



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:50 PM UTC

PDB ID : 4WFN / pdb_00004wfn
Title : Crystal structure of the large ribosomal subunit (50S) of *Deinococcus radiodurans* containing a three residue insertion in L22 in complex with erythromycin
Authors : Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on : 2014-09-16
Resolution : 3.54 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

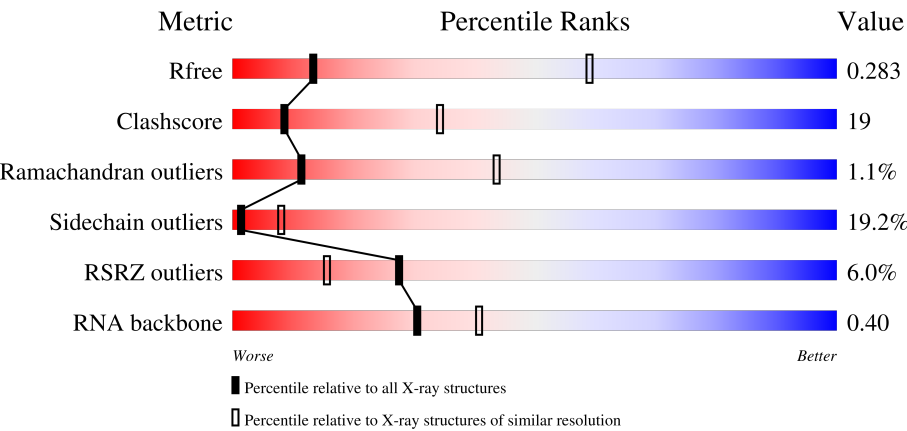
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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}	180053	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)
RNA backbone	3983	1006 (4.02-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	275	
2	B	211	
3	C	205	
4	D	180	

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Mol	Chain	Length	Quality of chain
5	E	185	
6	G	174	
7	H	134	
8	I	156	
9	J	141	
10	K	116	
11	L	114	
12	M	165	
13	N	118	
14	O	100	
15	P	137	
16	Q	95	
17	R	115	
18	S	237	
19	T	91	
20	U	81	
21	V	67	
22	W	55	
23	Z	60	
24	1	55	
25	2	47	
26	3	65	
27	X	2880	
28	Y	124	

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	MG	X	2904	-	-	-	X
29	MG	X	2914	-	-	-	X
29	MG	X	2915	-	-	-	X
29	MG	X	2916	-	-	-	X
29	MG	X	2918	-	-	-	X
29	MG	X	2926	-	-	-	X
29	MG	X	2935	-	-	-	X
29	MG	X	2943	-	-	-	X
29	MG	X	2965	-	-	-	X

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 84117 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1987	1235	399	350	3			

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L13.

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

- Molecule 7 is a protein called 50S ribosomal protein L14.

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

- Molecule 8 is a protein called 50S ribosomal protein L15.

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

- Molecule 9 is a protein called 50S ribosomal protein L16.

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

- Molecule 10 is a protein called 50S ribosomal protein L17.

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

- Molecule 11 is a protein called 50S ribosomal protein L18.

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

- Molecule 12 is a protein called 50S ribosomal protein L19.

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

- Molecule 13 is a protein called 50S ribosomal protein L20.

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

- Molecule 14 is a protein called 50S ribosomal protein L21.

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

- Molecule 15 is a protein called 50S ribosomal protein L22,50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	130	Total	C	N	O	S			
			1038	655	205	176	2	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	110	VAL	-	linker	UNP Q9RXJ7
P	111	PRO	-	linker	UNP Q9RXJ7
P	112	ARG	-	linker	UNP Q9RXJ7

- Molecule 16 is a protein called 50S ribosomal protein L23.

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

- Molecule 17 is a protein called 50S ribosomal protein L24.

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

- Molecule 18 is a protein called 50S ribosomal protein L25.

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

- Molecule 19 is a protein called 50S ribosomal protein L27.

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

- Molecule 20 is a protein called 50S ribosomal protein L28.

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

- Molecule 21 is a protein called 50S ribosomal protein L29.

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

- Molecule 22 is a protein called 50S ribosomal protein L30.

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

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	56	Total	C	N	O	S			
			443	272	91	75	5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	53	Total	C	N	O	S			
			431	274	80	76	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	46	Total	C	N	O	S			
			383	230	91	60	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	S			
			462	290	95	73	4	0	0	0

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	2680	Total	C	N	O	P	0	0	0
			57533	25663	10626	18564	2680			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

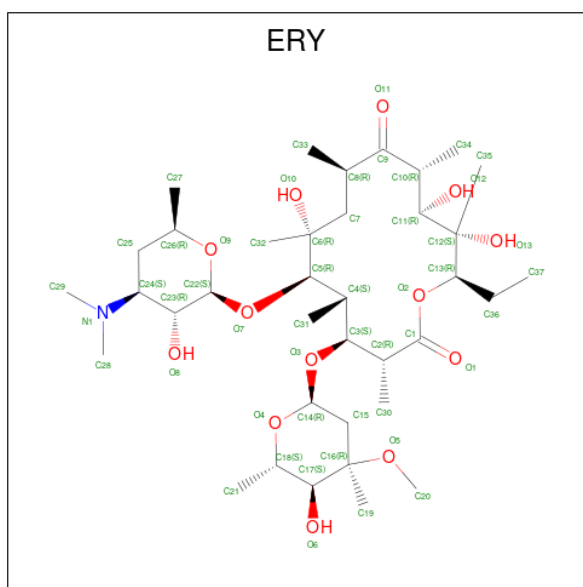
- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	1	Total	Mg	0	0
			1	1		
29	B	1	Total	Mg	0	0
			1	1		
29	K	2	Total	Mg	0	0
			2	2		
29	M	2	Total	Mg	0	0
			2	2		
29	X	64	Total	Mg	0	0
			64	64		

- Molecule 30 is ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃).

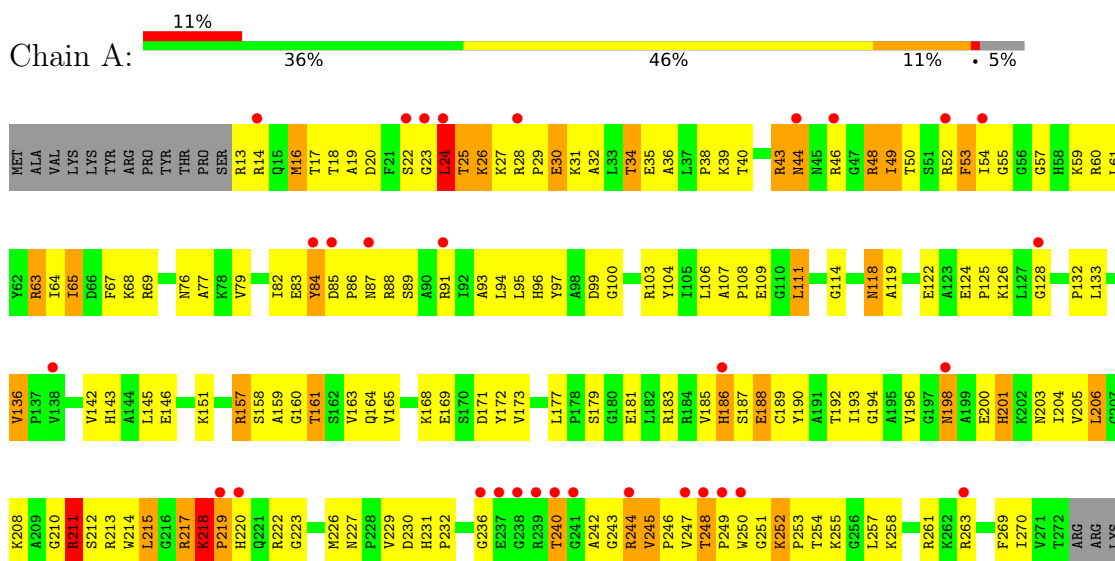


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	X	1	Total	C	N	O	0	0
			51	37	1	13		

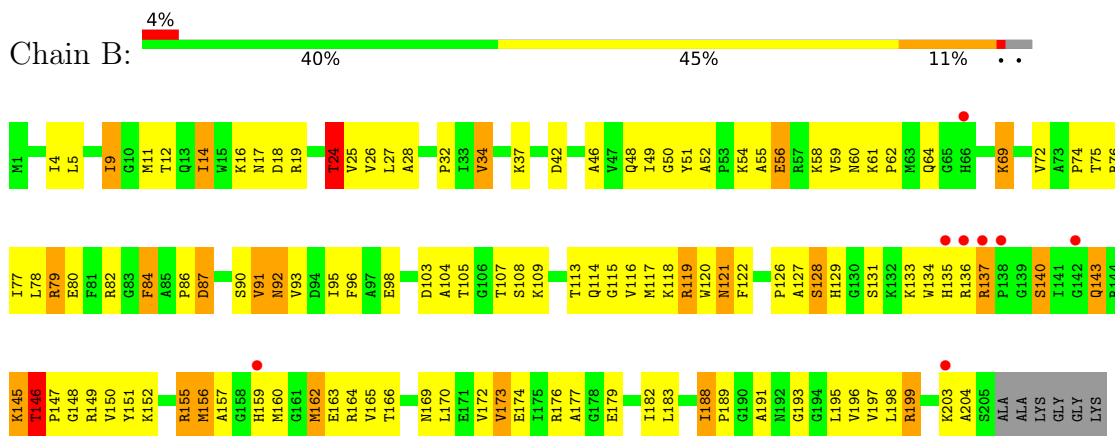
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: 50S ribosomal protein L2

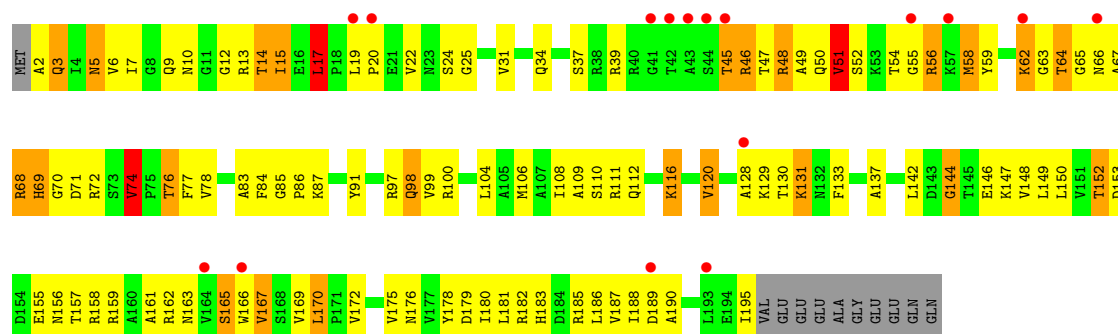


• Molecule 2: 50S ribosomal protein L3

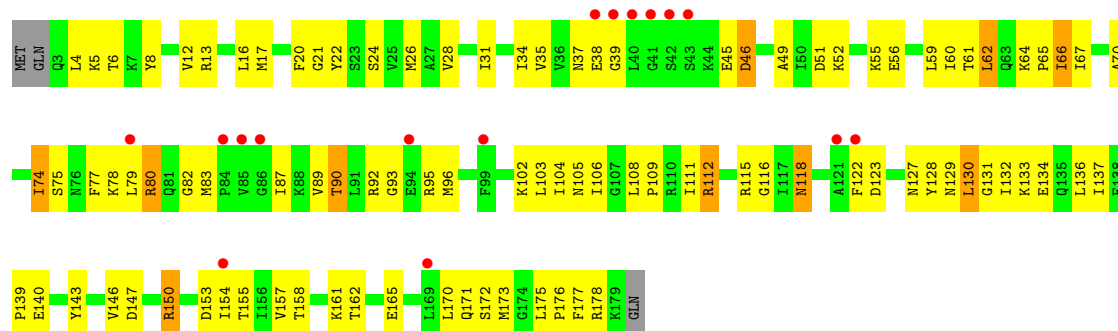
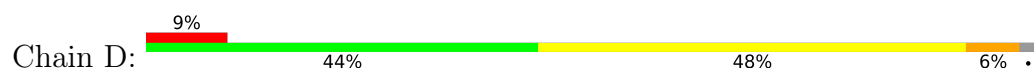


• Molecule 3: 50S ribosomal protein L4

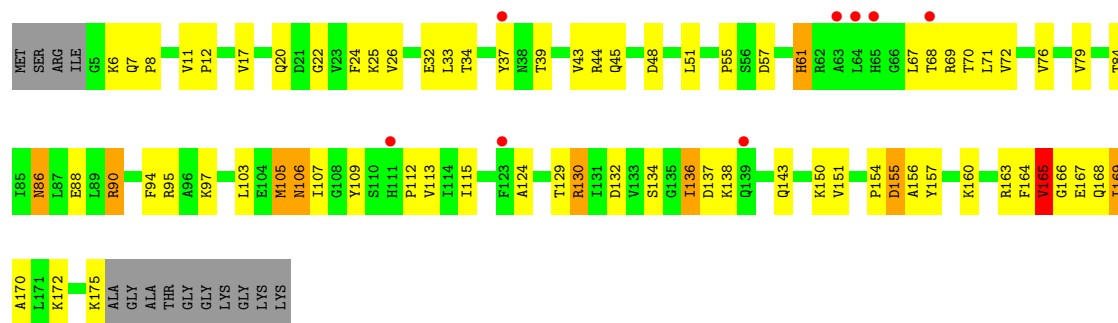




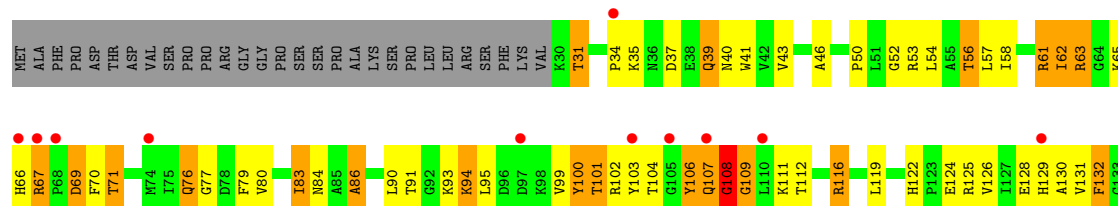
- Molecule 4: 50S ribosomal protein L5

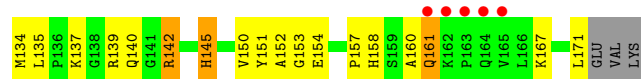


- Molecule 5: 50S ribosomal protein L6

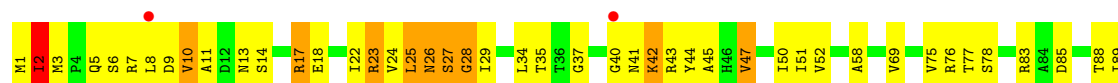
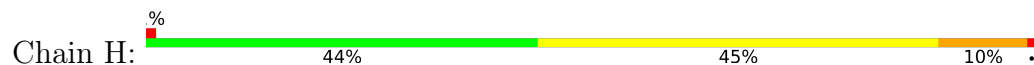


- Molecule 6: 50S ribosomal protein L13

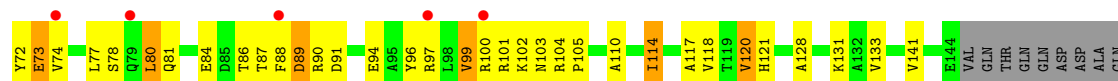
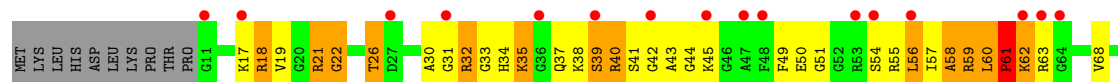
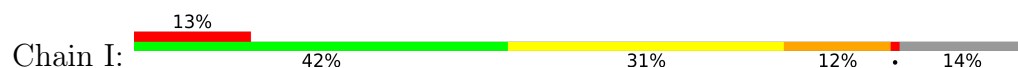




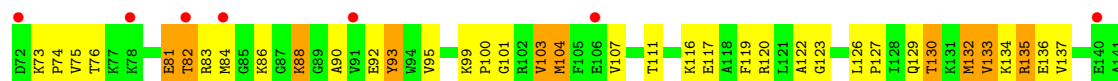
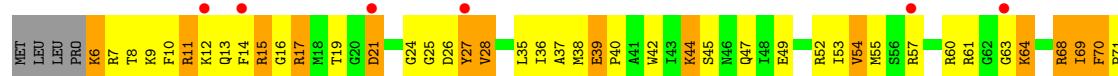
• Molecule 7: 50S ribosomal protein L14



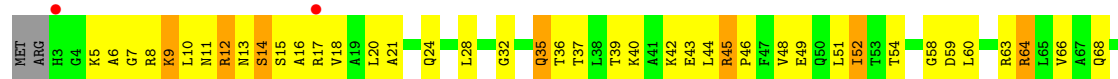
• Molecule 8: 50S ribosomal protein L15



• Molecule 9: 50S ribosomal protein L16

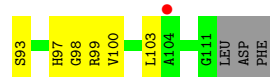
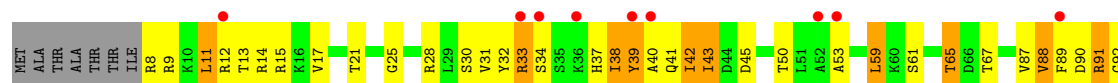


• Molecule 10: 50S ribosomal protein L17

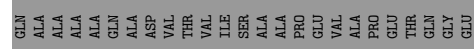
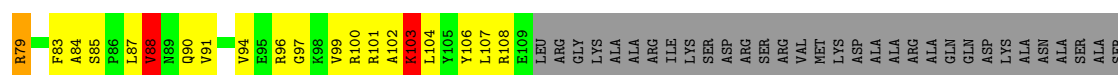
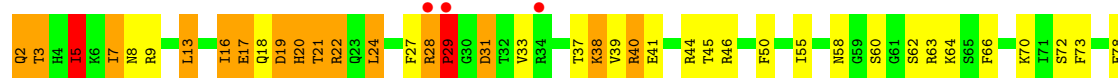
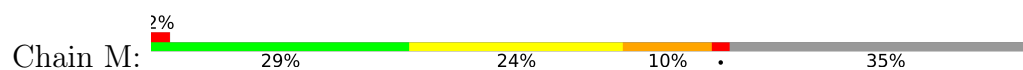




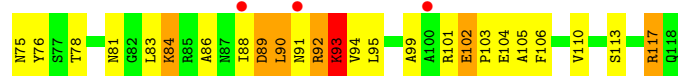
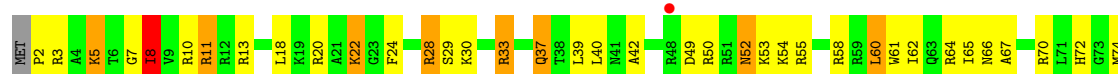
- Molecule 11: 50S ribosomal protein L18



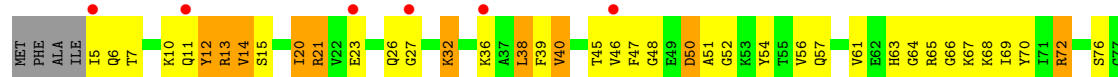
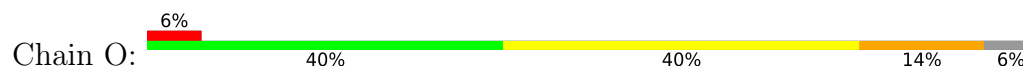
- Molecule 12: 50S ribosomal protein L19



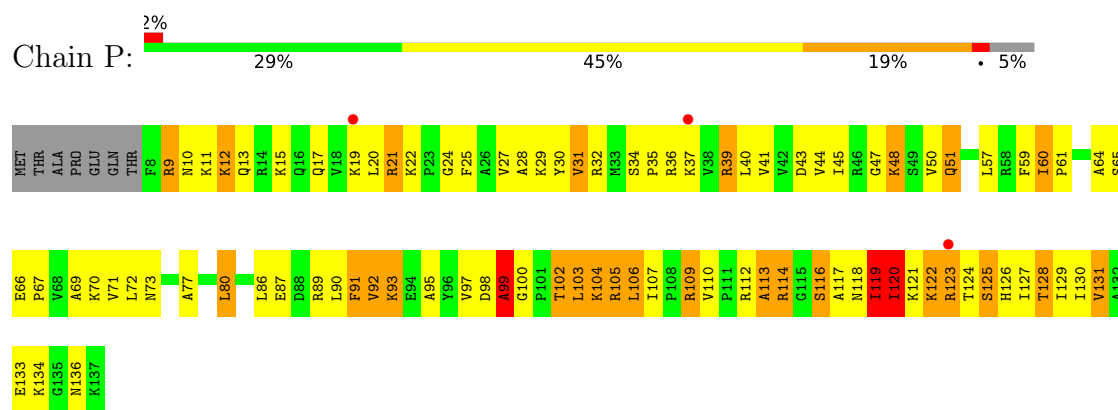
- Molecule 13: 50S ribosomal protein L20



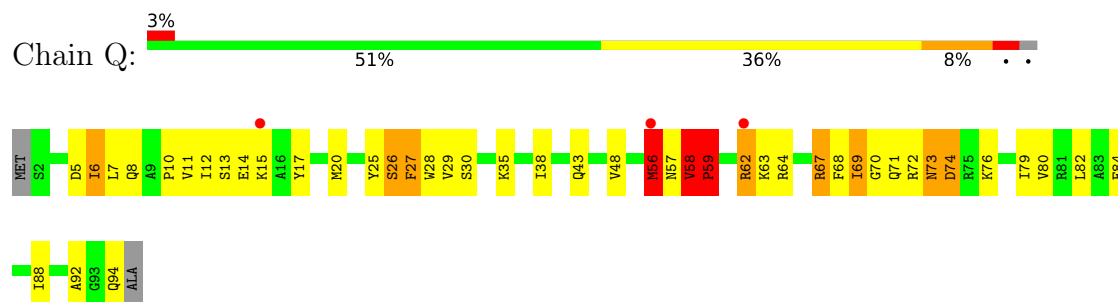
- Molecule 14: 50S ribosomal protein L21



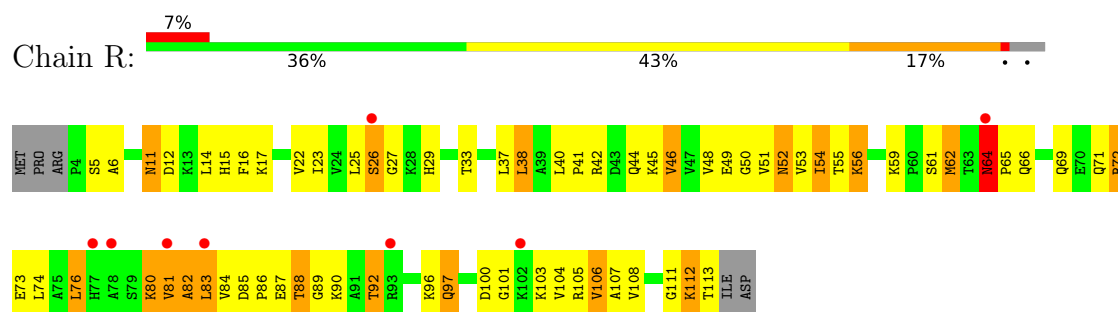
- Molecule 15: 50S ribosomal protein L22, 50S ribosomal protein L22



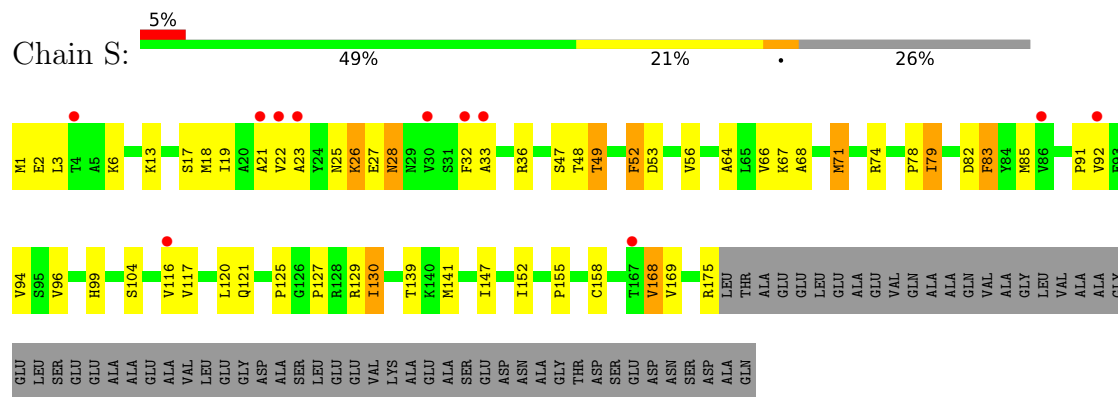
- Molecule 16: 50S ribosomal protein L23



- Molecule 17: 50S ribosomal protein L24

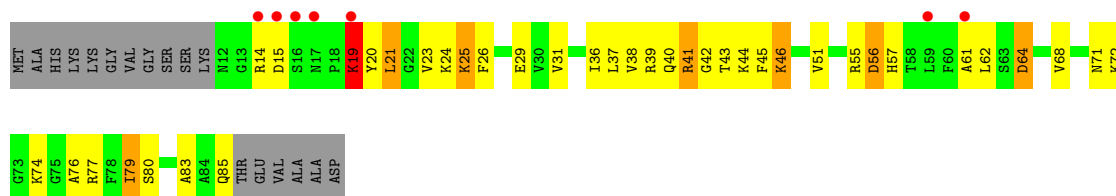


- Molecule 18: 50S ribosomal protein L25



- Molecule 19: 50S ribosomal protein L27

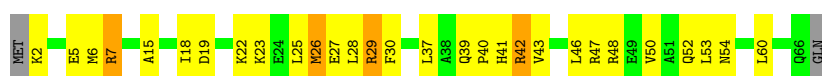




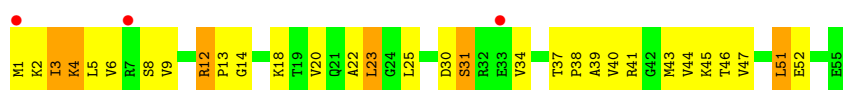
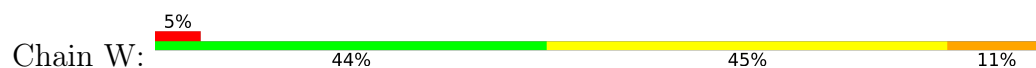
• Molecule 20: 50S ribosomal protein L28



• Molecule 21: 50S ribosomal protein L29



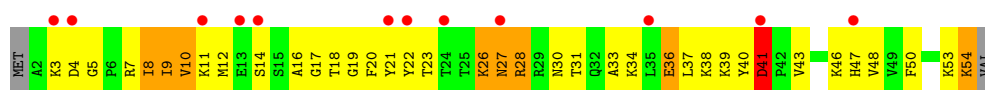
• Molecule 22: 50S ribosomal protein L30



• Molecule 23: 50S ribosomal protein L32



• Molecule 24: 50S ribosomal protein L33

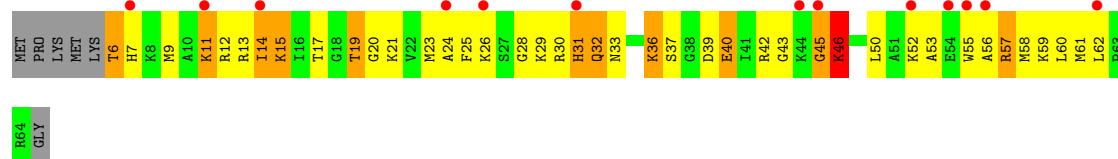


• Molecule 25: 50S ribosomal protein L34

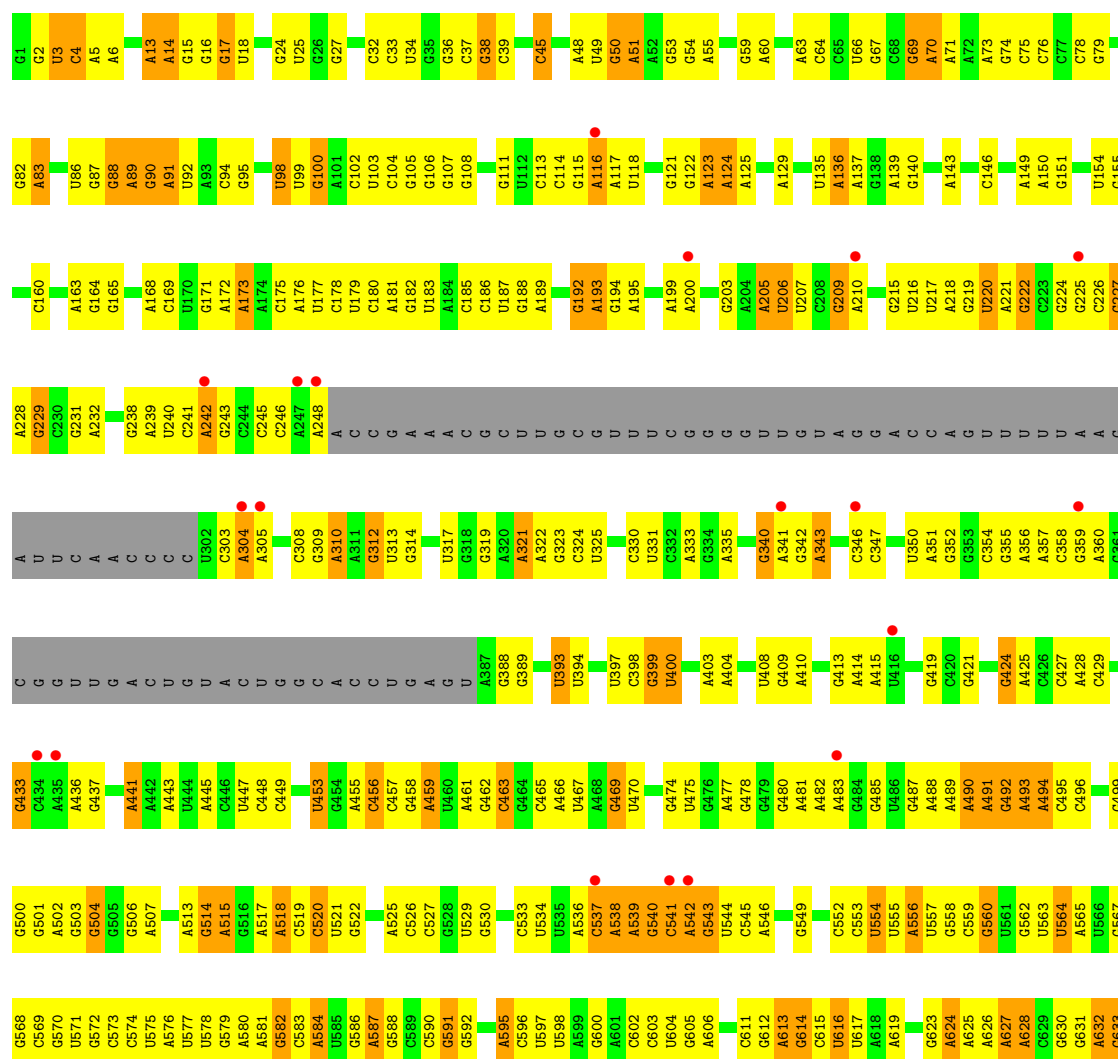




• Molecule 26: 50S ribosomal protein L35

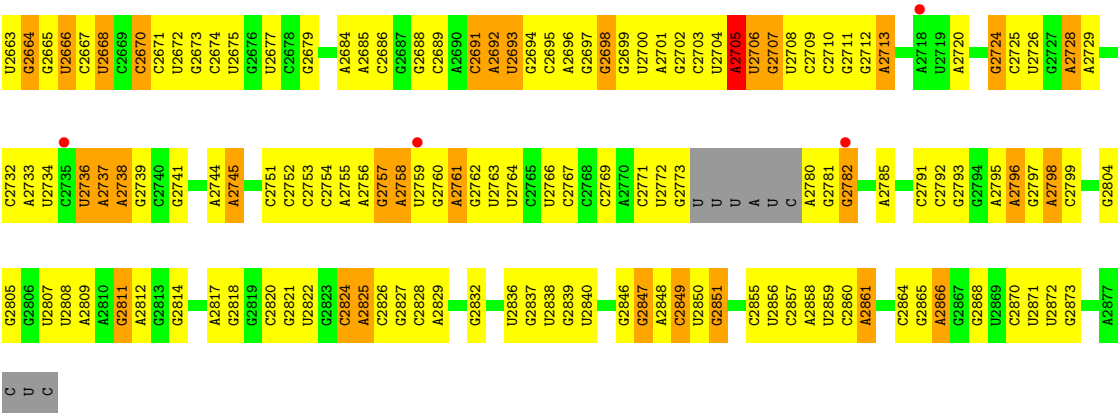


• Molecule 27: 23S ribosomal RNA

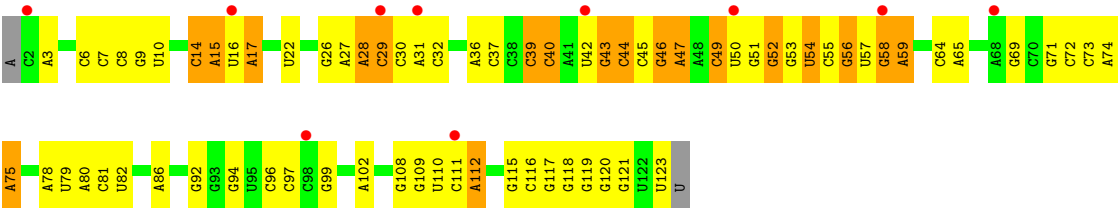


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A1597	U1505	G1435	U1365	A1287	U1217	G1142	G1069	A999	A929	G943	G772	C700	C635
C1598	A1506	G1436	A1366	A1288	C1218	C1145	U1071	G1000	A930	G844	A774	U701	G636
G1599	G1508	G1438	A1367	A1289	C1219	U1070	U1070	A1001	G931	U845	G773	G702	A637
U1600	G1514	G1439	G1291	G1291	G1220	G1147	G1073	U1005	G834	A846	U784	G704	A638
U1601	U1601	G1440	U1370	G1296	G1223	G1148	G1074	U1006	G935	U852	G787	C705	C640
G1602	A1603	A1441	G1371	G1296	A1224	G1149	A1080	A1007	C935	C853	A787	C711	G641
A1604	G1518	G1442	A1372	A1289	G1225	C1150	A1081	A1007	A936	G854	G788	A712	A642
U1607	G1519	G1444	G1374	A1290	A1226	U1151	G1082	U1010	C937	U857	A789	G713	G645
U1608	C1524	A1448	A1378	U1301	A1227	C1083	A1083	A1011	G939	G858	G791	G717	G646
U1609	A1525	U1448	A1379	C1302	G1228	A1154	A1084	U1014	G940	U859	U792	G717	G647
A1610	U1526	C1451	C1380	C1310	C1229	G1155	G1085	U1015	U941	C863	G793	C721	A648
C1614	C1528	U1452	C1381	C1311	C1230	U1159	C1086	U1016	U942	C864	A794	C721	G649
C1615	C1528	A1453	G1312	C1312	C1231	C1160	C1087	C1017	U943	A865	A796	C725	C651
C1616	C1531	U1454	U1313	U1313	G1236	U1161	A1088	C1018	G945	U871	G798	U727	G652
G1617	C1532	C1455	A1314	A1314	G1237	A1162	A1089	U1019	U946	C872	C799	U727	G653
C1623	A1533	C1456	C1385	A1315	A1238	C1163	U1093	A1020	C947	U873	C799	G728	A654
A1624	G1534	U1459	A1386	G1316	A1239	G1165	A1095	A1022	U951	G874	A801	C730	A655
A1625	U1539	G1461	G1387	G1317	G1240	A1166	A1096	U1023	G952	G875	A802	A731	A657
A1626	C1540	C1462	C1388	G1317	G1241	A1167	A1097	U1024	A952	A876	C803	G732	G658
G1629	G1541	U1465	A1321	A1321	U1247	U1171	G1098	U1025	U954	C877	C804	G733	G659
A1630	U1551	C1466	G1322	G1323	G1249	A1172	A1099	U1026	G955	C878	G805	G734	G660
C1631	C1552	U1467	U1324	U1325	A1250	U1173	U1101	C1027	A956	A879	A806	G735	C661
A1632	G1553	U1468	U1326	U1326	G1251	G1174	U1102	U1030	G957	C883	C808	G736	G662
G1633	U1554	U1469	C1327	C1327	C1252	A1175	C1103	U1031	G958	C884	C809	C737	G663
A1634	A1555	G1470	U1328	U1328	A1255	U1182	G1104	A1032	C959	A891	U810	G738	G664
G1635	A1556	U1471	G1329	U1329	C1256	C1183	U1105	G1033	U960	G891	G811	G739	A665
U1637	U1557	U1472	G1330	G1330	U1257	C1184	U1106	U1034	G961	G892	G812	G742	U666
C1640	G1562	C1473	G1331	G1331	G1258	C1185	U1107	G1035	C962	G893	G813	A743	A668
C1641	U1563	U1474	A1405	G1332	A1259	U1186	U1108	G1036	G963	G894	G814	G744	G669
G1642	U1564	G1475	A1406	A1334	A1261	A1187	U1109	U1037	A964	G895	G815	C745	U670
A1643	U1567	C1476	G1407	A1335	U1262	A1188	G1110	A1040	A866	G896	A817	G746	A671
G1644	A1568	U1477	A1408	G1336	G1263	G1189	C1111	G1041	C967	G897	G818	A747	C672
U1645	U1569	G1478	U1409	G1337	C1264	U1192	U1112	G1042	C968	U820	C819	A748	G673
G1646	G1570	U1481	U1410	C1340	G1265	U1194	A1114	A1043	U969	C898	U821	C750	C675
U1647	C1571	U1482	C1412	G1341	G1266	U1195	G1115	U1044	A970	A899	G822	G751	G676
C1648	C1572	G1483	U1413	U1342	A1267	G1196	U1116	G1045	A971	C899	C825	G752	G677
U1651	A1573	U1484	G1414	C1343	G1268	U1197	C1120	U1046	C972	A899	C826	U753	G682
G1652	U1574	U1485	C1344	C1344	C1270	G1200	G1121	U1051	U973	C897	C827	G754	A683
C1653	C1575	C1489	C1347	C1347	G1273	G1201	G1122	C1052	C976	C898	C828	C755	C684
A1654	U1580	U1490	C1348	C1348	C1274	U1202	G1123	G1053	U977	C899	C829	G758	U685
C1655	C1581	A1493	A1349	A1349	A1275	A1203	U1124	C1054	U978	A899	C830	G759	G686
U1656	U1582	U1494	G1350	G1350	U1276	G1204	C1127	A1055	A979	C899	C831	U760	G687
G1659	G1583	G1495	G1351	G1351	G1277	G1205	G1128	U1056	G980	A911	A832	G761	A690
C1661	A1586	C1497	A1352	A1352	U1278	G1206	G1133	A1057	C982	C914	A834	A762	C691
G1662	U1587	G1498	A1354	A1354	U1279	G1207	C1134	U1058	G983	C914	U835	A764	C692
C1663	A1588	C1501	U1357	U1357	A1281	G1209	C1137	A1059	G984	G920	G836	G765	A693
U1664	G1592	G1502	C1358	C1358	A1282	C1210	A1137	A1060	G985	A921	U837	A766	G694
C1665	U1592	G1503	G1359	G1359	C1283	U1212	A1139	A1065	A992	A922	A838	G767	G695
			A1433	A1360	A1285	U1213	A1140	G1067	C993	A923	U839	U768	U696
											U840	U770	A698

