



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:16 am GMT

PDB ID : 5JVH
Title : The crystal structure large ribosomal subunit (50S) of *Deinococcus radiodurans* in complex with evernimicin
Authors : Yonath, A.
Deposited on : 2016-05-11
Resolution : 3.58 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

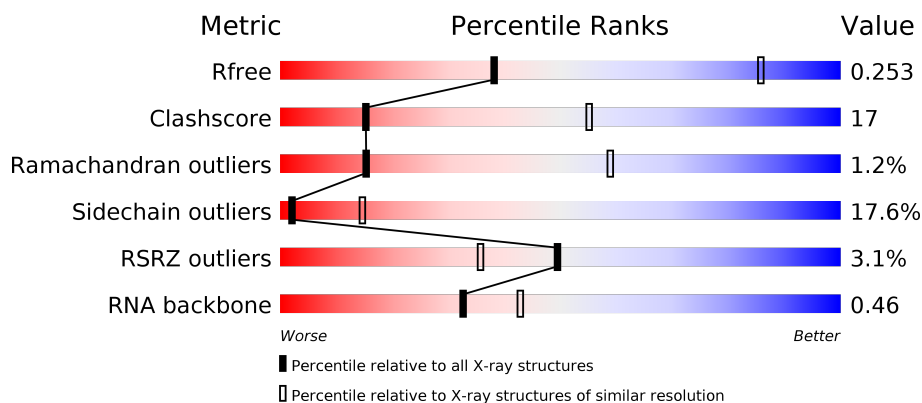
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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}	100719	1009 (3.70-3.46)
Clashscore	112137	1128 (3.70-3.46)
Ramachandran outliers	110173	1088 (3.70-3.46)
Sidechain outliers	110143	1088 (3.70-3.46)
RSRZ outliers	101464	1034 (3.70-3.46)
RNA backbone	2435	1005 (4.26-2.88)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>36% 40% 14% 8%</div> </div>
2	Y	123	<div> <div>2%</div> <div>46% 41% 11%</div> </div>
3	A	275	<div> <div>0%</div> <div>40% 45% 9% 6%</div> </div>
4	B	211	<div> <div>0%</div> <div>53% 38% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	G	174	
9	H	134	
10	I	156	
11	J	141	
12	K	116	
13	L	114	
14	M	166	
15	N	118	
16	O	100	
17	P	134	
18	Q	95	
19	R	115	
20	S	237	
21	T	91	
22	U	81	
23	V	67	
24	W	55	
25	Z	60	
26	1	54	
27	2	47	
28	3	66	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	6O1	X	2901	-	-	-	X
30	MG	K	201	-	-	-	X
30	MG	X	2903	-	-	-	X
30	MG	X	2906	-	-	-	X
30	MG	X	2907	-	-	-	X
30	MG	X	2910	-	-	-	X
30	MG	X	2911	-	-	-	X
30	MG	X	2912	-	-	-	X
30	MG	X	2915	-	-	-	X
30	MG	X	2916	-	-	-	X
30	MG	X	2918	-	-	-	X
30	MG	X	2921	-	-	-	X
30	MG	X	2924	-	-	-	X
30	MG	X	2925	-	-	-	X
30	MG	X	2926	-	-	-	X
30	MG	X	2931	-	-	-	X
30	MG	X	2935	-	-	-	X
30	MG	X	2936	-	-	-	X
30	MG	X	2939	-	-	-	X
30	MG	X	2941	-	-	-	X
30	MG	X	2946	-	-	-	X
30	MG	X	2947	-	-	-	X
30	MG	X	2952	-	-	-	X
30	MG	X	2953	-	-	-	X
30	MG	X	2954	-	-	-	X
30	MG	X	2957	-	-	-	X
30	MG	X	2959	-	-	-	X
30	MG	X	2963	-	-	-	X
30	MG	X	2964	-	-	-	X
30	MG	X	2969	-	-	-	X
30	MG	X	2970	-	-	-	X
30	MG	X	2975	-	-	-	X
30	MG	X	2977	-	-	-	X
30	MG	X	2978	-	-	-	X
30	MG	X	2980	-	-	-	X
30	MG	X	2981	-	-	-	X
30	MG	X	2983	-	-	-	X
30	MG	X	2990	-	-	-	X
30	MG	X	2992	-	-	-	X
30	MG	X	2993	-	-	-	X
30	MG	X	3008	-	-	-	X
30	MG	X	3011	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	3014	-	-	-	X
30	MG	X	3017	-	-	-	X
30	MG	X	3020	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 83681 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2658	Total	C	N	O	P	0	0	0
			57052	25450	10532	18413	2657			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073

- 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	259	Total	C	N	O	S	0	0	0
			1973	1226	395	349	3			

- 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 L13.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1078	690	196	185	7			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	108	Total	C	N	O	0	0	0
			859	537	166	156			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	179	Total	C	N	O	S	0	0	0
			1374	867	240	261	6			

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

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

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

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

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

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

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

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

- Molecule 25 is a protein called 50S ribosomal protein L32.

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

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	53	Total	C	N	O	S	0	0	0
			427	271	79	76	1			

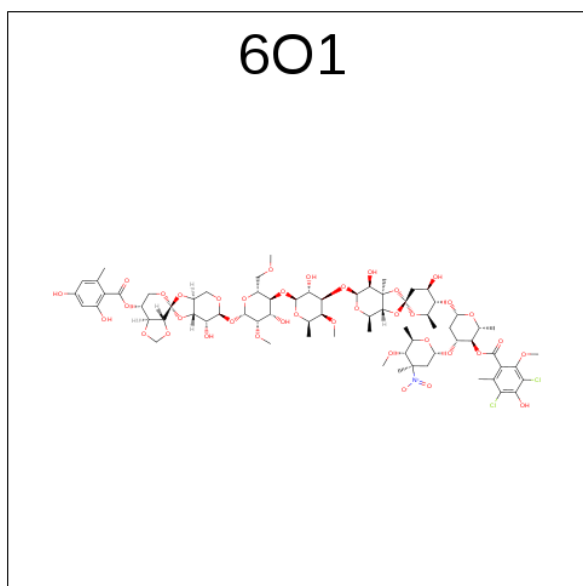
- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 29 is Evernimicin (three-letter code: 6O1) (formula: $C_{70}H_{97}Cl_2NO_{38}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	Cl	N	O	0	0
			111	70	2	1	38		

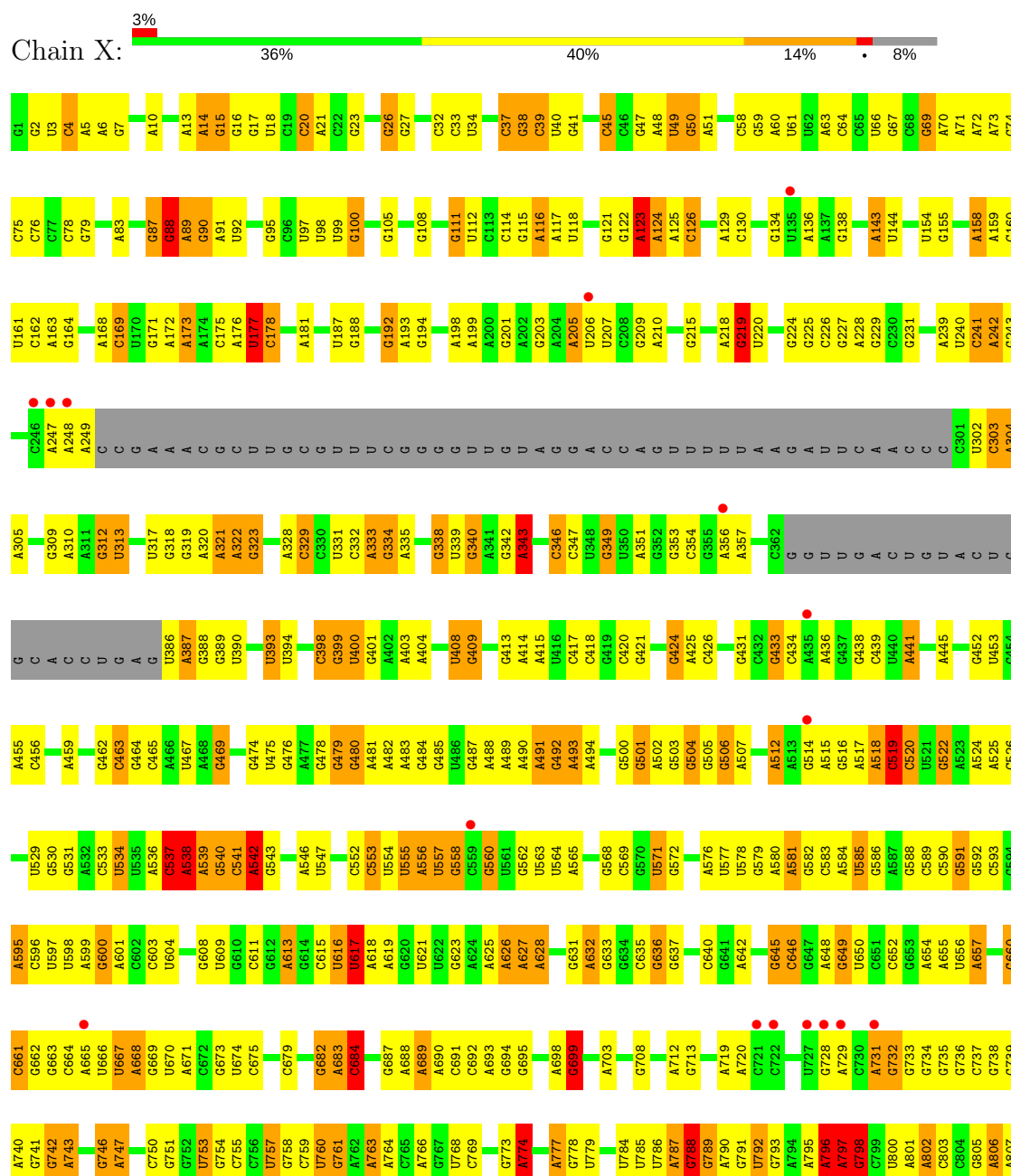
- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	119	Total	Mg	0	0
			119	119		
30	Y	1	Total	Mg	0	0
			1	1		
30	K	2	Total	Mg	0	0
			2	2		
30	M	1	Total	Mg	0	0
			1	1		

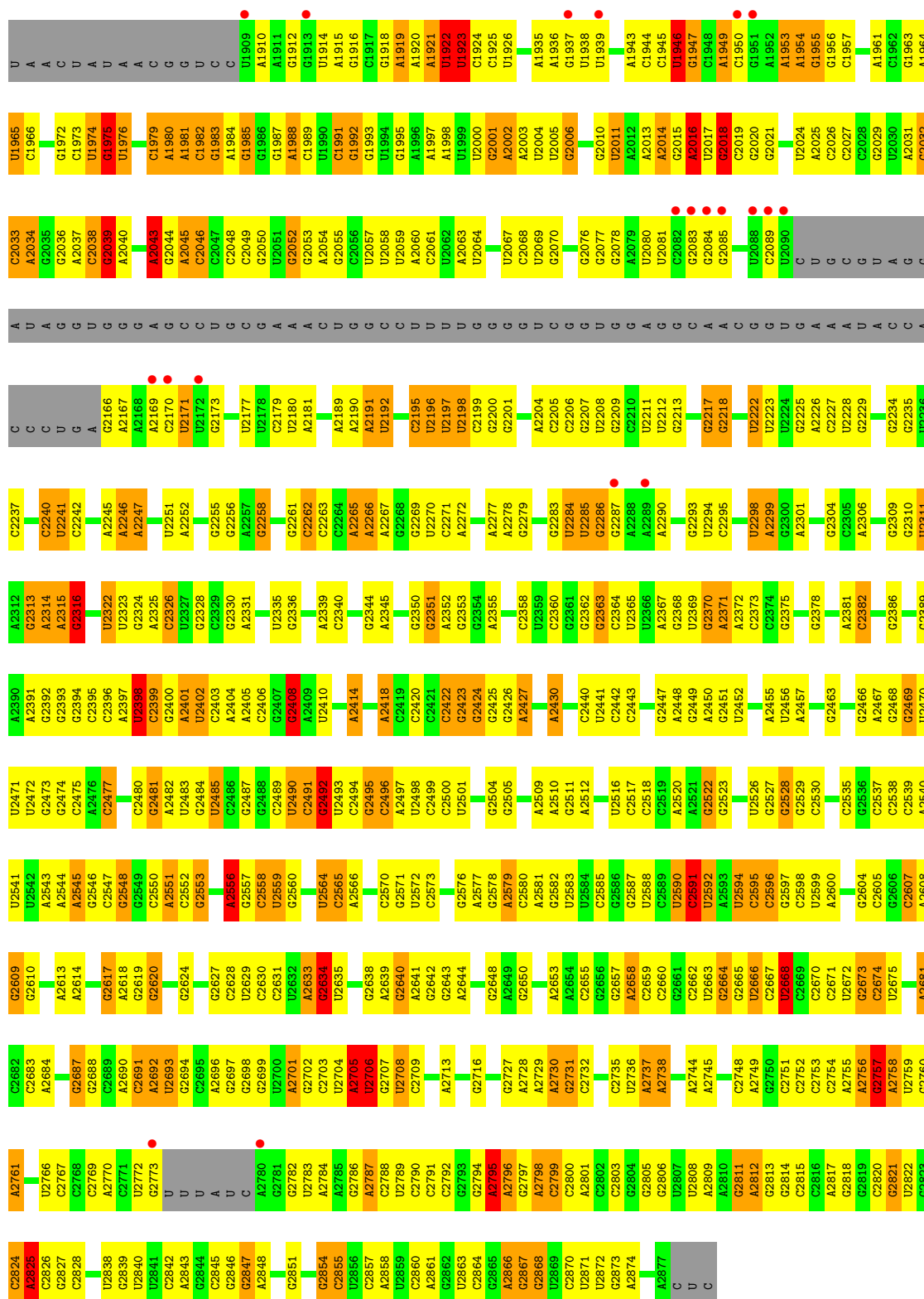
3 Residue-property plots

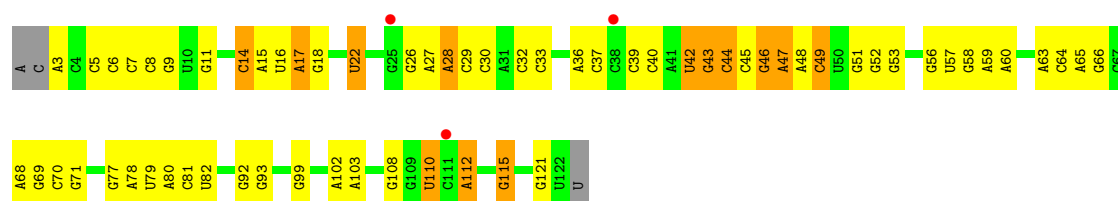
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S ribosomal RNA

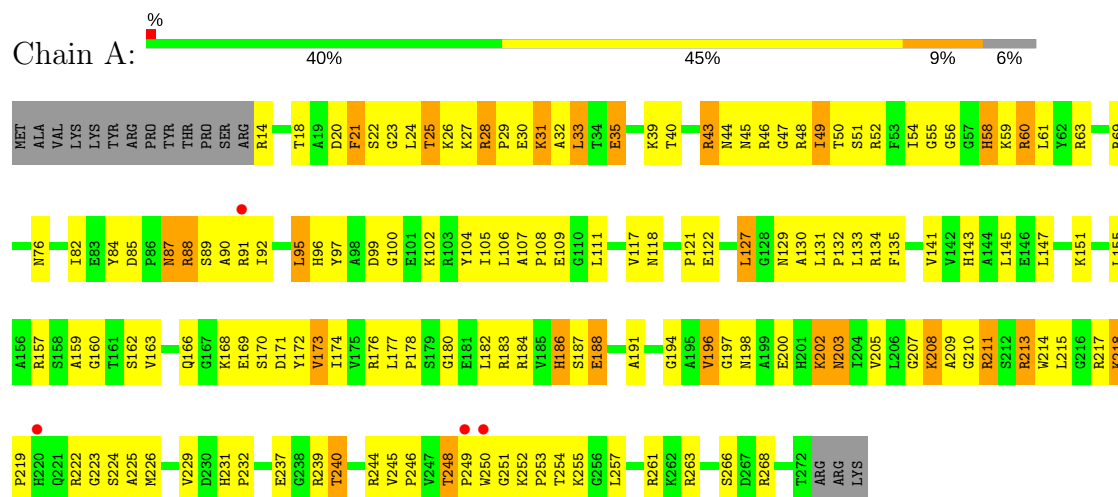


G1822	G1754	G1675	A1595	C1517	G1438	G1360	A1292	G1223	A1153	A	A1022	U946	A876	C808
G1823	G1755	U1676	G1599	U1520	G1439	G1361	A1293	A1224	A1154	C	U1023	C947	G877	C809
C1824	C1756	C1677	U1600	G1521	G1440	C1362	U1294	G1225	G1155	C	G1024	C948	C878	U810
C1825	C1757	G1678	U1601	C1522	C1441	C1363	U1295	A1226	U1161	U	C1029	G951	C880	G811
U1826	U1679	U1679	U1601	C1522	C1441	C1363	G1296	A1227	A1162	U	U1030	A952	C881	G812
G1827	A1759	A1682	G1602	C1524	C1443	G1371	A1299	G1228	A1163	C	G1031	G953	C882	G813
C1830	G1760	G1683	A1603	U1525	C1444	A1372	A1302	C1229	C1164	A	A1032	U954	U890	A817
G1831	G1761	G1684	A1604	U1526	A1448	G1373	U1304	C1230	C1165	A	G1033	U955	A	C818
G1832	G1762	A1685	A1605	G1527	U1454	G1374	U1304	A1231	A1166	A	U1034	A956	G	G819
U1833	A1764	C1686	C1606	C1528	U1455	A1378	U1304	C1235	A1167	G	G1035	G957	C	U820
G1834	C1765	C1687	U1608	U1531	C1455	A1378	G1310	G1236	G1173	G	G1036	G958	G	A821
C1835	U1766	U1688	A1610	A1532	U1459	G1381	C1311	G1237	G1174	U101	U1037	C959	G	G822
G1836	G1767	G1691	G1533	A1532	U1460	G1382	G1312	G1240	U1176	U102	U1038	A964	G	U823
G1837	U1768	C1692	G1534	U1533	C1461	G1384	U1313	A1241	U1177	C1103	A1040	C	G	U824
G1838	U1769	A1693	A1534	C1534	C1462	A1385	A1314	A1242	C1178	U105	G1041	G967	C	C825
A1839	U1770	A1694	C1615	G1542	A1463	A1386	A1315	G1245	C1179	A106	U1044	U969	U	C829
G1841	A1774	G1697	G1617	G1543	C1464	G1390	G1316	G1246	A1180	A107	U1045	A970	A	C830
G1842	A1775	U1697	C1623	A1544	C1465	A1391	G1317	U1247	C1181	U108	U1046	A971	C	G831
U1843	A1776	C1698	U1547	U1547	C1466	G1392	A1318	G1248	U1182	A109	U1047	A972	A	A832
G1844	U1777	A1699	U1548	U1548	U1467	G1393	A1321	G1249	C1183	G110	U1048	C972	G	A833
A1845	U1778	C1700	A1468	U1549	U1469	G1393	G1322	A1250	C1184	U112	C1049	U977	U	A834
G1846	C1779	C1701	U1470	G1550	G1470	A1397	G1323	G1251	C1185	U111	G1050	U978	C	U835
U1847	A1780	G1702	A1630	G1551	U1475	G1398	G1324	C1252	G1186	U113	U1051	A979	U	G836
U1848	C1781	C1631	C1632	U1551	C1476	C1399	U1325	A1255	A1187	A114	C1052	A984	A	U837
G1849	U1782	A1632	G1552	C1552	G1477	U1403	U1326	C1256	C1188	C115	G1053	G985	C	U840
G1850	A1783	C1633	G1553	G1553	C1478	U1404	U1327	G1260	C1189	U116	C1054	G986	C	G841
A1851	C1786	A1634	U1554	U1554	U1479	C1404	G1334	G1261	C1190	U117	A1055	G987	C	A842
G1854	U1787	G1635	A1555	G1555	G1480	G1407	A1334	G1265	C1191	U118	U1056	G988	C	U845
U1855	G1713	U1443	U1556	G1557	U1481	A1408	G1335	U1262	A1192	U119	G1058	G989	C	A846
G1856	A1714	G1646	C1558	C1558	U1482	U1409	G1336	G1263	C1193	C1123	A1059	C915	C	A847
A1859	U1715	U1647	G1559	U1559	G1483	U1410	G1337	G1264	U1194	G122	U1060	U919	C	A848
G1861	A1716	A1561	U1560	U1560	U1484	C1411	U1338	G1265	C1195	U124	G1063	U920	C	G849
C1862	A1717	C1648	A1561	C1412	A1486	C1412	A1335	U1266	U1197	G125	C	A921	C	C850
A1863	U1718	A1649	G1562	U1563	C1487	U1416	G1336	A1267	C1198	A126	A	A922	C	C851
U1864	G1721	G1652	U1564	U1564	U1490	C1417	G1337	U1268	G1201	C1127	G	A923	C	U852
C1865	U1722	C1653	G1565	G1565	C1491	C1418	U1338	G1269	U1202	G128	G	A924	C	C853
G1866	U1723	A1654	U1570	U1570	C1492	G1419	U1339	C1270	A1203	A129	A	A999	C	G854
A1867	C1724	C1655	C1570	C1570	A1493	A1420	G1340	G1271	U1197	U130	G	C1003	C	U857
U1868	U1727	U1656	G1573	G1573	G1494	U1421	G1342	G1272	G1205	U136	U1072	U1004	C	G858
A1869	A1728	A1657	A1574	A1574	G1495	C1422	C1343	C1273	G1206	A137	G1073	U1005	C	U859
G1870	C1734	G1658	C1575	C1575	G1496	A1423	C1344	A1275	U1207	A138	G1074	A929	C	U860
U1871	G1735	G1659	G1576	G1576	C1497	U1424	G1345	U1276	A1208	A139	C1075	A1007	C	G861
A1807	U1735	C1661	U1577	U1577	G1498	G1425	G1345	G1277	G1209	A140	U1076	C1008	C	A862
C1808	G1742	G1662	U1578	U1578	A1499	U1426	C	A1278	U1212	U141	U1077	C1009	C	C863
G1809	U1743	C1663	G1579	G1579	U1500	G1427	G1348	G1279	U1213	A142	A1078	G933	C	C864
U1810	C1743	G1664	U1582	U1582	C1501	G1428	G1350	C1283	G1214	G	U1079	G934	C	A865
G1814	G1744	C1665	A1583	A1583	U1505	A1429	G1351	A1284	C1215	C145	A1080	G938	C	U866
C1815	C1745	U1584	G1584	G1584	C1506	U1431	C1352	G1285	A1216	U1015	A1081	U1015	C	G870
G1816	A1746	A1585	C1584	C1584	U1507	G1432	A1353	A1286	G1217	G147	G1082	G940	C	G871
U1817	G1747	G1586	U1585	U1585	A1507	A1433	A1354	A1287	C1218	U148	C1083	U1016	C	U872
G1818	C1570	G1508	G1508	G1508	C1508	A1434	A1355	A1287	G1219	G149	A1084	C1017	C	G873
U1819	A1750	A1671	A1587	A1587	U1509	U1435	G1356	A1288	C1219	U150	C	C1018	C	U874
C1820	U1752	C1672	A1588	A1588	G1436	G1436	U1357	A1289	G1220	U151	G	U1019	C	A875
G	A1753	C1673	U1594	U1594	A1511	A1437	C1358	A1290	C1221	C152	C	A1020	C	G875

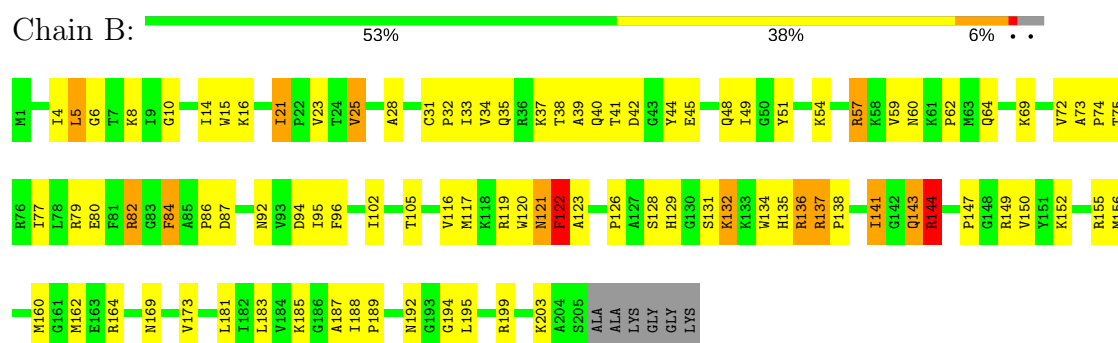




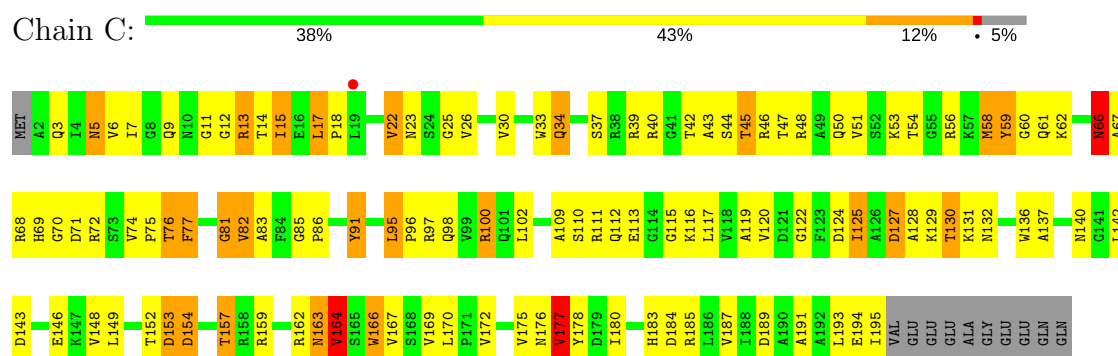
• Molecule 3: 50S ribosomal protein L2



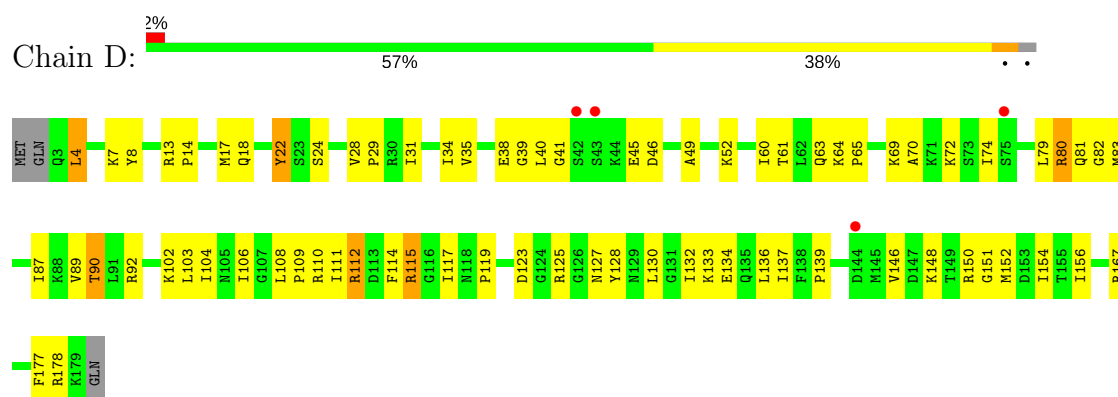
• Molecule 4: 50S ribosomal protein L3



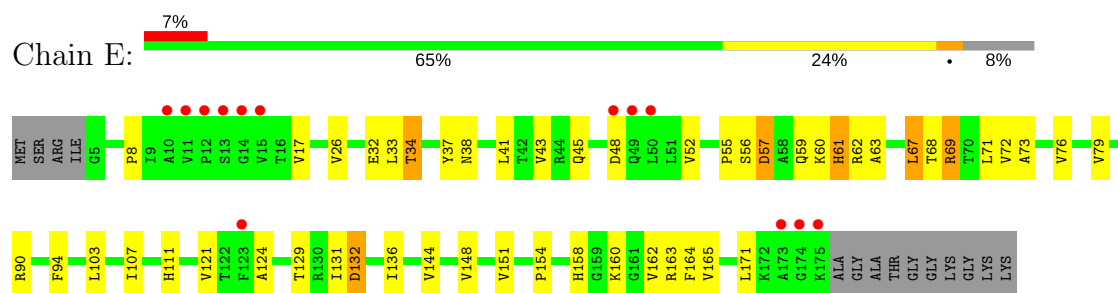
• Molecule 5: 50S ribosomal protein L4



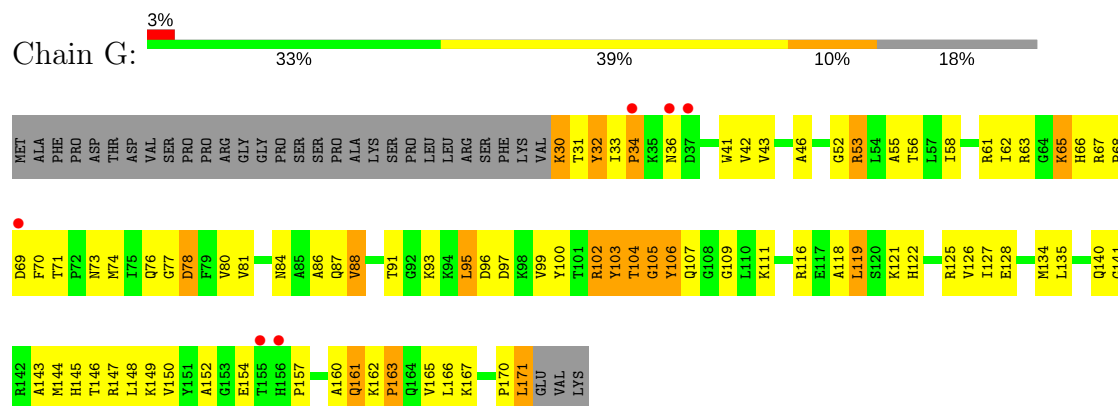
• Molecule 6: 50S ribosomal protein L5



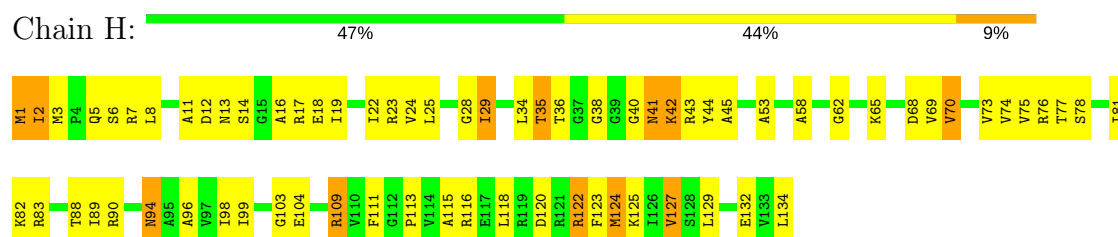
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L13



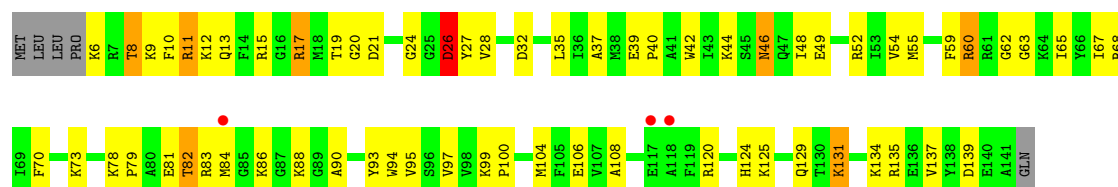
- Molecule 9: 50S ribosomal protein L14



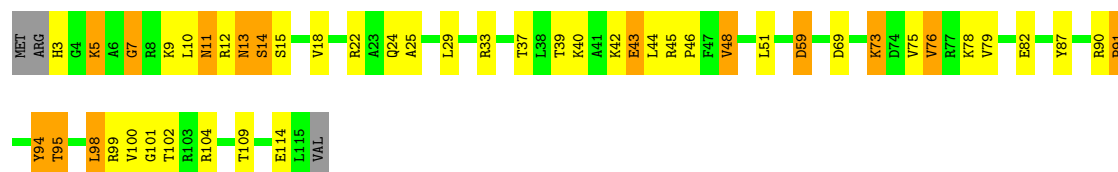
- Molecule 10: 50S ribosomal protein L15



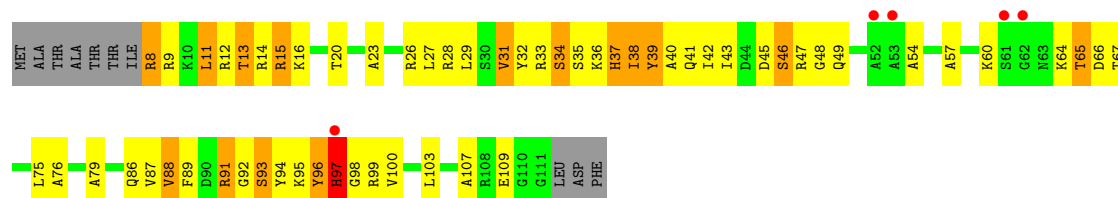
- Molecule 11: 50S ribosomal protein L16



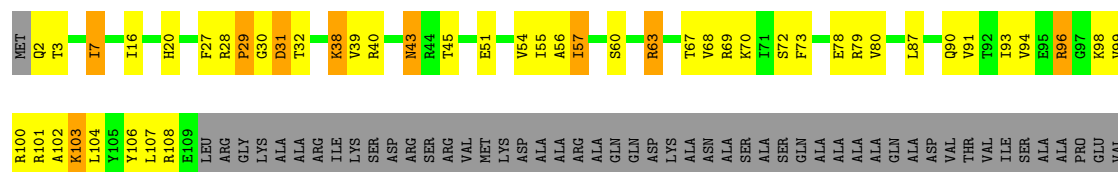
- Molecule 12: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L18

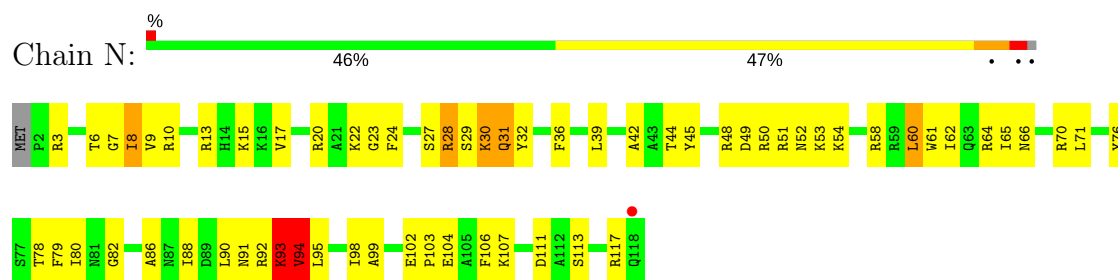


- Molecule 14: 50S ribosomal protein L19

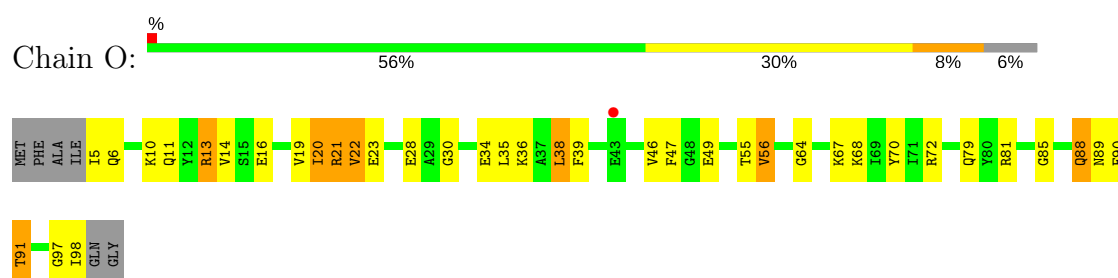


ALA
PRO
GLU
THR
GLN
GLY
GLU

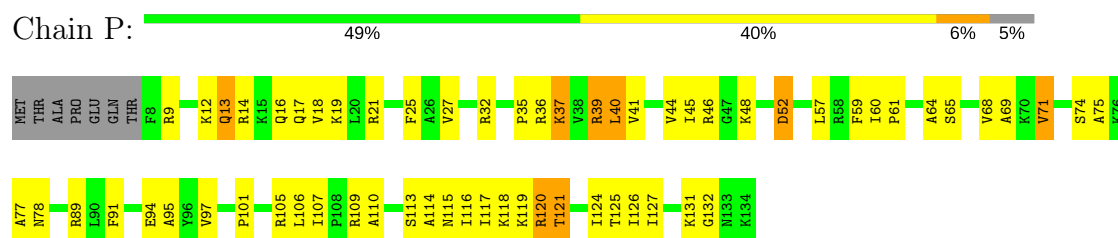
• Molecule 15: 50S ribosomal protein L20



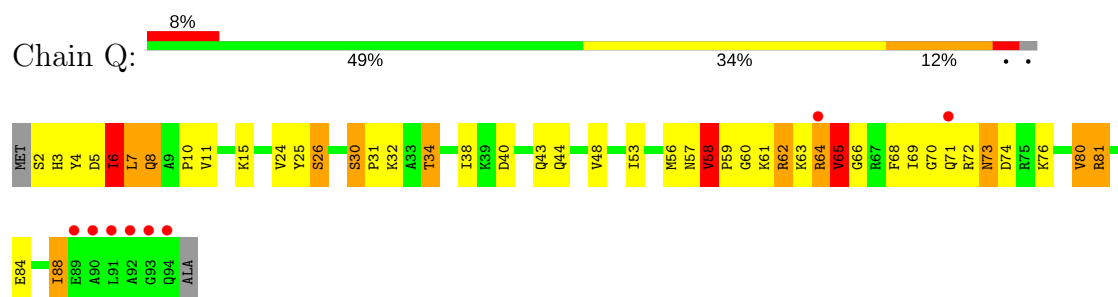
• Molecule 16: 50S ribosomal protein L21



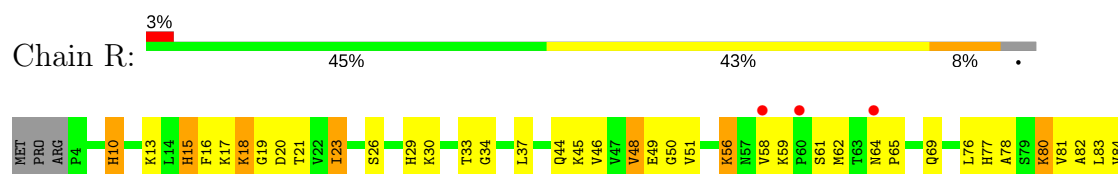
• Molecule 17: 50S ribosomal protein L22



