:G:HO2'	1:X:1745:C:H6	1.67	0.41
1:X:2000:U:O2	26:Z:10:LYS:HB2	2.19	0.41
1:X:2426:G:C8	1:X:2479:U:H6	2.39	0.41
1:X:1937:G:H1'	1:X:2530:C:H4'	2.02	0.41
1:X:2651:U:C2'	1:X:2652:G:O5'	2.68	0.41
1:X:1061:A:C2	1:X:2731:G:C2	3.08	0.41
1:X:459:A:H2	1:X:466:A:H2'	1.84	0.41
1:X:578:U:H5''	1:X:579:G:OP2	2.20	0.41
1:X:686:C:H2'	1:X:687:G:H5'	2.02	0.41
1:X:742:G:O2'	1:X:776:G:H4'	2.20	0.41
1:X:771:C:O2'	1:X:772:G:H5'	2.21	0.41
1:X:968:C:C4	1:X:970:A:C5	3.09	0.41
1:X:99:U:H3'	1:X:100:G:C5'	2.50	0.41
2:Y:45:C:O2	6:D:90:THR:HB	2.20	0.41
3:A:122:PRO:HG2	3:A:123:GLU:OE1	2.20	0.41
4:B:124:GLY:HA3	4:B:135:HIS:O	2.20	0.41
5:C:133:PHE:O	5:C:136:TRP:HB3	2.20	0.41
5:C:158:ARG:O	5:C:159:ARG:C	2.58	0.41
12:J:11:ARG:HB3	12:J:12:LYS:H	1.48	0.41
12:J:59:PHE:O	12:J:60:ARG:C	2.59	0.41
15:M:28:ARG:CB	15:M:29:PRO:CD	2.88	0.41
15:M:33:VAL:CG2	15:M:51:GLU:HB2	2.36	0.41
16:N:25:TRP:O	16:N:28:ARG:HB2	2.21	0.41
17:O:80:TYR:CE2	17:O:82:ARG:CZ	3.03	0.41
18:P:36:ARG:O	18:P:39:ARG:HB2	2.21	0.41
20:R:14:LEU:HD22	20:R:16:PHE:CZ	2.56	0.41
22:T:69:PHE:C	22:T:70:ILE:HG13	2.40	0.41
1:X:1128:G:H3'	1:X:1129:A:C5'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1313:U:H4'	1:X:1314:A:C5'	2.50	0.41
1:X:1380:C:H42	1:X:1799:A:H2	1.68	0.41
1:X:1885:C:C4'	3:A:245:ARG:HD2	2.50	0.41
1:X:201:G:H2'	1:X:202:A:C8	2.55	0.41
1:X:2572:U:H2'	1:X:2573:C:C6	2.56	0.41
31:X:2881:LMA:C12	31:X:2881:LMA:O55	2.68	0.41
1:X:404:A:N7	1:X:405:C:C4	2.89	0.41
1:X:30:G:C6	1:X:521:U:O2	2.74	0.41
1:X:788:G:C4	1:X:807:A:C8	3.09	0.41
1:X:88:G:C8	1:X:89:A:H8	2.37	0.41
30:4:15:LYS:HB2	30:4:26:ILE:CG1	2.50	0.41
1:X:1810:U:OP1	3:A:159:SER:HB3	2.21	0.41
4:B:5:LEU:HD13	4:B:49:ILE:HD13	2.03	0.41
5:C:117:LEU:HD23	5:C:117:LEU:C	2.41	0.41
7:E:7:GLN:H	7:E:8:PRO:CD	2.34	0.41
9:G:49:VAL:HG12	9:G:50:PRO:O	2.20	0.41
12:J:78:LYS:HA	12:J:88:LYS:NZ	2.36	0.41
20:R:22:VAL:HG13	20:R:81:VAL:C	2.38	0.41
20:R:24:VAL:HG11	20:R:28:LYS:O	2.20	0.41
24:V:15:ALA:O	24:V:18:ILE:HB	2.21	0.41
1:X:1049:C:C2	1:X:1129:A:C2	3.08	0.41
1:X:1373:G:H2'	1:X:1374:G:H5'	2.02	0.41
1:X:1467:U:H6	1:X:1467:U:C3'	2.34	0.41
1:X:1607:A:HO2'	1:X:1608:U:H6	1.68	0.41
1:X:1742:G:C6	1:X:1743:C:N4	2.89	0.41
1:X:1770:U:O2	1:X:1774:A:N6	2.54	0.41
1:X:1830:C:C4	1:X:1881:U:C5	3.09	0.41
1:X:2221:G:H2'	1:X:2222:U:O5'	2.20	0.41
1:X:2382:C:N3	1:X:2394:G:C2	2.88	0.41
1:X:2664:G:C2	1:X:2665:G:C8	3.09	0.41
1:X:2796:A:C2	1:X:2797:G:C5	3.08	0.41
1:X:459:A:H1'	1:X:461:A:H62	1.85	0.41
1:X:539:A:C6	1:X:2025:A:N3	2.88	0.41
1:X:614:G:C4	1:X:636:G:C2	3.09	0.41
1:X:814:G:OP2	5:C:56:ARG:CZ	2.69	0.41
1:X:931:G:H2'	1:X:932:G:O4'	2.20	0.41
3:A:211:GLY:C	3:A:213:SER:N	2.68	0.41
1:X:777:A:N3	3:A:214:ARG:NH1	2.68	0.41
3:A:220:PRO:O	3:A:221:HIS:O	2.38	0.41
3:A:247:PRO:HD3	3:A:253:LYS:HG3	2.03	0.41
4:B:116:VAL:CG2	4:B:136:ARG:CG	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:15:TRP:CD1	15:M:86:PRO:HD3	2.56	0.41
1:X:1268:U:H2'	5:C:66:ASN:HA	2.03	0.41
5:C:74:VAL:HA	5:C:75:PRO:HD3	1.84	0.41
7:E:136:ILE:N	7:E:136:ILE:HD12	2.35	0.41
7:E:156:ALA:O	7:E:157:TYR:CG	2.74	0.41
7:E:16:THR:O	7:E:26:VAL:HA	2.21	0.41
14:L:60:LYS:HZ2	14:L:64:LYS:CE	2.33	0.41
15:M:101:ARG:HH21	15:M:101:ARG:HG2	1.85	0.41
1:X:1276:U:C1'	26:Z:10:LYS:HG3	2.51	0.41
1:X:1290:A:H5''	13:K:40:LYS:NZ	2.35	0.41
1:X:1312:G:H5''	1:X:1313:U:P	2.61	0.41
1:X:173:A:O2'	1:X:2051:U:H5	2.03	0.41
1:X:1757:C:O2'	1:X:1758:C:H5'	2.20	0.41
1:X:1926:U:C1'	1:X:1928:G:H5'	2.51	0.41
1:X:1932:G:N2	1:X:1941:C:C2	2.89	0.41
1:X:1970:G:N2	1:X:1971:C:C2	2.89	0.41
1:X:2291:U:H2'	6:D:37:ASN:HD21	1.86	0.41
1:X:2405:A:H4'	1:X:2406:C:OP2	2.21	0.41
1:X:2863:U:O5'	1:X:2863:U:H6	2.04	0.41
1:X:2:G:O2'	1:X:3:U:H5'	2.20	0.41
1:X:646:C:O2'	1:X:650:U:H5''	2.21	0.41
11:I:61:PRO:CD	29:3:27:SER:HB3	2.46	0.41
3:A:178:LEU:C	3:A:180:SER:H	2.24	0.41
3:A:87:PRO:O	3:A:88:ASN:CB	2.65	0.41
4:B:101:LYS:HA	4:B:170:LEU:O	2.20	0.41
13:K:37:THR:OG1	13:K:40:LYS:HG3	2.20	0.41
13:K:54:THR:HG22	13:K:55:ALA:N	2.36	0.41
13:K:72:ASP:C	13:K:72:ASP:OD2	2.59	0.41
14:L:10:LYS:O	14:L:14:ARG:HG3	2.20	0.41
14:L:12:ARG:HG3	14:L:13:THR:HG23	2.02	0.41
14:L:73:LYS:O	14:L:74:ALA:C	2.59	0.41
19:Q:68:PHE:O	19:Q:69:ILE:O	2.38	0.41
22:T:43:THR:O	22:T:43:THR:CG2	2.55	0.41
1:X:1031:C:O2'	1:X:1032:A:OP2	2.30	0.41
1:X:1265:G:O2'	1:X:1266:G:C8	2.73	0.41
1:X:1974:U:C2'	1:X:1975:G:H5''	2.51	0.41
1:X:2441:U:H2'	1:X:2442:C:H6	1.83	0.41
1:X:2445:C:N4	1:X:2446:C:N4	2.69	0.41
1:X:2454:C:H42	1:X:2508:G:H22	1.68	0.41
1:X:1773:C:H1'	1:X:2588:U:C5'	2.51	0.41
1:X:2668:U:O2	1:X:2693:U:O5'	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:395:G:N3	1:X:406:G:N2	2.69	0.41
1:X:465:C:C2	1:X:467:U:C5	3.08	0.41
1:X:600:G:H2'	1:X:601:A:OP1	2.21	0.41
1:X:849:G:C5	1:X:850:C:C4	3.09	0.41
1:X:967:G:O6	12:J:17:ARG:CZ	2.69	0.41
2:Y:58:G:H5''	2:Y:59:A:P	2.60	0.41
27:1:14:SER:HB2	27:1:23:THR:N	2.35	0.41
1:X:696:U:H5'	28:2:30:ILE:HD11	2.02	0.41
4:B:50:GLY:HA2	4:B:77:ILE:O	2.21	0.41
1:X:334:G:C2	5:C:162:ARG:NH2	2.89	0.41
11:I:56:LEU:HB3	29:3:52:LYS:NZ	2.35	0.41
14:L:24:SER:C	14:L:26:ARG:H	2.23	0.41
15:M:5:ILE:N	15:M:5:ILE:HD12	2.36	0.41
21:S:13:LYS:HB2	21:S:13:LYS:HZ2	1.82	0.41
1:X:1042:G:H4'	30:4:6:SER:OG	2.21	0.41
1:X:105:G:H2'	1:X:106:G:H5'	2.02	0.41
1:X:123:A:C2	28:2:10:ARG:HA	2.56	0.41
1:X:1770:U:C2	1:X:1774:A:N7	2.89	0.41
1:X:1976:U:H4'	4:B:128:SER:HB3	2.02	0.41
1:X:2015:G:O4'	1:X:2015:G:P	2.79	0.41
1:X:2505:G:H1'	30:4:1:MET:CB	2.51	0.41
1:X:2594:U:H2'	1:X:2595:C:C6	2.56	0.41
1:X:2673:G:N3	1:X:2674:C:C6	2.89	0.41
1:X:496:C:H2'	1:X:497:C:H5'	2.02	0.41
1:X:579:G:H1'	1:X:994:A:N6	2.36	0.41
1:X:638:A:H4'	1:X:639:G:OP1	2.21	0.41
1:X:872:G:O2'	1:X:928:G:O6	2.36	0.41
3:A:146:LEU:HB3	3:A:156:LEU:HB2	2.02	0.41
3:A:39:PRO:HA	3:A:62:LEU:HD22	2.03	0.41
6:D:146:VAL:HB	6:D:147:ASP:H	1.62	0.41
15:M:13:LEU:HD12	15:M:13:LEU:N	2.35	0.41
15:M:83:PHE:N	15:M:83:PHE:HD1	2.19	0.41
16:N:14:HIS:CD2	16:N:32:TYR:CD2	3.09	0.41
18:P:37:LYS:O	18:P:40:LEU:N	2.54	0.41
19:Q:62:ARG:HB2	19:Q:63:LYS:H	1.74	0.41
21:S:149:ALA:HB1	21:S:160:LEU:HD13	2.02	0.41
22:T:12:ASN:HD22	22:T:14:ARG:HD3	1.86	0.41
22:T:18:PRO:O	22:T:19:LYS:O	2.38	0.41
1:X:1129:A:C5	1:X:1130:U:N3	2.89	0.41
1:X:1345:G:C5	1:X:1625:A:C6	3.08	0.41
1:X:1399:C:H2'	1:X:1400:A:C8	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1478:U:C2	1:X:1479:G:C8	3.09	0.41
1:X:1550:C:O2'	1:X:1551:U:H5''	2.20	0.41
1:X:1433:A:C5	1:X:1595:A:H2	2.39	0.41
1:X:1745:C:C2'	1:X:1746:A:O4'	2.66	0.41
1:X:1978:U:C2	1:X:1979:C:H5	2.34	0.41
1:X:2031:A:C6	1:X:2600:A:N1	2.89	0.41
1:X:2194:A:H3'	1:X:2195:C:C5'	2.41	0.41
1:X:2432:A:H2'	1:X:2433:G:C8	2.55	0.41
1:X:2477:C:O2'	1:X:2478:C:H5'	2.21	0.41
1:X:1938:U:O2'	1:X:2531:U:H5'	2.21	0.41
1:X:2691:C:O2'	1:X:2692:A:C5'	2.69	0.41
1:X:2736:U:C3'	30:4:19:ARG:HA	2.51	0.41
1:X:2762:G:H2'	1:X:2762:G:N3	2.35	0.41
1:X:2827:G:C6	1:X:2828:C:N3	2.88	0.41
1:X:14:A:C6	1:X:536:A:C2	3.08	0.41
26:Z:30:LEU:HD23	26:Z:30:LEU:HA	1.91	0.41
27:1:41:ASP:OD2	27:1:46:LYS:HD2	2.21	0.41
29:3:13:ARG:HG3	29:3:13:ARG:O	2.21	0.41
3:A:219:LYS:HD2	3:A:220:PRO:O	2.20	0.41