G1666	G1742	G1806	G1951	A2025	G	C	G2229	A2299	G2370	C2443	C2518	G2587
A1667	C1743	A1807	A1952	C2026	G	A	G2234	G2300	A2371	C2444	C2519	U2588
G1668	G1744	C1808	A1953	C2027	A	C	G2235	A2301	A2372	G	A2520	C2589
A1669	G1745	A1809	A1954	C2028	U	C	G2236	A2306	C2373	G2447	A2521	U2590
G1670	G1746	U1810	G1955	G2029	A	C	U2237	A2307	C2374	A2448	G2522	C2591
A1671	G1747	A1811	G1958	U2030	G	U	G	A2308	G2375	G2449	G2523	U2592
A1672	U1748	U1812	G1958	A2031	G	A2165	U2241	G2309	G2378	A2450	G2524	A2593
C1673	G1749	A1813	G1963	G2032	U	A2166	C2242	G2310	G2379	G2451	U2525	U2594
G1674	A1750	G1814	G1963	C2033	G	A2167	C2243	U2311	G2379	G2452	U2526	C2595
C1675	A1751	G1815	A1964	A2034	G	A2168	C2244	A2312	A2381	C2453	G2527	C2596
	U1752	G1816	U1965	G2035	G	A2169	A2245	A2313	A2381	C2454	G2528	C2597
	G1753	U1817	G1974	G2036	A	C2170	A2246	G2314	G2384	A2455	G2529	
U1679	U1754	G1818	G1975	A2037	G	U2171	A2247	A2315	U2385	U2456		A2600
U1680	G1755	U1819	G1976	C2038	C	U2172			G2386	A2457		C2601
A1681		A1820	U1977	G2039	U	G2173	G2250	C2321	G2389	G2460		C2605
G1682		A1821	U1978	A2040	C	G2174	U2251	U2322	A2390	G2463		C2606
G1684	G1761	C1825	U1978	A2041	G	A2175	A2252	U2323	G2394			A2614
A1685	C1762	U1826	U1978	A2042	G	A2176	A2253	G2324	C2395	U2470		U2615
A1686	G1763	A1827	A1980	A2043	G	A2182	C2254	A2325	C2396	U2471		U2616
G1687	A1764	A	A1981	G2044	A	C2183	G2255	A2326	C2397	U2472		G2617
U1688	G1765	U	A1982	A2045	A	C2184	G2256	U2327	A2397	G2473		
	U1766	A	G1985	C2046	A	U2185	A2257	G2328	G2398	U2474		
	G1767	C	G1986	C2047	C	G2186	G2258	G2329	U2398	C2475		
	U1768	G	G1987	G2048	U	A2187	G2259	G2330	C2399			
	U1769	U	A1988	C2049	G	A2188	C2260	A2331	G2400			
U1695	U1770	C		G2050	G	A2189	C2261	G2332	A2401			
C1696	A1771	C	C1991	U2051	C	A2190	C2262	U2333	U2402			
U1697	G1772	U1909	G1992	G2052	C	A2191	C2263	C2334	C2403			
G1698	C1773	A1910	G1992	G2053	U	U2185	C2264	U2335	A2404			
A1699	A1774	A1839	G1995	U2054	U	U2192	C2265	G2336	A2405			
C1700	A1775	A1840	A1996	G2055	U	C2193	A2266	A2337	C2406			
	U1776	G1841	A1997		U		A2267	C2338	G2407			
	G1777	G1842	A1997		G	U2196	G2268	A2339	G2408			
	U1778	U1914	U1999		G	U2197	G2269		A2409			
	C1779	G1844	U2000		U	U2198	U2270	C2340	U2410			
	A1780	A1845	A1919		U	G2200	G2271	A2341	A2413			
U1710	C1781	G1850	A2001		C	G2201	A2272	A2345				
G1712			A2002			G2202	C2273	G2346				
G1713			A2003		G	G2203		G2347				
A1714		G1854	U2004		U	G2204	A2278					
A1715	G1785	G1855	U2005		U	G2205	G2279	A2351				
G1716	C1786	U1856	U2006		G	C2205	A2280	A2352				
A1717	U1787	G1925	G2007		G		C2281	G2353				
U1718	C1788	U1926	C2008		A	G2209	G2282	A2354				
G1719	U1789	U1927	U2009		G		G2283	A2355				
	G1790	G1928	G2010		G	U2212	U2284	A2356				
	C1791	U1929	A2011		C	G2213	U2285	A2357				
	U1723	C1930	A2012		A	G2217	U2286	C2358				
C1724	A1794	A1867	A2013		A	G2218	G2287	U2359				
	A1868	U1869	A2014		C	U2219	A2288	C2360				
C1727	C1795	U1870	G2015		G	A2220	A2289	G2361				
A1728	U1796	G1871	A2016		U	G2221	A2290	C2362				
C1729	C1797	U1938	U2017		G	U2222	U2291	G2363				
G1730	G1798	U1939	G2018		U	U2223	C2292	C2364				
C1731	A1799	C1874	C2019		A	U2224	G2293	U2365				
U1732	A1800	C1875	G2020		A	U2225	U2294	U2366				
	C1801	C1876	G2021		A	A2226	G2295	A2367				
G1735	A1802	C1877	C2022		U	C2227	C2296	G2368				
C1736	G1803	C1878	C2023		A	U2228		U2369				
U1804	U1804	G1879	A1948		C							
G1737	G1805	G1880	C1950									



● Molecule 28: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.09Å 411.59Å 695.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.54 19.99 – 3.54	Depositor EDS
% Data completeness (in resolution range)	90.4 (19.99-3.54) 89.9 (19.99-3.54)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.234 , 0.282 0.235 , 0.283	Depositor DCC
R_{free} test set	13640 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	100.0	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	84117	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: ERY, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.60	0/2025	1.24	23/2726 (0.8%)
2	B	0.72	0/1567	1.14	6/2105 (0.3%)
3	C	0.61	0/1504	1.17	16/2036 (0.8%)
4	D	0.38	0/1419	0.89	2/1903 (0.1%)
5	E	0.40	0/1308	0.91	1/1771 (0.1%)
6	G	0.61	0/1138	1.24	14/1539 (0.9%)
7	H	0.79	1/1007 (0.1%)	1.21	8/1352 (0.6%)
8	I	0.63	0/1022	1.26	11/1366 (0.8%)
9	J	0.70	1/1113 (0.1%)	1.29	18/1486 (1.2%)
10	K	0.87	1/886 (0.1%)	1.30	8/1188 (0.7%)
11	L	0.46	0/785	0.93	1/1048 (0.1%)
12	M	0.86	0/884	1.33	8/1186 (0.7%)
13	N	0.55	0/994	1.06	6/1323 (0.5%)
14	O	0.52	0/750	1.07	8/1000 (0.8%)
15	P	0.78	0/1052	1.24	13/1409 (0.9%)
16	Q	0.57	0/737	1.21	8/988 (0.8%)
17	R	0.59	0/835	1.20	12/1121 (1.1%)
18	S	0.44	0/1370	0.93	1/1862 (0.1%)
19	T	0.55	0/563	1.13	4/747 (0.5%)
20	U	0.61	0/556	1.11	3/741 (0.4%)
21	V	0.36	0/529	0.91	2/704 (0.3%)
22	W	0.51	0/426	1.02	2/568 (0.4%)
23	Z	0.71	0/455	1.33	3/611 (0.5%)
24	1	0.56	0/438	1.19	5/583 (0.9%)
25	2	0.60	0/387	1.31	3/509 (0.6%)
26	3	0.65	0/468	1.36	6/614 (1.0%)
27	X	0.34	0/64429	0.55	3/100499 (0.0%)
28	Y	0.23	0/2907	0.42	0/4529
All	All	0.43	3/91554 (0.0%)	0.73	195/137514 (0.1%)

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
2	B	0	1
6	G	0	1
7	H	0	1
8	I	0	3
10	K	0	2
16	Q	0	1
17	R	0	1
19	T	0	1
20	U	0	1
23	Z	0	1
25	2	0	1
26	3	0	1
All	All	0	15

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	52	ILE	CA-CB	6.65	1.62	1.54
7	H	2	ILE	CA-CB	-5.75	1.46	1.54
9	J	19	THR	CA-C	5.41	1.58	1.52

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	92	GLY	N-CA-C	-12.79	95.74	110.96
25	2	38	GLY	N-CA-C	-11.94	96.42	111.70
6	G	106	TYR	N-CA-C	-11.74	90.24	109.96
1	A	245	VAL	CA-C-N	11.63	134.38	119.84
1	A	245	VAL	C-N-CA	11.63	134.38	119.84
16	Q	74	ASP	N-CA-C	10.47	123.17	110.91
25	2	43	THR	N-CA-C	10.04	123.15	111.11
1	A	218	LYS	CA-C-N	9.89	132.20	119.84
1	A	218	LYS	C-N-CA	9.89	132.20	119.84
2	B	193	GLY	N-CA-C	-9.47	102.90	115.21
8	I	22	GLY	CA-C-N	9.43	130.94	120.66
8	I	22	GLY	C-N-CA	9.43	130.94	120.66
3	C	56	ARG	N-CA-C	9.41	125.03	113.17
6	G	108	GLY	N-CA-C	-9.33	100.87	113.37
2	B	146	THR	CA-C-N	-9.10	108.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	146	THR	C-N-CA	-9.10	108.47	119.84
19	T	15	ASP	N-CA-C	9.01	121.45	110.91
3	C	68	ARG	N-CA-C	8.77	123.93	113.23
1	A	30	GLU	N-CA-C	8.69	121.08	110.91
9	J	82	THR	CB-CA-C	-8.63	104.50	115.89
16	Q	58	VAL	N-CA-C	8.47	117.12	107.89
16	Q	58	VAL	CA-C-N	8.40	130.34	119.84
16	Q	58	VAL	C-N-CA	8.40	130.34	119.84
12	M	58	ASN	N-CA-C	8.39	122.57	110.24
9	J	70	PHE	CA-C-N	8.29	129.50	120.13
9	J	70	PHE	C-N-CA	8.29	129.50	120.13
9	J	19	THR	N-CA-C	8.26	121.97	108.26
1	A	57	GLY	N-CA-C	8.21	119.75	111.95
26	3	14	ILE	N-CA-C	-8.01	104.90	112.83
6	G	109	GLY	N-CA-C	-7.94	104.37	114.37
8	I	56	LEU	N-CA-C	7.91	122.28	112.47
1	A	35	GLU	N-CA-C	7.89	120.88	111.02
12	M	103	LYS	N-CA-C	7.88	122.93	112.13
9	J	69	ILE	N-CA-C	7.84	119.66	112.29
10	K	83	VAL	N-CA-C	7.80	117.87	110.53
6	G	100	TYR	N-CA-C	-7.65	98.70	110.10
9	J	82	THR	N-CA-C	7.62	121.81	109.02
8	I	57	ILE	CB-CA-C	-7.57	105.28	111.71
15	P	60	ILE	CA-C-N	7.55	127.18	119.56
15	P	60	ILE	C-N-CA	7.55	127.18	119.56
13	N	90	LEU	N-CA-C	-7.54	103.98	113.02
1	A	211	ARG	N-CA-C	-7.52	103.09	111.82
1	A	34	THR	N-CA-C	7.51	120.65	108.34
17	R	64	ASN	CA-C-N	7.49	127.03	119.24
17	R	64	ASN	C-N-CA	7.49	127.03	119.24
3	C	17	LEU	CA-C-N	7.41	127.45	119.90
3	C	17	LEU	C-N-CA	7.41	127.45	119.90
1	A	179	SER	N-CA-C	-7.36	103.90	113.17
15	P	120	ILE	N-CA-C	7.34	124.62	109.34
4	D	118	ASN	CA-C-N	7.24	126.88	119.56
4	D	118	ASN	C-N-CA	7.24	126.88	119.56
12	M	17	GLU	N-CA-C	-7.22	95.43	110.80
1	A	242	ALA	N-CA-C	7.22	120.87	108.02
19	T	44	LYS	N-CA-C	-7.20	101.81	111.96
26	3	15	LYS	N-CA-C	7.13	120.30	110.24
9	J	101	GLY	N-CA-C	-7.10	106.24	114.69
9	J	25	GLY	N-CA-C	-7.09	102.52	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	50	GLU	N-CA-C	7.09	119.91	111.33
22	W	12	ARG	CA-C-N	7.06	127.48	119.92
22	W	12	ARG	C-N-CA	7.06	127.48	119.92
8	I	58	ALA	N-CA-C	-7.02	101.78	110.41
6	G	40	ASN	N-CA-C	6.90	120.38	110.10
26	3	45	GLY	N-CA-C	6.89	121.06	112.79
3	C	170	LEU	CA-C-N	6.75	127.14	119.92
3	C	170	LEU	C-N-CA	6.75	127.14	119.92
6	G	71	THR	CA-C-N	6.71	126.17	118.85
6	G	71	THR	C-N-CA	6.71	126.17	118.85
13	N	93	LYS	N-CA-C	6.70	120.09	110.24
26	3	46	LYS	N-CA-C	-6.58	100.47	110.14
6	G	86	ALA	N-CA-C	-6.57	104.20	111.36
17	R	59	LYS	CA-C-N	6.54	125.78	118.97
17	R	59	LYS	C-N-CA	6.54	125.78	118.97
8	I	57	ILE	N-CA-C	-6.52	105.35	111.48
1	A	44	ASN	N-CA-C	6.49	118.72	108.79
10	K	58	GLY	N-CA-C	6.48	124.15	115.59
24	1	5	GLY	CA-C-N	6.41	126.10	119.82
24	1	5	GLY	C-N-CA	6.41	126.10	119.82
23	Z	4	HIS	CA-C-N	6.41	127.85	119.84
23	Z	4	HIS	C-N-CA	6.41	127.85	119.84
9	J	15	ARG	N-CA-C	6.40	118.68	109.14
15	P	110	VAL	N-CA-C	6.37	114.41	107.60
27	X	1141	U	C2'-C3'-O3'	6.37	119.05	109.50
9	J	133	VAL	N-CA-C	6.36	116.28	108.53
12	M	5	ILE	N-CA-C	-6.35	99.08	108.85
21	V	39	GLN	CA-C-N	6.34	126.09	119.05
21	V	39	GLN	C-N-CA	6.34	126.09	119.05
10	K	95	THR	N-CA-C	-6.33	97.92	108.75
14	O	11	GLN	CB-CA-C	-6.30	107.52	116.34
17	R	26	SER	CB-CA-C	-6.28	109.31	116.54
18	S	96	VAL	N-CA-C	6.26	114.71	107.89
17	R	12	ASP	N-CA-C	-6.25	103.55	111.92
16	Q	67	ARG	N-CA-C	-6.23	105.54	113.02
1	A	53	PHE	N-CA-C	6.17	117.13	108.00
8	I	91	ASP	N-CA-C	6.17	120.96	113.38
15	P	93	LYS	N-CA-C	-6.14	103.91	111.40
13	N	52	ASN	N-CA-C	6.12	119.21	111.69
10	K	90	ARG	CA-C-N	6.11	127.48	119.84
10	K	90	ARG	C-N-CA	6.11	127.48	119.84
9	J	9	LYS	N-CA-C	6.05	119.86	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	107	GLN	N-CA-C	-6.04	100.45	109.15
24	1	37	LEU	N-CA-C	6.03	118.94	109.96
15	P	113	ALA	N-CA-C	5.97	117.56	108.07
1	A	20	ASP	N-CA-C	5.96	119.86	112.59
16	Q	56	MET	N-CA-C	5.93	116.93	108.74
2	B	127	ALA	N-CA-C	-5.89	106.08	113.20
15	P	59	PHE	N-CA-C	5.88	120.16	112.92
7	H	43	ARG	N-CA-C	5.88	119.71	112.54
1	A	240	THR	N-CA-C	5.86	115.58	107.73
9	J	92	GLU	N-CA-C	-5.85	102.62	111.34
19	T	21	LEU	CB-CA-C	-5.83	108.85	115.79
5	E	106	ASN	N-CA-C	5.82	118.39	108.02
20	U	33	LYS	N-CA-C	-5.81	104.58	111.03
15	P	119	ILE	N-CA-C	5.80	121.41	109.34
25	2	40	HIS	N-CA-C	-5.79	100.88	109.86
10	K	52	ILE	N-CA-CB	5.77	118.39	110.54
1	A	171	ASP	N-CA-C	-5.75	106.26	113.28
1	A	31	LYS	N-CA-C	5.75	118.04	109.25
14	O	61	VAL	N-CA-C	5.75	115.97	110.74
17	R	106	VAL	N-CA-C	5.74	116.63	108.42
26	3	40	GLU	N-CA-C	-5.70	105.05	112.23
9	J	39	GLU	CA-C-N	5.69	125.88	119.90
9	J	39	GLU	C-N-CA	5.69	125.88	119.90
10	K	108	VAL	CB-CA-C	-5.69	103.85	110.91
8	I	61	PRO	CA-C-N	-5.68	113.89	122.81
8	I	61	PRO	C-N-CA	-5.68	113.89	122.81
14	O	52	GLY	N-CA-C	-5.66	107.90	115.32
3	C	167	VAL	N-CA-C	5.66	117.06	108.80
15	P	116	SER	CB-CA-C	-5.64	110.06	116.54
7	H	27	SER	N-CA-C	5.62	118.04	111.02
2	B	90	SER	N-CA-C	5.61	117.92	107.99
14	O	14	VAL	N-CA-C	5.61	117.49	108.85
9	J	63	GLY	N-CA-C	-5.60	106.93	115.00
6	G	104	THR	N-CA-C	5.60	118.17	109.60
7	H	112	GLY	CA-C-N	5.60	125.60	119.89
7	H	112	GLY	C-N-CA	5.60	125.60	119.89
14	O	11	GLN	N-CA-C	5.60	116.28	108.00
9	J	11	ARG	N-CA-C	5.54	115.55	108.24
15	P	123	ARG	N-CA-C	-5.54	106.38	113.02
9	J	81	GLU	N-CA-C	5.53	115.54	108.24
20	U	17	SER	N-CA-C	5.53	117.65	109.69
14	O	95	ILE	CB-CA-C	-5.51	104.37	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	51	VAL	CB-CA-C	-5.51	104.92	111.97
17	R	6	ALA	N-CA-C	5.50	122.53	110.80
13	N	102	GLU	CA-C-N	5.49	124.68	118.97
13	N	102	GLU	C-N-CA	5.49	124.68	118.97
20	U	49	LYS	N-CA-C	5.49	118.40	109.24
17	R	46	VAL	CB-CA-C	-5.46	103.05	110.42
9	J	71	PRO	N-CA-C	5.45	119.44	110.55
13	N	89	ASP	N-CA-C	5.44	117.51	108.20
12	M	38	LYS	N-CA-C	5.44	117.26	108.34
15	P	119	ILE	CA-C-N	5.42	131.73	121.97
15	P	119	ILE	C-N-CA	5.42	131.73	121.97
26	3	36	LYS	N-CA-C	5.36	117.63	108.90
2	B	24	THR	N-CA-C	-5.35	99.71	108.76
24	1	41	ASP	CA-C-N	5.35	126.53	119.84
24	1	41	ASP	C-N-CA	5.35	126.53	119.84
6	G	94	LYS	N-CA-C	-5.34	103.38	111.56
1	A	24	LEU	N-CA-C	5.34	122.18	110.80
7	H	76	ARG	N-CA-C	5.32	117.32	108.02
3	C	3	GLN	N-CA-C	5.30	117.45	109.23
8	I	37	GLN	N-CA-C	5.29	115.83	108.00
12	M	28	ARG	CA-C-N	5.28	126.44	119.84
12	M	28	ARG	C-N-CA	5.28	126.44	119.84
6	G	112	THR	N-CA-C	5.28	117.57	109.07
17	R	82	ALA	N-CA-C	5.26	117.19	108.20
6	G	63	ARG	N-CA-C	-5.23	106.40	112.89
12	M	88	VAL	N-CA-C	5.23	115.65	108.12
7	H	26	ASN	N-CA-C	5.22	119.34	112.92
1	A	22	SER	N-CA-C	5.17	117.11	108.99
3	C	58	MET	N-CA-C	5.17	121.81	110.80
3	C	74	VAL	CA-C-N	5.17	124.83	119.56
3	C	74	VAL	C-N-CA	5.17	124.83	119.56
3	C	49	ALA	N-CA-C	-5.16	106.67	112.87
11	L	53	ALA	N-CA-C	5.15	116.94	110.91
1	A	261	ARG	N-CA-C	5.15	116.12	108.86
7	H	85	ASP	N-CA-C	-5.14	106.86	113.23
14	O	95	ILE	N-CA-C	5.13	114.14	106.85
3	C	69	HIS	N-CA-C	5.13	118.11	109.95
6	G	142	ARG	N-CA-C	-5.13	104.95	111.11
15	P	99	ALA	N-CA-C	5.13	121.73	110.80
17	R	76	LEU	N-CA-C	5.13	116.78	109.14
3	C	144	GLY	N-CA-C	-5.12	108.20	115.43
19	T	24	LYS	N-CA-C	5.12	116.72	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	131	LYS	N-CA-C	-5.12	105.39	111.69
23	Z	55	ARG	N-CA-C	5.11	117.78	109.24
14	O	50	ASP	N-CA-C	-5.08	107.08	113.28
16	Q	30	SER	CA-C-N	5.08	125.11	119.32
16	Q	30	SER	C-N-CA	5.08	125.11	119.32
27	X	1975	G	C2'-C3'-O3'	5.07	117.11	109.50
1	A	236	GLY	CA-C-O	-5.07	118.92	122.22
17	R	29	HIS	N-CA-C	-5.07	104.25	111.24
7	H	28	GLY	N-CA-C	5.06	125.16	113.18
1	A	136	VAL	CA-C-N	5.04	125.31	119.92
1	A	136	VAL	C-N-CA	5.04	125.31	119.92
27	X	2705	A	C4'-C3'-O3'	5.04	116.96	109.40

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	2	42	LEU	Peptide
26	3	45	GLY	Peptide
2	B	146	THR	Peptide
6	G	108	GLY	Peptide
7	H	26	ASN	Peptide
8	I	35	LYS	Peptide
8	I	40	ARG	Peptide
8	I	99	VAL	Peptide
10	K	93	GLY	Peptide
10	K	94	TYR	Peptide
16	Q	59	PRO	Peptide
17	R	64	ASN	Peptide
19	T	19	LYS	Peptide
20	U	30	VAL	Peptide
23	Z	4	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1987	0	2056	145	0
2	B	1539	0	1600	115	0
3	C	1481	0	1504	101	0
4	D	1400	0	1481	61	0
5	E	1286	0	1336	54	0
6	G	1114	0	1144	75	0
7	H	997	0	1046	57	0
8	I	1011	0	1047	74	0
9	J	1090	0	1125	64	0
10	K	878	0	930	47	0
11	L	779	0	820	36	0
12	M	871	0	894	61	0
13	N	978	0	1020	54	0
14	O	741	0	756	52	0
15	P	1038	0	1125	87	0
16	Q	726	0	753	35	0
17	R	825	0	881	54	0
18	S	1345	0	1372	42	0
19	T	556	0	579	30	0
20	U	552	0	604	36	0
21	V	525	0	546	21	0
22	W	424	0	470	18	0
23	Z	443	0	444	27	0
24	1	431	0	456	30	0
25	2	383	0	414	26	0
26	3	462	0	506	54	0
27	X	57533	0	28987	1345	0
28	Y	2601	0	1327	65	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	K	2	0	0	0	0
29	M	2	0	0	0	0
29	X	64	0	0	0	0
30	X	51	0	67	9	0
All	All	84117	0	55290	2511	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 19.