• Molecule 18: 50S ribosomal protein L23

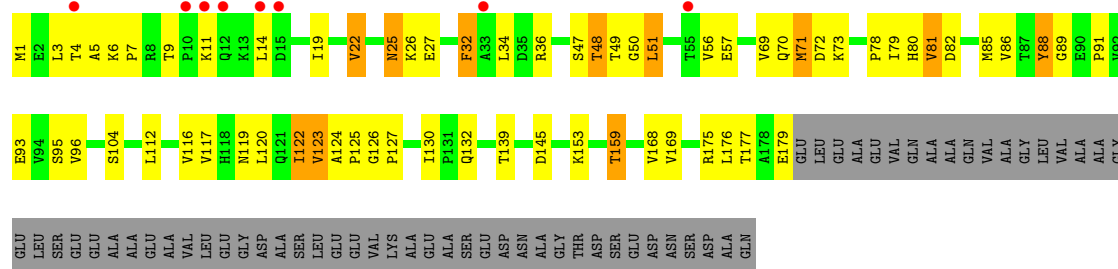


• Molecule 19: 50S ribosomal protein L24

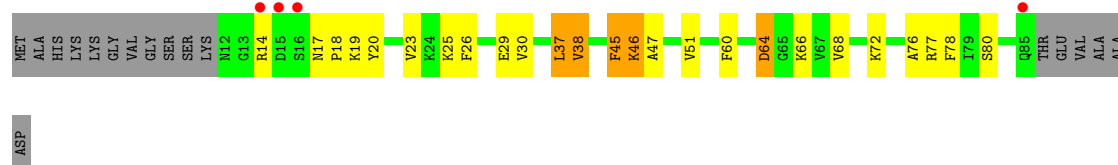




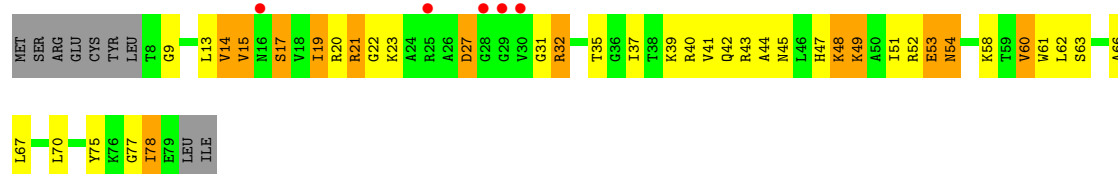
• Molecule 20: 50S ribosomal protein L25



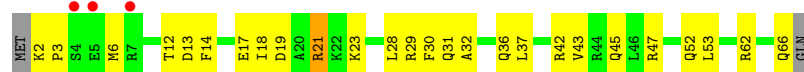
• Molecule 21: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L28



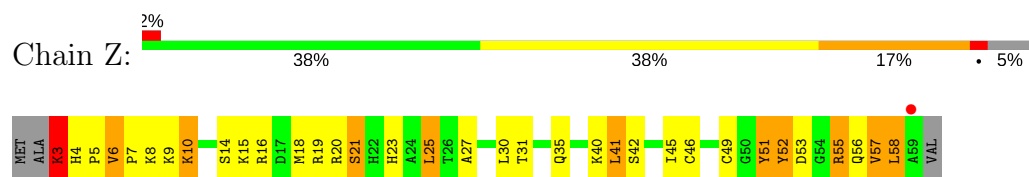
• Molecule 23: 50S ribosomal protein L29



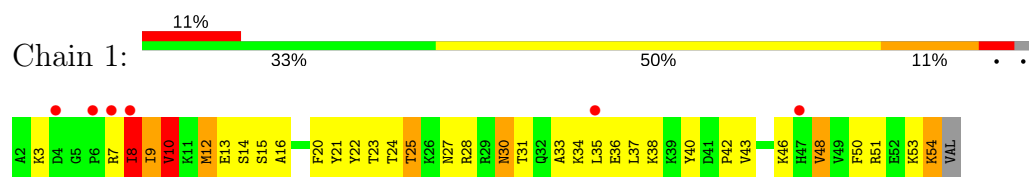
• Molecule 24: 50S ribosomal protein L30



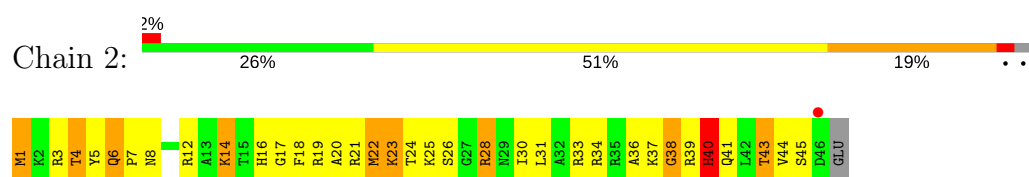
- Molecule 25: 50S ribosomal protein L32



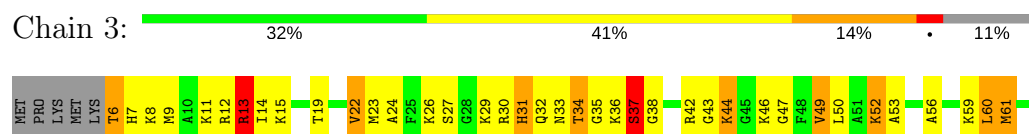
- Molecule 26: 50S ribosomal protein L33



- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.47Å 407.38Å 692.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.58 29.84 – 3.57	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.84-3.58) 94.2 (29.84-3.57)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.56Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.247 0.208 , 0.253	Depositor DCC
R_{free} test set	13342 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83681	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 6O1

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	20/63887 (0.0%)	1.25	500/99650 (0.5%)
2	Y	0.41	0/2863	0.93	0/4461
3	A	0.49	0/2011	0.79	4/2708 (0.1%)
4	B	0.58	0/1567	0.85	0/2105
5	C	0.49	0/1504	0.77	1/2036 (0.0%)
6	D	0.30	0/1419	0.51	0/1903
7	E	0.30	0/1308	0.54	0/1771
8	G	0.51	0/1138	0.81	1/1539 (0.1%)
9	H	0.56	0/1007	0.74	0/1352
10	I	0.61	0/1022	0.93	3/1366 (0.2%)
11	J	0.48	0/1101	0.71	0/1472
12	K	0.67	0/886	0.89	2/1188 (0.2%)
13	L	0.39	0/785	0.69	0/1048
14	M	0.67	1/872 (0.1%)	0.91	2/1172 (0.2%)
15	N	0.52	0/994	0.77	0/1323
16	O	0.46	0/750	0.81	2/1000 (0.2%)
17	P	0.58	0/1027	0.71	0/1373
18	Q	0.49	0/737	0.82	2/988 (0.2%)
19	R	0.45	0/835	0.75	0/1121
20	S	0.31	0/1399	0.57	0/1902
21	T	0.45	0/563	0.75	0/747
22	U	0.46	0/556	0.73	0/741
23	V	0.34	0/529	0.52	0/704
24	W	0.43	0/426	0.67	0/568
25	Z	0.56	0/464	0.77	0/622
26	1	0.55	0/434	0.83	0/579
27	2	0.58	0/387	1.04	2/509 (0.4%)
28	3	0.59	0/468	0.98	2/614 (0.3%)
All	All	0.63	21/90939 (0.0%)	1.14	521/136562 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
4	B	0	1
5	C	0	2
8	G	0	4
10	I	0	5
11	J	0	1
13	L	0	1
15	N	0	2
19	R	0	1
25	Z	0	1
27	2	0	3
28	3	0	2
All	All	0	24

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	774	A	C5-C4	7.18	1.43	1.38
1	X	542	A	N9-C4	-7.12	1.33	1.37
14	M	29	PRO	CA-C	6.60	1.66	1.52
1	X	540	G	C2-N3	6.49	1.38	1.32
1	X	2548	G	C6-O6	6.47	1.29	1.24
1	X	1278	A	N3-C4	-6.36	1.31	1.34
1	X	774	A	N7-C5	-6.11	1.35	1.39
1	X	1278	A	C6-N1	-5.86	1.31	1.35
1	X	540	G	N9-C4	5.80	1.42	1.38
1	X	1688	U	C2-N3	5.72	1.41	1.37
1	X	1333	G	N9-C4	-5.69	1.33	1.38
1	X	542	A	N3-C4	-5.66	1.31	1.34
1	X	512	A	N9-C4	-5.66	1.34	1.37
1	X	2795	A	N9-C4	5.46	1.41	1.37
1	X	1981	A	N3-C4	-5.45	1.31	1.34
1	X	2591	C	N1-C2	5.35	1.45	1.40
1	X	1672	A	N7-C5	-5.30	1.36	1.39
1	X	796	A	N9-C4	-5.19	1.34	1.37
1	X	1278	A	N9-C4	-5.18	1.34	1.37
1	X	1630	A	N7-C5	-5.13	1.36	1.39
1	X	2701	A	N9-C4	-5.07	1.34	1.37

All (521) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	774	A	N7-C8-N9	14.67	121.13	113.80
1	X	774	A	C8-N9-C4	-14.58	99.97	105.80
1	X	542	A	C2-N3-C4	-13.70	103.75	110.60
1	X	1333	G	N3-C4-N9	-12.51	118.49	126.00
1	X	2018	G	C4-C5-N7	11.72	115.49	110.80
1	X	537	C	N3-C2-O2	-11.52	113.84	121.90
1	X	540	G	N3-C4-C5	-11.45	122.88	128.60
1	X	1670	G	C8-N9-C4	11.16	110.86	106.40
1	X	1468	A	C8-N9-C4	-11.14	101.35	105.80
1	X	2548	G	C5-C6-N1	-10.99	106.00	111.50
1	X	542	A	N1-C2-N3	10.98	134.79	129.30
1	X	2705	A	N7-C8-N9	10.86	119.23	113.80
1	X	1333	G	N3-C4-C5	10.86	134.03	128.60
1	X	1278	A	C2-N3-C4	-10.68	105.26	110.60
1	X	774	A	C6-C5-N7	-10.52	124.94	132.30
1	X	346	C	C6-N1-C2	-10.48	116.11	120.30
1	X	540	G	N3-C2-N2	10.39	127.18	119.90
1	X	661	C	C6-N1-C2	-10.33	116.17	120.30
1	X	2018	G	O4'-C1'-N9	10.29	116.43	108.20
1	X	540	G	N1-C6-O6	-10.23	113.76	119.90
1	X	540	G	C5-C6-N1	10.10	116.55	111.50
1	X	774	A	C5-N7-C8	-9.75	99.03	103.90
1	X	1670	G	N9-C4-C5	-9.68	101.53	105.40
1	X	2033	C	C6-N1-C2	-9.62	116.45	120.30
1	X	2705	A	C8-N9-C4	-9.54	101.98	105.80
1	X	540	G	N1-C2-N2	-9.47	107.68	116.20
1	X	2690	A	C2-N3-C4	-9.33	105.93	110.60
1	X	1630	A	N1-C6-N6	9.31	124.19	118.60
1	X	2018	G	C5-N7-C8	-9.27	99.67	104.30
1	X	309	G	C4-C5-N7	9.15	114.46	110.80
1	X	2705	A	C2-N3-C4	-9.14	106.03	110.60
1	X	1333	G	C2-N3-C4	-9.11	107.34	111.90
1	X	2591	C	N1-C2-O2	9.10	124.36	118.90
1	X	537	C	C6-N1-C2	-9.01	116.69	120.30
1	X	2018	G	O5'-P-OP2	-9.00	97.60	105.70
1	X	2705	A	C5-N7-C8	-8.91	99.44	103.90
1	X	1770	U	C5-C6-N1	-8.87	118.26	122.70
1	X	699	G	C5-N7-C8	-8.76	99.92	104.30
1	X	479	G	N1-C6-O6	8.74	125.15	119.90
1	X	1278	A	N1-C2-N3	8.70	133.65	129.30
1	X	540	G	N3-C4-N9	8.68	131.21	126.00
1	X	1975	G	O5'-P-OP1	-8.65	97.91	105.70
1	X	538	A	C2-N3-C4	8.65	114.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1278	A	O5'-P-OP1	-8.58	97.98	105.70
1	X	1631	C	C2-N1-C1'	8.48	128.12	118.80
1	X	2045	A	N1-C6-N6	8.40	123.64	118.60
1	X	2820	C	C6-N1-C2	8.40	123.66	120.30
1	X	2246	A	N1-C6-N6	-8.39	113.57	118.60
1	X	2820	C	N3-C4-C5	8.37	125.25	121.90
1	X	774	A	C2-N3-C4	-8.35	106.42	110.60
1	X	2485	U	C2-N1-C1'	8.32	127.69	117.70
1	X	309	G	C5-N7-C8	-8.20	100.20	104.30
12	K	10	LEU	CA-CB-CG	8.17	134.08	115.30
1	X	1631	C	C5-C6-N1	8.14	125.07	121.00
1	X	1468	A	N1-C6-N6	-8.08	113.75	118.60
1	X	1746	A	N1-C2-N3	8.06	133.33	129.30
1	X	177	U	C5-C4-O4	-8.06	121.06	125.90
1	X	1630	A	C6-C5-N7	-8.05	126.67	132.30
1	X	2668	U	O5'-P-OP1	-8.03	98.48	105.70
1	X	1663	C	N1-C2-O2	8.01	123.70	118.90
1	X	1669	A	N1-C6-N6	7.98	123.39	118.60
1	X	699	G	C4-C5-N7	7.95	113.98	110.80
1	X	479	G	C5-C6-O6	-7.86	123.88	128.60
1	X	123	A	C8-N9-C4	7.86	108.94	105.80
1	X	1336	G	C4-C5-N7	7.85	113.94	110.80
1	X	774	A	N1-C6-N6	7.84	123.31	118.60
1	X	1336	G	N9-C4-C5	-7.80	102.28	105.40
1	X	343	A	C8-N9-C4	-7.72	102.71	105.80
1	X	841	G	N7-C8-N9	7.70	116.95	113.10
1	X	2553	G	N3-C4-C5	7.70	132.45	128.60
10	I	51	GLY	N-CA-C	7.64	132.20	113.10
1	X	774	A	C4-C5-C6	7.60	120.80	117.00
1	X	2490	U	N3-C2-O2	-7.46	116.98	122.20
1	X	542	A	C5-N7-C8	-7.45	100.17	103.90
1	X	2705	A	P-O3'-C3'	7.41	128.59	119.70
1	X	540	G	O4'-C1'-N9	7.41	114.12	108.20
28	3	60	LEU	CA-CB-CG	7.39	132.31	115.30
1	X	1770	U	C2-N1-C1'	-7.39	108.83	117.70
1	X	2820	C	C5-C6-N1	-7.38	117.31	121.00
1	X	537	C	N1-C2-O2	7.38	123.33	118.90
1	X	1992	G	C8-N9-C4	7.35	109.34	106.40
1	X	2018	G	N3-C4-C5	7.33	132.26	128.60
14	M	28	ARG	N-CA-C	-7.28	91.34	111.00
1	X	2018	G	C5-C6-O6	-7.27	124.24	128.60
1	X	689	A	C2-N3-C4	-7.27	106.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2815	C	C6-N1-C2	7.26	123.20	120.30
1	X	343	A	N7-C8-N9	7.23	117.42	113.80
1	X	522	G	N1-C6-O6	7.23	124.24	119.90
1	X	1688	U	N3-C4-C5	-7.22	110.27	114.60
1	X	522	G	C5-C6-O6	-7.22	124.27	128.60
1	X	2596	C	C6-N1-C2	7.22	123.19	120.30
1	X	2687	G	C8-N9-C4	7.19	109.28	106.40
1	X	2658	A	C8-N9-C4	7.18	108.67	105.80
1	X	540	G	C8-N9-C4	-7.18	103.53	106.40
1	X	774	A	C4-C5-N7	7.11	114.25	110.70
1	X	787	A	C2-N3-C4	-7.09	107.06	110.60
1	X	841	G	C5-N7-C8	-7.07	100.77	104.30
1	X	841	G	C8-N9-C4	-7.06	103.58	106.40
1	X	1006	C	N3-C2-O2	-7.03	116.98	121.90
1	X	617	U	N3-C2-O2	-7.00	117.30	122.20
1	X	540	G	C6-N1-C2	-7.00	120.90	125.10
1	X	462	G	C8-N9-C4	6.99	109.20	106.40
1	X	540	G	C2-N3-C4	6.96	115.38	111.90
1	X	542	A	C5-C6-N1	-6.95	114.22	117.70
1	X	1993	G	N1-C6-O6	6.94	124.06	119.90
1	X	1285	A	C2-N3-C4	-6.93	107.13	110.60
1	X	1277	G	N1-C6-O6	-6.92	115.75	119.90
1	X	88	G	C8-N9-C4	-6.92	103.63	106.40
1	X	542	A	N1-C6-N6	6.89	122.74	118.60
1	X	757	U	OP2-P-O3'	6.87	120.32	105.20
1	X	1338	G	N3-C4-N9	6.87	130.12	126.00
1	X	2553	G	N3-C4-N9	-6.87	121.88	126.00
1	X	923	A	C2-N3-C4	6.86	114.03	110.60
1	X	26	G	C8-N9-C4	-6.86	103.66	106.40
1	X	1975	G	N1-C6-O6	-6.86	115.78	119.90
1	X	1631	C	C4-C5-C6	-6.86	113.97	117.40
1	X	1630	A	C5-N7-C8	-6.85	100.47	103.90
1	X	2399	C	C6-N1-C2	6.81	123.02	120.30
1	X	1006	C	N1-C2-O2	6.81	122.98	118.90
1	X	1679	U	C5-C6-N1	-6.81	119.30	122.70
1	X	519	C	C6-N1-C2	-6.79	117.58	120.30
1	X	746	G	N3-C4-C5	-6.77	125.22	128.60
1	X	522	G	C4-C5-N7	6.74	113.50	110.80
1	X	955	G	C8-N9-C1'	-6.74	118.23	127.00
1	X	699	G	N7-C8-N9	6.73	116.46	113.10
1	X	699	G	C2-N3-C4	-6.73	108.54	111.90
1	X	2607	C	N3-C2-O2	-6.67	117.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	774	A	C5-C6-N1	-6.67	114.36	117.70
1	X	2423	G	O5'-P-OP2	-6.66	99.70	105.70
1	X	2547	C	N3-C4-C5	6.66	124.56	121.90
1	X	1333	G	C8-N9-C4	-6.63	103.75	106.40
1	X	1631	C	C6-N1-C1'	-6.62	112.85	120.80
1	X	1693	A	C8-N9-C4	-6.62	103.15	105.80
16	O	38	LEU	CA-CB-CG	6.60	130.48	115.30
1	X	413	G	C8-N9-C4	-6.59	103.76	106.40
1	X	2757	G	N1-C6-O6	6.58	123.85	119.90
1	X	542	A	C6-C5-N7	-6.58	127.70	132.30
1	X	661	C	N3-C4-C5	-6.56	119.28	121.90
1	X	540	G	P-O3'-C3'	6.56	127.57	119.70
1	X	1333	G	C5-N7-C8	-6.56	101.02	104.30
1	X	1304	U	C5-C6-N1	-6.56	119.42	122.70
1	X	763	A	N1-C6-N6	-6.55	114.67	118.60
1	X	837	U	C5-C6-N1	-6.53	119.44	122.70
1	X	1475	U	P-O3'-C3'	6.50	127.50	119.70
1	X	955	G	N3-C4-N9	6.50	129.90	126.00
1	X	2371	A	C4-C5-C6	6.47	120.23	117.00
1	X	1468	A	N7-C8-N9	6.45	117.02	113.80
1	X	309	G	C5-C6-O6	-6.45	124.73	128.60
1	X	2398	U	C6-N1-C2	-6.45	117.13	121.00
1	X	1688	U	N3-C4-O4	6.42	123.89	119.40
1	X	1647	U	N3-C4-C5	-6.41	110.75	114.60
16	O	30	GLY	N-CA-C	-6.41	97.07	113.10
1	X	689	A	O4'-C1'-N9	6.40	113.32	108.20
1	X	617	U	C4-C5-C6	6.39	123.54	119.70
1	X	955	G	C4-N9-C1'	6.39	134.81	126.50
1	X	1983	G	C8-N9-C4	6.38	108.95	106.40
1	X	1991	C	C5-C6-N1	-6.38	117.81	121.00
1	X	1985	G	C2-N3-C4	-6.37	108.71	111.90
1	X	1724	C	C6-N1-C2	6.37	122.85	120.30
1	X	1631	C	N1-C2-O2	6.37	122.72	118.90
1	X	1468	A	C5-C6-N1	6.36	120.88	117.70
1	X	2560	G	C8-N9-C4	-6.34	103.86	106.40
1	X	985	G	C4-C5-N7	6.34	113.34	110.80
1	X	309	G	N1-C6-O6	6.34	123.70	119.90
1	X	1746	A	C2-N3-C4	-6.33	107.44	110.60
1	X	2398	U	N3-C4-C5	-6.31	110.81	114.60
1	X	2485	U	C6-N1-C1'	-6.31	112.37	121.20
1	X	1141	U	C5-C6-N1	-6.30	119.55	122.70
1	X	993	C	N1-C2-O2	6.30	122.68	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1770	U	N1-C2-N3	6.30	118.68	114.90
1	X	1770	U	C5-C4-O4	6.30	129.68	125.90
1	X	1975	G	P-O3'-C3'	6.29	127.25	119.70
1	X	689	A	N1-C6-N6	6.29	122.37	118.60
1	X	88	G	N7-C8-N9	6.27	116.23	113.10
5	C	81	GLY	N-CA-C	-6.26	97.44	113.10
1	X	1647	U	N1-C2-O2	-6.25	118.42	122.80
1	X	860	U	C2-N1-C1'	6.25	125.20	117.70
1	X	1391	A	P-O3'-C3'	6.25	127.19	119.70
1	X	2820	C	C2-N3-C4	-6.24	116.78	119.90
1	X	746	G	N3-C4-N9	6.24	129.74	126.00
1	X	346	C	N3-C4-C5	-6.23	119.41	121.90
1	X	2553	G	C5-N7-C8	-6.23	101.18	104.30
1	X	2242	C	N3-C2-O2	-6.23	117.54	121.90
1	X	1974	U	O5'-P-OP2	-6.23	100.10	105.70
1	X	2705	A	C6-C5-N7	-6.22	127.94	132.30
1	X	1745	C	N1-C2-O2	-6.21	115.18	118.90
1	X	2655	C	C5-C6-N1	-6.21	117.90	121.00
1	X	2495	G	C5-C6-N1	6.20	114.60	111.50
1	X	2371	A	N7-C8-N9	6.20	116.90	113.80
1	X	746	G	C4-N9-C1'	6.20	134.56	126.50
1	X	1975	G	C8-N9-C4	-6.19	103.92	106.40
3	A	35	GLU	N-CA-C	6.18	127.69	111.00
1	X	1019	U	P-O3'-C3'	6.17	127.10	119.70
1	X	1664	G	N3-C4-C5	6.17	131.68	128.60
1	X	2624	G	C4-C5-N7	6.16	113.27	110.80
1	X	1923	U	P-O3'-C3'	6.15	127.08	119.70
1	X	796	A	C2-N3-C4	-6.15	107.52	110.60
1	X	2045	A	C5-C6-N6	-6.14	118.79	123.70
1	X	393	U	N3-C4-C5	-6.14	110.92	114.60
1	X	2541	U	N3-C2-O2	-6.14	117.90	122.20
12	K	7	GLY	N-CA-C	6.14	128.44	113.10
1	X	632	A	C2-N3-C4	-6.13	107.54	110.60
1	X	853	C	C6-N1-C2	6.13	122.75	120.30
1	X	2001	G	N1-C6-O6	-6.13	116.22	119.90
1	X	2854	G	N7-C8-N9	6.12	116.16	113.10
1	X	1630	A	C4-C5-N7	6.12	113.76	110.70
1	X	2698	G	OP1-P-O3'	6.11	118.65	105.20
1	X	2668	U	N3-C4-O4	-6.11	115.12	119.40
1	X	2371	A	C6-C5-N7	-6.11	128.03	132.30
1	X	661	C	C5-C6-N1	6.11	124.05	121.00
1	X	689	A	C5-N7-C8	-6.11	100.85	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1770	U	C6-N1-C1'	6.08	129.72	121.20
14	M	30	GLY	N-CA-C	-6.08	97.89	113.10
1	X	1775	A	C6-N1-C2	-6.08	114.95	118.60
1	X	1981	A	N1-C2-N3	6.07	132.34	129.30
1	X	742	G	N3-C4-N9	6.05	129.63	126.00
1	X	1683	G	O4'-C1'-N9	6.05	113.04	108.20
1	X	2559	U	O5'-P-OP1	-6.04	100.26	105.70
1	X	2043	A	OP2-P-O3'	6.03	118.47	105.20
1	X	1656	U	C5-C6-N1	-6.03	119.69	122.70
1	X	1991	C	N3-C4-C5	6.01	124.30	121.90
1	X	806	A	C8-N9-C4	6.00	108.20	105.80
1	X	2825	A	N1-C6-N6	6.00	122.20	118.60
1	X	1705	U	C2-N1-C1'	-6.00	110.50	117.70
1	X	2045	A	C6-C5-N7	-5.99	128.10	132.30
1	X	1304	U	C6-N1-C2	5.99	124.59	121.00
1	X	2496	C	C5-C4-N4	-5.99	116.01	120.20
1	X	123	A	N7-C8-N9	-5.96	110.82	113.80
1	X	2681	A	N1-C6-N6	5.96	122.18	118.60
1	X	2578	G	C4-N9-C1'	5.96	134.25	126.50
1	X	2668	U	C2-N1-C1'	-5.96	110.55	117.70
1	X	2490	U	N1-C2-N3	5.96	118.47	114.90
1	X	2705	A	N1-C2-N3	5.95	132.27	129.30
1	X	1570	C	N1-C2-O2	5.94	122.47	118.90
1	X	2002	A	N1-C6-N6	5.94	122.17	118.60
1	X	1975	G	N3-C4-C5	-5.94	125.63	128.60
1	X	1801	C	O5'-P-OP1	-5.93	100.36	105.70
1	X	660	G	N3-C4-N9	-5.93	122.44	126.00
1	X	699	G	C6-C5-N7	-5.92	126.85	130.40
1	X	2805	G	N3-C4-N9	5.91	129.54	126.00
1	X	1946	U	C2-N1-C1'	5.90	124.78	117.70
1	X	2634	G	O4'-C1'-N9	5.90	112.92	108.20
1	X	1278	A	O4'-C1'-N9	5.89	112.91	108.20
1	X	689	A	C6-C5-N7	-5.88	128.18	132.30
1	X	2655	C	C6-N1-C2	5.88	122.65	120.30
1	X	2668	U	C5-C4-O4	5.88	129.43	125.90
1	X	2548	G	C4-C5-N7	-5.87	108.45	110.80
1	X	797	A	P-O3'-C3'	5.86	126.73	119.70
1	X	177	U	N3-C4-O4	5.84	123.49	119.40
1	X	2258	G	C4-N9-C1'	-5.84	118.91	126.50
1	X	956	A	N1-C6-N6	5.84	122.10	118.60
1	X	955	G	C6-C5-N7	-5.83	126.90	130.40
1	X	1982	C	C5-C6-N1	-5.83	118.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2799	C	C6-N1-C2	-5.82	117.97	120.30
1	X	1670	G	N3-C2-N2	5.82	123.97	119.90
1	X	1669	A	C5-C6-N6	-5.82	119.05	123.70
1	X	1019	U	OP2-P-O3'	5.81	117.98	105.20
10	I	47	ALA	N-CA-C	5.79	126.64	111.00
1	X	219	G	P-O3'-C3'	5.78	126.64	119.70
1	X	1688	U	C2-N3-C4	5.78	130.47	127.00
1	X	2854	G	C4-N9-C1'	5.77	134.00	126.50
1	X	1468	A	N9-C4-C5	5.77	108.11	105.80
1	X	1666	G	C4-N9-C1'	-5.77	119.00	126.50
1	X	1283	C	N1-C2-O2	-5.75	115.45	118.90
1	X	798	G	N3-C4-C5	-5.75	125.72	128.60
1	X	581	A	O5'-P-OP1	-5.73	100.54	105.70
1	X	1702	C	C6-N1-C2	5.73	122.59	120.30
1	X	699	G	O4'-C1'-N9	-5.73	103.62	108.20
1	X	177	U	O4'-C1'-N1	5.72	112.78	108.20
1	X	788	G	P-O3'-C3'	5.72	126.57	119.70
1	X	1630	A	N7-C8-N9	5.72	116.66	113.80
1	X	699	G	N3-C4-C5	5.71	131.46	128.60
1	X	2812	A	C8-N9-C4	-5.71	103.52	105.80
1	X	850	C	C6-N1-C2	-5.71	118.02	120.30
1	X	1760	G	O5'-P-OP2	-5.70	100.57	105.70
1	X	2558	C	N3-C4-C5	5.70	124.18	121.90
1	X	1336	G	C5-C6-O6	-5.70	125.18	128.60
1	X	2591	C	C5-C6-N1	5.69	123.85	121.00
1	X	2039	G	C8-N9-C4	-5.69	104.12	106.40
1	X	2578	G	C8-N9-C1'	-5.68	119.61	127.00
1	X	2228	U	C6-N1-C2	-5.67	117.59	121.00
3	A	33	LEU	CA-CB-CG	5.67	128.35	115.30
1	X	2705	A	C4-C5-N7	5.66	113.53	110.70
1	X	2495	G	C6-N1-C2	-5.66	121.71	125.10
1	X	1335	A	C8-N9-C4	5.65	108.06	105.80
1	X	1468	A	N3-C4-C5	-5.65	122.84	126.80
1	X	2854	G	C4-C5-N7	5.65	113.06	110.80
1	X	571	U	C5-C6-N1	-5.65	119.88	122.70
1	X	1318	A	C8-N9-C4	5.65	108.06	105.80
1	X	1981	A	C6-N1-C2	-5.65	115.21	118.60
1	X	2673	G	C4-C5-N7	5.65	113.06	110.80
1	X	1454	U	N3-C4-O4	5.65	123.35	119.40
1	X	1688	U	C5-C6-N1	5.64	125.52	122.70
1	X	1780	A	N1-C6-N6	5.64	121.99	118.60
1	X	1982	C	C2-N3-C4	-5.63	117.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1975	G	O4'-C1'-N9	-5.63	103.69	108.20
1	X	1663	C	N3-C2-O2	-5.63	117.96	121.90
1	X	169	C	C6-N1-C2	5.63	122.55	120.30
1	X	2018	G	N1-C6-O6	5.63	123.28	119.90
1	X	2371	A	C8-N9-C4	-5.62	103.55	105.80
1	X	660	G	N3-C4-C5	5.62	131.41	128.60
1	X	1991	C	C6-N1-C2	5.62	122.55	120.30
1	X	2587	G	C5-C6-O6	-5.62	125.23	128.60
1	X	2756	A	P-O3'-C3'	5.61	126.43	119.70
1	X	177	U	P-O3'-C3'	5.61	126.43	119.70
1	X	1279	G	C8-N9-C4	5.61	108.64	106.40
1	X	1292	A	O5'-P-OP2	-5.61	100.65	105.70
3	A	21	PHE	N-CA-C	5.61	126.14	111.00
1	X	542	A	C4-C5-N7	5.61	113.50	110.70
1	X	1312	G	C5-N7-C8	-5.60	101.50	104.30
1	X	1333	G	N7-C8-N9	5.59	115.90	113.10
1	X	796	A	C5-N7-C8	-5.59	101.10	103.90
1	X	984	A	N1-C6-N6	5.59	121.95	118.60
1	X	309	G	N7-C8-N9	5.59	115.89	113.10
1	X	742	G	C4-N9-C1'	5.59	133.76	126.50
1	X	1991	C	C2-N3-C4	-5.59	117.11	119.90
1	X	1752	U	N1-C2-O2	-5.58	118.89	122.80
1	X	1939	U	N3-C2-O2	-5.58	118.29	122.20
1	X	1278	A	C5-C6-N1	-5.58	114.91	117.70
1	X	1647	U	C6-N1-C1'	5.58	129.00	121.20
1	X	874	A	C8-N9-C4	-5.57	103.57	105.80
1	X	1630	A	C5-C6-N1	-5.57	114.91	117.70
1	X	1939	U	N1-C2-O2	5.57	126.70	122.80
1	X	2825	A	N9-C4-C5	-5.57	103.57	105.80
1	X	338	G	C8-N9-C4	-5.56	104.17	106.40
1	X	1286	U	N3-C2-O2	-5.56	118.31	122.20
1	X	2490	U	C5-C4-O4	5.55	129.23	125.90
1	X	2590	U	N3-C2-O2	-5.55	118.31	122.20
1	X	2033	C	N3-C2-O2	-5.55	118.02	121.90
1	X	1269	G	C5-C6-O6	-5.55	125.27	128.60
1	X	2667	C	N1-C2-O2	5.54	122.22	118.90
1	X	747	A	N1-C6-N6	5.54	121.92	118.60
1	X	2252	A	C2-N3-C4	5.54	113.37	110.60
1	X	479	G	C4-C5-N7	5.53	113.01	110.80
1	X	1974	U	OP2-P-O3'	5.53	117.36	105.20
27	2	40	HIS	N-CA-C	-5.52	96.09	111.00
1	X	646	C	C6-N1-C2	-5.52	118.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1344	C	N1-C2-O2	5.52	122.21	118.90
1	X	504	G	C4-C5-N7	5.51	113.01	110.80
1	X	985	G	C5-N7-C8	-5.51	101.54	104.30
1	X	1664	G	C8-N9-C4	5.51	108.60	106.40
1	X	1304	U	C2-N3-C4	-5.51	123.69	127.00
1	X	742	G	C8-N9-C1'	-5.50	119.85	127.00
1	X	2528	G	C8-N9-C1'	-5.50	119.85	127.00
1	X	2550	C	C6-N1-C2	-5.50	118.10	120.30
1	X	1241	G	N3-C4-C5	-5.49	125.86	128.60
1	X	2240	C	N3-C2-O2	-5.49	118.06	121.90
1	X	2018	G	N9-C4-C5	-5.49	103.20	105.40
1	X	1467	U	C6-N1-C2	5.49	124.29	121.00
1	X	393	U	C6-N1-C2	-5.48	117.71	121.00
1	X	520	C	C6-N1-C2	-5.48	118.11	120.30
1	X	817	A	O4'-C1'-N9	5.48	112.58	108.20
1	X	1792	C	P-O3'-C3'	5.48	126.27	119.70
1	X	504	G	N1-C6-O6	5.47	123.19	119.90
1	X	2673	G	N1-C6-O6	5.47	123.19	119.90
1	X	2756	A	C8-N9-C4	-5.47	103.61	105.80
1	X	1269	G	C4-C5-N7	5.47	112.99	110.80
1	X	789	G	C4-N9-C1'	5.47	133.61	126.50
1	X	1468	A	C6-N1-C2	-5.47	115.32	118.60
1	X	2258	G	O4'-C1'-N9	5.46	112.57	108.20
18	Q	59	PRO	N-CA-C	5.45	126.28	112.10
1	X	841	G	C4-C5-N7	5.45	112.98	110.80
1	X	1670	G	C8-N9-C1'	-5.45	119.92	127.00
1	X	1946	U	N1-C2-O2	5.45	126.61	122.80
10	I	56	LEU	N-CA-C	5.45	125.70	111.00
1	X	1031	C	P-O3'-C3'	5.44	126.23	119.70
1	X	1979	C	N1-C2-O2	5.44	122.16	118.90
1	X	2749	A	N1-C6-N6	5.44	121.86	118.60
1	X	1705	U	C5-C4-O4	5.43	129.16	125.90
1	X	931	G	C8-N9-C4	5.43	108.57	106.40
1	X	2867	G	C4-C5-N7	5.42	112.97	110.80
1	X	1332	G	N1-C6-O6	5.41	123.15	119.90
1	X	1669	A	C6-C5-N7	-5.41	128.51	132.30
1	X	1632	A	C4-C5-C6	5.40	119.70	117.00
1	X	480	G	C5-C6-O6	-5.40	125.36	128.60
1	X	2617	G	N1-C6-O6	-5.40	116.66	119.90
1	X	957	G	N3-C4-C5	-5.40	125.90	128.60
1	X	1292	A	N1-C6-N6	-5.39	115.36	118.60
1	X	2854	G	C6-C5-N7	-5.39	127.17	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1676	U	O5'-P-OP2	-5.38	100.86	105.70
1	X	1302	C	C6-N1-C2	5.38	122.45	120.30
1	X	684	C	N1-C2-O2	-5.38	115.67	118.90
1	X	2016	A	N1-C6-N6	5.38	121.83	118.60
1	X	2857	C	C6-N1-C2	-5.38	118.15	120.30
1	X	537	C	C5-C4-N4	5.37	123.96	120.20
1	X	2414	A	O5'-P-OP1	-5.37	100.87	105.70
1	X	742	G	N1-C2-N2	-5.37	111.37	116.20
1	X	2027	C	C2-N1-C1'	5.36	124.70	118.80
1	X	2495	G	N3-C4-N9	5.36	129.22	126.00
1	X	2655	C	C2-N3-C4	-5.36	117.22	119.90
1	X	1313	U	P-O3'-C3'	5.36	126.13	119.70
1	X	2242	C	C6-N1-C2	-5.35	118.16	120.30
1	X	788	G	C5-C6-N1	5.35	114.17	111.50
1	X	20	C	C5-C4-N4	-5.34	116.47	120.20
1	X	1285	A	C5-C6-N1	-5.33	115.03	117.70
1	X	526	C	N3-C4-C5	5.33	124.03	121.90
1	X	2553	G	C4-C5-N7	5.32	112.93	110.80
1	X	585	U	N3-C4-O4	5.32	123.12	119.40
1	X	985	G	N7-C8-N9	5.32	115.76	113.10
1	X	2579	A	C8-N9-C4	5.32	107.93	105.80
1	X	2668	U	N1-C2-O2	-5.32	119.08	122.80
1	X	2821	G	C2-N3-C4	-5.32	109.24	111.90
1	X	1670	G	N7-C8-N9	-5.31	110.44	113.10
18	Q	58	VAL	C-N-CD	-5.31	108.92	120.60
1	X	746	G	C8-N9-C1'	-5.30	120.11	127.00
1	X	1975	G	C5-C6-O6	5.30	131.78	128.60
1	X	2620	G	C8-N9-C4	5.30	108.52	106.40
1	X	2418	A	N1-C6-N6	5.30	121.78	118.60
1	X	1312	G	C4-C5-N7	5.30	112.92	110.80
1	X	2634	G	C4-N9-C1'	-5.29	119.62	126.50
1	X	1975	G	N9-C4-C5	5.29	107.52	105.40
1	X	829	C	C5-C6-N1	-5.29	118.36	121.00
1	X	2607	C	N1-C2-O2	5.29	122.07	118.90
1	X	1770	U	C4-C5-C6	5.28	122.87	119.70
1	X	1980	A	OP1-P-OP2	5.28	127.51	119.60
1	X	2246	A	N9-C4-C5	5.27	107.91	105.80
1	X	2757	G	C8-N9-C4	5.27	108.51	106.40
1	X	2854	G	C5-N7-C8	-5.27	101.67	104.30
1	X	2673	G	C5-C6-O6	-5.27	125.44	128.60
1	X	1339	U	OP2-P-O3'	5.27	116.78	105.20
1	X	2382	C	C6-N1-C2	-5.26	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2570	C	N3-C2-O2	-5.26	118.22	121.90
1	X	538	A	N3-C4-C5	-5.26	123.12	126.80
1	X	1288	A	OP1-P-O3'	5.26	116.76	105.20
1	X	2228	U	N3-C4-C5	-5.25	111.45	114.60
28	3	37	SER	N-CA-C	5.25	125.18	111.00
1	X	1630	A	P-O3'-C3'	5.25	126.00	119.70
1	X	1983	G	N7-C8-N9	-5.25	110.48	113.10
1	X	2556	A	C8-N9-C4	-5.25	103.70	105.80
1	X	540	G	N7-C8-N9	5.24	115.72	113.10
1	X	689	A	C4-C5-N7	5.24	113.32	110.70
1	X	1746	A	N9-C4-C5	5.24	107.89	105.80
1	X	2674	C	C6-N1-C2	5.23	122.39	120.30
1	X	1203	A	OP1-P-O3'	5.23	116.71	105.20
1	X	2323	U	C5-C4-O4	5.23	129.04	125.90
1	X	1285	A	N1-C6-N6	5.22	121.73	118.60
1	X	1770	U	O4'-C1'-N1	5.22	112.38	108.20
1	X	38	G	C4-N9-C1'	5.22	133.29	126.50
1	X	2560	G	N7-C8-N9	5.22	115.71	113.10
1	X	2489	C	C6-N1-C2	-5.22	118.21	120.30
1	X	1217	U	C5-C6-N1	-5.22	120.09	122.70
1	X	583	C	C5-C6-N1	5.22	123.61	121.00
1	X	2487	G	N1-C6-O6	5.22	123.03	119.90
1	X	1285	A	C8-N9-C4	5.21	107.88	105.80
1	X	1744	G	N1-C6-O6	-5.20	116.78	119.90
1	X	522	G	N9-C4-C5	-5.20	103.32	105.40
1	X	1333	G	N9-C4-C5	5.20	107.48	105.40
1	X	1975	G	C2'-C3'-O3'	5.19	122.01	113.70
1	X	2624	G	C5-N7-C8	-5.19	101.70	104.30
1	X	1240	G	N3-C4-N9	5.19	129.11	126.00
1	X	1679	U	C2-N3-C4	-5.18	123.89	127.00
1	X	1284	G	N1-C6-O6	5.18	123.01	119.90
1	X	1496	G	OP1-P-O3'	5.17	116.58	105.20
1	X	2039	G	C6-N1-C2	-5.17	122.00	125.10
1	X	522	G	C5-N7-C8	-5.17	101.72	104.30
1	X	2756	A	N9-C4-C5	5.16	107.86	105.80
1	X	850	C	N3-C4-C5	-5.16	119.84	121.90
1	X	49	U	P-O3'-C3'	5.15	125.88	119.70
1	X	928	G	C5-C6-O6	-5.15	125.51	128.60
1	X	1630	A	C4-C5-C6	5.15	119.58	117.00
1	X	1574	A	O5'-P-OP1	5.15	116.88	110.70
1	X	1647	U	C5-C4-O4	5.14	128.99	125.90
1	X	537	C	N1-C2-N3	5.14	122.80	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	462	G	N7-C8-N9	-5.14	110.53	113.10
1	X	2706	U	O5'-P-OP2	-5.14	101.08	105.70
1	X	1012	A	N1-C6-N6	5.13	121.68	118.60
1	X	2371	A	N1-C6-N6	5.13	121.68	118.60
1	X	2430	A	C2-N3-C4	-5.13	108.03	110.60
1	X	977	G	C8-N9-C4	5.13	108.45	106.40
1	X	1336	G	C6-C5-N7	-5.12	127.33	130.40
3	A	24	LEU	N-CA-C	5.12	124.83	111.00
1	X	522	G	C6-C5-N7	-5.12	127.33	130.40
1	X	2658	A	N7-C8-N9	-5.12	111.24	113.80
1	X	689	A	N7-C8-N9	5.11	116.36	113.80
1	X	1292	A	C5-C6-N1	5.11	120.26	117.70
1	X	1278	A	C8-N9-C4	-5.11	103.75	105.80
1	X	2540	A	O4'-C1'-N9	5.11	112.29	108.20
1	X	2708	U	N3-C4-C5	5.11	117.67	114.60
1	X	699	G	N1-C6-O6	5.11	122.96	119.90
1	X	1336	G	C8-N9-C4	5.10	108.44	106.40
1	X	2050	G	N1-C6-O6	5.10	122.96	119.90
8	G	95	LEU	CA-CB-CG	5.10	127.02	115.30
1	X	636	G	N1-C6-O6	5.09	122.95	119.90
1	X	2705	A	C5-C6-N1	-5.08	115.16	117.70
1	X	1285	A	N3-C4-C5	5.08	130.36	126.80
1	X	2491	C	O5'-P-OP1	-5.08	101.13	105.70
1	X	833	A	N1-C6-N6	5.08	121.65	118.60
1	X	1705	U	C6-N1-C1'	5.08	128.31	121.20
1	X	2674	C	N3-C2-O2	5.07	125.45	121.90
1	X	1338	G	N3-C4-C5	-5.07	126.06	128.60
1	X	2316	G	N3-C4-N9	5.07	129.04	126.00
1	X	2489	C	N3-C4-C5	-5.07	119.87	121.90
1	X	1442	C	N1-C2-O2	5.06	121.94	118.90
1	X	2408	G	N3-C4-C5	-5.06	126.07	128.60
1	X	2039	G	N1-C2-N3	5.06	126.94	123.90
1	X	2687	G	N7-C8-N9	-5.06	110.57	113.10
1	X	632	A	N1-C2-N3	5.06	131.83	129.30
1	X	1397	A	N1-C6-N6	5.06	121.63	118.60
1	X	1241	G	N3-C4-N9	5.05	129.03	126.00
1	X	1333	G	C8-N9-C1'	5.05	133.57	127.00
1	X	553	C	C2-N1-C1'	5.04	124.35	118.80
1	X	2558	C	N3-C4-N4	-5.04	114.47	118.00
1	X	2371	A	C5-C6-N1	-5.04	115.18	117.70
1	X	1993	G	C6-C5-N7	-5.04	127.38	130.40
1	X	2495	G	N3-C4-C5	-5.04	126.08	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1467	U	O4'-C1'-N1	-5.03	104.17	108.20
1	X	1294	G	N1-C6-O6	5.03	122.92	119.90
1	X	329	C	C6-N1-C2	-5.03	118.29	120.30
1	X	2037	A	C2-N3-C4	-5.03	108.08	110.60
1	X	1673	C	C6-N1-C2	5.03	122.31	120.30
1	X	2492	G	N3-C4-C5	-5.03	126.09	128.60
27	2	38	GLY	N-CA-C	-5.03	100.54	113.10
1	X	1336	G	N3-C2-N2	5.02	123.42	119.90
1	X	1672	A	OP2-P-O3'	5.02	116.25	105.20
1	X	1922	U	N3-C2-O2	-5.02	118.69	122.20
1	X	787	A	N1-C2-N3	5.02	131.81	129.30
1	X	600	G	P-O3'-C3'	5.01	125.71	119.70
1	X	636	G	C6-C5-N7	-5.01	127.39	130.40
1	X	841	G	C6-C5-N7	-5.01	127.39	130.40
1	X	957	G	N1-C6-O6	-5.00	116.90	119.90
1	X	742	G	N3-C4-C5	-5.00	126.10	128.60