4:B:146:THR:CB	4:B:147:PRO:HD2	2.41	0.41
5:C:95:LEU:C	5:C:95:LEU:HD23	2.40	0.41
10:H:20:MET:O	10:H:53:ALA:HB1	2.21	0.41
12:J:68:ARG:O	12:J:102:ARG:NH2	2.54	0.41
12:J:17:ARG:O	12:J:18:MET:HB2	2.21	0.41
14:L:29:LEU:HD12	14:L:41:GLN:O	2.20	0.41
18:P:40:LEU:HD23	18:P:40:LEU:HA	1.87	0.41
20:R:16:PHE:HB3	20:R:82:ALA:HB1	2.02	0.41
24:V:25:LEU:HD13	24:V:46:LEU:CD1	2.48	0.41
1:X:1147:G:C4	1:X:1148:G:C8	3.09	0.41
1:X:1698:C:H1'	1:X:1753:A:H2'	2.03	0.41
1:X:1923:U:C4'	1:X:1924:C:O5'	2.69	0.41
1:X:2182:A:C2	1:X:2204:A:C2	3.09	0.41
1:X:965:G:O2'	1:X:2253:A:N1	2.45	0.41
1:X:82:G:H21	1:X:83:A:N6	2.20	0.41
1:X:934:G:H1'	22:T:26:PHE:CD1	2.56	0.41
2:Y:83:C:H2'	2:Y:84:G:O4'	2.21	0.41
6:D:30:ARG:O	6:D:158:THR:HB	2.20	0.40
4:B:152:LYS:HB2	9:G:106:TYR:HB3	2.01	0.40
10:H:73:VAL:O	10:H:96:ALA:HB1	2.21	0.40
1:X:1300:A:C8	13:K:106:ASP:OD2	2.74	0.40
16:N:72:HIS:CD2	16:N:110:VAL:HG21	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:13:ARG:O	16:N:16:LYS:HB2	2.21	0.40
17:O:5:ILE:HB	17:O:6:GLN:H	1.67	0.40
20:R:55:THR:OG1	20:R:56:LYS:N	2.53	0.40
20:R:5:SER:O	20:R:6:ALA:O	2.39	0.40
1:X:1033:G:N2	1:X:1035:G:N2	2.69	0.40
1:X:1174:G:N3	1:X:1175:A:C8	2.89	0.40
1:X:1625:A:H1'	1:X:1632:A:H1'	2.02	0.40
1:X:1672:A:O2'	4:B:115:GLY:HA2	2.20	0.40
1:X:1761:G:H2'	1:X:1762:C:H6	1.86	0.40
1:X:1950:C:C4	1:X:1951:G:N7	2.89	0.40
1:X:2043:A:C1'	1:X:2481:G:O4'	2.69	0.40
1:X:2705:A:N6	1:X:2707:G:N2	2.69	0.40
2:Y:26:G:N3	2:Y:58:G:C6	2.90	0.40
27:1:12:MET:HB2	27:1:27:ASN:OD1	2.20	0.40
3:A:54:PHE:HA	3:A:218:ARG:HH21	1.86	0.40
5:C:23:ASN:HB3	5:C:26:VAL:CG2	2.52	0.40
14:L:99:ARG:HG3	14:L:100:VAL:N	2.36	0.40
15:M:66:PHE:HD2	15:M:83:PHE:HE1	1.65	0.40
18:P:62:ARG:O	18:P:65:SER:HB2	2.20	0.40
20:R:16:PHE:CZ	20:R:46:VAL:CG2	3.04	0.40
1:X:1202:U:O2'	1:X:1203:A:H5'	2.21	0.40
1:X:573:C:HO2'	1:X:1266:G:H1	1.69	0.40
1:X:1281:A:H2'	1:X:1282:A:O4'	2.21	0.40
1:X:1475:U:H3'	1:X:1475:U:H6	1.86	0.40
1:X:1978:U:C2'	1:X:1979:C:OP1	2.69	0.40
1:X:2002:A:N7	26:Z:9:LYS:NZ	2.63	0.40
1:X:2041:A:N1	31:X:2881:LMA:C40	2.84	0.40
1:X:2043:A:O2'	1:X:2044:G:H5'	2.20	0.40
1:X:2282:G:N3	1:X:2293:G:N2	2.69	0.40
1:X:2756:A:OP1	1:X:2756:A:H3'	2.21	0.40
1:X:334:G:H4'	1:X:335:A:C5'	2.51	0.40
1:X:59:G:O6	1:X:62:U:N3	2.55	0.40
1:X:760:U:C5	26:Z:3:LYS:CE	3.03	0.40
1:X:769:C:C4	1:X:770:U:C4	3.09	0.40
1:X:824:U:H1'	1:X:1264:C:O4'	2.21	0.40
4:B:136:ARG:NH2	4:B:157:ALA:HB2	2.37	0.40
1:X:2753:C:H5''	4:B:164:ARG:HG2	2.02	0.40
11:I:108:LEU:HD22	11:I:120:VAL:HG11	2.03	0.40
12:J:29:ALA:O	12:J:106:GLU:HG3	2.21	0.40
13:K:29:LEU:HD23	13:K:29:LEU:HA	1.90	0.40
1:X:2273:C:OP1	14:L:95:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:24:LEU:HD11	15:M:34:ARG:NH2	2.37	0.40
20:R:83:LEU:O	20:R:90:LYS:HE2	2.20	0.40
21:S:163:ASP:HA	21:S:164:PRO:HD3	1.88	0.40
24:V:2:LYS:N	24:V:3:PRO:CD	2.84	0.40
1:X:1814:G:H2'	1:X:1815:G:H8	1.86	0.40
1:X:2013:A:H5''	1:X:2014:A:OP1	2.21	0.40
1:X:2665:G:C6	1:X:2666:U:C4	3.09	0.40
1:X:2765:C:O2'	1:X:2766:U:H5'	2.21	0.40
1:X:2609:G:N3	1:X:2868:G:C2	2.89	0.40
1:X:514:G:N3	1:X:514:G:C2'	2.84	0.40
1:X:617:U:O4'	1:X:617:U:O2	2.40	0.40
1:X:75:C:C2'	1:X:76:C:H5'	2.51	0.40
1:X:2264:C:C4	27:1:28:ARG:NH2	2.89	0.40
29:3:13:ARG:HH12	29:3:26:LYS:N	2.19	0.40
3:A:132:LEU:HD23	3:A:132:LEU:N	2.36	0.40
3:A:207:LEU:O	3:A:212:ARG:HB3	2.21	0.40
3:A:234:HIS:CE1	3:A:253:LYS:NZ	2.90	0.40
3:A:69:LYS:HG2	3:A:70:ARG:N	2.36	0.40
5:C:149:LEU:HD11	5:C:170:LEU:HB2	2.02	0.40
5:C:39:ARG:HH21	5:C:91:TYR:HB2	1.87	0.40
9:G:46:ALA:HB1	9:G:54:LEU:HD22	2.03	0.40
9:G:90:LEU:HD12	9:G:90:LEU:N	2.36	0.40
10:H:134:LEU:HD23	10:H:134:LEU:HA	1.81	0.40
10:H:4:PRO:O	10:H:5:GLN:CB	2.69	0.40
12:J:64:LYS:HZ1	12:J:110:VAL:HG13	1.84	0.40
17:O:36:LYS:HE3	17:O:55:THR:C	2.41	0.40
20:R:44:GLN:HE21	20:R:78:ALA:HB2	1.86	0.40
20:R:48:VAL:O	20:R:50:GLY:N	2.54	0.40
22:T:32:LYS:N	22:T:35:ASN:HD22	2.20	0.40
23:U:39:LYS:O	23:U:40:ARG:HB2	2.22	0.40
1:X:1468:A:O5'	1:X:1468:A:H8	2.05	0.40
1:X:1537:U:O2'	1:X:1538:A:H5'	2.22	0.40
1:X:1609:G:H2'	1:X:1610:A:O4'	2.21	0.40
1:X:1652:G:H2'	1:X:1653:C:C6	2.56	0.40
1:X:1683:G:C2'	1:X:1684:G:H5'	2.51	0.40
1:X:1725:C:H42	1:X:1741:G:H1	1.70	0.40
1:X:1841:G:H2'	1:X:1842:G:H5'	2.04	0.40
1:X:1947:G:N1	1:X:1950:C:C4	2.89	0.40
1:X:2059:U:H5	1:X:2575:U:O2	2.05	0.40
1:X:2348:A:O2'	1:X:2349:G:H5'	2.21	0.40
1:X:2625:U:H2'	1:X:2626:U:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2614:A:C2	1:X:2764:U:N3	2.90	0.40
1:X:2817:A:C2	1:X:2851:G:C2	3.10	0.40
1:X:2819:G:H2'	1:X:2820:C:C6	2.55	0.40
1:X:448:C:C5	1:X:449:C:C4	3.03	0.40
1:X:521:U:C4	1:X:522:G:C2	3.10	0.40
1:X:688:A:N6	1:X:689:A:N6	2.69	0.40
1:X:784:U:H2'	1:X:785:U:C6	2.57	0.40
2:Y:55:C:H2'	2:Y:56:G:O4'	2.21	0.40
28:2:34:ARG:HH11	28:2:42:LEU:CG	2.34	0.40
29:3:49:VAL:HB	29:3:52:LYS:HG2	2.03	0.40
4:B:116:VAL:CG2	4:B:136:ARG:HG3	2.52	0.40
4:B:49:ILE:HD13	4:B:49:ILE:HG21	1.85	0.40
6:D:41:GLY:HA2	6:D:44:LYS:O	2.21	0.40
9:G:75:ILE:HG23	9:G:140:GLN:HE21	1.86	0.40
10:H:55:VAL:HG12	10:H:56:LYS:N	2.36	0.40
11:I:45:LYS:HE3	11:I:47:ALA:HB3	2.03	0.40
11:I:77:LEU:HD22	11:I:110:ALA:HA	2.03	0.40
12:J:64:LYS:CD	12:J:108:ALA:O	2.70	0.40
1:X:1261:G:O2'	16:N:3:ARG:HA	2.22	0.40
18:P:42:VAL:O	18:P:44:VAL:N	2.55	0.40
1:X:1742:G:C2	1:X:1743:C:N3	2.89	0.40
1:X:177:U:H4'	23:U:40:ARG:HG3	2.03	0.40
1:X:1951:G:O2'	1:X:1952:A:O5'	2.30	0.40
1:X:2046:C:C5	1:X:2047:C:C4	3.09	0.40
1:X:2557:G:O2'	1:X:2558:C:H5'	2.21	0.40
1:X:2659:C:C2	1:X:2660:C:C5	3.09	0.40
1:X:2751:C:H2'	1:X:2752:C:H6	1.87	0.40
1:X:5:A:C2	1:X:2873:G:C2	3.10	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	251/274 (92%)	195 (78%)	44 (18%)	12 (5%)	2	15
4	B	203/211 (96%)	160 (79%)	29 (14%)	14 (7%)	1	7
5	C	192/205 (94%)	143 (74%)	37 (19%)	12 (6%)	1	9
6	D	175/180 (97%)	137 (78%)	32 (18%)	6 (3%)	3	22
7	E	169/185 (91%)	142 (84%)	20 (12%)	7 (4%)	3	18
8	F	61/144 (42%)	48 (79%)	12 (20%)	1 (2%)	9	40
9	G	140/174 (80%)	104 (74%)	27 (19%)	9 (6%)	1	9
10	H	132/134 (98%)	111 (84%)	17 (13%)	4 (3%)	4	25
11	I	132/156 (85%)	82 (62%)	31 (24%)	19 (14%)	0	1
12	J	134/141 (95%)	96 (72%)	27 (20%)	11 (8%)	1	5
13	K	111/116 (96%)	89 (80%)	14 (13%)	8 (7%)	1	6
14	L	102/114 (90%)	73 (72%)	26 (26%)	3 (3%)	4	25
15	M	106/166 (64%)	82 (77%)	18 (17%)	6 (6%)	1	12
16	N	115/118 (98%)	95 (83%)	16 (14%)	4 (4%)	3	21
17	O	92/100 (92%)	68 (74%)	17 (18%)	7 (8%)	1	6
18	P	124/134 (92%)	101 (82%)	18 (14%)	5 (4%)	3	18
19	Q	91/95 (96%)	63 (69%)	19 (21%)	9 (10%)	0	3
20	R	108/115 (94%)	70 (65%)	26 (24%)	12 (11%)	0	2
21	S	173/237 (73%)	135 (78%)	32 (18%)	6 (4%)	3	21
22	T	72/91 (79%)	53 (74%)	18 (25%)	1 (1%)	11	43
23	U	70/81 (86%)	50 (71%)	13 (19%)	7 (10%)	0	3
24	V	63/67 (94%)	55 (87%)	5 (8%)	3 (5%)	2	15
25	W	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
26	Z	55/60 (92%)	42 (76%)	9 (16%)	4 (7%)	1	6
27	1	51/55 (93%)	30 (59%)	15 (29%)	6 (12%)	0	2
28	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	2	16
29	3	57/66 (86%)	34 (60%)	18 (32%)	5 (9%)	1	4
30	4	35/37 (95%)	29 (83%)	6 (17%)	0	100	100
All	All	3111/3558 (87%)	2371 (76%)	557 (18%)	183 (6%)	1	11