All (2511) 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)
2:B:116:VAL:HG22	2:B:136:ARG:HG3	1.32	1.11
23:Z:19:ARG:NH2	27:X:1277:G:OP1	1.90	1.04
13:N:66:ASN:HB3	13:N:76:TYR:HB2	1.46	0.97
27:X:854:G:H1	27:X:948:C:H42	1.04	0.96
7:H:40:GLY:HA3	27:X:2545:A:H61	1.29	0.95
8:I:21:ARG:HE	8:I:22:GLY:H	1.08	0.95
6:G:109:GLY:HA2	6:G:111:LYS:HE3	1.46	0.95
27:X:517:A:H5''	27:X:518:A:H5'	1.50	0.94
1:A:250:TRP:O	1:A:255:LYS:NZ	2.01	0.93
27:X:2447:G:HO2'	27:X:2448:A:H8	1.07	0.92
9:J:82:THR:HA	27:X:2474:G:H5''	1.53	0.90
27:X:4:C:H42	27:X:2873:G:H1	1.17	0.89
1:A:55:GLY:H	1:A:217:ARG:HB2	1.38	0.88
27:X:571:U:HO2'	27:X:581:A:H8	1.21	0.87
10:K:60:LEU:HG	10:K:64:ARG:HD2	1.55	0.86
27:X:2281:C:H42	27:X:2293:G:H1	1.23	0.86
20:U:38:THR:HB	27:X:2063:A:H5'	1.58	0.85
15:P:80:LEU:HD11	15:P:87:GLU:HB3	1.58	0.85
8:I:21:ARG:HE	8:I:22:GLY:N	1.75	0.85
24:1:41:ASP:HB2	24:1:46:LYS:HE3	1.56	0.85
27:X:538:A:H62	27:X:2026:C:H5'	1.40	0.84
27:X:832:A:OP2	27:X:1201:G:N2	2.10	0.84
1:A:218:LYS:NZ	1:A:219:PRO:O	2.10	0.84
27:X:2016:A:O2'	27:X:2018:G:OP2	1.95	0.84
27:X:833:A:N3	27:X:954:U:O2'	2.10	0.83
27:X:2225:G:H2'	27:X:2226:A:H8	1.41	0.83
9:J:83:ARG:HH22	27:X:971:A:H61	1.22	0.83
27:X:2757:G:H5''	27:X:2758:A:H5'	1.60	0.83
26:3:13:ARG:HE	26:3:25:PHE:H	1.27	0.83
15:P:100:GLY:HA3	15:P:124:THR:HA	1.58	0.83
2:B:14:ILE:HG12	12:M:20:HIS:HD2	1.43	0.82
27:X:2811:G:H2'	27:X:2812:A:C8	2.13	0.82
2:B:146:THR:HG1	27:X:2550:C:HO2'	1.12	0.81
14:O:12:TYR:HB3	14:O:40:VAL:H	1.45	0.81
27:X:649:G:H22	27:X:661:C:H1'	1.45	0.81
22:W:8:SER:HB2	27:X:999:A:H5''	1.62	0.81
1:A:243:GLY:C	1:A:244:ARG:HE	1.89	0.80
27:X:1173:G:H2'	27:X:1174:G:H8	1.46	0.80
6:G:37:ASP:O	6:G:39:GLN:NE2	2.15	0.79
27:X:841:G:H2'	27:X:842:A:C8	2.16	0.79
27:X:2259:G:H4'	27:X:2306:A:H5'	1.65	0.79
27:X:415:A:H61	27:X:436:A:H61	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:H	1:A:252:LYS:HZ2	1.28	0.78
15:P:99:ALA:HB2	27:X:24:G:O2'	1.83	0.78
2:B:82:ARG:NH2	27:X:2617:G:OP2	2.16	0.78
26:3:26:LYS:HD3	26:3:28:GLY:H	1.45	0.78
9:J:17:ARG:NH1	27:X:966:A:OP2	2.17	0.78
15:P:30:TYR:H	15:P:126:HIS:HD2	1.32	0.78
14:O:57:GLN:H	14:O:97:GLY:HA3	1.47	0.78
27:X:538:A:O2'	27:X:539:A:O5'	2.00	0.78
2:B:51:TYR:HE2	12:M:3:THR:HG21	1.49	0.77
18:S:125:PRO:O	18:S:129:ARG:NH1	2.18	0.77
1:A:157:ARG:NH1	27:X:1810:U:OP2	2.17	0.77
9:J:100:PRO:HB2	18:S:74:ARG:HG2	1.67	0.77
7:H:23:ARG:NH1	27:X:2526:U:O2	2.17	0.77
27:X:2796:A:H2'	27:X:2797:G:C8	2.19	0.77
27:X:89:A:H4'	27:X:90:G:H5'	1.68	0.76
27:X:1856:U:OP1	27:X:2389:G:O2'	2.02	0.76
3:C:163:ASN:HD21	3:C:167:VAL:H	1.31	0.76
27:X:215:G:H21	27:X:632:A:H8	1.30	0.76
27:X:1882:G:N2	27:X:1885:C:H41	1.83	0.76
20:U:21:ARG:HD3	20:U:23:LYS:HG2	1.66	0.76
3:C:162:ARG:NH1	3:C:162:ARG:O	2.19	0.76
27:X:1329:U:H2'	27:X:1330:G:H8	1.49	0.76
27:X:2002:A:N6	27:X:2018:G:O6	2.19	0.76
1:A:14:ARG:HG3	1:A:24:LEU:HG	1.68	0.76
8:I:40:ARG:NH2	27:X:820:U:OP1	2.18	0.76
2:B:176:ARG:HH21	12:M:16:ILE:HG23	1.51	0.75
3:C:161:ALA:HB1	3:C:167:VAL:HG21	1.69	0.75
27:X:2543:A:H5'	27:X:2627:G:H4'	1.66	0.75
27:X:2761:A:H5''	27:X:2762:G:H5'	1.67	0.75
1:A:24:LEU:HB2	1:A:205:VAL:HG22	1.68	0.75
15:P:45:ILE:HD11	15:P:57:LEU:HD11	1.68	0.75
27:X:965:G:O2'	27:X:2253:A:N1	2.20	0.75
3:C:137:ALA:HB1	3:C:142:LEU:HB2	1.68	0.75
1:A:210:GLY:HA2	1:A:213:ARG:HG2	1.69	0.75
16:Q:14:GLU:OE2	27:X:1405:A:N6	2.18	0.75
17:R:56:LYS:HB3	17:R:69:GLN:HG2	1.69	0.75
24:1:27:ASN:ND2	24:1:36:GLU:OE1	2.20	0.75
27:X:1327:C:H42	27:X:1351:G:H1	1.32	0.75
26:3:32:GLN:HB3	27:X:2400:G:N7	2.02	0.75
27:X:27:G:N2	27:X:522:G:H1'	2.02	0.75
27:X:2225:G:H2'	27:X:2226:A:C8	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2796:A:H2'	27:X:2797:G:H8	1.50	0.74
11:L:90:ASP:OD2	11:L:91:ARG:N	2.20	0.74
1:A:91:ARG:HB2	1:A:107:ALA:HB3	1.69	0.74
9:J:15:ARG:HH21	9:J:73:LYS:HZ2	1.33	0.74
15:P:30:TYR:H	15:P:126:HIS:CD2	2.05	0.74
2:B:91:VAL:HB	2:B:93:VAL:HG12	1.70	0.74
27:X:1278:A:H2	27:X:1997:A:H62	1.35	0.74
27:X:1673:C:H2'	27:X:1674:C:H6	1.52	0.74
27:X:591:G:H3'	27:X:592:G:H8	1.51	0.74
27:X:1922:U:H3'	27:X:1923:U:H5'	1.70	0.74
6:G:34:PRO:HB3	6:G:71:THR:HG21	1.69	0.74
9:J:117:GLU:OE1	9:J:120:ARG:NH1	2.21	0.74
12:M:60:SER:HA	12:M:64:LYS:HB2	1.69	0.74
27:X:2757:G:OP2	27:X:2761:A:O2'	2.06	0.74
22:W:5:LEU:HB2	22:W:25:LEU:HD13	1.68	0.74
25:2:19:ARG:HG2	27:X:123:A:H5'	1.68	0.74
27:X:465:C:O2'	27:X:483:A:N6	2.21	0.74
27:X:2820:C:H2'	27:X:2821:G:H8	1.52	0.73
11:L:65:THR:OG1	28:Y:52:G:OP1	2.06	0.73
27:X:1337:G:N2	27:X:1343:C:O2	2.20	0.73
2:B:137:ARG:NH2	27:X:2034:A:OP1	2.19	0.73
27:X:854:G:N2	27:X:948:C:N3	2.32	0.73
2:B:9:ILE:HD11	2:B:27:LEU:HB2	1.70	0.73
27:X:872:G:O2'	27:X:928:G:O6	2.07	0.73
2:B:128:SER:HB3	27:X:1976:U:H4'	1.71	0.73
12:M:100:ARG:HD2	27:X:1744:G:OP1	1.89	0.73
27:X:115:G:OP2	27:X:117:A:O2'	2.07	0.73
27:X:613:A:N6	27:X:668:A:O2'	2.22	0.73
4:D:116:GLY:HA2	4:D:176:PRO:HB2	1.71	0.73
27:X:1963:G:O2'	27:X:1965:U:OP2	2.07	0.73
15:P:35:PRO:HD3	15:P:124:THR:OG1	1.89	0.73
27:X:2708:U:H2'	27:X:2709:C:C6	2.23	0.73
17:R:17:LYS:NZ	27:X:83:A:OP2	2.16	0.72
27:X:2484:G:H22	30:X:2902:ERY:H191	1.54	0.72
17:R:105:ARG:HH22	17:R:113:THR:H	1.37	0.72
27:X:313:U:H2'	27:X:314:G:H8	1.54	0.72
1:A:63:ARG:HH21	1:A:86:PRO:HD2	1.55	0.72
2:B:152:LYS:HB3	6:G:106:TYR:HB2	1.71	0.72
16:Q:35:LYS:NZ	27:X:1615:C:OP2	2.23	0.72
27:X:1399:C:OP2	27:X:1409:U:N3	2.21	0.72
14:O:68:LYS:NZ	27:X:1238:A:OP1	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:16:ARG:NH1	23:Z:17:ASP:OD2	2.22	0.72
27:X:1744:G:N2	27:X:1747:G:OP2	2.18	0.72
24:1:28:ARG:NH1	27:X:2264:C:OP2	2.22	0.72
27:X:1643:A:H61	27:X:1656:U:H3	1.38	0.72
1:A:54:ILE:HA	1:A:217:ARG:H	1.55	0.71
27:X:168:A:H2'	27:X:169:C:C6	2.24	0.71
27:X:209:G:N2	27:X:433:G:OP1	2.22	0.71
3:C:6:VAL:HG13	3:C:7:ILE:HG12	1.72	0.71
14:O:66:GLY:O	14:O:87:ARG:NH2	2.23	0.71
27:X:1030:U:H3	27:X:1153:A:H62	1.38	0.71
16:Q:64:ARG:NH2	27:X:1348:C:O2'	2.22	0.71
26:3:30:ARG:HE	26:3:31:HIS:CE1	2.09	0.71
27:X:2048:C:O2	27:X:2428:U:N3	2.20	0.71
9:J:16:GLY:HA2	9:J:17:ARG:HH11	1.55	0.71
27:X:2020:G:H2'	27:X:2021:G:C8	2.26	0.71
27:X:1551:U:OP2	27:X:1553:G:N2	2.24	0.71
3:C:149:LEU:HD11	3:C:170:LEU:HB2	1.73	0.71
6:G:56:THR:HA	6:G:134:MET:HE1	1.73	0.71
8:I:38:LYS:NZ	27:X:954:U:OP2	2.20	0.71
22:W:25:LEU:HD22	22:W:30:ASP:HB3	1.73	0.71
27:X:2354:G:N2	27:X:2357:A:OP2	2.22	0.71
8:I:31:GLY:O	8:I:32:ARG:NH2	2.23	0.71
27:X:1466:C:H2'	27:X:1467:U:O4'	1.91	0.71
6:G:116:ARG:HA	6:G:119:LEU:HD23	1.73	0.70
8:I:18:ARG:NH2	8:I:18:ARG:O	2.23	0.70
27:X:1845:A:N3	27:X:2212:U:O2'	2.24	0.70
28:Y:51:G:H2'	28:Y:52:G:H8	1.56	0.70
6:G:100:TYR:HB2	6:G:116:ARG:NH1	2.06	0.70
27:X:1361:G:H1	27:X:1614:C:H42	1.39	0.70
7:H:28:GLY:HA3	7:H:35:THR:OG1	1.91	0.70
8:I:17:LYS:HG3	8:I:19:VAL:H	1.57	0.70
24:1:41:ASP:OD1	24:1:41:ASP:N	2.24	0.70
5:E:33:LEU:HD21	5:E:136:ILE:HB	1.73	0.70
26:3:13:ARG:NE	26:3:25:PHE:H	1.89	0.70
1:A:96:HIS:NE2	27:X:1517:C:O2'	2.21	0.69
27:X:113:C:HO2'	27:X:125:A:HO2'	1.40	0.69
27:X:538:A:HO2'	27:X:539:A:P	2.15	0.69
27:X:661:C:H2'	27:X:662:G:C8	2.27	0.69
5:E:124:ALA:HB3	5:E:132:ASP:HB3	1.73	0.69
10:K:24:GLN:HB3	10:K:44:LEU:HD22	1.74	0.69
27:X:27:G:H22	27:X:522:G:HI1'	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2241:U:H2'	27:X:2242:C:H6	1.56	0.69
1:A:231:HIS:CD2	1:A:232:PRO:HD2	2.26	0.69
1:A:249:PRO:HD3	27:X:2218:G:H5'	1.73	0.69
27:X:793:G:H21	27:X:796:A:H62	1.38	0.69
27:X:1089:C:O2'	27:X:1099:A:OP1	2.10	0.69
27:X:2237:C:O2'	27:X:2406:C:OP2	2.11	0.69
12:M:31:ASP:HB2	12:M:94:VAL:HB	1.75	0.69
14:O:23:GLU:HB2	14:O:91:THR:HG21	1.75	0.69
27:X:953:G:O2'	27:X:1203:A:N3	2.24	0.69
6:G:106:TYR:CD2	6:G:108:GLY:HA2	2.28	0.68
27:X:1030:U:O2	27:X:1155:G:N2	2.26	0.68
27:X:1082:G:O6	27:X:1103:C:N4	2.26	0.68
27:X:2617:G:H1	27:X:2755:A:H2'	1.58	0.68
27:X:224:G:OP2	27:X:226:C:N4	2.26	0.68
27:X:105:G:H21	27:X:357:A:H61	1.42	0.68
11:L:28:ARG:NH1	11:L:90:ASP:OD1	2.27	0.68
27:X:1342:U:H5''	27:X:1343:C:H5	1.57	0.68
4:D:66:ILE:HD11	28:Y:43:G:H3'	1.75	0.68
19:T:41:ARG:HH12	27:X:2366:U:H1'	1.59	0.68
21:V:48:ARG:NH2	27:X:76:C:OP1	2.27	0.68
6:G:50:PRO:HG2	6:G:53:ARG:HB2	1.76	0.68
1:A:55:GLY:N	1:A:217:ARG:HB2	2.07	0.68
8:I:51:GLY:HA3	26:3:59:LYS:HE3	1.74	0.68
8:I:56:LEU:HB3	26:3:52:LYS:HZ1	1.60	0.68
9:J:61:ARG:HH11	18:S:175:ARG:HB2	1.58	0.68
11:L:39:TYR:OH	28:Y:118:G:N3	2.27	0.68
25:2:33:ARG:NE	27:X:478:G:OP1	2.25	0.68
26:3:19:THR:OG1	27:X:661:C:OP1	2.12	0.67
27:X:226:C:OP2	27:X:2373:C:O2'	2.12	0.67
27:X:2200:G:H2'	27:X:2201:G:C8	2.29	0.67
2:B:78:LEU:O	2:B:79:ARG:NE	2.27	0.67
3:C:48:ARG:NH1	3:C:51:VAL:HG13	2.09	0.67
9:J:81:GLU:HG2	9:J:82:THR:HG23	1.76	0.67
27:X:1573:G:O6	27:X:1574:A:N6	2.27	0.67
3:C:111:ARG:NH1	3:C:180:ILE:O	2.27	0.67
27:X:540:G:HO2'	27:X:542:A:H2	1.40	0.67
10:K:12:ARG:HD3	10:K:16:ALA:HB1	1.77	0.67
2:B:26:VAL:HB	2:B:182:ILE:HG23	1.77	0.67
15:P:28:ALA:HB2	15:P:71:VAL:HG21	1.76	0.67
27:X:578:U:O2'	27:X:994:A:N1	2.26	0.67
27:X:1202:U:H2'	27:X:1203:A:H8	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:760:U:O2'	27:X:761:G:OP2	2.12	0.67
27:X:2672:U:H2'	27:X:2673:G:H8	1.60	0.67
4:D:115:ARG:HH22	4:D:178:ARG:HH12	1.43	0.67
7:H:40:GLY:HA3	27:X:2545:A:N6	2.08	0.67
23:Z:36:CYS:SG	23:Z:49:CYS:N	2.67	0.67
27:X:203:G:O2'	27:X:205:A:N1	2.23	0.67
27:X:2040:A:H2'	27:X:2041:A:C8	2.29	0.67
3:C:59:TYR:OH	3:C:67:ALA:HB1	1.93	0.67
15:P:99:ALA:HB1	27:X:25:U:H5'	1.76	0.67
4:D:62:LEU:O	4:D:95:ARG:NH1	2.28	0.66
10:K:28:LEU:HD21	10:K:115:LEU:HG	1.78	0.66
14:O:10:LYS:HG3	14:O:13:ARG:HH22	1.60	0.66
18:S:47:SER:OG	18:S:48:THR:N	2.18	0.66
27:X:1287:A:N1	27:X:1661:C:O2'	2.26	0.66
9:J:38:MET:HB2	9:J:129:GLN:HB2	1.76	0.66
27:X:1278:A:N6	27:X:1996:A:H5''	2.10	0.66
25:2:16:HIS:HB3	25:2:43:THR:HG21	1.77	0.66
27:X:18:U:O2'	27:X:563:U:OP1	2.14	0.66
27:X:571:U:O2'	27:X:581:A:H8	1.77	0.66
27:X:617:U:H5	27:X:632:A:C2	2.12	0.66
27:X:1173:G:H2'	27:X:1174:G:C8	2.30	0.66
23:Z:31:THR:OG1	27:X:2861:A:O2'	2.12	0.66
27:X:2324:G:O2'	27:X:2360:C:O2'	2.13	0.66
27:X:854:G:H1	27:X:948:C:N4	1.86	0.66
27:X:1850:G:O2'	27:X:1867:A:N6	2.29	0.66
3:C:46:ARG:HB3	3:C:51:VAL:HB	1.77	0.66
12:M:101:ARG:NH2	27:X:1745:C:OP1	2.29	0.66
17:R:61:SER:HA	17:R:65:PRO:HG3	1.77	0.66
27:X:2298:U:O2	27:X:2299:A:N6	2.28	0.66
2:B:77:ILE:HD13	2:B:195:LEU:HD22	1.77	0.66
27:X:2324:G:N3	27:X:2360:C:H2'	2.10	0.66
5:E:150:LYS:HZ1	27:X:2741:G:H21	1.44	0.66
6:G:122:HIS:HB3	6:G:125:ARG:HB2	1.78	0.66
27:X:2284:U:H5'	27:X:2286:G:H1	1.59	0.66
27:X:2324:G:HO2'	27:X:2360:C:HO2'	1.41	0.66
3:C:83:ALA:HB3	27:X:595:A:H5'	1.77	0.65
7:H:13:ASN:HD21	7:H:109:ARG:HG2	1.61	0.65
17:R:84:VAL:HG11	17:R:90:LYS:H	1.59	0.65
27:X:1283:C:H5''	27:X:1284:G:H5'	1.78	0.65
28:Y:46:G:N3	28:Y:49:C:N4	2.44	0.65
1:A:183:ARG:NH1	27:X:1790:G:O2'	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:103:TYR:CG	6:G:111:LYS:HB2	2.31	0.65
9:J:36:ILE:HG12	9:J:103:VAL:HA	1.78	0.65
27:X:1329:U:H2'	27:X:1330:G:C8	2.30	0.65
6:G:130:ALA:O	27:X:1148:G:O2'	2.14	0.65
7:H:13:ASN:ND2	7:H:109:ARG:HG2	2.11	0.65
19:T:74:LYS:HA	19:T:77:ARG:HG3	1.77	0.65
1:A:52:ARG:HD3	27:X:1816:G:OP1	1.96	0.65
6:G:61:ARG:HH12	6:G:66:HIS:H	1.45	0.65
13:N:93:LYS:HE2	14:O:10:LYS:HD3	1.76	0.65
27:X:1109:A:H3'	27:X:1110:G:H8	1.62	0.65
27:X:1466:C:H42	27:X:1476:G:H1	1.45	0.65
27:X:2015:G:OP2	27:X:2433:G:O2'	2.09	0.65
27:X:1562:G:H5'	27:X:1563:U:H5'	1.78	0.65
2:B:140:SER:HB3	27:X:2554:C:O2'	1.96	0.65
23:Z:6:VAL:HG22	23:Z:7:PRO:HD2	1.79	0.65
27:X:840:U:H4'	27:X:841:G:C2	2.32	0.65
27:X:1082:G:O2'	27:X:1100:G:OP2	2.14	0.65
2:B:76:ARG:NH2	27:X:2804:G:O3'	2.30	0.65
17:R:56:LYS:HD2	27:X:494:A:C8	2.31	0.65
27:X:219:G:HO2'	27:X:231:G:H1	1.44	0.65
27:X:1742:G:HO2'	27:X:2836:U:HO2'	1.43	0.65
27:X:87:G:H2'	27:X:88:G:H5''	1.77	0.65
3:C:163:ASN:ND2	3:C:167:VAL:H	1.95	0.65
15:P:105:ARG:NE	15:P:105:ARG:O	2.29	0.65
27:X:545:C:H2'	27:X:546:A:C8	2.32	0.65
27:X:812:G:H3'	27:X:813:A:H2'	1.79	0.65
27:X:1067:G:H5''	27:X:1068:A:H5'	1.77	0.65
27:X:308:C:O2	27:X:352:G:N2	2.23	0.65
27:X:403:A:H4'	27:X:404:A:H5'	1.79	0.65
3:C:9:GLN:HG2	3:C:120:VAL:HG21	1.79	0.64
6:G:132:PHE:CZ	6:G:145:HIS:HB2	2.32	0.64
27:X:1225:G:O2'	27:X:1250:A:N6	2.30	0.64
8:I:40:ARG:NH1	27:X:576:A:O3'	2.30	0.64
10:K:87:TYR:HE1	10:K:94:TYR:HD1	1.46	0.64
11:L:38:ILE:HD11	11:L:40:ALA:HB2	1.77	0.64
19:T:40:GLN:NE2	19:T:42:GLY:O	2.30	0.64
27:X:304:A:N6	27:X:356:A:N7	2.44	0.64
27:X:1373:G:H22	27:X:2192:U:H3	1.45	0.64
27:X:2432:A:H61	27:X:2479:U:H3	1.45	0.64
2:B:16:LYS:HD3	2:B:173:VAL:HG12	1.80	0.64
5:E:94:PHE:HB3	5:E:107:ILE:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:47:HIS:ND1	27:X:410:A:OP1	2.30	0.64
27:X:759:C:H5''	27:X:761:G:H1'	1.79	0.64
27:X:800:U:H5''	27:X:801:A:H5'	1.79	0.64
2:B:5:LEU:HD11	2:B:79:ARG:HB2	1.79	0.64
27:X:1225:G:H2'	27:X:1249:G:N2	2.12	0.64
4:D:92:ARG:CZ	28:Y:47:A:H1'	2.27	0.64
7:H:104:GLU:OE2	7:H:125:LYS:NZ	2.31	0.64
10:K:68:GLN:NE2	27:X:2686:C:O3'	2.28	0.64
10:K:102:THR:HA	10:K:109:THR:HA	1.80	0.64
27:X:542:A:OP1	27:X:570:G:N2	2.29	0.64
27:X:1017:C:H2'	27:X:1018:C:H6	1.60	0.64
9:J:84:MET:HG2	27:X:2229:G:H5'	1.80	0.64
16:Q:56:MET:HE3	16:Q:57:ASN:H	1.62	0.64
17:R:90:LYS:HG3	17:R:108:VAL:HG21	1.79	0.64
27:X:1504:G:N2	27:X:1517:C:O2	2.31	0.64
9:J:15:ARG:HD3	9:J:74:PRO:HD2	1.79	0.64
12:M:103:LYS:HG2	27:X:2698:G:H4'	1.79	0.64
27:X:1882:G:H21	27:X:1885:C:H41	1.45	0.64
1:A:254:THR:OG1	27:X:1835:C:O2'	2.15	0.64
3:C:2:ALA:HA	3:C:13:ARG:HA	1.80	0.64
27:X:5:A:H2'	27:X:6:A:C8	2.33	0.64
27:X:2811:G:H2'	27:X:2812:A:H8	1.58	0.64
2:B:14:ILE:HG12	12:M:20:HIS:CD2	2.29	0.63
5:E:8:PRO:HD2	5:E:69:ARG:HH11	1.62	0.63
6:G:70:PHE:HB3	13:N:64:ARG:HG2	1.78	0.63
2:B:92:ASN:HA	2:B:95:ILE:HB	1.78	0.63
5:E:90:ARG:HH21	5:E:163:ARG:HD2	1.64	0.63
16:Q:48:VAL:HG21	16:Q:82:LEU:HD13	1.79	0.63
27:X:619:A:N6	27:X:630:G:O2'	2.31	0.63
27:X:874:A:H2'	27:X:875:G:O4'	1.99	0.63
14:O:5:ILE:HG23	14:O:13:ARG:NH1	2.13	0.63
16:Q:88:ILE:HG13	16:Q:92:ALA:HB2	1.80	0.63
1:A:159:ALA:HB3	27:X:1812:U:H3'	1.80	0.63
3:C:58:MET:HG2	3:C:59:TYR:CD1	2.33	0.63
27:X:1827:G:H1	27:X:1888:C:H42	1.45	0.63
7:H:123:PHE:HB3	7:H:126:ILE:HG13	1.80	0.63
26:3:17:THR:HG22	26:3:21:LYS:H	1.62	0.63
27:X:584:A:OP2	27:X:2038:C:N4	2.31	0.63
27:X:826:U:H2'	27:X:827:C:C6	2.33	0.63
27:X:1422:C:H2'	27:X:1423:A:H8	1.63	0.63
27:X:1030:U:H2'	27:X:1032:A:H2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:86:LYS:NZ	27:X:2256:G:OP2	2.29	0.63
27:X:2039:G:C2	27:X:2040:A:C8	2.87	0.63
27:X:646:C:O2'	27:X:650:U:OP1	2.17	0.63
27:X:748:A:H5'	27:X:749:C:OP2	1.99	0.63
14:O:21:ARG:HH22	27:X:1005:U:H1'	1.64	0.62
19:T:51:VAL:HG21	19:T:79:ILE:HG22	1.80	0.62
27:X:160:C:O2'	27:X:445:A:N3	2.28	0.62
27:X:1502:G:H22	27:X:1518:C:H42	1.46	0.62
27:X:1554:G:H2'	27:X:1555:A:H8	1.64	0.62
28:Y:27:A:O2'	28:Y:28:A:O5'	2.17	0.62
4:D:16:LEU:O	4:D:20:PHE:N	2.27	0.62
6:G:119:LEU:HD12	6:G:122:HIS:HB2	1.80	0.62
8:I:61:PRO:HB2	26:3:30:ARG:HD3	1.80	0.62
15:P:70:LYS:NZ	27:X:500:G:O6	2.31	0.62
18:S:91:PRO:HD3	18:S:127:PRO:HD3	1.80	0.62
27:X:661:C:H2'	27:X:662:G:H8	1.62	0.62
28:Y:42:U:O2'	28:Y:47:A:N6	2.32	0.62
1:A:46:ARG:NE	27:X:1383:C:OP1	2.32	0.62
2:B:51:TYR:CE2	12:M:3:THR:HG21	2.33	0.62
8:I:59:ARG:HB2	27:X:2371:A:H8	1.63	0.62
27:X:725:C:O2	27:X:732:G:N2	2.26	0.62
27:X:2200:G:H2'	27:X:2201:G:H8	1.63	0.62
8:I:59:ARG:HB2	27:X:2371:A:C8	2.34	0.62
9:J:15:ARG:NH2	9:J:73:LYS:HZ2	1.97	0.62
15:P:57:LEU:HD13	15:P:69:ALA:HA	1.82	0.62
27:X:772:G:H2'	27:X:773:G:H8	1.65	0.62
27:X:2679:G:H1	27:X:2686:C:H42	1.48	0.62
4:D:39:GLY:O	4:D:150:ARG:NH2	2.33	0.62
6:G:157:PRO:O	6:G:161:GLN:NE2	2.32	0.62
7:H:25:LEU:HD21	7:H:52:VAL:HG23	1.81	0.62
27:X:313:U:H2'	27:X:314:G:C8	2.35	0.62
27:X:1919:A:N6	27:X:1946:U:H3	1.97	0.62
5:E:45:GLN:NE2	5:E:48:ASP:O	2.32	0.62
27:X:588:G:O2'	27:X:2002:A:OP1	2.14	0.62
2:B:115:GLY:HA2	2:B:136:ARG:HD2	1.81	0.62
17:R:22:VAL:HG22	17:R:82:ALA:HA	1.81	0.62
19:T:74:LYS:C	19:T:76:ALA:H	2.07	0.62
27:X:1361:G:H1	27:X:1614:C:N4	1.97	0.62
8:I:102:LYS:O	8:I:104:ARG:N	2.32	0.62
20:U:53:GLU:HB3	20:U:58:LYS:H	1.65	0.62
23:Z:51:TYR:CE1	23:Z:55:ARG:HB2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:41:ARG:NH2	27:X:2366:U:O2'	2.25	0.61
27:X:2617:G:N1	27:X:2755:A:H2'	2.15	0.61
4:D:4:LEU:HG	4:D:5:LYS:H	1.66	0.61
10:K:6:ALA:HB1	27:X:2848:A:H2	1.63	0.61
13:N:66:ASN:ND2	27:X:1021:A:OP1	2.33	0.61
27:X:2417:U:O2'	27:X:2419:C:OP1	2.16	0.61
1:A:89:SER:C	1:A:198:ASN:HD21	2.08	0.61
1:A:252:LYS:H	1:A:252:LYS:NZ	1.97	0.61
4:D:106:ILE:HG21	4:D:139:PRO:HB3	1.81	0.61
5:E:86:ASN:HB2	5:E:165:VAL:HG13	1.82	0.61
15:P:25:PHE:HD1	15:P:130:ILE:HD11	1.66	0.61
27:X:605:G:H2'	27:X:606:A:H8	1.66	0.61
28:Y:78:A:H2'	28:Y:79:U:O4'	2.01	0.61
7:H:13:ASN:OD1	7:H:108:THR:N	2.32	0.61
12:M:18:GLN:HA	12:M:21:THR:HB	1.82	0.61
13:N:50:ARG:HA	13:N:53:LYS:HE2	1.83	0.61
27:X:1440:G:H5''	27:X:1441:A:H2'	1.83	0.61
27:X:2191:A:OP1	27:X:2193:C:N4	2.32	0.61
2:B:189:PRO:HA	27:X:2659:C:H5'	1.82	0.61
12:M:17:GLU:HG3	12:M:62:SER:H	1.65	0.61
14:O:36:LYS:HB2	14:O:51:ALA:HB1	1.82	0.61
27:X:165:G:H1	27:X:185:C:H42	1.47	0.61
2:B:136:ARG:HB3	27:X:1673:C:H5''	1.81	0.61
12:M:66:PHE:HB3	12:M:83:PHE:HE1	1.66	0.61
22:W:4:LYS:HG3	22:W:52:GLU:HB3	1.83	0.61
25:2:7:PRO:HB2	27:X:1322:G:H4'	1.81	0.61
27:X:1070:G:H5''	27:X:1071:U:H2'	1.82	0.61
1:A:246:PRO:HD3	1:A:252:LYS:HE3	1.82	0.61
6:G:35:LYS:N	6:G:69:ASP:OD2	2.34	0.61
13:N:5:LYS:HG2	13:N:7:GLY:H	1.64	0.61
20:U:51:ILE:HG23	20:U:59:THR:HA	1.82	0.61
21:V:15:ALA:HA	21:V:18:ILE:HD12	1.83	0.61
27:X:1514:C:H4'	27:X:1592:U:O2'	2.01	0.61
27:X:635:C:O2'	27:X:670:U:OP1	2.17	0.61
2:B:174:GLU:HB3	2:B:183:LEU:HD12	1.82	0.61
7:H:1:MET:HE2	27:X:1682:A:H1'	1.82	0.61
17:R:42:ARG:NH2	27:X:86:U:OP2	2.33	0.61
27:X:810:U:H2'	27:X:811:G:O4'	2.01	0.61
1:A:252:LYS:HZ2	1:A:252:LYS:N	1.98	0.60
7:H:99:ILE:HD12	7:H:103:GLY:HA2	1.83	0.60
11:L:28:ARG:NH2	28:Y:10:U:O3'	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:49:LYS:HD3	20:U:61:TRP:CE2	2.36	0.60
27:X:2820:C:H2'	27:X:2821:G:C8	2.36	0.60
3:C:15:ILE:HD11	3:C:195:ILE:H	1.66	0.60
27:X:2591:C:H2'	27:X:2592:U:H5	1.65	0.60
7:H:47:VAL:HG23	7:H:77:THR:HG23	1.83	0.60
8:I:81:GLN:HB3	8:I:114:ILE:HG23	1.84	0.60
11:L:50:THR:N	28:Y:116:C:O2'	2.33	0.60
20:U:52:ARG:HD2	20:U:79:GLU:HA	1.82	0.60
27:X:1073:G:H22	27:X:1087:C:H42	1.48	0.60
27:X:1301:U:O2'	27:X:1664:G:N2	2.34	0.60
27:X:2191:A:H5''	27:X:2192:U:H5	1.66	0.60
8:I:62:LYS:HB3	26:3:12:ARG:HA	1.83	0.60
18:S:117:VAL:HB	18:S:168:VAL:HG22	1.82	0.60
21:V:6:MET:HE1	21:V:52:GLN:HB3	1.83	0.60
27:X:2591:C:H2'	27:X:2592:U:C5	2.35	0.60
4:D:45:GLU:OE1	4:D:78:LYS:NZ	2.30	0.60
5:E:103:LEU:HD23	5:E:115:ILE:HD12	1.83	0.60
13:N:13:ARG:NH1	27:X:1264:C:H5''	2.17	0.60
27:X:482:A:H2'	27:X:483:A:O4'	2.02	0.60
27:X:623:G:C2	27:X:624:A:H1'	2.37	0.60
2:B:169:ASN:HD21	2:B:204:ALA:HB2	1.66	0.60
15:P:118:ASN:HA	27:X:1996:A:O2'	2.01	0.60
16:Q:13:SER:OG	16:Q:14:GLU:N	2.32	0.60
18:S:28:ASN:OD1	18:S:28:ASN:N	2.34	0.60
27:X:1430:G:H1	27:X:1598:C:H42	1.50	0.60
28:Y:3:A:N6	28:Y:121:G:O6	2.34	0.60
1:A:68:LYS:HD3	1:A:68:LYS:H	1.67	0.60
2:B:52:ALA:O	2:B:76:ARG:N	2.25	0.60
3:C:71:ASP:OD1	3:C:72:ARG:N	2.34	0.60
7:H:11:ALA:O	7:H:111:PHE:N	2.30	0.60
9:J:6:LYS:HB3	9:J:45:SER:HB2	1.84	0.60
18:S:26:LYS:HG3	18:S:27:GLU:HG3	1.83	0.60
27:X:663:G:H3'	27:X:664:C:H5''	1.84	0.60
3:C:48:ARG:HB2	3:C:50:GLN:HB3	1.82	0.60
7:H:9:ASP:O	7:H:96:ALA:N	2.34	0.60
27:X:615:C:O2	27:X:670:U:O2'	2.17	0.60
27:X:1451:C:H2'	27:X:1452:U:H6	1.67	0.60
2:B:105:THR:HB	2:B:166:THR:HG23	1.84	0.60
3:C:158:ARG:HB3	3:C:169:VAL:HG11	1.83	0.60
4:D:133:LYS:HE2	27:X:2284:U:H4'	1.83	0.60
6:G:62:ILE:O	6:G:77:GLY:HA3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:17:THR:HG23	26:3:19:THR:H	1.67	0.60
27:X:2707:G:H2'	27:X:2708:U:C6	2.36	0.60
1:A:63:ARG:HE	1:A:85:ASP:HB3	1.67	0.60
12:M:3:THR:HG22	12:M:5:ILE:HG13	1.84	0.60
12:M:27:PHE:HA	12:M:96:ARG:NH2	2.16	0.60
27:X:1350:G:H2'	27:X:1351:G:H8	1.66	0.60
10:K:10:LEU:HD11	10:K:17:ARG:HE	1.66	0.59
18:S:71:MET:HA	18:S:78:PRO:HA	1.84	0.59
27:X:705:C:HO2'	27:X:1367:A:HO2'	1.46	0.59
27:X:1777:A:H1'	27:X:1921:A:N6	2.17	0.59
27:X:2330:G:H21	27:X:2345:A:H62	1.50	0.59
4:D:171:GLN:HE21	4:D:177:PHE:HE1	1.49	0.59
27:X:242:A:N6	27:X:441:A:N7	2.50	0.59
27:X:1997:A:H2'	27:X:1998:A:C8	2.37	0.59
27:X:2279:G:N2	27:X:2295:C:O2	2.33	0.59
4:D:70:ALA:HB3	4:D:82:GLY:HA2	1.83	0.59
4:D:112:ARG:NH2	4:D:134:GLU:OE2	2.35	0.59
13:N:93:LYS:HE3	14:O:6:GLN:HG3	1.84	0.59
14:O:85:GLY:O	27:X:1237:G:H4'	2.02	0.59
28:Y:7:C:O2'	28:Y:29:C:O2	2.14	0.59
1:A:163:VAL:HG22	1:A:177:LEU:HA	1.84	0.59
2:B:136:ARG:HD3	27:X:1673:C:H5'	1.84	0.59
8:I:26:THR:OG1	27:X:676:G:OP1	2.15	0.59
13:N:20:ARG:HD2	13:N:39:LEU:HD13	1.84	0.59
27:X:2174:G:H2'	27:X:2175:A:H8	1.68	0.59
2:B:56:GLU:HG2	2:B:74:PRO:HG3	1.83	0.59
8:I:30:ALA:CA	27:X:824:U:H2'	2.33	0.59
25:2:3:ARG:O	25:2:6:GLN:NE2	2.30	0.59
27:X:721:C:H42	27:X:736:G:H1	1.51	0.59
1:A:168:LYS:HD3	1:A:173:VAL:HG22	1.83	0.59
2:B:60:ASN:HB3	2:B:62:PRO:HD2	1.85	0.59
5:E:22:GLY:HA3	5:E:39:THR:HG22	1.85	0.59
7:H:2:ILE:HD12	7:H:8:LEU:HD21	1.85	0.59
14:O:70:TYR:OH	27:X:1236:G:O6	2.21	0.59
27:X:1563:U:H2'	27:X:1564:U:C6	2.38	0.59
27:X:2684:A:O2'	27:X:2827:G:OP1	2.20	0.59
27:X:2837:G:H2'	27:X:2838:U:H6	1.67	0.59
5:E:107:ILE:HD11	5:E:151:VAL:HG12	1.85	0.59
17:R:107:ALA:HB2	17:R:111:GLY:HA2	1.83	0.59
27:X:711:C:O2'	27:X:747:A:N6	2.36	0.59
27:X:2283:G:H1	27:X:2291:U:H3	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:LYS:C	3:C:131:LYS:H	2.11	0.59
27:X:1141:U:H6	27:X:1141:U:O5'	1.86	0.59
27:X:1479:G:H2'	27:X:1480:G:C8	2.38	0.59
2:B:128:SER:OG	27:X:1976:U:O3'	2.21	0.59
16:Q:26:SER:HB3	16:Q:79:ILE:HG12	1.85	0.59
24:1:14:SER:HB2	24:1:23:THR:H	1.68	0.59
27:X:1937:G:O2'	27:X:1939:U:O4	2.14	0.59
27:X:2849:C:H2'	27:X:2850:U:H6	1.68	0.59
1:A:172:TYR:HA	1:A:186:HIS:HA	1.84	0.59
13:N:49:ASP:HA	13:N:52:ASN:HB2	1.85	0.59
3:C:48:ARG:NE	3:C:51:VAL:HG22	2.18	0.58
3:C:68:ARG:NH1	27:X:687:G:H1'	2.18	0.58
10:K:79:VAL:HA	10:K:83:VAL:HB	1.85	0.58
15:P:30:TYR:O	15:P:123:ARG:NE	2.27	0.58
27:X:2201:G:H2'	27:X:2202:G:H8	1.68	0.58
27:X:2767:C:HO2'	27:X:2785:A:HO2'	1.50	0.58
2:B:5:LEU:HD22	2:B:195:LEU:HD11	1.85	0.58
27:X:139:A:H2'	27:X:140:G:H8	1.68	0.58
27:X:1854:G:H2'	27:X:1855:G:H8	1.69	0.58
27:X:2522:G:H2'	27:X:2523:G:C8	2.38	0.58
2:B:76:ARG:HH22	27:X:2805:G:P	2.25	0.58
2:B:128:SER:CB	27:X:1976:U:H4'	2.34	0.58
2:B:133:LYS:HG3	2:B:137:ARG:HB3	1.85	0.58
10:K:10:LEU:HD23	10:K:13:ASN:O	2.03	0.58
13:N:24:PHE:CE1	27:X:543:G:H5'	2.38	0.58
17:R:26:SER:OG	17:R:27:GLY:N	2.34	0.58
1:A:245:VAL:HB	1:A:249:PRO:HA	1.85	0.58
4:D:122:PHE:HA	27:X:2282:G:H4'	1.85	0.58
20:U:51:ILE:HG12	20:U:59:THR:HB	1.84	0.58
27:X:154:U:H3'	27:X:155:G:H8	1.68	0.58
27:X:1785:A:H2'	27:X:1786:C:H6	1.66	0.58
1:A:16:MET:SD	1:A:17:THR:N	2.74	0.58
17:R:84:VAL:HG21	17:R:89:GLY:HA2	1.85	0.58
27:X:500:G:C2	27:X:501:G:H1'	2.39	0.58
27:X:1210:C:H2'	27:X:1211:G:H8	1.68	0.58
27:X:1468:A:H8	27:X:1468:A:O5'	1.87	0.58
1:A:76:ASN:ND2	1:A:118:ASN:OD1	2.37	0.58
2:B:156:MET:HE1	27:X:2033:C:H1'	1.85	0.58
6:G:61:ARG:NH1	6:G:65:LYS:HB3	2.19	0.58
7:H:75:VAL:HG22	7:H:96:ALA:HA	1.84	0.58
9:J:61:ARG:HB3	18:S:175:ARG:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:68:GLN:HG2	27:X:2686:C:O2'	2.04	0.58
27:X:1554:G:H2'	27:X:1555:A:C8	2.38	0.58
27:X:2245:A:H4'	27:X:2246:A:N3	2.18	0.58
27:X:1019:U:O2'	27:X:1020:A:O5'	2.19	0.58
27:X:1501:C:H42	27:X:1519:G:H1	1.50	0.58
4:D:64:LYS:O	28:Y:44:C:O2'	2.20	0.58
27:X:1919:A:H2	27:X:1926:U:H3	1.52	0.58
2:B:176:ARG:HH21	12:M:16:ILE:CG2	2.17	0.58
6:G:84:ASN:O	6:G:152:ALA:HA	2.03	0.58
6:G:103:TYR:CD2	6:G:111:LYS:HB2	2.39	0.58
13:N:37:GLN:HB3	27:X:1265:G:H1	1.69	0.58
27:X:712:A:H2'	27:X:713:G:O4'	2.04	0.58
12:M:7:ILE:HD12	12:M:8:ASN:H	1.68	0.58
27:X:70:A:H4'	27:X:71:A:H5''	1.85	0.58
27:X:163:A:H2'	27:X:164:G:C8	2.39	0.58
27:X:670:U:H2'	27:X:671:A:C8	2.38	0.58
27:X:2006:G:H5'	27:X:2596:C:H4'	1.85	0.58
19:T:68:VAL:HB	19:T:80:SER:HB2	1.86	0.57
19:T:72:LYS:HD3	28:Y:14:C:H5''	1.85	0.57
27:X:705:C:O2'	27:X:1367:A:O2'	2.21	0.57
27:X:1699:A:H61	27:X:1723:U:H3	1.52	0.57
27:X:2492:G:C2	27:X:2493:U:C2	2.92	0.57
3:C:176:ASN:HB3	3:C:179:ASP:H	1.68	0.57
8:I:73:GLU:HG3	8:I:101:ARG:HG3	1.84	0.57
15:P:95:ALA:HB2	15:P:129:ILE:HG23	1.86	0.57
26:3:15:LYS:O	26:3:23:MET:N	2.35	0.57
27:X:1443:G:H2'	27:X:1444:C:C6	2.39	0.57
27:X:1454:U:H2'	27:X:1455:C:C6	2.40	0.57
2:B:143:GLN:O	27:X:2035:G:H4'	2.03	0.57
6:G:69:ASP:H	6:G:76:GLN:HE22	1.51	0.57
6:G:134:MET:HE3	27:X:1017:C:H1'	1.86	0.57
27:X:2594:U:H2'	27:X:2595:C:H6	1.69	0.57
3:C:69:HIS:HE2	27:X:1270:C:P	2.27	0.57
4:D:60:ILE:HG13	4:D:61:THR:HG23	1.86	0.57
5:E:6:LYS:HB2	5:E:69:ARG:HG3	1.85	0.57
11:L:32:TYR:CZ	11:L:34:SER:HB3	2.39	0.57
18:S:3:LEU:HD23	18:S:56:VAL:HG13	1.86	0.57
27:X:346:C:H2'	27:X:347:C:C6	2.40	0.57
28:Y:17:A:H1'	28:Y:112:A:C8	2.39	0.57
27:X:303:C:H3'	27:X:304:A:H5''	1.86	0.57
27:X:1310:C:H2'	27:X:1311:C:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1342:U:H5''	27:X:1343:C:C5	2.37	0.57
13:N:78:THR:HG23	13:N:117:ARG:CZ	2.34	0.57
13:N:105:ALA:HB2	14:O:45:THR:HG21	1.86	0.57
27:X:222:G:O2'	27:X:397:U:O2	2.18	0.57
27:X:1422:C:H2'	27:X:1423:A:C8	2.38	0.57
2:B:121:ASN:O	2:B:122:PHE:HB2	2.03	0.57
27:X:2528:G:H2'	27:X:2529:G:H8	1.69	0.57
27:X:2570:C:H2'	27:X:2571:G:C8	2.40	0.57
17:R:92:THR:O	17:R:92:THR:OG1	2.21	0.57
27:X:554:U:H5''	27:X:556:A:C2	2.39	0.57
27:X:751:G:H2'	27:X:752:G:C8	2.40	0.57
27:X:1185:C:H2'	27:X:1186:G:H2'	1.85	0.57
27:X:1373:G:N2	27:X:2192:U:H3	2.03	0.57
27:X:2493:U:H2'	27:X:2494:C:C6	2.40	0.57
1:A:158:SER:OG	1:A:159:ALA:N	2.35	0.57
6:G:132:PHE:HZ	6:G:142:ARG:HA	1.70	0.57
9:J:81:GLU:HB2	27:X:2473:G:O2'	2.05	0.57
10:K:32:GLY:HA2	10:K:115:LEU:HD12	1.86	0.57
10:K:36:THR:OG1	27:X:1291:G:OP1	2.16	0.57
22:W:3:ILE:HD11	22:W:44:VAL:HG11	1.86	0.57
24:1:16:ALA:HB2	24:1:50:PHE:CZ	2.40	0.57
27:X:772:G:H2'	27:X:773:G:C8	2.40	0.57
27:X:859:U:H3	27:X:944:A:N6	2.03	0.57
27:X:992:A:N1	27:X:2010:G:O2'	2.32	0.57
27:X:1645:U:H2'	27:X:1646:G:C8	2.40	0.57
27:X:2590:U:H1'	30:X:2902:ERY:H361	1.85	0.57
1:A:223:GLY:HA2	1:A:226:MET:HG3	1.87	0.57
1:A:252:LYS:O	27:X:1787:U:O2'	2.22	0.57
2:B:136:ARG:HB3	27:X:1673:C:C5'	2.34	0.57
10:K:76:VAL:HA	10:K:79:VAL:HG12	1.87	0.57
10:K:87:TYR:CE1	10:K:94:TYR:HD1	2.23	0.57
18:S:64:ALA:HB2	18:S:85:MET:HG2	1.86	0.57
27:X:436:A:H5''	27:X:437:G:H5''	1.85	0.57
27:X:638:A:H4'	27:X:639:G:H5'	1.86	0.57
8:I:30:ALA:HA	27:X:824:U:H2'	1.87	0.56
27:X:1333:G:N7	27:X:1342:U:H5'	2.20	0.56
27:X:1455:C:H2'	27:X:1456:C:H6	1.70	0.56
27:X:1774:A:H5'	27:X:2587:G:H4'	1.87	0.56
27:X:1982:C:H5''	27:X:2703:C:O2'	2.05	0.56
9:J:26:ASP:OD1	9:J:27:TYR:N	2.38	0.56
12:M:17:GLU:OE2	12:M:63:ARG:NH2	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:13:ARG:HH12	27:X:1264:C:H5''	1.70	0.56
27:X:1033:G:H22	27:X:1153:A:H2	1.53	0.56
27:X:2025:A:H5''	27:X:2026:C:OP2	2.05	0.56
27:X:2085:G:H22	27:X:2171:U:H1'	1.69	0.56
27:X:2222:U:H2'	27:X:2223:U:C6	2.39	0.56
27:X:2336:G:N2	27:X:2339:A:OP2	2.38	0.56
9:J:86:LYS:O	9:J:88:LYS:HE3	2.05	0.56
27:X:540:G:C6	27:X:2005:U:H5''	2.40	0.56
27:X:726:G:H21	27:X:731:A:H2	1.53	0.56
27:X:1017:C:H2'	27:X:1018:C:C6	2.40	0.56
27:X:1830:C:N4	27:X:1882:G:OP2	2.39	0.56
27:X:2708:U:H2'	27:X:2709:C:H6	1.70	0.56
27:X:2736:U:H1'	27:X:2737:A:H5''	1.87	0.56
27:X:2763:U:H2'	27:X:2764:U:H6	1.70	0.56
4:D:13:ARG:HG3	4:D:28:VAL:HG11	1.87	0.56
9:J:26:ASP:H	9:J:103:VAL:HG12	1.70	0.56
12:M:22:ARG:HB2	12:M:84:ALA:HB2	1.87	0.56
19:T:21:LEU:HD11	19:T:41:ARG:HG2	1.87	0.56
20:U:63:SER:O	20:U:67:LEU:N	2.38	0.56
27:X:1327:C:N4	27:X:1351:G:H1	2.02	0.56
1:A:43:ARG:NH1	27:X:704:G:O2'	2.39	0.56
2:B:87:ASP:OD2	2:B:87:ASP:N	2.38	0.56
12:M:22:ARG:NH1	12:M:83:PHE:O	2.39	0.56
27:X:1674:C:H2'	27:X:1675:C:C6	2.41	0.56
27:X:2431:C:H2'	27:X:2432:A:C8	2.40	0.56
27:X:2871:U:H2'	27:X:2872:U:C6	2.40	0.56
15:P:117:ALA:HB3	27:X:1997:A:H5''	1.87	0.56
15:P:117:ALA:O	15:P:118:ASN:ND2	2.38	0.56
27:X:2174:G:H2'	27:X:2175:A:C8	2.41	0.56
2:B:176:ARG:NH2	12:M:16:ILE:HG23	2.18	0.56
3:C:54:THR:HG21	3:C:72:ARG:HB2	1.88	0.56
10:K:7:GLY:N	27:X:2848:A:N3	2.52	0.56
13:N:104:GLU:N	13:N:104:GLU:OE2	2.37	0.56
17:R:54:ILE:HG12	17:R:71:GLN:HG3	1.86	0.56
27:X:597:U:H2'	27:X:598:U:C6	2.41	0.56
27:X:1467:U:C6	27:X:1468:A:H5'	2.41	0.56
27:X:2492:G:H2'	27:X:2493:U:C6	2.40	0.56
12:M:28:ARG:HB2	12:M:29:PRO:HD3	1.87	0.56
27:X:75:C:H2'	27:X:76:C:C6	2.41	0.56
27:X:1174:G:H2'	27:X:1175:A:H8	1.71	0.56
15:P:44:VAL:HG11	23:Z:27:ALA:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:9:ILE:HA	24:1:28:ARG:HA	1.87	0.56
24:1:12:MET:HB2	24:1:27:ASN:ND2	2.21	0.56
27:X:388:G:H2'	27:X:389:G:C8	2.41	0.56
27:X:1501:C:H2'	27:X:1502:G:O4'	2.06	0.56
28:Y:51:G:H2'	28:Y:52:G:C8	2.38	0.56
1:A:43:ARG:HH21	1:A:55:GLY:HA2	1.71	0.55
7:H:117:GLU:O	7:H:120:ASP:HB2	2.05	0.55
21:V:23:LYS:O	21:V:27:GLU:HG2	2.06	0.55
2:B:143:GLN:NE2	2:B:151:TYR:OH	2.39	0.55
3:C:144:GLY:HA3	3:C:166:TRP:CD1	2.42	0.55
3:C:152:THR:OG1	3:C:153:ASP:O	2.22	0.55
13:N:58:ARG:O	13:N:62:ILE:HG13	2.07	0.55
25:2:39:ARG:O	27:X:469:G:H3'	2.07	0.55
27:X:82:G:H1	27:X:100:G:HO2'	1.53	0.55
27:X:1795:C:H2'	27:X:1796:A:H8	1.71	0.55
6:G:132:PHE:CZ	6:G:142:ARG:HA	2.41	0.55
23:Z:42:SER:O	23:Z:44:HIS:HD2	1.88	0.55
17:R:16:PHE:CZ	17:R:46:VAL:HG22	2.42	0.55
25:2:1:MET:HB3	25:2:3:ARG:HH12	1.71	0.55
27:X:388:G:H2'	27:X:389:G:H8	1.72	0.55
27:X:533:C:O2	27:X:563:U:O2'	2.23	0.55
27:X:1918:G:H1'	27:X:1947:G:N2	2.22	0.55
24:1:30:ASN:ND2	27:X:2264:C:OP2	2.40	0.55
27:X:1481:U:O2'	27:X:1562:G:O2'	2.18	0.55
1:A:28:ARG:HD2	27:X:1583:A:N6	2.22	0.55
2:B:159:HIS:NE2	2:B:162:MET:HE2	2.21	0.55
6:G:151:TYR:CE1	6:G:160:ALA:HB3	2.41	0.55
17:R:83:LEU:HD13	17:R:113:THR:HB	1.87	0.55
18:S:3:LEU:HB3	18:S:56:VAL:HA	1.88	0.55
27:X:1336:G:H2'	27:X:1337:G:H5'	1.88	0.55
27:X:1348:C:H2'	27:X:1349:A:C8	2.41	0.55
2:B:4:ILE:HD13	2:B:28:ALA:HB1	1.88	0.55
15:P:90:LEU:HD22	15:P:131:VAL:HG12	1.88	0.55
17:R:11:ASN:O	17:R:11:ASN:ND2	2.36	0.55
27:X:542:A:O2'	27:X:543:G:OP1	2.25	0.55
27:X:1825:C:O2'	27:X:1952:A:N1	2.33	0.55
1:A:48:ARG:H	1:A:48:ARG:HD2	1.72	0.55
15:P:27:VAL:HG13	27:X:504:G:H4'	1.88	0.55
27:X:2828:C:H2'	27:X:2829:A:H8	1.71	0.55
28:Y:39:C:N4	28:Y:51:G:O4'	2.40	0.55
3:C:48:ARG:HB2	3:C:50:GLN:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:123:ASP:HB3	4:D:127:ASN:H	1.71	0.55
10:K:96:ARG:NE	27:X:2857:C:OP1	2.39	0.55
15:P:47:GLY:H	15:P:92:VAL:HG23	1.71	0.55
27:X:1480:G:C2	27:X:1481:U:O2	2.59	0.55
13:N:54:LYS:NZ	27:X:1006:C:OP2	2.40	0.55
14:O:12:TYR:HD2	14:O:40:VAL:HB	1.72	0.55
18:S:168:VAL:HG12	18:S:169:VAL:HG23	1.89	0.55
27:X:1810:U:HO2'	27:X:1811:A:P	2.29	0.55
27:X:2594:U:H2'	27:X:2595:C:C6	2.42	0.55
27:X:2856:U:H2'	27:X:2857:C:C6	2.41	0.55
1:A:60:ARG:HD3	1:A:86:PRO:HB2	1.89	0.54
11:L:8:ARG:HG3	11:L:9:ARG:H	1.71	0.54
14:O:83:ARG:NH2	27:X:1239:A:OP1	2.40	0.54
19:T:40:GLN:HE22	19:T:43:THR:HA	1.71	0.54
27:X:2235:G:N2	27:X:2254:C:C4	2.75	0.54
27:X:2860:C:H2'	27:X:2861:A:O4'	2.07	0.54
2:B:104:ALA:HB3	2:B:170:LEU:HD12	1.88	0.54
2:B:118:LYS:HG2	2:B:160:MET:SD	2.48	0.54
3:C:66:ASN:HA	27:X:1268:U:H2'	1.89	0.54
4:D:74:ILE:HA	4:D:79:LEU:HB3	1.89	0.54
4:D:130:LEU:HD13	4:D:131:GLY:H	1.71	0.54
27:X:188:G:H2'	27:X:189:A:C8	2.43	0.54
27:X:228:A:C5	27:X:229:G:H1'	2.42	0.54
27:X:1412:C:O2'	27:X:1413:U:O5'	2.25	0.54
27:X:1454:U:H3	27:X:1567:A:H61	1.53	0.54
28:Y:58:G:H4'	28:Y:59:A:O5'	2.07	0.54
1:A:44:ASN:HB3	1:A:49:ILE:HA	1.89	0.54
5:E:86:ASN:HB3	5:E:130:ARG:HH21	1.72	0.54
13:N:93:LYS:HB3	27:X:1007:A:H4'	1.89	0.54
27:X:540:G:N1	27:X:2005:U:OP1	2.40	0.54
27:X:946:U:H2'	27:X:947:C:H6	1.72	0.54
27:X:1279:G:O2'	27:X:1995:G:O6	2.11	0.54
27:X:1919:A:H2	27:X:1926:U:N3	2.04	0.54
1:A:93:ALA:HB2	1:A:107:ALA:HB2	1.88	0.54
1:A:146:GLU:HB2	1:A:189:CYS:HB3	1.88	0.54
3:C:65:GLY:HA3	27:X:2042:A:H5''	1.90	0.54
23:Z:51:TYR:CE1	23:Z:55:ARG:HD3	2.43	0.54
27:X:2384:G:N2	27:X:2390:A:N7	2.56	0.54
3:C:34:GLN:O	3:C:37:SER:OG	2.19	0.54
12:M:29:PRO:HB3	12:M:99:VAL:HG12	1.90	0.54
15:P:13:GLN:O	15:P:17:GLN:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:219:G:N2	27:X:231:G:H2'	2.23	0.54
27:X:627:A:H2'	27:X:628:A:C8	2.43	0.54
27:X:825:C:H5''	27:X:1263:G:O2'	2.07	0.54
27:X:1673:C:H2'	27:X:1674:C:C6	2.38	0.54
27:X:1785:A:H2'	27:X:1786:C:C6	2.42	0.54
28:Y:27:A:N6	28:Y:56:G:OP2	2.41	0.54
9:J:21:ASP:C	9:J:99:LYS:HG2	2.33	0.54
11:L:32:TYR:CE2	28:Y:9:G:H5'	2.43	0.54
15:P:116:SER:OG	15:P:117:ALA:N	2.40	0.54
27:X:317:U:O2'	27:X:1224:A:N7	2.40	0.54
27:X:963:G:H1	27:X:976:C:H42	1.56	0.54
27:X:1141:U:O2	27:X:2008:C:H5''	2.08	0.54
27:X:1787:U:H2'	27:X:1788:C:C6	2.43	0.54
27:X:1827:G:H1'	27:X:1914:U:C2	2.43	0.54
27:X:1991:C:H2'	27:X:1992:G:H8	1.72	0.54
1:A:244:ARG:O	1:A:252:LYS:NZ	2.20	0.54
2:B:62:PRO:O	27:X:2766:U:O2'	2.22	0.54
4:D:17:MET:HA	4:D:21:GLY:H	1.72	0.54
25:2:12:ARG:NH2	25:2:46:ASP:O	2.36	0.54
27:X:312:G:HO2'	27:X:313:U:H6	1.56	0.54
27:X:490:A:H1'	27:X:491:A:H5'	1.89	0.54
27:X:653:G:H2'	27:X:654:A:H5''	1.89	0.54
27:X:838:A:H4'	27:X:2407:G:C5	2.42	0.54
27:X:1790:G:H5'	27:X:1811:A:N6	2.23	0.54
27:X:2054:A:H2'	27:X:2055:G:H8	1.71	0.54
3:C:48:ARG:HD2	3:C:50:GLN:HB3	1.90	0.54
3:C:106:MET:O	3:C:110:SER:OG	2.19	0.54
14:O:5:ILE:HG23	14:O:13:ARG:HH12	1.73	0.54
15:P:19:LYS:NZ	27:X:507:A:OP2	2.23	0.54
25:2:26:SER:O	25:2:30:ILE:HG13	2.08	0.54
27:X:343:A:H1'	27:X:346:C:H41	1.73	0.54
27:X:684:C:H2'	27:X:685:U:C6	2.42	0.54
27:X:2705:A:H1'	27:X:2706:U:H2'	1.89	0.54
5:E:44:ARG:HH22	5:E:51:LEU:HB3	1.72	0.54
15:P:97:VAL:HG22	15:P:127:ILE:HA	1.90	0.54
27:X:1484:G:H2'	27:X:1485:U:C6	2.43	0.54
27:X:2791:C:O2'	27:X:2792:C:H5'	2.08	0.54
1:A:61:LEU:HG	27:X:1584:G:H5''	1.90	0.54
3:C:74:VAL:HG23	3:C:76:THR:H	1.72	0.54
3:C:128:ALA:C	3:C:130:THR:H	2.16	0.54
4:D:93:GLY:H	4:D:96:MET:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:33:ALA:O	24:1:34:LYS:HD2	2.08	0.54
27:X:774:A:H8	27:X:774:A:O5'	1.90	0.54
27:X:946:U:H2'	27:X:947:C:C6	2.43	0.54
27:X:1296:G:H22	27:X:1299:A:H5'	1.73	0.54
27:X:1974:U:H2'	27:X:1975:G:H5''	1.90	0.54
27:X:2707:G:H2'	27:X:2708:U:H6	1.72	0.54
3:C:48:ARG:O	3:C:51:VAL:HG23	2.07	0.53
3:C:67:ALA:HB2	15:P:112:ARG:HH22	1.73	0.53
8:I:62:LYS:H	26:3:12:ARG:HG3	1.72	0.53
9:J:16:GLY:C	9:J:17:ARG:HD3	2.33	0.53
13:N:93:LYS:HB3	27:X:1007:A:O3'	2.08	0.53
17:R:56:LYS:HD3	17:R:69:GLN:HE21	1.73	0.53
27:X:171:G:H2'	27:X:172:A:O4'	2.08	0.53
27:X:455:A:H2	27:X:1258:G:N3	2.06	0.53
27:X:2378:G:H1	27:X:2396:C:H42	1.56	0.53
27:X:2555:G:N2	27:X:2555:G:OP2	2.41	0.53
1:A:16:MET:HE1	1:A:23:GLY:HA2	1.89	0.53
1:A:27:LYS:HZ3	1:A:29:PRO:HB3	1.71	0.53
5:E:160:LYS:HZ1	27:X:2637:C:H5'	1.72	0.53
20:U:21:ARG:HH12	27:X:400:U:H2'	1.74	0.53
3:C:50:GLN:HE22	3:C:56:ARG:HH12	1.56	0.53
25:2:19:ARG:HG2	27:X:123:A:C5'	2.36	0.53
27:X:1374:G:N2	27:X:1384:G:H1'	2.23	0.53
27:X:2241:U:H2'	27:X:2242:C:C6	2.38	0.53
4:D:75:SER:H	4:D:79:LEU:HD12	1.73	0.53
10:K:14:SER:HB3	27:X:2693:U:OP1	2.08	0.53
10:K:40:LYS:NZ	27:X:1290:A:OP1	2.42	0.53
25:2:41:GLN:NE2	27:X:470:U:OP1	2.36	0.53
27:X:75:C:H2'	27:X:76:C:H6	1.73	0.53
27:X:1854:G:H2'	27:X:1855:G:C8	2.44	0.53
27:X:2374:C:H42	27:X:2400:G:H1	1.56	0.53
27:X:2572:U:H3	27:X:2579:A:H61	1.57	0.53
8:I:89:ASP:HB2	8:I:120:VAL:HG13	1.90	0.53
12:M:102:ALA:C	12:M:103:LYS:HD2	2.33	0.53
17:R:52:ASN:HA	17:R:74:LEU:H	1.72	0.53
18:S:68:ALA:HB3	18:S:82:ASP:HB2	1.91	0.53
27:X:605:G:H2'	27:X:606:A:C8	2.44	0.53
27:X:978:U:H2'	27:X:979:A:C8	2.43	0.53
27:X:1714:A:OP2	27:X:1715:A:O2'	2.26	0.53
1:A:50:THR:HG21	27:X:1805:G:N3	2.24	0.53
3:C:148:VAL:HB	3:C:167:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:155:ASP:OD1	5:E:155:ASP:N	2.36	0.53
10:K:81:ASP:O	10:K:85:PRO:HG2	2.09	0.53
13:N:84:LYS:HB2	13:N:92:ARG:HH12	1.74	0.53
17:R:26:SER:HB2	27:X:321:A:H5''	1.90	0.53
18:S:6:LYS:HD3	18:S:32:PHE:HD2	1.73	0.53
27:X:538:A:H62	27:X:2026:C:C5'	2.16	0.53
28:Y:16:U:H1'	28:Y:109:G:H21	1.74	0.53
6:G:132:PHE:CE2	6:G:145:HIS:HB2	2.44	0.53
15:P:122:LYS:HB3	15:P:124:THR:HG23	1.90	0.53
27:X:542:A:H62	27:X:2002:A:H2	1.55	0.53
27:X:746:G:OP2	27:X:774:A:N6	2.32	0.53
27:X:1184:G:H1	27:X:1190:C:H42	1.57	0.53
1:A:25:THR:HG22	1:A:26:LYS:H	1.74	0.53
1:A:28:ARG:HD3	1:A:84:TYR:HB3	1.90	0.53
3:C:112:GLN:HE22	3:C:116:LYS:HG3	1.73	0.53
9:J:44:LYS:HA	9:J:95:VAL:HG12	1.91	0.53
11:L:91:ARG:HG2	11:L:92:GLY:O	2.08	0.53
12:M:63:ARG:HD3	27:X:2661:G:H4'	1.90	0.53
27:X:746:G:N7	27:X:774:A:C5	2.76	0.53
27:X:2870:C:H2'	27:X:2871:U:C6	2.44	0.53
1:A:186:HIS:HB2	1:A:188:GLU:HG2	1.91	0.53
27:X:5:A:H2'	27:X:6:A:H8	1.71	0.53
27:X:2083:G:H1	27:X:2172:U:H3	1.56	0.53
27:X:2633:A:N1	27:X:2644:A:H5''	2.23	0.53
28:Y:7:C:H2'	28:Y:8:C:H6	1.74	0.53