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	2	4	THR	Peptide
27	2	40	HIS	Peptide
27	2	6	GLN	Peptide
28	3	37	SER	Peptide
28	3	44	LYS	Peptide
3	A	58	HIS	Peptide
4	B	122	PHE	Peptide
5	C	176	ASN	Peptide
5	C	66	ASN	Peptide
8	G	105	GLY	Peptide
8	G	109	GLY	Peptide
8	G	111	LYS	Peptide
8	G	34	PRO	Peptide
10	I	31	GLY	Peptide
10	I	36	GLY	Peptide
10	I	38	LYS	Peptide
10	I	53	ARG	Peptide
10	I	55	ARG	Peptide
11	J	26	ASP	Peptide
13	L	97	HIS	Peptide
15	N	93	LYS	Peptide

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Mol	Chain	Res	Type	Group
15	N	94	VAL	Peptide
19	R	64	ASN	Peptide
25	Z	3	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57052	0	28750	1265	0
2	Y	2561	0	1306	59	0
3	A	1973	0	2034	131	0
4	B	1539	0	1600	81	0
5	C	1481	0	1504	97	0
6	D	1400	0	1481	60	0
7	E	1286	0	1336	31	0
8	G	1114	0	1144	83	0
9	H	997	0	1046	55	0
10	I	1011	0	1047	76	0
11	J	1078	0	1103	47	0
12	K	878	0	930	34	0
13	L	779	0	820	49	0
14	M	859	0	872	35	0
15	N	978	0	1020	66	0
16	O	741	0	756	34	0
17	P	1014	0	1096	49	0
18	Q	726	0	753	29	0
19	R	825	0	881	57	0
20	S	1374	0	1401	44	0
21	T	556	0	579	24	0
22	U	552	0	604	42	0
23	V	525	0	546	14	0
24	W	424	0	470	16	0
25	Z	452	0	457	34	0
26	1	427	0	445	35	0
27	2	383	0	414	37	0
28	3	462	0	506	36	0
29	X	111	0	0	2	0
30	K	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	M	1	0	0	0	0
30	X	119	0	0	0	0
30	Y	1	0	0	0	0
All	All	83681	0	54901	2278	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 17.