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	220	PRO
3	A	221	HIS
3	A	248	VAL
4	B	135	HIS
4	B	147	PRO
4	B	148	GLY
4	B	202	ALA
5	C	9	GLN
5	C	68	ARG
10	H	42	LYS
10	H	115	ALA
11	I	36	GLY
11	I	58	ALA
12	J	21	ASP
13	K	6	ALA
13	K	91	PRO
13	K	100	VAL
15	M	17	GLU
16	N	5	LYS
16	N	94	VAL
19	Q	59	PRO
19	Q	61	LYS
19	Q	69	ILE
19	Q	83	ALA
20	R	6	ALA
20	R	60	PRO
24	V	3	PRO
27	1	9	ILE
27	1	30	ASN
28	2	42	LEU
29	3	14	ILE
29	3	60	LEU
3	A	47	ARG
3	A	48	GLY
3	A	152	LYS
4	B	123	ALA
4	B	132	LYS
5	C	22	VAL
5	C	121	ASP
7	E	165	VAL
8	F	120	VAL
9	G	68	PRO
9	G	170	PRO

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Mol	Chain	Res	Type
11	I	38	LYS
11	I	44	GLY
11	I	53	ARG
11	I	86	THR
11	I	88	PHE
12	J	13	GLN
12	J	26	ASP
12	J	83	ARG
12	J	136	GLU
13	K	20	LEU
13	K	93	GLY
14	L	45	ASP
15	M	28	ARG
15	M	105	TYR
16	N	8	ILE
17	O	8	GLY
17	O	80	TYR
18	P	32	ARG
18	P	46	ARG
19	Q	63	LYS
19	Q	74	ASP
19	Q	87	SER
20	R	26	SER
20	R	63	THR
20	R	94	VAL
21	S	26	LYS
21	S	91	PRO
22	T	19	LYS
23	U	16	ASN
23	U	31	GLY
23	U	60	VAL
26	Z	37	HIS
27	1	34	LYS
27	1	42	PRO
29	3	31	HIS
3	A	157	ALA
5	C	128	ALA
5	C	159	ARG
7	E	55	PRO
7	E	173	ALA
10	H	27	SER
10	H	116	ARG

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Mol	Chain	Res	Type
11	I	33	GLY
12	J	10	PHE
12	J	17	ARG
13	K	7	GLY
15	M	29	PRO
16	N	92	ARG
17	O	25	LEU
17	O	79	GLN
18	P	43	ASP
20	R	5	SER
21	S	87	THR
21	S	88	TYR
23	U	15	VAL
27	1	31	THR
28	2	8	ASN
29	3	32	GLN
3	A	56	GLY
3	A	126	PRO
3	A	253	LYS
4	B	14	ILE
4	B	122	PHE
4	B	137	ARG
5	C	10	ASN
5	C	67	ALA
6	D	146	VAL
7	E	7	GLN
7	E	12	PRO
9	G	67	ARG
9	G	97	ASP
11	I	30	ALA
11	I	65	PHE
11	I	81	GLN
11	I	91	ASP
12	J	79	PRO
12	J	139	ASP
13	K	13	ASN
14	L	60	LYS
15	M	25	PRO
17	O	24	SER
19	Q	65	VAL
20	R	49	GLU
20	R	85	ASP

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Mol	Chain	Res	Type
21	S	7	PRO
21	S	156	GLU
23	U	30	VAL
23	U	39	LYS
24	V	10	GLN
3	A	55	ILE
3	A	113	THR
4	B	43	GLY
4	B	95	ILE
4	B	115	GLY
4	B	136	ARG
5	C	15	ILE
6	D	21	GLY
6	D	52	LYS
9	G	107	GLN
9	G	108	GLY
9	G	118	ALA
9	G	163	PRO
11	I	37	GLN
11	I	57	ILE
11	I	68	VAL
12	J	111	THR
13	K	56	LYS
14	L	53	ALA
17	O	10	LYS
18	P	20	LEU
20	R	7	GLY
20	R	83	LEU
29	3	13	ARG
6	D	77	PHE
6	D	122	PHE
11	I	63	ARG
12	J	18	MET
15	M	83	PHE
17	O	66	GLY
26	Z	53	ASP
11	I	31	GLY
11	I	61	PRO
18	P	132	GLY
4	B	124	GLY
5	C	78	VAL
6	D	174	GLY

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Mol	Chain	Res	Type
7	E	118	PRO
9	G	64	GLY
23	U	14	VAL
24	V	18	ILE
5	C	175	VAL
20	R	51	VAL
20	R	65	PRO
26	Z	4	HIS
26	Z	5	PRO
5	C	103	GLY
7	E	107	ILE
11	I	122	VAL
19	Q	60	GLY
27	1	49	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	194/215 (90%)	184 (95%)	10 (5%)	23	56
4	B	155/157 (99%)	149 (96%)	6 (4%)	32	65
5	C	154/163 (94%)	147 (96%)	7 (4%)	27	61
6	D	153/156 (98%)	150 (98%)	3 (2%)	55	78
7	E	136/144 (94%)	136 (100%)	0	100	100
8	F	46/107 (43%)	46 (100%)	0	100	100
9	G	118/146 (81%)	115 (98%)	3 (2%)	47	74
10	H	103/103 (100%)	94 (91%)	9 (9%)	10	35
11	I	101/121 (84%)	97 (96%)	4 (4%)	31	64
12	J	110/115 (96%)	108 (98%)	2 (2%)	59	80
13	K	90/93 (97%)	82 (91%)	8 (9%)	9	34
14	L	74/82 (90%)	68 (92%)	6 (8%)	11	39
15	M	94/134 (70%)	87 (93%)	7 (7%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	96/97 (99%)	93 (97%)	3 (3%)	40	70
17	O	75/79 (95%)	72 (96%)	3 (4%)	31	64
18	P	108/115 (94%)	101 (94%)	7 (6%)	17	49
19	Q	75/76 (99%)	70 (93%)	5 (7%)	16	47
20	R	91/96 (95%)	84 (92%)	7 (8%)	13	41
21	S	149/192 (78%)	146 (98%)	3 (2%)	55	78
22	T	55/67 (82%)	53 (96%)	2 (4%)	35	66
23	U	57/66 (86%)	55 (96%)	2 (4%)	36	67
24	V	53/55 (96%)	53 (100%)	0	100	100
25	W	48/48 (100%)	48 (100%)	0	100	100
26	Z	51/53 (96%)	47 (92%)	4 (8%)	12	41
27	1	46/48 (96%)	41 (89%)	5 (11%)	6	25
28	2	39/40 (98%)	33 (85%)	6 (15%)	2	12
29	3	46/52 (88%)	43 (94%)	3 (6%)	17	49
30	4	35/35 (100%)	35 (100%)	0	100	100
All	All	2552/2855 (89%)	2437 (96%)	115 (4%)	27	61

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	44	ARG
3	A	49	ARG
3	A	69	LYS
3	A	165	GLN
3	A	199	ASN
3	A	202	HIS
3	A	209	LYS
3	A	219	LYS
3	A	245	ARG
3	A	246	VAL
4	B	44	TYR
4	B	75	THR
4	B	87	ASP
4	B	119	ARG
4	B	137	ARG
4	B	154	LYS
5	C	31	VAL