1:A:108:PRO:HB3	1:A:143:HIS:CE1	2.45	0.52
5:E:7:GLN:N	5:E:7:GLN:OE1	2.42	0.52
6:G:100:TYR:HB2	6:G:116:ARG:HH11	1.72	0.52
15:P:24:GLY:O	15:P:130:ILE:HA	2.09	0.52
27:X:754:G:H2'	27:X:755:C:H6	1.74	0.52
27:X:1348:C:H2'	27:X:1349:A:H8	1.73	0.52
13:N:39:LEU:HA	13:N:42:ALA:HB3	1.92	0.52
24:1:7:ARG:NH2	27:X:2262:C:OP1	2.42	0.52
27:X:88:G:H3'	27:X:89:A:H5''	1.91	0.52
27:X:2245:A:H4'	27:X:2246:A:C2	2.44	0.52
1:A:91:ARG:NH1	1:A:109:GLU:OE1	2.43	0.52
9:J:83:ARG:HH22	27:X:971:A:N6	1.99	0.52
21:V:7:ARG:HB2	21:V:60:LEU:HD11	1.91	0.52
21:V:28:LEU:HD21	21:V:42:ARG:HG2	1.91	0.52
26:3:6:THR:OG1	26:3:7:HIS:N	2.42	0.52
27:X:90:G:H3'	27:X:91:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:732:G:H2'	27:X:733:G:H8	1.74	0.52
27:X:872:G:OP2	27:X:872:G:H8	1.91	0.52
27:X:1250:A:H5'	27:X:1250:A:H8	1.73	0.52
27:X:1744:G:N2	27:X:1746:A:H3'	2.25	0.52
27:X:2837:G:H2'	27:X:2838:U:C6	2.45	0.52
27:X:2856:U:H2'	27:X:2857:C:H6	1.74	0.52
1:A:108:PRO:HB3	1:A:143:HIS:HE1	1.75	0.52
15:P:104:LYS:HE2	15:P:119:ILE:HD12	1.90	0.52
18:S:74:ARG:HH22	28:Y:94:G:H5''	1.75	0.52
27:X:1333:G:N2	27:X:1344:C:H41	2.08	0.52
27:X:1556:A:H2'	27:X:1557:G:H8	1.74	0.52
27:X:2014:A:C6	27:X:2477:C:H1'	2.44	0.52
1:A:212:SER:O	1:A:215:LEU:HD12	2.10	0.52
1:A:227:ASN:ND2	27:X:797:A:H5''	2.24	0.52
9:J:70:PHE:C	9:J:70:PHE:CD2	2.87	0.52
11:L:89:PHE:O	11:L:91:ARG:NH2	2.43	0.52
17:R:51:VAL:HG12	17:R:74:LEU:HD21	1.91	0.52
19:T:23:VAL:HB	19:T:26:PHE:HE2	1.74	0.52
19:T:64:ASP:OD1	19:T:64:ASP:N	2.41	0.52
27:X:2062:U:H2'	27:X:2063:A:C8	2.45	0.52
28:Y:64:C:H2'	28:Y:65:A:H8	1.75	0.52
2:B:120:TRP:CD2	2:B:155:ARG:HD2	2.44	0.52
5:E:76:VAL:HA	5:E:79:VAL:HG22	1.91	0.52
10:K:45:ARG:HD3	10:K:95:THR:HG22	1.91	0.52
16:Q:71:GLN:NE2	27:X:64:C:OP1	2.42	0.52
28:Y:36:A:H61	28:Y:46:G:H2'	1.74	0.52
1:A:48:ARG:HB2	27:X:792:U:P	2.49	0.52
2:B:55:ALA:HB3	2:B:58:LYS:HD2	1.92	0.52
12:M:5:ILE:HD12	12:M:5:ILE:H	1.75	0.52
15:P:31:VAL:N	15:P:125:SER:OG	2.43	0.52
20:U:48:LYS:HE3	27:X:2074:U:H1'	1.92	0.52
27:X:447:U:O2'	27:X:449:C:N4	2.42	0.52
27:X:1350:G:H2'	27:X:1351:G:C8	2.45	0.52
27:X:2306:A:O2'	27:X:2307:A:O4'	2.26	0.52
1:A:16:MET:HE2	1:A:24:LEU:HD12	1.90	0.52
4:D:4:LEU:C	4:D:6:THR:H	2.18	0.52
7:H:44:TYR:OH	27:X:1978:U:O2	2.28	0.52
16:Q:29:VAL:HG21	16:Q:38:ILE:HD11	1.91	0.52
27:X:1441:A:H4'	27:X:1442:C:O5'	2.10	0.52
27:X:1762:C:H2'	27:X:1763:G:C8	2.45	0.52
27:X:2335:U:H2'	27:X:2336:G:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HD11	1:A:52:ARG:HA	1.92	0.52
1:A:94:LEU:HD12	1:A:95:LEU:H	1.75	0.52
5:E:67:LEU:HD21	27:X:2738:A:C4	2.45	0.52
8:I:55:ARG:HH21	27:X:846:A:H4'	1.74	0.52
12:M:29:PRO:HG2	12:M:97:GLY:H	1.75	0.52
14:O:36:LYS:HE2	14:O:56:VAL:HB	1.92	0.52
20:U:39:LYS:HA	27:X:2063:A:H4'	1.92	0.52
27:X:1655:C:H5''	27:X:2689:C:O2'	2.10	0.52
27:X:2309:G:H2'	27:X:2310:G:O4'	2.10	0.52
1:A:43:ARG:O	27:X:1805:G:O2'	2.28	0.52
3:C:187:VAL:HG12	3:C:189:ASP:HB2	1.92	0.52
7:H:116:ARG:NH2	12:M:41:GLU:OE2	2.35	0.52
16:Q:17:TYR:HA	16:Q:20:MET:HB2	1.92	0.52
27:X:188:G:H2'	27:X:189:A:H8	1.73	0.52
27:X:1316:G:H5'	27:X:1659:G:H21	1.75	0.52
27:X:2299:A:H4'	27:X:2300:G:O5'	2.09	0.52
2:B:52:ALA:HB3	2:B:76:ARG:HB2	1.91	0.51
6:G:43:VAL:HG21	6:G:158:HIS:HE1	1.75	0.51
7:H:42:LYS:HA	27:X:2653:A:O3'	2.10	0.51
8:I:35:LYS:NZ	27:X:575:U:H5''	2.25	0.51
14:O:36:LYS:NZ	14:O:54:TYR:HB3	2.25	0.51
25:2:34:ARG:HD3	25:2:37:LYS:HD2	1.92	0.51
27:X:1573:G:O5'	27:X:1574:A:H5''	2.10	0.51
27:X:1662:G:H5''	27:X:1663:C:H5'	1.92	0.51
27:X:2234:G:H2'	27:X:2235:G:O4'	2.10	0.51
11:L:91:ARG:NH2	27:X:2355:A:H61	2.08	0.51
12:M:55:ILE:O	12:M:103:LYS:O	2.28	0.51
15:P:50:VAL:HG23	15:P:91:PHE:HA	1.92	0.51
15:P:103:LEU:HB2	15:P:121:LYS:O	2.10	0.51
16:Q:62:ARG:O	16:Q:70:GLY:HA2	2.09	0.51
26:3:20:GLY:O	26:3:57:ARG:NH1	2.43	0.51
27:X:185:C:H2'	27:X:186:C:H6	1.74	0.51
27:X:1296:G:N2	27:X:1299:A:H5'	2.25	0.51
28:Y:96:C:H2'	28:Y:97:C:H6	1.76	0.51
7:H:129:LEU:O	7:H:131:PRO:HD3	2.11	0.51
20:U:61:TRP:O	20:U:62:LEU:HD12	2.10	0.51
26:3:62:LEU:HD13	27:X:603:C:H5''	1.91	0.51
27:X:939:C:OP2	27:X:940:G:H8	1.94	0.51
27:X:2007:G:C2	27:X:2023:C:C2	2.98	0.51
27:X:2451:G:O2'	27:X:2457:A:N6	2.42	0.51
3:C:19:LEU:HA	3:C:20:PRO:C	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:LYS:NZ	4:D:140:GLU:OE2	2.33	0.51
8:I:102:LYS:C	8:I:104:ARG:H	2.17	0.51
18:S:17:SER:HB2	18:S:36:ARG:HB3	1.93	0.51
27:X:503:G:H2'	27:X:504:G:O4'	2.10	0.51
27:X:2171:U:H2'	27:X:2172:U:C5	2.46	0.51
27:X:2826:C:H2'	27:X:2827:G:O4'	2.11	0.51
1:A:159:ALA:HA	1:A:198:ASN:CG	2.35	0.51
5:E:24:PHE:HB2	5:E:37:TYR:CD1	2.45	0.51
6:G:58:ILE:HG12	6:G:80:VAL:HG11	1.93	0.51
15:P:36:ARG:HD3	27:X:1279:G:N7	2.26	0.51
27:X:2:G:O2'	27:X:3:U:H5'	2.10	0.51
27:X:636:G:O2'	27:X:669:G:H4'	2.10	0.51
27:X:746:G:C8	27:X:774:A:C6	2.98	0.51
27:X:2824:C:H4'	27:X:2825:A:O5'	2.10	0.51
2:B:54:LYS:HD3	2:B:59:VAL:HG22	1.92	0.51
4:D:46:ASP:HB2	4:D:49:ALA:H	1.75	0.51
6:G:61:ARG:HH22	6:G:65:LYS:H	1.59	0.51
14:O:12:TYR:CD2	14:O:40:VAL:HB	2.46	0.51
17:R:100:ASP:HB3	17:R:103:LYS:HB2	1.93	0.51
23:Z:4:HIS:HB2	23:Z:5:PRO:HD3	1.93	0.51
27:X:3:U:O2'	27:X:4:C:O5'	2.26	0.51
7:H:27:SER:HB2	7:H:50:ILE:HB	1.93	0.51
12:M:50:PHE:HE2	12:M:70:LYS:HB2	1.76	0.51
27:X:474:G:N2	27:X:477:A:OP2	2.38	0.51
27:X:1316:G:N2	27:X:1317:G:H1'	2.26	0.51
27:X:1599:G:C2	27:X:1600:U:H1'	2.46	0.51
27:X:2250:G:H2'	27:X:2251:U:C6	2.45	0.51
3:C:39:ARG:HG3	27:X:455:A:C8	2.46	0.51
19:T:26:PHE:HD1	27:X:934:G:H1'	1.76	0.51
21:V:40:PRO:HD2	27:X:94:C:H1'	1.92	0.51
23:Z:35:GLN:HG3	23:Z:51:TYR:HB3	1.91	0.51
26:3:15:LYS:HZ3	26:3:60:LEU:HD11	1.75	0.51
27:X:13:A:O2'	27:X:15:G:N7	2.35	0.51
27:X:959:C:H42	27:X:980:G:H1	1.59	0.51
27:X:1692:C:N4	27:X:1976:U:O4'	2.44	0.51
27:X:2167:A:H2	27:X:2168:A:H62	1.59	0.51
3:C:48:ARG:CZ	3:C:51:VAL:HG13	2.41	0.51
3:C:67:ALA:HB2	15:P:112:ARG:HH12	1.76	0.51
5:E:109:TYR:HD2	27:X:2646:C:H1'	1.75	0.51
5:E:154:PRO:HA	5:E:160:LYS:O	2.10	0.51
6:G:67:ARG:CG	6:G:70:PHE:HA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:577:U:O5'	27:X:956:A:N6	2.44	0.51
27:X:796:A:C8	27:X:797:A:H4'	2.45	0.51
3:C:25:GLY:HA3	8:I:18:ARG:NH1	2.26	0.51
3:C:58:MET:HG2	3:C:59:TYR:HD1	1.76	0.51
6:G:56:THR:CA	6:G:134:MET:HE1	2.41	0.51
15:P:36:ARG:NH2	27:X:1279:G:O5'	2.44	0.51
20:U:20:ARG:HB2	20:U:43:ARG:HD2	1.92	0.51
27:X:1443:G:H2'	27:X:1444:C:H6	1.75	0.51
3:C:162:ARG:HH21	27:X:333:A:H2'	1.76	0.50
11:L:15:ARG:HH21	27:X:2272:A:P	2.34	0.50
15:P:119:ILE:HG13	15:P:120:ILE:H	1.76	0.50
18:S:25:ASN:HD22	18:S:85:MET:HB2	1.75	0.50
27:X:541:C:H4'	27:X:542:A:H5''	1.92	0.50
27:X:2270:U:O2'	27:X:2353:G:N3	2.43	0.50
2:B:117:MET:HA	2:B:121:ASN:O	2.11	0.50
3:C:149:LEU:HD23	3:C:180:ILE:HG22	1.92	0.50
5:E:136:ILE:HD12	5:E:137:ASP:H	1.76	0.50
6:G:101:THR:HG23	6:G:103:TYR:CE1	2.46	0.50
16:Q:56:MET:HG2	27:X:1354:A:H4'	1.93	0.50
17:R:15:HIS:CE1	17:R:80:LYS:HE2	2.45	0.50
18:S:13:LYS:HA	18:S:18:MET:HB2	1.93	0.50
20:U:46:LEU:O	27:X:2209:G:O2'	2.28	0.50
25:2:17:GLY:O	25:2:21:ARG:HG2	2.11	0.50
27:X:493:A:H5''	27:X:494:A:OP1	2.10	0.50
27:X:943:U:H2'	27:X:944:A:C8	2.46	0.50
27:X:1539:U:H2'	27:X:1540:C:C6	2.45	0.50
6:G:53:ARG:NH2	27:X:1150:C:O3'	2.43	0.50
8:I:90:ARG:HG2	8:I:121:HIS:CE1	2.47	0.50
11:L:30:SER:HB2	11:L:43:ILE:HD11	1.93	0.50
15:P:35:PRO:HD3	15:P:124:THR:CB	2.41	0.50
19:T:39:ARG:NH2	27:X:2334:C:O2	2.44	0.50
26:3:6:THR:N	26:3:9:MET:HG2	2.26	0.50
27:X:116:A:N3	27:X:155:G:H1'	2.26	0.50
27:X:1843:U:H3	27:X:1874:G:H1	1.58	0.50
27:X:1870:U:H3'	27:X:1871:G:H21	1.77	0.50
27:X:2020:G:H2'	27:X:2021:G:H8	1.76	0.50
27:X:2380:U:H3	27:X:2394:G:H1	1.58	0.50
27:X:2664:G:H2'	27:X:2665:G:H8	1.74	0.50
2:B:11:MET:HG2	2:B:24:THR:OG1	2.10	0.50
6:G:84:ASN:HD21	6:G:154:GLU:HG2	1.74	0.50
7:H:10:VAL:HA	7:H:96:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:68:ARG:CZ	9:J:103:VAL:HG11	2.42	0.50
15:P:134:LYS:HG3	15:P:136:ASN:H	1.75	0.50
19:T:23:VAL:HG13	19:T:38:VAL:HG22	1.92	0.50
27:X:633:G:H2'	27:X:634:G:H8	1.77	0.50
1:A:63:ARG:O	1:A:65:ILE:HG22	2.12	0.50
10:K:35:GLN:HB3	10:K:112:LEU:HD23	1.94	0.50
27:X:163:A:H2'	27:X:164:G:H8	1.76	0.50
27:X:461:A:C4	27:X:462:G:C8	2.99	0.50
27:X:700:C:H2'	27:X:701:U:O4'	2.11	0.50
27:X:1332:G:O2'	27:X:1333:G:H5'	2.11	0.50
27:X:1770:U:H5	27:X:1775:A:N7	2.10	0.50
27:X:1867:A:O2'	27:X:1868:A:H8	1.95	0.50
27:X:2067:U:H2'	27:X:2068:C:C6	2.47	0.50
27:X:2674:C:H2'	27:X:2675:U:C6	2.46	0.50
6:G:106:TYR:CE2	6:G:108:GLY:HA2	2.47	0.50
9:J:44:LYS:HB2	9:J:47:GLN:NE2	2.26	0.50
15:P:28:ALA:HB2	15:P:71:VAL:CG2	2.42	0.50
21:V:42:ARG:O	21:V:46:LEU:HG	2.11	0.50
22:W:20:VAL:HG23	22:W:47:VAL:HG11	1.94	0.50
26:3:30:ARG:HE	26:3:31:HIS:HE1	1.57	0.50
1:A:244:ARG:HD2	27:X:1884:A:O2'	2.11	0.50
4:D:170:LEU:HB2	4:D:175:LEU:HD22	1.92	0.50
14:O:64:GLY:HA3	14:O:90:PHE:CZ	2.46	0.50
27:X:358:C:H2'	27:X:359:G:O4'	2.11	0.50
27:X:857:U:H2'	27:X:858:G:O4'	2.11	0.50
3:C:163:ASN:HD21	3:C:167:VAL:N	2.03	0.50
6:G:125:ARG:HD2	6:G:129:HIS:CE1	2.45	0.50
8:I:38:LYS:HE3	8:I:41:SER:OG	2.12	0.50
11:L:32:TYR:CE1	11:L:34:SER:HB3	2.46	0.50
12:M:85:SER:O	12:M:88:VAL:N	2.42	0.50
15:P:66:GLU:HB3	15:P:67:PRO:HD3	1.93	0.50
21:V:5:GLU:HA	21:V:7:ARG:HH21	1.77	0.50
27:X:806:A:OP2	27:X:806:A:H8	1.94	0.50
27:X:1001:A:H1'	27:X:1167:A:N3	2.26	0.50
27:X:1399:C:H2'	27:X:1400:A:H8	1.77	0.50
27:X:2482:A:H4'	27:X:2483:U:OP1	2.10	0.50
27:X:2828:C:H2'	27:X:2829:A:C8	2.47	0.50
1:A:161:THR:H	1:A:196:VAL:HG23	1.76	0.50
2:B:115:GLY:CA	2:B:136:ARG:HD2	2.42	0.50
3:C:146:GLU:OE2	3:C:185:ARG:NH2	2.45	0.50
15:P:21:ARG:HG3	15:P:22:LYS:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:51:ILE:O	20:U:52:ARG:HD3	2.11	0.50
26:3:11:LYS:H	26:3:11:LYS:HD2	1.77	0.50
27:X:121:G:H2'	27:X:122:G:O4'	2.12	0.50
27:X:958:G:H2'	27:X:959:C:H6	1.77	0.50
27:X:1059:A:O2'	27:X:1060:C:OP1	2.26	0.50
27:X:1098:G:N2	27:X:1114:A:H1'	2.27	0.50
27:X:1148:G:H5''	27:X:1149:G:OP2	2.11	0.50
27:X:2557:G:H2'	27:X:2558:C:H6	1.77	0.50
27:X:2628:C:H2'	27:X:2629:U:H6	1.77	0.50
28:Y:43:G:H5'	28:Y:44:C:H5''	1.94	0.50
1:A:169:GLU:N	1:A:172:TYR:O	2.36	0.49
10:K:39:THR:O	10:K:42:LYS:N	2.45	0.49
16:Q:20:MET:HE1	16:Q:94:GLN:HB2	1.94	0.49
17:R:105:ARG:NH2	17:R:111:GLY:O	2.43	0.49
27:X:820:U:H2'	27:X:821:A:H8	1.76	0.49
27:X:1060:C:O2	27:X:1124:U:H4'	2.12	0.49
27:X:1383:C:H3'	27:X:1384:G:H8	1.76	0.49
27:X:2528:G:H2'	27:X:2529:G:C8	2.47	0.49
1:A:132:PRO:HD3	1:A:190:TYR:CE2	2.47	0.49
1:A:160:GLY:HA3	27:X:1812:U:C4	2.47	0.49
1:A:244:ARG:HD3	27:X:1885:C:O4'	2.12	0.49
3:C:14:THR:HG22	3:C:15:ILE:H	1.77	0.49
6:G:103:TYR:HD2	27:X:1142:G:O4'	1.94	0.49
15:P:102:THR:HA	15:P:123:ARG:H	1.76	0.49
27:X:1665:C:H42	27:X:1992:G:H1	1.59	0.49
1:A:145:LEU:HD21	1:A:185:VAL:HG11	1.93	0.49
1:A:169:GLU:HB3	1:A:172:TYR:HB2	1.94	0.49
4:D:111:ILE:HG23	4:D:137:ILE:HG21	1.94	0.49
16:Q:63:LYS:HD3	16:Q:69:ILE:H	1.78	0.49
27:X:50:G:O2'	27:X:51:A:OP2	2.30	0.49
27:X:116:A:OP2	27:X:117:A:H2'	2.12	0.49
27:X:520:C:H2'	27:X:521:U:O4'	2.13	0.49
27:X:1310:C:H2'	27:X:1311:C:H6	1.76	0.49
27:X:1938:U:H5	27:X:2536:G:N2	2.10	0.49
28:Y:6:C:H2'	28:Y:7:C:C6	2.47	0.49
3:C:56:ARG:NE	27:X:814:G:OP2	2.45	0.49
6:G:103:TYR:O	6:G:107:GLN:NE2	2.46	0.49
15:P:41:VAL:HG21	15:P:64:ALA:HB3	1.94	0.49
16:Q:15:LYS:HG2	27:X:1404:C:O2	2.13	0.49
16:Q:73:ASN:OD1	16:Q:73:ASN:N	2.44	0.49
24:1:8:ILE:HG12	24:1:9:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:562:G:H2'	27:X:563:U:O4'	2.12	0.49
27:X:1035:G:C6	27:X:1036:G:C6	3.00	0.49
27:X:1277:G:H2'	27:X:1997:A:N6	2.28	0.49
27:X:1313:U:H4'	27:X:1314:A:H5'	1.93	0.49
27:X:1703:C:H2'	27:X:1704:G:O4'	2.12	0.49
27:X:2484:G:N2	30:X:2902:ERY:H191	2.26	0.49
1:A:226:MET:HB3	1:A:230:ASP:HB2	1.93	0.49
2:B:50:GLY:HA3	2:B:75:THR:HG21	1.93	0.49
3:C:3:GLN:N	3:C:12:GLY:O	2.30	0.49
4:D:37:ASN:ND2	27:X:2291:U:O2'	2.39	0.49
10:K:6:ALA:HB1	27:X:2848:A:C2	2.47	0.49
13:N:20:ARG:NH1	14:O:83:ARG:HH11	2.11	0.49
14:O:10:LYS:HE3	14:O:13:ARG:HH22	1.77	0.49
17:R:45:LYS:HA	17:R:76:LEU:O	2.12	0.49
23:Z:44:HIS:N	23:Z:44:HIS:CD2	2.80	0.49
27:X:1255:A:H2'	27:X:1256:C:C6	2.48	0.49
27:X:1640:C:H2'	27:X:1641:C:H6	1.78	0.49
27:X:1790:G:H5'	27:X:1811:A:H62	1.77	0.49
27:X:1922:U:H1'	27:X:2571:G:O4'	2.12	0.49
27:X:2189:A:H3'	27:X:2190:A:H5''	1.93	0.49
27:X:2457:A:C8	27:X:2508:G:C5	3.01	0.49
27:X:2520:A:H2	27:X:2745:A:H61	1.58	0.49
27:X:2557:G:H2'	27:X:2558:C:C6	2.47	0.49
27:X:2839:G:H2'	27:X:2840:U:C6	2.48	0.49
28:Y:58:G:O2'	28:Y:59:A:H5''	2.13	0.49
1:A:32:ALA:HB3	1:A:83:GLU:CD	2.38	0.49
1:A:48:ARG:HD3	27:X:1797:C:H4'	1.94	0.49
8:I:72:TYR:CE2	8:I:105:PRO:HG2	2.48	0.49
12:M:27:PHE:HA	12:M:96:ARG:HH22	1.78	0.49
17:R:37:LEU:HD11	17:R:49:GLU:HG2	1.95	0.49
27:X:32:C:O2'	27:X:33:C:H5'	2.13	0.49
27:X:828:C:H2'	27:X:829:C:C6	2.47	0.49
27:X:1787:U:H2'	27:X:1788:C:H6	1.75	0.49
27:X:1979:C:H4'	27:X:1980:A:OP1	2.13	0.49
27:X:2053:G:H2'	27:X:2054:A:C8	2.48	0.49
28:Y:73:C:H2'	28:Y:74:A:O4'	2.13	0.49
1:A:38:PRO:HA	1:A:61:LEU:HD22	1.93	0.49
1:A:252:LYS:H	1:A:252:LYS:CE	2.26	0.49
2:B:37:LYS:HB2	2:B:46:ALA:HB3	1.95	0.49
3:C:111:ARG:NH1	3:C:183:HIS:O	2.45	0.49
7:H:10:VAL:HG23	7:H:17:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:9:ILE:HB	24:1:27:ASN:O	2.13	0.49
24:1:38:LYS:HE2	24:1:40:TYR:HE1	1.78	0.49
27:X:2226:A:H2'	27:X:2227:C:C6	2.47	0.49
27:X:2512:A:OP1	27:X:2644:A:O2'	2.26	0.49
27:X:2605:C:H2'	27:X:2606:G:H8	1.76	0.49
1:A:161:THR:O	1:A:196:VAL:HG22	2.13	0.49
2:B:104:ALA:HB1	2:B:188:ILE:HD11	1.93	0.49
8:I:42:GLY:N	8:I:45:LYS:HE3	2.27	0.49
17:R:84:VAL:HG11	17:R:89:GLY:HA2	1.95	0.49
18:S:155:PRO:HG2	18:S:158:CYS:SG	2.53	0.49
20:U:46:LEU:C	20:U:47:HIS:CG	2.90	0.49
26:3:42:ARG:NE	27:X:2328:G:OP1	2.46	0.49
27:X:104:C:H2'	27:X:105:G:H8	1.78	0.49
27:X:346:C:C6	27:X:347:C:H5	2.30	0.49
27:X:538:A:N6	27:X:2025:A:H3'	2.28	0.49
27:X:960:U:H2'	27:X:961:G:C8	2.47	0.49
27:X:1184:G:H3'	27:X:1185:C:H5''	1.95	0.49
27:X:1699:A:H2'	27:X:1700:C:C6	2.48	0.49
27:X:2198:U:C2	27:X:2199:C:H1'	2.48	0.49
27:X:2553:G:N1	27:X:2554:C:O2	2.45	0.49
1:A:143:HIS:ND1	1:A:194:GLY:O	2.35	0.49
1:A:206:LEU:HD23	1:A:211:ARG:HD2	1.94	0.49
4:D:56:GLU:HA	4:D:59:LEU:HD12	1.95	0.49
5:E:24:PHE:HB2	5:E:37:TYR:HD1	1.76	0.49
9:J:15:ARG:HH21	9:J:73:LYS:NZ	2.07	0.49
10:K:12:ARG:HG2	10:K:12:ARG:HH11	1.78	0.49
17:R:62:MET:O	17:R:65:PRO:HA	2.12	0.49
26:3:14:ILE:HG23	26:3:60:LEU:HD22	1.95	0.49
26:3:30:ARG:HB3	26:3:31:HIS:ND1	2.28	0.49
27:X:1672:A:C6	27:X:1673:C:C2	3.00	0.49
4:D:38:GLU:HB3	4:D:87:ILE:HB	1.95	0.49
7:H:28:GLY:O	7:H:35:THR:HG23	2.13	0.49
27:X:830:C:O2'	27:X:852:U:H5''	2.13	0.49
27:X:1802:A:H2'	27:X:1803:G:O4'	2.13	0.49
28:Y:15:A:O2'	28:Y:16:U:H5''	2.12	0.49
28:Y:39:C:H5'	28:Y:40:C:OP2	2.12	0.49
2:B:136:ARG:HG2	2:B:137:ARG:N	2.27	0.48
6:G:67:ARG:HG2	6:G:70:PHE:HA	1.95	0.48
6:G:69:ASP:H	6:G:76:GLN:NE2	2.10	0.48
11:L:32:TYR:O	11:L:38:ILE:HA	2.13	0.48
12:M:104:LEU:HA	12:M:106:TYR:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:86:PRO:HG2	17:R:90:LYS:HE2	1.95	0.48
27:X:1351:G:H2'	27:X:1352:G:C8	2.48	0.48
27:X:2543:A:C2	27:X:2626:U:H4'	2.47	0.48
28:Y:96:C:H2'	28:Y:97:C:C6	2.47	0.48
2:B:145:LYS:HB2	27:X:2551:A:N7	2.29	0.48
4:D:24:SER:OG	28:Y:57:U:O3'	2.29	0.48
8:I:33:GLY:HA2	14:O:79:GLN:HG3	1.95	0.48
13:N:66:ASN:HB2	13:N:70:ARG:NH1	2.28	0.48
14:O:85:GLY:N	27:X:1238:A:H5'	2.27	0.48
15:P:41:VAL:HG11	15:P:65:SER:HA	1.95	0.48
18:S:1:MET:HE2	18:S:52:PHE:HB3	1.94	0.48
27:X:836:G:H2'	27:X:837:U:H6	1.78	0.48
27:X:2204:A:H4'	27:X:2205:C:O5'	2.13	0.48
27:X:2261:G:H5''	27:X:2262:C:O4'	2.14	0.48
1:A:251:GLY:HA3	1:A:255:LYS:NZ	2.27	0.48
2:B:203:LYS:HG2	27:X:2713:A:H61	1.78	0.48
3:C:163:ASN:HD21	3:C:166:TRP:HB2	1.78	0.48
6:G:43:VAL:HG12	6:G:167:LYS:HE3	1.96	0.48
18:S:104:SER:HA	18:S:139:THR:HA	1.95	0.48
19:T:41:ARG:HD2	19:T:41:ARG:HA	1.52	0.48
27:X:38:G:H1	27:X:453:U:H3	1.61	0.48
27:X:346:C:H2'	27:X:347:C:C5	2.48	0.48
27:X:514:G:H4'	27:X:515:A:OP2	2.11	0.48
27:X:543:G:C5	27:X:544:U:C4	3.02	0.48
27:X:558:G:C8	27:X:560:G:C8	3.01	0.48
27:X:1283:C:H5''	27:X:1284:G:C5'	2.42	0.48
27:X:2532:G:C2	27:X:2533:U:H1'	2.47	0.48
4:D:80:ARG:NE	4:D:83:MET:SD	2.81	0.48
11:L:21:THR:O	11:L:25:GLY:N	2.33	0.48
24:1:30:ASN:OD1	24:1:31:THR:N	2.47	0.48
26:3:26:LYS:NZ	26:3:28:GLY:HA3	2.28	0.48
27:X:165:G:H1	27:X:185:C:N4	2.11	0.48
27:X:736:G:H2'	27:X:737:C:O4'	2.14	0.48
27:X:2040:A:H2'	27:X:2041:A:H8	1.73	0.48
27:X:2278:A:H2'	27:X:2279:G:C8	2.47	0.48
27:X:2407:G:H5''	27:X:2408:G:O5'	2.12	0.48
27:X:2498:U:C5	27:X:2520:A:C6	3.01	0.48
27:X:2655:C:O2	27:X:2712:G:N2	2.38	0.48
1:A:30:GLU:HB2	1:A:82:ILE:O	2.14	0.48
2:B:128:SER:HB2	2:B:129:HIS:ND1	2.29	0.48
2:B:172:VAL:HG22	2:B:182:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:182:ARG:NH1	3:C:183:HIS:HE1	2.10	0.48
9:J:99:LYS:HG3	9:J:100:PRO:HD2	1.94	0.48
16:Q:62:ARG:NH1	16:Q:73:ASN:HD21	2.11	0.48
26:3:58:MET:HA	26:3:61:MET:HB2	1.94	0.48
27:X:224:G:H4'	27:X:399:G:C5	2.48	0.48
27:X:459:A:H4'	27:X:461:A:N7	2.28	0.48
27:X:1019:U:HO2'	27:X:1020:A:P	2.35	0.48
27:X:1437:A:H2'	27:X:1438:G:C8	2.47	0.48
27:X:1623:C:H4'	27:X:1624:A:O5'	2.13	0.48
28:Y:7:C:H2'	28:Y:8:C:C6	2.49	0.48
1:A:226:MET:HE2	27:X:795:A:C6	2.49	0.48
3:C:104:LEU:O	3:C:108:ILE:HG13	2.12	0.48
5:E:37:TYR:CZ	5:E:72:VAL:HG22	2.48	0.48
5:E:143:GLN:NE2	27:X:2724:G:H21	2.12	0.48
7:H:14:SER:OG	7:H:98:ILE:HD12	2.13	0.48
16:Q:28:TRP:HZ3	16:Q:58:VAL:HG21	1.78	0.48
27:X:936:A:H2'	27:X:937:C:O4'	2.13	0.48
3:C:62:LYS:HD2	27:X:2044:G:OP1	2.13	0.48
9:J:57:ARG:NE	27:X:2448:A:O2'	2.38	0.48
15:P:39:ARG:HD2	15:P:97:VAL:HB	1.94	0.48
20:U:20:ARG:N	20:U:41:VAL:O	2.38	0.48
20:U:20:ARG:HH21	20:U:43:ARG:HG2	1.79	0.48
27:X:537:C:O2'	27:X:538:A:C4	2.66	0.48
27:X:764:A:H2	27:X:802:A:HO2'	1.59	0.48
27:X:1653:C:H2'	27:X:1654:A:C8	2.49	0.48
27:X:1815:G:H2'	27:X:1816:G:H8	1.79	0.48
27:X:2013:A:H4'	27:X:2014:A:C8	2.49	0.48
8:I:94:GLU:HA	8:I:97:ARG:NE	2.28	0.48
10:K:82:GLU:O	10:K:85:PRO:HD2	2.14	0.48
16:Q:58:VAL:HA	16:Q:59:PRO:HD2	1.61	0.48
17:R:61:SER:HA	17:R:65:PRO:CG	2.42	0.48
24:1:28:ARG:HB2	24:1:30:ASN:ND2	2.28	0.48
27:X:492:G:H2'	27:X:517:A:N1	2.29	0.48
27:X:603:C:H2'	27:X:604:U:H6	1.79	0.48
27:X:1333:G:N2	27:X:1344:C:N4	2.61	0.48
27:X:1404:C:C2	27:X:1406:A:N7	2.81	0.48
27:X:1451:C:H2'	27:X:1452:U:C6	2.47	0.48
27:X:1586:A:H2'	27:X:1587:A:C8	2.49	0.48
27:X:2199:C:H2'	27:X:2200:G:H8	1.79	0.48
27:X:2590:U:C1'	30:X:2902:ERY:H361	2.44	0.48
27:X:2657:G:H2'	27:X:2658:A:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:ARG:CZ	3:C:77:PHE:HE2	2.27	0.48
4:D:134:GLU:HG2	4:D:136:LEU:H	1.79	0.48
5:E:24:PHE:CD1	5:E:37:TYR:HB2	2.49	0.48
5:E:165:VAL:HB	5:E:166:GLY:H	1.46	0.48
6:G:137:LYS:HD2	27:X:2022:C:OP2	2.14	0.48
14:O:48:GLY:C	14:O:50:ASP:H	2.22	0.48
15:P:70:LYS:HE2	27:X:499:G:O2'	2.14	0.48
25:2:36:ALA:C	25:2:38:GLY:H	2.21	0.48
27:X:568:G:H2'	27:X:569:C:O4'	2.14	0.48
27:X:732:G:H2'	27:X:733:G:C8	2.48	0.48
27:X:2260:C:O2'	27:X:2261:G:H5'	2.14	0.48
1:A:200:GLU:HB2	1:A:203:ASN:ND2	2.29	0.48
1:A:206:LEU:HA	1:A:211:ARG:HH11	1.79	0.48
5:E:143:GLN:HG2	27:X:2725:C:H1'	1.95	0.48
23:Z:7:PRO:HA	27:X:2594:U:C6	2.49	0.48
27:X:227:G:C6	27:X:228:A:C6	3.01	0.48
27:X:2190:A:H61	27:X:2196:U:H3	1.60	0.48
1:A:212:SER:OG	1:A:213:ARG:N	2.48	0.47
3:C:62:LYS:HE2	3:C:63:GLY:N	2.29	0.47
8:I:31:GLY:HA3	8:I:34:HIS:ND1	2.29	0.47
8:I:38:LYS:HG3	27:X:954:U:OP2	2.14	0.47
13:N:81:ASN:HD22	13:N:117:ARG:HH12	1.61	0.47
24:1:36:GLU:HG3	24:1:53:LYS:HA	1.96	0.47
27:X:114:C:O2'	27:X:124:A:N3	2.43	0.47
27:X:773:G:H2'	27:X:774:A:H5'	1.95	0.47
27:X:824:U:O2	27:X:1263:G:H3'	2.14	0.47
27:X:825:C:H5''	27:X:1263:G:HO2'	1.77	0.47
27:X:1107:A:H3'	27:X:1108:U:H5''	1.96	0.47
27:X:1417:C:H2'	27:X:1418:C:H6	1.78	0.47
2:B:108:SER:HB3	2:B:163:GLU:H	1.79	0.47
8:I:38:LYS:HG3	27:X:954:U:P	2.53	0.47
9:J:28:VAL:HG11	9:J:135:ARG:HB3	1.95	0.47
13:N:74:MET:HE1	13:N:113:SER:HB3	1.95	0.47
18:S:67:LYS:NZ	18:S:92:VAL:HG21	2.28	0.47
27:X:66:U:H2'	27:X:67:G:C8	2.49	0.47
30:X:2902:ERY:H312	30:X:2902:ERY:H2	1.63	0.47
1:A:97:TYR:HE2	1:A:103:ARG:HB2	1.79	0.47
7:H:11:ALA:N	7:H:96:ALA:O	2.37	0.47
8:I:62:LYS:HB3	26:3:13:ARG:H	1.77	0.47
16:Q:59:PRO:HA	16:Q:74:ASP:OD1	2.15	0.47
19:T:56:ASP:OD1	27:X:2343:C:H4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:83:ALA:HB1	19:T:85:GLN:HE21	1.79	0.47
21:V:46:LEU:O	21:V:50:VAL:HG23	2.14	0.47
27:X:1074:G:H1	27:X:1086:C:N4	2.12	0.47
27:X:1636:G:H2'	27:X:1637:U:C6	2.49	0.47
27:X:1655:C:H4'	27:X:2689:C:O2	2.14	0.47
27:X:1672:A:H3'	27:X:1673:C:C6	2.49	0.47
27:X:2542:U:O2	27:X:2544:A:H8	1.98	0.47
2:B:136:ARG:HH21	2:B:157:ALA:H	1.62	0.47
8:I:56:LEU:CB	26:3:52:LYS:HZ1	2.25	0.47
8:I:128:ALA:HA	8:I:131:LYS:HB3	1.95	0.47
9:J:16:GLY:HA2	9:J:17:ARG:NH1	2.25	0.47
21:V:54:ASN:HB3	27:X:71:A:C5	2.49	0.47
27:X:91:A:H2'	27:X:92:U:C6	2.49	0.47
27:X:333:A:H5'	27:X:351:A:H1'	1.95	0.47
27:X:760:U:OP1	27:X:2591:C:H1'	2.15	0.47
27:X:1052:C:N4	27:X:1053:G:N7	2.63	0.47
27:X:1171:A:H2'	27:X:1172:U:C6	2.49	0.47
27:X:2184:C:H2'	27:X:2185:U:O4'	2.14	0.47
27:X:2258:G:C2	27:X:2259:G:C8	3.02	0.47
27:X:2691:C:O2'	27:X:2693:U:H5'	2.13	0.47
27:X:2701:A:C2	27:X:2848:A:C4	3.03	0.47
10:K:63:ARG:HA	10:K:80:MET:HE3	1.97	0.47
13:N:81:ASN:CG	27:X:1162:A:H4'	2.39	0.47
23:Z:45:ILE:HD13	23:Z:57:VAL:HG23	1.96	0.47
27:X:525:A:N1	27:X:1273:G:O2'	2.40	0.47
27:X:540:G:C5	27:X:2005:U:H5''	2.49	0.47
27:X:2363:G:H3'	27:X:2365:U:OP1	2.14	0.47
4:D:31:ILE:HA	4:D:158:THR:HA	1.97	0.47
4:D:153:ASP:OD1	27:X:2283:G:O2'	2.28	0.47
15:P:21:ARG:HH21	27:X:506:G:H5'	1.79	0.47
15:P:122:LYS:HB3	15:P:124:THR:CG2	2.45	0.47
27:X:552:C:H2'	27:X:553:C:H5''	1.96	0.47
27:X:682:G:H3'	27:X:683:A:C8	2.50	0.47
27:X:1468:A:H8	27:X:1468:A:P	2.38	0.47
27:X:1750:A:H4'	27:X:2695:C:O4'	2.14	0.47
27:X:2368:G:H5''	27:X:2369:U:H5'	1.97	0.47
27:X:2576:G:C6	27:X:2577:A:C6	3.03	0.47
1:A:79:VAL:HB	1:A:114:GLY:H	1.80	0.47
2:B:131:SER:C	2:B:134:TRP:HE1	2.19	0.47
7:H:23:ARG:HD2	7:H:24:VAL:O	2.15	0.47
7:H:110:VAL:HB	7:H:129:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:60:LEU:HD11	10:K:64:ARG:HH11	1.80	0.47
15:P:47:GLY:H	15:P:92:VAL:CG2	2.27	0.47
17:R:62:MET:H	17:R:65:PRO:HA	1.79	0.47
27:X:136:A:H2'	27:X:137:A:O4'	2.15	0.47
27:X:469:G:N2	27:X:480:G:H2'	2.30	0.47
27:X:536:A:N6	27:X:2605:C:H4'	2.30	0.47
27:X:582:G:O2'	27:X:583:C:H3'	2.14	0.47
27:X:742:G:H2'	27:X:1766:U:H1'	1.96	0.47
27:X:1164:C:H2'	27:X:1165:G:O4'	2.15	0.47
27:X:1353:A:H4'	27:X:1407:G:H1'	1.95	0.47
27:X:1419:G:H2'	27:X:1420:A:C8	2.50	0.47
27:X:1673:C:C2	27:X:1674:C:C5	3.02	0.47
27:X:1779:C:O5'	27:X:1779:C:H6	1.97	0.47
27:X:2524:G:C6	27:X:2525:U:C4	3.02	0.47
27:X:2670:C:H5'	27:X:2847:G:H5''	1.97	0.47
27:X:2684:A:H2'	27:X:2685:A:O4'	2.14	0.47
1:A:181:GLU:HG3	1:A:270:ILE:HA	1.95	0.47
2:B:32:PRO:O	2:B:49:ILE:HA	2.15	0.47
5:E:138:LYS:HG2	27:X:2726:U:H5''	1.97	0.47
11:L:8:ARG:HE	11:L:9:ARG:HG2	1.79	0.47
11:L:59:LEU:HD23	11:L:61:SER:HB3	1.97	0.47
15:P:34:SER:O	15:P:37:LYS:HB3	2.15	0.47
16:Q:57:ASN:HD21	16:Q:76:LYS:HE3	1.80	0.47
27:X:343:A:H1'	27:X:346:C:N4	2.29	0.47
27:X:835:U:H2'	27:X:836:G:C8	2.50	0.47
27:X:1332:G:C6	27:X:1333:G:N1	2.82	0.47
27:X:1838:G:N2	27:X:1878:C:N3	2.63	0.47
27:X:2280:A:H2'	27:X:2281:C:C6	2.49	0.47
28:Y:16:U:O2'	28:Y:110:U:H1'	2.15	0.47
1:A:38:PRO:HG3	27:X:1586:A:H5'	1.97	0.47
3:C:54:THR:HG22	3:C:55:GLY:O	2.15	0.47
11:L:33:ARG:HH21	11:L:103:LEU:HD12	1.79	0.47
17:R:22:VAL:HG13	17:R:81:VAL:O	2.15	0.47
19:T:46:LYS:HE3	19:T:76:ALA:HA	1.96	0.47
26:3:23:MET:HB3	26:3:25:PHE:CE2	2.49	0.47
26:3:30:ARG:HB2	27:X:2372:A:OP1	2.15	0.47
27:X:393:U:H2'	27:X:394:U:C6	2.49	0.47
27:X:640:C:H1'	27:X:650:U:H1'	1.97	0.47
27:X:1727:C:H2'	27:X:1728:A:C8	2.50	0.47
27:X:1813:A:H5''	27:X:1814:G:OP2	2.15	0.47
1:A:118:ASN:HD22	1:A:119:ALA:N	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LYS:C	2:B:134:TRP:CD1	2.93	0.47
3:C:129:LYS:O	3:C:131:LYS:N	2.47	0.47
6:G:151:TYR:HE1	6:G:161:GLN:HE21	1.63	0.47
9:J:28:VAL:HG21	9:J:135:ARG:HB3	1.97	0.47
14:O:88:GLN:HE21	14:O:88:GLN:HB3	1.48	0.47
15:P:9:ARG:HD2	15:P:13:GLN:HG3	1.96	0.47
18:S:1:MET:N	18:S:53:ASP:O	2.42	0.47
20:U:64:ALA:O	20:U:67:LEU:HB3	2.15	0.47
23:Z:42:SER:O	23:Z:44:HIS:CD2	2.67	0.47
27:X:203:G:H21	27:X:205:A:H62	1.63	0.47
27:X:649:G:C5	27:X:650:U:C5	3.02	0.47
27:X:879:A:H2'	27:X:879:A:N3	2.30	0.47
27:X:1643:A:N6	27:X:1656:U:H3	2.08	0.47
27:X:2266:A:H5''	27:X:2267:A:OP1	2.15	0.47
27:X:2781:G:H2'	27:X:2782:G:H5''	1.96	0.47
28:Y:53:G:N3	28:Y:53:G:H2'	2.29	0.47
4:D:103:LEU:HG	4:D:108:LEU:HG	1.97	0.46
6:G:83:ILE:HG22	6:G:153:GLY:O	2.15	0.46
7:H:29:ILE:HB	7:H:34:LEU:HD23	1.96	0.46
7:H:132:GLU:HB2	12:M:73:PHE:CE1	2.49	0.46
9:J:21:ASP:OD1	9:J:21:ASP:N	2.36	0.46
11:L:11:LEU:HD21	27:X:2273:C:H5''	1.97	0.46
15:P:45:ILE:O	15:P:48:LYS:HG2	2.15	0.46
26:3:6:THR:N	26:3:59:LYS:HB3	2.30	0.46
27:X:1301:U:C2	27:X:1340:C:O2	2.68	0.46
27:X:1448:A:H61	27:X:1574:A:H61	1.61	0.46
27:X:1467:U:H3'	27:X:1467:U:H6	1.80	0.46
27:X:2170:C:H3'	27:X:2171:U:H5''	1.97	0.46
1:A:18:THR:HG22	1:A:19:ALA:H	1.79	0.46
1:A:133:LEU:HB3	1:A:173:VAL:HG21	1.97	0.46
5:E:84:THR:HG22	5:E:134:SER:OG	2.15	0.46
8:I:31:GLY:O	8:I:32:ARG:HD2	2.15	0.46
10:K:13:ASN:OD1	10:K:15:SER:N	2.43	0.46
10:K:78:LYS:O	10:K:83:VAL:HG23	2.15	0.46
12:M:99:VAL:HG21	12:M:104:LEU:HD11	1.97	0.46
27:X:179:U:H2'	27:X:180:C:O4'	2.15	0.46
27:X:218:A:H61	27:X:232:A:H5''	1.80	0.46
27:X:522:G:OP1	27:X:1247:U:O2'	2.23	0.46
27:X:540:G:O2'	27:X:542:A:H2	1.97	0.46
27:X:687:G:N2	27:X:2423:G:O3'	2.48	0.46
27:X:747:A:H2'	27:X:748:A:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:758:G:H2'	27:X:759:C:H5'	1.98	0.46
27:X:1141:U:O2'	27:X:1142:G:O5'	2.23	0.46
27:X:1407:G:C6	27:X:1408:A:C6	3.03	0.46
27:X:1781:C:H2'	27:X:1782:A:C5	2.50	0.46
27:X:1919:A:C6	27:X:1928:G:C4	3.03	0.46
27:X:2312:A:H4'	27:X:2313:G:O5'	2.15	0.46
1:A:25:THR:HG22	1:A:26:LYS:N	2.30	0.46
1:A:222:ARG:HD3	27:X:1820:G:O6	2.16	0.46
2:B:162:MET:SD	27:X:2796:A:H4'	2.55	0.46
3:C:5:ASN:N	3:C:5:ASN:OD1	2.48	0.46
5:E:68:THR:O	5:E:72:VAL:HG23	2.15	0.46
7:H:5:GLN:HG2	27:X:1685:A:H5''	1.97	0.46
9:J:37:ALA:O	9:J:100:PRO:HA	2.14	0.46
12:M:22:ARG:HH22	12:M:24:LEU:HD23	1.80	0.46
12:M:90:GLN:OE1	12:M:90:GLN:N	2.34	0.46
16:Q:8:GLN:O	21:V:29:ARG:HG2	2.15	0.46
26:3:6:THR:N	26:3:59:LYS:HD3	2.31	0.46
27:X:1388:C:H2'	27:X:1389:C:C6	2.50	0.46
27:X:1840:A:H2'	27:X:1841:G:O4'	2.15	0.46
27:X:2020:G:C6	27:X:2021:G:C6	3.03	0.46
6:G:31:THR:HG21	13:N:61:TRP:HE1	1.81	0.46
9:J:6:LYS:HE2	9:J:6:LYS:HB2	1.57	0.46
9:J:116:LYS:HE2	9:J:132:MET:HE2	1.97	0.46
15:P:28:ALA:O	15:P:126:HIS:HA	2.16	0.46
22:W:2:LYS:HZ3	22:W:31:SER:HB2	1.80	0.46
27:X:835:U:H2'	27:X:836:G:H8	1.80	0.46
27:X:962:C:H2'	27:X:963:G:H8	1.81	0.46
27:X:1159:U:H2'	27:X:1160:C:C6	2.51	0.46
27:X:1975:G:H22	27:X:1979:C:H6	1.63	0.46
27:X:2026:C:H2'	27:X:2027:C:H6	1.80	0.46
27:X:2226:A:H2'	27:X:2227:C:H6	1.81	0.46
27:X:2605:C:H2'	27:X:2606:G:C8	2.50	0.46
7:H:2:ILE:HG22	7:H:6:SER:HB3	1.98	0.46
13:N:74:MET:SD	13:N:110:VAL:HG13	2.55	0.46
14:O:5:ILE:N	14:O:10:LYS:HE2	2.30	0.46
14:O:20:ILE:HG22	14:O:21:ARG:H	1.80	0.46
14:O:68:LYS:HA	14:O:87:ARG:HG2	1.97	0.46
17:R:40:LEU:HB2	17:R:45:LYS:HB2	1.98	0.46
18:S:94:VAL:O	18:S:121:GLN:HA	2.15	0.46
19:T:74:LYS:HG2	19:T:77:ARG:NE	2.30	0.46
27:X:89:A:H4'	27:X:90:G:C5'	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:104:C:H2'	27:X:105:G:C8	2.50	0.46
27:X:571:U:C2	27:X:581:A:C8	3.03	0.46
27:X:769:C:C4	27:X:770:U:C4	3.03	0.46
27:X:958:G:H2'	27:X:959:C:C6	2.51	0.46
27:X:2030:U:H2'	27:X:2031:A:H8	1.81	0.46
27:X:2406:C:H5''	27:X:2407:G:OP1	2.15	0.46
27:X:2425:G:C2	27:X:2480:C:C4	3.03	0.46
3:C:46:ARG:HD3	27:X:463:C:OP1	2.15	0.46
8:I:118:VAL:HG23	8:I:133:VAL:HG13	1.98	0.46
9:J:37:ALA:HB2	9:J:104:MET:SD	2.55	0.46
13:N:84:LYS:NZ	27:X:1163:C:OP1	2.45	0.46
14:O:15:SER:N	14:O:95:ILE:O	2.49	0.46
18:S:19:ILE:HG23	18:S:79:ILE:O	2.16	0.46
19:T:25:LYS:HD3	19:T:31:VAL:HG12	1.98	0.46
22:W:12:ARG:HG2	22:W:12:ARG:HH11	1.81	0.46
27:X:54:G:O2'	27:X:125:A:N1	2.43	0.46
27:X:817:A:H2'	27:X:819:C:C4	2.50	0.46
27:X:824:U:H1'	27:X:1264:C:O4'	2.15	0.46
27:X:1018:C:H5''	27:X:1019:U:H5''	1.98	0.46
27:X:1030:U:H2'	27:X:1032:A:C2	2.48	0.46
27:X:1040:A:C8	27:X:1041:G:C8	3.04	0.46
27:X:1073:G:OP2	27:X:1073:G:H8	1.99	0.46
27:X:1806:G:H5''	27:X:1807:A:H2'	1.97	0.46
27:X:2197:U:H2'	27:X:2198:U:C5	2.51	0.46
27:X:2485:U:O2	27:X:2485:U:H2'	2.15	0.46
27:X:2522:G:H2'	27:X:2523:G:H8	1.79	0.46
27:X:2692:A:H5''	27:X:2693:U:OP2	2.16	0.46
2:B:98:GLU:HA	2:B:172:VAL:HG12	1.97	0.46
3:C:58:MET:HB2	3:C:70:GLY:O	2.16	0.46
5:E:90:ARG:HB3	5:E:160:LYS:HA	1.97	0.46
5:E:169:ILE:HD13	5:E:170:ALA:H	1.81	0.46
8:I:35:LYS:HZ3	27:X:575:U:H5''	1.81	0.46
10:K:28:LEU:HD12	10:K:113:ILE:HG23	1.96	0.46
12:M:31:ASP:OD2	12:M:31:ASP:N	2.49	0.46
15:P:89:ARG:HB3	15:P:133:GLU:HB3	1.97	0.46
15:P:105:ARG:HG3	15:P:107:ILE:HB	1.97	0.46
25:2:21:ARG:O	25:2:28:ARG:HD3	2.16	0.46
27:X:308:C:H2'	27:X:309:G:O4'	2.15	0.46
27:X:603:C:H2'	27:X:604:U:C6	2.51	0.46
27:X:971:A:N1	27:X:2474:G:O2'	2.47	0.46
27:X:1412:C:H6	27:X:1412:C:H2'	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2051:U:H3	27:X:2409:A:H62	1.63	0.46
2:B:129:HIS:CD2	27:X:1692:C:C2	3.03	0.46
4:D:22:TYR:OH	4:D:165:GLU:OE1	2.34	0.46
6:G:94:LYS:HE3	6:G:95:LEU:HG	1.98	0.46
7:H:132:GLU:HB2	12:M:73:PHE:HE1	1.80	0.46
18:S:13:LYS:N	18:S:18:MET:HE2	2.30	0.46
26:3:29:LYS:HD2	26:3:33:ASN:O	2.16	0.46
27:X:82:G:N1	27:X:100:G:O2'	2.42	0.46
27:X:839:U:H5''	27:X:2408:G:P	2.56	0.46
27:X:1681:A:C2	27:X:2706:U:C2	3.04	0.46
27:X:2516:U:H2'	27:X:2517:C:C6	2.51	0.46
27:X:2546:G:H2'	27:X:2547:C:C6	2.51	0.46
27:X:2696:A:O2'	27:X:2697:G:H5'	2.15	0.46
27:X:2753:C:H2'	27:X:2754:C:H6	1.81	0.46
1:A:201:HIS:HA	1:A:204:ILE:HD12	1.97	0.46
3:C:59:TYR:CD2	3:C:64:THR:HG21	2.51	0.46
7:H:100:ASN:C	7:H:100:ASN:OD1	2.59	0.46
13:N:24:PHE:HB3	13:N:28:ARG:HB2	1.97	0.46
15:P:97:VAL:HG13	15:P:125:SER:O	2.16	0.46
16:Q:11:VAL:HG23	16:Q:27:PHE:HA	1.97	0.46
26:3:13:ARG:HG3	26:3:13:ARG:O	2.16	0.46
27:X:312:G:C4	27:X:313:U:C5	3.04	0.46
27:X:330:C:H2'	27:X:331:U:O4'	2.16	0.46
27:X:1096:A:H5''	27:X:1116:U:H4'	1.98	0.46
27:X:1223:G:H5'	27:X:1225:G:O4'	2.16	0.46
27:X:1770:U:C5	27:X:1775:A:N7	2.84	0.46
27:X:2309:G:H1	27:X:2364:C:H42	1.63	0.46
27:X:2453:C:H5'	27:X:2454:C:OP2	2.16	0.46
27:X:2526:U:H2'	27:X:2527:G:C8	2.50	0.46
1:A:252:LYS:NZ	1:A:253:PRO:HD2	2.31	0.46
3:C:34:GLN:NE2	3:C:176:ASN:OD1	2.49	0.46
12:M:16:ILE:H	12:M:16:ILE:HD12	1.81	0.46
27:X:650:U:H2'	27:X:651:C:C6	2.51	0.46
27:X:820:U:H2'	27:X:821:A:C8	2.51	0.46
27:X:1981:A:O3'	27:X:2704:U:H4'	2.15	0.46
27:X:1998:A:O5'	27:X:1998:A:H8	1.99	0.46
27:X:2372:A:H62	27:X:2401:A:N6	2.14	0.46
27:X:2434:G:H2'	27:X:2435:C:C6	2.51	0.46
1:A:24:LEU:O	1:A:25:THR:OG1	2.34	0.45
2:B:164:ARG:HD2	27:X:2753:C:H5''	1.98	0.45
10:K:89:GLU:O	10:K:91:PRO:HD3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:104:LEU:HD23	12:M:106:TYR:CZ	2.51	0.45
27:X:658:G:H2'	27:X:659:G:H8	1.81	0.45
27:X:666:U:H2'	27:X:667:U:H5''	1.98	0.45
27:X:746:G:N7	27:X:774:A:C6	2.85	0.45
27:X:939:C:OP2	27:X:940:G:C8	2.70	0.45
27:X:984:A:O4'	27:X:1202:U:C6	2.69	0.45
27:X:1478:U:H2'	27:X:1479:G:C8	2.51	0.45
27:X:1782:A:N6	27:X:1820:G:O2'	2.49	0.45
27:X:1793:A:H2'	27:X:1794:A:C8	2.51	0.45
27:X:2048:C:H1'	27:X:2428:U:H3	1.81	0.45
28:Y:16:U:H4'	28:Y:72:C:O2	2.16	0.45
1:A:252:LYS:HD3	27:X:1817:U:O4'	2.16	0.45
2:B:52:ALA:HB2	12:M:3:THR:HG23	1.98	0.45
2:B:119:ARG:HA	2:B:160:MET:HE3	1.97	0.45
7:H:91:PHE:N	7:H:91:PHE:CD1	2.84	0.45
13:N:8:ILE:HG22	13:N:11:ARG:NH2	2.31	0.45
16:Q:10:PRO:HA	16:Q:27:PHE:HB3	1.98	0.45
24:1:12:MET:HE3	24:1:54:LYS:HD3	1.98	0.45
27:X:88:G:C3'	27:X:89:A:H5''	2.47	0.45
27:X:982:C:H2'	27:X:983:G:O4'	2.16	0.45
27:X:2736:U:H4'	27:X:2737:A:OP1	2.17	0.45
27:X:2797:G:H2'	27:X:2798:A:H5''	1.99	0.45
27:X:2849:C:H2'	27:X:2850:U:C6	2.51	0.45
2:B:9:ILE:HD11	2:B:27:LEU:CB	2.43	0.45
2:B:37:LYS:NZ	2:B:80:GLU:OE2	2.42	0.45
4:D:80:ARG:HG3	4:D:83:MET:HE3	1.99	0.45
8:I:59:ARG:CB	27:X:2371:A:H8	2.30	0.45
8:I:94:GLU:HA	8:I:97:ARG:HG3	1.97	0.45
9:J:82:THR:HA	27:X:2474:G:C5'	2.34	0.45
15:P:99:ALA:CB	27:X:25:U:H5'	2.43	0.45
15:P:104:LYS:HG3	15:P:106:LEU:H	1.82	0.45
16:Q:68:PHE:O	16:Q:70:GLY:N	2.42	0.45
24:1:39:LYS:NZ	24:1:47:HIS:HA	2.31	0.45
25:2:38:GLY:HA3	27:X:469:G:H8	1.82	0.45
26:3:15:LYS:HZ3	26:3:60:LEU:HD21	1.82	0.45
27:X:239:A:N3	27:X:443:A:O2'	2.43	0.45
27:X:324:C:H2'	27:X:325:U:O4'	2.17	0.45
27:X:1230:C:H2'	27:X:1231:A:C8	2.52	0.45
27:X:1763:G:H2'	27:X:1764:A:H4'	1.97	0.45
27:X:2477:C:O2'	27:X:2478:C:H5'	2.15	0.45
27:X:2640:G:H2'	27:X:2641:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD22	1:A:211:ARG:HB3	1.98	0.45
2:B:69:LYS:HE2	2:B:69:LYS:HB3	1.80	0.45
2:B:136:ARG:O	2:B:137:ARG:C	2.59	0.45
3:C:133:PHE:CE1	3:C:161:ALA:HB2	2.51	0.45
5:E:44:ARG:NH2	5:E:51:LEU:HB3	2.32	0.45
9:J:13:GLN:HG3	9:J:14:PHE:CD1	2.51	0.45
12:M:50:PHE:CE2	12:M:70:LYS:HB2	2.52	0.45
27:X:577:U:H2'	27:X:579:G:OP2	2.17	0.45
27:X:768:U:C4	27:X:769:C:C4	3.05	0.45
27:X:2044:G:C8	27:X:2482:A:C8	3.04	0.45
27:X:2590:U:C5	30:X:2902:ERY:H312	2.51	0.45
27:X:2645:C:H3'	27:X:2646:C:H6	1.82	0.45
27:X:2674:C:H2'	27:X:2675:U:H6	1.81	0.45
28:Y:43:G:OP1	28:Y:45:C:N4	2.40	0.45
2:B:152:LYS:HB3	6:G:106:TYR:CB	2.44	0.45
7:H:24:VAL:HG22	7:H:45:ALA:HB2	1.97	0.45
8:I:56:LEU:HD21	8:I:59:ARG:HH21	1.82	0.45
9:J:42:TRP:CZ2	27:X:969:U:H5	2.35	0.45
17:R:105:ARG:HH22	17:R:112:LYS:HA	1.82	0.45
26:3:14:ILE:HD11	26:3:56:ALA:HB1	1.98	0.45
27:X:90:G:H3'	27:X:91:A:H8	1.80	0.45
27:X:172:A:H5''	27:X:173:A:OP2	2.17	0.45
27:X:1083:C:H42	27:X:1103:C:N4	2.15	0.45
27:X:1225:G:H2'	27:X:1249:G:H22	1.81	0.45
27:X:1724:C:N3	27:X:1747:G:C6	2.85	0.45
27:X:1751:A:H2'	27:X:1752:U:C6	2.51	0.45
27:X:2499:C:C4	27:X:2546:G:C8	3.04	0.45
27:X:2519:C:O2	27:X:2720:A:H2	2.00	0.45
1:A:43:ARG:NH1	1:A:43:ARG:H	2.14	0.45
1:A:208:LYS:HD3	27:X:1782:A:H1'	1.99	0.45
1:A:231:HIS:CG	1:A:232:PRO:HD2	2.52	0.45
3:C:86:PRO:C	3:C:87:LYS:HD2	2.42	0.45
9:J:76:THR:HB	9:J:88:LYS:O	2.17	0.45
10:K:43:GLU:O	10:K:46:PRO:HD2	2.17	0.45
13:N:64:ARG:O	13:N:67:ALA:HB3	2.16	0.45
21:V:6:MET:HE3	21:V:53:LEU:HD23	1.99	0.45
25:2:25:LYS:HD3	25:2:25:LYS:HA	1.74	0.45
26:3:52:LYS:O	26:3:56:ALA:HB2	2.17	0.45
27:X:16:G:H2'	27:X:17:G:H8	1.80	0.45
27:X:725:C:H2'	27:X:726:G:C8	2.52	0.45
27:X:1223:G:N2	27:X:1249:G:O2'	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1646:G:C5	27:X:1647:U:C5	3.04	0.45
27:X:1736:C:H2'	27:X:1737:G:C8	2.52	0.45
27:X:2220:A:H2'	27:X:2221:G:H8	1.81	0.45
27:X:2579:A:H2'	27:X:2580:C:H6	1.81	0.45
28:Y:71:G:C6	28:Y:72:C:C4	3.05	0.45
2:B:145:LYS:HB2	27:X:2551:A:C8	2.51	0.45
4:D:129:ASN:ND2	27:X:2282:G:O2'	2.49	0.45
24:1:16:ALA:HB2	24:1:50:PHE:CE1	2.51	0.45
27:X:36:G:N3	27:X:462:G:O2'	2.50	0.45
2:B:114:GLN:C	27:X:1672:A:H4'	2.42	0.45
3:C:65:GLY:O	15:P:112:ARG:NH2	2.50	0.45
5:E:25:LYS:HG3	5:E:34:THR:HG22	1.98	0.45
7:H:23:ARG:HH11	27:X:2541:U:H1'	1.82	0.45
10:K:98:LEU:O	10:K:111:ALA:HB1	2.17	0.45
20:U:78:ILE:HG12	20:U:79:GLU:H	1.81	0.45
21:V:15:ALA:O	21:V:18:ILE:HB	2.17	0.45
22:W:14:GLY:O	22:W:18:LYS:HG2	2.17	0.45
26:3:62:LEU:HD12	26:3:62:LEU:HA	1.86	0.45
27:X:186:C:H2'	27:X:187:U:O4'	2.17	0.45
27:X:231:G:H4'	27:X:397:U:H5''	1.99	0.45
27:X:242:A:C8	27:X:441:A:N6	2.84	0.45
27:X:346:C:H2'	27:X:347:C:H6	1.80	0.45
27:X:742:G:N2	27:X:1766:U:O4'	2.50	0.45
27:X:809:C:H2'	27:X:810:U:C6	2.52	0.45
27:X:828:C:H2'	27:X:829:C:H6	1.82	0.45
27:X:838:A:H2'	27:X:839:U:O4'	2.17	0.45
27:X:1098:G:C5	27:X:1100:G:H1'	2.51	0.45
27:X:1286:U:O2	27:X:1985:G:O2'	2.35	0.45
27:X:1982:C:OP1	27:X:2704:U:H5'	2.16	0.45
27:X:2368:G:H5''	27:X:2369:U:C5'	2.47	0.45
27:X:2513:A:C2	27:X:2514:G:H1'	2.50	0.45
27:X:2668:U:OP2	27:X:2847:G:N2	2.36	0.45
27:X:2859:U:C5	27:X:2860:C:C2	3.05	0.45
1:A:107:ALA:HA	1:A:108:PRO:HD2	1.82	0.45
6:G:124:GLU:O	6:G:128:GLU:HG2	2.17	0.45
11:L:88:VAL:HG11	27:X:2357:A:H1'	1.99	0.45
15:P:120:ILE:HG12	27:X:1996:A:OP1	2.17	0.45
17:R:38:LEU:HD22	17:R:40:LEU:HG	1.99	0.45
17:R:105:ARG:HH22	17:R:113:THR:N	2.10	0.45
21:V:26:MET:HE3	21:V:26:MET:HB3	1.68	0.45
26:3:7:HIS:NE2	27:X:220:U:OP2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:658:G:H1'	27:X:2330:G:OP1	2.17	0.45
27:X:659:G:H2'	27:X:660:G:C8	2.51	0.45
27:X:1418:C:H2'	27:X:1419:G:C8	2.52	0.45
27:X:1987:G:C6	27:X:1988:A:C4	3.05	0.45
27:X:2579:A:H2'	27:X:2580:C:C6	2.52	0.45
27:X:2656:G:H1	27:X:2710:C:H42	1.63	0.45
27:X:2706:U:OP1	27:X:2706:U:C6	2.70	0.45
27:X:2738:A:H2'	27:X:2739:G:O4'	2.17	0.45
2:B:95:ILE:HD13	2:B:95:ILE:HA	1.82	0.45
2:B:109:LYS:NZ	27:X:2703:C:OP2	2.50	0.45
2:B:177:ALA:C	2:B:179:GLU:H	2.25	0.45
3:C:17:LEU:HG	3:C:109:ALA:HB2	1.99	0.45
5:E:109:TYR:CD2	27:X:2646:C:H1'	2.51	0.45