All (2278) 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:356:A:HO2'	1:X:357:A:H8	1.10	0.99
8:G:100:TYR:HB2	8:G:116:ARG:HE	1.25	0.96
10:I:56:LEU:H	10:I:59:ARG:HD3	1.30	0.94
1:X:1277:G:OP1	25:Z:19:ARG:NH2	2.01	0.93
1:X:1264:C:H5''	15:N:13:ARG:HH12	1.34	0.93
15:N:66:ASN:HB3	15:N:76:TYR:HB2	1.48	0.92
1:X:608:G:H1'	10:I:21:ARG:HG3	1.52	0.91
1:X:971:A:H61	11:J:83:ARG:HH22	1.16	0.89
1:X:177:U:O2'	1:X:178:C:O5'	1.90	0.88
1:X:2598:C:OP1	4:B:152:LYS:NZ	2.07	0.87
1:X:1030:U:H3	1:X:1153:A:H62	1.23	0.87
1:X:2016:A:O2'	1:X:2018:G:OP2	1.94	0.85
26:1:12:MET:SD	26:1:13:GLU:N	2.50	0.85
1:X:796:A:H8	1:X:797:A:H4'	1.40	0.85
1:X:640:C:H4'	1:X:660:G:H21	1.40	0.85
4:B:77:ILE:HD13	4:B:195:LEU:HD22	1.59	0.85
1:X:538:A:O2'	1:X:539:A:O5'	1.95	0.84
1:X:1882:G:H21	1:X:1885:C:H41	1.26	0.83
17:P:45:ILE:HD11	17:P:57:LEU:HD11	1.58	0.83
1:X:1562:G:H5'	1:X:1563:U:H5'	1.61	0.82
1:X:1322:G:H4'	27:2:7:PRO:HB2	1.61	0.82
1:X:824:U:H2'	10:I:30:ALA:HA	1.59	0.82
1:X:2039:G:N2	25:Z:4:HIS:O	2.12	0.82
19:R:84:VAL:HG11	19:R:90:LYS:H	1.44	0.82
1:X:2757:G:H5''	1:X:2758:A:H5'	1.60	0.82
15:N:95:LEU:HA	15:N:98:ILE:HD13	1.62	0.81
16:O:5:ILE:HG23	16:O:10:LYS:HZ2	1.45	0.81
10:I:41:SER:OG	10:I:45:LYS:NZ	2.12	0.81
1:X:332:C:O2	5:C:159:ARG:NH2	2.14	0.81
3:A:145:LEU:HB3	3:A:155:LEU:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2653:A:O2'	9:H:41:ASN:ND2	2.14	0.81
1:X:339:U:H4'	19:R:77:HIS:CD2	2.16	0.80
1:X:339:U:H4'	19:R:77:HIS:HD2	1.45	0.80
1:X:2218:G:H5'	3:A:249:PRO:HD3	1.62	0.80
1:X:2796:A:OP2	12:K:3:HIS:NE2	2.15	0.79
1:X:215:G:H21	1:X:632:A:H8	1.27	0.79
19:R:80:LYS:NZ	19:R:81:VAL:O	2.13	0.79
8:G:73:ASN:O	8:G:140:GLN:NE2	2.16	0.78
1:X:2638:G:OP1	7:E:158:HIS:NE2	2.17	0.78
28:3:37:SER:OG	28:3:38:GLY:N	2.16	0.78
4:B:194:GLY:HA2	14:M:2:GLN:HB3	1.65	0.78
6:D:13:ARG:HG3	6:D:28:VAL:HG21	1.63	0.78
7:E:56:SER:HG	7:E:61:HIS:HD1	1.26	0.78
4:B:143:GLN:HB2	4:B:147:PRO:HG3	1.65	0.78
1:X:596:C:N3	10:I:37:GLN:NE2	2.32	0.78
1:X:841:G:H2'	1:X:842:A:C8	2.19	0.78
1:X:1007:A:H4'	15:N:93:LYS:HZ3	1.49	0.77
13:L:26:ARG:NH1	13:L:86:GLN:O	2.17	0.77
1:X:89:A:O2'	1:X:91:A:N6	2.18	0.77
1:X:2237:C:O2'	1:X:2406:C:OP2	2.00	0.77
13:L:11:LEU:HD12	13:L:93:SER:HB3	1.65	0.77
1:X:1337:G:OP2	17:P:105:ARG:NH1	2.18	0.77
1:X:1278:A:H2	1:X:1997:A:H62	1.32	0.77
9:H:88:THR:HB	14:M:80:VAL:HB	1.67	0.76
1:X:2660:C:H42	1:X:2705:A:H2	1.31	0.76
1:X:923:A:N7	11:J:12:LYS:HG2	1.99	0.76
1:X:1617:G:OP2	18:Q:57:ASN:ND2	2.18	0.76
1:X:1834:G:O2'	3:A:244:ARG:NH2	2.19	0.76
3:A:246:PRO:HD2	3:A:251:GLY:H	1.49	0.76
9:H:29:ILE:HG21	9:H:122:ARG:HB2	1.68	0.76
10:I:33:GLY:HA2	16:O:79:GLN:HG3	1.68	0.76
19:R:59:LYS:HB3	19:R:62:MET:HB2	1.68	0.76
3:A:172:TYR:HA	3:A:186:HIS:HA	1.68	0.76
9:H:124:MET:HA	9:H:127:VAL:HB	1.68	0.75
2:Y:46:G:N3	2:Y:49:C:N4	2.34	0.75
8:G:31:THR:HG22	15:N:61:TRP:CH2	2.22	0.75
8:G:67:ARG:HB2	8:G:70:PHE:HA	1.69	0.75
16:O:34:GLU:HB2	16:O:56:VAL:HG23	1.69	0.75
1:X:2672:U:H2'	1:X:2673:G:H8	1.50	0.75
17:P:101:PRO:O	17:P:121:THR:OG1	2.05	0.74
1:X:1373:G:H22	1:X:2192:U:H3	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2474:G:H5''	11:J:82:THR:HA	1.69	0.74
2:Y:57:U:HO2'	6:D:24:SER:HG	1.32	0.74
1:X:989:G:HO2'	1:X:1013:G:HO2'	1.29	0.74
2:Y:42:U:O2'	2:Y:47:A:N6	2.20	0.74
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.69	0.74
15:N:92:ARG:HB3	15:N:95:LEU:HD22	1.69	0.74
1:X:2043:A:H62	5:C:68:ARG:HH12	1.36	0.74
1:X:1348:C:OP2	18:Q:62:ARG:NH1	2.21	0.74
24:W:2:LYS:HB3	24:W:54:GLN:HB3	1.69	0.74
1:X:1222:G:O2'	1:X:1250:A:N6	2.21	0.74
20:S:69:VAL:HG13	20:S:81:VAL:HG22	1.70	0.73
1:X:954:U:OP2	10:I:38:LYS:NZ	2.17	0.73
3:A:205:VAL:HG12	3:A:207:GLY:H	1.50	0.73
9:H:76:ARG:NH1	9:H:113:PRO:O	2.20	0.73
3:A:108:PRO:HA	3:A:196:VAL:HA	1.71	0.73
1:X:1769:U:H2'	1:X:1775:A:H62	1.53	0.73
1:X:2551:A:H5''	1:X:2553:G:H4'	1.68	0.73
3:A:250:TRP:O	3:A:255:LYS:NZ	2.19	0.73
19:R:37:LEU:HD11	19:R:49:GLU:HG3	1.71	0.72
1:X:1283:C:H5''	1:X:1284:G:H5'	1.71	0.72
1:X:2059:U:OP2	1:X:2217:G:N2	2.20	0.72
1:X:2556:A:H5''	1:X:2557:G:H5'	1.71	0.72
1:X:492:G:O2'	1:X:517:A:N6	2.22	0.72
4:B:60:ASN:HB3	4:B:62:PRO:HD2	1.70	0.72
1:X:2170:C:H3'	1:X:2171:U:H5''	1.70	0.72
9:H:70:VAL:HG21	9:H:98:ILE:HG23	1.72	0.72
22:U:19:ILE:HA	22:U:42:GLN:HA	1.72	0.72
2:Y:27:A:N6	2:Y:56:G:OP2	2.23	0.72
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.71	0.71
1:X:168:A:H2'	1:X:169:C:C6	2.25	0.71
1:X:2450:A:N3	29:X:2901:6O1:O30	2.23	0.71
1:X:558:G:H8	1:X:560:G:C8	2.08	0.71
3:A:45:ASN:OD1	3:A:46:ARG:NH1	2.22	0.71
9:H:113:PRO:HD3	14:M:73:PHE:HB2	1.72	0.71
1:X:1264:C:H5''	15:N:13:ARG:NH1	2.05	0.71
20:S:47:SER:OG	20:S:48:THR:N	2.20	0.71
1:X:2545:A:H61	9:H:40:GLY:HA3	1.56	0.71
16:O:11:GLN:HE22	16:O:38:LEU:HB3	1.55	0.71
1:X:2716:G:H1	1:X:2748:C:H42	1.39	0.71
5:C:54:THR:HG21	5:C:72:ARG:HB2	1.72	0.71
12:K:29:LEU:HD13	12:K:79:VAL:HG11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:23:VAL:HG13	21:T:38:VAL:HG23	1.71	0.71
22:U:31:GLY:HA2	22:U:32:ARG:HH11	1.56	0.71
1:X:349:G:OP1	19:R:13:LYS:NZ	2.20	0.71
1:X:160:C:O2'	1:X:445:A:N3	2.24	0.71
1:X:89:A:H4'	1:X:90:G:H5'	1.73	0.71
1:X:408:U:H2'	1:X:409:G:C8	2.26	0.71
1:X:1079:G:N2	1:X:1106:A:O2'	2.24	0.71
8:G:157:PRO:O	8:G:161:GLN:NE2	2.24	0.70
15:N:88:ILE:HG12	16:O:49:GLU:HB2	1.71	0.70
1:X:1333:G:N2	1:X:1344:C:H41	1.88	0.70
1:X:2516:U:H2'	1:X:2517:C:C6	2.26	0.70
12:K:13:ASN:OD1	12:K:14:SER:N	2.24	0.70
22:U:27:ASP:HB3	22:U:32:ARG:HA	1.73	0.70
18:Q:62:ARG:O	18:Q:70:GLY:HA3	1.90	0.70
3:A:168:LYS:HB3	3:A:173:VAL:HG13	1.73	0.70
1:X:2634:G:O2'	1:X:2635:U:OP2	2.09	0.70
1:X:346:C:H2'	1:X:347:C:H6	1.55	0.70
1:X:1007:A:H2'	1:X:1008:G:H8	1.55	0.70
1:X:1551:U:OP2	1:X:1553:G:N2	2.24	0.70
1:X:242:A:N6	1:X:441:A:OP2	2.24	0.70
1:X:1922:U:OP1	1:X:2583:U:O2'	2.08	0.70
1:X:2029:G:OP1	25:Z:15:LYS:NZ	2.16	0.69
20:S:93:GLU:HG3	20:S:123:VAL:HG23	1.74	0.69
6:D:38:GLU:HB3	6:D:87:ILE:HB	1.73	0.69
1:X:304:A:N6	1:X:356:A:N7	2.39	0.69
1:X:2400:G:N7	28:3:32:GLN:HB3	2.07	0.69
28:3:14:ILE:HD13	28:3:56:ALA:HB1	1.74	0.69
2:Y:30:C:OP1	13:L:37:HIS:ND1	2.25	0.69
1:X:797:A:C5	3:A:229:VAL:HG21	2.27	0.69
3:A:218:LYS:NZ	3:A:219:PRO:O	2.25	0.69
4:B:122:PHE:HE2	4:B:138:PRO:HB3	1.58	0.69
5:C:163:ASN:HB3	5:C:166:TRP:HB2	1.73	0.69
1:X:588:G:O2'	1:X:2002:A:OP1	2.07	0.69
10:I:18:ARG:HB3	10:I:21:ARG:HB2	1.74	0.69
1:X:1422:C:H2'	1:X:1423:A:H8	1.58	0.69
8:G:149:LYS:NZ	8:G:160:ALA:O	2.26	0.69
17:P:25:PHE:HD1	17:P:127:ILE:HD11	1.58	0.69
1:X:854:G:H1	1:X:948:C:H42	1.39	0.69
1:X:1810:U:OP2	3:A:157:ARG:NH1	2.25	0.68
1:X:1329:U:H2'	1:X:1330:G:H8	1.58	0.68
1:X:1386:A:OP1	1:X:2191:A:N6	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:25:PHE:HA	17:P:127:ILE:HG12	1.74	0.68
20:S:25:ASN:HB3	20:S:85:MET:HB2	1.74	0.68
22:U:53:GLU:HB3	22:U:58:LYS:H	1.57	0.68
1:X:1542:G:H22	1:X:1562:G:H1	1.39	0.68
13:L:15:ARG:HA	13:L:15:ARG:HH11	1.58	0.68
1:X:1296:G:H22	1:X:1299:A:H5'	1.58	0.68
22:U:54:ASN:HA	22:U:78:ILE:HG22	1.75	0.68
1:X:863:C:HO2'	24:W:19:THR:HG1	1.38	0.68
1:X:1124:U:H2'	1:X:1125:G:H8	1.58	0.68
3:A:14:ARG:HH11	3:A:27:LYS:HB3	1.59	0.68
9:H:75:VAL:HG12	9:H:118:LEU:HD21	1.76	0.68
20:S:3:LEU:HD13	20:S:32:PHE:HB3	1.75	0.68
1:X:673:G:N3	10:I:21:ARG:NH2	2.41	0.68
3:A:245:VAL:HA	3:A:251:GLY:HA2	1.75	0.68
7:E:8:PRO:O	7:E:69:ARG:NH1	2.26	0.68
13:L:8:ARG:HG3	13:L:9:ARG:H	1.59	0.68
1:X:203:G:O2'	1:X:205:A:N6	2.26	0.68
1:X:2838:U:H2'	1:X:2839:G:H8	1.58	0.68
1:X:2659:C:H5'	4:B:189:PRO:HA	1.77	0.68
1:X:2551:A:C8	4:B:144:ARG:HG2	2.29	0.68
26:1:30:ASN:HD22	26:1:31:THR:H	1.41	0.67
1:X:2786:G:H5''	4:B:60:ASN:HD22	1.59	0.67
1:X:2672:U:H2'	1:X:2673:G:C8	2.29	0.67
8:G:41:TRP:HZ3	8:G:149:LYS:HD2	1.58	0.67
1:X:1054:C:H42	1:X:1123:G:H1	1.40	0.67
1:X:1850:G:O2'	1:X:1867:A:N6	2.27	0.67
1:X:2663:U:H3	1:X:2705:A:H62	1.39	0.67
1:X:346:C:H2'	1:X:347:C:C6	2.28	0.67
2:Y:52:G:OP1	13:L:65:THR:OG1	2.11	0.67
1:X:1882:G:N2	1:X:1885:C:H41	1.93	0.67
1:X:1684:G:O2'	1:X:1974:U:O4	2.11	0.67
1:X:1678:G:H1	1:X:1982:C:H42	1.42	0.67
1:X:646:C:O2'	1:X:650:U:OP1	2.09	0.67
1:X:64:C:OP1	18:Q:71:GLN:HB2	1.95	0.67
1:X:492:G:H1'	1:X:516:G:N2	2.10	0.67
10:I:18:ARG:NH2	10:I:18:ARG:O	2.27	0.67
10:I:56:LEU:HB3	28:3:52:LYS:NZ	2.09	0.67
13:L:76:ALA:HB2	13:L:107:ALA:HA	1.75	0.67
1:X:1800:A:H4'	1:X:1801:C:OP1	1.95	0.67
3:A:176:ARG:HH11	3:A:180:GLY:HA2	1.60	0.67
1:X:791:G:H5''	3:A:48:ARG:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:504:G:H4'	17:P:27:VAL:HG12	1.76	0.67
18:Q:63:LYS:HE3	18:Q:65:VAL:HA	1.77	0.67
1:X:1340:C:O3'	12:K:104:ARG:NH2	2.28	0.67
1:X:1429:A:H1'	1:X:1603:A:C6	2.30	0.67
1:X:2372:A:H62	1:X:2401:A:H62	1.43	0.67
1:X:812:G:H3'	1:X:813:A:H2'	1.75	0.67
6:D:119:PRO:HD3	6:D:178:ARG:HG3	1.77	0.66
6:D:72:LYS:HA	6:D:81:GLN:HA	1.77	0.66
1:X:953:G:O2'	1:X:1203:A:N3	2.27	0.66
1:X:712:A:H2'	1:X:713:G:O4'	1.94	0.66
5:C:136:TRP:O	5:C:140:ASN:ND2	2.27	0.66
1:X:746:G:N7	1:X:774:A:C6	2.63	0.66
2:Y:115:G:N2	13:L:48:GLY:O	2.28	0.66
3:A:244:ARG:HD2	3:A:253:PRO:HD3	1.78	0.66
5:C:129:LYS:O	5:C:131:LYS:N	2.28	0.66
13:L:54:ALA:H	13:L:75:LEU:HD13	1.60	0.66
2:Y:27:A:O2'	2:Y:28:A:O5'	2.12	0.66
1:X:1264:C:OP1	15:N:13:ARG:NH1	2.29	0.66
1:X:920:G:H21	11:J:11:ARG:HH22	1.44	0.66
25:Z:6:VAL:HG22	25:Z:7:PRO:HD2	1.77	0.66
4:B:131:SER:O	4:B:134:TRP:NE1	2.26	0.66
22:U:21:ARG:HA	22:U:39:LYS:HB2	1.77	0.66
1:X:1431:U:H4'	1:X:1604:A:H4'	1.78	0.66
1:X:761:G:H5''	17:P:110:ALA:HB2	1.78	0.66
1:X:88:G:H3'	1:X:89:A:H5''	1.78	0.66
15:N:24:PHE:HB2	15:N:29:SER:HB3	1.77	0.65
1:X:83:A:H3'	19:R:17:LYS:HG2	1.78	0.65
22:U:48:LYS:HE2	22:U:49:LYS:H	1.61	0.65
1:X:1332:G:O2'	1:X:1333:G:H5'	1.96	0.65
1:X:1675:C:H2'	1:X:1676:U:C6	2.30	0.65
11:J:21:ASP:HA	11:J:99:LYS:HE2	1.79	0.65
13:L:26:ARG:HH11	13:L:88:VAL:HG22	1.61	0.65
1:X:318:G:N2	1:X:321:A:OP2	2.28	0.65
5:C:3:GLN:H	5:C:12:GLY:HA3	1.62	0.65
8:G:100:TYR:CB	8:G:116:ARG:HE	2.06	0.65
1:X:2064:U:H5'	22:U:41:VAL:HG21	1.78	0.65
1:X:595:A:H5'	5:C:83:ALA:HB3	1.79	0.65
1:X:814:G:OP2	5:C:56:ARG:NH2	2.29	0.65
1:X:786:U:H4'	3:A:47:GLY:HA2	1.78	0.65
3:A:43:ARG:HB3	3:A:54:ILE:HG13	1.78	0.65
21:T:26:PHE:N	21:T:29:GLU:OE1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:11:GLY:O	5:C:13:ARG:NH1	2.30	0.65
10:I:80:LEU:O	10:I:116:ARG:NH2	2.30	0.65
3:A:56:GLY:H	3:A:217:ARG:HB2	1.60	0.65
15:N:61:TRP:CE2	15:N:94:VAL:HG22	2.32	0.65
5:C:95:LEU:O	5:C:100:ARG:NH2	2.30	0.65
1:X:1184:G:H3'	1:X:1185:C:H5''	1.79	0.65
1:X:540:G:C5	1:X:2005:U:H5''	2.32	0.65
1:X:679:C:H5''	10:I:49:PHE:HB3	1.77	0.65
21:T:45:PHE:HB3	21:T:77:ARG:HB2	1.79	0.65
26:1:35:LEU:HA	26:1:53:LYS:HD2	1.78	0.65
1:X:1270:C:H5'	5:C:69:HIS:CE1	2.32	0.65
10:I:88:PHE:HE1	10:I:118:VAL:HA	1.62	0.64
1:X:1342:U:H5''	1:X:1343:C:H5	1.62	0.64
1:X:692:C:H2'	1:X:693:A:H8	1.61	0.64
1:X:2481:G:H5'	1:X:2482:A:H5''	1.79	0.64
1:X:87:G:H2'	1:X:88:G:H5''	1.79	0.64
10:I:81:GLN:HG2	10:I:116:ARG:HB3	1.78	0.64
13:L:33:ARG:HH11	13:L:38:ILE:HG21	1.62	0.64
3:A:143:HIS:ND1	3:A:194:GLY:O	2.27	0.64
19:R:84:VAL:HG21	19:R:89:GLY:HA2	1.78	0.64
1:X:1443:G:H2'	1:X:1444:C:C6	2.33	0.64
1:X:332:C:HO2'	1:X:351:A:HO2'	1.42	0.64
13:L:27:LEU:HB2	13:L:87:VAL:HG22	1.79	0.64
1:X:2556:A:H1'	25:Z:4:HIS:HB3	1.79	0.64
1:X:2838:U:H2'	1:X:2839:G:C8	2.33	0.64
11:J:78:LYS:HD2	11:J:81:GLU:HA	1.80	0.64
3:A:203:ASN:N	3:A:203:ASN:OD1	2.28	0.64
1:X:1345:G:N7	1:X:1625:A:O2'	2.26	0.64
1:X:2766:U:OP1	4:B:69:LYS:NZ	2.28	0.64
6:D:60:ILE:HG13	6:D:61:THR:HG23	1.79	0.64
8:G:84:ASN:O	8:G:152:ALA:HA	1.97	0.64
19:R:97:GLN:HB3	19:R:101:GLY:HA2	1.80	0.64
1:X:1685:A:O2'	1:X:1691:G:N7	2.28	0.64
1:X:2811:G:H2'	1:X:2812:A:C8	2.32	0.64
1:X:1674:C:H2'	1:X:1675:C:C6	2.33	0.63
1:X:1744:G:N2	1:X:1747:G:OP2	2.30	0.63
22:U:47:HIS:ND1	22:U:48:LYS:O	2.32	0.63
1:X:1296:G:N2	1:X:1299:A:H5'	2.13	0.63
1:X:1746:A:H2	1:X:2696:A:HO2'	1.47	0.63
1:X:2371:A:C8	10:I:59:ARG:HG2	2.33	0.63
1:X:1007:A:H1'	16:O:6:GLN:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1791:C:OP1	3:A:261:ARG:NH2	2.29	0.63
1:X:946:U:H2'	1:X:947:C:C6	2.33	0.63
22:U:21:ARG:HE	22:U:40:ARG:HG2	1.64	0.63
10:I:62:LYS:HD3	10:I:63:ARG:H	1.64	0.63
19:R:81:VAL:HG12	19:R:82:ALA:H	1.64	0.63
1:X:2324:G:N3	1:X:2360:C:H2'	2.14	0.63
2:Y:7:C:O2'	2:Y:29:C:O2	2.16	0.63
1:X:2222:U:H2'	1:X:2223:U:C6	2.34	0.63
1:X:2796:A:H2'	1:X:2797:G:H8	1.64	0.63
1:X:796:A:C8	1:X:797:A:H4'	2.28	0.63
26:1:51:ARG:NH2	26:1:53:LYS:O	2.32	0.63
7:E:103:LEU:HD21	7:E:131:ILE:HD13	1.80	0.63
16:O:56:VAL:HG12	16:O:97:GLY:HA3	1.79	0.63
1:X:876:A:H2	1:X:926:C:H41	1.46	0.63
1:X:1003:C:H2'	1:X:1004:A:H8	1.63	0.63
1:X:1223:G:H5'	1:X:1225:G:O4'	1.98	0.63
1:X:2240:C:N4	21:T:14:ARG:O	2.32	0.62
1:X:649:G:C6	1:X:662:G:N2	2.67	0.62
1:X:938:G:H4'	1:X:939:C:H5'	1.81	0.62
8:G:61:ARG:NH1	8:G:66:HIS:H	1.97	0.62
25:Z:18:MET:O	25:Z:21:SER:HB3	1.98	0.62
3:A:25:THR:HG23	3:A:211:ARG:HH12	1.65	0.62
4:B:117:MET:HA	4:B:121:ASN:O	1.99	0.62
4:B:37:LYS:NZ	4:B:80:GLU:OE2	2.29	0.62
19:R:16:PHE:HZ	19:R:46:VAL:HG21	1.64	0.62
19:R:48:VAL:HG13	19:R:50:GLY:H	1.64	0.62
1:X:830:C:O2'	1:X:852:U:OP1	2.17	0.62
20:S:51:LEU:H	20:S:51:LEU:HD23	1.64	0.62
1:X:824:U:C2'	10:I:30:ALA:HA	2.30	0.62
2:Y:11:G:OP2	13:L:16:LYS:NZ	2.26	0.62
5:C:39:ARG:HH21	5:C:91:TYR:HB2	1.64	0.62
6:D:74:ILE:HA	6:D:79:LEU:HB3	1.81	0.62
16:O:5:ILE:HG23	16:O:10:LYS:NZ	2.14	0.62
1:X:564:U:H2'	1:X:565:A:C8	2.34	0.62
3:A:96:HIS:HE1	3:A:100:GLY:HA2	1.65	0.62
1:X:824:U:H2'	10:I:30:ALA:CA	2.27	0.62
20:S:50:GLY:HA2	20:S:130:ILE:HD12	1.82	0.62
29:X:2901:6O1:O52	29:X:2901:6O1:O57	2.15	0.62
1:X:172:A:H61	1:X:175:C:H3'	1.65	0.62
1:X:2579:A:H2'	1:X:2580:C:C6	2.35	0.62
1:X:403:A:H4'	1:X:404:A:H5'	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:103:TYR:C	8:G:107:GLN:HG3	2.21	0.61
10:I:56:LEU:HD22	28:3:52:LYS:HZ2	1.65	0.61
21:T:64:ASP:N	21:T:64:ASP:OD1	2.32	0.61
1:X:2693:U:OP1	12:K:14:SER:HB3	2.00	0.61
5:C:149:LEU:HD11	5:C:170:LEU:HB2	1.83	0.61
4:B:35:GLN:HB3	4:B:48:GLN:HB3	1.82	0.61
1:X:825:C:H5''	10:I:30:ALA:HB1	1.82	0.61
22:U:19:ILE:HG22	22:U:42:GLN:HG3	1.82	0.61
22:U:52:ARG:HG3	22:U:62:LEU:HD22	1.81	0.61
1:X:1052:C:N4	1:X:1053:G:N7	2.48	0.61
1:X:2372:A:H62	1:X:2401:A:N6	1.99	0.61
3:A:184:ARG:HD2	3:A:266:SER:HA	1.82	0.61
14:M:31:ASP:OD1	14:M:31:ASP:N	2.31	0.61
1:X:1584:G:H5''	3:A:61:LEU:HG	1.82	0.61
11:J:49:GLU:OE2	11:J:52:ARG:NH2	2.34	0.61
20:S:104:SER:HA	20:S:139:THR:HA	1.81	0.61
1:X:872:G:O2'	1:X:928:G:O6	2.17	0.61
2:Y:9:G:H5'	13:L:32:TYR:CE2	2.35	0.61
13:L:40:ALA:HB2	13:L:103:LEU:HD11	1.82	0.61
22:U:47:HIS:CG	22:U:48:LYS:H	2.19	0.61
1:X:171:G:H2'	1:X:172:A:O4'	2.00	0.61
1:X:517:A:H5''	1:X:518:A:H5'	1.83	0.61
27:2:41:GLN:NE2	27:2:41:GLN:HA	2.14	0.61
1:X:1279:G:O2'	1:X:1995:G:O6	2.12	0.61
26:1:25:THR:O	26:1:27:ASN:ND2	2.34	0.61
28:3:26:LYS:HE2	28:3:43:GLY:HA3	1.81	0.61
6:D:46:ASP:HB2	6:D:49:ALA:HB3	1.83	0.61
13:L:89:PHE:O	13:L:91:ARG:NH2	2.33	0.61
1:X:1008:G:OP1	15:N:93:LYS:HB2	2.01	0.61
1:X:1182:U:H3	1:X:1192:A:H61	1.48	0.61
1:X:943:U:O2'	1:X:944:A:O4'	2.10	0.61
8:G:70:PHE:HB3	15:N:64:ARG:HG2	1.83	0.60
20:S:9:THR:HG22	20:S:11:LYS:H	1.65	0.60
1:X:2696:A:O2'	1:X:2697:G:H5'	2.01	0.60
8:G:31:THR:HG22	15:N:61:TRP:HH2	1.65	0.60
12:K:33:ARG:HG3	12:K:114:GLU:HB3	1.83	0.60
22:U:63:SER:O	22:U:67:LEU:N	2.33	0.60
1:X:1250:A:H4'	1:X:1250:A:OP1	1.99	0.60
1:X:1468:A:H5''	1:X:1468:A:C8	2.36	0.60
25:Z:35:GLN:HG3	25:Z:51:TYR:CD2	2.36	0.60
1:X:1279:G:O5'	17:P:36:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:119:LEU:HD13	8:G:122:HIS:CE1	2.36	0.60
1:X:2873:G:H2'	1:X:2874:A:C8	2.35	0.60
1:X:603:C:H2'	1:X:604:U:C6	2.36	0.60
20:S:70:GLN:HB2	20:S:80:HIS:HB3	1.82	0.60
1:X:2466:G:H2'	1:X:2467:A:H8	1.65	0.60
1:X:537:C:O2'	1:X:538:A:C4	2.54	0.60
26:1:28:ARG:HB2	26:1:30:ASN:OD1	2.02	0.60
22:U:22:GLY:HA3	22:U:39:LYS:NZ	2.15	0.60
1:X:1196:G:H2'	1:X:1197:U:O4'	2.01	0.60
1:X:1313:U:H4'	1:X:1314:A:H5''	1.84	0.60
1:X:1915:A:H3'	1:X:1916:G:H8	1.66	0.60
1:X:2335:U:H4'	21:T:20:TYR:CD2	2.37	0.60
17:P:14:ARG:HA	17:P:17:GLN:HG2	1.82	0.60
8:G:84:ASN:HD22	8:G:87:GLN:HG3	1.66	0.60
9:H:12:ASP:OD1	9:H:14:SER:OG	2.14	0.60
2:Y:52:G:OP2	13:L:65:THR:HG21	2.02	0.60
1:X:806:A:OP2	1:X:2054:A:O2'	2.20	0.60
1:X:2757:G:OP2	1:X:2761:A:O2'	2.19	0.60
1:X:37:C:O2	5:C:44:SER:OG	2.19	0.60
2:Y:57:U:O2'	6:D:24:SER:OG	2.17	0.60
26:1:14:SER:HB2	26:1:22:TYR:HA	1.84	0.60
1:X:478:G:OP1	27:2:33:ARG:HD2	2.01	0.60
10:I:32:ARG:O	10:I:32:ARG:HD2	2.02	0.60
18:Q:61:LYS:H	18:Q:72:ARG:HA	1.66	0.60
1:X:863:C:O2'	24:W:19:THR:OG1	2.13	0.60
24:W:38:PRO:HD3	24:W:41:ARG:HH21	1.66	0.60
5:C:76:THR:O	5:C:76:THR:OG1	2.15	0.59
9:H:28:GLY:O	9:H:35:THR:N	2.29	0.59
12:K:87:TYR:HE1	12:K:94:TYR:HD1	1.49	0.59
1:X:415:A:H61	1:X:436:A:H61	1.50	0.59
1:X:627:A:H2'	1:X:628:A:C8	2.36	0.59
26:1:30:ASN:ND2	26:1:31:THR:H	1.99	0.59
6:D:74:ILE:HG12	6:D:80:ARG:HA	1.83	0.59
1:X:1422:C:H2'	1:X:1423:A:C8	2.38	0.59
1:X:1643:A:H61	1:X:1656:U:H3	1.49	0.59
1:X:2245:A:H4'	1:X:2246:A:C2	2.37	0.59
1:X:636:G:H5'	1:X:637:G:OP2	2.01	0.59
3:A:133:LEU:HB2	3:A:187:SER:HA	1.84	0.59
14:M:56:ALA:HB3	14:M:67:THR:HB	1.84	0.59
24:W:23:LEU:HD21	24:W:43:MET:HB3	1.84	0.59
6:D:8:TYR:HH	6:D:31:ILE:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:8:TYR:OH	6:D:31:ILE:N	2.29	0.59
1:X:1333:G:N7	1:X:1342:U:H5'	2.17	0.59
1:X:1058:G:O2'	1:X:1122:A:N6	2.36	0.59
1:X:1154:A:OP1	1:X:1154:A:H8	1.85	0.59
1:X:48:A:H61	1:X:154:U:H2'	1.67	0.59
1:X:417:C:H4'	1:X:418:C:H5'	1.83	0.59
1:X:1673:C:OP1	4:B:136:ARG:HG2	2.02	0.59
6:D:13:ARG:HA	6:D:28:VAL:HG11	1.85	0.59
1:X:2038:C:H5'	1:X:2039:G:H5''	1.84	0.59
2:Y:17:A:H1'	2:Y:112:A:C8	2.37	0.59
2:Y:22:U:O2'	2:Y:66:G:N2	2.36	0.59
26:1:35:LEU:HD13	26:1:37:LEU:HD12	1.83	0.59
1:X:742:G:C6	3:A:208:LYS:HB3	2.37	0.59
6:D:167:ARG:HG3	6:D:177:PHE:CZ	2.38	0.59
1:X:1963:G:O2'	1:X:1965:U:OP2	2.20	0.59
3:A:170:SER:OG	3:A:171:ASP:N	2.35	0.59
4:B:122:PHE:CE2	4:B:138:PRO:HB3	2.36	0.59
4:B:5:LEU:HD13	4:B:51:TYR:HB2	1.84	0.59
6:D:132:ILE:HG13	6:D:154:ILE:HD13	1.85	0.59
1:X:2226:A:H2'	1:X:2227:C:C6	2.37	0.59
27:2:1:MET:HG3	27:2:3:ARG:NH1	2.18	0.59
3:A:14:ARG:HD2	3:A:27:LYS:HB3	1.84	0.59
9:H:77:THR:HA	9:H:94:ASN:HB3	1.84	0.59
1:X:1983:G:HO2'	1:X:2668:U:H6	1.51	0.59
1:X:2285:U:O4'	6:D:150:ARG:NH1	2.36	0.58
1:X:1179:A:H2'	1:X:1180:A:C8	2.37	0.58
1:X:2491:C:OP1	4:B:123:ALA:HB2	2.03	0.58
9:H:23:ARG:HG2	9:H:25:LEU:HD23	1.84	0.58
2:Y:9:G:H21	13:L:41:GLN:HE22	1.49	0.58
1:X:1225:G:H2'	1:X:1249:G:H22	1.68	0.58
1:X:2298:U:O2	1:X:2299:A:N6	2.36	0.58
1:X:2607:C:H1'	1:X:2761:A:H2'	1.85	0.58
3:A:60:ARG:HD3	3:A:87:ASN:HD22	1.68	0.58
1:X:1839:A:HO2'	1:X:1840:A:H8	1.49	0.58
1:X:492:G:H1'	1:X:516:G:H21	1.67	0.58
9:H:41:ASN:HD22	9:H:42:LYS:H	1.52	0.58
21:T:18:PRO:O	21:T:19:LYS:HG2	2.02	0.58
1:X:1212:U:H2'	1:X:1213:U:C6	2.38	0.58
1:X:2634:G:O2'	1:X:2643:G:N1	2.36	0.58
1:X:1745:C:O2	1:X:2697:G:H4'	2.04	0.58
1:X:1582:A:OP1	3:A:211:ARG:NH1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1594:U:H2'	1:X:1595:A:H8	1.68	0.58
1:X:2262:C:O2	1:X:2304:G:N2	2.26	0.58
1:X:691:C:H2'	1:X:692:C:C6	2.39	0.58
1:X:1268:U:H2'	5:C:66:ASN:HA	1.85	0.58
1:X:178:C:O5'	22:U:40:ARG:NH2	2.36	0.58
1:X:1264:C:OP1	15:N:10:ARG:HG3	2.02	0.58
1:X:1332:G:C6	1:X:1333:G:N1	2.71	0.58
1:X:834:A:H5'	1:X:835:U:C6	2.39	0.58
1:X:930:A:N3	2:Y:82:U:O2'	2.33	0.58
21:T:25:LYS:HB2	21:T:37:LEU:HA	1.86	0.58
1:X:1047:G:H1	1:X:1130:U:H3	1.52	0.58
1:X:1770:U:H5	1:X:1775:A:N7	2.01	0.58
4:B:92:ASN:HA	4:B:95:ILE:HB	1.84	0.58
11:J:48:ILE:O	11:J:52:ARG:N	2.26	0.58
1:X:1261:G:C4	15:N:3:ARG:HG2	2.39	0.58
1:X:1350:G:H2'	1:X:1351:G:H8	1.69	0.58
1:X:2494:C:H42	1:X:2548:G:H1	1.50	0.58
1:X:774:A:H8	1:X:774:A:O5'	1.86	0.58
26:1:8:ILE:HG12	26:1:9:ILE:HG23	1.86	0.58
1:X:1586:A:H2'	1:X:1587:A:C8	2.39	0.58
1:X:537:C:H1'	1:X:538:A:C6	2.39	0.58
3:A:182:LEU:HB2	3:A:268:ARG:O	2.04	0.58
6:D:60:ILE:O	6:D:102:LYS:NZ	2.31	0.58
15:N:78:THR:HG23	15:N:117:ARG:CZ	2.34	0.58
1:X:1922:U:H3'	1:X:1923:U:H5'	1.84	0.58
1:X:1919:A:H2	1:X:1926:U:H3	1.51	0.58
26:1:46:LYS:O	26:1:48:VAL:HG12	2.04	0.57
3:A:231:HIS:CD2	3:A:232:PRO:HD2	2.38	0.57
6:D:134:GLU:HG2	6:D:136:LEU:H	1.69	0.57
19:R:92:THR:HA	19:R:108:VAL:HG22	1.85	0.57
18:Q:10:PRO:HD3	23:V:30:PHE:CD2	2.38	0.57
1:X:2594:U:C6	25:Z:7:PRO:HA	2.39	0.57
6:D:70:ALA:HB3	6:D:82:GLY:HA2	1.86	0.57
10:I:81:GLN:HA	10:I:116:ARG:HD2	1.86	0.57
20:S:117:VAL:HG22	20:S:168:VAL:HA	1.86	0.57
1:X:2212:U:H2'	1:X:2213:G:C8	2.39	0.57
1:X:2772:U:H2'	1:X:2773:G:C8	2.38	0.57
1:X:753:U:H2'	1:X:754:G:C8	2.39	0.57
1:X:636:G:O2'	1:X:669:G:H4'	2.03	0.57
4:B:38:THR:HB	4:B:41:THR:HG23	1.86	0.57
6:D:111:ILE:HG12	6:D:137:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:44:C:O2'	6:D:64:LYS:O	2.18	0.57
10:I:90:ARG:HA	10:I:121:HIS:H	1.69	0.57
14:M:78:GLU:OE1	14:M:108:ARG:NH2	2.35	0.57
15:N:66:ASN:ND2	15:N:70:ARG:HH12	2.01	0.57
1:X:2234:G:H2'	1:X:2235:G:O4'	2.04	0.57
1:X:2269:G:H22	1:X:2322:U:H1'	1.70	0.57
1:X:487:G:H4'	1:X:512:A:N1	2.18	0.57
1:X:829:C:H2'	1:X:830:C:C6	2.39	0.57
8:G:31:THR:OG1	8:G:32:TYR:N	2.37	0.57
1:X:2398:U:H5'	26:1:24:THR:HG21	1.86	0.57
8:G:122:HIS:ND1	8:G:122:HIS:O	2.38	0.57
1:X:1974:U:O2'	1:X:1975:G:H5'	2.04	0.57
1:X:2708:U:H2'	1:X:2709:C:C6	2.39	0.57
1:X:1886:G:H2'	1:X:1887:G:H8	1.69	0.57
1:X:408:U:H2'	1:X:409:G:H8	1.67	0.57
26:1:13:GLU:HG2	26:1:24:THR:HA	1.86	0.57
3:A:246:PRO:HD2	3:A:251:GLY:N	2.19	0.57
4:B:120:TRP:CD1	4:B:155:ARG:HB3	2.40	0.57
9:H:109:ARG:HA	9:H:129:LEU:HD13	1.86	0.57
1:X:398:C:H42	1:X:424:G:H1	1.52	0.57
9:H:19:ILE:O	9:H:19:ILE:HG13	2.05	0.57
15:N:17:VAL:HG21	15:N:32:TYR:HE1	1.69	0.57
14:M:104:LEU:HD23	14:M:106:TYR:CE2	2.40	0.57
1:X:1030:U:H3	1:X:1153:A:N6	1.98	0.57
1:X:1336:G:O6	1:X:1337:G:C6	2.58	0.57
1:X:2006:G:H5'	1:X:2596:C:H4'	1.86	0.57
1:X:2795:A:N3	1:X:2795:A:H2'	2.18	0.57
28:3:29:LYS:NZ	28:3:36:LYS:O	2.36	0.56
1:X:2034:A:H4'	4:B:141:ILE:HG12	1.85	0.56
19:R:16:PHE:CZ	19:R:46:VAL:HG21	2.40	0.56
1:X:1333:G:N2	1:X:1344:C:N4	2.52	0.56
1:X:143:A:H2'	1:X:144:U:C6	2.39	0.56
1:X:394:U:OP2	22:U:21:ARG:NH2	2.38	0.56
1:X:1443:G:H2'	1:X:1444:C:H6	1.68	0.56
1:X:16:G:H2'	1:X:17:G:H8	1.69	0.56
2:Y:7:C:H2'	2:Y:8:C:H6	1.70	0.56
1:X:1976:U:C5'	4:B:128:SER:HB3	2.35	0.56
1:X:1046:U:H5'	7:E:59:GLN:HG2	1.87	0.56
4:B:14:ILE:HG12	14:M:20:HIS:CD2	2.39	0.56
1:X:1321:A:H5'	1:X:1322:G:OP2	2.05	0.56
5:C:152:THR:OG1	5:C:153:ASP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:2:ILE:HD12	9:H:8:LEU:HD21	1.87	0.56
1:X:1834:G:H2'	1:X:1835:C:C6	2.41	0.56
1:X:2020:G:H2'	1:X:2021:G:C8	2.40	0.56
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.88	0.56
4:B:39:ALA:HB2	4:B:45:GLU:HG2	1.87	0.56
1:X:2313:G:C2	13:L:13:THR:HG22	2.41	0.56
1:X:1831:G:H2'	1:X:1832:G:H8	1.71	0.56
1:X:2372:A:N6	1:X:2401:A:H62	2.02	0.56
19:R:26:SER:O	19:R:30:LYS:HB2	2.05	0.56
20:S:3:LEU:HD23	20:S:56:VAL:HG13	1.87	0.56
1:X:2225:G:H2'	1:X:2226:A:H8	1.68	0.56
15:N:20:ARG:NH1	16:O:72:ARG:HD2	2.21	0.56
1:X:1223:G:H4'	1:X:1224:A:H5''	1.87	0.56
1:X:1448:A:H61	1:X:1574:A:H61	1.53	0.56
1:X:1919:A:H62	1:X:1946:U:H3	1.53	0.56
1:X:1883:A:H1'	1:X:1953:A:H2'	1.88	0.56
1:X:693:A:H2'	1:X:694:G:C8	2.40	0.56
1:X:568:G:N2	15:N:49:ASP:OD1	2.38	0.56
1:X:1183:C:N4	1:X:1189:G:O6	2.39	0.56
1:X:1360:G:N2	1:X:1615:C:O2	2.34	0.56
2:Y:59:A:H5'	2:Y:60:A:OP2	2.05	0.56
1:X:2797:G:OP2	12:K:3:HIS:NE2	2.38	0.56
1:X:708:G:OP1	1:X:1393:G:O2'	2.24	0.56
1:X:1792:C:OP1	3:A:263:ARG:NH2	2.39	0.56
1:X:2272:A:OP2	13:L:15:ARG:NH2	2.39	0.56
1:X:682:G:H3'	1:X:683:A:H5''	1.88	0.56
4:B:8:LYS:HG2	4:B:192:ASN:HA	1.88	0.56
1:X:1727:C:H2'	1:X:1728:A:C8	2.40	0.56
1:X:2352:A:H2'	1:X:2353:G:C8	2.41	0.56
1:X:539:A:H4'	1:X:539:A:OP1	2.06	0.56
5:C:127:ASP:OD2	5:C:129:LYS:NZ	2.39	0.56
10:I:88:PHE:HB3	10:I:90:ARG:NH2	2.21	0.56
19:R:23:ILE:HG23	19:R:33:THR:HB	1.87	0.56
20:S:72:ASP:HB2	20:S:79:ILE:HD13	1.88	0.56
6:D:130:LEU:HD13	6:D:132:ILE:HD11	1.88	0.55
11:J:55:MET:HB3	11:J:65:ILE:HD11	1.88	0.55
13:L:31:VAL:HA	13:L:40:ALA:HA	1.88	0.55
9:H:116:ARG:CZ	14:M:38:LYS:HD3	2.36	0.55
1:X:1250:A:H2'	1:X:1251:G:O4'	2.06	0.55
1:X:1919:A:H1'	1:X:1923:U:C2	2.41	0.55
1:X:854:G:H1	1:X:948:C:N4	2.02	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:141:GLY:O	8:G:144:MET:N	2.39	0.55
9:H:89:ILE:HG23	14:M:79:ARG:HD3	1.89	0.55
1:X:2226:A:H2'	1:X:2227:C:H6	1.71	0.55
1:X:27:G:N2	1:X:522:G:H1'	2.21	0.55
1:X:832:A:OP2	1:X:1201:G:N2	2.34	0.55
1:X:953:G:H5''	10:I:38:LYS:HA	1.88	0.55
26:1:38:LYS:HD2	26:1:40:TYR:HE1	1.71	0.55
1:X:954:U:P	10:I:38:LYS:HZ3	2.28	0.55
1:X:642:A:O2'	10:I:65:PHE:HB2	2.06	0.55
18:Q:73:ASN:OD1	18:Q:73:ASN:N	2.39	0.55
1:X:1482:U:H2'	1:X:1483:G:H8	1.72	0.55
8:G:140:GLN:O	8:G:144:MET:HG3	2.07	0.55
1:X:1482:U:H2'	1:X:1483:G:C8	2.41	0.55
1:X:2526:U:H2'	1:X:2527:G:H8	1.71	0.55
1:X:2705:A:H1'	1:X:2706:U:H2'	1.89	0.55
1:X:542:A:C2	1:X:2004:U:H2'	2.41	0.55
1:X:617:U:H5	1:X:632:A:C2	2.24	0.55
2:Y:44:C:N3	6:D:90:THR:OG1	2.40	0.55
8:G:41:TRP:CZ3	8:G:149:LYS:HD2	2.41	0.55
1:X:2708:U:H2'	1:X:2709:C:H6	1.71	0.55
2:Y:45:C:O2	6:D:92:ARG:NH2	2.40	0.55
7:E:37:TYR:CZ	7:E:72:VAL:HG22	2.42	0.55
8:G:61:ARG:HH12	8:G:66:HIS:HB2	1.72	0.55
10:I:32:ARG:HH12	10:I:34:HIS:HE1	1.55	0.55
17:P:57:LEU:HD13	17:P:69:ALA:HB2	1.88	0.55
18:Q:34:THR:O	18:Q:38:ILE:HG12	2.06	0.55
8:G:103:TYR:HB3	8:G:107:GLN:CG	2.37	0.55
17:P:95:ALA:HB2	17:P:126:ILE:HG13	1.89	0.55
22:U:54:ASN:CG	22:U:78:ILE:H	2.10	0.55
1:X:2195:C:H5'	1:X:2196:U:OP1	2.07	0.55
1:X:603:C:H4'	28:3:61:MET:HG2	1.88	0.55
1:X:75:C:H2'	1:X:76:C:H6	1.70	0.55
1:X:787:A:H2	1:X:800:U:HO2'	1.53	0.55
6:D:4:LEU:HD11	6:D:7:LYS:HB2	1.88	0.55
1:X:2469:G:OP2	1:X:2469:G:H8	1.89	0.55
2:Y:39:C:H5'	2:Y:40:C:OP2	2.08	0.55
1:X:1809:G:H3'	3:A:157:ARG:HH12	1.71	0.54
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.88	0.54
5:C:58:MET:HG2	5:C:70:GLY:O	2.07	0.54
7:E:154:PRO:HA	7:E:160:LYS:O	2.07	0.54
14:M:43:ASN:N	14:M:43:ASN:OD1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1630:A:O2'	1:X:1631:C:OP1	2.24	0.54
1:X:1785:A:H2'	1:X:1786:C:C6	2.41	0.54
1:X:219:G:N2	1:X:231:G:H2'	2.22	0.54
1:X:617:U:C5	1:X:632:A:C2	2.96	0.54
1:X:793:G:H21	1:X:796:A:H62	1.54	0.54
3:A:168:LYS:HA	3:A:173:VAL:HA	1.89	0.54
8:G:67:ARG:HG3	8:G:70:PHE:CD1	2.42	0.54
19:R:56:LYS:HA	19:R:69:GLN:HG2	1.88	0.54
1:X:2674:C:H2'	1:X:2675:U:H6	1.73	0.54
1:X:2756:A:H3'	1:X:2756:A:OP1	2.07	0.54
2:Y:46:G:H1'	2:Y:49:C:H41	1.72	0.54
1:X:2753:C:H5''	4:B:164:ARG:HG2	1.88	0.54
10:I:34:HIS:O	10:I:35:LYS:HD3	2.07	0.54
10:I:89:ASP:HB2	10:I:120:VAL:HG12	1.88	0.54
1:X:1005:U:H1'	16:O:21:ARG:HH22	1.72	0.54
20:S:116:VAL:HG12	20:S:117:VAL:HG13	1.90	0.54
1:X:1288:A:H4'	1:X:1289:A:OP1	2.06	0.54
1:X:1547:U:H3	1:X:1556:A:H61	1.55	0.54
1:X:1973:C:H2'	1:X:1974:U:O4'	2.07	0.54
1:X:224:G:H4'	1:X:399:G:C5	2.43	0.54
1:X:834:A:H5'	1:X:835:U:H6	1.72	0.54
2:Y:51:G:H2'	2:Y:52:G:H8	1.73	0.54
6:D:103:LEU:HG	6:D:108:LEU:HG	1.89	0.54
1:X:14:A:H5''	1:X:15:G:OP2	2.06	0.54
1:X:1687:C:O2	4:B:129:HIS:HE1	1.90	0.54
1:X:20:C:H2'	1:X:21:A:H8	1.72	0.54
1:X:319:G:N7	17:P:12:LYS:NZ	2.54	0.54
2:Y:40:C:H5'	13:L:97:HIS:CE1	2.43	0.54
1:X:475:U:O3'	27:2:12:ARG:NH2	2.41	0.54
1:X:2368:G:H5''	1:X:2369:U:H5'	1.89	0.54
1:X:2522:G:H2'	1:X:2523:G:C8	2.42	0.54
1:X:2572:U:H2'	1:X:2573:C:H6	1.71	0.54
1:X:320:A:N3	1:X:340:G:O2'	2.37	0.54
2:Y:7:C:H2'	2:Y:8:C:C6	2.43	0.54
9:H:28:GLY:HA3	9:H:34:LEU:HD22	1.88	0.54
1:X:1261:G:C5	15:N:3:ARG:HG2	2.42	0.54
16:O:89:ASN:OD1	16:O:89:ASN:N	2.40	0.54
17:P:40:LEU:HB3	25:Z:25:LEU:HD22	1.90	0.54
18:Q:6:ILE:HA	18:Q:30:SER:OG	2.07	0.54
1:X:2528:G:H2'	1:X:2529:G:H8	1.73	0.54
11:J:99:LYS:HE3	11:J:100:PRO:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:39:THR:O	12:K:42:LYS:N	2.41	0.54
1:X:1329:U:H2'	1:X:1330:G:C8	2.40	0.54
1:X:2466:G:H2'	1:X:2467:A:C8	2.41	0.54
1:X:2597:G:H21	4:B:150:VAL:HG21	1.73	0.54
1:X:2736:U:H1'	1:X:2737:A:H5''	1.88	0.54
1:X:847:C:H2'	1:X:848:A:H8	1.72	0.54
1:X:1782:A:O2'	3:A:207:GLY:O	2.18	0.54
3:A:43:ARG:HB3	3:A:54:ILE:O	2.08	0.54
17:P:39:ARG:HD2	17:P:97:VAL:HB	1.90	0.54
19:R:92:THR:O	19:R:92:THR:OG1	2.17	0.54
20:S:25:ASN:H	20:S:25:ASN:HD22	1.56	0.54
24:W:12:ARG:HG2	24:W:12:ARG:HH11	1.72	0.54
1:X:1845:A:N6	1:X:1871:G:O2'	2.41	0.54
1:X:1856:U:OP1	1:X:2389:G:O2'	2.21	0.54
1:X:530:G:H2'	1:X:531:G:H8	1.72	0.54
1:X:613:A:H8	1:X:636:G:H21	1.54	0.54
1:X:758:G:H2'	1:X:759:C:H5'	1.90	0.54
28:3:6:THR:HG23	28:3:8:LYS:H	1.73	0.54
3:A:134:ARG:HG3	3:A:135:PHE:CD2	2.43	0.54
17:P:37:LYS:HZ3	17:P:64:ALA:H	1.56	0.54
18:Q:11:VAL:HB	18:Q:26:SER:HB2	1.90	0.54
1:X:1991:C:H2'	1:X:1992:G:H8	1.73	0.54
1:X:2043:A:H62	5:C:68:ARG:NH1	2.04	0.54
1:X:2729:A:N1	1:X:2730:A:N6	2.56	0.54
1:X:2767:C:H1'	4:B:62:PRO:HG3	1.89	0.54
1:X:2293:G:H5'	6:D:35:VAL:HG11	1.89	0.54
7:E:43:VAL:HA	7:E:52:VAL:HG22	1.90	0.54
9:H:16:ALA:HB3	9:H:98:ILE:HD11	1.90	0.54
1:X:1121:G:H2'	1:X:1122:A:H8	1.72	0.54
1:X:2579:A:H2'	1:X:2580:C:H6	1.71	0.54
3:A:160:GLY:N	3:A:196:VAL:O	2.41	0.53
3:A:44:ASN:HA	3:A:49:ILE:HA	1.90	0.53
1:X:2806:G:OP1	4:B:57:ARG:NH1	2.41	0.53
13:L:46:SER:OG	13:L:47:ARG:N	2.38	0.53
1:X:1496:G:H4'	1:X:1497:C:OP1	2.07	0.53
1:X:177:U:H1'	1:X:178:C:OP1	2.08	0.53
1:X:2195:C:H2'	1:X:2196:U:C5	2.44	0.53
3:A:209:ALA:C	3:A:211:ARG:H	2.11	0.53
1:X:1816:G:OP1	3:A:52:ARG:HD3	2.07	0.53
1:X:852:U:H1'	1:X:1205:G:H1'	1.91	0.53
1:X:1820:G:OP2	3:A:239:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2591:C:O2'	1:X:2592:U:OP1	2.25	0.53
1:X:388:G:H2'	1:X:389:G:H8	1.73	0.53
13:L:95:LYS:HG3	13:L:96:TYR:H	1.73	0.53
21:T:46:LYS:NZ	21:T:76:ALA:HA	2.24	0.53
21:T:46:LYS:HB2	21:T:78:PHE:CE2	2.43	0.53
1:X:611:C:O2	1:X:615:C:H4'	2.09	0.53
1:X:667:U:O2'	1:X:668:A:H8	1.91	0.53
1:X:691:C:H2'	1:X:692:C:H6	1.71	0.53
1:X:1744:G:OP1	14:M:100:ARG:HD2	2.08	0.53
1:X:492:G:OP2	19:R:56:LYS:HG2	2.09	0.53
11:J:32:ASP:H	11:J:108:ALA:HB2	1.74	0.53
14:M:103:LYS:O	14:M:104:LEU:HB2	2.08	0.53
14:M:29:PRO:HB2	14:M:99:VAL:HG11	1.91	0.53
1:X:1385:C:H2'	1:X:1386:A:O4'	2.09	0.53
1:X:1674:C:H2'	1:X:1675:C:H6	1.74	0.53
1:X:1693:A:H2'	1:X:1694:A:O4'	2.08	0.53
1:X:2526:U:H2'	1:X:2527:G:C8	2.44	0.53
1:X:608:G:H2'	1:X:609:U:H6	1.73	0.53
28:3:13:ARG:HG3	28:3:14:ILE:HG13	1.90	0.53
4:B:33:ILE:HD11	4:B:86:PRO:HB2	1.91	0.53
8:G:67:ARG:CB	8:G:70:PHE:HA	2.38	0.53
12:K:90:ARG:HD2	12:K:94:TYR:HB2	1.90	0.53
22:U:49:LYS:HD3	22:U:61:TRP:CE2	2.44	0.53
1:X:742:G:H2'	1:X:1766:U:H1'	1.90	0.53
1:X:1884:A:O2'	3:A:244:ARG:HD3	2.08	0.53
1:X:1777:A:H1'	1:X:1921:A:N6	2.24	0.53
1:X:2043:A:H1'	1:X:2481:G:H1'	1.89	0.53
1:X:1046:U:H4'	7:E:60:LYS:HE2	1.91	0.53
1:X:1517:C:H4'	3:A:96:HIS:NE2	2.24	0.53
1:X:2245:A:H4'	1:X:2246:A:N3	2.24	0.53
28:3:52:LYS:O	28:3:56:ALA:HB2	2.08	0.53
3:A:246:PRO:HG2	3:A:248:THR:O	2.09	0.53
5:C:125:ILE:HG12	5:C:157:THR:HA	1.91	0.53
5:C:154:ASP:HB3	5:C:157:THR:HB	1.91	0.53
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.91	0.53
13:L:32:TYR:HB3	13:L:39:TYR:HB2	1.89	0.53
19:R:16:PHE:HE2	19:R:80:LYS:HZ3	1.57	0.53
1:X:1059:A:H2	1:X:1123:G:H21	1.55	0.53
1:X:1184:G:O6	1:X:1190:C:N4	2.41	0.53
1:X:1479:G:H2'	1:X:1480:G:C8	2.44	0.53
1:X:70:A:H4'	1:X:71:A:H5''	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:9:ILE:O	26:1:10:VAL:HB	2.08	0.53
3:A:111:LEU:HD23	3:A:127:LEU:HD13	1.91	0.53
1:X:1692:C:N3	4:B:128:SER:OG	2.39	0.53
1:X:2054:A:H2'	1:X:2055:G:H8	1.73	0.53
12:K:100:VAL:HG12	12:K:101:GLY:N	2.24	0.53
14:M:29:PRO:HA	14:M:54:VAL:HG13	1.91	0.53
1:X:1177:U:H2'	1:X:1178:C:O4'	2.09	0.53
1:X:1418:C:H2'	1:X:1419:G:C8	2.44	0.53
1:X:857:U:H2'	1:X:858:G:O4'	2.09	0.53
1:X:99:U:H3'	1:X:100:G:H5'	1.91	0.53
1:X:1816:G:H21	3:A:252:LYS:HG3	1.73	0.52
1:X:1342:U:H5''	1:X:1343:C:C5	2.43	0.52
1:X:1819:U:H2'	1:X:1820:G:O4'	2.08	0.52
27:2:26:SER:O	27:2:30:ILE:HG13	2.09	0.52
10:I:77:LEU:HD12	10:I:108:LEU:HD11	1.92	0.52
16:O:19:VAL:HG13	16:O:90:PHE:CD1	2.44	0.52
1:X:2639:A:H2'	1:X:2640:G:O4'	2.09	0.52
1:X:863:C:H42	1:X:940:G:H1	1.57	0.52
5:C:76:THR:O	5:C:77:PHE:HD1	1.92	0.52
8:G:103:TYR:HB3	8:G:107:GLN:HG2	1.91	0.52
9:H:29:ILE:HD13	9:H:123:PHE:CE1	2.44	0.52
10:I:62:LYS:CB	28:3:12:ARG:HA	2.39	0.52
19:R:84:VAL:CG1	19:R:90:LYS:H	2.17	0.52
24:W:46:THR:HG22	24:W:47:VAL:HG13	1.91	0.52
1:X:1204:G:H2'	1:X:1205:G:C8	2.45	0.52
1:X:1781:C:H4'	3:A:209:ALA:HB2	1.90	0.52
1:X:2440:C:H2'	1:X:2441:U:C6	2.44	0.52
3:A:186:HIS:HB2	3:A:188:GLU:HG2	1.92	0.52
5:C:6:VAL:HG12	5:C:7:ILE:HG12	1.91	0.52
14:M:70:LYS:HE2	14:M:72:SER:HB3	1.90	0.52
1:X:1870:U:P	1:X:1871:G:H22	2.32	0.52
1:X:469:G:N2	1:X:480:G:H2'	2.25	0.52
5:C:112:GLN:OE1	5:C:112:GLN:HA	2.08	0.52
10:I:62:LYS:HD3	10:I:63:ARG:N	2.24	0.52
1:X:2855:C:H1'	12:K:91:PRO:HB2	1.92	0.52
1:X:394:U:OP1	22:U:19:ILE:HG12	2.10	0.52
1:X:503:G:H2'	1:X:504:G:O4'	2.10	0.52
1:X:692:C:H2'	1:X:693:A:C8	2.43	0.52
10:I:78:SER:HB3	10:I:112:GLY:HA3	1.92	0.52
11:J:42:TRP:CD1	11:J:97:VAL:HG12	2.44	0.52
13:L:75:LEU:O	13:L:79:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:7:LEU:HD22	18:Q:7:LEU:H	1.75	0.52
19:R:105:ARG:NH2	19:R:111:GLY:O	2.42	0.52
22:U:17:SER:OG	22:U:45:ASN:N	2.42	0.52
1:X:1223:G:H5''	1:X:1224:A:H3'	1.92	0.52
1:X:1454:U:H2'	1:X:1455:C:C6	2.44	0.52
1:X:502:A:H2'	1:X:503:G:O4'	2.10	0.52
1:X:1673:C:H5''	4:B:136:ARG:HB3	1.91	0.52
8:G:46:ALA:HB1	8:G:88:VAL:HG23	1.92	0.52
9:H:83:ARG:HG2	14:M:40:ARG:NH2	2.24	0.52
15:N:66:ASN:HB3	15:N:76:TYR:CB	2.33	0.52
23:V:32:ALA:HB2	23:V:37:LEU:HD13	1.92	0.52
1:X:47:G:N2	1:X:154:U:OP2	2.29	0.52
1:X:2441:U:H1'	1:X:2470:U:O4	2.09	0.52
1:X:2824:C:H4'	1:X:2825:A:O5'	2.10	0.52
1:X:761:G:H2'	1:X:763:A:N7	2.25	0.52
1:X:940:G:H4'	24:W:37:THR:HG21	1.92	0.52
2:Y:9:G:H5'	13:L:32:TYR:CZ	2.45	0.52
9:H:73:VAL:HG21	9:H:123:PHE:CE2	2.44	0.52
22:U:15:VAL:HA	22:U:45:ASN:O	2.10	0.52
1:X:2078:G:H1	1:X:2177:U:H3	1.57	0.52
1:X:2668:U:P	1:X:2699:G:H22	2.33	0.52
1:X:580:A:H4'	1:X:581:A:OP1	2.10	0.52
1:X:615:C:H41	10:I:100:ARG:NH1	2.07	0.52
5:C:47:THR:HA	5:C:82:VAL:HG13	1.90	0.52
13:L:37:HIS:HD2	13:L:57:ALA:HA	1.75	0.52
1:X:1004:A:H1'	16:O:88:GLN:HG3	1.92	0.52
1:X:1558:C:H2'	1:X:1559:G:O4'	2.10	0.52
1:X:2451:G:H22	1:X:2456:U:H5'	1.74	0.52
1:X:2716:G:H1	1:X:2748:C:N4	2.07	0.52
1:X:538:A:H2'	1:X:538:A:N3	2.24	0.52
26:1:12:MET:HG3	26:1:54:LYS:HB3	1.92	0.52
5:C:26:VAL:HG11	5:C:102:LEU:HD22	1.91	0.52
6:D:65:PRO:HA	6:D:89:VAL:HG22	1.92	0.52
9:H:99:ILE:HD12	9:H:103:GLY:HA2	1.91	0.52
15:N:58:ARG:O	15:N:62:ILE:HG13	2.10	0.52
15:N:86:ALA:HB1	15:N:88:ILE:HB	1.92	0.52
20:S:19:ILE:HD11	20:S:36:ARG:HG3	1.91	0.52
1:X:1787:U:H2'	1:X:1788:C:C6	2.44	0.52
9:H:73:VAL:HG21	9:H:123:PHE:HE2	1.75	0.51
19:R:29:HIS:NE2	19:R:51:VAL:HG13	2.25	0.51
20:S:7:PRO:HB2	20:S:9:THR:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1225:G:HO2'	1:X:1226:A:H8	1.59	0.51
1:X:2269:G:N2	1:X:2322:U:H1'	2.24	0.51
19:R:33:THR:OG1	19:R:34:GLY:N	2.43	0.51
1:X:1033:G:H4'	1:X:1034:U:H5'	1.92	0.51
1:X:1128:G:H3'	1:X:1129:A:H5''	1.93	0.51
2:Y:16:U:O2'	2:Y:17:A:OP2	2.28	0.51
5:C:45:THR:HG23	5:C:47:THR:H	1.74	0.51
7:E:17:VAL:HG13	7:E:26:VAL:HG22	1.91	0.51
7:E:41:LEU:HD22	7:E:68:THR:HG21	1.93	0.51
8:G:68:PRO:HD2	8:G:76:GLN:HB3	1.91	0.51
19:R:77:HIS:CG	19:R:78:ALA:H	2.29	0.51
1:X:1825:C:O2	1:X:1955:G:N2	2.35	0.51
1:X:608:G:H2'	1:X:609:U:C6	2.45	0.51
26:1:30:ASN:HD22	26:1:31:THR:HG23	1.75	0.51
6:D:110:ARG:O	6:D:111:ILE:HG13	2.10	0.51
24:W:4:LYS:HG2	24:W:52:GLU:HB3	1.92	0.51
1:X:1429:A:H1'	1:X:1603:A:C5	2.46	0.51
1:X:2692:A:H5''	1:X:2693:U:OP2	2.10	0.51
1:X:346:C:C6	1:X:347:C:H5	2.29	0.51
1:X:967:G:N2	1:X:971:A:OP2	2.43	0.51
8:G:33:ILE:HB	8:G:34:PRO:HD2	1.92	0.51
17:P:35:PRO:HD3	17:P:121:THR:O	2.10	0.51
1:X:1599:G:C2	1:X:1600:U:H1'	2.45	0.51
1:X:1886:G:H2'	1:X:1887:G:C8	2.45	0.51
1:X:1714:A:O2'	1:X:1961:A:OP1	2.23	0.51
1:X:977:G:H1'	1:X:2246:A:H62	1.75	0.51
1:X:224:G:OP2	1:X:226:C:N4	2.42	0.51
4:B:102:ILE:N	4:B:169:ASN:O	2.43	0.51
14:M:60:SER:HB3	14:M:63:ARG:HH12	1.75	0.51
15:N:39:LEU:HA	15:N:42:ALA:HB3	1.93	0.51
15:N:7:GLY:O	15:N:8:ILE:HG12	2.11	0.51
20:S:6:LYS:HE2	20:S:56:VAL:HG11	1.93	0.51
1:X:1686:A:H5''	1:X:1687:C:OP2	2.10	0.51
1:X:1769:U:H2'	1:X:1775:A:N6	2.24	0.51
1:X:334:G:C8	5:C:164:VAL:HG13	2.46	0.51
1:X:845:U:OP1	10:I:41:SER:HB3	2.11	0.51
25:Z:4:HIS:HB2	25:Z:5:PRO:HD3	1.92	0.51
1:X:2766:U:O2'	4:B:62:PRO:O	2.24	0.51
5:C:119:ALA:HB3	5:C:189:ASP:HA	1.92	0.51
1:X:1101:U:H2'	1:X:1102:G:C8	2.45	0.51
1:X:1724:C:N3	1:X:1747:G:C6	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:617:U:H5	1:X:632:A:H2	1.58	0.51
1:X:938:G:O2'	1:X:939:C:O5'	2.28	0.51
1:X:2371:A:H8	10:I:59:ARG:HG2	1.76	0.51
1:X:1770:U:C2	1:X:1774:A:N7	2.79	0.51
1:X:2043:A:N3	1:X:2481:G:C4	2.79	0.51
1:X:2594:U:H2'	1:X:2595:C:H6	1.75	0.51
1:X:542:A:H5'	15:N:28:ARG:HH21	1.74	0.51
4:B:41:THR:OG1	4:B:42:ASP:N	2.41	0.51
8:G:128:GLU:HG3	8:G:150:VAL:HG21	1.93	0.51
8:G:96:ASP:HB3	8:G:97:ASP:OD1	2.10	0.51
9:H:13:ASN:HD21	9:H:109:ARG:HG2	1.75	0.51
1:X:1846:A:H2'	1:X:1847:G:O4'	2.11	0.51
1:X:2270:U:H2'	1:X:2271:C:C6	2.46	0.51
1:X:836:G:H2'	1:X:837:U:H6	1.76	0.51
26:1:8:ILE:O	26:1:9:ILE:HG12	2.11	0.51
3:A:88:ARG:HG3	3:A:90:ALA:HB3	1.93	0.51
17:P:59:PHE:CD1	25:Z:41:LEU:HD22	2.45	0.51
1:X:1173:G:H5''	16:O:22:VAL:HG22	1.93	0.51
1:X:455:A:H1'	1:X:1215:A:O4'	2.11	0.51
1:X:1348:C:H2'	1:X:1349:A:H8	1.76	0.51
1:X:1469:U:H5'	1:X:1470:G:OP2	2.11	0.51
1:X:590:C:H2'	1:X:591:G:H8	1.76	0.51
28:3:22:VAL:HG21	28:3:53:ALA:HA	1.92	0.50
3:A:108:PRO:HB3	3:A:143:HIS:CE1	2.46	0.50
5:C:153:ASP:OD1	5:C:172:VAL:HA	2.11	0.50
10:I:94:GLU:HA	10:I:97:ARG:NE	2.25	0.50
20:S:88:TYR:O	20:S:127:PRO:HB3	2.11	0.50
1:X:1486:A:H2'	1:X:1487:C:C6	2.46	0.50
6:D:34:ILE:HD12	6:D:156:ILE:HG12	1.92	0.50
1:X:1048:U:H3	1:X:1129:A:H61	1.59	0.50
1:X:1919:A:H1'	1:X:1923:U:N3	2.25	0.50
1:X:2372:A:H5''	10:I:61:PRO:HB3	1.92	0.50
1:X:2474:G:H5''	11:J:82:THR:CA	2.40	0.50
1:X:2640:G:H2'	1:X:2641:A:C8	2.46	0.50
1:X:50:G:H4'	1:X:51:A:H5'	1.93	0.50
1:X:558:G:OP2	1:X:558:G:N2	2.42	0.50
1:X:2283:G:O2'	6:D:130:LEU:O	2.28	0.50
7:E:33:LEU:HD22	7:E:136:ILE:HG22	1.92	0.50
1:X:1935:A:N3	1:X:2539:C:O2'	2.38	0.50
1:X:2558:C:H2'	1:X:2559:U:O4'	2.10	0.50
1:X:740:A:C6	1:X:741:G:C6	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:875:G:H2'	1:X:876:A:O4'	2.11	0.50
26:1:14:SER:HB3	26:1:50:PHE:CD2	2.47	0.50
27:2:36:ALA:C	27:2:38:GLY:H	2.15	0.50
27:2:34:ARG:HG2	27:2:40:HIS:HD2	1.75	0.50
5:C:47:THR:OG1	5:C:85:GLY:N	2.38	0.50
6:D:63:GLN:NE2	6:D:90:THR:O	2.24	0.50
8:G:67:ARG:HB2	8:G:76:GLN:NE2	2.26	0.50
20:S:91:PRO:HG2	20:S:125:PRO:HD2	1.93	0.50
1:X:1573:G:H3'	1:X:1574:A:H5''	1.92	0.50
1:X:1997:A:H2'	1:X:1998:A:C8	2.47	0.50
1:X:2620:G:P	8:G:102:ARG:HH21	2.34	0.50
1:X:2705:A:C8	1:X:2706:U:H2'	2.47	0.50
1:X:399:G:H5'	1:X:401:G:H22	1.75	0.50
1:X:489:A:O3'	19:R:45:LYS:NZ	2.44	0.50
1:X:754:G:H2'	1:X:755:C:H6	1.77	0.50
10:I:88:PHE:HB3	10:I:90:ARG:CZ	2.41	0.50
12:K:11:ASN:ND2	12:K:11:ASN:H	2.07	0.50
1:X:1850:G:H1'	1:X:1867:A:H62	1.77	0.50
1:X:719:A:H2'	1:X:720:A:O4'	2.12	0.50
15:N:90:LEU:O	15:N:92:ARG:HG3	2.11	0.50
1:X:1441:A:H4'	1:X:1442:C:O5'	2.12	0.50
1:X:1578:U:H2'	1:X:1579:G:H8	1.77	0.50
1:X:1870:U:O5'	1:X:1871:G:N2	2.45	0.50
1:X:761:G:C8	1:X:763:A:C8	2.99	0.50
1:X:877:G:H1	1:X:924:C:H42	1.58	0.50
28:3:34:THR:OG1	28:3:35:GLY:N	2.43	0.50
1:X:2627:G:O2'	9:H:38:GLY:HA2	2.12	0.50
10:I:86:THR:OG1	10:I:116:ARG:NE	2.45	0.50
15:N:49:ASP:HA	15:N:52:ASN:HB2	1.92	0.50
17:P:97:VAL:HG22	17:P:124:ILE:HG23	1.94	0.50
18:Q:2:SER:OG	18:Q:3:HIS:N	2.45	0.50
19:R:90:LYS:HG3	19:R:108:VAL:HG21	1.93	0.50
1:X:1427:G:N1	1:X:1603:A:OP1	2.45	0.50
1:X:2262:C:H2'	1:X:2263:C:O4'	2.11	0.50
1:X:409:G:H1'	22:U:45:ASN:ND2	2.27	0.50
1:X:734:G:H2'	1:X:735:G:H8	1.76	0.50
3:A:244:ARG:O	3:A:244:ARG:HG2	2.12	0.50
17:P:52:ASP:OD1	17:P:52:ASP:N	2.43	0.50
1:X:123:A:H1'	27:2:14:LYS:HD3	1.93	0.50
1:X:1614:C:H2'	1:X:1615:C:H6	1.77	0.50
1:X:919:U:O3'	11:J:24:GLY:HA3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:56:GLN:N	25:Z:56:GLN:OE1	2.45	0.50
14:M:102:ALA:C	14:M:103:LYS:HD2	2.32	0.50
1:X:1235:C:H42	1:X:1240:G:H1	1.60	0.50
1:X:1481:U:O2'	1:X:1562:G:H1'	2.12	0.50
1:X:615:C:O2	1:X:670:U:O2'	2.30	0.50
1:X:971:A:H61	11:J:83:ARG:NH2	1.98	0.50
1:X:2036:G:H5'	4:B:144:ARG:O	2.12	0.49
9:H:70:VAL:CG2	9:H:98:ILE:HG23	2.38	0.49
1:X:542:A:H8	15:N:28:ARG:NH2	2.10	0.49
1:X:1949:A:H1'	1:X:2572:U:H5'	1.93	0.49
1:X:332:C:H5''	1:X:333:A:OP2	2.12	0.49
1:X:399:G:H5'	1:X:401:G:N2	2.28	0.49
1:X:542:A:C5'	15:N:28:ARG:HH21	2.26	0.49
1:X:825:C:H1'	1:X:1263:G:C2	2.46	0.49
27:2:22:MET:HA	27:2:28:ARG:HD3	1.94	0.49
5:C:53:LYS:O	5:C:54:THR:OG1	2.23	0.49
10:I:18:ARG:HB3	10:I:21:ARG:CB	2.42	0.49
11:J:44:LYS:HA	11:J:95:VAL:HG12	1.92	0.49
24:W:25:LEU:HD23	24:W:30:ASP:HB3	1.94	0.49
1:X:1223:G:N2	1:X:1249:G:O2'	2.45	0.49
1:X:558:G:H8	1:X:560:G:N7	2.10	0.49
1:X:667:U:H2'	1:X:668:A:H5''	1.94	0.49
1:X:922:A:N7	1:X:923:A:C6	2.80	0.49
2:Y:42:U:HO2'	2:Y:47:A:N6	2.10	0.49
5:C:47:THR:OG1	5:C:82:VAL:HG22	2.12	0.49
1:X:592:G:O5'	15:N:10:ARG:NH1	2.45	0.49
15:N:82:GLY:HA3	15:N:113:SER:OG	2.12	0.49
19:R:15:HIS:N	19:R:15:HIS:CD2	2.81	0.49
1:X:1236:G:O6	16:O:70:TYR:OH	2.29	0.49
1:X:1390:G:H8	1:X:1390:G:O5'	1.95	0.49
1:X:1750:A:C8	1:X:2675:U:H1'	2.47	0.49
1:X:2498:U:C5	1:X:2520:A:C6	3.00	0.49
1:X:2854:G:H4'	1:X:2855:C:OP1	2.12	0.49
27:2:41:GLN:HE21	27:2:41:GLN:HA	1.76	0.49
5:C:5:ASN:ND2	5:C:9:GLN:HG3	2.27	0.49
1:X:1006:C:N3	8:G:31:THR:HG23	2.26	0.49
9:H:83:ARG:HH12	14:M:38:LYS:HE2	1.77	0.49
17:P:35:PRO:O	17:P:39:ARG:HD3	2.12	0.49
1:X:2335:U:H2'	1:X:2336:G:C8	2.48	0.49
27:2:38:GLY:O	27:2:40:HIS:N	2.45	0.49
6:D:115:ARG:HH22	6:D:178:ARG:HH12	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:78:ASP:N	8:G:78:ASP:OD1	2.45	0.49
22:U:60:VAL:O	22:U:61:TRP:HD1	1.95	0.49
1:X:1034:U:OP2	1:X:1036:G:O2'	2.31	0.49
1:X:1468:A:OP2	1:X:1468:A:C8	2.66	0.49
1:X:1827:G:H1'	1:X:1914:U:C2	2.48	0.49
1:X:2018:G:H4'	1:X:2019:C:OP2	2.13	0.49
1:X:2314:A:O2'	1:X:2316:G:N7	2.32	0.49
1:X:420:C:H2'	1:X:421:G:C8	2.47	0.49
1:X:946:U:H2'	1:X:947:C:H6	1.73	0.49
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.95	0.49
1:X:1816:G:H2'	1:X:1817:U:C6	2.48	0.49
1:X:1918:G:H1'	1:X:1947:G:N2	2.28	0.49
1:X:871:U:O2	1:X:2247:A:H2'	2.12	0.49
1:X:2311:U:O2'	1:X:2315:A:N7	2.45	0.49
1:X:585:U:H4'	1:X:2481:G:C8	2.48	0.49
1:X:2500:C:H2'	1:X:2501:U:C6	2.47	0.49
1:X:746:G:C8	1:X:774:A:N1	2.80	0.49
27:2:1:MET:HE2	27:2:3:ARG:HH12	1.77	0.49
8:G:58:ILE:HG12	8:G:80:VAL:HG11	1.95	0.49
14:M:104:LEU:HA	14:M:106:TYR:CE2	2.48	0.49
1:X:1834:G:H2'	1:X:1835:C:H6	1.77	0.49
1:X:2084:G:H2'	1:X:2085:G:C8	2.47	0.49
1:X:426:C:O2'	1:X:1863:U:O2'	2.16	0.49
1:X:386:U:H5'	1:X:436:A:N3	2.27	0.49
1:X:518:A:O2'	1:X:519:C:OP1	2.28	0.49
1:X:667:U:HO2'	1:X:668:A:H8	1.60	0.49
25:Z:57:VAL:HG12	25:Z:58:LEU:HD23	1.95	0.49
8:G:43:VAL:HB	8:G:167:LYS:HG2	1.94	0.49
1:X:1675:C:H2'	1:X:1676:U:H6	1.76	0.49
1:X:1974:U:C2'	1:X:1975:G:H5'	2.42	0.49
1:X:2206:C:H2'	1:X:2207:G:O4'	2.12	0.49
1:X:645:G:H2'	1:X:646:C:C6	2.47	0.49
1:X:635:C:O2'	1:X:670:U:OP1	2.29	0.49
1:X:687:G:H4'	5:C:68:ARG:O	2.13	0.49
3:A:76:ASN:HA	3:A:118:ASN:HA	1.94	0.49
5:C:22:VAL:HG22	5:C:110:SER:HA	1.94	0.49
1:X:1023:U:C4	8:G:53:ARG:HG3	2.47	0.49
10:I:56:LEU:HB3	28:3:52:LYS:HZ2	1.76	0.49
11:J:60:ARG:HE	11:J:60:ARG:HA	1.77	0.49
1:X:1004:A:OP1	15:N:50:ARG:NH1	2.41	0.49
23:V:2:LYS:HB2	23:V:3:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1742:G:H2'	1:X:1743:C:C6	2.47	0.49
1:X:1746:A:C2	1:X:2696:A:H1'	2.47	0.49
1:X:1779:C:H2'	1:X:1780:A:C8	2.48	0.49
1:X:227:G:OP2	28:3:8:LYS:HG2	2.13	0.49
1:X:2598:C:O2'	1:X:2599:U:H5'	2.12	0.49
1:X:493:A:H4'	19:R:56:LYS:HG3	1.95	0.49
1:X:1791:C:OP2	3:A:183:ARG:NH1	2.44	0.49
5:C:128:ALA:O	5:C:130:THR:N	2.38	0.49
12:K:73:LYS:O	12:K:76:VAL:HG12	2.13	0.49
13:L:33:ARG:NH1	13:L:38:ILE:HG21	2.28	0.49
20:S:80:HIS:NE2	20:S:82:ASP:OD2	2.43	0.49
1:X:870:C:H5''	21:T:77:ARG:HH22	1.78	0.49
1:X:1225:G:O6	17:P:12:LYS:HB2	2.12	0.49
1:X:1272:G:H2'	1:X:1273:G:C8	2.48	0.49
1:X:1350:G:H2'	1:X:1351:G:C8	2.46	0.49
1:X:1448:A:N6	1:X:1574:A:H61	2.11	0.49
1:X:1578:U:H2'	1:X:1579:G:C8	2.48	0.49
1:X:2326:C:OP1	1:X:2326:C:H4'	2.13	0.49
1:X:2572:U:H2'	1:X:2573:C:C6	2.47	0.49
1:X:58:C:H1'	1:X:72:A:H2'	1.93	0.49
8:G:71:THR:N	8:G:76:GLN:HE22	2.10	0.48
8:G:62:ILE:O	8:G:77:GLY:HA3	2.13	0.48
22:U:17:SER:HB2	22:U:44:ALA:HA	1.95	0.48
1:X:1468:A:H8	1:X:1468:A:OP2	1.96	0.48
1:X:2516:U:H2'	1:X:2517:C:H6	1.75	0.48
1:X:321:A:C6	1:X:323:G:C4	3.01	0.48
1:X:38:G:O2'	1:X:39:C:O5'	2.23	0.48
1:X:591:G:C6	1:X:592:G:C6	3.00	0.48
1:X:89:A:H4'	1:X:90:G:C5'	2.40	0.48
2:Y:3:A:N6	2:Y:121:G:O6	2.46	0.48
4:B:16:LYS:H	4:B:21:ILE:HD11	1.78	0.48
1:X:2619:G:OP1	8:G:125:ARG:NH2	2.46	0.48
16:O:10:LYS:HE2	16:O:13:ARG:NH2	2.27	0.48
17:P:71:VAL:HG13	17:P:126:ILE:HG22	1.95	0.48
22:U:23:LYS:HB2	22:U:35:THR:HG23	1.94	0.48
1:X:865:A:H5'	24:W:42:GLY:HA3	1.94	0.48
1:X:121:G:H2'	1:X:122:G:O4'	2.13	0.48
1:X:1699:A:H61	1:X:1723:U:H3	1.61	0.48
1:X:2211:U:OP1	22:U:43:ARG:NH1	2.22	0.48
1:X:2225:G:H2'	1:X:2226:A:C8	2.47	0.48
1:X:2796:A:H4'	4:B:162:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:40:U:H2'	1:X:41:G:C8	2.48	0.48
1:X:590:C:H2'	1:X:591:G:C8	2.48	0.48
1:X:5:A:H2'	1:X:6:A:C8	2.48	0.48
1:X:70:A:H5''	1:X:71:A:H2'	1.95	0.48
1:X:977:G:C1'	1:X:2246:A:H62	2.26	0.48
4:B:119:ARG:HA	4:B:160:MET:SD	2.53	0.48
5:C:26:VAL:O	5:C:30:VAL:HG23	2.12	0.48
14:M:32:THR:O	14:M:51:GLU:HA	2.13	0.48
1:X:1269:G:H2'	1:X:1269:G:N3	2.28	0.48
1:X:2240:C:C2'	1:X:2241:U:H5'	2.43	0.48
1:X:2370:G:O6	1:X:2406:C:H1'	2.13	0.48
1:X:2596:C:H2'	1:X:2597:G:H8	1.77	0.48
1:X:318:G:N1	1:X:321:A:OP2	2.45	0.48
1:X:577:U:H2'	1:X:579:G:OP2	2.12	0.48
1:X:596:C:C4	1:X:684:C:C2	3.02	0.48
1:X:824:U:H2'	10:I:30:ALA:N	2.29	0.48
11:J:11:ARG:NE	11:J:15:ARG:HH12	2.11	0.48
20:S:3:LEU:HD22	20:S:32:PHE:CD2	2.48	0.48
23:V:31:GLN:O	23:V:36:GLN:HB3	2.12	0.48
1:X:1466:C:H2'	1:X:1467:U:C1'	2.43	0.48
1:X:1510:A:H2'	1:X:1511:A:O4'	2.13	0.48
1:X:1630:A:OP1	1:X:1633:C:N4	2.40	0.48
1:X:1982:C:O2	1:X:2666:U:O2'	2.29	0.48
1:X:2031:A:H2'	1:X:2032:G:O4'	2.13	0.48
1:X:2571:G:C6	1:X:2572:U:N3	2.82	0.48
1:X:331:U:H2'	5:C:130:THR:HG21	1.93	0.48
5:C:47:THR:HG1	5:C:85:GLY:H	1.58	0.48
6:D:13:ARG:O	6:D:17:MET:HG3	2.13	0.48
7:E:121:VAL:HG11	7:E:144:VAL:HG21	1.95	0.48
9:H:62:GLY:O	9:H:65:LYS:NZ	2.36	0.48
11:J:15:ARG:HD3	11:J:73:LYS:HE3	1.96	0.48
16:O:11:GLN:HA	16:O:38:LEU:O	2.13	0.48
1:X:1075:C:H2'	1:X:1076:U:O4'	2.13	0.48
1:X:154:U:H3'	1:X:155:G:H8	1.78	0.48
1:X:1678:G:H1	1:X:1982:C:N4	2.07	0.48
1:X:540:G:C6	1:X:2005:U:H5''	2.48	0.48
1:X:2200:G:H2'	1:X:2201:G:C8	2.47	0.48
1:X:2691:C:O2'	1:X:2693:U:H5'	2.14	0.48
1:X:343:A:O2'	1:X:346:C:N4	2.42	0.48
25:Z:16:ARG:HD3	25:Z:20:ARG:CZ	2.44	0.48
26:1:37:LEU:HD23	26:1:51:ARG:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:14:ARG:NH1	3:A:27:LYS:O	2.47	0.48
1:X:1023:U:O4	8:G:56:THR:OG1	2.23	0.48
1:X:1151:U:O4	8:G:93:LYS:HE3	2.14	0.48
1:X:1029:C:H42	1:X:1155:G:H1	1.62	0.48
1:X:1310:C:H2'	1:X:1311:C:H6	1.79	0.48
1:X:1705:U:O2	1:X:1717:A:H5'	2.13	0.48
1:X:2670:C:H2'	1:X:2671:C:H6	1.79	0.48
1:X:2751:C:H2'	1:X:2752:C:C6	2.48	0.48
1:X:2787:A:H2'	1:X:2788:C:H6	1.78	0.48
6:D:17:MET:HG2	6:D:22:TYR:HB2	1.94	0.48
7:E:67:LEU:O	7:E:71:LEU:HG	2.13	0.48
9:H:13:ASN:ND2	9:H:109:ARG:HG2	2.29	0.48
15:N:76:TYR:CZ	15:N:80:ILE:HG13	2.48	0.48
22:U:32:ARG:HE	22:U:32:ARG:N	2.10	0.48
1:X:1603:A:OP2	1:X:1603:A:H8	1.96	0.48
1:X:2738:A:C5	7:E:67:LEU:HD11	2.49	0.48
1:X:438:G:H2'	1:X:439:C:C6	2.49	0.48
1:X:507:A:OP2	17:P:19:LYS:NZ	2.36	0.48
1:X:546:A:H2'	1:X:547:U:C6	2.48	0.48
1:X:810:U:H2'	1:X:811:G:O4'	2.12	0.48
5:C:117:LEU:HB3	5:C:187:VAL:HA	1.94	0.48
5:C:71:ASP:OD1	5:C:72:ARG:N	2.44	0.48
1:X:1148:G:O2'	8:G:134:MET:HG3	2.13	0.48
19:R:18:LYS:HE2	19:R:19:GLY:N	2.28	0.48
1:X:1269:G:O3'	5:C:69:HIS:CE1	2.67	0.48
1:X:1398:G:O2'	1:X:1399:C:O4'	2.21	0.48
1:X:1426:U:H2'	1:X:1427:G:O4'	2.14	0.48
1:X:1563:U:H2'	1:X:1564:U:C6	2.48	0.48
1:X:1984:A:H2'	1:X:1985:G:O4'	2.14	0.48
1:X:542:A:H2	1:X:2004:U:H2'	1.78	0.48
1:X:303:C:H3'	1:X:304:A:H5''	1.95	0.48
1:X:649:G:C5	1:X:650:U:C5	3.01	0.48
1:X:688:A:H4'	5:C:61:GLN:OE1	2.12	0.48
1:X:736:G:H2'	1:X:737:C:O4'	2.13	0.48
1:X:1276:U:O4'	25:Z:10:LYS:HG3	2.13	0.48
28:3:15:LYS:HB2	28:3:23:MET:HB2	1.96	0.48
6:D:14:PRO:HA	6:D:17:MET:HB2	1.96	0.48
11:J:42:TRP:HB3	11:J:95:VAL:HG11	1.95	0.48
20:S:168:VAL:HG12	20:S:169:VAL:HG23	1.95	0.48
1:X:115:G:OP2	1:X:117:A:O2'	2.32	0.48
1:X:1202:U:H2'	1:X:1203:A:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1442:C:O2'	1:X:1585:A:OP2	2.22	0.48
1:X:1782:A:N3	3:A:208:LYS:HE2	2.29	0.48
1:X:1816:G:H2'	1:X:1817:U:H6	1.78	0.48
1:X:1816:G:N2	3:A:252:LYS:HG3	2.28	0.48
1:X:227:G:C6	1:X:228:A:C6	3.02	0.48
1:X:2370:G:C6	1:X:2406:C:H1'	2.49	0.48
1:X:536:A:N6	1:X:2605:C:H4'	2.28	0.48
1:X:401:G:OP1	22:U:35:THR:HB	2.13	0.48
2:Y:63:A:H2'	2:Y:64:C:H6	1.79	0.48
3:A:208:LYS:O	3:A:211:ARG:HB3	2.14	0.48
1:X:2551:A:N7	4:B:144:ARG:HG2	2.28	0.48
5:C:149:LEU:HB2	5:C:183:HIS:ND1	2.29	0.48