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Mol	Chain	Res	Type
5	C	62	LYS
5	C	71	ASP
5	C	74	VAL
5	C	91	TYR
5	C	163	ASN
5	C	180	ILE
6	D	51	ASP
6	D	80	ARG
6	D	112	ARG
9	G	104	THR
9	G	113	GLU
9	G	154	GLU
10	H	1	MET
10	H	8	LEU
10	H	9	ASP
10	H	10	VAL
10	H	23	ARG
10	H	29	ILE
10	H	41	ASN
10	H	81	ILE
10	H	109	ARG
11	I	39	SER
11	I	49	PHE
11	I	53	ARG
11	I	60	LEU
12	J	8	THR
12	J	64	LYS
13	K	3	HIS
13	K	5	LYS
13	K	37	THR
13	K	48	VAL
13	K	71	HIS
13	K	91	PRO
13	K	95	THR
13	K	96	ARG
14	L	31	VAL
14	L	38	ILE
14	L	42	ILE
14	L	45	ASP
14	L	60	LYS
14	L	91	ARG
15	M	5	ILE

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Mol	Chain	Res	Type
15	M	20	HIS
15	M	25	PRO
15	M	31	ASP
15	M	85	SER
15	M	92	THR
15	M	98	LYS
16	N	22	LYS
16	N	30	LYS
16	N	93	LYS
17	O	5	ILE
17	O	18	ASP
17	O	87	ARG
18	P	32	ARG
18	P	36	ARG
18	P	39	ARG
18	P	65	SER
18	P	124	ILE
18	P	125	THR
18	P	126	ILE
19	Q	5	ASP
19	Q	7	LEU
19	Q	12	ILE
19	Q	36	THR
19	Q	62	ARG
20	R	10	HIS
20	R	11	ASN
20	R	15	HIS
20	R	18	LYS
20	R	55	THR
20	R	71	GLN
20	R	112	LYS
21	S	34	LEU
21	S	71	MET
21	S	82	ASP
22	T	15	ASP
22	T	64	ASP
23	U	32	ARG
23	U	78	ILE
26	Z	12	SER
26	Z	23	HIS
26	Z	41	LEU
26	Z	58	LEU

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Mol	Chain	Res	Type
27	1	8	ILE
27	1	15	SER
27	1	34	LYS
27	1	51	ARG
27	1	54	LYS
28	2	5	TYR
28	2	10	ARG
28	2	12	ARG
28	2	14	LYS
28	2	15	THR
28	2	44	VAL
29	3	31	HIS
29	3	39	ASP
29	3	46	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	155	GLN
3	A	167	GLN
3	A	199	ASN
5	C	132	ASN
5	C	163	ASN
5	C	176	ASN
6	D	37	ASN
7	E	61	HIS
9	G	73	ASN
9	G	107	GLN
9	G	129	HIS
9	G	145	HIS
10	H	46	HIS
12	J	46	ASN
12	J	47	GLN
13	K	24	GLN
14	L	41	GLN
14	L	97	HIS
16	N	14	HIS
16	N	37	GLN
16	N	72	HIS
16	N	81	ASN
17	O	88	GLN
18	P	73	ASN

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Mol	Chain	Res	Type
18	P	81	HIS
18	P	82	ASN
20	R	29	HIS
20	R	71	GLN
21	S	121	GLN
22	T	12	ASN
22	T	35	ASN
26	Z	29	ASN
26	Z	44	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2647/2880 (91%)	473 (17%)	54 (2%)
2	Y	119/123 (96%)	18 (15%)	0
All	All	2766/3003 (92%)	491 (17%)	54 (1%)

All (491) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	13	A
1	X	14	A
1	X	34	U
1	X	35	G
1	X	39	C
1	X	45	C
1	X	49	U
1	X	59	G
1	X	63	A
1	X	70	A
1	X	74	G
1	X	76	C
1	X	83	A
1	X	87	G
1	X	88	G
1	X	89	A
1	X	90	G
1	X	98	U
1	X	100	G
1	X	101	A

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Mol	Chain	Res	Type
1	X	111	G
1	X	116	A
1	X	118	U
1	X	123	A
1	X	129	A
1	X	136	A
1	X	143	A
1	X	155	G
1	X	157	G
1	X	158	A
1	X	173	A
1	X	176	A
1	X	177	U
1	X	178	C
1	X	193	A
1	X	199	A
1	X	206	U
1	X	210	A
1	X	219	G
1	X	225	G
1	X	226	C
1	X	229	G
1	X	242	A
1	X	243	G
1	X	304	A
1	X	305	A
1	X	312	G
1	X	318	G
1	X	323	G
1	X	333	A
1	X	334	G
1	X	335	A
1	X	340	G
1	X	342	G
1	X	343	A
1	X	399	G
1	X	400	U
1	X	414	A
1	X	418	C
1	X	424	G
1	X	425	A
1	X	441	A

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Mol	Chain	Res	Type
1	X	456	C
1	X	460	U
1	X	463	C
1	X	467	U
1	X	468	A
1	X	469	G
1	X	482	A
1	X	484	G
1	X	491	A
1	X	492	G
1	X	497	C
1	X	515	A
1	X	537	C
1	X	538	A
1	X	539	A
1	X	540	G
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	556	A
1	X	557	U
1	X	572	G
1	X	578	U
1	X	581	A
1	X	582	G
1	X	583	C
1	X	584	A
1	X	587	A
1	X	595	A
1	X	602	C
1	X	613	A
1	X	614	G
1	X	624	A
1	X	625	A
1	X	626	A
1	X	627	A
1	X	628	A
1	X	631	G
1	X	633	G
1	X	636	G

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Mol	Chain	Res	Type
1	X	648	A
1	X	649	G
1	X	652	C
1	X	654	A
1	X	655	A
1	X	657	A
1	X	662	G
1	X	665	A
1	X	666	U
1	X	669	G
1	X	682	G
1	X	683	A
1	X	699	G
1	X	741	G
1	X	743	A
1	X	748	A
1	X	751	G
1	X	752	G
1	X	753	U
1	X	759	C
1	X	760	U
1	X	761	G
1	X	765	C
1	X	766	A
1	X	777	A
1	X	781	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	797	A
1	X	798	G
1	X	803	C
1	X	804	C
1	X	805	G
1	X	806	A
1	X	807	A
1	X	818	G
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	859	U

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Mol	Chain	Res	Type
1	X	919	U
1	X	921	A
1	X	922	A
1	X	926	C
1	X	939	C
1	X	940	G
1	X	944	A
1	X	952	A
1	X	956	A
1	X	957	G
1	X	969	U
1	X	970	A
1	X	972	C
1	X	983	G
1	X	984	A
1	X	985	G
1	X	994	A
1	X	1006	C
1	X	1007	A
1	X	1016	C
1	X	1019	U
1	X	1023	U
1	X	1032	A
1	X	1033	G
1	X	1037	U
1	X	1044	U
1	X	1051	U
1	X	1054	C
1	X	1056	U
1	X	1057	A
1	X	1058	G
1	X	1060	C
1	X	1070	G
1	X	1078	A
1	X	1081	A
1	X	1082	G
1	X	1087	C
1	X	1090	C
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1108	U

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Mol	Chain	Res	Type
1	X	1119	U
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1142	G
1	X	1145	C
1	X	1146	G
1	X	1148	G
1	X	1149	G
1	X	1152	C
1	X	1153	A
1	X	1167	A
1	X	1168	G
1	X	1183	C
1	X	1192	A
1	X	1220	G
1	X	1223	G
1	X	1224	A
1	X	1249	G
1	X	1250	A
1	X	1266	G
1	X	1269	G
1	X	1275	A
1	X	1278	A
1	X	1279	G
1	X	1282	A
1	X	1284	G
1	X	1285	A
1	X	1288	A
1	X	1289	A
1	X	1299	A
1	X	1301	U
1	X	1313	U
1	X	1314	A
1	X	1325	U
1	X	1326	U
1	X	1340	C
1	X	1342	U
1	X	1345	G
1	X	1358	C
1	X	1359	G
1	X	1378	A

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Mol	Chain	Res	Type
1	X	1381	G
1	X	1391	A
1	X	1392	U
1	X	1393	G
1	X	1398	G
1	X	1405	A
1	X	1409	U
1	X	1413	U
1	X	1428	G
1	X	1430	G
1	X	1432	G
1	X	1434	U
1	X	1440	G
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1475	U
1	X	1476	G
1	X	1482	U
1	X	1490	U
1	X	1497	C
1	X	1498	G
1	X	1506	C
1	X	1528	C
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1563	U
1	X	1570	C
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1585	A
1	X	1601	U
1	X	1602	G
1	X	1608	U

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Mol	Chain	Res	Type
1	X	1619	A
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1632	A
1	X	1634	A
1	X	1635	G
1	X	1648	C
1	X	1651	U
1	X	1656	U
1	X	1657	A
1	X	1665	C
1	X	1668	G
1	X	1677	C
1	X	1686	A
1	X	1691	G
1	X	1692	C
1	X	1701	C
1	X	1710	U
1	X	1712	G
1	X	1714	A
1	X	1717	A
1	X	1718	A
1	X	1747	G
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1775	A
1	X	1782	A
1	X	1790	G
1	X	1791	C
1	X	1793	A
1	X	1801	C
1	X	1802	A
1	X	1807	A
1	X	1808	C
1	X	1812	U
1	X	1821	A
1	X	1825	C
1	X	1831	G
1	X	1842	G
1	X	1868	A

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Mol	Chain	Res	Type
1	X	1884	A
1	X	1910	A
1	X	1919	A
1	X	1920	A
1	X	1921	A
1	X	1922	U
1	X	1923	U
1	X	1924	C
1	X	1927	U
1	X	1928	G
1	X	1938	U
1	X	1939	U
1	X	1947	G
1	X	1949	A
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1965	U
1	X	1975	G
1	X	1976	U
1	X	1979	C
1	X	1980	A
1	X	1988	A
1	X	2006	G
1	X	2009	U
1	X	2014	A
1	X	2015	G
1	X	2016	A
1	X	2017	U
1	X	2019	C
1	X	2026	C
1	X	2029	G
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2075	U
1	X	2083	G

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Mol	Chain	Res	Type
1	X	2171	U
1	X	2181	A
1	X	2190	A
1	X	2191	A
1	X	2192	U
1	X	2195	C
1	X	2199	C
1	X	2200	G
1	X	2205	C
1	X	2218	G
1	X	2238	G
1	X	2241	U
1	X	2242	C
1	X	2246	A
1	X	2247	A
1	X	2259	G
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2272	A
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2298	U
1	X	2300	G
1	X	2301	A
1	X	2306	A
1	X	2313	G
1	X	2315	A
1	X	2324	G
1	X	2325	A
1	X	2326	C
1	X	2362	G
1	X	2364	C
1	X	2386	G
1	X	2396	C
1	X	2398	U
1	X	2402	U
1	X	2404	A
1	X	2405	A

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Mol	Chain	Res	Type
1	X	2407	G
1	X	2410	U
1	X	2418	A
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2452	U
1	X	2455	A
1	X	2458	U
1	X	2470	U
1	X	2471	U
1	X	2477	C
1	X	2481	G
1	X	2482	A
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2497	A
1	X	2498	U
1	X	2501	U
1	X	2528	G
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	X	2553	G
1	X	2561	G
1	X	2564	U
1	X	2565	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2591	C
1	X	2594	U
1	X	2608	A
1	X	2609	G
1	X	2613	A
1	X	2634	G
1	X	2650	G
1	X	2664	G
1	X	2668	U
1	X	2691	C
1	X	2692	A