14:O:83:ARG:HG2	27:X:1238:A:H4'	1.99	0.45
17:R:62:MET:HE3	17:R:62:MET:HB3	1.86	0.45
19:T:29:GLU:HG2	27:X:935:C:H1'	1.98	0.45
24:1:9:ILE:HG13	24:1:10:VAL:N	2.32	0.45
27:X:513:A:H5''	27:X:514:G:H5'	1.99	0.45
27:X:699:G:H5''	27:X:699:G:H8	1.82	0.45
27:X:1141:U:HO2'	27:X:1142:G:P	2.38	0.45
27:X:2034:A:H2	27:X:2035:G:O6	1.99	0.45
27:X:2792:C:C2	27:X:2805:G:C2	3.05	0.45
2:B:115:GLY:O	2:B:119:ARG:HB2	2.17	0.44
2:B:152:LYS:CB	6:G:106:TYR:HB2	2.45	0.44
6:G:94:LYS:HB3	6:G:94:LYS:HE2	1.48	0.44
8:I:22:GLY:HA3	27:X:674:U:O2'	2.17	0.44
13:N:93:LYS:H	13:N:93:LYS:HG3	1.49	0.44
20:U:37:ILE:HD12	27:X:177:U:O2'	2.17	0.44
20:U:49:LYS:HB2	20:U:61:TRP:HA	1.99	0.44
22:W:12:ARG:HA	22:W:13:PRO:HD3	1.83	0.44
27:X:310:A:N3	27:X:330:C:O2'	2.50	0.44
27:X:613:A:N7	27:X:668:A:H1'	2.31	0.44
27:X:649:G:C8	27:X:650:U:H5	2.35	0.44
27:X:1121:G:H2'	27:X:1122:A:C8	2.52	0.44
27:X:1468:A:C8	27:X:1468:A:OP2	2.69	0.44
27:X:2053:G:C2	27:X:2054:A:C4	3.05	0.44
27:X:2269:G:N2	27:X:2322:U:H1'	2.32	0.44
27:X:2495:G:C6	27:X:2548:G:C2	3.05	0.44
27:X:2864:C:H2'	27:X:2865:G:C8	2.52	0.44
28:Y:56:G:H8	28:Y:56:G:O5'	2.00	0.44
28:Y:80:A:H2'	28:Y:81:C:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:HG12	1:A:193:ILE:HA	1.98	0.44
2:B:134:TRP:HB2	2:B:135:HIS:CD2	2.52	0.44
4:D:83:MET:HE3	4:D:83:MET:HB2	1.92	0.44
4:D:115:ARG:HH22	4:D:178:ARG:NH1	2.12	0.44
7:H:116:ARG:CZ	12:M:38:LYS:HD2	2.47	0.44
8:I:100:ARG:NH1	27:X:614:G:N7	2.64	0.44
15:P:11:LYS:HD2	27:X:1225:G:N7	2.32	0.44
16:Q:10:PRO:HD3	21:V:30:PHE:CD2	2.52	0.44
17:R:14:LEU:HD21	17:R:41:PRO:HA	1.99	0.44
17:R:23:ILE:HG22	17:R:33:THR:HB	1.98	0.44
17:R:105:ARG:NH2	17:R:112:LYS:HA	2.32	0.44
27:X:205:A:H2'	27:X:206:U:H5'	1.99	0.44
27:X:495:C:H2'	27:X:496:C:C6	2.52	0.44
27:X:1210:C:C2	27:X:1211:G:C8	3.05	0.44
27:X:1329:U:O2'	27:X:1330:G:H5'	2.17	0.44
27:X:2058:U:C4	27:X:2217:G:C6	3.05	0.44
27:X:2451:G:H22	27:X:2456:U:H5''	1.81	0.44
27:X:2728:A:H2'	27:X:2729:A:C8	2.51	0.44
1:A:24:LEU:HB3	1:A:25:THR:H	1.61	0.44
1:A:99:ASP:HB3	27:X:1507:A:O4'	2.17	0.44
8:I:54:SER:HB3	8:I:55:ARG:HE	1.82	0.44
11:L:88:VAL:HG12	11:L:89:PHE:H	1.82	0.44
11:L:91:ARG:HH22	27:X:2355:A:H61	1.66	0.44
13:N:60:LEU:O	13:N:64:ARG:HG3	2.17	0.44
13:N:75:ASN:H	13:N:78:THR:HB	1.83	0.44
27:X:354:C:H2'	27:X:355:G:H8	1.82	0.44
27:X:588:G:C2	27:X:1275:A:C4	3.05	0.44
27:X:748:A:H5''	27:X:749:C:C5	2.52	0.44
27:X:2044:G:N2	27:X:2046:C:C2	2.85	0.44
27:X:2372:A:H62	27:X:2401:A:H61	1.65	0.44
27:X:2406:C:H5'	27:X:2408:G:H5'	1.99	0.44
28:Y:39:C:H5''	28:Y:40:C:C5	2.53	0.44
1:A:246:PRO:HG2	1:A:248:THR:O	2.18	0.44
3:C:39:ARG:HE	3:C:91:TYR:HD2	1.65	0.44
3:C:47:THR:N	3:C:51:VAL:HG21	2.32	0.44
4:D:106:ILE:C	4:D:109:PRO:HD2	2.43	0.44
5:E:156:ALA:O	5:E:172:LYS:N	2.43	0.44
5:E:160:LYS:NZ	27:X:2637:C:H5'	2.32	0.44
8:I:73:GLU:N	8:I:73:GLU:OE2	2.50	0.44
16:Q:72:ARG:NH2	27:X:1324:G:O2'	2.51	0.44
18:S:3:LEU:HD11	18:S:33:ALA:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:51:TYR:CD1	23:Z:55:ARG:HD3	2.53	0.44
27:X:787:A:H2	27:X:800:U:HO2'	1.60	0.44
27:X:1482:U:OP2	27:X:1562:G:O2'	2.35	0.44
27:X:1686:A:O3'	27:X:2528:G:H5'	2.17	0.44
27:X:2510:A:C2'	27:X:2511:G:H5'	2.48	0.44
27:X:2797:G:O2'	27:X:2799:C:OP2	2.25	0.44
1:A:208:LYS:O	1:A:211:ARG:HB2	2.18	0.44
5:E:88:GLU:HG3	5:E:130:ARG:HG2	1.99	0.44
6:G:134:MET:HG3	27:X:1148:G:O2'	2.17	0.44
6:G:151:TYR:HB2	6:G:157:PRO:HB3	1.99	0.44
7:H:8:LEU:HD22	7:H:94:ASN:HB3	2.00	0.44
8:I:41:SER:OG	8:I:41:SER:O	2.35	0.44
12:M:22:ARG:NH1	12:M:22:ARG:HB3	2.32	0.44
13:N:86:ALA:C	13:N:88:ILE:N	2.73	0.44
15:P:39:ARG:NH2	27:X:527:C:O2'	2.47	0.44
23:Z:4:HIS:HB3	27:X:2039:G:H22	1.83	0.44
27:X:98:U:H4'	27:X:99:U:H5''	1.99	0.44
27:X:494:A:N7	27:X:507:A:H2	2.16	0.44
27:X:763:A:H2'	27:X:764:A:H5''	1.98	0.44
27:X:1329:U:C2	27:X:1330:G:N7	2.85	0.44
27:X:1816:G:H2'	27:X:1817:U:H6	1.83	0.44
27:X:1882:G:N2	27:X:1885:C:N4	2.60	0.44
27:X:2495:G:O2'	27:X:2496:C:H5'	2.18	0.44
2:B:61:LYS:HB3	2:B:62:PRO:HD3	1.99	0.44
2:B:105:THR:CG2	2:B:197:VAL:HB	2.48	0.44
2:B:116:VAL:CG2	2:B:136:ARG:HG3	2.23	0.44
2:B:118:LYS:NZ	27:X:2704:U:OP1	2.24	0.44
6:G:62:ILE:HG13	6:G:80:VAL:HG23	2.00	0.44
19:T:20:TYR:CD2	27:X:2335:U:H4'	2.52	0.44
19:T:26:PHE:CD1	27:X:934:G:H1'	2.53	0.44
26:3:57:ARG:O	26:3:61:MET:N	2.50	0.44
27:X:245:C:H42	27:X:437:G:H1	1.64	0.44
27:X:748:A:H3'	27:X:749:C:C6	2.52	0.44
27:X:1065:A:H2'	27:X:1066:G:H8	1.83	0.44
27:X:2058:U:H1'	27:X:2576:G:H21	1.81	0.44
27:X:2251:U:H5''	27:X:2252:A:OP1	2.18	0.44
27:X:2351:G:C2	27:X:2352:A:C5	3.06	0.44
3:C:112:GLN:NE2	3:C:116:LYS:HD2	2.33	0.44
6:G:35:LYS:HD3	6:G:35:LYS:HA	1.44	0.44
7:H:17:ARG:H	7:H:58:ALA:HA	1.82	0.44
7:H:83:ARG:HD2	7:H:89:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:38:LYS:HG2	8:I:40:ARG:O	2.18	0.44
10:K:49:GLU:O	10:K:52:ILE:HG12	2.18	0.44
12:M:78:GLU:OE2	12:M:108:ARG:NE	2.48	0.44
16:Q:35:LYS:HB2	27:X:1614:C:H5''	2.00	0.44
23:Z:16:ARG:HD3	23:Z:20:ARG:CZ	2.48	0.44
27:X:448:C:H2'	27:X:449:C:O4'	2.18	0.44
27:X:580:A:H4'	27:X:581:A:OP1	2.17	0.44
27:X:840:U:H4'	27:X:841:G:N2	2.32	0.44
27:X:1296:G:N2	27:X:1299:A:C8	2.85	0.44
27:X:1935:A:C6	27:X:1936:A:N1	2.85	0.44
27:X:2528:G:C2	27:X:2529:G:N7	2.85	0.44
27:X:2578:G:N2	27:X:2579:A:C4	2.86	0.44
1:A:59:LYS:HG3	1:A:59:LYS:O	2.18	0.44
3:C:112:GLN:HE22	3:C:116:LYS:HD2	1.83	0.44
3:C:176:ASN:ND2	3:C:178:TYR:HB3	2.32	0.44
6:G:84:ASN:C	6:G:86:ALA:H	2.26	0.44
15:P:25:PHE:CD2	15:P:25:PHE:C	2.95	0.44
15:P:44:VAL:O	15:P:48:LYS:HD3	2.18	0.44
18:S:66:VAL:HG22	18:S:83:PHE:CE2	2.53	0.44
22:W:18:LYS:HB2	27:X:863:C:H4'	1.99	0.44
22:W:23:LEU:HD23	22:W:43:MET:HE2	1.99	0.44
27:X:586:G:C6	27:X:587:A:N6	2.86	0.44
27:X:616:U:O2'	27:X:671:A:H4'	2.18	0.44
27:X:753:U:H2'	27:X:754:G:C8	2.52	0.44
27:X:1679:U:O2	27:X:2666:U:H5''	2.18	0.44
27:X:1773:C:H1'	27:X:2588:U:C5'	2.48	0.44
27:X:1777:A:C4	27:X:1921:A:C6	3.06	0.44
27:X:1795:C:H2'	27:X:1796:A:C8	2.52	0.44
27:X:2474:G:H2'	27:X:2475:C:O4'	2.18	0.44
27:X:2493:U:H2'	27:X:2494:C:H6	1.81	0.44
27:X:2634:G:O2'	27:X:2643:G:O6	2.28	0.44
3:C:48:ARG:C	3:C:50:GLN:H	2.25	0.44
5:E:17:VAL:HG13	5:E:26:VAL:HG22	1.98	0.44
5:E:55:PRO:HD2	5:E:61:HIS:CD2	2.53	0.44
6:G:158:HIS:HA	6:G:161:GLN:HE22	1.83	0.44
8:I:56:LEU:HD22	26:3:52:LYS:HZ1	1.82	0.44
15:P:27:VAL:CG1	27:X:504:G:H4'	2.48	0.44
15:P:29:LYS:HB3	15:P:30:TYR:CD2	2.52	0.44
27:X:14:A:N6	27:X:15:G:C2	2.86	0.44
27:X:226:C:H4'	27:X:227:G:O5'	2.18	0.44
27:X:796:A:H8	27:X:797:A:H4'	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1359:G:C6	27:X:1617:G:C6	3.06	0.44
27:X:1597:A:H2'	27:X:1598:C:C6	2.52	0.44
27:X:1698:C:O2'	27:X:1753:A:N3	2.42	0.44
27:X:2198:U:N3	27:X:2199:C:H1'	2.32	0.44
27:X:2201:G:H2'	27:X:2202:G:C8	2.51	0.44
27:X:2363:G:HO2'	27:X:2364:C:P	2.40	0.44
1:A:133:LEU:HB2	1:A:187:SER:HA	2.00	0.43
1:A:222:ARG:HG3	27:X:1780:A:OP1	2.17	0.43
2:B:120:TRP:CE3	2:B:155:ARG:HD2	2.53	0.43
2:B:133:LYS:C	2:B:134:TRP:HD1	2.26	0.43
9:J:35:LEU:HD11	9:J:130:THR:HB	2.00	0.43
9:J:54:VAL:O	9:J:57:ARG:HB2	2.18	0.43
11:L:32:TYR:CZ	28:Y:9:G:H5'	2.53	0.43
17:R:97:GLN:NE2	17:R:101:GLY:HA2	2.33	0.43
27:X:500:G:H2'	27:X:501:G:O4'	2.18	0.43
27:X:748:A:H3'	27:X:749:C:H6	1.83	0.43
27:X:957:G:H2'	27:X:958:G:H8	1.83	0.43
27:X:1026:U:H2'	27:X:1027:C:C6	2.53	0.43
27:X:1043:A:H2	27:X:1133:G:H22	1.65	0.43
27:X:1098:G:H22	27:X:1114:A:H1'	1.82	0.43
27:X:1580:C:H2'	27:X:1581:C:C6	2.53	0.43
27:X:1670:G:H5'	27:X:2797:G:N2	2.33	0.43
27:X:1835:C:H2'	27:X:1836:C:C6	2.52	0.43
27:X:2670:C:H2'	27:X:2671:C:H6	1.83	0.43
2:B:95:ILE:HG22	2:B:96:PHE:CD1	2.53	0.43
2:B:122:PHE:CE1	27:X:2491:C:H4'	2.53	0.43
3:C:129:LYS:C	3:C:131:LYS:N	2.77	0.43
4:D:12:VAL:HG22	4:D:172:SER:HB2	2.00	0.43
8:I:80:LEU:HD21	8:I:89:ASP:OD2	2.18	0.43
27:X:649:G:H2'	27:X:650:U:H6	1.84	0.43
27:X:773:G:C2'	27:X:774:A:H5'	2.48	0.43
27:X:1219:C:H2'	27:X:1220:G:O4'	2.18	0.43
27:X:1399:C:H2'	27:X:1400:A:C8	2.53	0.43
27:X:2041:A:H61	30:X:2902:ERY:H282	1.83	0.43
27:X:2307:A:H2'	27:X:2308:A:C8	2.53	0.43
27:X:2310:G:N2	27:X:2364:C:C4	2.86	0.43
28:Y:64:C:H2'	28:Y:65:A:C8	2.52	0.43
1:A:108:PRO:HG2	1:A:111:LEU:HD12	2.00	0.43
1:A:254:THR:O	27:X:1836:C:H5'	2.19	0.43
8:I:63:ARG:HD3	26:3:30:ARG:HH22	1.82	0.43
11:L:8:ARG:HB2	11:L:8:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:81:ASN:ND2	27:X:1162:A:H4'	2.33	0.43
14:O:32:LYS:HA	14:O:32:LYS:HD3	1.77	0.43
14:O:39:PHE:CE2	14:O:46:VAL:HB	2.53	0.43
17:R:48:VAL:HG13	17:R:50:GLY:H	1.83	0.43
27:X:1014:G:O2'	27:X:1021:A:N1	2.45	0.43
27:X:1336:G:O6	27:X:1337:G:C6	2.72	0.43
27:X:1573:G:H3'	27:X:1574:A:H5''	2.00	0.43
27:X:1880:G:C6	27:X:1881:U:C4	3.06	0.43
27:X:2555:G:OP1	27:X:2555:G:H3'	2.19	0.43
2:B:34:VAL:HG11	2:B:78:LEU:HD21	2.00	0.43
5:E:150:LYS:NZ	27:X:2741:G:H21	2.13	0.43
10:K:107:GLY:HA3	27:X:1992:G:H1'	2.00	0.43
21:V:41:HIS:CD2	27:X:95:G:H4'	2.52	0.43
27:X:485:G:C6	27:X:520:C:N4	2.86	0.43
27:X:1255:A:H2'	27:X:1256:C:H6	1.82	0.43
27:X:1712:G:H3'	27:X:1712:G:N3	2.34	0.43
27:X:1974:U:O5'	27:X:1974:U:H6	2.01	0.43
27:X:2017:U:H2'	27:X:2018:G:H5''	2.00	0.43
27:X:2048:C:H1'	27:X:2428:U:N3	2.33	0.43
27:X:2470:U:H2'	27:X:2470:U:O2	2.17	0.43
27:X:2511:G:C6	27:X:2512:A:C5	3.07	0.43
28:Y:27:A:N6	28:Y:55:C:H5''	2.34	0.43
28:Y:30:C:H2'	28:Y:31:A:C8	2.53	0.43
8:I:59:ARG:HA	27:X:2371:A:H8	1.81	0.43
13:N:22:LYS:C	13:N:24:PHE:H	2.25	0.43
18:S:125:PRO:HA	18:S:158:CYS:SG	2.58	0.43
22:W:39:ALA:O	27:X:864:C:O2'	2.37	0.43
23:Z:10:LYS:HG3	27:X:1276:U:O4'	2.18	0.43
23:Z:18:MET:HB2	23:Z:18:MET:HE3	1.85	0.43
24:1:3:LYS:HB3	24:1:3:LYS:HE2	1.83	0.43
26:3:40:GLU:C	26:3:43:GLY:H	2.26	0.43
27:X:529:U:H2'	27:X:530:G:H8	1.83	0.43
27:X:611:C:N4	27:X:612:G:C5	2.86	0.43
27:X:754:G:H2'	27:X:755:C:C6	2.53	0.43
27:X:859:U:H3	27:X:944:A:H61	1.66	0.43
27:X:956:A:C4	27:X:2427:A:C2	3.06	0.43
27:X:1493:A:H2'	27:X:1494:G:O4'	2.19	0.43
27:X:2027:C:C2'	27:X:2028:C:H5'	2.48	0.43
27:X:2451:G:H2'	27:X:2454:C:H42	1.83	0.43
1:A:63:ARG:HH22	27:X:1584:G:P	2.42	0.43
1:A:258:LYS:HG3	27:X:1790:G:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LYS:HB3	2:B:74:PRO:HB2	2.00	0.43
4:D:52:LYS:HE3	4:D:147:ASP:HB2	2.01	0.43
4:D:66:ILE:HD12	28:Y:44:C:C6	2.54	0.43
5:E:103:LEU:HD21	5:E:105:MET:HG3	1.99	0.43
6:G:46:ALA:HB2	6:G:54:LEU:HD22	2.00	0.43
7:H:104:GLU:HB3	7:H:125:LYS:HD2	1.99	0.43
11:L:32:TYR:CG	28:Y:9:G:H4'	2.54	0.43
12:M:101:ARG:HG2	12:M:101:ARG:HH21	1.84	0.43
14:O:15:SER:OG	14:O:96:LEU:HD13	2.18	0.43
18:S:130:ILE:H	18:S:130:ILE:HD12	1.84	0.43
19:T:74:LYS:C	19:T:76:ALA:N	2.73	0.43
20:U:48:LYS:HE2	20:U:48:LYS:HB2	1.76	0.43
25:2:8:ASN:HB3	25:2:11:LYS:HB3	2.00	0.43
25:2:42:LEU:H	25:2:42:LEU:HD12	1.83	0.43
27:X:240:U:H2'	27:X:241:C:O4'	2.19	0.43
27:X:617:U:C5	27:X:632:A:N1	2.87	0.43
27:X:632:A:C2	27:X:633:G:C4	3.07	0.43
27:X:1574:A:H2'	27:X:1575:C:H5''	2.00	0.43
27:X:2224:U:H5''	27:X:2225:G:H5'	2.00	0.43
1:A:188:GLU:HG2	1:A:188:GLU:H	1.46	0.43
4:D:26:MET:HE2	28:Y:56:G:H21	1.83	0.43
15:P:60:ILE:HA	15:P:61:PRO:HD3	1.67	0.43
19:T:57:HIS:CD2	19:T:57:HIS:N	2.87	0.43
24:1:54:LYS:HE2	24:1:54:LYS:HB2	1.76	0.43
26:3:25:PHE:CG	26:3:46:LYS:HA	2.54	0.43
27:X:734:G:C2	27:X:735:G:C8	3.07	0.43
27:X:1398:G:O2'	27:X:1399:C:O5'	2.36	0.43
27:X:1949:A:O2'	27:X:2572:U:H5'	2.18	0.43
27:X:2234:G:C6	27:X:2235:G:C4	3.06	0.43
27:X:2367:A:N7	27:X:2368:G:C5	2.87	0.43
1:A:91:ARG:NH1	1:A:109:GLU:HA	2.34	0.43
1:A:248:THR:HG22	1:A:249:PRO:HD2	2.01	0.43
7:H:7:ARG:HB3	7:H:18:GLU:OE2	2.18	0.43
11:L:33:ARG:HH11	11:L:99:ARG:HD2	1.84	0.43
12:M:104:LEU:HD23	12:M:106:TYR:CE2	2.54	0.43
15:P:109:ARG:HD2	15:P:109:ARG:O	2.19	0.43
18:S:49:THR:O	18:S:49:THR:OG1	2.37	0.43
27:X:187:U:H2'	27:X:188:G:C8	2.54	0.43
27:X:577:U:O2'	27:X:579:G:N7	2.42	0.43
27:X:883:A:H2'	27:X:884:C:O4'	2.19	0.43
27:X:1408:A:C6	27:X:1411:C:C2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1429:A:N6	27:X:1600:U:H4'	2.33	0.43
27:X:1769:U:H2'	27:X:1775:A:H62	1.83	0.43
27:X:1810:U:O2'	27:X:1811:A:O5'	2.36	0.43
27:X:2262:C:C2	27:X:2368:G:C2	3.06	0.43
1:A:24:LEU:HD22	1:A:205:VAL:HG13	2.00	0.43
1:A:124:GLU:HA	1:A:125:PRO:HD3	1.80	0.43
8:I:17:LYS:HB3	8:I:17:LYS:HE2	1.81	0.43
8:I:42:GLY:H	8:I:45:LYS:HE3	1.84	0.43
8:I:77:LEU:HB2	8:I:110:ALA:HA	2.01	0.43
9:J:136:GLU:OE1	9:J:137:VAL:HB	2.19	0.43
15:P:9:ARG:HB3	15:P:10:ASN:H	1.46	0.43
15:P:99:ALA:O	15:P:124:THR:HG22	2.19	0.43
18:S:21:ALA:HB3	18:S:32:PHE:C	2.44	0.43
23:Z:6:VAL:HG13	23:Z:7:PRO:O	2.19	0.43
24:1:9:ILE:O	24:1:10:VAL:HB	2.17	0.43
27:X:17:G:H1	27:X:533:C:H42	1.66	0.43
27:X:78:C:H2'	27:X:79:G:H8	1.84	0.43
27:X:172:A:H61	27:X:175:C:H3'	1.84	0.43
27:X:194:G:H3'	27:X:195:A:H8	1.84	0.43
27:X:1154:A:H8	27:X:1154:A:OP1	2.01	0.43
27:X:1370:U:H2'	27:X:1371:G:C8	2.53	0.43
27:X:1845:A:N1	27:X:2070:G:H1'	2.34	0.43
27:X:2574:G:N1	27:X:2578:G:C6	2.86	0.43
27:X:2596:C:HO2'	27:X:2597:G:H5'	1.84	0.43
1:A:39:LYS:HE2	1:A:87:ASN:HD21	1.84	0.43
1:A:87:ASN:O	27:X:1809:G:H5''	2.19	0.43
4:D:51:ASP:O	4:D:55:LYS:HG2	2.18	0.43
6:G:71:THR:HG22	6:G:76:GLN:OE1	2.17	0.43
9:J:15:ARG:HE	9:J:73:LYS:NZ	2.17	0.43
9:J:126:LEU:HA	9:J:127:PRO:HD3	1.86	0.43
12:M:38:LYS:HE2	12:M:38:LYS:HB3	1.78	0.43
13:N:20:ARG:HH22	14:O:72:ARG:HD3	1.83	0.43
13:N:101:ARG:O	13:N:103:PRO:HD3	2.18	0.43
19:T:40:GLN:HE21	19:T:57:HIS:HB3	1.84	0.43
23:Z:40:LYS:HD3	23:Z:46:CYS:HB2	1.99	0.43
26:3:9:MET:N	26:3:9:MET:SD	2.92	0.43
26:3:13:ARG:HD2	26:3:24:ALA:HA	2.01	0.43
27:X:1196:G:H2'	27:X:1197:U:O4'	2.19	0.43
1:A:218:LYS:HD2	1:A:219:PRO:HD2	2.00	0.42
3:C:46:ARG:HD2	3:C:51:VAL:HG11	2.01	0.42
4:D:65:PRO:HA	4:D:89:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:ILE:HD13	4:D:173:MET:HB3	2.01	0.42
5:E:175:LYS:HD3	5:E:175:LYS:HA	1.74	0.42
7:H:3:MET:O	7:H:6:SER:HB3	2.19	0.42
9:J:61:ARG:NH1	18:S:175:ARG:HD3	2.34	0.42
15:P:122:LYS:C	15:P:124:THR:H	2.27	0.42
18:S:141:MET:SD	18:S:147:ILE:HG12	2.59	0.42
20:U:17:SER:CB	20:U:44:ALA:HA	2.49	0.42
22:W:46:THR:HG22	22:W:47:VAL:HG13	2.01	0.42
26:3:23:MET:HB3	26:3:25:PHE:HE2	1.82	0.42
27:X:69:G:H5''	27:X:111:G:H1'	2.01	0.42
27:X:149:A:H2'	27:X:150:A:C8	2.54	0.42
27:X:1281:A:H2'	27:X:1282:A:O4'	2.19	0.42
27:X:2044:G:H2'	27:X:2480:C:O2'	2.19	0.42
27:X:2331:A:C4	27:X:2345:A:C2	3.06	0.42
3:C:97:ARG:HA	3:C:100:ARG:HB2	2.00	0.42
5:E:157:TYR:CZ	27:X:2510:A:H5'	2.53	0.42
9:J:40:PRO:HB3	9:J:99:LYS:HD2	2.00	0.42
10:K:20:LEU:HD23	10:K:21:ALA:N	2.35	0.42
12:M:104:LEU:HD22	12:M:107:LEU:HD11	2.01	0.42
13:N:24:PHE:O	13:N:29:SER:HB3	2.19	0.42
13:N:65:ILE:HD13	13:N:95:LEU:HD22	2.01	0.42
14:O:39:PHE:HE2	14:O:46:VAL:HB	1.84	0.42
14:O:72:ARG:HA	14:O:82:ARG:O	2.18	0.42
20:U:15:VAL:HG23	20:U:16:ASN:H	1.83	0.42
20:U:20:ARG:HD3	20:U:43:ARG:HD2	2.01	0.42
27:X:565:A:H8	27:X:565:A:O5'	2.02	0.42
27:X:745:C:H2'	27:X:746:G:O4'	2.19	0.42
27:X:820:U:H1'	27:X:2424:G:OP1	2.19	0.42
27:X:1260:A:C6	27:X:1262:U:C2	3.07	0.42
27:X:1330:G:H2'	27:X:1331:G:O4'	2.19	0.42
27:X:2559:U:C2'	27:X:2560:G:H5'	2.49	0.42
1:A:133:LEU:HD23	1:A:133:LEU:HA	1.91	0.42
1:A:183:ARG:NH2	1:A:263:ARG:HB3	2.34	0.42
1:A:210:GLY:HA2	1:A:213:ARG:CG	2.45	0.42
5:E:106:ASN:HD22	5:E:112:PRO:HB3	1.84	0.42
7:H:109:ARG:HA	7:H:129:LEU:HD22	2.00	0.42
7:H:129:LEU:HD23	7:H:129:LEU:HA	1.74	0.42
11:L:39:TYR:OH	28:Y:117:G:N2	2.52	0.42
14:O:85:GLY:H	27:X:1238:A:H5'	1.84	0.42
17:R:25:LEU:H	17:R:80:LYS:HA	1.83	0.42
20:U:68:ARG:O	20:U:72:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:8:ILE:HD13	24:1:8:ILE:H	1.85	0.42
27:X:105:G:C2	27:X:106:G:C8	3.07	0.42
27:X:475:U:C2	27:X:801:A:C6	3.07	0.42
27:X:488:A:H8	27:X:488:A:OP1	2.02	0.42
27:X:725:C:H2'	27:X:726:G:H8	1.84	0.42
27:X:764:A:C2	27:X:802:A:C4	3.07	0.42
27:X:795:A:OP2	27:X:1768:U:O2'	2.26	0.42
27:X:877:G:H1	27:X:924:C:H42	1.67	0.42
27:X:1032:A:O2'	27:X:1134:C:H5''	2.19	0.42
27:X:1466:C:N4	27:X:1476:G:H1	2.16	0.42
27:X:1603:A:H2'	27:X:1604:A:H8	1.84	0.42
27:X:1742:G:C2	27:X:1743:C:C4	3.07	0.42
27:X:1832:G:H1	27:X:1885:C:H42	1.65	0.42
27:X:2011:U:H2'	27:X:2012:A:C8	2.54	0.42
27:X:2221:G:H22	27:X:2413:A:H2	1.67	0.42
27:X:2328:G:H1	27:X:2347:C:H42	1.66	0.42
2:B:147:PRO:HD3	27:X:1141:U:C5	2.54	0.42
4:D:4:LEU:CG	4:D:5:LYS:H	2.27	0.42
4:D:90:THR:OG1	28:Y:44:C:N3	2.42	0.42
7:H:3:MET:HE1	27:X:1683:G:H21	1.85	0.42
14:O:26:GLN:HG2	14:O:27:GLY:N	2.34	0.42
15:P:73:ASN:O	15:P:77:ALA:N	2.42	0.42
15:P:119:ILE:HG13	15:P:120:ILE:N	2.35	0.42
25:2:44:VAL:HG11	27:X:124:A:OP1	2.19	0.42
27:X:930:A:C2	28:Y:82:U:H4'	2.55	0.42
27:X:1227:A:H4'	27:X:1252:C:H4'	2.02	0.42
27:X:1469:U:H5'	27:X:1470:G:OP2	2.20	0.42
27:X:2780:A:H2'	27:X:2780:A:N3	2.35	0.42
28:Y:39:C:N4	28:Y:50:U:O2'	2.53	0.42
28:Y:42:U:O2'	28:Y:45:C:N4	2.53	0.42
3:C:156:ASN:HA	3:C:159:ARG:HH21	1.84	0.42
4:D:118:ASN:HB3	4:D:122:PHE:HZ	1.85	0.42
6:G:119:LEU:HA	6:G:119:LEU:HD13	1.64	0.42
8:I:90:ARG:HA	8:I:121:HIS:CG	2.54	0.42
9:J:53:ILE:O	9:J:57:ARG:HG2	2.20	0.42
10:K:60:LEU:CG	10:K:64:ARG:HD2	2.36	0.42
14:O:6:GLN:HB2	14:O:7:THR:H	1.66	0.42
15:P:64:ALA:O	15:P:67:PRO:HD2	2.20	0.42
16:Q:43:GLN:HG2	16:Q:48:VAL:O	2.20	0.42
17:R:52:ASN:HB2	17:R:73:GLU:HA	2.01	0.42
27:X:14:A:C5	27:X:536:A:C2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:54:G:H2'	27:X:55:A:H8	1.83	0.42
27:X:398:C:N4	27:X:424:G:H1	2.18	0.42
27:X:564:U:H2'	27:X:565:A:C8	2.54	0.42
27:X:748:A:H5''	27:X:749:C:H5	1.84	0.42
27:X:1086:C:H2'	27:X:1087:C:H5''	2.01	0.42
27:X:2284:U:H5'	27:X:2286:G:N1	2.32	0.42
27:X:2432:A:O2'	27:X:2551:A:H1'	2.19	0.42
27:X:2817:A:H2'	27:X:2818:G:O4'	2.19	0.42
1:A:143:HIS:HD1	1:A:194:GLY:C	2.23	0.42
2:B:5:LEU:CD2	2:B:195:LEU:HD11	2.49	0.42
3:C:48:ARG:H	3:C:48:ARG:HG3	1.45	0.42
3:C:128:ALA:O	3:C:130:THR:N	2.51	0.42
4:D:105:ASN:O	4:D:109:PRO:HG2	2.19	0.42
4:D:161:LYS:HG3	4:D:162:THR:HG23	2.02	0.42
6:G:103:TYR:CD2	27:X:1142:G:O4'	2.73	0.42
8:I:17:LYS:HG3	8:I:19:VAL:N	2.31	0.42
9:J:123:GLY:HA2	9:J:126:LEU:HD12	2.01	0.42
14:O:26:GLN:HG3	14:O:63:HIS:HD2	1.85	0.42
15:P:109:ARG:H	15:P:109:ARG:HG3	1.64	0.42
17:R:52:ASN:HB2	17:R:72:ARG:O	2.20	0.42
20:U:68:ARG:NH1	27:X:413:G:N7	2.67	0.42
22:W:38:PRO:HB2	27:X:865:A:O2'	2.20	0.42
27:X:340:G:O4'	27:X:488:A:H1'	2.20	0.42
27:X:427:C:H2'	27:X:428:A:C8	2.54	0.42
27:X:788:G:C4	27:X:807:A:C8	3.08	0.42
27:X:802:A:H8	27:X:802:A:OP2	2.02	0.42
27:X:1016:C:C2	27:X:1154:A:C5	3.07	0.42
27:X:1437:A:H2'	27:X:1438:G:H8	1.85	0.42
27:X:1562:G:H8	27:X:1562:G:OP2	2.03	0.42
27:X:2424:G:O2'	27:X:2425:G:H5'	2.19	0.42
1:A:94:LEU:HD12	1:A:95:LEU:N	2.35	0.42
1:A:96:HIS:HE1	1:A:100:GLY:HA2	1.84	0.42
10:K:39:THR:OG1	27:X:1668:G:H5'	2.20	0.42
12:M:19:ASP:OD2	12:M:19:ASP:N	2.33	0.42
13:N:89:ASP:HB3	13:N:91:ASN:HB2	2.02	0.42
14:O:6:GLN:HG2	27:X:1007:A:O2'	2.19	0.42
14:O:10:LYS:HE3	14:O:13:ARG:NH2	2.35	0.42
14:O:82:ARG:HA	14:O:82:ARG:HD3	1.56	0.42
17:R:15:HIS:HE1	17:R:80:LYS:HE2	1.84	0.42
24:1:17:GLY:O	24:1:19:GLY:N	2.51	0.42
27:X:102:C:C4	27:X:103:U:C4	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:590:C:H2'	27:X:591:G:H8	1.84	0.42
27:X:964:A:H2'	27:X:965:G:O4'	2.19	0.42
27:X:1454:U:H2'	27:X:1455:C:H6	1.83	0.42
27:X:2327:U:O5'	27:X:2327:U:H6	2.03	0.42
2:B:103:ASP:O	2:B:199:ARG:HG3	2.20	0.42
3:C:45:THR:HG21	3:C:85:GLY:HA3	2.00	0.42
3:C:48:ARG:C	3:C:50:GLN:N	2.74	0.42
5:E:130:ARG:CZ	5:E:130:ARG:HB3	2.49	0.42
6:G:43:VAL:HG21	6:G:158:HIS:CE1	2.53	0.42
11:L:97:HIS:CG	11:L:98:GLY:N	2.85	0.42
12:M:103:LYS:O	12:M:104:LEU:HB2	2.18	0.42
13:N:72:HIS:CD2	13:N:110:VAL:HG21	2.55	0.42
14:O:64:GLY:HA3	14:O:90:PHE:CE1	2.54	0.42
18:S:127:PRO:C	18:S:129:ARG:H	2.27	0.42
24:1:8:ILE:O	24:1:9:ILE:HG12	2.20	0.42
25:2:3:ARG:HA	25:2:3:ARG:HD3	1.51	0.42
27:X:459:A:N1	27:X:466:A:O2'	2.45	0.42
27:X:591:G:H3'	27:X:592:G:C8	2.42	0.42
27:X:1730:G:N2	27:X:1736:C:O2	2.51	0.42
27:X:1812:U:O2	27:X:1812:U:H2'	2.20	0.42
27:X:2043:A:O4'	27:X:2481:G:H1'	2.20	0.42
27:X:2263:C:O2'	27:X:2267:A:N6	2.53	0.42
27:X:2696:A:H2'	27:X:2697:G:H8	1.84	0.42
1:A:67:PHE:CE2	1:A:106:LEU:HD11	2.54	0.42
1:A:252:LYS:HZ2	1:A:253:PRO:HD2	1.84	0.42
2:B:195:LEU:HB3	12:M:2:GLN:HE21	1.84	0.42
9:J:64:LYS:O	9:J:107:VAL:HA	2.19	0.42
14:O:78:VAL:HG22	27:X:1202:U:H5'	2.02	0.42
16:Q:64:ARG:HH21	27:X:1349:A:H5'	1.84	0.42
27:X:459:A:O4'	27:X:461:A:N6	2.53	0.42
27:X:485:G:C5	27:X:520:C:N4	2.88	0.42
27:X:615:C:H1'	27:X:670:U:H1'	2.00	0.42
27:X:762:A:H4'	27:X:1284:G:N3	2.34	0.42
27:X:797:A:N7	27:X:805:G:C4	2.88	0.42
27:X:1484:G:H2'	27:X:1485:U:H6	1.85	0.42
27:X:1505:U:H1'	27:X:1506:C:C5	2.55	0.42
28:Y:58:G:H5''	28:Y:59:A:OP1	2.20	0.42
3:C:176:ASN:HD22	3:C:178:TYR:HB3	1.85	0.42
5:E:44:ARG:HH22	5:E:51:LEU:HD23	1.85	0.42
6:G:116:ARG:HE	6:G:126:VAL:HG13	1.85	0.42
8:I:84:GLU:OE2	8:I:87:THR:OG1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:119:PHE:CD1	9:J:132:MET:HB2	2.55	0.42
13:N:10:ARG:HG3	27:X:1264:C:OP1	2.19	0.42
17:R:65:PRO:O	17:R:66:GLN:C	2.63	0.42
22:W:1:MET:HE1	22:W:41:ARG:HG2	2.02	0.42
25:2:4:THR:O	27:X:700:C:H5'	2.19	0.42
27:X:48:A:H61	27:X:154:U:H2'	1.85	0.42
27:X:1212:U:H2'	27:X:1213:U:C6	2.55	0.42
27:X:2321:C:O2'	27:X:2353:G:H5''	2.20	0.42
1:A:69:ARG:NH1	1:A:128:GLY:O	2.40	0.41
1:A:118:ASN:HD22	1:A:119:ALA:H	1.68	0.41
2:B:17:ASN:HB3	2:B:18:ASP:H	1.57	0.41
2:B:48:GLN:NE2	27:X:2614:A:O2'	2.53	0.41
9:J:39:GLU:CD	28:Y:92:G:H22	2.28	0.41
12:M:44:ARG:NH2	12:M:46:ARG:HE	2.18	0.41
18:S:79:ILE:HD11	28:Y:78:A:O2'	2.19	0.41
20:U:49:LYS:HB3	20:U:61:TRP:CE3	2.55	0.41
25:2:24:THR:OG1	25:2:25:LYS:N	2.53	0.41
25:2:25:LYS:O	25:2:29:ASN:HB2	2.20	0.41
27:X:502:A:H2'	27:X:503:G:O4'	2.19	0.41
27:X:742:G:C2	27:X:1766:U:C6	3.08	0.41
27:X:753:U:H2'	27:X:754:G:H8	1.85	0.41
27:X:1788:C:C4	27:X:1789:U:C4	3.07	0.41
27:X:2048:C:H1'	27:X:2428:U:C2	2.55	0.41
27:X:2189:A:H61	27:X:2190:A:N6	2.18	0.41
27:X:2338:C:H2'	27:X:2339:A:C8	2.55	0.41
27:X:2553:G:C2	27:X:2554:C:O2	2.73	0.41
28:Y:75:A:OP1	28:Y:75:A:H4'	2.19	0.41
1:A:133:LEU:HD23	1:A:136:VAL:HG21	2.01	0.41
3:C:10:ASN:OD1	3:C:13:ARG:NH1	2.53	0.41
6:G:116:ARG:HD2	6:G:119:LEU:HG	2.02	0.41
7:H:101:ASN:N	7:H:101:ASN:HD22	2.18	0.41
9:J:12:LYS:HD3	27:X:923:A:N7	2.34	0.41
9:J:75:VAL:HG21	9:J:93:TYR:HE1	1.86	0.41
13:N:66:ASN:HB2	13:N:70:ARG:HH11	1.85	0.41
15:P:35:PRO:O	15:P:39:ARG:HD3	2.20	0.41
17:R:96:LYS:O	17:R:104:VAL:HA	2.20	0.41
22:W:22:ALA:HA	27:X:942:U:O2'	2.20	0.41
26:3:50:LEU:HD23	26:3:53:ALA:CB	2.50	0.41
27:X:627:A:C6	27:X:628:A:C6	3.08	0.41
27:X:837:U:H2'	27:X:838:A:C8	2.54	0.41
27:X:1137:A:H4'	27:X:1138:A:O5'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1615:C:H2'	27:X:1616:C:C6	2.55	0.41
27:X:1793:A:N1	27:X:1814:G:H1'	2.35	0.41
27:X:2188:A:H2'	27:X:2189:A:N7	2.36	0.41
3:C:162:ARG:NH2	27:X:331:U:O2'	2.54	0.41
3:C:178:TYR:OH	27:X:1216:G:O2'	2.32	0.41
3:C:180:ILE:HG22	3:C:186:LEU:HD13	2.03	0.41
4:D:102:LYS:O	4:D:106:ILE:HB	2.21	0.41
5:E:11:VAL:HA	5:E:12:PRO:HD2	1.95	0.41
8:I:44:GLY:HA2	27:X:684:C:H5	1.84	0.41
8:I:86:THR:HG21	8:I:117:ALA:O	2.20	0.41
12:M:8:ASN:HA	27:X:2851:G:O5'	2.21	0.41
14:O:93:ILE:HG13	14:O:95:ILE:HD11	2.02	0.41
16:Q:68:PHE:C	16:Q:69:ILE:HG13	2.45	0.41
17:R:84:VAL:HB	17:R:88:THR:O	2.20	0.41
18:S:23:ALA:HB1	18:S:85:MET:HE3	2.02	0.41
24:1:28:ARG:O	24:1:33:ALA:HB2	2.20	0.41
27:X:182:G:HO2'	27:X:183:U:P	2.44	0.41
27:X:1030:U:C4	27:X:1031:C:H5	2.38	0.41
27:X:2499:C:N3	27:X:2546:G:C8	2.88	0.41
27:X:2578:G:C2	27:X:2579:A:C4	3.08	0.41
27:X:2705:A:H8	27:X:2706:U:O2'	2.03	0.41
28:Y:53:G:H2'	28:Y:54:U:H5''	2.02	0.41
1:A:49:ILE:HG22	27:X:792:U:OP1	2.20	0.41
1:A:257:LEU:HB3	27:X:1794:A:O3'	2.21	0.41
4:D:79:LEU:HD23	4:D:79:LEU:HA	1.92	0.41
9:J:49:GLU:OE2	9:J:52:ARG:NH2	2.54	0.41
10:K:28:LEU:CD2	10:K:115:LEU:HG	2.49	0.41
10:K:73:LYS:HA	10:K:76:VAL:HG12	2.03	0.41
17:R:40:LEU:HA	17:R:41:PRO:HD2	1.95	0.41
23:Z:36:CYS:HB3	23:Z:49:CYS:HB3	1.94	0.41
27:X:640:C:H5''	27:X:660:G:O2'	2.20	0.41
27:X:671:A:H2'	27:X:672:C:O4'	2.20	0.41
27:X:1228:G:C6	27:X:1229:C:C4	3.08	0.41
27:X:1841:G:H1	27:X:1876:C:H42	1.68	0.41
27:X:2046:C:O2	27:X:2430:A:C2	2.74	0.41
27:X:2283:G:H2'	27:X:2283:G:N3	2.35	0.41
27:X:2447:G:O2'	27:X:2448:A:H8	1.85	0.41
27:X:2705:A:O2'	27:X:2706:U:O5'	2.33	0.41
1:A:157:ARG:HB2	1:A:157:ARG:HH11	1.85	0.41
5:E:86:ASN:O	5:E:165:VAL:HG22	2.20	0.41
5:E:95:ARG:HH22	5:E:97:LYS:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:67:ARG:HH11	6:G:67:ARG:HB2	1.86	0.41
7:H:37:GLY:O	27:X:2542:U:H5''	2.20	0.41
8:I:62:LYS:HB3	26:3:13:ARG:N	2.35	0.41
8:I:62:LYS:HG3	8:I:63:ARG:N	2.35	0.41
8:I:74:VAL:HG11	27:X:638:A:C8	2.56	0.41
9:J:14:PHE:HE1	9:J:90:ALA:HA	1.86	0.41
11:L:14:ARG:HE	11:L:14:ARG:HB2	1.50	0.41
13:N:99:ALA:HB2	13:N:106:PHE:CE1	2.56	0.41
19:T:23:VAL:HB	19:T:26:PHE:CE2	2.54	0.41
19:T:37:LEU:HD11	19:T:61:ALA:HB2	2.03	0.41
23:Z:15:LYS:O	23:Z:18:MET:HB3	2.19	0.41
27:X:525:A:C8	27:X:526:C:C6	3.09	0.41
27:X:726:G:H1'	27:X:731:A:H61	1.86	0.41
27:X:1010:U:O2'	27:X:1011:A:H5'	2.20	0.41
27:X:1024:G:H2'	27:X:1025:A:C8	2.55	0.41
27:X:1278:A:H2	27:X:1997:A:N6	2.09	0.41
27:X:1462:C:C2	27:X:1480:G:N2	2.89	0.41
27:X:1642:G:O5'	27:X:1642:G:H8	2.03	0.41
27:X:2667:C:N4	27:X:2700:U:OP2	2.41	0.41
1:A:124:GLU:O	1:A:126:LYS:N	2.52	0.41
2:B:5:LEU:HD21	2:B:79:ARG:CG	2.50	0.41
2:B:62:PRO:HG3	27:X:2767:C:H1'	2.01	0.41
3:C:152:THR:OG1	3:C:153:ASP:N	2.53	0.41
4:D:132:ILE:HG13	4:D:154:ILE:HD13	2.03	0.41
8:I:33:GLY:CA	14:O:79:GLN:HG3	2.49	0.41
11:L:12:ARG:HG3	11:L:13:THR:N	2.35	0.41
14:O:38:LEU:HD13	14:O:39:PHE:C	2.46	0.41
15:P:27:VAL:HG23	15:P:128:THR:HG22	2.02	0.41
15:P:72:LEU:HA	15:P:129:ILE:HD12	2.01	0.41
16:Q:64:ARG:NH1	27:X:1348:C:H4'	2.35	0.41
21:V:41:HIS:ND1	27:X:94:C:O2'	2.33	0.41
27:X:645:G:H2'	27:X:646:C:C6	2.55	0.41
27:X:828:C:C2	27:X:1207:G:C2	3.08	0.41
27:X:1031:C:OP1	27:X:1045:G:N2	2.30	0.41
27:X:2511:G:O2'	27:X:2636:A:N1	2.54	0.41
27:X:2557:G:OP1	27:X:2593:A:N6	2.53	0.41
27:X:2733:A:H2'	27:X:2734:U:O4'	2.20	0.41
30:X:2902:ERY:H71	30:X:2902:ERY:H4	1.92	0.41
1:A:44:ASN:CB	1:A:49:ILE:HA	2.51	0.41
1:A:77:ALA:HB2	1:A:97:TYR:CD1	2.56	0.41
1:A:89:SER:O	1:A:198:ASN:ND2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:GLN:HE21	3:C:98:GLN:HB3	1.56	0.41
6:G:41:TRP:CZ3	6:G:79:PHE:CG	3.09	0.41
8:I:30:ALA:N	27:X:824:U:H2'	2.35	0.41
8:I:58:ALA:HA	26:3:12:ARG:NH1	2.35	0.41
8:I:58:ALA:C	8:I:60:LEU:H	2.28	0.41
9:J:39:GLU:HA	9:J:40:PRO:HD3	1.79	0.41
12:M:9:ARG:O	12:M:13:LEU:HB2	2.21	0.41
15:P:119:ILE:O	15:P:120:ILE:HG12	2.21	0.41
20:U:46:LEU:C	27:X:2209:G:H4'	2.46	0.41
27:X:665:A:N7	27:X:666:U:H1'	2.36	0.41
27:X:754:G:C2	27:X:755:C:C4	3.08	0.41
27:X:922:A:N7	27:X:923:A:C6	2.89	0.41
27:X:944:A:C2	27:X:945:G:C8	3.09	0.41
27:X:1391:A:O2'	27:X:1393:G:N7	2.46	0.41
27:X:1398:G:O2'	27:X:1399:C:O4'	2.25	0.41
27:X:2042:A:C6	27:X:2482:A:C2	3.08	0.41
27:X:2510:A:H2'	27:X:2511:G:H5'	2.02	0.41
27:X:2522:G:H2'	27:X:2523:G:O4'	2.21	0.41
27:X:2679:G:H1	27:X:2686:C:N4	2.16	0.41
27:X:2751:C:H2'	27:X:2752:C:C6	2.55	0.41
2:B:84:PHE:C	2:B:86:PRO:HD3	2.46	0.41
3:C:68:ARG:HH12	27:X:687:G:H1'	1.83	0.41
7:H:2:ILE:HG12	7:H:45:ALA:O	2.21	0.41
8:I:99:VAL:O	8:I:101:ARG:HG2	2.21	0.41
11:L:15:ARG:HA	11:L:15:ARG:HD3	1.57	0.41
11:L:39:TYR:HD2	11:L:41:GLN:HG3	1.86	0.41
14:O:23:GLU:CB	14:O:91:THR:HG21	2.48	0.41
14:O:65:ARG:NH2	27:X:1237:G:OP2	2.53	0.41
15:P:41:VAL:O	15:P:44:VAL:HG22	2.21	0.41
17:R:85:ASP:O	17:R:87:GLU:N	2.46	0.41
19:T:45:PHE:HE2	19:T:77:ARG:CZ	2.33	0.41
21:V:2:LYS:HE3	21:V:2:LYS:HB2	1.90	0.41
21:V:43:VAL:O	21:V:47:ARG:HG2	2.21	0.41
27:X:457:C:O2'	27:X:458:G:H5'	2.21	0.41
27:X:998:C:O2	27:X:1011:A:H2	2.04	0.41
27:X:1533:G:H2'	27:X:1534:A:H8	1.85	0.41
27:X:2050:G:C6	27:X:2423:G:C6	3.09	0.41
27:X:2394:G:C2	27:X:2395:C:C2	3.08	0.41
27:X:2663:U:H3	27:X:2705:A:H62	1.66	0.41
1:A:36:ALA:CB	1:A:63:ARG:HA	2.50	0.41
1:A:69:ARG:NH2	1:A:192:THR:OG1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ILE:HG13	2:B:25:VAL:O	2.21	0.41
2:B:59:VAL:CG1	2:B:64:GLN:HG3	2.51	0.41
4:D:77:PHE:HB2	27:X:2289:A:N1	2.36	0.41
6:G:62:ILE:HG22	6:G:135:LEU:HD21	2.02	0.41
6:G:111:LYS:HG2	27:X:1142:G:H5''	2.01	0.41
7:H:113:PRO:HD3	12:M:73:PHE:HB2	2.03	0.41
8:I:41:SER:HB2	27:X:844:G:O3'	2.21	0.41
9:J:55:MET:HG3	9:J:122:ALA:HB2	2.03	0.41
10:K:12:ARG:HG2	10:K:12:ARG:NH1	2.36	0.41
11:L:42:ILE:HD13	11:L:42:ILE:HA	1.90	0.41
13:N:33:ARG:H	13:N:33:ARG:HG2	1.46	0.41
13:N:72:HIS:HD2	13:N:110:VAL:HG21	1.86	0.41
15:P:113:ALA:HB1	15:P:114:ARG:HD2	2.02	0.41
17:R:56:LYS:HD3	17:R:69:GLN:NE2	2.35	0.41
20:U:51:ILE:HG23	20:U:59:THR:HG22	2.03	0.41
27:X:216:U:H2'	27:X:217:U:C6	2.56	0.41
27:X:224:G:H4'	27:X:399:G:C6	2.56	0.41
27:X:242:A:N6	27:X:441:A:C8	2.89	0.41
27:X:474:G:C6	27:X:478:G:O6	2.74	0.41
27:X:481:A:H3'	27:X:482:A:C8	2.56	0.41
27:X:487:G:N2	27:X:489:A:H3'	2.35	0.41
27:X:534:U:P	27:X:549:G:H21	2.43	0.41
27:X:717:G:N3	27:X:739:G:C2	2.89	0.41
27:X:1250:A:H5'	27:X:1250:A:C8	2.54	0.41
27:X:1365:U:O2'	27:X:1586:A:N3	2.43	0.41
27:X:1385:C:H2'	27:X:1386:A:O4'	2.21	0.41
27:X:1609:G:H2'	27:X:1610:A:O4'	2.21	0.41
27:X:1779:C:H2'	27:X:1780:A:C8	2.56	0.41
27:X:1816:G:H2'	27:X:1817:U:C6	2.56	0.41
27:X:1869:A:H2'	27:X:1870:U:O4'	2.21	0.41
27:X:1991:C:H2'	27:X:1992:G:C8	2.53	0.41
27:X:2185:U:H2'	27:X:2186:G:C8	2.56	0.41
27:X:2355:A:H8	27:X:2355:A:OP1	2.04	0.41
27:X:2432:A:N6	27:X:2479:U:H3	2.15	0.41
27:X:2443:C:H2'	27:X:2444:C:H6	1.86	0.41
27:X:2501:U:O2'	27:X:2626:U:OP1	2.32	0.41
27:X:2579:A:O2'	27:X:2580:C:H5'	2.21	0.41
27:X:2702:G:H2'	27:X:2703:C:O4'	2.21	0.41
27:X:2772:U:H2'	27:X:2773:G:C8	2.56	0.41
27:X:2838:U:H2'	27:X:2839:G:H8	1.86	0.41
3:C:65:GLY:CA	27:X:2042:A:H5''	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:56:THR:HG21	27:X:1016:C:O2'	2.21	0.41
7:H:116:ARG:HD3	12:M:40:ARG:HB2	2.03	0.41
7:H:127:VAL:HG22	7:H:133:VAL:HG21	2.03	0.41
9:J:24:GLY:HA3	27:X:920:G:P	2.61	0.41
24:1:10:VAL:HG22	24:1:11:LYS:N	2.36	0.41
27:X:215:G:H1'	27:X:619:A:H1'	2.03	0.41
27:X:617:U:H5	27:X:632:A:N1	2.19	0.41
27:X:830:C:H3'	27:X:831:G:H8	1.86	0.41
27:X:923:A:N3	27:X:2243:C:H1'	2.36	0.41
27:X:1123:G:C6	27:X:1124:U:N3	2.89	0.41
27:X:1417:C:H2'	27:X:1418:C:C6	2.56	0.41
27:X:1717:A:H5'	27:X:1718:A:OP2	2.20	0.41
27:X:2712:G:H3'	27:X:2713:A:O4'	2.21	0.41
28:Y:32:C:H6	28:Y:32:C:O5'	2.03	0.41
2:B:148:GLY:HA3	27:X:2036:G:C4'	2.51	0.40
3:C:17:LEU:HD12	3:C:17:LEU:HA	1.78	0.40
3:C:165:SER:HB3	3:C:166:TRP:CE3	2.56	0.40
10:K:96:ARG:HB2	27:X:2857:C:H5'	2.03	0.40
12:M:101:ARG:HH22	27:X:1745:C:P	2.43	0.40
16:Q:56:MET:HE3	16:Q:57:ASN:N	2.32	0.40
17:R:14:LEU:HD23	17:R:14:LEU:HA	1.85	0.40
20:U:28:GLY:HA3	20:U:32:ARG:HG2	2.03	0.40
23:Z:52:TYR:CE1	27:X:2859:U:N3	2.88	0.40
25:2:35:ARG:NH1	27:X:53:G:H1'	2.36	0.40
27:X:877:G:C6	27:X:878:C:N4	2.89	0.40
27:X:1671:A:O4'	27:X:2798:A:H5'	2.21	0.40
27:X:1754:G:OP1	27:X:1754:G:H4'	2.21	0.40
27:X:2220:A:H2'	27:X:2221:G:C8	2.56	0.40
27:X:2288:A:C5	27:X:2289:A:N7	2.89	0.40
27:X:2616:U:H5''	27:X:2617:G:OP2	2.21	0.40
2:B:126:PRO:C	2:B:128:SER:H	2.28	0.40
3:C:163:ASN:ND2	3:C:166:TRP:HB2	2.36	0.40
3:C:189:ASP:HB3	3:C:190:ALA:H	1.65	0.40
4:D:35:VAL:HB	4:D:155:THR:OG1	2.21	0.40
6:G:52:GLY:HA3	27:X:1150:C:H5'	2.04	0.40
6:G:139:ARG:HB2	27:X:567:G:OP1	2.21	0.40
7:H:88:THR:O	12:M:79:ARG:HG2	2.22	0.40
8:I:56:LEU:HD22	26:3:52:LYS:NZ	2.37	0.40
9:J:26:ASP:OD1	9:J:28:VAL:N	2.52	0.40
13:N:2:PRO:HD3	27:X:456:C:O5'	2.22	0.40
13:N:52:ASN:O	13:N:55:ARG:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:89:ASP:C	13:N:91:ASN:H	2.29	0.40
15:P:125:SER:OG	15:P:126:HIS:N	2.53	0.40
18:S:1:MET:HB3	18:S:2:GLU:H	1.70	0.40
18:S:152:ILE:HD11	18:S:168:VAL:HB	2.03	0.40
20:U:10:LYS:HD3	20:U:11:LYS:N	2.37	0.40
20:U:33:LYS:HD3	20:U:33:LYS:HA	1.72	0.40
22:W:47:VAL:HG23	22:W:51:LEU:HD21	2.03	0.40
26:3:15:LYS:HA	26:3:15:LYS:HD3	1.70	0.40
27:X:350:U:H6	27:X:350:U:O5'	2.04	0.40
27:X:825:C:C6	27:X:1263:G:C5	3.10	0.40
27:X:951:G:N3	27:X:1205:G:H4'	2.35	0.40
27:X:1251:G:O2'	27:X:1252:C:H5'	2.21	0.40
27:X:1531:C:H5'	27:X:1532:A:OP1	2.21	0.40
27:X:1882:G:N2	27:X:1886:G:C6	2.89	0.40
27:X:2609:G:H21	27:X:2866:A:H1'	1.85	0.40
28:Y:31:A:N3	28:Y:58:G:N2	2.69	0.40
2:B:37:LYS:HD2	2:B:42:ASP:OD1	2.22	0.40
3:C:84:PHE:CD2	27:X:597:U:H1'	2.57	0.40
3:C:147:LYS:O	3:C:185:ARG:N	2.50	0.40
8:I:43:ALA:HB1	27:X:684:C:H41	1.85	0.40
15:P:30:TYR:HB3	15:P:123:ARG:CZ	2.51	0.40
26:3:32:GLN:H	26:3:32:GLN:HG3	1.67	0.40
27:X:45:C:OP2	27:X:192:G:H2'	2.21	0.40
27:X:312:G:O2'	27:X:313:U:H6	2.03	0.40
27:X:494:A:C8	27:X:495:C:C5	3.09	0.40
27:X:538:A:N3	27:X:2025:A:C6	2.89	0.40
27:X:676:G:C6	27:X:677:G:C5	3.10	0.40
27:X:1026:U:H2'	27:X:1027:C:H6	1.86	0.40
27:X:1080:A:N7	27:X:1084:A:N6	2.69	0.40
27:X:1742:G:H2'	27:X:1743:C:C6	2.56	0.40
27:X:1850:G:C1'	27:X:1867:A:H62	2.35	0.40
27:X:2013:A:H4'	27:X:2014:A:H8	1.87	0.40
27:X:2262:C:H2'	27:X:2263:C:O4'	2.21	0.40
27:X:2455:A:N3	27:X:2460:G:N1	2.62	0.40
27:X:2609:G:N3	27:X:2866:A:O2'	2.53	0.40
28:Y:36:A:N6	28:Y:46:G:H2'	2.36	0.40
1:A:222:ARG:NH2	27:X:1819:U:OP2	2.53	0.40
2:B:109:LYS:HE2	2:B:191:ALA:HB2	2.02	0.40
2:B:136:ARG:CZ	2:B:157:ALA:HB2	2.51	0.40
5:E:67:LEU:O	5:E:71:LEU:HG	2.22	0.40
5:E:143:GLN:HE21	27:X:2724:G:H21	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:111:LYS:HE2	27:X:1142:G:H5''	2.03	0.40
7:H:3:MET:HG2	7:H:44:TYR:CE1	2.57	0.40
8:I:56:LEU:HD21	8:I:59:ARG:NH2	2.35	0.40
12:M:103:LYS:HD2	12:M:103:LYS:N	2.36	0.40
13:N:13:ARG:NH2	27:X:1264:C:OP1	2.53	0.40
15:P:51:GLN:HE22	23:Z:39:LYS:NZ	2.20	0.40
16:Q:20:MET:HG3	16:Q:25:TYR:CD1	2.57	0.40
20:U:53:GLU:HB2	20:U:56:GLN:O	2.21	0.40
24:1:11:LYS:HE3	24:1:26:LYS:HD3	2.03	0.40
25:2:19:ARG:O	25:2:22:MET:HB3	2.22	0.40
26:3:25:PHE:CD2	26:3:25:PHE:N	2.88	0.40
27:X:192:G:H4'	27:X:193:A:H4'	2.04	0.40
27:X:200:A:O2'	27:X:433:G:O2'	2.26	0.40
27:X:573:C:H2'	27:X:574:C:O4'	2.21	0.40
27:X:600:G:C6	27:X:602:C:C4	3.09	0.40
27:X:692:C:H2'	27:X:693:A:C8	2.56	0.40
27:X:836:G:C4	27:X:837:U:C5	3.10	0.40
27:X:1354:A:H2'	27:X:1410:U:O2	2.21	0.40
27:X:1473:U:O2	27:X:1474:A:N6	2.55	0.40
27:X:1773:C:H2'	27:X:2587:G:O2'	2.22	0.40
27:X:2030:U:H2'	27:X:2031:A:C8	2.57	0.40
27:X:2281:C:N4	27:X:2293:G:H1	2.04	0.40
27:X:2533:U:H2'	27:X:2534:U:C6	2.56	0.40
27:X:2827:G:C6	27:X:2828:C:N3	2.90	0.40
28:Y:119:G:C6	28:Y:120:G:C5	3.10	0.40
2:B:147:PRO:HB2	2:B:149:ARG:HG2	2.03	0.40
6:G:131:VAL:O	6:G:134:MET:N	2.41	0.40
9:J:6:LYS:HB2	9:J:7:ARG:H	1.68	0.40
10:K:9:LYS:HE2	27:X:1669:A:OP1	2.22	0.40
10:K:45:ARG:O	10:K:49:GLU:HG3	2.21	0.40
10:K:66:VAL:HG21	10:K:80:MET:HE1	2.04	0.40
15:P:12:LYS:HA	15:P:15:LYS:HB2	2.04	0.40
15:P:31:VAL:O	15:P:125:SER:HB3	2.21	0.40
17:R:14:LEU:HD13	17:R:16:PHE:CZ	2.57	0.40
18:S:116:VAL:N	18:S:168:VAL:O	2.49	0.40
21:V:18:ILE:HG23	21:V:22:LYS:HE2	2.04	0.40
23:Z:8:LYS:O	27:X:2000:U:H4'	2.21	0.40
27:X:354:C:H2'	27:X:355:G:C8	2.55	0.40
27:X:759:C:C2	30:X:2902:ERY:H371	2.56	0.40
27:X:1174:G:N2	27:X:1175:A:C5	2.89	0.40
27:X:1413:U:H2'	27:X:1414:G:H8	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1662:G:O5'	27:X:1662:G:H8	2.04	0.40
27:X:1695:U:H2'	27:X:1696:C:O4'	2.21	0.40
27:X:2212:U:H2'	27:X:2213:G:C8	2.56	0.40
27:X:2528:G:C2	27:X:2529:G:C5	3.09	0.40
27:X:2662:C:C4	27:X:2663:U:C5	3.10	0.40
27:X:2698:G:H2'	27:X:2699:G:O4'	2.21	0.40
27:X:2763:U:H2'	27:X:2764:U:C6	2.51	0.40
27:X:2821:G:H2'	27:X:2822:U:O4'	2.20	0.40
27:X:2825:A:N3	27:X:2825:A:H2'	2.35	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	
1	A	258/275 (94%)	221 (86%)	34 (13%)	3 (1%)	10	42
2	B	203/211 (96%)	178 (88%)	24 (12%)	1 (0%)	24	58
3	C	192/205 (94%)	164 (85%)	26 (14%)	2 (1%)	12	45
4	D	175/180 (97%)	155 (89%)	19 (11%)	1 (1%)	21	55
5	E	169/185 (91%)	157 (93%)	11 (6%)	1 (1%)	21	55
6	G	140/174 (80%)	127 (91%)	13 (9%)	0	100	100
7	H	132/134 (98%)	120 (91%)	11 (8%)	1 (1%)	16	50
8	I	132/156 (85%)	102 (77%)	26 (20%)	4 (3%)	3	25
9	J	134/141 (95%)	113 (84%)	21 (16%)	0	100	100
10	K	111/116 (96%)	102 (92%)	8 (7%)	1 (1%)	14	47
11	L	102/114 (90%)	86 (84%)	16 (16%)	0	100	100
12	M	106/165 (64%)	99 (93%)	6 (6%)	1 (1%)	14	47
13	N	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	O	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
15	P	128/137 (93%)	109 (85%)	15 (12%)	4 (3%)	3	24
16	Q	91/95 (96%)	76 (84%)	12 (13%)	3 (3%)	3	23
17	R	108/115 (94%)	91 (84%)	16 (15%)	1 (1%)	14	47
18	S	173/237 (73%)	154 (89%)	19 (11%)	0	100	100
19	T	72/91 (79%)	62 (86%)	9 (12%)	1 (1%)	9	38
20	U	70/81 (86%)	52 (74%)	14 (20%)	4 (6%)	1	13
21	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
22	W	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
23	Z	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
24	1	51/55 (93%)	38 (74%)	10 (20%)	3 (6%)	1	12
25	2	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
26	3	57/65 (88%)	46 (81%)	10 (18%)	1 (2%)	6	34
All	All	3025/3379 (90%)	2632 (87%)	359 (12%)	34 (1%)	11	44