11:J:131:LYS:HB2	11:J:131:LYS:NZ	2.28	0.48
13:L:60:LYS:HD2	13:L:60:LYS:HA	1.58	0.48
15:N:49:ASP:O	15:N:53:LYS:HG2	2.14	0.48
15:N:92:ARG:O	15:N:93:LYS:HD3	2.12	0.48
16:O:5:ILE:N	16:O:10:LYS:HD3	2.28	0.48
1:X:1163:C:H2'	1:X:1164:C:H6	1.78	0.48
1:X:1337:G:N2	1:X:1344:C:C2	2.82	0.48
1:X:240:U:H2'	1:X:241:C:O4'	2.14	0.48
1:X:2674:C:H2'	1:X:2675:U:C6	2.49	0.48
1:X:2821:G:H2'	1:X:2822:U:O4'	2.14	0.48
1:X:2825:A:N7	1:X:2843:A:O2'	2.36	0.48
1:X:2784:A:C6	1:X:2866:A:C8	3.02	0.48
1:X:613:A:N6	1:X:668:A:O4'	2.46	0.48
1:X:69:G:H1'	1:X:72:A:H1'	1.95	0.48
1:X:809:C:H2'	1:X:810:U:C6	2.49	0.48
26:1:13:GLU:O	26:1:14:SER:OG	2.27	0.47
12:K:3:HIS:HB3	12:K:5:LYS:HD2	1.96	0.47
16:O:11:GLN:HB2	16:O:13:ARG:HH21	1.78	0.47
18:Q:31:PRO:HA	18:Q:76:LYS:CB	2.44	0.47
21:T:17:ASN:HA	21:T:18:PRO:HD3	1.64	0.47
23:V:42:ARG:NH1	23:V:45:GLN:OE1	2.47	0.47
1:X:1003:C:H2'	1:X:1004:A:C8	2.46	0.47
1:X:1024:G:N2	1:X:1161:U:O2	2.47	0.47
1:X:1054:C:N4	1:X:1123:G:H1	2.10	0.47
1:X:1653:C:H2'	1:X:1654:A:C8	2.49	0.47
1:X:2060:A:H2'	1:X:2061:C:H6	1.78	0.47
1:X:2378:G:H1	1:X:2396:C:H42	1.61	0.47
1:X:469:G:H5'	27:2:39:ARG:O	2.14	0.47
1:X:785:U:H2'	1:X:786:U:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:4:ILE:HG22	4:B:96:PHE:HE1	1.79	0.47
8:G:81:VAL:HG21	8:G:161:GLN:HG2	1.96	0.47
12:K:11:ASN:O	12:K:12:ARG:HG2	2.13	0.47
15:N:79:PHE:HE2	15:N:95:LEU:HD21	1.79	0.47
19:R:10:HIS:HD2	19:R:44:GLN:NE2	2.12	0.47
1:X:2492:G:H2'	1:X:2493:U:C6	2.48	0.47
1:X:2798:A:C5	1:X:2799:C:C5	3.02	0.47
1:X:824:U:H2'	10:I:30:ALA:H	1.78	0.47
4:B:38:THR:HG22	4:B:40:GLN:H	1.79	0.47
1:X:2614:A:O2'	4:B:48:GLN:NE2	2.47	0.47
7:E:56:SER:OG	7:E:61:HIS:ND1	2.26	0.47
11:J:82:THR:HG23	11:J:84:MET:H	1.79	0.47
17:P:94:GLU:HG3	17:P:127:ILE:HB	1.96	0.47
18:Q:31:PRO:HA	18:Q:76:LYS:HB2	1.97	0.47
1:X:125:A:H5''	1:X:126:C:O4'	2.14	0.47
1:X:1357:U:H4'	1:X:1397:A:C6	2.49	0.47
1:X:1988:A:H5''	1:X:1989:C:OP2	2.14	0.47
3:A:198:ASN:ND2	3:A:198:ASN:O	2.48	0.47
3:A:96:HIS:HB2	3:A:102:LYS:NZ	2.29	0.47
1:X:1976:U:H5''	4:B:128:SER:HB3	1.96	0.47
5:C:43:ALA:HB3	5:C:86:PRO:HB2	1.96	0.47
21:T:38:VAL:HG21	21:T:45:PHE:CE1	2.50	0.47
1:X:1348:C:H2'	1:X:1349:A:C8	2.49	0.47
1:X:1854:G:H1	1:X:1863:U:H3	1.62	0.47
1:X:2382:C:N4	1:X:2393:G:H1	2.11	0.47
1:X:2477:C:H5'	1:X:2477:C:H6	1.79	0.47
1:X:557:U:O4	1:X:560:G:N2	2.47	0.47
1:X:1884:A:OP2	3:A:252:LYS:HE3	2.14	0.47
5:C:3:GLN:HB2	5:C:116:LYS:HZ2	1.79	0.47
5:C:58:MET:HE2	5:C:59:TYR:HB2	1.97	0.47
8:G:162:LYS:N	8:G:163:PRO:HD2	2.30	0.47
11:J:137:VAL:HG11	20:S:71:MET:SD	2.55	0.47
19:R:59:LYS:HD2	19:R:62:MET:HG3	1.96	0.47
20:S:122:ILE:HB	20:S:123:VAL:H	1.58	0.47
20:S:25:ASN:OD1	20:S:27:GLU:HB2	2.14	0.47
1:X:1779:C:H2'	1:X:1780:A:H8	1.78	0.47
1:X:2826:C:H2'	1:X:2827:G:O4'	2.15	0.47
1:X:2860:C:H2'	1:X:2861:A:O4'	2.14	0.47
1:X:2871:U:H2'	1:X:2872:U:C6	2.49	0.47
1:X:830:C:O2'	1:X:852:U:H5''	2.15	0.47
4:B:188:ILE:HG12	4:B:189:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:18:PRO:HD2	5:C:109:ALA:HB2	1.96	0.47
5:C:25:GLY:HA3	10:I:18:ARG:NH1	2.30	0.47
11:J:46:ASN:C	11:J:48:ILE:H	2.17	0.47
11:J:8:THR:HG23	11:J:70:PHE:HE2	1.79	0.47
13:L:27:LEU:C	13:L:87:VAL:HG13	2.35	0.47
17:P:59:PHE:CG	25:Z:30:LEU:HD21	2.50	0.47
18:Q:53:ILE:HD13	18:Q:80:VAL:HG13	1.97	0.47
22:U:31:GLY:HA2	22:U:32:ARG:HE	1.80	0.47
1:X:1260:A:C6	1:X:1262:U:C2	3.02	0.47
1:X:1283:C:H5''	1:X:1284:G:C5'	2.44	0.47
1:X:1348:C:H4'	18:Q:64:ARG:HH12	1.79	0.47
1:X:1399:C:OP2	1:X:1409:U:N3	2.46	0.47
1:X:1494:G:H2'	1:X:1495:G:H8	1.78	0.47
1:X:1785:A:H2'	1:X:1786:C:H6	1.79	0.47
1:X:1746:A:H2	1:X:2696:A:H1'	1.80	0.47
1:X:485:G:C6	1:X:520:C:N4	2.83	0.47
1:X:788:G:C4	1:X:807:A:C8	3.02	0.47
1:X:792:U:OP1	3:A:48:ARG:HA	2.14	0.47
1:X:87:G:C2'	1:X:88:G:H5''	2.43	0.47
3:A:108:PRO:HG2	3:A:111:LEU:HB2	1.95	0.47
4:B:96:PHE:CD2	4:B:102:ILE:HG21	2.48	0.47
5:C:5:ASN:N	5:C:5:ASN:OD1	2.47	0.47
9:H:17:ARG:H	9:H:58:ALA:HA	1.78	0.47
10:I:107:LYS:HG3	10:I:125:ALA:HA	1.96	0.47
12:K:98:LEU:HA	12:K:98:LEU:HD13	1.60	0.47
21:T:38:VAL:HG21	21:T:45:PHE:CZ	2.49	0.47
1:X:1349:A:H2'	1:X:1350:G:H8	1.79	0.47
1:X:340:G:O4'	1:X:488:A:H1'	2.15	0.47
1:X:597:U:H2'	1:X:598:U:C6	2.49	0.47
1:X:836:G:H2'	1:X:837:U:C6	2.49	0.47
2:Y:36:A:N6	2:Y:46:G:H2'	2.29	0.47
1:X:875:G:O2'	2:Y:80:A:N3	2.47	0.47
3:A:246:PRO:CD	3:A:251:GLY:H	2.21	0.47
4:B:37:LYS:HD2	4:B:42:ASP:OD1	2.14	0.47
8:G:116:ARG:NH1	8:G:126:VAL:HG13	2.29	0.47
8:G:55:ALA:C	8:G:134:MET:HE1	2.35	0.47
10:I:102:LYS:C	10:I:104:ARG:H	2.18	0.47
14:M:55:ILE:O	14:M:103:LYS:O	2.32	0.47
15:N:45:TYR:O	15:N:49:ASP:HB2	2.15	0.47
19:R:29:HIS:CG	19:R:51:VAL:HG22	2.50	0.47
19:R:45:LYS:HA	19:R:76:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:137:VAL:HG21	20:S:71:MET:SD	2.54	0.47
1:X:2258:G:O6	21:T:14:ARG:HG3	2.15	0.47
1:X:1330:G:O6	1:X:1349:A:N6	2.48	0.47
1:X:1437:A:H2'	1:X:1438:G:C8	2.49	0.47
1:X:2067:U:H2'	1:X:2068:C:C6	2.49	0.47
1:X:2084:G:H1	1:X:2171:U:H3	1.62	0.47
1:X:105:G:H21	1:X:357:A:H61	1.62	0.47
1:X:474:G:N2	1:X:476:G:H3'	2.30	0.47
1:X:239:A:H5''	1:X:621:U:H5'	1.96	0.47
1:X:652:C:H42	1:X:657:A:H61	1.63	0.47
1:X:865:A:H2'	1:X:866:U:C6	2.50	0.47
4:B:84:PHE:O	4:B:86:PRO:HD3	2.14	0.47
7:E:94:PHE:HB3	7:E:107:ILE:HG22	1.95	0.47
8:G:55:ALA:HB1	8:G:134:MET:HE1	1.97	0.47
13:L:33:ARG:NH2	13:L:103:LEU:HB2	2.29	0.47
16:O:39:PHE:HE2	16:O:46:VAL:HB	1.78	0.47
19:R:15:HIS:CD2	19:R:15:HIS:H	2.33	0.47
1:X:1219:C:H2'	1:X:1220:G:O4'	2.14	0.47
1:X:1631:C:O2	1:X:1631:C:H2'	2.15	0.47
1:X:1850:G:HO2'	1:X:1851:A:H8	1.61	0.47
1:X:1975:G:O2'	1:X:1976:U:OP2	2.24	0.47
1:X:2171:U:H4'	1:X:2171:U:OP1	2.15	0.47
1:X:2284:U:H3'	1:X:2286:G:N2	2.29	0.47
1:X:2537:C:H2'	1:X:2538:C:O4'	2.14	0.47
1:X:37:C:O2'	5:C:44:SER:HB3	2.15	0.47
1:X:768:U:H2'	1:X:769:C:O4'	2.15	0.47
1:X:876:A:O2'	1:X:877:G:H5'	2.14	0.47
2:Y:80:A:H2'	2:Y:81:C:O4'	2.15	0.47
28:3:26:LYS:HG2	28:3:43:GLY:O	2.15	0.47
8:G:63:ARG:HA	8:G:144:MET:HE1	1.97	0.47
1:X:1669:A:OP1	12:K:9:LYS:HE2	2.15	0.47
1:X:1757:C:O2'	1:X:1758:C:H5'	2.15	0.47
1:X:17:G:H2'	1:X:18:U:C6	2.50	0.47
1:X:187:U:H2'	1:X:188:G:C8	2.50	0.47
1:X:2817:A:H2'	1:X:2818:G:O4'	2.15	0.47
1:X:321:A:N6	1:X:323:G:N3	2.63	0.47
1:X:353:G:H2'	1:X:354:C:C6	2.50	0.47
1:X:39:C:H1'	5:C:42:THR:HG21	1.96	0.47
1:X:469:G:H3'	27:2:39:ARG:O	2.14	0.47
3:A:163:VAL:HG22	3:A:177:LEU:HA	1.97	0.47
5:C:112:GLN:HE22	5:C:116:LYS:HZ2	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:825:C:H5''	10:I:30:ALA:CB	2.45	0.47
11:J:62:GLY:N	11:J:63:GLY:HA2	2.30	0.47
19:R:61:SER:HA	19:R:65:PRO:HG3	1.97	0.47
20:S:3:LEU:HB3	20:S:56:VAL:HA	1.96	0.47
1:X:2367:A:N7	1:X:2368:G:C6	2.83	0.47
1:X:2660:C:C2	1:X:2704:U:O4	2.68	0.47
1:X:2769:C:H1'	1:X:2866:A:H2	1.79	0.47
25:Z:40:LYS:HD3	25:Z:46:CYS:HB2	1.97	0.47
6:D:111:ILE:HG22	6:D:114:PHE:HB2	1.96	0.46
4:B:183:LEU:HD21	14:M:16:ILE:HG12	1.97	0.46
14:M:57:ILE:HD12	14:M:57:ILE:H	1.81	0.46
22:U:20:ARG:HB2	22:U:20:ARG:HE	1.47	0.46
1:X:757:U:H2'	1:X:758:G:O4'	2.14	0.46
3:A:188:GLU:H	3:A:188:GLU:HG2	1.42	0.46
3:A:63:ARG:HG3	3:A:85:ASP:OD1	2.15	0.46
8:G:65:LYS:NZ	15:N:70:ARG:HD2	2.30	0.46
1:X:494:A:O4'	19:R:56:LYS:HB2	2.14	0.46
20:S:95:SER:HB3	20:S:119:ASN:HB3	1.97	0.46
23:V:62:ARG:O	23:V:66:GLN:N	2.45	0.46
1:X:2265:A:OP1	26:1:31:THR:OG1	2.21	0.46
1:X:956:A:C4	1:X:2427:A:C2	3.03	0.46
3:A:245:VAL:HB	3:A:249:PRO:HA	1.97	0.46
3:A:91:ARG:O	3:A:107:ALA:N	2.33	0.46
6:D:104:ILE:HG12	6:D:108:LEU:HD12	1.98	0.46
11:J:54:VAL:HG21	11:J:125:LYS:HE3	1.97	0.46
15:N:102:GLU:HA	15:N:103:PRO:HD3	1.69	0.46
21:T:47:ALA:HB1	21:T:51:VAL:HB	1.96	0.46
1:X:1584:G:H4'	3:A:59:LYS:HG3	1.97	0.46
1:X:1673:C:H2'	1:X:1674:C:H6	1.80	0.46
1:X:1802:A:H2'	1:X:1803:G:O4'	2.15	0.46
1:X:1827:G:H1	1:X:1888:C:H42	1.63	0.46
1:X:2394:G:C2	1:X:2395:C:C2	3.03	0.46
1:X:2629:U:H2'	1:X:2630:C:H6	1.81	0.46
1:X:32:C:O2'	1:X:33:C:H5'	2.16	0.46
1:X:538:A:HO2'	1:X:539:A:P	2.34	0.46
1:X:811:G:OP2	5:C:56:ARG:HG2	2.15	0.46
2:Y:51:G:OP1	13:L:99:ARG:N	2.41	0.46
4:B:14:ILE:HA	14:M:20:HIS:CD2	2.49	0.46
6:D:112:ARG:CZ	6:D:137:ILE:HG22	2.46	0.46
7:E:34:THR:OG1	7:E:34:THR:O	2.34	0.46
11:J:79:PRO:CD	11:J:88:LYS:HD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:20:ARG:HD2	22:U:43:ARG:NE	2.30	0.46
1:X:1609:G:H2'	1:X:1610:A:O4'	2.16	0.46
1:X:1761:G:C5	1:X:1762:C:C5	3.03	0.46
1:X:224:G:H4'	1:X:399:G:C6	2.50	0.46
1:X:623:G:H21	1:X:626:A:H2	1.61	0.46
2:Y:14:C:H4'	2:Y:17:A:H62	1.79	0.46
9:H:134:LEU:HA	9:H:134:LEU:HD23	1.78	0.46
11:J:20:GLY:O	11:J:99:LYS:HG2	2.16	0.46
15:N:66:ASN:HD22	15:N:70:ARG:HH12	1.63	0.46
18:Q:4:TYR:CE2	23:V:23:LYS:HB2	2.51	0.46
19:R:81:VAL:HG12	19:R:82:ALA:N	2.30	0.46
27:2:28:ARG:HD2	27:2:28:ARG:HA	1.75	0.46
3:A:117:VAL:HG13	3:A:129:ASN:HD22	1.80	0.46
4:B:188:ILE:HG12	4:B:189:PRO:CD	2.46	0.46
6:D:133:LYS:O	6:D:151:GLY:HA3	2.15	0.46
1:X:1046:U:C5'	7:E:59:GLN:HG2	2.45	0.46
9:H:2:ILE:HB	9:H:45:ALA:HB3	1.97	0.46
17:P:44:VAL:HG21	25:Z:27:ALA:HB2	1.98	0.46
19:R:18:LYS:HD3	19:R:18:LYS:H	1.79	0.46
19:R:61:SER:HA	19:R:65:PRO:HB3	1.97	0.46
1:X:1925:C:H2'	1:X:1926:U:C5	2.50	0.46
1:X:2309:G:H2'	1:X:2310:G:O4'	2.15	0.46
1:X:2663:U:H3	1:X:2705:A:N6	2.09	0.46
1:X:2707:G:H2'	1:X:2708:U:C6	2.50	0.46
1:X:670:U:H2'	1:X:671:A:C8	2.50	0.46
1:X:753:U:H2'	1:X:754:G:H8	1.80	0.46
2:Y:46:G:H1'	2:Y:49:C:N4	2.31	0.46
26:1:42:PRO:HG3	26:1:50:PHE:CE1	2.51	0.46
3:A:244:ARG:NH1	3:A:253:PRO:HG3	2.31	0.46
7:E:90:ARG:CZ	7:E:163:ARG:HD2	2.46	0.46
8:G:140:GLN:O	8:G:143:ALA:HB3	2.15	0.46
1:X:1004:A:N3	16:O:88:GLN:NE2	2.63	0.46
1:X:1104:G:H1'	1:X:1110:G:N2	2.31	0.46
1:X:1231:A:C2	1:X:1245:G:C2	3.04	0.46
1:X:1349:A:H2'	1:X:1350:G:C8	2.50	0.46
1:X:2272:A:P	13:L:15:ARG:HH21	2.38	0.46
1:X:388:G:H2'	1:X:389:G:C8	2.51	0.46
1:X:529:U:H2'	1:X:530:G:H8	1.80	0.46
1:X:568:G:H2'	1:X:569:C:O4'	2.16	0.46
27:2:18:PHE:H	27:2:44:VAL:CG2	2.29	0.46
3:A:218:LYS:HD2	3:A:218:LYS:HA	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:42:VAL:HA	8:G:166:LEU:O	2.16	0.46
8:G:170:PRO:O	8:G:171:LEU:HB2	2.15	0.46
13:L:15:ARG:HA	13:L:15:ARG:HD3	1.70	0.46
16:O:36:LYS:NZ	16:O:56:VAL:HG13	2.31	0.46
16:O:67:LYS:HG3	16:O:68:LYS:N	2.30	0.46
1:X:1361:G:H2'	1:X:1362:A:C8	2.51	0.46
1:X:1606:C:N4	1:X:1607:A:H62	2.14	0.46
1:X:162:C:H2'	1:X:163:A:C8	2.51	0.46
1:X:2057:U:H2'	1:X:2058:U:C6	2.51	0.46
1:X:20:C:H2'	1:X:21:A:C8	2.50	0.46
1:X:2363:G:H8	1:X:2363:G:OP2	1.99	0.46
1:X:2474:G:H2'	1:X:2475:C:O4'	2.16	0.46
1:X:742:G:C5	3:A:208:LYS:HB3	2.50	0.46
2:Y:16:U:HO2'	2:Y:17:A:P	2.39	0.46
2:Y:70:C:H2'	2:Y:71:G:O4'	2.15	0.46
2:Y:77:G:H1'	20:S:22:VAL:HG21	1.97	0.46
9:H:23:ARG:HG3	9:H:24:VAL:N	2.31	0.46
13:L:8:ARG:HG3	13:L:9:ARG:N	2.30	0.46
1:X:1583:A:H2	3:A:31:LYS:HE2	1.80	0.46
1:X:1845:A:N3	1:X:2212:U:O2'	2.43	0.46
1:X:1987:G:C5	1:X:1988:A:C8	3.04	0.46
1:X:2448:A:H2'	1:X:2449:G:O4'	2.16	0.46
1:X:2845:C:C4	1:X:2846:G:N7	2.84	0.46
1:X:464:G:H2'	1:X:465:C:C6	2.51	0.46
1:X:627:A:H2'	1:X:628:A:H8	1.78	0.46
27:2:1:MET:HG3	27:2:3:ARG:HH12	1.80	0.46
27:2:21:ARG:HE	27:2:43:THR:HG21	1.81	0.46
9:H:29:ILE:CG2	9:H:122:ARG:HB2	2.44	0.46
13:L:20:THR:HG21	13:L:23:ALA:HB3	1.97	0.46
1:X:18:U:O2'	15:N:23:GLY:HA2	2.16	0.46
15:N:62:ILE:HG23	15:N:76:TYR:CE1	2.51	0.46
17:P:89:ARG:HD3	17:P:132:GLY:HA2	1.98	0.46
18:Q:66:GLY:HA3	18:Q:68:PHE:CD2	2.51	0.46
1:X:1439:G:H2'	1:X:1440:G:C8	2.51	0.46
1:X:1494:G:C4	1:X:1495:G:C8	3.04	0.46
1:X:1710:U:H5''	1:X:1711:C:H5	1.81	0.46
1:X:2039:G:C2	1:X:2040:A:C8	3.04	0.46
1:X:2200:G:H2'	1:X:2201:G:H8	1.80	0.46
1:X:2707:G:H2'	1:X:2708:U:H6	1.81	0.46
1:X:2796:A:H2'	1:X:2797:G:C8	2.47	0.46
1:X:334:G:OP1	1:X:349:G:N2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:78:A:H2'	2:Y:79:U:O4'	2.16	0.46
6:D:112:ARG:HD2	6:D:112:ARG:N	2.31	0.45
9:H:11:ALA:O	9:H:111:PHE:N	2.41	0.45
1:X:1407:G:C6	1:X:1408:A:N6	2.84	0.45
1:X:2197:U:H5'	1:X:2198:U:OP1	2.16	0.45
1:X:2447:G:OP1	11:J:120:ARG:NH2	2.49	0.45
1:X:78:C:O2'	1:X:357:A:N3	2.46	0.45
1:X:562:G:C6	1:X:563:U:C4	3.04	0.45
1:X:732:G:H2'	1:X:733:G:C8	2.51	0.45
1:X:750:C:H2'	1:X:751:G:H5'	1.98	0.45
1:X:849:G:C5	1:X:850:C:C4	3.04	0.45
3:A:222:ARG:HH11	3:A:225:ALA:HB2	1.81	0.45
7:E:45:GLN:NE2	7:E:48:ASP:O	2.48	0.45
7:E:69:ARG:HH21	7:E:73:ALA:HB2	1.81	0.45
8:G:66:HIS:CD2	15:N:71:LEU:HD13	2.51	0.45
1:X:2229:G:C6	11:J:83:ARG:HG2	2.52	0.45
1:X:1008:G:H5'	15:N:93:LYS:HG3	1.98	0.45
1:X:1459:U:O2	1:X:1475:U:H5''	2.15	0.45
1:X:1715:A:C8	1:X:1717:A:O4'	2.70	0.45
1:X:1981:A:O2'	1:X:2704:U:O2'	2.23	0.45
1:X:2468:G:C6	1:X:2469:G:C6	3.05	0.45
1:X:2495:G:O2'	1:X:2496:C:H5'	2.16	0.45
1:X:746:G:C8	1:X:774:A:C6	3.04	0.45
1:X:938:G:H2'	1:X:940:G:N7	2.32	0.45
25:Z:58:LEU:HG	25:Z:58:LEU:O	2.16	0.45
28:3:13:ARG:HD2	28:3:24:ALA:HA	1.98	0.45
9:H:3:MET:O	9:H:6:SER:HB3	2.16	0.45
10:I:75:VAL:HG22	10:I:99:VAL:HG21	1.97	0.45
11:J:6:LYS:HB3	11:J:6:LYS:HE2	1.69	0.45
19:R:96:LYS:O	19:R:104:VAL:HA	2.16	0.45
1:X:1745:C:C5	1:X:1746:A:C5	3.04	0.45
1:X:2262:C:OP1	26:1:7:ARG:NH1	2.48	0.45
1:X:2422:C:H2'	1:X:2423:G:H8	1.81	0.45
1:X:66:U:H2'	1:X:67:G:H8	1.82	0.45
2:Y:27:A:HO2'	2:Y:28:A:P	2.38	0.45
1:X:2594:U:N1	25:Z:7:PRO:HA	2.31	0.45
3:A:169:GLU:N	3:A:172:TYR:O	2.34	0.45
3:A:169:GLU:OE2	3:A:184:ARG:NH1	2.49	0.45
3:A:96:HIS:NE2	3:A:97:TYR:O	2.49	0.45
5:C:191:ALA:HA	5:C:194:GLU:HB2	1.99	0.45
9:H:29:ILE:HB	9:H:123:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:25:ALA:HB1	12:K:48:VAL:HG23	1.99	0.45
17:P:89:ARG:HG2	17:P:131:LYS:H	1.81	0.45
18:Q:8:GLN:O	23:V:29:ARG:HD2	2.16	0.45
1:X:1121:G:H2'	1:X:1122:A:C8	2.52	0.45
1:X:1164:C:H2'	1:X:1165:G:O4'	2.17	0.45
1:X:1781:C:OP1	3:A:219:PRO:HB2	2.16	0.45
1:X:1922:U:H5''	1:X:1922:U:O2	2.16	0.45
1:X:2058:U:H2'	1:X:2217:G:N2	2.32	0.45
1:X:2401:A:N3	1:X:2401:A:H2'	2.31	0.45
1:X:2442:C:H2'	1:X:2443:C:C6	2.52	0.45
1:X:2662:C:H2'	1:X:2663:U:C6	2.52	0.45
1:X:400:U:H4'	1:X:401:G:O5'	2.16	0.45
1:X:764:A:C6	1:X:802:A:C5	3.04	0.45
25:Z:51:TYR:CE1	25:Z:55:ARG:HG2	2.52	0.45
27:2:4:THR:OG1	27:2:4:THR:O	2.34	0.45
4:B:32:PRO:O	4:B:49:ILE:HA	2.17	0.45
4:B:5:LEU:H	4:B:5:LEU:HD12	1.80	0.45
1:X:1374:G:N2	1:X:1384:G:H1'	2.31	0.45
1:X:824:U:H1'	1:X:1264:C:O4'	2.15	0.45
26:1:28:ARG:O	26:1:33:ALA:HB2	2.17	0.45
3:A:96:HIS:CE1	3:A:100:GLY:HA2	2.47	0.45
7:E:57:ASP:HB3	7:E:62:ARG:HH11	1.82	0.45
1:X:969:U:O4'	11:J:17:ARG:NH1	2.50	0.45
13:L:97:HIS:HB3	13:L:98:GLY:H	1.60	0.45
17:P:114:ALA:O	17:P:115:ASN:ND2	2.43	0.45
1:X:999:A:OP1	24:W:7:ARG:HD3	2.16	0.45
1:X:1007:A:H2'	1:X:1008:G:C8	2.44	0.45
1:X:1008:G:C2	1:X:1009:C:C5	3.05	0.45
1:X:1227:A:H4'	1:X:1252:C:H4'	1.98	0.45
1:X:1462:C:H2'	1:X:1463:A:C8	2.52	0.45
1:X:1935:A:C6	1:X:1936:A:N1	2.85	0.45
1:X:2255:G:H2'	1:X:2256:G:H8	1.82	0.45
1:X:2576:G:C6	1:X:2577:A:N6	2.84	0.45
1:X:88:G:C3'	1:X:89:A:H5''	2.45	0.45
27:2:17:GLY:O	27:2:21:ARG:HG2	2.17	0.45
28:3:29:LYS:HD2	28:3:33:ASN:O	2.17	0.45
4:B:137:ARG:HG3	4:B:138:PRO:HD2	1.99	0.45
5:C:97:ARG:O	5:C:100:ARG:HG2	2.15	0.45
10:I:31:GLY:HA2	10:I:34:HIS:HB2	1.99	0.45
11:J:124:HIS:CD2	11:J:124:HIS:H	2.34	0.45
15:N:92:ARG:CA	15:N:95:LEU:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:35:PRO:HB2	17:P:39:ARG:NH1	2.32	0.45
17:P:75:ALA:HB2	17:P:126:ILE:HG23	1.98	0.45
1:X:111:G:H8	1:X:111:G:OP2	2.00	0.45
1:X:1050:G:H1	1:X:1127:C:H42	1.64	0.45
1:X:1330:G:C6	1:X:1349:A:C6	3.05	0.45
1:X:177:U:O2'	1:X:178:C:O4'	2.35	0.45
1:X:2067:U:H2'	1:X:2068:C:H6	1.82	0.45
1:X:2309:G:N2	1:X:2365:U:C2	2.85	0.45
1:X:2371:A:C4	1:X:2408:G:C6	3.05	0.45
1:X:2014:A:C6	1:X:2477:C:H1'	2.52	0.45
1:X:746:G:N7	1:X:774:A:C5	2.85	0.45
27:2:1:MET:HG3	27:2:3:ARG:CZ	2.46	0.45
28:3:11:LYS:HD2	28:3:11:LYS:N	2.32	0.45
3:A:143:HIS:CD2	3:A:196:VAL:HG13	2.52	0.45
3:A:200:GLU:HG3	3:A:202:LYS:HG3	1.97	0.45
3:A:85:ASP:CG	3:A:92:ILE:HD12	2.37	0.45
3:A:89:SER:O	3:A:159:ALA:HB2	2.17	0.45
1:X:2033:C:H1'	4:B:156:MET:CE	2.47	0.45
10:I:32:ARG:HH22	10:I:34:HIS:CE1	2.34	0.45
11:J:35:LEU:HD12	11:J:131:LYS:O	2.17	0.45
1:X:1189:G:H2'	1:X:1190:C:C6	2.51	0.45
1:X:1652:G:H2'	1:X:1653:C:H6	1.82	0.45
1:X:1818:G:OP1	3:A:224:SER:OG	2.27	0.45
1:X:1949:A:H1'	1:X:2572:U:C5'	2.47	0.45
1:X:2727:G:O6	1:X:2735:C:H5''	2.17	0.45
1:X:750:C:C2'	1:X:751:G:H5'	2.47	0.45
1:X:2340:C:O5'	28:3:27:SER:OG	2.35	0.45
7:E:107:ILE:HD11	7:E:151:VAL:HG12	1.99	0.45
8:G:97:ASP:O	8:G:99:VAL:HG23	2.16	0.45
11:J:46:ASN:HA	11:J:49:GLU:HB2	1.99	0.45
1:X:2579:A:O2'	1:X:2580:C:H5'	2.16	0.45
1:X:2754:C:H2'	1:X:2755:A:O4'	2.17	0.45
1:X:2827:G:H2'	1:X:2828:C:O4'	2.17	0.45
1:X:469:G:H22	1:X:480:G:H2'	1.82	0.45
1:X:481:A:C6	1:X:482:A:C6	3.05	0.45
1:X:603:C:H2'	1:X:604:U:H6	1.82	0.45
1:X:920:G:P	11:J:24:GLY:HA3	2.57	0.45
1:X:938:G:O2'	1:X:939:C:P	2.75	0.45
1:X:978:U:H2'	1:X:979:A:C8	2.52	0.45
1:X:1517:C:H4'	3:A:96:HIS:CE1	2.52	0.45
8:G:88:VAL:HG21	8:G:127:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:35:SER:OG	13:L:36:LYS:N	2.50	0.45
13:L:8:ARG:HB2	13:L:8:ARG:CZ	2.46	0.45
14:M:32:THR:HG22	14:M:93:ILE:HA	1.99	0.45
16:O:36:LYS:HZ1	16:O:56:VAL:HG13	1.82	0.45
18:Q:6:ILE:HG22	18:Q:7:LEU:HD13	1.99	0.45
20:S:153:LYS:HA	20:S:153:LYS:HD3	1.79	0.45
21:T:66:LYS:HB3	21:T:66:LYS:HE2	1.78	0.45
1:X:1398:G:O2'	1:X:1399:C:O5'	2.34	0.45
1:X:1692:C:N4	1:X:1976:U:O4'	2.49	0.45
1:X:2662:C:H2'	1:X:2663:U:H6	1.81	0.45
1:X:2691:C:O2'	1:X:2692:A:P	2.75	0.45
1:X:389:G:H2'	1:X:390:U:C6	2.52	0.45
1:X:481:A:N3	1:X:481:A:H2'	2.32	0.45
1:X:576:A:H4'	1:X:821:A:OP1	2.16	0.45
2:Y:5:C:H2'	2:Y:6:C:O4'	2.16	0.45
1:X:1786:C:O2	3:A:252:LYS:HD2	2.17	0.44
3:A:31:LYS:HE3	3:A:32:ALA:H	1.82	0.44
5:C:177:VAL:HB	5:C:178:TYR:H	1.59	0.44
8:G:118:ALA:O	8:G:121:LYS:HB3	2.17	0.44
8:G:67:ARG:HD3	8:G:70:PHE:HA	1.99	0.44
8:G:84:ASN:C	8:G:86:ALA:H	2.20	0.44
9:H:75:VAL:HG22	9:H:96:ALA:HA	1.98	0.44
9:H:83:ARG:HG2	14:M:40:ARG:HH22	1.83	0.44
12:K:75:VAL:O	12:K:79:VAL:HG13	2.17	0.44
13:L:11:LEU:HA	13:L:14:ARG:NH1	2.32	0.44
13:L:27:LEU:HD13	13:L:87:VAL:HG22	1.99	0.44
18:Q:60:GLY:HA3	18:Q:73:ASN:H	1.81	0.44
19:R:84:VAL:HG11	19:R:90:LYS:N	2.23	0.44
1:X:2344:G:H4'	21:T:60:PHE:CE1	2.52	0.44
22:U:42:GLN:OE1	22:U:42:GLN:N	2.51	0.44
1:X:1287:A:N1	1:X:1661:C:O2'	2.34	0.44
1:X:1479:G:H2'	1:X:1480:G:H8	1.81	0.44
1:X:1552:C:O2	1:X:1553:G:N2	2.50	0.44
1:X:1778:U:H2'	1:X:1779:C:H6	1.82	0.44
1:X:2398:U:H4'	26:I:13:GLU:OE1	2.17	0.44
1:X:2543:A:C6	1:X:2544:A:N1	2.85	0.44
1:X:854:G:N2	1:X:948:C:N3	2.58	0.44
2:Y:64:C:H2'	2:Y:65:A:H8	1.82	0.44
3:A:121:PRO:HA	3:A:132:PRO:HD2	1.98	0.44
6:D:106:ILE:HG21	6:D:139:PRO:HB3	1.99	0.44
1:X:596:C:N4	10:I:36:GLY:HA3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:37:ALA:O	11:J:100:PRO:HA	2.17	0.44
11:J:39:GLU:HA	11:J:40:PRO:HD3	1.86	0.44
14:M:107:LEU:HA	14:M:107:LEU:HD23	1.73	0.44
17:P:106:LEU:O	17:P:106:LEU:HD23	2.17	0.44
1:X:934:G:H1'	21:T:26:PHE:CD1	2.52	0.44
1:X:1032:A:H62	1:X:1151:U:H3	1.65	0.44
1:X:1658:A:H2'	1:X:1659:G:O4'	2.17	0.44
1:X:2339:A:P	28:3:49:VAL:HG11	2.57	0.44
1:X:2396:C:H2'	1:X:2397:A:O4'	2.17	0.44
1:X:2526:U:C4	1:X:2545:A:N7	2.85	0.44
1:X:2630:C:H2'	1:X:2631:C:C6	2.52	0.44
1:X:353:G:H2'	1:X:354:C:H6	1.82	0.44
2:Y:63:A:H2'	2:Y:64:C:C6	2.53	0.44
28:3:30:ARG:HB3	28:3:31:HIS:ND1	2.33	0.44
5:C:129:LYS:C	5:C:131:LYS:H	2.16	0.44
12:K:59:ASP:N	12:K:59:ASP:OD2	2.51	0.44
13:L:88:VAL:HG12	13:L:89:PHE:H	1.82	0.44
1:X:1212:U:H2'	1:X:1213:U:H6	1.81	0.44
1:X:1353:A:H2'	18:Q:56:MET:SD	2.57	0.44
1:X:1430:G:H2'	1:X:1431:U:C6	2.52	0.44
1:X:1713:G:C5	1:X:1714:A:C8	3.06	0.44
1:X:2024:U:H2'	1:X:2025:A:O4'	2.18	0.44
1:X:2701:A:H2'	1:X:2702:G:O4'	2.16	0.44
1:X:2848:A:N3	12:K:7:GLY:N	2.61	0.44
1:X:321:A:N1	1:X:323:G:H1'	2.32	0.44
1:X:75:C:H2'	1:X:76:C:C6	2.52	0.44
2:Y:11:G:OP1	13:L:28:ARG:NH1	2.50	0.44
25:Z:41:LEU:HA	25:Z:41:LEU:HD13	1.70	0.44
3:A:23:GLY:HA3	3:A:205:VAL:HG11	1.99	0.44
3:A:39:LYS:HA	3:A:39:LYS:HD2	1.66	0.44
4:B:173:VAL:HG23	4:B:185:LYS:HB2	1.98	0.44
5:C:122:GLY:O	5:C:125:ILE:HB	2.18	0.44
8:G:104:THR:OG1	8:G:105:GLY:N	2.48	0.44
12:K:43:GLU:O	12:K:46:PRO:HD2	2.17	0.44
15:N:50:ARG:HA	15:N:53:LYS:HD3	1.99	0.44
20:S:36:ARG:HH21	20:S:78:PRO:HD2	1.83	0.44
1:X:1727:C:H2'	1:X:1728:A:H8	1.81	0.44
1:X:1847:G:H2'	1:X:1848:U:C6	2.52	0.44
1:X:1919:A:OP2	1:X:1944:C:N4	2.46	0.44
1:X:2633:A:N1	1:X:2644:A:H5''	2.32	0.44
1:X:433:G:N2	1:X:434:C:H1'	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:490:A:H1'	1:X:491:A:H5''	2.00	0.44
1:X:836:G:C5	1:X:837:U:C5	3.05	0.44
6:D:128:TYR:HB3	6:D:156:ILE:HB	1.98	0.44
8:G:141:GLY:O	8:G:145:HIS:HD2	2.00	0.44
15:N:27:SER:HB2	15:N:31:GLN:HG3	1.98	0.44
15:N:60:LEU:O	15:N:64:ARG:HG3	2.17	0.44
17:P:45:ILE:HD11	17:P:57:LEU:CD1	2.40	0.44
1:X:2010:G:C6	1:X:2011:U:C4	3.06	0.44
1:X:2529:G:C6	1:X:2530:C:C4	3.06	0.44
1:X:2630:C:H2'	1:X:2631:C:H6	1.83	0.44
1:X:593:C:OP2	15:N:6:THR:OG1	2.36	0.44
2:Y:51:G:H2'	2:Y:52:G:C8	2.53	0.44
2:Y:52:G:C2	2:Y:53:G:C8	3.06	0.44
5:C:60:GLY:C	5:C:62:LYS:H	2.21	0.44
7:E:68:THR:O	7:E:72:VAL:HG23	2.18	0.44
8:G:52:GLY:O	8:G:55:ALA:HB3	2.18	0.44
15:N:61:TRP:O	15:N:65:ILE:HG12	2.17	0.44
16:O:20:ILE:HG13	16:O:21:ARG:N	2.27	0.44
1:X:1316:G:N2	1:X:1317:G:H1'	2.33	0.44
1:X:1919:A:H2	1:X:1926:U:N3	2.15	0.44
1:X:2261:G:H5''	1:X:2262:C:O4'	2.17	0.44
1:X:2545:A:H61	9:H:40:GLY:CA	2.28	0.44
1:X:2595:C:H5''	1:X:2596:C:OP2	2.17	0.44
1:X:2736:U:H4'	1:X:2737:A:OP1	2.18	0.44
1:X:452:G:H2'	1:X:453:U:O4'	2.17	0.44
1:X:1998:A:N3	25:Z:6:VAL:HG23	2.32	0.44
1:X:2265:A:H61	26:1:25:THR:HG21	1.83	0.44
6:D:108:LEU:HD22	6:D:117:ILE:HD11	1.99	0.44
7:E:61:HIS:C	7:E:63:ALA:H	2.21	0.44
1:X:1041:G:OP2	11:J:129:GLN:NE2	2.50	0.44
14:M:27:PHE:HA	14:M:96:ARG:NH2	2.33	0.44
19:R:23:ILE:O	19:R:80:LYS:HB2	2.17	0.44
20:S:96:VAL:O	20:S:119:ASN:HA	2.17	0.44
20:S:70:GLN:CB	20:S:80:HIS:HB3	2.48	0.44
22:U:54:ASN:HD21	22:U:77:GLY:HA2	1.82	0.44
1:X:1018:C:OP2	1:X:1019:U:O2'	2.15	0.44
1:X:1430:G:H2'	1:X:1431:U:H6	1.83	0.44
1:X:1594:U:H2'	1:X:1595:A:C8	2.52	0.44
1:X:21:A:C6	1:X:530:G:C6	3.05	0.44
1:X:2285:U:H2'	1:X:2286:G:H5'	1.98	0.44
1:X:530:G:H2'	1:X:531:G:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:703:A:O2'	1:X:793:G:OP1	2.36	0.44
3:A:29:PRO:HB2	3:A:30:GLU:CD	2.38	0.44
4:B:59:VAL:HG12	4:B:64:GLN:HG3	1.99	0.44
9:H:1:MET:HB2	9:H:44:TYR:HB3	1.98	0.44
9:H:83:ARG:HD2	9:H:89:ILE:HD11	1.99	0.44
23:V:21:ARG:NH1	23:V:53:LEU:HD11	2.33	0.44
1:X:1775:A:H4'	1:X:1776:A:O5'	2.18	0.44
1:X:187:U:H2'	1:X:188:G:H8	1.82	0.44
1:X:2418:A:N1	1:X:2564:U:O2'	2.48	0.44
1:X:2839:G:H2'	1:X:2840:U:C6	2.53	0.44
1:X:386:U:H5'	1:X:436:A:C2	2.52	0.44
1:X:66:U:H2'	1:X:67:G:C8	2.52	0.44
17:P:13:GLN:O	17:P:16:GLN:HG2	2.18	0.44
17:P:41:VAL:O	17:P:44:VAL:HG12	2.18	0.44
18:Q:25:TYR:CZ	18:Q:88:ILE:HG23	2.53	0.44
1:X:1175:A:C2	1:X:1176:U:C2	3.06	0.44
1:X:1193:G:H2'	1:X:1194:U:C6	2.53	0.44
1:X:1652:G:H2'	1:X:1653:C:C6	2.53	0.44
1:X:178:C:P	22:U:40:ARG:CZ	3.06	0.44
1:X:1966:C:H4'	1:X:2585:C:H4'	2.00	0.44
1:X:2399:C:H41	28:3:31:HIS:HB2	1.82	0.44
1:X:2491:C:H2'	1:X:2492:G:O4'	2.18	0.44
1:X:2610:G:N2	1:X:2767:C:O2	2.44	0.44
1:X:312:G:HO2'	1:X:313:U:H6	1.64	0.44
1:X:778:G:H2'	1:X:779:U:H6	1.83	0.44
1:X:998:C:H2'	1:X:999:A:O4'	2.18	0.44
26:1:14:SER:HB2	26:1:23:THR:H	1.82	0.43
26:1:9:ILE:HG22	26:1:30:ASN:OD1	2.17	0.43
4:B:14:ILE:HG12	14:M:20:HIS:NE2	2.32	0.43
5:C:17:LEU:HA	5:C:17:LEU:HD12	1.73	0.43
5:C:50:GLN:NE2	5:C:56:ARG:HH12	2.16	0.43
11:J:13:GLN:HE21	11:J:90:ALA:HB1	1.82	0.43
15:N:92:ARG:HB3	15:N:95:LEU:HB2	2.00	0.43
16:O:35:LEU:HD23	16:O:55:THR:HG22	1.98	0.43
17:P:60:ILE:HA	17:P:61:PRO:HD3	1.45	0.43
1:X:2010:G:H1	1:X:2019:C:H42	1.66	0.43
1:X:2295:C:O2'	6:D:125:ARG:NH2	2.50	0.43
1:X:2609:G:H2'	1:X:2610:G:C8	2.52	0.43
1:X:2812:A:H2'	1:X:2813:G:C8	2.53	0.43
1:X:504:G:H4'	17:P:27:VAL:CG1	2.47	0.43
1:X:518:A:HO2'	1:X:519:C:P	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:14:A:C6	1:X:536:A:C2	3.06	0.43
1:X:556:A:O2'	1:X:557:U:OP2	2.32	0.43
1:X:661:C:O2	1:X:662:G:N2	2.51	0.43
2:Y:16:U:O2'	2:Y:110:U:O2	2.36	0.43
4:B:38:THR:HB	4:B:41:THR:H	1.83	0.43
1:X:814:G:OP1	5:C:50:GLN:HB2	2.17	0.43
5:C:45:THR:HB	5:C:86:PRO:O	2.17	0.43
8:G:36:ASN:HB3	8:G:74:MET:HG3	2.00	0.43
10:I:62:LYS:HB3	28:3:12:ARG:HA	2.00	0.43
13:L:89:PHE:HZ	13:L:100:VAL:HG22	1.83	0.43
1:X:1635:G:O2'	27:2:1:MET:HB2	2.17	0.43
1:X:2069:U:H2'	1:X:2070:G:C8	2.52	0.43
1:X:2222:U:H2'	1:X:2223:U:H6	1.80	0.43
1:X:2787:A:H2'	1:X:2788:C:C6	2.53	0.43
1:X:463:C:P	5:C:46:ARG:HG2	2.59	0.43
1:X:540:G:N1	1:X:2005:U:OP1	2.51	0.43
2:Y:14:C:O5'	21:T:72:LYS:NZ	2.51	0.43
25:Z:19:ARG:O	25:Z:21:SER:N	2.51	0.43
4:B:122:PHE:HE2	4:B:138:PRO:CB	2.30	0.43
10:I:103:ASN:O	10:I:103:ASN:ND2	2.52	0.43
14:M:87:LEU:HD23	14:M:87:LEU:HA	1.61	0.43
1:X:1216:G:C6	1:X:1217:U:C4	3.06	0.43
1:X:1228:G:C6	1:X:1229:C:C4	3.05	0.43
1:X:1672:A:C6	1:X:1673:C:C2	3.06	0.43
1:X:1721:G:H2'	1:X:1722:G:O4'	2.18	0.43
1:X:2758:A:HO2'	1:X:2760:G:HO2'	1.57	0.43
27:2:24:THR:OG1	27:2:25:LYS:N	2.51	0.43
27:2:21:ARG:HD2	27:2:30:ILE:HD12	2.00	0.43
28:3:24:ALA:N	28:3:47:GLY:O	2.37	0.43
3:A:186:HIS:H	3:A:186:HIS:CD2	2.34	0.43
4:B:10:GLY:O	4:B:25:VAL:HG23	2.19	0.43
5:C:97:ARG:HA	5:C:100:ARG:HD3	1.99	0.43
5:C:111:ARG:O	5:C:115:GLY:O	2.37	0.43
6:D:14:PRO:O	6:D:18:GLN:HG2	2.17	0.43
8:G:84:ASN:HD21	8:G:154:GLU:HG2	1.84	0.43
1:X:5:A:O2'	8:G:162:LYS:HE3	2.18	0.43
8:G:67:ARG:HD3	8:G:70:PHE:C	2.39	0.43
9:H:115:ALA:O	9:H:118:LEU:HB2	2.19	0.43
17:P:17:GLN:HG3	17:P:18:VAL:HG23	2.01	0.43
1:X:2169:A:H2'	1:X:2170:C:C6	2.53	0.43
1:X:2077:G:N2	1:X:2179:C:H1'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2504:G:C2	1:X:2518:C:C2	3.07	0.43
1:X:2657:G:H2'	1:X:2658:A:O4'	2.18	0.43
1:X:662:G:H2'	1:X:663:G:O4'	2.19	0.43
3:A:217:ARG:HG2	3:A:218:LYS:HB2	2.00	0.43
10:I:73:GLU:OE2	10:I:104:ARG:HB2	2.18	0.43
12:K:45:ARG:HD3	12:K:95:THR:HG22	2.01	0.43
16:O:64:GLY:HA3	16:O:90:PHE:CZ	2.54	0.43
17:P:45:ILE:HD13	17:P:45:ILE:HG21	1.77	0.43
22:U:63:SER:HB2	22:U:66:ALA:H	1.84	0.43
1:X:125:A:H5''	1:X:126:C:C1'	2.49	0.43
1:X:1507:A:O4'	3:A:99:ASP:HB3	2.18	0.43
1:X:2424:G:O2'	1:X:2425:G:H5'	2.18	0.43
1:X:2576:G:C6	1:X:2577:A:C6	3.07	0.43
1:X:2751:C:H2'	1:X:2752:C:H6	1.84	0.43
1:X:328:A:H2'	1:X:329:C:C6	2.53	0.43
1:X:26:G:H1'	1:X:524:A:N6	2.33	0.43
26:1:9:ILE:HG13	26:1:10:VAL:N	2.34	0.43
26:1:42:PRO:HG3	26:1:50:PHE:HE1	1.82	0.43
28:3:13:ARG:HH12	28:3:49:VAL:CG2	2.32	0.43
8:G:106:TYR:HD1	8:G:106:TYR:HA	1.50	0.43
8:G:67:ARG:CG	8:G:70:PHE:HA	2.49	0.43
8:G:67:ARG:HD3	8:G:70:PHE:O	2.18	0.43
13:L:47:ARG:C	13:L:49:GLN:H	2.20	0.43
19:R:108:VAL:HB	19:R:109:ALA:H	1.66	0.43
1:X:494:A:H5''	19:R:58:VAL:HG22	2.00	0.43
1:X:1586:A:C6	1:X:1587:A:C6	3.07	0.43
1:X:1693:A:C2	1:X:1976:U:H5'	2.53	0.43
1:X:1699:A:C2	1:X:1700:C:C2	3.07	0.43
1:X:1944:C:H2'	1:X:1945:C:O4'	2.18	0.43
1:X:2788:C:H2'	1:X:2789:U:H6	1.84	0.43
1:X:393:U:H2'	1:X:394:U:C6	2.53	0.43
1:X:518:A:N3	1:X:518:A:H5''	2.34	0.43
1:X:608:G:H1'	10:I:21:ARG:CG	2.36	0.43
1:X:661:C:OP1	28:3:19:THR:OG1	2.20	0.43
28:3:9:MET:SD	28:3:59:LYS:HG3	2.58	0.43
3:A:177:LEU:HB3	3:A:178:PRO:HD2	2.00	0.43
4:B:79:ARG:HA	4:B:79:ARG:HD3	1.71	0.43
5:C:3:GLN:HB2	5:C:116:LYS:NZ	2.34	0.43
7:E:76:VAL:HA	7:E:79:VAL:HG22	2.00	0.43
8:G:71:THR:N	8:G:76:GLN:NE2	2.67	0.43
24:W:7:ARG:HB2	24:W:50:LEU:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:116:A:N3	1:X:155:G:H1'	2.34	0.43
1:X:1746:A:H2	1:X:2696:A:O2'	2.00	0.43
1:X:2528:G:C2	1:X:2529:G:N7	2.87	0.43
1:X:694:G:H2'	1:X:695:G:O4'	2.18	0.43
3:A:56:GLY:N	3:A:217:ARG:HB2	2.29	0.43
3:A:223:GLY:HA2	3:A:226:MET:HG3	2.01	0.43
5:C:102:LEU:HD23	5:C:102:LEU:O	2.18	0.43
10:I:43:ALA:O	10:I:45:LYS:HG2	2.17	0.43
11:J:26:ASP:HB2	11:J:68:ARG:HH22	1.84	0.43
15:N:36:PHE:O	15:N:39:LEU:HB2	2.18	0.43
23:V:2:LYS:HB3	23:V:52:GLN:HE22	1.84	0.43
1:X:1954:A:H1'	3:A:240:THR:HA	2.01	0.43
1:X:2033:C:H2'	1:X:2034:A:O4'	2.19	0.43
1:X:2048:C:H2'	1:X:2049:C:C6	2.54	0.43
1:X:2271:C:H2'	1:X:2272:A:C8	2.53	0.43
1:X:618:A:H2'	1:X:619:A:C8	2.54	0.43
1:X:874:A:H2'	1:X:875:G:O4'	2.18	0.43
1:X:914:C:H2'	1:X:915:C:C6	2.54	0.43
1:X:861:G:N3	1:X:944:A:H1'	2.34	0.43
1:X:699:G:C6	27:2:12:ARG:HA	2.53	0.43
4:B:44:TYR:HB2	4:B:82:ARG:NH1	2.34	0.43
1:X:687:G:H21	5:C:68:ARG:NH2	2.15	0.43
19:R:29:HIS:CE1	19:R:51:VAL:HA	2.54	0.43
1:X:1031:C:O2'	1:X:1032:A:OP2	2.33	0.43
1:X:1174:G:H2'	1:X:1175:A:H8	1.84	0.43
1:X:1198:C:OP1	24:W:26:ARG:NH1	2.52	0.43
1:X:1371:G:O2'	1:X:1386:A:N6	2.47	0.43
1:X:1419:G:H2'	1:X:1420:A:C8	2.54	0.43
1:X:1646:G:C5	1:X:1647:U:N3	2.87	0.43
1:X:2442:C:H2'	1:X:2443:C:H6	1.84	0.43
1:X:2681:A:OP1	12:K:73:LYS:NZ	2.52	0.43
1:X:2687:G:H2'	1:X:2688:G:H8	1.83	0.43
1:X:589:C:H2'	1:X:590:C:C6	2.54	0.43
1:X:764:A:C6	1:X:802:A:C6	3.06	0.43
1:X:824:U:C4	10:I:29:THR:HB	2.53	0.43
26:1:16:ALA:HB2	26:1:50:PHE:HA	2.01	0.43
27:2:36:ALA:C	27:2:38:GLY:N	2.73	0.43
4:B:59:VAL:CG1	4:B:64:GLN:HG3	2.49	0.43
6:D:130:LEU:HD23	6:D:130:LEU:HA	1.80	0.43
8:G:103:TYR:HB3	8:G:107:GLN:HG3	2.01	0.43
16:O:23:GLU:HG3	16:O:91:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:23:ILE:HD11	19:R:84:VAL:HG21	2.01	0.43
19:R:77:HIS:CG	19:R:78:ALA:N	2.87	0.43
1:X:1278:A:H2	1:X:1997:A:N6	2.08	0.43
1:X:1495:G:OP1	1:X:1576:G:O2'	2.28	0.43
1:X:1751:A:H2'	1:X:1752:U:C6	2.53	0.43
1:X:1774:A:C2	1:X:2566:A:C5	3.07	0.43
1:X:2000:U:H4'	25:Z:8:LYS:O	2.18	0.43
1:X:2304:G:P	1:X:2304:G:H8	2.41	0.43
1:X:589:C:H4'	15:N:31:GLN:NE2	2.34	0.43
1:X:599:A:O2'	1:X:600:G:H5'	2.19	0.43
3:A:166:GLN:HB2	3:A:174:ILE:HB	2.00	0.42
3:A:250:TRP:N	3:A:250:TRP:CD1	2.87	0.42
1:X:1583:A:C2	3:A:31:LYS:HE2	2.54	0.42
4:B:21:ILE:HG12	4:B:21:ILE:H	1.60	0.42
4:B:31:CYS:HA	4:B:32:PRO:HD3	1.79	0.42
4:B:59:VAL:HG21	4:B:74:PRO:HB3	2.01	0.42
5:C:54:THR:CG2	5:C:72:ARG:HB2	2.46	0.42
10:I:119:THR:HG22	10:I:139:ARG:HB3	2.01	0.42
10:I:14:LYS:HD2	10:I:14:LYS:HA	1.90	0.42
19:R:97:GLN:CB	19:R:101:GLY:HA2	2.49	0.42
1:X:1246:G:C5	1:X:1247:U:C5	3.07	0.42
1:X:1351:G:H2'	1:X:1352:G:C8	2.54	0.42
1:X:1407:G:O6	1:X:1408:A:N6	2.52	0.42
1:X:689:A:H1'	1:X:2422:C:H1'	2.01	0.42
1:X:2863:U:H2'	1:X:2864:C:O4'	2.18	0.42
1:X:661:C:C2	1:X:662:G:N1	2.87	0.42
1:X:760:U:C4	1:X:2592:U:C4	3.06	0.42
1:X:79:G:HO2'	1:X:356:A:H2	1.65	0.42
3:A:31:LYS:HA	3:A:31:LYS:HD2	1.72	0.42
10:I:57:ILE:N	10:I:58:ALA:O	2.52	0.42
1:X:123:A:O5'	27:2:19:ARG:HG2	2.19	0.42
1:X:1370:U:H2'	1:X:1371:G:C8	2.54	0.42
1:X:1544:A:C4	1:X:1560:A:C6	3.08	0.42
1:X:1647:U:H6	1:X:1649:A:OP2	2.02	0.42
1:X:1710:U:H5''	1:X:1711:C:C5	2.54	0.42
1:X:1810:U:H2'	3:A:157:ARG:HD3	2.01	0.42
1:X:2006:G:H4'	1:X:2596:C:O3'	2.19	0.42
1:X:2052:G:C2	1:X:2053:G:C8	3.08	0.42
1:X:2371:A:H2	1:X:2403:C:H42	1.67	0.42
1:X:555:U:H3'	1:X:556:A:H8	1.84	0.42
26:1:8:ILE:H	26:1:8:ILE:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:699:G:C2	27:2:12:ARG:HB2	2.55	0.42
6:D:17:MET:HG2	6:D:22:TYR:CB	2.49	0.42
8:G:67:ARG:O	8:G:70:PHE:CG	2.72	0.42
9:H:68:ASP:O	9:H:70:VAL:HG12	2.19	0.42
10:I:60:LEU:HA	10:I:61:PRO:HD3	1.85	0.42
22:U:27:ASP:OD2	22:U:32:ARG:HG3	2.19	0.42
1:X:1466:C:H2'	1:X:1467:U:H1'	1.99	0.42
1:X:1777:A:C4	1:X:1921:A:C6	3.07	0.42
1:X:1859:A:H2'	1:X:1860:A:C8	2.54	0.42
1:X:500:G:C2	1:X:501:G:H1'	2.54	0.42
1:X:571:U:C2	1:X:581:A:C8	3.07	0.42
1:X:733:G:H2'	1:X:734:G:H8	1.84	0.42
1:X:2328:G:OP2	28:3:42:ARG:HG3	2.18	0.42
4:B:149:ARG:HG3	4:B:150:VAL:N	2.34	0.42
4:B:96:PHE:CE2	4:B:102:ILE:HG21	2.54	0.42
5:C:187:VAL:HG12	5:C:189:ASP:HB2	2.02	0.42
5:C:74:VAL:HG23	5:C:76:THR:H	1.83	0.42
1:X:1630:A:N6	17:P:113:SER:O	2.48	0.42
1:X:1429:A:N3	1:X:1429:A:H2'	2.34	0.42
1:X:1548:U:H2'	1:X:1549:C:C6	2.54	0.42
1:X:1698:C:O2	1:X:1753:A:H2'	2.19	0.42
1:X:1982:C:H5''	1:X:2703:C:O2'	2.19	0.42
1:X:1991:C:H2'	1:X:1992:G:C8	2.53	0.42
1:X:2046:C:O2	1:X:2430:A:C2	2.72	0.42
1:X:2350:G:C2	1:X:2351:G:C5	3.07	0.42
1:X:2664:G:C2'	1:X:2665:G:H5'	2.49	0.42
1:X:2800:C:H3'	1:X:2801:A:H8	1.85	0.42
1:X:320:A:H1'	1:X:340:G:N3	2.33	0.42
1:X:524:A:H2'	1:X:525:A:O4'	2.19	0.42
1:X:859:U:O2'	1:X:860:U:O5'	2.30	0.42
1:X:954:U:OP2	10:I:38:LYS:HG2	2.20	0.42
3:A:109:GLU:OE1	3:A:197:GLY:HA3	2.19	0.42
8:G:65:LYS:HZ3	15:N:70:ARG:HD2	1.85	0.42
17:P:35:PRO:HD2	17:P:120:ARG:HB2	2.00	0.42
18:Q:57:ASN:O	18:Q:58:VAL:HG23	2.19	0.42
19:R:107:ALA:HB2	19:R:111:GLY:HA3	2.02	0.42
20:S:4:THR:HA	20:S:57:GLU:HG3	2.02	0.42
1:X:1013:G:C5	1:X:1014:G:C8	3.07	0.42
1:X:1164:C:H2'	1:X:1165:G:C8	2.53	0.42
1:X:114:C:O2'	1:X:124:A:N3	2.45	0.42
1:X:1349:A:H5'	18:Q:64:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1766:U:H2'	1:X:1767:G:O4'	2.19	0.42
1:X:1956:G:C6	1:X:1957:C:N4	2.87	0.42
1:X:2505:G:N1	1:X:2517:C:C2	2.88	0.42
1:X:491:A:N3	1:X:491:A:H2'	2.34	0.42
1:X:552:C:H2'	1:X:553:C:H5''	2.02	0.42
2:Y:58:G:H4'	2:Y:59:A:C5'	2.49	0.42
1:X:2039:G:H22	25:Z:4:HIS:HA	1.85	0.42
1:X:699:G:N2	27:2:12:ARG:HB2	2.35	0.42
10:I:62:LYS:HB2	28:3:12:ARG:HA	2.02	0.42
6:D:119:PRO:HB2	6:D:167:ARG:HH22	1.83	0.42
6:D:80:ARG:HD3	6:D:83:MET:CB	2.49	0.42
10:I:133:VAL:HG11	10:I:140:VAL:HG23	2.01	0.42
11:J:19:THR:HG23	11:J:99:LYS:HD3	2.01	0.42
1:X:346:C:H5''	19:R:91:ALA:HB2	2.02	0.42
22:U:9:GLY:H	22:U:14:VAL:HG21	1.85	0.42
24:W:27:LYS:HE2	24:W:27:LYS:HB3	1.83	0.42
1:X:1102:G:N2	1:X:1112:U:H1'	2.35	0.42
1:X:1187:A:H2'	1:X:1188:A:C8	2.55	0.42
1:X:1416:A:H2'	1:X:1417:C:C6	2.55	0.42
1:X:1755:G:C6	1:X:1972:G:C2	3.08	0.42
1:X:540:G:C2	1:X:2005:U:OP1	2.73	0.42
1:X:2054:A:H2'	1:X:2055:G:C8	2.54	0.42
1:X:2691:C:O2'	1:X:2692:A:OP2	2.31	0.42
1:X:507:A:P	17:P:21:ARG:HE	2.42	0.42
1:X:538:A:N3	1:X:538:A:C2'	2.82	0.42
1:X:753:U:O4'	1:X:1964:A:C4	2.73	0.42
1:X:2861:A:O2'	25:Z:31:THR:HG23	2.19	0.42
1:X:777:A:H5'	3:A:210:GLY:HA3	2.01	0.42
5:C:59:TYR:HE1	5:C:67:ALA:HA	1.85	0.42
9:H:7:ARG:HD3	9:H:18:GLU:OE2	2.19	0.42
11:J:83:ARG:HD3	11:J:83:ARG:HA	1.94	0.42
16:O:14:VAL:N	16:O:16:GLU:OE2	2.53	0.42
1:X:1336:G:H2'	1:X:1337:G:H5'	2.00	0.42
1:X:1480:G:N3	1:X:1561:A:H2	2.18	0.42
1:X:175:C:H5'	1:X:2223:U:OP1	2.18	0.42
1:X:2284:U:P	1:X:2286:G:H22	2.42	0.42
1:X:2293:G:H2'	1:X:2294:U:C6	2.54	0.42
1:X:2796:A:C4	1:X:2797:G:C8	3.07	0.42
1:X:585:U:H2'	1:X:586:G:C8	2.55	0.42
1:X:615:C:H1'	1:X:670:U:H1'	2.00	0.42
1:X:731:A:H2'	1:X:732:G:H4'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:820:U:P	10:I:40:ARG:NH2	2.93	0.42
25:Z:52:TYR:HB3	25:Z:56:GLN:NE2	2.34	0.42
3:A:69:ARG:NH1	3:A:130:ALA:HB2	2.35	0.42
3:A:30:GLU:HB2	3:A:82:ILE:O	2.20	0.42
4:B:132:LYS:HE3	4:B:132:LYS:HB2	1.71	0.42
5:C:125:ILE:HD12	5:C:125:ILE:HA	1.87	0.42
1:X:2284:U:H3	6:D:39:GLY:HA3	1.84	0.42
9:H:104:GLU:HG3	9:H:125:LYS:HG3	2.02	0.42
10:I:96:TYR:HD2	10:I:96:TYR:HA	1.65	0.42
13:L:12:ARG:HG3	13:L:92:GLY:HA2	2.02	0.42
1:X:2266:A:HO2'	1:X:2267:A:P	2.43	0.42
1:X:2355:A:H8	1:X:2355:A:OP1	2.03	0.42
1:X:2471:U:H2'	1:X:2472:U:C6	2.55	0.42
1:X:2604:G:H2'	1:X:2605:C:C6	2.55	0.42
1:X:2729:A:C6	1:X:2730:A:N6	2.88	0.42
1:X:60:A:C6	1:X:61:U:C4	3.08	0.42
3:A:130:ALA:HA	3:A:191:ALA:O	2.19	0.42
8:G:34:PRO:HA	8:G:69:ASP:CB	2.49	0.42
9:H:22:ILE:H	9:H:53:ALA:HA	1.84	0.42
19:R:95:ARG:HB2	19:R:104:VAL:HB	2.02	0.42
20:S:123:VAL:HG13	20:S:124:ALA:HB3	2.01	0.42
20:S:71:MET:HB2	20:S:78:PRO:HA	2.01	0.42
20:S:89:GLY:O	20:S:126:GLY:HA2	2.20	0.42
1:X:1147:G:H2'	1:X:1148:G:C8	2.55	0.42
1:X:2080:U:H2'	1:X:2081:U:C6	2.55	0.42
1:X:674:U:H2'	1:X:675:C:O4'	2.20	0.42
1:X:788:G:C5	1:X:807:A:C8	3.08	0.42
2:Y:103:A:H8	2:Y:103:A:O5'	2.03	0.42
2:Y:33:C:H1'	2:Y:56:G:N2	2.35	0.42
27:2:25:LYS:HD3	27:2:25:LYS:HA	1.72	0.42
9:H:132:GLU:HB2	14:M:73:PHE:CE1	2.54	0.42
15:N:107:LYS:HE3	15:N:111:ASP:OD2	2.20	0.42
1:X:1005:U:H3'	15:N:54:LYS:HE3	2.02	0.42
19:R:48:VAL:HG12	19:R:51:VAL:H	1.85	0.42
1:X:161:U:H1'	1:X:194:G:O2'	2.20	0.42
1:X:1745:C:H5	1:X:1746:A:C5	2.37	0.42
1:X:333:A:H5'	1:X:351:A:H1'	2.01	0.42
1:X:88:G:OP2	1:X:89:A:H3'	2.20	0.42
1:X:984:A:O4'	1:X:1202:U:C6	2.73	0.42
2:Y:92:G:N7	2:Y:93:G:H1'	2.35	0.42
1:X:1794:A:O2'	3:A:257:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:23:ASN:ND2	5:C:26:VAL:HG23	2.34	0.41
5:C:33:TRP:CZ3	5:C:34:GLN:HG2	2.55	0.41
5:C:50:GLN:OE1	5:C:56:ARG:NH1	2.53	0.41
7:E:55:PRO:HB2	7:E:61:HIS:CE1	2.55	0.41
10:I:126:SER:O	10:I:130:ILE:HG13	2.19	0.41
1:X:673:G:H21	10:I:21:ARG:HG2	1.84	0.41
11:J:93:TYR:CE1	11:J:95:VAL:HG13	2.55	0.41
12:K:15:SER:O	12:K:18:VAL:HB	2.20	0.41
12:K:73:LYS:HE2	12:K:73:LYS:HB3	1.86	0.41
22:U:31:GLY:HA2	22:U:32:ARG:NH1	2.30	0.41
1:X:1796:A:N3	3:A:50:THR:HB	2.35	0.41
1:X:1865:C:H2'	1:X:1866:G:O4'	2.20	0.41
1:X:2019:C:O2'	1:X:2020:G:H5'	2.20	0.41
1:X:617:U:H3'	1:X:617:U:O2	2.20	0.41
1:X:876:A:H2	1:X:926:C:N4	2.16	0.41
1:X:987:G:C2	1:X:988:G:C8	3.08	0.41
28:3:26:LYS:CE	28:3:43:GLY:HA3	2.46	0.41
3:A:50:THR:OG1	3:A:51:SER:N	2.53	0.41
4:B:102:ILE:O	4:B:102:ILE:HG13	2.19	0.41
5:C:146:GLU:HG3	5:C:185:ARG:HH22	1.84	0.41
5:C:47:THR:HA	5:C:82:VAL:H	1.85	0.41
8:G:103:TYR:CE1	8:G:107:GLN:O	2.73	0.41
8:G:34:PRO:HA	8:G:69:ASP:CG	2.41	0.41
20:S:49:THR:HB	20:S:132:GLN:HA	2.02	0.41
1:X:1269:G:O3'	5:C:69:HIS:HE1	2.03	0.41
1:X:1290:A:OP1	12:K:40:LYS:NZ	2.53	0.41
1:X:1314:A:O2'	1:X:1315:A:H3'	2.19	0.41
1:X:1476:G:C6	1:X:1477:C:C4	3.08	0.41
1:X:2490:U:H2'	1:X:2491:C:C6	2.55	0.41
1:X:2495:G:C6	1:X:2496:C:N4	2.88	0.41
1:X:741:G:O2'	1:X:743:A:H8	2.03	0.41
27:2:20:ALA:HA	27:2:23:LYS:HD2	2.03	0.41
3:A:31:LYS:NZ	3:A:84:TYR:H	2.19	0.41
1:X:2659:C:H1'	4:B:187:ALA:HB1	2.02	0.41
1:X:2394:G:H4'	10:I:64:GLY:O	2.21	0.41
1:X:1216:G:C5	1:X:1217:U:C5	3.08	0.41
1:X:129:A:H2'	1:X:130:C:C6	2.56	0.41
1:X:1332:G:C2	1:X:1333:G:C2	3.09	0.41
1:X:1499:A:H2'	1:X:1500:U:C6	2.55	0.41
1:X:1509:A:H8	1:X:1510:A:N7	2.18	0.41
1:X:1656:U:C2'	1:X:1657:A:H5''	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1837:G:H2'	1:X:1838:G:C8	2.55	0.41
1:X:2277:A:H2'	1:X:2278:A:O4'	2.20	0.41
1:X:2394:G:C6	1:X:2395:C:C4	3.09	0.41
1:X:649:G:N1	1:X:660:G:N1	2.68	0.41
1:X:732:G:H2'	1:X:733:G:H8	1.86	0.41
3:A:25:THR:CG2	3:A:211:ARG:HH12	2.31	0.41
1:X:1788:C:H5'	3:A:254:THR:HA	2.01	0.41
4:B:126:PRO:HG2	4:B:131:SER:HB3	2.01	0.41
4:B:25:VAL:HG12	4:B:181:LEU:HD22	2.01	0.41
4:B:6:GLY:HA3	4:B:28:ALA:HA	2.02	0.41
5:C:124:ASP:OD1	5:C:136:TRP:NE1	2.49	0.41
5:C:13:ARG:HD2	5:C:13:ARG:H	1.85	0.41
5:C:95:LEU:HD23	5:C:96:PRO:HD2	2.03	0.41
8:G:70:PHE:CA	8:G:76:GLN:HE22	2.33	0.41
1:X:2628:C:O3'	9:H:35:THR:HG21	2.20	0.41
10:I:31:GLY:O	10:I:32:ARG:HG3	2.20	0.41
12:K:22:ARG:HG2	12:K:69:ASP:HB3	2.03	0.41
12:K:78:LYS:O	12:K:82:GLU:HB2	2.20	0.41
12:K:99:ARG:HG2	12:K:99:ARG:HH11	1.86	0.41
15:N:91:ASN:O	15:N:93:LYS:HB3	2.20	0.41
1:X:1016:C:C2	1:X:1154:A:C5	3.08	0.41
1:X:1329:U:C2	1:X:1330:G:C8	3.09	0.41
1:X:1355:A:N1	1:X:1358:C:C2	2.88	0.41
1:X:13:A:N3	1:X:15:G:C6	2.87	0.41
1:X:1408:A:C6	1:X:1411:C:C2	3.08	0.41
1:X:1448:A:H61	1:X:1574:A:N6	2.18	0.41
1:X:14:A:C5	1:X:536:A:C2	3.08	0.41
1:X:1497:C:H42	1:X:1527:G:H1	1.69	0.41
1:X:1682:A:O2'	9:H:1:MET:N	2.50	0.41
1:X:616:U:O2'	1:X:671:A:H4'	2.19	0.41
3:A:32:ALA:O	3:A:33:LEU:HB3	2.20	0.41
5:C:15:ILE:HD11	5:C:195:ILE:H	1.84	0.41
6:D:41:GLY:HA2	6:D:45:GLU:HB2	2.01	0.41
6:D:79:LEU:HA	6:D:79:LEU:HD23	1.86	0.41
16:O:11:GLN:CB	16:O:13:ARG:HH21	2.34	0.41
17:P:57:LEU:HD13	17:P:69:ALA:CB	2.49	0.41
20:S:25:ASN:H	20:S:25:ASN:ND2	2.16	0.41
1:X:1776:A:C8	1:X:1778:U:C5	3.08	0.41
1:X:2208:U:H2'	1:X:2209:G:C8	2.56	0.41
1:X:2331:A:C4	1:X:2345:A:C2	3.08	0.41
1:X:2509:A:H2'	1:X:2510:A:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2702:G:H2'	1:X:2703:C:O4'	2.20	0.41
1:X:539:A:C2	1:X:2006:G:C8	3.09	0.41
1:X:91:A:H2'	1:X:92:U:C6	2.56	0.41
1:X:958:G:H2'	1:X:959:C:C6	2.55	0.41
25:Z:3:LYS:HD2	25:Z:3:LYS:HA	1.63	0.41
1:X:2402:U:OP2	26:1:3:LYS:HG3	2.20	0.41
28:3:6:THR:HG23	28:3:8:LYS:N	2.35	0.41
1:X:792:U:P	3:A:48:ARG:HA	2.61	0.41
3:A:55:GLY:C	3:A:217:ARG:HD3	2.40	0.41
1:X:463:C:OP2	5:C:46:ARG:HG2	2.20	0.41
6:D:52:LYS:HD2	6:D:148:LYS:HE2	2.02	0.41
12:K:76:VAL:O	12:K:79:VAL:HG22	2.20	0.41
15:N:44:THR:O	15:N:48:ARG:HG3	2.21	0.41
18:Q:43:GLN:HG2	18:Q:48:VAL:O	2.20	0.41
21:T:19:LYS:O	21:T:20:TYR:CG	2.73	0.41
1:X:951:G:N3	1:X:1205:G:H4'	2.35	0.41
1:X:1313:U:H4'	1:X:1314:A:C5'	2.51	0.41
1:X:1412:C:OP1	18:Q:81:ARG:NH1	2.54	0.41
1:X:1623:C:H4'	1:X:1624:A:O5'	2.21	0.41
1:X:2039:G:H2'	1:X:2039:G:N3	2.36	0.41
1:X:2450:A:N6	1:X:2451:G:C2	2.89	0.41
1:X:474:G:C6	1:X:478:G:O6	2.74	0.41
1:X:738:G:C6	1:X:739:G:N1	2.89	0.41
1:X:787:A:H2	1:X:800:U:O2'	2.02	0.41
1:X:797:A:HO2'	1:X:798:G:P	2.44	0.41
1:X:945:G:C4	1:X:946:U:C5	3.09	0.41
1:X:1583:A:H2'	3:A:84:TYR:HE1	1.85	0.41
1:X:1685:A:H5''	9:H:5:GLN:HG2	2.02	0.41
16:O:23:GLU:HB2	16:O:91:THR:HG21	2.02	0.41
17:P:44:VAL:O	17:P:48:LYS:HD3	2.19	0.41
19:R:100:ASP:OD1	19:R:102:LYS:HB3	2.20	0.41
21:T:25:LYS:HA	21:T:25:LYS:HD3	1.88	0.41
21:T:45:PHE:CD1	21:T:45:PHE:N	2.87	0.41
23:V:6:MET:HE2	23:V:6:MET:HB3	1.73	0.41
1:X:1372:A:H2'	1:X:1373:G:O4'	2.21	0.41
1:X:2324:G:H4'	1:X:2325:A:H5''	2.03	0.41
1:X:2391:A:H2'	1:X:2392:G:H8	1.85	0.41
1:X:2511:G:H2'	1:X:2512:A:O4'	2.21	0.41
1:X:2564:U:H4'	1:X:2565:C:OP2	2.18	0.41
17:P:59:PHE:CZ	25:Z:40:LYS:HA	2.55	0.41
5:C:75:PRO:HA	5:C:81:GLY:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:28:VAL:HA	6:D:29:PRO:HD3	1.96	0.41
9:H:28:GLY:O	9:H:34:LEU:HA	2.20	0.41
15:N:86:ALA:C	15:N:88:ILE:N	2.74	0.41
17:P:117:ILE:HA	17:P:117:ILE:HD13	1.63	0.41
1:X:1235:C:N4	1:X:1240:G:H1	2.19	0.41
1:X:1781:C:H4'	3:A:209:ALA:CB	2.50	0.41
1:X:226:C:OP2	1:X:2373:C:O2'	2.38	0.41
1:X:2279:G:N2	1:X:2295:C:O2	2.33	0.41
1:X:2631:C:C2	1:X:2648:G:C2	3.09	0.41
1:X:26:G:C6	1:X:27:G:N1	2.89	0.41
1:X:2791:C:O2'	1:X:2792:C:H5'	2.21	0.41
1:X:2870:C:H2'	1:X:2871:U:C6	2.56	0.41
2:Y:48:A:H2'	2:Y:49:C:O4'	2.20	0.41
1:X:699:G:N1	27:2:12:ARG:HB2	2.35	0.41
5:C:34:GLN:O	5:C:37:SER:OG	2.34	0.41
5:C:62:LYS:HA	5:C:62:LYS:HD3	1.87	0.41
6:D:123:ASP:HB3	6:D:127:ASN:H	1.85	0.41
2:Y:53:G:C5'	13:L:64:LYS:HG3	2.51	0.41
14:M:7:ILE:HD12	14:M:7:ILE:HA	1.88	0.41
14:M:90:GLN:OE1	14:M:91:VAL:N	2.42	0.41
19:R:103:LYS:HE2	19:R:103:LYS:HB3	1.92	0.41
20:S:89:GLY:HA2	20:S:127:PRO:HB3	2.03	0.41
23:V:13:ASP:O	23:V:17:GLU:HG2	2.21	0.41
1:X:1007:A:H4'	15:N:93:LYS:NZ	2.29	0.41
1:X:1237:G:O3'	16:O:85:GLY:HA3	2.21	0.41
1:X:1255:A:H2'	1:X:1256:C:H6	1.86	0.41
1:X:1418:C:H2'	1:X:1419:G:H8	1.85	0.41
1:X:1469:U:H5''	1:X:1470:G:N7	2.35	0.41
1:X:2262:C:C2	1:X:2368:G:C2	3.09	0.41
1:X:2310:G:H2'	1:X:2311:U:O4'	2.20	0.41
1:X:2557:G:N2	1:X:2558:C:C2	2.89	0.41
1:X:2790:C:H42	1:X:2806:G:H1	1.66	0.41
1:X:538:A:C2	1:X:2025:A:C6	3.09	0.41
1:X:881:U:C4	1:X:882:C:N4	2.89	0.41
25:Z:45:ILE:HD11	25:Z:56:GLN:HG2	2.02	0.41
8:G:128:GLU:HG2	8:G:148:LEU:HD23	2.03	0.41
8:G:154:GLU:C	8:G:157:PRO:HD2	2.41	0.41
8:G:62:ILE:HG21	8:G:135:LEU:HD11	2.02	0.41
10:I:31:GLY:O	10:I:32:ARG:NH2	2.54	0.41
18:Q:66:GLY:HA3	18:Q:68:PHE:CE2	2.56	0.41
20:S:123:VAL:HG12	20:S:159:THR:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:3:LEU:HD11	20:S:5:ALA:O	2.21	0.41
24:W:4:LYS:HE3	24:W:52:GLU:HB3	2.03	0.41
1:X:1270:C:H4'	5:C:77:PHE:CE1	2.56	0.41
1:X:1533:G:H2'	1:X:1534:A:H8	1.85	0.41
1:X:1564:U:H2'	1:X:1565:G:H8	1.86	0.41
1:X:158:A:H2'	1:X:159:A:C8	2.55	0.41
1:X:1742:G:H2'	1:X:1743:C:H6	1.86	0.41
1:X:45:C:OP2	1:X:192:G:H2'	2.21	0.41
1:X:2847:G:C2	1:X:2848:A:N6	2.88	0.41
1:X:822:G:C6	1:X:823:U:C4	3.09	0.41
1:X:870:C:C2'	1:X:871:U:H5'	2.51	0.41
26:1:34:LYS:HG3	26:1:35:LEU:H	1.85	0.41
1:X:699:G:N2	27:2:7:PRO:O	2.53	0.41
28:3:13:ARG:HB2	28:3:23:MET:O	2.21	0.41
6:D:106:ILE:O	6:D:109:PRO:HD2	2.20	0.41
2:Y:43:G:H1	6:D:69:LYS:HZ1	1.68	0.41
7:E:94:PHE:CB	7:E:107:ILE:HG22	2.50	0.41
8:G:93:LYS:HD3	8:G:93:LYS:HA	1.80	0.41
10:I:77:LEU:HB2	10:I:111:SER:H	1.85	0.41
23:V:43:VAL:O	23:V:47:ARG:HG2	2.21	0.41
1:X:1039:A:N6	1:X:1136:G:H2'	2.36	0.41
1:X:1179:A:H2'	1:X:1180:A:H8	1.85	0.41
1:X:1500:U:H2'	1:X:1501:C:C6	2.56	0.41
1:X:1814:G:H2'	1:X:1815:G:H8	1.86	0.41
1:X:2794:G:C2	1:X:2803:C:C2	3.09	0.41
1:X:506:G:C6	1:X:507:A:C4	3.09	0.41
1:X:533:C:H2'	1:X:534:U:O4'	2.21	0.41
1:X:540:G:H4'	1:X:541:C:OP1	2.21	0.41
1:X:661:C:C2	1:X:662:G:C2	3.09	0.41
1:X:941:U:H2'	1:X:942:U:O4'	2.21	0.41
25:Z:14:SER:O	25:Z:18:MET:HB2	2.21	0.41
27:2:37:LYS:O	27:2:37:LYS:HG2	2.21	0.40
3:A:95:LEU:HG	3:A:105:ILE:HD12	2.02	0.40
7:E:124:ALA:HB3	7:E:132:ASP:HB2	2.02	0.40
7:E:148:VAL:HG12	7:E:162:VAL:HG11	2.03	0.40
15:N:99:ALA:HB2	15:N:106:PHE:CD1	2.56	0.40
21:T:23:VAL:HA	21:T:38:VAL:HG23	2.03	0.40
22:U:47:HIS:CG	22:U:48:LYS:N	2.89	0.40
22:U:51:ILE:O	22:U:52:ARG:NH2	2.37	0.40
1:X:1204:G:H2'	1:X:1205:G:H8	1.84	0.40
1:X:1500:U:H3	1:X:1520:G:H1	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:163:A:H2'	1:X:164:G:H8	1.87	0.40
1:X:1669:A:N7	1:X:1670:G:C6	2.89	0.40
1:X:580:A:C8	1:X:2013:A:N6	2.89	0.40
1:X:2867:G:H4'	1:X:2868:G:O4'	2.22	0.40
1:X:312:G:C4	1:X:313:U:C5	3.10	0.40
4:B:122:PHE:HB3	4:B:123:ALA:H	1.64	0.40
8:G:100:TYR:CD2	8:G:119:LEU:HD12	2.55	0.40
8:G:30:LYS:O	8:G:31:THR:OG1	2.26	0.40
11:J:73:LYS:H	11:J:94:TRP:HD1	1.69	0.40
15:N:104:GLU:OE2	15:N:104:GLU:N	2.54	0.40
16:O:68:LYS:HE3	16:O:70:TYR:CZ	2.56	0.40
17:P:68:VAL:HG22	17:P:124:ILE:HG21	2.02	0.40
22:U:13:LEU:O	22:U:14:VAL:HG13	2.22	0.40
23:V:14:PHE:O	23:V:18:ILE:HG13	2.21	0.40
1:X:1273:G:H2'	1:X:1274:C:O4'	2.21	0.40
1:X:2001:G:C6	1:X:2002:A:C6	3.08	0.40
1:X:2043:A:C2	1:X:2481:G:C5	3.09	0.40
1:X:841:G:N2	1:X:2225:G:O2'	2.46	0.40
1:X:2422:C:H2'	1:X:2423:G:C8	2.56	0.40
1:X:2482:A:H4'	1:X:2483:U:OP1	2.20	0.40
1:X:2658:A:H2'	1:X:2659:C:O4'	2.20	0.40
1:X:322:A:H62	1:X:339:U:H2'	1.86	0.40
1:X:698:A:H5''	1:X:801:A:H62	1.85	0.40
1:X:734:G:H2'	1:X:735:G:C8	2.56	0.40
25:Z:8:LYS:O	25:Z:9:LYS:HD2	2.21	0.40
3:A:176:ARG:NH1	3:A:180:GLY:HA2	2.31	0.40
4:B:54:LYS:HD3	4:B:59:VAL:HG22	2.03	0.40
15:N:30:LYS:HA	15:N:30:LYS:HD2	1.82	0.40
16:O:36:LYS:HE2	16:O:56:VAL:HG22	2.03	0.40
19:R:10:HIS:N	19:R:10:HIS:ND1	2.69	0.40
20:S:71:MET:CB	20:S:78:PRO:HA	2.52	0.40
1:X:1915:A:N1	1:X:1956:G:H1'	2.36	0.40
1:X:2166:G:H2'	1:X:2167:A:C8	2.57	0.40
1:X:2340:C:P	28:3:27:SER:HG	2.44	0.40
1:X:2594:U:C2	1:X:2595:C:C5	3.08	0.40
1:X:317:U:H2'	1:X:318:G:O4'	2.22	0.40
1:X:478:G:H2'	1:X:479:G:O4'	2.20	0.40
1:X:932:G:H2'	1:X:933:G:H8	1.86	0.40
27:2:36:ALA:O	27:2:38:GLY:N	2.54	0.40
5:C:112:GLN:HE22	5:C:116:LYS:NZ	2.20	0.40
10:I:73:GLU:OE2	10:I:101:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:34:SER:HB3	13:L:35:SER:H	1.77	0.40
1:X:1424:U:H2'	1:X:1425:G:C8	2.57	0.40
1:X:1643:A:N6	1:X:1656:U:H3	2.18	0.40
1:X:1671:A:H1'	1:X:2798:A:H5'	2.02	0.40
1:X:173:A:H2'	1:X:173:A:N3	2.36	0.40
1:X:1697:U:N3	1:X:1755:G:OP2	2.55	0.40
1:X:2039:G:N2	1:X:2040:A:N9	2.70	0.40
1:X:2060:A:H2'	1:X:2061:C:C6	2.57	0.40
1:X:2597:G:O2'	4:B:149:ARG:HB2	2.21	0.40
1:X:2730:A:O2'	1:X:2731:G:N2	2.54	0.40
1:X:2617:G:O2'	1:X:2755:A:N1	2.50	0.40
1:X:3:U:O2'	1:X:4:C:P	2.80	0.40
1:X:505:G:O2'	17:P:78:ASN:HB3	2.22	0.40
1:X:625:A:H4'	1:X:626:A:OP1	2.21	0.40
2:Y:44:C:OP2	6:D:64:LYS:NZ	2.48	0.40
1:X:475:U:O2'	27:2:16:HIS:NE2	2.50	0.40
3:A:28:ARG:HA	3:A:29:PRO:HD3	1.85	0.40
5:C:154:ASP:O	5:C:157:THR:N	2.54	0.40
12:K:45:ARG:HD3	12:K:95:THR:CG2	2.51	0.40
17:P:74:SER:HA	17:P:77:ALA:HB3	2.04	0.40
1:X:1208:A:H2'	1:X:1209:G:O4'	2.21	0.40
1:X:1267:A:H5''	1:X:1268:U:H5''	2.03	0.40
1:X:1327:C:H42	1:X:1351:G:H1	1.69	0.40
1:X:1465:G:N3	1:X:1466:C:O2	2.54	0.40
1:X:1919:A:N6	1:X:1946:U:N3	2.69	0.40
1:X:2691:C:H2'	1:X:2694:G:H5''	2.03	0.40
1:X:2728:A:C6	1:X:2729:A:C6	3.10	0.40
1:X:2867:G:O5'	1:X:2867:G:H8	2.04	0.40
1:X:387:A:H2'	1:X:387:A:N3	2.36	0.40
1:X:540:G:O2'	1:X:542:A:C2	2.63	0.40
1:X:787:A:C2	1:X:800:U:O2'	2.74	0.40
1:X:861:G:N2	1:X:943:U:H1'	2.36	0.40
1:X:977:G:H5'	1:X:2251:U:O2	2.22	0.40
25:Z:3:LYS:O	25:Z:4:HIS:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	257/275 (94%)	219 (85%)	37 (14%)	1 (0%)	38	76
4	B	203/211 (96%)	183 (90%)	15 (7%)	5 (2%)	6	44
5	C	192/205 (94%)	161 (84%)	25 (13%)	6 (3%)	5	39
6	D	175/180 (97%)	151 (86%)	24 (14%)	0	100	100
7	E	169/185 (91%)	155 (92%)	13 (8%)	1 (1%)	28	70
8	G	140/174 (80%)	124 (89%)	15 (11%)	1 (1%)	25	68
9	H	132/134 (98%)	123 (93%)	8 (6%)	1 (1%)	22	65
10	I	132/156 (85%)	98 (74%)	30 (23%)	4 (3%)	5	40
11	J	134/141 (95%)	117 (87%)	16 (12%)	1 (1%)	25	68
12	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	20	64
13	L	102/114 (90%)	80 (78%)	22 (22%)	0	100	100
14	M	106/166 (64%)	100 (94%)	6 (6%)	0	100	100
15	N	115/118 (98%)	100 (87%)	13 (11%)	2 (2%)	11	52
16	O	92/100 (92%)	83 (90%)	9 (10%)	0	100	100
17	P	125/134 (93%)	121 (97%)	4 (3%)	0	100	100
18	Q	91/95 (96%)	69 (76%)	19 (21%)	3 (3%)	4	38
19	R	108/115 (94%)	80 (74%)	28 (26%)	0	100	100
20	S	177/237 (75%)	150 (85%)	25 (14%)	2 (1%)	17	61
21	T	72/91 (79%)	63 (88%)	9 (12%)	0	100	100
22	U	70/81 (86%)	51 (73%)	17 (24%)	2 (3%)	5	41
23	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
24	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
25	Z	55/60 (92%)	45 (82%)	10 (18%)	0	100	100
26	1	51/54 (94%)	36 (71%)	12 (24%)	3 (6%)	2	23
27	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	3	57/66 (86%)	44 (77%)	11 (19%)	2 (4%)	4	37
All	All	3026/3377 (90%)	2598 (86%)	391 (13%)	37 (1%)	15	59