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Mol	Chain	Res	Type
1	X	2693	U
1	X	2694	G
1	X	2706	U
1	X	2713	A
1	X	2730	A
1	X	2731	G
1	X	2732	C
1	X	2737	A
1	X	2744	A
1	X	2745	A
1	X	2757	G
1	X	2758	A
1	X	2759	U
1	X	2760	G
1	X	2761	A
1	X	2770	A
1	X	2771	C
1	X	2782	G
1	X	2783	U
1	X	2792	C
1	X	2795	A
1	X	2796	A
1	X	2807	U
1	X	2808	U
1	X	2809	A
1	X	2814	G
1	X	2825	A
1	X	2842	C
1	X	2847	G
1	X	2850	U
1	X	2867	G
1	X	2868	G
2	Y	4	C
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	26	G
2	Y	27	A
2	Y	28	A
2	Y	43	G
2	Y	44	C

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Mol	Chain	Res	Type
2	Y	46	G
2	Y	47	A
2	Y	59	A
2	Y	69	G
2	Y	102	A
2	Y	110	U
2	Y	111	C
2	Y	112	A

All (54) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	33	C
1	X	38	G
1	X	48	A
1	X	62	U
1	X	334	G
1	X	342	G
1	X	467	U
1	X	538	A
1	X	751	G
1	X	759	C
1	X	760	U
1	X	780	U
1	X	788	G
1	X	789	G
1	X	969	U
1	X	983	G
1	X	984	A
1	X	1031	C
1	X	1053	G
1	X	1096	A
1	X	1141	U
1	X	1182	U
1	X	1223	G
1	X	1312	G
1	X	1313	U
1	X	1357	U
1	X	1391	A
1	X	1441	A
1	X	1442	C
1	X	1496	G

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Mol	Chain	Res	Type
1	X	1601	U
1	X	1607	A
1	X	1623	C
1	X	1685	A
1	X	1781	C
1	X	1790	G
1	X	1811	A
1	X	1923	U
1	X	1938	U
1	X	1975	G
1	X	2015	G
1	X	2018	G
1	X	2044	G
1	X	2045	A
1	X	2204	A
1	X	2312	A
1	X	2404	A
1	X	2409	A
1	X	2426	G
1	X	2692	A
1	X	2705	A
1	X	2736	U
1	X	2756	A
1	X	2824	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 212 ligands modelled in this entry, 211 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMA	X	2881	-	58,60,60	4.94	26 (44%)	75,90,90	1.30	5 (6%)

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
31	LMA	X	2881	-	-	20/80/115/115	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	2881	LMA	C30-C2	-19.79	1.10	1.53
31	X	2881	LMA	C2-C1	-17.00	1.13	1.51
31	X	2881	LMA	O53-C8	-10.30	1.25	1.43
31	X	2881	LMA	O2-C13	8.52	1.57	1.44
31	X	2881	LMA	C35-C12	-8.22	1.36	1.53
31	X	2881	LMA	C33-C8	-7.31	1.41	1.52
31	X	2881	LMA	C7-C6	-7.19	1.44	1.54
31	X	2881	LMA	C19-C16	-6.15	1.38	1.52
31	X	2881	LMA	C32-C6	-6.04	1.38	1.53
31	X	2881	LMA	C8-C9	-5.87	1.41	1.54
31	X	2881	LMA	O5-C16	-5.24	1.34	1.44
31	X	2881	LMA	C16-C17	-5.20	1.41	1.53
31	X	2881	LMA	C40-C23	-4.85	1.43	1.53
31	X	2881	LMA	O55-C54	4.79	1.38	1.20
31	X	2881	LMA	C6-C5	4.54	1.61	1.53
31	X	2881	LMA	O52-C51	4.44	1.37	1.20
31	X	2881	LMA	O51-C17	-4.17	1.37	1.45
31	X	2881	LMA	O2-C1	3.76	1.43	1.34
31	X	2881	LMA	C2-C3	3.71	1.63	1.55
31	X	2881	LMA	C12-C13	-3.68	1.44	1.54
31	X	2881	LMA	O17-C24	3.15	1.51	1.43
31	X	2881	LMA	O3-C3	2.72	1.50	1.43
31	X	2881	LMA	O4-C18	2.24	1.49	1.44
31	X	2881	LMA	C4-C5	2.18	1.59	1.54
31	X	2881	LMA	C15-C16	2.08	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	2881	LMA	O12-C54	2.02	1.39	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X	2881	LMA	O12-C54-C56	4.58	119.52	111.09
31	X	2881	LMA	O51-C51-C53	4.56	119.48	111.09
31	X	2881	LMA	O7-C5-C4	3.88	112.90	108.22
31	X	2881	LMA	C3-C2-C1	-2.76	104.38	110.01
31	X	2881	LMA	C25-C24-C23	-2.45	106.55	113.08

There are no chirality outliers.

All (20) torsion outliers are listed below:

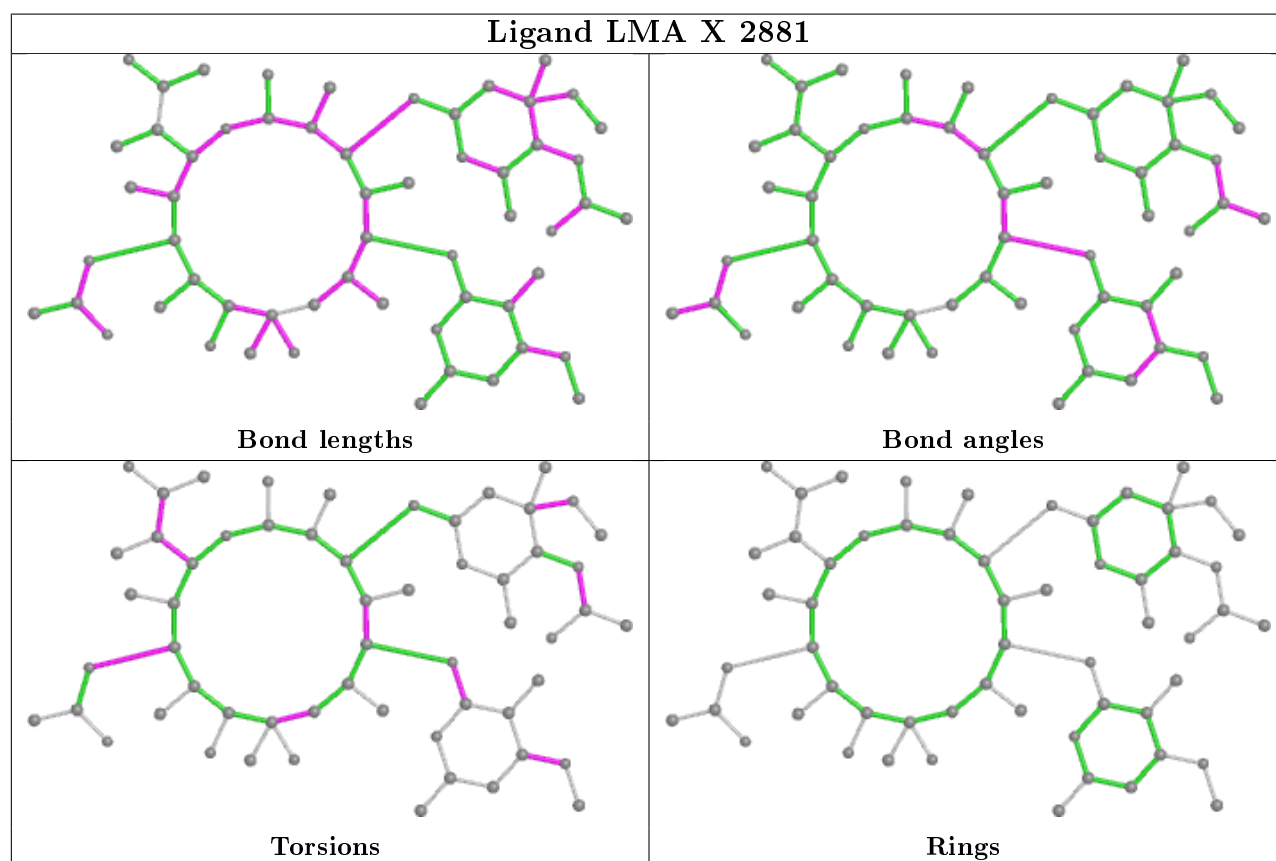
Mol	Chain	Res	Type	Atoms
31	X	2881	LMA	C3-C4-C5-C6
31	X	2881	LMA	C3-C4-C5-O7
31	X	2881	LMA	C31-C4-C5-C6
31	X	2881	LMA	C12-C11-O12-C54
31	X	2881	LMA	C13-C36-C57-O57
31	X	2881	LMA	C13-C36-C57-C58
31	X	2881	LMA	C37-C36-C57-O57
31	X	2881	LMA	C37-C36-C57-C58
31	X	2881	LMA	C53-C51-O51-C17
31	X	2881	LMA	O52-C51-O51-C17
31	X	2881	LMA	C31-C4-C5-O7
31	X	2881	LMA	C25-C24-O17-C29
31	X	2881	LMA	C10-C11-O12-C54
31	X	2881	LMA	C6-C7-C8-C9
31	X	2881	LMA	C12-C13-C36-C57
31	X	2881	LMA	O9-C22-O7-C5
31	X	2881	LMA	C6-C7-C8-C33
31	X	2881	LMA	C15-C16-O5-C20
31	X	2881	LMA	C19-C16-O5-C20
31	X	2881	LMA	C6-C7-C8-O53

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	X	2881	LMA	13	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](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	X	2657/2880 (92%)	-0.13	75 (2%) 53 41	32, 91, 207, 392	0
2	Y	120/123 (97%)	0.08	2 (1%) 70 60	85, 155, 211, 300	0
3	A	253/274 (92%)	0.42	15 (5%) 22 15	54, 119, 183, 297	0
4	B	205/211 (97%)	-0.34	3 (1%) 73 64	22, 64, 130, 298	0
5	C	194/205 (94%)	0.19	14 (7%) 15 10	44, 117, 220, 268	0
6	D	177/180 (98%)	0.88	25 (14%) 2 2	146, 209, 280, 370	0
7	E	171/185 (92%)	0.24	11 (6%) 19 13	86, 149, 209, 245	0
8	F	63/144 (43%)	3.09	43 (68%) 0 0	180, 261, 394, 440	0
9	G	142/174 (81%)	0.27	8 (5%) 24 15	55, 101, 188, 266	0
10	H	134/134 (100%)	-0.48	1 (0%) 87 83	35, 61, 108, 204	0
11	I	134/156 (85%)	0.65	15 (11%) 5 4	64, 145, 237, 367	0
12	J	136/141 (96%)	0.17	7 (5%) 28 18	76, 108, 190, 272	0
13	K	113/116 (97%)	-0.65	0 100 100	27, 46, 79, 105	0
14	L	104/114 (91%)	0.54	11 (10%) 6 5	117, 160, 248, 306	0
15	M	108/166 (65%)	-0.33	3 (2%) 53 41	36, 60, 135, 241	0
16	N	117/118 (99%)	-0.12	4 (3%) 45 33	44, 88, 156, 279	0
17	O	94/100 (94%)	0.15	6 (6%) 19 13	58, 119, 195, 238	0
18	P	126/134 (94%)	-0.40	0 100 100	29, 59, 118, 200	0
19	Q	93/95 (97%)	0.04	2 (2%) 62 52	59, 107, 182, 273	0
20	R	110/115 (95%)	0.66	21 (19%) 1 1	68, 127, 234, 359	0
21	S	175/237 (73%)	0.93	34 (19%) 1 1	112, 169, 237, 314	0
22	T	74/91 (81%)	0.63	13 (17%) 1 1	82, 123, 199, 271	0
23	U	72/81 (88%)	1.79	20 (27%) 0 0	89, 155, 302, 332	0
24	V	65/67 (97%)	0.29	4 (6%) 20 13	94, 126, 205, 256	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	55/55 (100%)	0.08	2 (3%) 42 31	73, 102, 166, 177	0
26	Z	57/60 (95%)	-0.15	2 (3%) 44 32	31, 63, 108, 191	0
27	1	53/55 (96%)	1.55	17 (32%) 0 0	106, 171, 261, 319	0
28	2	46/47 (97%)	0.22	3 (6%) 18 12	56, 85, 154, 195	0
29	3	59/66 (89%)	1.58	21 (35%) 0 0	97, 150, 276, 316	0
30	4	37/37 (100%)	6.38	35 (94%) 0 0	133, 223, 289, 323	0
All	All	5944/6561 (90%)	0.16	417 (7%) 16 11	22, 105, 230, 440	0