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	120	ILE
16	Q	6	ILE
16	Q	69	ILE
1	A	24	LEU
1	A	25	THR
13	N	94	VAL
16	Q	59	PRO
24	1	9	ILE
24	1	10	VAL
15	P	125	SER
20	U	60	VAL
5	E	165	VAL
7	H	42	LYS
8	I	39	SER
8	I	103	ASN
15	P	119	ILE
20	U	15	VAL
20	U	39	LYS
10	K	18	VAL

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Mol	Chain	Res	Type
15	P	99	ALA
19	T	19	LYS
24	1	18	THR
2	B	121	ASN
4	D	8	TYR
13	N	8	ILE
17	R	80	LYS
26	3	37	SER
1	A	219	PRO
3	C	15	ILE
12	M	29	PRO
20	U	30	VAL
3	C	22	VAL
8	I	61	PRO
8	I	68	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	
1	A	202/216 (94%)	161 (80%)	41 (20%)	1	7
2	B	155/157 (99%)	123 (79%)	32 (21%)	1	7
3	C	154/163 (94%)	126 (82%)	28 (18%)	2	10
4	D	153/156 (98%)	138 (90%)	15 (10%)	7	30
5	E	136/144 (94%)	117 (86%)	19 (14%)	3	19
6	G	118/146 (81%)	94 (80%)	24 (20%)	1	7
7	H	103/103 (100%)	83 (81%)	20 (19%)	1	8
8	I	101/121 (84%)	83 (82%)	18 (18%)	2	10
9	J	110/115 (96%)	86 (78%)	24 (22%)	1	6
10	K	90/93 (97%)	72 (80%)	18 (20%)	1	7
11	L	74/82 (90%)	56 (76%)	18 (24%)	1	4
12	M	94/133 (71%)	70 (74%)	24 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	N	96/97 (99%)	77 (80%)	19 (20%)	1	8
14	O	75/79 (95%)	58 (77%)	17 (23%)	1	5
15	P	112/118 (95%)	84 (75%)	28 (25%)	0	4
16	Q	75/76 (99%)	62 (83%)	13 (17%)	2	12
17	R	91/96 (95%)	72 (79%)	19 (21%)	1	6
18	S	149/192 (78%)	137 (92%)	12 (8%)	11	35
19	T	55/67 (82%)	43 (78%)	12 (22%)	1	6
20	U	57/66 (86%)	43 (75%)	14 (25%)	1	4
21	V	53/55 (96%)	46 (87%)	7 (13%)	4	21
22	W	48/48 (100%)	37 (77%)	11 (23%)	1	5
23	Z	50/53 (94%)	42 (84%)	8 (16%)	2	14
24	1	46/48 (96%)	33 (72%)	13 (28%)	0	3
25	2	39/40 (98%)	27 (69%)	12 (31%)	0	2
26	3	46/51 (90%)	36 (78%)	10 (22%)	1	6
All	All	2482/2715 (91%)	2006 (81%)	476 (19%)	1	8