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	94	VAL
18	Q	6	ILE
5	C	177	VAL
20	S	122	ILE
26	1	9	ILE
26	1	10	VAL
4	B	136	ARG
11	J	82	THR
22	U	60	VAL
27	2	5	TYR
3	A	21	PHE
4	B	144	ARG
5	C	130	THR
7	E	165	VAL
10	I	103	ASN
12	K	91	PRO
18	Q	69	ILE
22	U	15	VAL
4	B	121	ASN
5	C	113	GLU
5	C	164	VAL
10	I	38	LYS
27	2	8	ASN
4	B	137	ARG
9	H	42	LYS
18	Q	65	VAL
28	3	13	ARG
28	3	61	MET
8	G	163	PRO
4	B	73	ALA
5	C	15	ILE
15	N	8	ILE
26	1	8	ILE
5	C	22	VAL
10	I	19	VAL
10	I	68	VAL

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Mol	Chain	Res	Type
20	S	81	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	200/216 (93%)	160 (80%)	40 (20%)	1	10
4	B	155/157 (99%)	132 (85%)	23 (15%)	3	23
5	C	154/163 (94%)	117 (76%)	37 (24%)	1	6
6	D	153/156 (98%)	144 (94%)	9 (6%)	23	62
7	E	136/144 (94%)	124 (91%)	12 (9%)	12	47
8	G	118/146 (81%)	100 (85%)	18 (15%)	3	22
9	H	103/103 (100%)	83 (81%)	20 (19%)	1	11
10	I	101/121 (84%)	77 (76%)	24 (24%)	1	6
11	J	108/115 (94%)	89 (82%)	19 (18%)	2	15
12	K	90/93 (97%)	74 (82%)	16 (18%)	2	14
13	L	74/82 (90%)	50 (68%)	24 (32%)	0	2
14	M	92/134 (69%)	76 (83%)	16 (17%)	2	15
15	N	96/97 (99%)	87 (91%)	9 (9%)	10	44
16	O	75/79 (95%)	64 (85%)	11 (15%)	3	24
17	P	109/115 (95%)	90 (83%)	19 (17%)	2	15
18	Q	75/76 (99%)	53 (71%)	22 (29%)	0	3
19	R	91/96 (95%)	77 (85%)	14 (15%)	3	21
20	S	152/192 (79%)	130 (86%)	22 (14%)	4	24
21	T	55/67 (82%)	47 (86%)	8 (14%)	4	24
22	U	57/66 (86%)	43 (75%)	14 (25%)	1	5
23	V	53/55 (96%)	49 (92%)	4 (8%)	16	53
24	W	48/48 (100%)	42 (88%)	6 (12%)	5	30
25	Z	51/53 (96%)	36 (71%)	15 (29%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	1	45/47 (96%)	33 (73%)	12 (27%)	0	4
27	2	39/40 (98%)	29 (74%)	10 (26%)	0	5
28	3	46/52 (88%)	34 (74%)	12 (26%)	0	5
All	All	2476/2713 (91%)	2040 (82%)	436 (18%)	2	15