All (417) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	28	GLY	25.4
30	4	25	VAL	14.2
8	F	113	PRO	14.0
30	4	17	VAL	13.9
30	4	24	LEU	12.9
30	4	13	ASN	12.7
3	A	204	ASN	12.4
8	F	114	ASP	11.2
21	S	91	PRO	10.0
30	4	6	SER	9.4
30	4	23	VAL	9.3
23	U	27	ASP	9.2
27	1	35	LEU	9.1
30	4	35	ARG	8.9
8	F	125	ASN	8.5
6	D	75	SER	8.4
21	S	15	ASP	8.4
1	X	1095	A	8.2
30	4	4	ARG	8.2
6	D	43	SER	8.1
23	U	26	ALA	7.9
23	U	29	GLY	7.8
30	4	34	GLN	7.8
8	F	112	MET	7.6
5	C	19	LEU	7.2
30	4	5	SER	7.0
30	4	27	CYS	7.0
23	U	47	HIS	7.0
30	4	12	ASP	7.0

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Mol	Chain	Res	Type	RSRZ
19	Q	64	ARG	7.0
8	F	97	GLY	6.8
30	4	26	ILE	6.7
30	4	21	GLY	6.5
30	4	16	VAL	6.5
1	X	1080	A	6.4
30	4	3	VAL	6.4
30	4	28	SER	6.3
1	X	1085	G	6.2
30	4	29	ASN	6.0
22	T	73	GLY	6.0
29	3	50	LEU	6.0
1	X	665	A	5.9
30	4	36	GLN	5.8
3	A	251	TRP	5.8
30	4	11	CYS	5.8
1	X	1115	C	5.7
4	B	205	SER	5.7
8	F	123	ALA	5.7
1	X	1106	A	5.7
6	D	145	MET	5.6
30	4	1	MET	5.6
30	4	37	GLY	5.6
6	D	45	GLU	5.6
1	X	1107	A	5.5
6	D	76	ASN	5.4
27	1	45	LYS	5.4
6	D	147	ASP	5.3
21	S	23	ALA	5.2
30	4	7	VAL	5.2
5	C	165	SER	5.1
9	G	156	HIS	5.1
27	1	32	GLN	5.1
30	4	20	HIS	5.1
11	I	56	LEU	5.0
30	4	33	LYS	5.0
1	X	248	A	5.0
6	D	142	THR	5.0
30	4	14	CYS	5.0
21	S	92	VAL	5.0
20	R	57	ASN	5.0
30	4	10	MET	5.0

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Mol	Chain	Res	Type	RSRZ
30	4	22	ARG	4.9
30	4	15	LYS	4.8
20	R	102	LYS	4.8
8	F	120	VAL	4.8
22	T	85	GLN	4.8
12	J	84	MET	4.8
6	D	71	LYS	4.8
21	S	31	SER	4.7
6	D	74	ILE	4.7
1	X	1086	C	4.7
29	3	9	MET	4.7
11	I	54	SER	4.7
1	X	2287	G	4.7
27	1	23	THR	4.7
3	A	250	PRO	4.7
6	D	143	TYR	4.6
24	V	66	GLN	4.6
3	A	243	ALA	4.6
16	N	88	ILE	4.6
3	A	161	GLY	4.6
23	U	12	ASN	4.5
8	F	101	TRP	4.5
8	F	136	VAL	4.5
21	S	12	GLN	4.4
17	O	64	GLY	4.4
20	R	67	GLY	4.4
1	X	1114	A	4.4
1	X	1104	G	4.4
22	T	18	PRO	4.4
30	4	32	HIS	4.4
27	1	47	HIS	4.3
21	S	128	ARG	4.3
29	3	55	TRP	4.3
8	F	85	GLY	4.2
27	1	27	ASN	4.2
1	X	1072	U	4.2
22	T	15	ASP	4.2
22	T	16	SER	4.2
11	I	36	GLY	4.1
27	1	52	GLU	4.1
21	S	76	ARG	4.1
1	X	558	G	4.1

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Mol	Chain	Res	Type	RSRZ
9	G	97	ASP	4.0
21	S	94	VAL	4.0
21	S	30	VAL	4.0
23	U	52	ARG	4.0
23	U	30	VAL	4.0
23	U	13	LEU	4.0
8	F	76	TYR	3.9
6	D	120	ASN	3.9
14	L	35	SER	3.9
20	R	58	VAL	3.8
1	X	1089	C	3.8
8	F	90	THR	3.8
22	T	13	GLY	3.8
7	E	25	LYS	3.7
1	X	1079	G	3.7
27	1	13	GLU	3.7
8	F	94	ALA	3.7
1	X	2190	A	3.7
16	N	91	ASN	3.7
1	X	1068	A	3.6
1	X	1077	U	3.6
21	S	22	VAL	3.6
1	X	1057	A	3.6
20	R	112	LYS	3.6
21	S	55	THR	3.6
11	I	74	VAL	3.6
29	3	33	ASN	3.6
23	U	46	LEU	3.5
30	4	2	LYS	3.5
8	F	99	LEU	3.5
24	V	4	SER	3.5
12	J	27	TYR	3.5
5	C	44	SER	3.5
27	1	14	SER	3.5
3	A	220	PRO	3.5
29	3	44	LYS	3.5
1	X	358	C	3.5
8	F	111	LYS	3.4
27	1	36	GLU	3.4
6	D	81	GLN	3.4
21	S	113	VAL	3.4
3	A	85	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
8	F	119	SER	3.4
22	T	71	ASN	3.4
8	F	132	ARG	3.4
6	D	42	SER	3.4
8	F	121	GLU	3.3
6	D	125	ARG	3.3
29	3	21	LYS	3.3
5	C	48	ARG	3.3
6	D	144	ASP	3.3
23	U	16	ASN	3.3
5	C	167	VAL	3.3
3	A	268	ASP	3.3
20	R	66	GLN	3.3
6	D	18	GLN	3.2
1	X	1081	A	3.2
11	I	52	GLY	3.2
21	S	14	LEU	3.2
21	S	21	ALA	3.2
29	3	61	MET	3.2
8	F	91	PRO	3.2
20	R	52	ASN	3.2
20	R	94	VAL	3.2
27	1	31	THR	3.2
10	H	27	SER	3.2
1	X	1108	U	3.2
8	F	129	GLY	3.2
7	E	51	LEU	3.1
8	F	92	ASN	3.1
5	C	193	LEU	3.1
9	G	159	SER	3.1
22	T	17	ASN	3.1
11	I	57	ILE	3.1
29	3	43	GLY	3.1
20	R	100	ASP	3.1
8	F	133	SER	3.1
1	X	1552	C	3.1
1	X	1105	U	3.1
14	L	63	ASN	3.1
27	1	24	THR	3.0
21	S	83	PHE	3.0
8	F	78	ILE	3.0
3	A	32	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
5	C	47	THR	3.0
3	A	203	LYS	3.0
1	X	1734	C	3.0
1	X	1120	C	3.0
1	X	2290	A	3.0
17	O	36	LYS	3.0
1	X	1037	U	3.0
30	4	18	ARG	3.0
12	J	136	GLU	3.0
3	A	221	HIS	3.0
1	X	1067	G	3.0
1	X	1913	G	3.0
1	X	1191	G	2.9
14	L	62	GLY	2.9
22	T	14	ARG	2.9
21	S	173	PRO	2.9
1	X	732	G	2.9
29	3	10	ALA	2.9
6	D	20	PHE	2.9
7	E	23	VAL	2.9
17	O	46	VAL	2.9
21	S	77	ALA	2.9
7	E	62	ARG	2.9
1	X	1184	G	2.9
29	3	39	ASP	2.9
14	L	64	LYS	2.9
11	I	31	GLY	2.9
29	3	48	PHE	2.9
6	D	72	LYS	2.9
29	3	54	GLU	2.9
21	S	11	LYS	2.9
1	X	601	A	2.9
5	C	192	ALA	2.9
6	D	46	ASP	2.8
17	O	39	PHE	2.8
4	B	135	HIS	2.8
8	F	96	VAL	2.8
1	X	2015	G	2.8
24	V	5	GLU	2.8
25	W	33	GLU	2.8
8	F	81	ALA	2.8
21	S	24	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
22	T	20	TYR	2.8
29	3	14	ILE	2.8
21	S	147	ILE	2.8
2	Y	68	A	2.8
8	F	95	LYS	2.8
29	3	51	ALA	2.8
23	U	61	TRP	2.8
8	F	77	LEU	2.8
29	3	38	GLY	2.8
14	L	55	SER	2.7
20	R	61	SER	2.7
21	S	165	GLU	2.7
8	F	80	LYS	2.7
8	F	84	ILE	2.7
27	1	2	ALA	2.7
8	F	127	VAL	2.7
30	4	9	LYS	2.7
20	R	60	PRO	2.7
1	X	1602	G	2.7
3	A	153	GLY	2.7
8	F	108	ALA	2.7
6	D	40	LEU	2.6
1	X	304	A	2.6
1	X	1119	U	2.6
21	S	32	PHE	2.6
8	F	104	VAL	2.6
12	J	28	VAL	2.6
21	S	86	VAL	2.6
1	X	1912	G	2.6
1	X	1076	U	2.6
23	U	8	THR	2.6
8	F	122	ALA	2.6
1	X	2289	A	2.6
8	F	110	THR	2.6
2	Y	4	C	2.6
20	R	71	GLN	2.6
7	E	37	TYR	2.6
5	C	45	THR	2.6
30	4	30	VAL	2.6
8	F	105	LEU	2.6
1	X	247	A	2.6
1	X	1522	C	2.6