All (476) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	16	MET
1	A	26	LYS
1	A	34	THR
1	A	40	THR
1	A	43	ARG
1	A	48	ARG
1	A	49	ILE
1	A	53	PHE
1	A	63	ARG
1	A	64	ILE
1	A	65	ILE
1	A	84	TYR
1	A	88	ARG
1	A	104	TYR
1	A	111	LEU
1	A	118	ASN
1	A	122	GLU

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Mol	Chain	Res	Type
1	A	151	LYS
1	A	157	ARG
1	A	161	THR
1	A	164	GLN
1	A	165	VAL
1	A	186	HIS
1	A	188	GLU
1	A	198	ASN
1	A	201	HIS
1	A	206	LEU
1	A	211	ARG
1	A	214	TRP
1	A	215	LEU
1	A	217	ARG
1	A	218	LYS
1	A	220	HIS
1	A	229	VAL
1	A	240	THR
1	A	244	ARG
1	A	247	VAL
1	A	248	THR
1	A	252	LYS
1	A	269	PHE
2	B	9	ILE
2	B	12	THR
2	B	14	ILE
2	B	19	ARG
2	B	24	THR
2	B	34	VAL
2	B	56	GLU
2	B	69	LYS
2	B	72	VAL
2	B	79	ARG
2	B	84	PHE
2	B	87	ASP
2	B	91	VAL
2	B	92	ASN
2	B	107	THR
2	B	113	THR
2	B	119	ARG
2	B	128	SER
2	B	137	ARG