All (436) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	18	THR
3	A	20	ASP
3	A	22	SER
3	A	25	THR
3	A	26	LYS
3	A	28	ARG
3	A	31	LYS
3	A	35	GLU
3	A	40	THR
3	A	43	ARG
3	A	49	ILE
3	A	58	HIS
3	A	60	ARG
3	A	87	ASN
3	A	88	ARG
3	A	95	LEU
3	A	104	TYR
3	A	106	LEU
3	A	122	GLU
3	A	127	LEU
3	A	131	LEU
3	A	141	VAL
3	A	147	LEU
3	A	151	LYS
3	A	162	SER
3	A	173	VAL
3	A	186	HIS
3	A	188	GLU
3	A	196	VAL
3	A	202	LYS
3	A	203	ASN
3	A	208	LYS
3	A	211	ARG

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Mol	Chain	Res	Type
3	A	213	ARG
3	A	214	TRP
3	A	215	LEU
3	A	218	LYS
3	A	237	GLU
3	A	240	THR
3	A	248	THR
4	B	5	LEU
4	B	15	TRP
4	B	21	ILE
4	B	23	VAL
4	B	25	VAL
4	B	34	VAL
4	B	57	ARG
4	B	72	VAL
4	B	75	THR
4	B	82	ARG
4	B	84	PHE
4	B	87	ASP
4	B	94	ASP
4	B	105	THR
4	B	116	VAL
4	B	122	PHE
4	B	132	LYS
4	B	135	HIS
4	B	141	ILE
4	B	143	GLN
4	B	144	ARG
4	B	199	ARG
4	B	203	LYS
5	C	5	ASN
5	C	13	ARG
5	C	14	THR
5	C	17	LEU
5	C	34	GLN
5	C	40	ARG
5	C	45	THR
5	C	58	MET
5	C	59	TYR
5	C	66	ASN
5	C	76	THR
5	C	77	PHE

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Mol	Chain	Res	Type
5	C	82	VAL
5	C	91	TYR
5	C	95	LEU
5	C	98	GLN
5	C	100	ARG
5	C	120	VAL
5	C	125	ILE
5	C	127	ASP
5	C	132	ASN
5	C	143	ASP
5	C	148	VAL
5	C	153	ASP
5	C	154	ASP
5	C	157	THR
5	C	162	ARG
5	C	163	ASN
5	C	164	VAL
5	C	166	TRP
5	C	167	VAL
5	C	169	VAL
5	C	175	VAL
5	C	177	VAL
5	C	180	ILE
5	C	184	ASP
5	C	193	LEU
6	D	4	LEU
6	D	22	TYR
6	D	40	LEU
6	D	80	ARG
6	D	90	THR
6	D	112	ARG
6	D	115	ARG
6	D	146	VAL
6	D	152	MET
7	E	32	GLU
7	E	34	THR
7	E	38	ASN
7	E	57	ASP
7	E	61	HIS
7	E	67	LEU
7	E	69	ARG
7	E	111	HIS

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Mol	Chain	Res	Type
7	E	129	THR
7	E	132	ASP
7	E	164	PHE
7	E	171	LEU
8	G	30	LYS
8	G	32	TYR
8	G	53	ARG
8	G	65	LYS
8	G	78	ASP
8	G	88	VAL
8	G	91	THR
8	G	95	LEU
8	G	102	ARG
8	G	103	TYR
8	G	104	THR
8	G	106	TYR
8	G	119	LEU
8	G	146	THR
8	G	147	ARG
8	G	161	GLN
8	G	165	VAL
8	G	171	LEU
9	H	1	MET
9	H	2	ILE
9	H	29	ILE
9	H	35	THR
9	H	36	THR
9	H	41	ASN
9	H	43	ARG
9	H	69	VAL
9	H	70	VAL
9	H	74	VAL
9	H	78	SER
9	H	81	ILE
9	H	82	LYS
9	H	90	ARG
9	H	94	ASN
9	H	109	ARG
9	H	120	ASP
9	H	122	ARG
9	H	124	MET
9	H	127	VAL

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Mol	Chain	Res	Type
10	I	18	ARG
10	I	26	THR
10	I	28	LYS
10	I	32	ARG
10	I	37	GLN
10	I	39	SER
10	I	40	ARG
10	I	49	PHE
10	I	53	ARG
10	I	55	ARG
10	I	65	PHE
10	I	71	THR
10	I	83	LEU
10	I	88	PHE
10	I	89	ASP
10	I	90	ARG
10	I	96	TYR
10	I	98	LEU
10	I	99	VAL
10	I	103	ASN
10	I	120	VAL
10	I	126	SER
10	I	141	VAL
10	I	142	LEU
11	J	8	THR
11	J	9	LYS
11	J	10	PHE
11	J	11	ARG
11	J	17	ARG
11	J	26	ASP
11	J	27	TYR
11	J	28	VAL
11	J	46	ASN
11	J	59	PHE
11	J	60	ARG
11	J	67	ILE
11	J	86	LYS
11	J	104	MET
11	J	106	GLU
11	J	131	LYS
11	J	134	LYS
11	J	135	ARG