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Mol	Chain	Res	Type	RSRZ
21	S	174	PRO	2.6
9	G	39	GLN	2.5
27	1	22	TYR	2.5
1	X	302	U	2.5
9	G	129	HIS	2.5
6	D	146	VAL	2.5
23	U	54	ASN	2.5
14	L	65	THR	2.5
14	L	111	GLY	2.5
1	X	667	U	2.5
11	I	55	ARG	2.5
11	I	97	ARG	2.5
23	U	25	ARG	2.5
27	1	51	ARG	2.5
12	J	112	GLU	2.5
1	X	1078	A	2.5
1	X	1109	A	2.5
11	I	33	GLY	2.5
29	3	13	ARG	2.5
15	M	29	PRO	2.5
21	S	85	MET	2.5
1	X	1055	A	2.5
21	S	145	ASP	2.5
20	R	69	GLN	2.5
22	T	66	LYS	2.5
8	F	124	ALA	2.5
5	C	59	TYR	2.5
29	3	7	HIS	2.5
1	X	1098	G	2.4
29	3	45	GLY	2.4
22	T	84	ALA	2.4
1	X	2085	G	2.4
21	S	125	PRO	2.4
8	F	86	LYS	2.4
8	F	102	ASP	2.4
17	O	47	PHE	2.4
14	L	56	SER	2.4
20	R	81	VAL	2.4
1	X	1909	U	2.4
1	X	1090	C	2.4
7	E	119	ALA	2.4
1	X	1733	U	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
21	S	124	ALA	2.4
1	X	1084	A	2.3
9	G	109	GLY	2.3
1	X	2087	U	2.3
7	E	5	GLY	2.3
26	Z	37	HIS	2.3
4	B	94	ASP	2.3
17	O	23	GLU	2.3
7	E	61	HIS	2.3
1	X	2082	C	2.3
8	F	107	ILE	2.3
29	3	63	PRO	2.3
5	C	166	TRP	2.3
20	R	77	HIS	2.3
15	M	40	ARG	2.3
1	X	2174	G	2.3
27	1	19	GLY	2.3
21	S	93	GLU	2.3
11	I	46	GLY	2.3
23	U	73	GLY	2.3
1	X	2044	G	2.3
3	A	163	SER	2.3
1	X	1093	U	2.3
12	J	21	ASP	2.3
5	C	172	VAL	2.2
1	X	1074	G	2.2
21	S	69	VAL	2.2
26	Z	5	PRO	2.2
9	G	167	LYS	2.2
11	I	100	ARG	2.2
20	R	113	THR	2.2
1	X	1553	G	2.2
21	S	123	VAL	2.2
1	X	1099	A	2.2
1	X	1841	G	2.2
11	I	24	GLY	2.2
21	S	58	GLY	2.2
24	V	65	GLU	2.2
6	D	136	LEU	2.2
28	2	38	GLY	2.2
20	R	83	LEU	2.2
8	F	109	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
28	2	39	ARG	2.2
25	W	54	GLN	2.2
7	E	174	GLY	2.2
8	F	100	ASN	2.2
21	S	114	ASP	2.2
1	X	1551	U	2.1
20	R	95	ARG	2.1
9	G	66	HIS	2.1
14	L	58	ALA	2.1
3	A	92	ARG	2.1
3	A	272	VAL	2.1
14	L	34	SER	2.1
20	R	103	LYS	2.1
23	U	57	VAL	2.1
29	3	20	GLY	2.1
12	J	72	ASP	2.1
7	E	68	THR	2.1
7	E	82	GLY	2.1
23	U	50	ALA	2.1
11	I	50	GLU	2.1
19	Q	65	VAL	2.1
16	N	23	GLY	2.1
22	T	61	ALA	2.1
5	C	164	VAL	2.1
8	F	79	ARG	2.1
11	I	53	ARG	2.1
16	N	89	ASP	2.1
1	X	1019	U	2.1
1	X	1116	U	2.1
1	X	2169	A	2.1
5	C	21	GLU	2.1
20	R	29	HIS	2.1
6	D	151	GLY	2.1
6	D	11	GLN	2.1
1	X	871	U	2.1
14	L	107	ALA	2.1
1	X	1094	C	2.1
27	1	50	PHE	2.0
6	D	90	THR	2.0
23	U	65	ASN	2.0
1	X	69	G	2.0
30	4	31	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
28	2	46	ASP	2.0
8	F	130	THR	2.0
15	M	28	ARG	2.0
29	3	25	PHE	2.0
1	X	1073	G	2.0
1	X	1121	G	2.0
1	X	1556	A	2.0
1	X	2299	A	2.0
23	U	49	LYS	2.0
20	R	99	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
33	NA	X	3064	1/1	0.72	0.27	58,58,58,58	0
34	K	X	3074	1/1	0.75	0.67	171,171,171,171	0
34	K	X	3076	1/1	0.76	0.36	100,100,100,100	0
32	MG	X	2891	1/1	0.78	0.20	56,56,56,56	0
33	NA	Y	126	1/1	0.80	0.40	85,85,85,85	0
33	NA	X	3061	1/1	0.81	0.55	62,62,62,62	0
32	MG	X	2939	1/1	0.83	0.56	79,79,79,79	0
32	MG	X	2931	1/1	0.83	0.59	48,48,48,48	0
33	NA	A	277	1/1	0.83	0.43	72,72,72,72	0
33	NA	X	3037	1/1	0.83	0.26	53,53,53,53	0
33	NA	X	3053	1/1	0.83	0.53	62,62,62,62	0
32	MG	X	2992	1/1	0.84	0.23	44,44,44,44	0
33	NA	X	3069	1/1	0.84	0.94	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	X	3023	1/1	0.85	0.32	73,73,73,73	0
32	MG	X	2903	1/1	0.86	0.45	51,51,51,51	0
32	MG	X	2975	1/1	0.86	0.23	73,73,73,73	0
32	MG	X	2952	1/1	0.86	0.44	57,57,57,57	0
32	MG	X	2901	1/1	0.87	0.49	30,30,30,30	0
32	MG	X	2966	1/1	0.87	0.29	60,60,60,60	0
32	MG	X	2997	1/1	0.88	0.20	50,50,50,50	0
32	MG	X	2970	1/1	0.88	0.21	51,51,51,51	0
32	MG	X	2937	1/1	0.88	0.24	46,46,46,46	0
32	MG	X	3015	1/1	0.88	0.45	77,77,77,77	0
32	MG	I	157	1/1	0.88	0.35	50,50,50,50	0
33	NA	X	3036	1/1	0.88	0.26	79,79,79,79	0
32	MG	X	2978	1/1	0.89	0.42	48,48,48,48	0
33	NA	X	3046	1/1	0.89	0.59	80,80,80,80	0
32	MG	X	2928	1/1	0.89	0.40	41,41,41,41	0
33	NA	X	3058	1/1	0.89	0.35	69,69,69,69	0
32	MG	X	2934	1/1	0.90	0.20	62,62,62,62	0
32	MG	X	2918	1/1	0.90	0.21	60,60,60,60	0
33	NA	K	117	1/1	0.90	0.16	28,28,28,28	0
32	MG	X	3000	1/1	0.90	0.25	65,65,65,65	0
33	NA	X	3038	1/1	0.90	0.39	59,59,59,59	0
32	MG	X	2887	1/1	0.90	0.31	37,37,37,37	0
32	MG	X	3004	1/1	0.90	0.39	71,71,71,71	0
31	LMA	X	2881	58/58	0.90	0.27	22,83,114,128	0
33	NA	X	3067	1/1	0.91	0.29	47,47,47,47	0
33	NA	X	3063	1/1	0.91	0.38	50,50,50,50	0
32	MG	X	3019	1/1	0.91	0.41	74,74,74,74	0
32	MG	X	2894	1/1	0.91	0.24	33,33,33,33	0
33	NA	X	3057	1/1	0.91	0.89	75,75,75,75	0
32	MG	X	2988	1/1	0.91	0.29	63,63,63,63	0
33	NA	X	3050	1/1	0.91	0.30	40,40,40,40	0
32	MG	X	3014	1/1	0.91	0.36	54,54,54,54	0
34	K	X	3070	1/1	0.91	0.53	72,72,72,72	0
32	MG	X	2979	1/1	0.92	0.60	50,50,50,50	0
33	NA	X	3052	1/1	0.92	0.25	43,43,43,43	0
32	MG	X	2940	1/1	0.92	0.25	34,34,34,34	0
32	MG	X	3022	1/1	0.92	0.14	43,43,43,43	0
32	MG	X	2883	1/1	0.92	0.33	34,34,34,34	0
32	MG	X	2910	1/1	0.92	0.29	47,47,47,47	0
32	MG	X	2961	1/1	0.92	0.36	61,61,61,61	0
32	MG	X	2916	1/1	0.92	0.30	51,51,51,51	0
33	NA	X	3066	1/1	0.92	0.42	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	X	3018	1/1	0.92	0.40	59,59,59,59	0
32	MG	X	3010	1/1	0.92	0.43	73,73,73,73	0
32	MG	X	2923	1/1	0.92	0.52	66,66,66,66	0
32	MG	X	2985	1/1	0.92	0.17	50,50,50,50	0
32	MG	X	2907	1/1	0.93	0.48	66,66,66,66	0
33	NA	X	3062	1/1	0.93	0.14	47,47,47,47	0
32	MG	X	2949	1/1	0.93	0.41	48,48,48,48	0
32	MG	X	2925	1/1	0.93	0.35	72,72,72,72	0
32	MG	X	2930	1/1	0.93	0.53	51,51,51,51	0
32	MG	X	2950	1/1	0.93	0.25	49,49,49,49	0
33	NA	X	3039	1/1	0.93	0.28	51,51,51,51	0
32	MG	X	2914	1/1	0.93	0.61	60,60,60,60	0
32	MG	X	3032	1/1	0.93	0.37	74,74,74,74	0
32	MG	X	3028	1/1	0.93	0.18	65,65,65,65	0
33	NA	X	3056	1/1	0.93	0.70	76,76,76,76	0
33	NA	X	3049	1/1	0.93	0.49	68,68,68,68	0
34	K	X	3077	1/1	0.93	0.45	80,80,80,80	0
32	MG	X	2945	1/1	0.93	0.46	32,32,32,32	0
32	MG	X	3007	1/1	0.93	0.20	37,37,37,37	0
32	MG	X	3027	1/1	0.93	0.17	51,51,51,51	0
32	MG	X	2968	1/1	0.93	0.26	56,56,56,56	0
32	MG	X	2942	1/1	0.93	0.20	74,74,74,74	0
34	K	X	3079	1/1	0.93	0.47	97,97,97,97	0
32	MG	X	2963	1/1	0.94	0.27	69,69,69,69	0
32	MG	X	2921	1/1	0.94	0.23	52,52,52,52	0
33	NA	X	3044	1/1	0.94	0.09	48,48,48,48	0
32	MG	X	2953	1/1	0.94	0.21	59,59,59,59	0
32	MG	X	2984	1/1	0.94	0.29	62,62,62,62	0
32	MG	X	2895	1/1	0.94	0.35	19,19,19,19	0
32	MG	X	2957	1/1	0.94	0.40	35,35,35,35	0
33	NA	X	3035	1/1	0.94	0.30	50,50,50,50	0
34	K	X	3082	1/1	0.94	0.29	98,98,98,98	0
32	MG	X	2999	1/1	0.94	0.18	49,49,49,49	0
33	NA	X	3047	1/1	0.94	0.59	75,75,75,75	0
32	MG	X	2969	1/1	0.94	0.24	31,31,31,31	0
32	MG	X	2943	1/1	0.94	0.52	29,29,29,29	0
32	MG	X	2995	1/1	0.94	0.63	42,42,42,42	0
32	MG	X	2909	1/1	0.94	0.43	44,44,44,44	0
32	MG	X	2972	1/1	0.94	0.21	65,65,65,65	0
32	MG	X	2911	1/1	0.94	0.47	83,83,83,83	0
33	NA	Z	61	1/1	0.94	0.30	48,48,48,48	0
32	MG	X	2987	1/1	0.94	0.46	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	X	3029	1/1	0.94	0.41	63,63,63,63	0
32	MG	X	2908	1/1	0.94	0.32	55,55,55,55	0
32	MG	X	3005	1/1	0.95	0.15	58,58,58,58	0
32	MG	X	2935	1/1	0.95	0.32	55,55,55,55	0
32	MG	X	3024	1/1	0.95	0.28	68,68,68,68	0
32	MG	X	2993	1/1	0.95	0.36	51,51,51,51	0
33	NA	X	3055	1/1	0.95	0.28	70,70,70,70	0
32	MG	X	2989	1/1	0.95	0.40	83,83,83,83	0
32	MG	X	2885	1/1	0.95	0.50	21,21,21,21	0
33	NA	X	3048	1/1	0.95	0.26	71,71,71,71	0
32	MG	X	3002	1/1	0.95	0.22	34,34,34,34	0
32	MG	X	2960	1/1	0.95	0.36	33,33,33,33	0
32	MG	X	2912	1/1	0.95	0.34	24,24,24,24	0
32	MG	X	2893	1/1	0.95	0.48	25,25,25,25	0
33	NA	X	3042	1/1	0.95	0.48	45,45,45,45	0
32	MG	X	2956	1/1	0.95	0.66	71,71,71,71	0
32	MG	X	2936	1/1	0.95	0.27	26,26,26,26	0
32	MG	X	2941	1/1	0.95	0.43	46,46,46,46	0
32	MG	X	3030	1/1	0.95	0.10	66,66,66,66	0
32	MG	X	3026	1/1	0.95	0.33	37,37,37,37	0
32	MG	X	2900	1/1	0.95	0.41	37,37,37,37	0
32	MG	X	2913	1/1	0.95	0.43	56,56,56,56	0
34	K	X	3072	1/1	0.95	0.21	104,104,104,104	0
32	MG	X	2983	1/1	0.95	0.26	23,23,23,23	0
34	K	X	3078	1/1	0.95	0.32	91,91,91,91	0
34	K	X	3075	1/1	0.95	0.22	68,68,68,68	0
33	NA	X	3059	1/1	0.95	0.13	66,66,66,66	0
32	MG	X	3008	1/1	0.95	0.25	45,45,45,45	0
32	MG	X	3003	1/1	0.95	0.48	55,55,55,55	0
32	MG	X	2922	1/1	0.95	0.18	19,19,19,19	0
32	MG	X	2998	1/1	0.96	0.38	29,29,29,29	0
32	MG	X	2964	1/1	0.96	0.44	50,50,50,50	0
32	MG	X	2994	1/1	0.96	0.10	41,41,41,41	0
32	MG	X	2920	1/1	0.96	0.36	31,31,31,31	0
32	MG	X	2944	1/1	0.96	0.35	59,59,59,59	0
33	NA	X	3051	1/1	0.96	0.24	43,43,43,43	0
32	MG	X	2947	1/1	0.96	0.39	47,47,47,47	0
32	MG	Y	124	1/1	0.96	0.11	40,40,40,40	0
32	MG	X	3021	1/1	0.96	0.54	70,70,70,70	0
33	NA	X	3034	1/1	0.96	0.31	50,50,50,50	0
32	MG	X	2976	1/1	0.96	0.24	32,32,32,32	0
32	MG	X	2892	1/1	0.96	0.22	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	X	2990	1/1	0.96	0.39	31,31,31,31	0
32	MG	X	2919	1/1	0.96	0.35	61,61,61,61	0
34	K	X	3071	1/1	0.96	0.23	86,86,86,86	0
32	MG	X	2971	1/1	0.96	0.24	44,44,44,44	0
33	NA	X	3065	1/1	0.96	0.38	58,58,58,58	0
32	MG	X	2977	1/1	0.96	0.32	51,51,51,51	0
33	NA	X	3041	1/1	0.96	0.30	37,37,37,37	0
32	MG	X	2933	1/1	0.96	0.49	59,59,59,59	0
32	MG	X	3012	1/1	0.96	0.57	45,45,45,45	0
34	K	X	3083	1/1	0.96	0.28	103,103,103,103	0
32	MG	X	2974	1/1	0.96	0.18	37,37,37,37	0
32	MG	X	2982	1/1	0.96	0.48	51,51,51,51	0
32	MG	X	2962	1/1	0.96	0.13	70,70,70,70	0
32	MG	X	2897	1/1	0.96	0.36	37,37,37,37	0
34	K	X	3081	1/1	0.97	0.36	91,91,91,91	0
32	MG	X	3001	1/1	0.97	0.46	84,84,84,84	0
32	MG	X	3020	1/1	0.97	0.35	42,42,42,42	0
33	NA	X	3043	1/1	0.97	0.31	48,48,48,48	0
32	MG	X	2981	1/1	0.97	0.47	65,65,65,65	0
32	MG	X	2926	1/1	0.97	0.17	35,35,35,35	0
32	MG	X	2927	1/1	0.97	0.21	55,55,55,55	0
32	MG	X	3013	1/1	0.97	0.11	60,60,60,60	0
32	MG	X	2884	1/1	0.97	0.54	38,38,38,38	0
32	MG	X	2965	1/1	0.97	0.31	42,42,42,42	0
34	K	X	3080	1/1	0.97	0.49	94,94,94,94	0
33	NA	Y	125	1/1	0.97	0.44	62,62,62,62	0
32	MG	X	3011	1/1	0.97	0.55	45,45,45,45	0
32	MG	X	2955	1/1	0.97	0.37	54,54,54,54	0
33	NA	X	3054	1/1	0.97	0.38	49,49,49,49	0
32	MG	X	2882	1/1	0.97	0.33	5,5,5,5	0
34	K	X	3073	1/1	0.97	0.39	57,57,57,57	0
33	NA	X	3033	1/1	0.97	0.44	38,38,38,38	0
32	MG	X	2905	1/1	0.97	0.37	57,57,57,57	0
32	MG	X	2899	1/1	0.97	0.30	57,57,57,57	0
32	MG	X	2948	1/1	0.97	0.43	40,40,40,40	0
32	MG	X	2902	1/1	0.97	0.35	39,39,39,39	0
32	MG	X	3016	1/1	0.97	0.35	39,39,39,39	0
32	MG	X	2889	1/1	0.97	0.26	26,26,26,26	0
32	MG	X	2915	1/1	0.97	0.55	47,47,47,47	0
34	K	M	167	1/1	0.97	0.38	44,44,44,44	0
32	MG	X	2958	1/1	0.97	0.10	29,29,29,29	0
32	MG	X	3009	1/1	0.97	0.24	53,53,53,53	0