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Mol	Chain	Res	Type
11	J	139	ASP
12	K	5	LYS
12	K	11	ASN
12	K	13	ASN
12	K	14	SER
12	K	37	THR
12	K	43	GLU
12	K	48	VAL
12	K	51	LEU
12	K	59	ASP
12	K	73	LYS
12	K	76	VAL
12	K	94	TYR
12	K	95	THR
12	K	98	LEU
12	K	102	THR
12	K	109	THR
13	L	8	ARG
13	L	11	LEU
13	L	13	THR
13	L	15	ARG
13	L	29	LEU
13	L	31	VAL
13	L	34	SER
13	L	37	HIS
13	L	38	ILE
13	L	39	TYR
13	L	42	ILE
13	L	43	ILE
13	L	45	ASP
13	L	46	SER
13	L	65	THR
13	L	66	ASP
13	L	67	THR
13	L	88	VAL
13	L	91	ARG
13	L	93	SER
13	L	94	TYR
13	L	96	TYR
13	L	97	HIS
13	L	109	GLU
14	M	3	THR

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Mol	Chain	Res	Type
14	M	7	ILE
14	M	31	ASP
14	M	38	LYS
14	M	39	VAL
14	M	43	ASN
14	M	45	THR
14	M	57	ILE
14	M	63	ARG
14	M	68	VAL
14	M	69	ARG
14	M	94	VAL
14	M	96	ARG
14	M	98	LYS
14	M	101	ARG
14	M	103	LYS
15	N	9	VAL
15	N	15	LYS
15	N	22	LYS
15	N	28	ARG
15	N	30	LYS
15	N	31	GLN
15	N	51	ARG
15	N	60	LEU
15	N	93	LYS
16	O	13	ARG
16	O	20	ILE
16	O	21	ARG
16	O	22	VAL
16	O	28	GLU
16	O	47	PHE
16	O	56	VAL
16	O	81	ARG
16	O	88	GLN
16	O	91	THR
16	O	98	ILE
17	P	9	ARG
17	P	13	GLN
17	P	32	ARG
17	P	37	LYS
17	P	39	ARG
17	P	40	LEU
17	P	46	ARG

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Mol	Chain	Res	Type
17	P	52	ASP
17	P	65	SER
17	P	71	VAL
17	P	91	PHE
17	P	107	ILE
17	P	109	ARG
17	P	116	ILE
17	P	118	LYS
17	P	119	LYS
17	P	120	ARG
17	P	121	THR
17	P	125	THR
18	Q	5	ASP
18	Q	6	ILE
18	Q	7	LEU
18	Q	8	GLN
18	Q	15	LYS
18	Q	24	VAL
18	Q	26	SER
18	Q	30	SER
18	Q	32	LYS
18	Q	34	THR
18	Q	40	ASP
18	Q	44	GLN
18	Q	58	VAL
18	Q	62	ARG
18	Q	64	ARG
18	Q	65	VAL
18	Q	73	ASN
18	Q	74	ASP
18	Q	80	VAL
18	Q	81	ARG
18	Q	84	GLU
18	Q	88	ILE
19	R	10	HIS
19	R	15	HIS
19	R	18	LYS
19	R	20	ASP
19	R	21	THR
19	R	23	ILE
19	R	48	VAL
19	R	56	LYS

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Mol	Chain	Res	Type
19	R	80	LYS
19	R	83	LEU
19	R	94	VAL
19	R	95	ARG
19	R	97	GLN
19	R	110	SER
20	S	1	MET
20	S	14	LEU
20	S	22	VAL
20	S	25	ASN
20	S	26	LYS
20	S	32	PHE
20	S	34	LEU
20	S	48	THR
20	S	51	LEU
20	S	71	MET
20	S	73	LYS
20	S	86	VAL
20	S	88	TYR
20	S	112	LEU
20	S	120	LEU
20	S	123	VAL
20	S	145	ASP
20	S	159	THR
20	S	175	ARG
20	S	176	LEU
20	S	177	THR
20	S	179	GLU
21	T	30	VAL
21	T	37	LEU
21	T	38	VAL
21	T	45	PHE
21	T	46	LYS
21	T	64	ASP
21	T	68	VAL
21	T	80	SER
22	U	14	VAL
22	U	17	SER
22	U	19	ILE
22	U	21	ARG
22	U	27	ASP
22	U	32	ARG

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Mol	Chain	Res	Type
22	U	37	ILE
22	U	48	LYS
22	U	49	LYS
22	U	53	GLU
22	U	54	ASN
22	U	70	LEU
22	U	75	TYR
22	U	78	ILE
23	V	12	THR
23	V	19	ASP
23	V	21	ARG
23	V	28	LEU
24	W	3	ILE
24	W	4	LYS
24	W	9	VAL
24	W	12	ARG
24	W	32	ARG
24	W	36	ASP
25	Z	3	LYS
25	Z	6	VAL
25	Z	10	LYS
25	Z	21	SER
25	Z	23	HIS
25	Z	25	LEU
25	Z	41	LEU
25	Z	42	SER
25	Z	49	CYS
25	Z	51	TYR
25	Z	52	TYR
25	Z	53	ASP
25	Z	55	ARG
25	Z	57	VAL
25	Z	58	LEU
26	1	8	ILE
26	1	10	VAL
26	1	12	MET
26	1	15	SER
26	1	20	PHE
26	1	21	TYR
26	1	25	THR
26	1	30	ASN
26	1	36	GLU

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Mol	Chain	Res	Type
26	1	43	VAL
26	1	48	VAL
26	1	54	LYS
27	2	1	MET
27	2	6	GLN
27	2	14	LYS
27	2	22	MET
27	2	23	LYS
27	2	28	ARG
27	2	31	LEU
27	2	40	HIS
27	2	43	THR
27	2	45	SER
28	3	6	THR
28	3	7	HIS
28	3	13	ARG
28	3	22	VAL
28	3	31	HIS
28	3	34	THR
28	3	44	LYS
28	3	46	LYS
28	3	49	VAL
28	3	50	LEU
28	3	52	LYS
28	3	60	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	87	ASN
3	A	129	ASN
3	A	198	ASN
4	B	48	GLN
4	B	60	ASN
4	B	129	HIS
5	C	101	GLN
5	C	112	GLN
5	C	163	ASN
6	D	118	ASN
6	D	135	GLN
7	E	20	GLN
7	E	38	ASN

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Mol	Chain	Res	Type
7	E	74	ASN
8	G	76	GLN
8	G	84	ASN
8	G	140	GLN
8	G	145	HIS
8	G	158	HIS
9	H	41	ASN
10	I	34	HIS
10	I	103	ASN
11	J	47	GLN
11	J	58	HIS
11	J	124	HIS
12	K	11	ASN
12	K	35	GLN
13	L	41	GLN
13	L	97	HIS
15	N	66	ASN
16	O	6	GLN
16	O	11	GLN
16	O	79	GLN
19	R	10	HIS
19	R	44	GLN
19	R	77	HIS
20	S	25	ASN
20	S	46	GLN
20	S	146	HIS
22	U	45	ASN
23	V	52	GLN
24	W	49	HIS
24	W	54	GLN
25	Z	44	HIS
26	1	30	ASN
27	2	6	GLN
27	2	29	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2649/2880 (91%)	580 (21%)	0
2	Y	119/123 (96%)	23 (19%)	0
All	All	2768/3003 (92%)	603 (21%)	0

All (603) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	4	C
1	X	7	G
1	X	10	A
1	X	14	A
1	X	15	G
1	X	23	G
1	X	34	U
1	X	37	C
1	X	39	C
1	X	45	C
1	X	49	U
1	X	50	G
1	X	59	G
1	X	63	A
1	X	69	G
1	X	73	A
1	X	74	G
1	X	87	G
1	X	88	G
1	X	89	A
1	X	90	G
1	X	95	G
1	X	97	U
1	X	98	U
1	X	100	G
1	X	108	G
1	X	111	G
1	X	112	U
1	X	116	A
1	X	118	U
1	X	123	A
1	X	124	A
1	X	126	C
1	X	134	G
1	X	136	A
1	X	138	G
1	X	143	A
1	X	158	A
1	X	173	A
1	X	176	A
1	X	177	U

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Mol	Chain	Res	Type
1	X	178	C
1	X	181	A
1	X	192	G
1	X	193	A
1	X	198	A
1	X	199	A
1	X	201	G
1	X	205	A
1	X	206	U
1	X	207	U
1	X	209	G
1	X	210	A
1	X	218	A
1	X	219	G
1	X	220	U
1	X	225	G
1	X	229	G
1	X	241	C
1	X	242	A
1	X	243	G
1	X	247	A
1	X	248	A
1	X	249	A
1	X	302	U
1	X	303	C
1	X	304	A
1	X	305	A
1	X	310	A
1	X	312	G
1	X	313	U
1	X	321	A
1	X	322	A
1	X	323	G
1	X	333	A
1	X	334	G
1	X	335	A
1	X	338	G
1	X	340	G
1	X	342	G
1	X	343	A
1	X	349	G
1	X	387	A

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Mol	Chain	Res	Type
1	X	398	C
1	X	399	G
1	X	400	U
1	X	408	U
1	X	409	G
1	X	414	A
1	X	424	G
1	X	425	A
1	X	431	G
1	X	433	G
1	X	441	A
1	X	456	C
1	X	459	A
1	X	463	C
1	X	467	U
1	X	469	G
1	X	483	A
1	X	484	G
1	X	491	A
1	X	492	G
1	X	493	A
1	X	501	G
1	X	506	G
1	X	514	G
1	X	515	A
1	X	518	A
1	X	519	C
1	X	534	U
1	X	537	C
1	X	538	A
1	X	539	A
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	558	G
1	X	560	G
1	X	572	G
1	X	578	U

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Mol	Chain	Res	Type
1	X	582	G
1	X	584	A
1	X	591	G
1	X	595	A
1	X	601	A
1	X	613	A
1	X	616	U
1	X	617	U
1	X	626	A
1	X	627	A
1	X	628	A
1	X	631	G
1	X	633	G
1	X	645	G
1	X	648	A
1	X	649	G
1	X	654	A
1	X	655	A
1	X	656	U
1	X	657	A
1	X	664	C
1	X	665	A
1	X	666	U
1	X	667	U
1	X	668	A
1	X	682	G
1	X	683	A
1	X	684	C
1	X	690	A
1	X	699	G
1	X	728	G
1	X	729	A
1	X	731	A
1	X	732	G
1	X	743	A
1	X	747	A
1	X	753	U
1	X	760	U
1	X	761	G
1	X	766	A
1	X	773	G
1	X	774	A

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Mol	Chain	Res	Type
1	X	777	A
1	X	784	U
1	X	788	G
1	X	789	G
1	X	790	A
1	X	792	U
1	X	795	A
1	X	796	A
1	X	797	A
1	X	798	G
1	X	802	A
1	X	803	C
1	X	805	G
1	X	818	G
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	846	A
1	X	859	U
1	X	871	U
1	X	872	G
1	X	879	A
1	X	922	A
1	X	926	C
1	X	931	G
1	X	939	C
1	X	940	G
1	X	941	U
1	X	943	U
1	X	944	A
1	X	952	A
1	X	957	G
1	X	964	A
1	X	970	A
1	X	972	C
1	X	985	G
1	X	994	A
1	X	996	C
1	X	999	A
1	X	1006	C
1	X	1007	A

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Mol	Chain	Res	Type
1	X	1014	G
1	X	1016	C
1	X	1018	C
1	X	1020	A
1	X	1021	A
1	X	1022	A
1	X	1023	U
1	X	1031	C
1	X	1032	A
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1044	U
1	X	1046	U
1	X	1049	C
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1058	G
1	X	1073	G
1	X	1076	U
1	X	1077	U
1	X	1081	A
1	X	1082	G
1	X	1083	C
1	X	1108	U
1	X	1120	C
1	X	1121	G
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1139	A
1	X	1141	U
1	X	1142	G
1	X	1145	C
1	X	1146	G
1	X	1149	G
1	X	1152	C
1	X	1153	A
1	X	1154	A
1	X	1166	A

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Mol	Chain	Res	Type
1	X	1167	A
1	X	1176	U
1	X	1183	C
1	X	1185	C
1	X	1189	G
1	X	1192	A
1	X	1194	U
1	X	1207	G
1	X	1240	G
1	X	1242	A
1	X	1249	G
1	X	1250	A
1	X	1263	G
1	X	1266	G
1	X	1267	A
1	X	1269	G
1	X	1278	A
1	X	1284	G
1	X	1285	A
1	X	1286	U
1	X	1289	A
1	X	1313	U
1	X	1314	A
1	X	1324	G
1	X	1325	U
1	X	1334	A
1	X	1342	U
1	X	1344	C
1	X	1345	G
1	X	1351	G
1	X	1363	C
1	X	1372	A
1	X	1378	A
1	X	1381	G
1	X	1391	A
1	X	1392	U
1	X	1398	G
1	X	1403	U
1	X	1404	C
1	X	1409	U
1	X	1428	G
1	X	1429	A

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Mol	Chain	Res	Type
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1435	G
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1467	U
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	1505	U
1	X	1506	C
1	X	1524	C
1	X	1525	A
1	X	1526	U
1	X	1528	C
1	X	1531	C
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1570	C
1	X	1574	A
1	X	1575	C
1	X	1582	A
1	X	1585	A
1	X	1594	U
1	X	1602	G
1	X	1603	A
1	X	1608	U
1	X	1614	C
1	X	1623	C
1	X	1624	A

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Mol	Chain	Res	Type
1	X	1625	A
1	X	1630	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1648	C
1	X	1656	U
1	X	1657	A
1	X	1661	C
1	X	1665	C
1	X	1671	A
1	X	1685	A
1	X	1686	A
1	X	1691	G
1	X	1710	U
1	X	1714	A
1	X	1717	A
1	X	1718	A
1	X	1735	G
1	X	1743	C
1	X	1747	G
1	X	1754	G
1	X	1755	G
1	X	1760	G
1	X	1764	A
1	X	1767	G
1	X	1775	A
1	X	1782	A
1	X	1788	C
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1801	C
1	X	1802	A
1	X	1807	A
1	X	1808	C
1	X	1819	U
1	X	1821	A
1	X	1822	C
1	X	1824	C

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Mol	Chain	Res	Type
1	X	1825	C
1	X	1830	C
1	X	1831	G
1	X	1840	A
1	X	1850	G
1	X	1861	G
1	X	1864	G
1	X	1867	A
1	X	1868	A
1	X	1882	G
1	X	1886	G
1	X	1910	A
1	X	1912	G
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	1937	G
1	X	1938	U
1	X	1943	A
1	X	1946	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	2003	A
1	X	2006	G
1	X	2011	U
1	X	2014	A
1	X	2015	G
1	X	2016	A
1	X	2017	U

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Mol	Chain	Res	Type
1	X	2018	G
1	X	2026	C
1	X	2032	G
1	X	2034	A
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	2063	A
1	X	2076	G
1	X	2083	G
1	X	2089	C
1	X	2171	U
1	X	2173	G
1	X	2180	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2192	U
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2198	U
1	X	2199	C
1	X	2204	A
1	X	2205	C
1	X	2217	G
1	X	2218	G
1	X	2222	U
1	X	2241	U
1	X	2247	A
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G

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Mol	Chain	Res	Type
1	X	2290	A
1	X	2298	U
1	X	2299	A
1	X	2301	A
1	X	2306	A
1	X	2311	U
1	X	2313	G
1	X	2314	A
1	X	2315	A
1	X	2316	G
1	X	2322	U
1	X	2326	C
1	X	2330	G
1	X	2351	G
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2370	G
1	X	2375	G
1	X	2381	A
1	X	2386	G
1	X	2398	U
1	X	2401	A
1	X	2402	U
1	X	2404	A
1	X	2405	A
1	X	2408	G
1	X	2410	U
1	X	2414	A
1	X	2420	C
1	X	2422	C
1	X	2424	G
1	X	2426	G
1	X	2427	A
1	X	2452	U
1	X	2455	A
1	X	2457	A
1	X	2463	G
1	X	2469	G
1	X	2473	G
1	X	2477	C

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Mol	Chain	Res	Type
1	X	2480	C
1	X	2481	G
1	X	2484	G
1	X	2485	U
1	X	2492	G
1	X	2497	A
1	X	2499	C
1	X	2522	G
1	X	2535	C
1	X	2545	A
1	X	2546	G
1	X	2551	A
1	X	2552	C
1	X	2556	A
1	X	2564	U
1	X	2565	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2590	U
1	X	2591	C
1	X	2592	U
1	X	2594	U
1	X	2595	C
1	X	2600	A
1	X	2608	A
1	X	2609	G
1	X	2613	A
1	X	2618	A
1	X	2633	A
1	X	2634	G
1	X	2640	G
1	X	2642	G
1	X	2650	G
1	X	2664	G
1	X	2666	U
1	X	2668	U
1	X	2683	C
1	X	2684	A
1	X	2691	C
1	X	2692	A
1	X	2693	U

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Mol	Chain	Res	Type
1	X	2705	A
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	2738	A
1	X	2744	A
1	X	2745	A
1	X	2757	G
1	X	2758	A
1	X	2759	U
1	X	2761	A
1	X	2770	A
1	X	2782	G
1	X	2783	U
1	X	2787	A
1	X	2795	A
1	X	2796	A
1	X	2798	A
1	X	2808	U
1	X	2809	A
1	X	2811	G
1	X	2814	G
1	X	2824	C
1	X	2825	A
1	X	2842	C
1	X	2847	G
1	X	2851	G
1	X	2855	C
1	X	2858	A
1	X	2866	A
1	X	2868	G
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	22	U
2	Y	26	G
2	Y	28	A
2	Y	32	C

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Mol	Chain	Res	Type
2	Y	37	C
2	Y	42	U
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	49	C
2	Y	68	A
2	Y	69	G
2	Y	99	G
2	Y	102	A
2	Y	108	G
2	Y	110	U
2	Y	112	A
2	Y	115	G

There are no RNA pucker outliers to report.

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 124 ligands modelled in this entry, 123 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	$\# Z > 2$
29	6O1	X	2901	-	116,123,123	1.61	13 (11%)	154,191,191	1.86	28 (18%)

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
29	6O1	X	2901	-	-	0/50/234/234	0/13/13/13

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	2901	6O1	C08-C05	-5.99	1.39	1.51
29	X	2901	6O1	C62-C61	-5.36	1.40	1.51
29	X	2901	6O1	C04-C09	-4.19	1.40	1.50
29	X	2901	6O1	C56-C55	-3.69	1.41	1.50
29	X	2901	6O1	C51-C50	-2.79	1.48	1.53
29	X	2901	6O1	C65-N65	-2.46	1.47	1.52
29	X	2901	6O1	O26-C22	2.32	1.47	1.41
29	X	2901	6O1	O50-C54	2.56	1.45	1.41
29	X	2901	6O1	O25-C16	2.59	1.46	1.41
29	X	2901	6O1	O20-C16	2.73	1.44	1.41
29	X	2901	6O1	O51-C54	3.34	1.47	1.41
29	X	2901	6O1	O53-C49	5.15	1.45	1.40
29	X	2901	6O1	O71-N65	7.75	1.36	1.21

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	6O1	O50-C50-C51	-10.81	97.90	106.55
29	X	2901	6O1	O51-C51-C50	-6.18	98.11	106.36
29	X	2901	6O1	C44-O44-C36	-5.04	105.27	114.37
29	X	2901	6O1	C36-C37-C38	-4.76	102.16	110.37
29	X	2901	6O1	C29-O33-C33	-3.59	107.33	113.67
29	X	2901	6O1	O25-C25-C24	-3.14	98.32	103.98
29	X	2901	6O1	C29-C30-C31	-3.12	104.61	110.04
29	X	2901	6O1	C45-C46-C47	-3.05	106.00	113.33
29	X	2901	6O1	O47-C47-C46	-2.97	98.50	103.45
29	X	2901	6O1	C15-C14-C13	-2.89	108.91	113.36
29	X	2901	6O1	C16-O20-C20	-2.83	109.56	112.11
29	X	2901	6O1	C13-O13-C09	-2.82	112.64	117.24
29	X	2901	6O1	C30-C31-C32	-2.75	105.28	111.65
29	X	2901	6O1	C48-C47-C46	-2.53	107.37	112.57
29	X	2901	6O1	C28-C26-C25	-2.53	108.52	113.58
29	X	2901	6O1	C53-O53-C49	-2.42	110.07	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	6O1	C10-O19-C19	-2.16	110.22	114.68
29	X	2901	6O1	C08-C05-C06	-2.15	118.54	121.55
29	X	2901	6O1	C34-O32-C32	-2.15	108.67	114.54
29	X	2901	6O1	C42-C40-C39	-2.11	108.06	113.30
29	X	2901	6O1	C69-O66-C66	-2.09	110.42	114.29
29	X	2901	6O1	O57-C57-C56	-2.08	117.17	121.14
29	X	2901	6O1	O20-C20-C21	2.13	108.50	105.81
29	X	2901	6O1	O31-C31-C32	2.19	113.14	107.50
29	X	2901	6O1	O39-C29-O33	2.27	116.21	110.70
29	X	2901	6O1	O53-C49-O47	2.43	114.45	109.91
29	X	2901	6O1	C03-C02-CL1	3.00	123.84	118.88
29	X	2901	6O1	C02-C01-C06	4.70	122.20	117.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	2901	6O1	2	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2658/2880 (92%)	-0.12	96 (3%) 43 31	30, 77, 204, 337	0
2	Y	120/123 (97%)	-0.07	3 (2%) 58 43	80, 150, 187, 207	0
3	A	259/275 (94%)	-0.19	4 (1%) 74 60	50, 105, 160, 212	0
4	B	205/211 (97%)	-0.49	0 100 100	30, 51, 113, 199	0
5	C	194/205 (94%)	-0.38	1 (0%) 90 83	35, 103, 180, 254	0
6	D	177/180 (98%)	-0.14	4 (2%) 61 46	128, 183, 249, 280	0
7	E	171/185 (92%)	-0.08	13 (7%) 15 11	70, 142, 203, 254	0
8	G	142/174 (81%)	-0.12	6 (4%) 37 26	38, 78, 188, 245	0
9	H	134/134 (100%)	-0.43	0 100 100	40, 55, 108, 175	0
10	I	134/156 (85%)	-0.10	2 (1%) 74 60	50, 120, 191, 236	0
11	J	136/141 (96%)	-0.04	3 (2%) 62 47	65, 106, 170, 225	0
12	K	113/116 (97%)	-0.53	0 100 100	30, 37, 91, 200	0
13	L	104/114 (91%)	0.01	5 (4%) 31 22	120, 154, 189, 241	0
14	M	108/166 (65%)	-0.66	0 100 100	37, 50, 117, 169	0
15	N	117/118 (99%)	-0.47	1 (0%) 84 72	42, 82, 136, 279	0
16	O	94/100 (94%)	-0.37	1 (1%) 80 67	48, 101, 170, 216	0
17	P	127/134 (94%)	-0.53	0 100 100	34, 53, 105, 192	0
18	Q	93/95 (97%)	-0.28	8 (8%) 11 9	49, 88, 174, 215	0
19	R	110/115 (95%)	-0.28	4 (3%) 43 31	62, 117, 213, 259	0
20	S	179/237 (75%)	-0.10	8 (4%) 34 24	97, 158, 213, 289	0
21	T	74/91 (81%)	-0.09	4 (5%) 26 19	67, 104, 157, 206	0
22	U	72/81 (88%)	0.10	5 (6%) 18 12	70, 125, 187, 215	0
23	V	65/67 (97%)	-0.23	3 (4%) 33 23	83, 125, 197, 216	0
24	W	55/55 (100%)	-0.61	0 100 100	68, 90, 135, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/60 (95%)	-0.28	1 (1%) 69 54	32, 43, 104, 182	0
26	1	53/54 (98%)	0.36	6 (11%) 6 5	101, 129, 224, 259	0
27	2	46/47 (97%)	-0.29	1 (2%) 62 47	44, 59, 103, 162	0
28	3	59/66 (89%)	0.04	0 100 100	72, 100, 161, 239	0
All	All	5856/6380 (91%)	-0.19	179 (3%) 49 36	30, 91, 201, 337	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	1523	A	15.4
6	D	43	SER	8.2
22	U	29	GLY	6.4
1	X	1522	C	6.3
1	X	1073	G	6.0
11	J	84	MET	5.8
1	X	1553	G	5.6
1	X	2780	A	5.4
1	X	1186	G	5.3
1	X	1187	A	5.3
8	G	156	HIS	5.3
1	X	1115	C	5.2
1	X	514	G	5.2
1	X	1552	C	4.9
18	Q	64	ARG	4.9
1	X	1117	G	4.9
1	X	1109	A	4.9
1	X	1074	G	4.8
1	X	248	A	4.8
1	X	1188	A	4.8
1	X	731	A	4.5
1	X	2287	G	4.5
1	X	1524	C	4.5
20	S	15	ASP	4.4
7	E	13	SER	4.4
6	D	42	SER	4.4
1	X	1845	A	4.4
1	X	1525	A	4.2
19	R	60	PRO	4.2
1	X	911	A	4.0
23	V	4	SER	4.0
20	S	14	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
21	T	16	SER	3.8
20	S	11	LYS	3.7
19	R	58	VAL	3.7
3	A	249	PRO	3.6
1	X	1951	G	3.6
1	X	1734	C	3.6
1	X	1121	G	3.6
1	X	1076	U	3.5
1	X	728	G	3.5
1	X	1044	U	3.5
1	X	1841	G	3.5
1	X	1077	U	3.5
1	X	1078	A	3.5
13	L	97	HIS	3.5
1	X	1114	A	3.4
2	Y	25	G	3.4
22	U	30	VAL	3.4
7	E	174	GLY	3.4
25	Z	59	ALA	3.4
18	Q	92	ALA	3.3
1	X	2083	G	3.3
22	U	28	GLY	3.3
1	X	1909	U	3.3
7	E	12	PRO	3.3
8	G	155	THR	3.3
1	X	1913	G	3.2
13	L	62	GLY	3.2
1	X	1110	G	3.2
1	X	1075	C	3.2
7	E	10	ALA	3.2
1	X	1842	G	3.1
1	X	727	U	3.1
5	C	19	LEU	3.1
1	X	1588	A	3.1
1	X	1847	G	3.1
6	D	144	ASP	3.1
1	X	435	A	3.1
1	X	665	A	3.1
1	X	1871	G	3.1
3	A	250	TRP	3.0
18	Q	90	ALA	3.0
1	X	1554	G	3.0

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Mol	Chain	Res	Type	RSRZ
1	X	1189	G	3.0
1	X	1548	U	3.0
1	X	1185	C	2.9
1	X	206	U	2.9
20	S	4	THR	2.9
7	E	123	PHE	2.9
1	X	1848	U	2.8
16	O	43	GLU	2.8
1	X	1556	A	2.8
1	X	1843	U	2.8
1	X	1844	C	2.8
1	X	2088	U	2.8
1	X	2773	G	2.8
19	R	99	VAL	2.8
13	L	61	SER	2.8
1	X	1184	G	2.8
8	G	69	ASP	2.8
13	L	53	ALA	2.8
1	X	1477	C	2.7
1	X	2085	G	2.7
1	X	1803	G	2.7
1	X	2082	C	2.7
1	X	2084	G	2.7
18	Q	93	GLY	2.7
1	X	1116	U	2.7
1	X	2169	A	2.7
26	1	47	HIS	2.7
13	L	52	ALA	2.7
22	U	25	ARG	2.6
1	X	729	A	2.6
1	X	1084	A	2.6
21	T	85	GLN	2.6
1	X	1498	G	2.6
1	X	2170	C	2.6
1	X	1434	U	2.6
1	X	1937	G	2.6
26	1	4	ASP	2.6
1	X	1104	G	2.6
23	V	5	GLU	2.5
1	X	1082	G	2.5
26	1	6	PRO	2.5
18	Q	71	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
6	D	75	SER	2.5
19	R	64	ASN	2.4
18	Q	91	LEU	2.4
10	I	52	GLY	2.4
21	T	14	ARG	2.4
26	1	35	LEU	2.4
26	1	8	ILE	2.4
20	S	33	ALA	2.4
3	A	220	HIS	2.4
7	E	50	LEU	2.4
10	I	23	PRO	2.4
15	N	118	GLN	2.4
18	Q	94	GLN	2.4
3	A	91	ARG	2.4
7	E	175	LYS	2.4
1	X	1555	A	2.3
1	X	356	A	2.3
1	X	1138	A	2.3
1	X	1939	U	2.3
1	X	2089	C	2.3
18	Q	89	GLU	2.3
7	E	173	ALA	2.3
8	G	37	ASP	2.3
20	S	10	PRO	2.3
1	X	2289	A	2.3
2	Y	38	C	2.3
21	T	15	ASP	2.3
20	S	12	GLN	2.3
27	2	46	ASP	2.3
1	X	1547	U	2.3
7	E	11	VAL	2.3
1	X	1888	C	2.3
23	V	7	ARG	2.3
1	X	1846	A	2.3
1	X	1492	A	2.2
1	X	1950	C	2.2
1	X	912	A	2.2
26	1	7	ARG	2.2
1	X	721	C	2.2
2	Y	111	C	2.2
7	E	15	VAL	2.2
7	E	49	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	1840	A	2.2
1	X	1118	G	2.2
1	X	246	C	2.2
8	G	36	ASN	2.2
1	X	2172	U	2.2
1	X	2090	U	2.1
11	J	117	GLU	2.1
1	X	722	C	2.1
7	E	14	GLY	2.1
7	E	48	ASP	2.1
1	X	1190	C	2.1
8	G	34	PRO	2.1
20	S	55	THR	2.1
1	X	135	U	2.1
11	J	118	ALA	2.1
1	X	1057	A	2.0
1	X	1839	A	2.0
22	U	16	ASN	2.0
1	X	247	A	2.0
1	X	559	C	2.0
1	X	1557	G	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	MG	X	2977	1/1	0.96	1.03	85.12	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	MG	X	2935	1/1	0.88	2.21	66.25	41,41,41,41	0
30	MG	X	2952	1/1	0.97	1.28	43.51	54,54,54,54	0
30	MG	X	2992	1/1	0.90	1.05	42.15	34,34,34,34	0
30	MG	X	2970	1/1	0.94	1.03	33.37	63,63,63,63	0
30	MG	X	2947	1/1	0.94	1.18	32.51	52,52,52,52	0
30	MG	X	2921	1/1	0.96	0.98	30.70	37,37,37,37	0
30	MG	X	2975	1/1	0.89	1.38	30.37	49,49,49,49	0
30	MG	X	3020	1/1	0.54	1.57	29.07	64,64,64,64	0
30	MG	X	2910	1/1	0.94	0.62	27.03	34,34,34,34	0
30	MG	X	3008	1/1	0.94	0.62	23.65	39,39,39,39	0
30	MG	X	2911	1/1	0.97	0.66	19.97	46,46,46,46	0
30	MG	X	2906	1/1	0.91	0.87	19.73	42,42,42,42	0
30	MG	X	2916	1/1	0.82	1.05	18.56	51,51,51,51	0
30	MG	X	2912	1/1	0.95	0.46	16.76	34,34,34,34	0
30	MG	X	2939	1/1	0.96	0.61	15.65	30,30,30,30	0
30	MG	X	2907	1/1	0.90	1.25	14.61	49,49,49,49	0
30	MG	K	201	1/1	0.83	0.69	14.53	31,31,31,31	0
30	MG	X	2963	1/1	0.98	0.67	14.51	71,71,71,71	0
30	MG	X	2925	1/1	0.92	0.53	11.43	43,43,43,43	0
30	MG	X	2918	1/1	0.98	0.47	10.87	45,45,45,45	0
30	MG	X	2969	1/1	0.99	0.64	10.71	43,43,43,43	0
30	MG	X	2964	1/1	0.92	0.53	10.70	60,60,60,60	0
30	MG	X	2946	1/1	0.98	0.43	10.65	34,34,34,34	0
30	MG	X	2993	1/1	0.98	0.42	10.22	44,44,44,44	0
30	MG	X	2959	1/1	0.96	0.69	9.95	54,54,54,54	0
30	MG	X	2990	1/1	0.96	0.63	9.85	39,39,39,39	0
30	MG	X	2924	1/1	0.99	0.39	9.74	30,30,30,30	0
30	MG	X	2931	1/1	0.96	0.58	9.73	32,32,32,32	0
30	MG	X	2941	1/1	0.97	0.43	9.41	55,55,55,55	0
30	MG	X	2915	1/1	0.98	0.36	9.06	36,36,36,36	0
30	MG	X	2978	1/1	0.92	0.42	9.04	49,49,49,49	0
30	MG	X	2903	1/1	0.95	0.61	8.38	37,37,37,37	0
30	MG	X	2936	1/1	0.98	0.48	7.90	53,53,53,53	0
30	MG	X	2954	1/1	0.99	0.56	7.77	41,41,41,41	0
30	MG	X	2980	1/1	0.97	0.44	5.83	49,49,49,49	0
30	MG	X	3017	1/1	0.88	0.76	5.60	52,52,52,52	0
30	MG	X	2981	1/1	0.92	0.61	5.30	99,99,99,99	0
30	MG	X	2983	1/1	0.98	0.30	4.80	63,63,63,63	0
30	MG	X	2926	1/1	0.97	0.32	4.77	32,32,32,32	0
30	MG	X	2957	1/1	0.96	0.33	4.75	42,42,42,42	0
30	MG	X	3014	1/1	0.97	0.29	3.61	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
29	6O1	X	2901	111/111	0.91	0.39	3.50	106,116,136,139	0
30	MG	X	3011	1/1	0.94	0.34	3.27	58,58,58,58	0
30	MG	X	2953	1/1	0.97	0.29	2.01	38,38,38,38	0
30	MG	X	2943	1/1	0.95	0.29	1.75	33,33,33,33	0
30	MG	X	2942	1/1	0.91	0.25	1.23	31,31,31,31	0
30	MG	X	3018	1/1	0.96	0.28	0.90	32,32,32,32	0
30	MG	X	2917	1/1	0.94	0.21	0.73	33,33,33,33	0
30	MG	X	2951	1/1	0.97	0.22	0.71	35,35,35,35	0
30	MG	X	2998	1/1	0.94	0.22	0.47	35,35,35,35	0
30	MG	X	2996	1/1	0.98	0.19	0.03	43,43,43,43	0
30	MG	K	202	1/1	0.95	0.19	-0.39	31,31,31,31	0
30	MG	X	2932	1/1	0.95	0.32	-	53,53,53,53	0
30	MG	X	2902	1/1	0.94	1.16	-	32,32,32,32	0
30	MG	X	2967	1/1	0.90	0.37	-	55,55,55,55	0
30	MG	X	3013	1/1	0.98	0.49	-	47,47,47,47	0
30	MG	X	2973	1/1	0.94	0.35	-	52,52,52,52	0
30	MG	X	3005	1/1	0.96	0.92	-	66,66,66,66	0
30	MG	X	3002	1/1	0.95	0.31	-	44,44,44,44	0
30	MG	X	2965	1/1	0.97	0.48	-	40,40,40,40	0
30	MG	X	2997	1/1	0.99	0.36	-	38,38,38,38	0
30	MG	X	2999	1/1	0.80	0.77	-	74,74,74,74	0
30	MG	X	2955	1/1	0.96	0.39	-	31,31,31,31	0
30	MG	Y	201	1/1	0.96	0.90	-	77,77,77,77	0
30	MG	X	2909	1/1	0.94	0.72	-	36,36,36,36	0
30	MG	X	3001	1/1	0.79	1.63	-	86,86,86,86	0
30	MG	X	2950	1/1	0.97	0.51	-	36,36,36,36	0
30	MG	X	2961	1/1	0.96	0.68	-	68,68,68,68	0
30	MG	X	3006	1/1	0.74	0.50	-	34,34,34,34	0
30	MG	X	2940	1/1	0.92	0.41	-	34,34,34,34	0
30	MG	X	2982	1/1	0.89	0.86	-	31,31,31,31	0
30	MG	X	2937	1/1	0.93	0.73	-	32,32,32,32	0
30	MG	X	2986	1/1	0.96	0.48	-	46,46,46,46	0
30	MG	X	2987	1/1	0.93	0.46	-	43,43,43,43	0
30	MG	X	2908	1/1	0.95	0.67	-	34,34,34,34	0
30	MG	X	2974	1/1	0.87	0.85	-	30,30,30,30	0
30	MG	X	2920	1/1	0.95	0.74	-	34,34,34,34	0
30	MG	X	3016	1/1	0.71	1.26	-	74,74,74,74	0
30	MG	X	2938	1/1	0.94	0.33	-	36,36,36,36	0
30	MG	X	2968	1/1	0.94	0.26	-	35,35,35,35	0
30	MG	X	3009	1/1	0.99	0.33	-	41,41,41,41	0
30	MG	X	2923	1/1	0.98	0.38	-	30,30,30,30	0
30	MG	X	3019	1/1	0.83	1.06	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MG	X	2928	1/1	0.91	0.17	-	41,41,41,41	0
30	MG	X	2995	1/1	0.93	0.82	-	83,83,83,83	0
30	MG	X	2966	1/1	0.98	0.34	-	37,37,37,37	0
30	MG	X	2930	1/1	0.97	0.64	-	46,46,46,46	0
30	MG	X	2913	1/1	0.91	0.63	-	36,36,36,36	0
30	MG	X	2976	1/1	0.94	0.49	-	53,53,53,53	0
30	MG	X	3015	1/1	0.89	0.55	-	98,98,98,98	0
30	MG	X	2945	1/1	0.93	1.19	-	55,55,55,55	0
30	MG	X	3012	1/1	0.74	0.39	-	52,52,52,52	0
30	MG	X	2985	1/1	0.98	0.27	-	55,55,55,55	0
30	MG	X	2905	1/1	0.97	0.82	-	30,30,30,30	0
30	MG	X	2933	1/1	0.88	1.35	-	38,38,38,38	0
30	MG	X	3004	1/1	0.96	0.30	-	54,54,54,54	0
30	MG	X	3007	1/1	0.88	0.50	-	40,40,40,40	0
30	MG	X	2948	1/1	0.97	0.26	-	30,30,30,30	0
30	MG	X	2927	1/1	0.79	0.54	-	57,57,57,57	0
30	MG	X	2971	1/1	0.92	0.62	-	33,33,33,33	0
30	MG	X	3010	1/1	0.97	0.27	-	41,41,41,41	0
30	MG	X	2972	1/1	0.92	0.63	-	36,36,36,36	0
30	MG	X	3000	1/1	0.98	0.28	-	39,39,39,39	0
30	MG	X	2962	1/1	0.98	0.20	-	41,41,41,41	0
30	MG	X	2922	1/1	0.95	0.45	-	35,35,35,35	0
30	MG	X	3003	1/1	0.95	0.87	-	63,63,63,63	0
30	MG	X	2984	1/1	0.97	0.56	-	49,49,49,49	0
30	MG	X	2956	1/1	0.95	0.58	-	32,32,32,32	0
30	MG	X	2904	1/1	0.91	1.01	-	32,32,32,32	0
30	MG	X	2989	1/1	0.96	0.67	-	56,56,56,56	0
30	MG	X	2979	1/1	0.90	0.29	-	46,46,46,46	0
30	MG	X	2994	1/1	0.94	0.37	-	77,77,77,77	0
30	MG	X	2949	1/1	0.96	0.35	-	32,32,32,32	0
30	MG	X	2914	1/1	0.96	0.46	-	43,43,43,43	0
30	MG	X	2944	1/1	0.93	0.88	-	37,37,37,37	0
30	MG	X	2991	1/1	0.96	0.69	-	72,72,72,72	0
30	MG	M	201	1/1	0.92	1.59	-	35,35,35,35	0
30	MG	X	2934	1/1	0.98	0.81	-	39,39,39,39	0
30	MG	X	2958	1/1	0.96	0.86	-	38,38,38,38	0
30	MG	X	2988	1/1	0.94	0.64	-	55,55,55,55	0
30	MG	X	2929	1/1	0.98	0.73	-	39,39,39,39	0
30	MG	X	2960	1/1	0.80	0.88	-	34,34,34,34	0
30	MG	X	2919	1/1	0.98	0.31	-	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.