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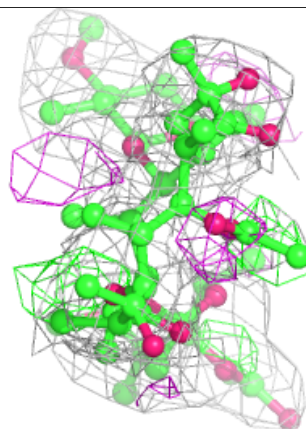
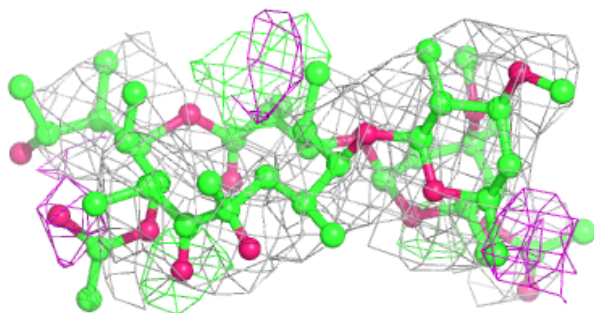
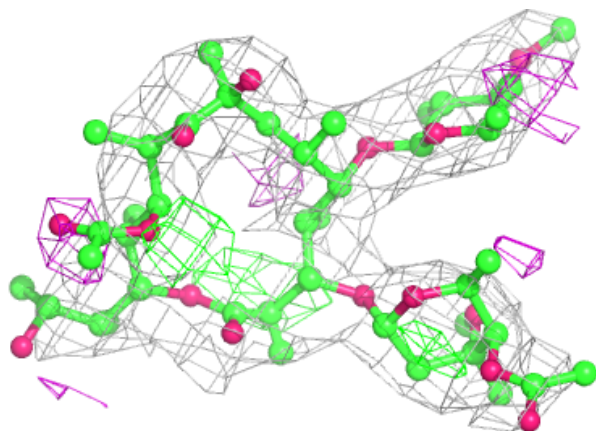
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	X	2906	1/1	0.97	0.39	43,43,43,43	0
32	MG	X	3017	1/1	0.97	0.51	70,70,70,70	0
32	MG	X	2924	1/1	0.98	0.31	26,26,26,26	0
32	MG	X	3025	1/1	0.98	0.19	62,62,62,62	0
32	MG	X	2904	1/1	0.98	0.49	39,39,39,39	0
33	NA	X	3068	1/1	0.98	0.31	64,64,64,64	0
32	MG	X	2896	1/1	0.98	0.41	28,28,28,28	0
32	MG	X	2959	1/1	0.98	0.40	33,33,33,33	0
32	MG	X	2946	1/1	0.98	0.45	38,38,38,38	0
32	MG	X	2886	1/1	0.98	0.36	16,16,16,16	0
33	NA	X	3060	1/1	0.98	0.70	73,73,73,73	0
32	MG	X	3006	1/1	0.98	0.07	59,59,59,59	0
32	MG	X	2938	1/1	0.98	0.40	34,34,34,34	0
33	NA	X	3045	1/1	0.98	0.45	31,31,31,31	0
32	MG	X	2954	1/1	0.98	0.30	31,31,31,31	0
32	MG	X	2991	1/1	0.98	0.38	51,51,51,51	0
32	MG	X	2967	1/1	0.98	0.31	50,50,50,50	0
32	MG	X	3031	1/1	0.98	0.15	48,48,48,48	0
32	MG	X	2986	1/1	0.98	0.26	54,54,54,54	0
32	MG	C	206	1/1	0.98	0.20	37,37,37,37	0
33	NA	X	3040	1/1	0.98	0.41	70,70,70,70	0
32	MG	X	2973	1/1	0.98	0.22	30,30,30,30	0
32	MG	X	2888	1/1	0.98	0.46	36,36,36,36	0
32	MG	X	2996	1/1	0.98	0.08	42,42,42,42	0
32	MG	X	2980	1/1	0.99	0.12	42,42,42,42	0
32	MG	X	2929	1/1	0.99	0.32	10,10,10,10	0
32	MG	X	2890	1/1	0.99	0.24	38,38,38,38	0
32	MG	X	2898	1/1	0.99	0.39	8,8,8,8	0
32	MG	X	2932	1/1	0.99	0.36	31,31,31,31	0
32	MG	X	2917	1/1	0.99	0.27	52,52,52,52	0
32	MG	X	2951	1/1	0.99	0.36	28,28,28,28	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.

**Electron density around LMA X 2881:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.