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Mol	Chain	Res	Type
2	B	140	SER
2	B	143	GLN
2	B	145	LYS
2	B	150	VAL
2	B	155	ARG
2	B	156	MET
2	B	162	MET
2	B	165	VAL
2	B	173	VAL
2	B	188	ILE
2	B	196	VAL
2	B	198	LEU
2	B	199	ARG
3	C	5	ASN
3	C	14	THR
3	C	17	LEU
3	C	24	SER
3	C	31	VAL
3	C	45	THR
3	C	46	ARG
3	C	48	ARG
3	C	51	VAL
3	C	52	SER
3	C	62	LYS
3	C	64	THR
3	C	74	VAL
3	C	76	THR
3	C	78	VAL
3	C	98	GLN
3	C	99	VAL
3	C	116	LYS
3	C	120	VAL
3	C	150	LEU
3	C	152	THR
3	C	155	GLU
3	C	157	THR
3	C	165	SER
3	C	172	VAL
3	C	175	VAL
3	C	181	LEU
3	C	188	ILE
4	D	34	ILE

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Mol	Chain	Res	Type
4	D	46	ASP
4	D	62	LEU
4	D	66	ILE
4	D	67	ILE
4	D	74	ILE
4	D	80	ARG
4	D	90	THR
4	D	112	ARG
4	D	128	TYR
4	D	130	LEU
4	D	143	TYR
4	D	146	VAL
4	D	150	ARG
4	D	157	VAL
5	E	20	GLN
5	E	32	GLU
5	E	43	VAL
5	E	57	ASP
5	E	61	HIS
5	E	70	THR
5	E	86	ASN
5	E	90	ARG
5	E	105	MET
5	E	113	VAL
5	E	129	THR
5	E	130	ARG
5	E	136	ILE
5	E	155	ASP
5	E	164	PHE
5	E	165	VAL
5	E	167	GLU
5	E	168	GLN
5	E	169	ILE
6	G	31	THR
6	G	39	GLN
6	G	56	THR
6	G	57	LEU
6	G	61	ARG
6	G	62	ILE
6	G	63	ARG
6	G	67	ARG
6	G	69	ASP

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Mol	Chain	Res	Type
6	G	76	GLN
6	G	83	ILE
6	G	90	LEU
6	G	91	THR
6	G	93	LYS
6	G	99	VAL
6	G	101	THR
6	G	102	ARG
6	G	116	ARG
6	G	132	PHE
6	G	140	GLN
6	G	145	HIS
6	G	150	VAL
6	G	161	GLN
6	G	171	LEU
7	H	2	ILE
7	H	10	VAL
7	H	17	ARG
7	H	22	ILE
7	H	23	ARG
7	H	25	LEU
7	H	41	ASN
7	H	47	VAL
7	H	51	ILE
7	H	69	VAL
7	H	78	SER
7	H	93	ARG
7	H	102	GLN
7	H	104	GLU
7	H	108	THR
7	H	114	VAL
7	H	117	GLU
7	H	119	ARG
7	H	126	ILE
7	H	127	VAL
8	I	18	ARG
8	I	21	ARG
8	I	26	THR
8	I	32	ARG
8	I	39	SER
8	I	49	PHE
8	I	59	ARG

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Mol	Chain	Res	Type
8	I	60	LEU
8	I	62	LYS
8	I	73	GLU
8	I	78	SER
8	I	80	LEU
8	I	88	PHE
8	I	89	ASP
8	I	96	TYR
8	I	114	ILE
8	I	120	VAL
8	I	141	VAL
9	J	6	LYS
9	J	8	THR
9	J	10	PHE
9	J	11	ARG
9	J	17	ARG
9	J	21	ASP
9	J	27	TYR
9	J	28	VAL
9	J	44	LYS
9	J	54	VAL
9	J	60	ARG
9	J	64	LYS
9	J	68	ARG
9	J	69	ILE
9	J	88	LYS
9	J	93	TYR
9	J	103	VAL
9	J	104	MET
9	J	111	THR
9	J	130	THR
9	J	132	MET
9	J	133	VAL
9	J	134	LYS
9	J	135	ARG
10	K	5	LYS
10	K	8	ARG
10	K	9	LYS
10	K	11	ASN
10	K	12	ARG
10	K	14	SER
10	K	35	GLN

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Mol	Chain	Res	Type
10	K	37	THR
10	K	45	ARG
10	K	48	VAL
10	K	51	LEU
10	K	54	THR
10	K	59	ASP
10	K	64	ARG
10	K	95	THR
10	K	98	LEU
10	K	109	THR
10	K	112	LEU
11	L	11	LEU
11	L	17	VAL
11	L	31	VAL
11	L	33	ARG
11	L	37	HIS
11	L	38	ILE
11	L	39	TYR
11	L	42	ILE
11	L	43	ILE
11	L	45	ASP
11	L	59	LEU
11	L	65	THR
11	L	67	THR
11	L	87	VAL
11	L	88	VAL
11	L	91	ARG
11	L	93	SER
11	L	100	VAL
12	M	2	GLN
12	M	3	THR
12	M	5	ILE
12	M	7	ILE
12	M	13	LEU
12	M	16	ILE
12	M	19	ASP
12	M	20	HIS
12	M	21	THR
12	M	22	ARG
12	M	24	LEU
12	M	29	PRO
12	M	31	ASP

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Mol	Chain	Res	Type
12	M	33	VAL
12	M	37	THR
12	M	39	VAL
12	M	40	ARG
12	M	45	THR
12	M	72	SER
12	M	79	ARG
12	M	87	LEU
12	M	88	VAL
12	M	91	VAL
12	M	103	LYS
13	N	3	ARG
13	N	5	LYS
13	N	8	ILE
13	N	11	ARG
13	N	18	LEU
13	N	22	LYS
13	N	28	ARG
13	N	30	LYS
13	N	33	ARG
13	N	37	GLN
13	N	40	LEU
13	N	60	LEU
13	N	83	LEU
13	N	84	LYS
13	N	90	LEU
13	N	92	ARG
13	N	93	LYS
13	N	102	GLU
13	N	117	ARG
14	O	12	TYR
14	O	13	ARG
14	O	14	VAL
14	O	20	ILE
14	O	21	ARG
14	O	32	LYS
14	O	38	LEU
14	O	40	VAL
14	O	47	PHE
14	O	67	LYS
14	O	69	ILE
14	O	72	ARG

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Mol	Chain	Res	Type
14	O	76	SER
14	O	81	ARG
14	O	82	ARG
14	O	88	GLN
14	O	91	THR
15	P	9	ARG
15	P	12	LYS
15	P	20	LEU
15	P	21	ARG
15	P	31	VAL
15	P	32	ARG
15	P	39	ARG
15	P	40	LEU
15	P	43	ASP
15	P	48	LYS
15	P	51	GLN
15	P	80	LEU
15	P	86	LEU
15	P	91	PHE
15	P	92	VAL
15	P	93	LYS
15	P	98	ASP
15	P	102	THR
15	P	103	LEU
15	P	104	LYS
15	P	105	ARG
15	P	106	LEU
15	P	109	ARG
15	P	114	ARG
15	P	120	ILE
15	P	122	LYS
15	P	128	THR
15	P	131	VAL
16	Q	5	ASP
16	Q	6	ILE
16	Q	7	LEU
16	Q	12	ILE
16	Q	26	SER
16	Q	27	PHE
16	Q	56	MET
16	Q	58	VAL
16	Q	62	ARG

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Mol	Chain	Res	Type
16	Q	67	ARG
16	Q	73	ASN
16	Q	80	VAL
16	Q	84	GLU
17	R	5	SER
17	R	11	ASN
17	R	38	LEU
17	R	44	GLN
17	R	52	ASN
17	R	53	VAL
17	R	54	ILE
17	R	55	THR
17	R	56	LYS
17	R	62	MET
17	R	64	ASN
17	R	72	ARG
17	R	81	VAL
17	R	83	LEU
17	R	88	THR
17	R	92	THR
17	R	97	GLN
17	R	106	VAL
17	R	112	LYS
18	S	22	VAL
18	S	26	LYS
18	S	28	ASN
18	S	49	THR
18	S	52	PHE
18	S	71	MET
18	S	79	ILE
18	S	83	PHE
18	S	99	HIS
18	S	120	LEU
18	S	130	ILE
18	S	168	VAL
19	T	14	ARG
19	T	19	LYS
19	T	25	LYS
19	T	36	ILE
19	T	41	ARG
19	T	46	LYS
19	T	55	ARG

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Mol	Chain	Res	Type
19	T	56	ASP
19	T	62	LEU
19	T	64	ASP
19	T	71	ASN
19	T	79	ILE
20	U	8	THR
20	U	13	LEU
20	U	19	ILE
20	U	21	ARG
20	U	23	LYS
20	U	32	ARG
20	U	34	THR
20	U	35	THR
20	U	37	ILE
20	U	43	ARG
20	U	47	HIS
20	U	62	LEU
20	U	63	SER
20	U	70	LEU
21	V	7	ARG
21	V	19	ASP
21	V	25	LEU
21	V	26	MET
21	V	29	ARG
21	V	37	LEU
21	V	42	ARG
22	W	3	ILE
22	W	4	LYS
22	W	6	VAL
22	W	9	VAL
22	W	23	LEU
22	W	31	SER
22	W	34	VAL
22	W	37	THR
22	W	40	VAL
22	W	45	LYS
22	W	51	LEU
23	Z	6	VAL
23	Z	11	THR
23	Z	19	ARG
23	Z	23	HIS
23	Z	25	LEU

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Mol	Chain	Res	Type
23	Z	29	ASN
23	Z	41	LEU
23	Z	44	HIS
24	1	4	ASP
24	1	8	ILE
24	1	20	PHE
24	1	21	TYR
24	1	22	TYR
24	1	26	LYS
24	1	27	ASN
24	1	28	ARG
24	1	36	GLU
24	1	41	ASP
24	1	43	VAL
24	1	48	VAL
24	1	54	LYS
25	2	3	ARG
25	2	4	THR
25	2	10	ARG
25	2	14	LYS
25	2	19	ARG
25	2	22	MET
25	2	23	LYS
25	2	28	ARG
25	2	29	ASN
25	2	40	HIS
25	2	42	LEU
25	2	44	VAL
26	3	6	THR
26	3	11	LYS
26	3	19	THR
26	3	31	HIS
26	3	32	GLN
26	3	36	LYS
26	3	39	ASP
26	3	46	LYS
26	3	55	TRP
26	3	57	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	198	ASN
1	A	201	HIS
1	A	227	ASN
2	B	35	GLN
2	B	48	GLN
2	B	135	HIS
2	B	169	ASN
2	B	192	ASN
3	C	34	GLN
3	C	50	GLN
3	C	98	GLN
3	C	112	GLN
3	C	132	ASN
3	C	156	ASN
3	C	163	ASN
4	D	37	ASN
4	D	129	ASN
4	D	135	GLN
4	D	171	GLN
5	E	61	HIS
5	E	65	HIS
5	E	74	ASN
5	E	86	ASN
5	E	106	ASN
5	E	168	GLN
6	G	39	GLN
6	G	66	HIS
6	G	76	GLN
6	G	84	ASN
6	G	158	HIS
6	G	161	GLN
7	H	79	HIS
7	H	101	ASN
8	I	79	GLN
8	I	103	ASN
9	J	114	GLN
10	K	3	HIS
10	K	24	GLN
10	K	61	HIS
11	L	37	HIS
11	L	86	GLN
12	M	2	GLN

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Mol	Chain	Res	Type
12	M	20	HIS
13	N	31	GLN
13	N	37	GLN
13	N	41	ASN
13	N	52	ASN
13	N	63	GLN
13	N	72	HIS
13	N	81	ASN
14	O	11	GLN
14	O	88	GLN
15	P	16	GLN
15	P	51	GLN
15	P	78	ASN
15	P	81	HIS
15	P	118	ASN
16	Q	3	HIS
16	Q	44	GLN
16	Q	57	ASN
16	Q	71	GLN
16	Q	73	ASN
17	R	10	HIS
17	R	15	HIS
17	R	32	GLN
17	R	44	GLN
17	R	69	GLN
17	R	71	GLN
17	R	97	GLN
18	S	46	GLN
18	S	118	HIS
18	S	121	GLN
19	T	71	ASN
19	T	85	GLN
20	U	54	ASN
21	V	54	ASN
22	W	15	ASN
22	W	49	HIS
23	Z	29	ASN
23	Z	44	HIS
24	1	32	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2673/2880 (92%)	640 (23%)	40 (1%)
28	Y	121/124 (97%)	29 (23%)	1 (0%)
All	All	2794/3004 (93%)	669 (23%)	41 (1%)

All (669) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	X	3	U
27	X	4	C
27	X	13	A
27	X	14	A
27	X	17	G
27	X	34	U
27	X	37	C
27	X	39	C
27	X	45	C
27	X	49	U
27	X	50	G
27	X	51	A
27	X	59	G
27	X	60	A
27	X	63	A
27	X	69	G
27	X	70	A
27	X	73	A
27	X	74	G
27	X	83	A
27	X	88	G
27	X	89	A
27	X	90	G
27	X	91	A
27	X	98	U
27	X	100	G
27	X	107	G
27	X	108	G
27	X	116	A
27	X	118	U
27	X	123	A
27	X	124	A
27	X	129	A
27	X	135	U
27	X	136	A
27	X	143	A

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Mol	Chain	Res	Type
27	X	146	C
27	X	151	G
27	X	173	A
27	X	176	A
27	X	178	C
27	X	181	A
27	X	192	G
27	X	193	A
27	X	199	A
27	X	205	A
27	X	206	U
27	X	207	U
27	X	209	G
27	X	210	A
27	X	220	U
27	X	221	A
27	X	222	G
27	X	225	G
27	X	227	G
27	X	229	G
27	X	238	G
27	X	242	A
27	X	243	G
27	X	246	C
27	X	248	A
27	X	304	A
27	X	305	A
27	X	310	A
27	X	312	G
27	X	319	G
27	X	321	A
27	X	322	A
27	X	323	G
27	X	335	A
27	X	340	G
27	X	341	A
27	X	342	G
27	X	343	A
27	X	360	A
27	X	393	U
27	X	399	G
27	X	400	U

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Mol	Chain	Res	Type
27	X	408	U
27	X	409	G
27	X	414	A
27	X	419	G
27	X	421	G
27	X	424	G
27	X	425	A
27	X	429	C
27	X	433	G
27	X	441	A
27	X	453	U
27	X	456	C
27	X	459	A
27	X	463	C
27	X	467	U
27	X	469	G
27	X	490	A
27	X	491	A
27	X	492	G
27	X	493	A
27	X	494	A
27	X	504	G
27	X	514	G
27	X	515	A
27	X	518	A
27	X	519	C
27	X	520	C
27	X	537	C
27	X	538	A
27	X	539	A
27	X	540	G
27	X	541	C
27	X	542	A
27	X	543	G
27	X	554	U
27	X	555	U
27	X	556	A
27	X	557	U
27	X	559	C
27	X	560	G
27	X	564	U
27	X	572	G

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Mol	Chain	Res	Type
27	X	582	G
27	X	584	A
27	X	587	A
27	X	591	G
27	X	595	A
27	X	596	C
27	X	613	A
27	X	614	G
27	X	616	U
27	X	624	A
27	X	625	A
27	X	626	A
27	X	627	A
27	X	628	A
27	X	631	G
27	X	632	A
27	X	633	G
27	X	642	A
27	X	645	G
27	X	648	A
27	X	649	G
27	X	651	C
27	X	654	A
27	X	655	A
27	X	656	U
27	X	657	A
27	X	658	G
27	X	664	C
27	X	665	A
27	X	666	U
27	X	667	U
27	X	668	A
27	X	677	G
27	X	682	G
27	X	690	A
27	X	695	G
27	X	697	G
27	X	699	G
27	X	703	A
27	X	725	C
27	X	729	A
27	X	731	A

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Mol	Chain	Res	Type
27	X	732	G
27	X	743	A
27	X	749	C
27	X	753	U
27	X	759	C
27	X	760	U
27	X	761	G
27	X	766	A
27	X	774	A
27	X	784	U
27	X	789	G
27	X	790	A
27	X	795	A
27	X	797	A
27	X	798	G
27	X	801	A
27	X	802	A
27	X	803	C
27	X	804	C
27	X	805	G
27	X	806	A
27	X	814	G
27	X	818	G
27	X	824	U
27	X	825	C
27	X	830	C
27	X	832	A
27	X	840	U
27	X	841	G
27	X	843	G
27	X	859	U
27	X	872	G
27	X	879	A
27	X	891	A
27	X	914	C
27	X	922	A
27	X	931	G
27	X	938	G
27	X	939	C
27	X	940	G
27	X	943	U
27	X	944	A

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Mol	Chain	Res	Type
27	X	952	A
27	X	956	A
27	X	957	G
27	X	966	A
27	X	967	G
27	X	969	U
27	X	972	C
27	X	973	U
27	X	976	C
27	X	979	A
27	X	985	G
27	X	992	A
27	X	999	A
27	X	1000	G
27	X	1006	C
27	X	1007	A
27	X	1016	C
27	X	1018	C
27	X	1019	U
27	X	1020	A
27	X	1022	A
27	X	1023	U
27	X	1024	G
27	X	1033	G
27	X	1034	U
27	X	1035	G
27	X	1037	U
27	X	1044	U
27	X	1046	U
27	X	1051	U
27	X	1054	C
27	X	1055	A
27	X	1056	U
27	X	1058	G
27	X	1060	C
27	X	1071	U
27	X	1073	G
27	X	1081	A
27	X	1082	G
27	X	1083	C
27	X	1086	C
27	X	1087	C

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Mol	Chain	Res	Type
27	X	1096	A
27	X	1097	A
27	X	1099	A
27	X	1101	U
27	X	1105	U
27	X	1108	U
27	X	1109	A
27	X	1113	C
27	X	1120	C
27	X	1121	G
27	X	1123	G
27	X	1127	C
27	X	1128	G
27	X	1140	A
27	X	1142	G
27	X	1145	C
27	X	1146	G
27	X	1149	G
27	X	1152	C
27	X	1153	A
27	X	1183	C
27	X	1185	C
27	X	1187	A
27	X	1189	G
27	X	1194	U
27	X	1195	U
27	X	1200	G
27	X	1203	A
27	X	1208	A
27	X	1209	G
27	X	1217	U
27	X	1223	G
27	X	1225	G
27	X	1240	G
27	X	1249	G
27	X	1250	A
27	X	1251	G
27	X	1260	A
27	X	1261	G
27	X	1262	U
27	X	1263	G
27	X	1266	G

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Mol	Chain	Res	Type
27	X	1269	G
27	X	1278	A
27	X	1279	G
27	X	1284	G
27	X	1285	A
27	X	1286	U
27	X	1288	A
27	X	1289	A
27	X	1301	U
27	X	1302	C
27	X	1313	U
27	X	1314	A
27	X	1315	A
27	X	1321	A
27	X	1325	U
27	X	1332	G
27	X	1334	A
27	X	1341	G
27	X	1342	U
27	X	1347	C
27	X	1349	A
27	X	1354	A
27	X	1358	C
27	X	1365	U
27	X	1378	A
27	X	1379	A
27	X	1381	G
27	X	1391	A
27	X	1392	U
27	X	1393	G
27	X	1397	A
27	X	1398	G
27	X	1404	C
27	X	1408	A
27	X	1409	U
27	X	1413	U
27	X	1428	G
27	X	1429	A
27	X	1430	G
27	X	1432	G
27	X	1433	A
27	X	1434	U

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Mol	Chain	Res	Type
27	X	1435	G
27	X	1441	A
27	X	1442	C
27	X	1443	G
27	X	1459	U
27	X	1460	G
27	X	1465	G
27	X	1467	U
27	X	1468	A
27	X	1469	U
27	X	1470	G
27	X	1475	U
27	X	1482	U
27	X	1490	U
27	X	1497	C
27	X	1498	G
27	X	1508	G
27	X	1517	C
27	X	1518	C
27	X	1524	C
27	X	1525	A
27	X	1527	G
27	X	1528	C
27	X	1541	G
27	X	1551	U
27	X	1552	C
27	X	1553	G
27	X	1554	G
27	X	1562	G
27	X	1571	G
27	X	1574	A
27	X	1575	C
27	X	1582	A
27	X	1585	A
27	X	1600	U
27	X	1601	U
27	X	1602	G
27	X	1603	A
27	X	1608	U
27	X	1624	A
27	X	1625	A
27	X	1626	A

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Mol	Chain	Res	Type
27	X	1629	G
27	X	1631	C
27	X	1632	A
27	X	1634	A
27	X	1641	C
27	X	1648	C
27	X	1651	U
27	X	1656	U
27	X	1661	C
27	X	1664	G
27	X	1665	C
27	X	1666	G
27	X	1667	A
27	X	1668	G
27	X	1682	A
27	X	1688	U
27	X	1691	G
27	X	1710	U
27	X	1711	C
27	X	1713	G
27	X	1719	G
27	X	1732	U
27	X	1735	G
27	X	1747	G
27	X	1754	G
27	X	1755	G
27	X	1760	G
27	X	1764	A
27	X	1771	A
27	X	1775	A
27	X	1776	A
27	X	1782	A
27	X	1790	G
27	X	1791	C
27	X	1792	C
27	X	1793	A
27	X	1799	A
27	X	1801	C
27	X	1807	A
27	X	1808	C
27	X	1811	A
27	X	1812	U

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Mol	Chain	Res	Type
27	X	1813	A
27	X	1819	U
27	X	1821	A
27	X	1830	C
27	X	1831	G
27	X	1859	A
27	X	1861	G
27	X	1867	A
27	X	1868	A
27	X	1882	G
27	X	1884	A
27	X	1910	A
27	X	1912	G
27	X	1919	A
27	X	1920	A
27	X	1921	A
27	X	1922	U
27	X	1923	U
27	X	1924	C
27	X	1930	C
27	X	1938	U
27	X	1946	U
27	X	1947	G
27	X	1948	C
27	X	1949	A
27	X	1950	C
27	X	1951	G
27	X	1953	A
27	X	1954	A
27	X	1955	G
27	X	1958	G
27	X	1965	U
27	X	1974	U
27	X	1976	U
27	X	1980	A
27	X	2001	G
27	X	2003	A
27	X	2004	U
27	X	2006	G
27	X	2014	A
27	X	2015	G
27	X	2016	A

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Mol	Chain	Res	Type
27	X	2018	G
27	X	2023	C
27	X	2025	A
27	X	2026	C
27	X	2028	C
27	X	2032	G
27	X	2035	G
27	X	2038	C
27	X	2039	G
27	X	2043	A
27	X	2044	G
27	X	2045	A
27	X	2052	G
27	X	2059	U
27	X	2075	U
27	X	2083	G
27	X	2089	C
27	X	2171	U
27	X	2172	U
27	X	2182	A
27	X	2189	A
27	X	2190	A
27	X	2191	A
27	X	2192	U
27	X	2193	C
27	X	2196	U
27	X	2197	U
27	X	2198	U
27	X	2199	C
27	X	2200	G
27	X	2204	A
27	X	2205	C
27	X	2217	G
27	X	2218	G
27	X	2247	A
27	X	2252	A
27	X	2259	G
27	X	2262	C
27	X	2265	A
27	X	2266	A
27	X	2267	A
27	X	2272	A

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Mol	Chain	Res	Type
27	X	2284	U
27	X	2285	U
27	X	2286	G
27	X	2287	G
27	X	2290	A
27	X	2291	U
27	X	2298	U
27	X	2299	A
27	X	2300	G
27	X	2301	A
27	X	2306	A
27	X	2307	A
27	X	2311	U
27	X	2312	A
27	X	2313	G
27	X	2315	A
27	X	2324	G
27	X	2326	C
27	X	2327	U
27	X	2330	G
27	X	2333	A
27	X	2351	G
27	X	2358	C
27	X	2362	G
27	X	2364	C
27	X	2367	A
27	X	2368	G
27	X	2369	U
27	X	2375	G
27	X	2381	A
27	X	2385	U
27	X	2386	G
27	X	2397	A
27	X	2398	U
27	X	2401	A
27	X	2402	U
27	X	2404	A
27	X	2405	A
27	X	2406	C
27	X	2407	G
27	X	2408	G
27	X	2410	U

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Mol	Chain	Res	Type
27	X	2413	A
27	X	2420	C
27	X	2424	G
27	X	2426	G
27	X	2427	A
27	X	2429	A
27	X	2441	U
27	X	2449	G
27	X	2452	U
27	X	2453	C
27	X	2455	A
27	X	2460	G
27	X	2463	G
27	X	2470	U
27	X	2471	U
27	X	2477	C
27	X	2480	C
27	X	2481	G
27	X	2482	A
27	X	2484	G
27	X	2485	U
27	X	2497	A
27	X	2498	U
27	X	2504	G
27	X	2508	G
27	X	2511	G
27	X	2521	A
27	X	2545	A
27	X	2546	G
27	X	2552	C
27	X	2553	G
27	X	2557	G
27	X	2564	U
27	X	2581	A
27	X	2582	G
27	X	2588	U
27	X	2591	C
27	X	2593	A
27	X	2594	U
27	X	2600	A
27	X	2601	C
27	X	2608	A

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Mol	Chain	Res	Type
27	X	2617	G
27	X	2624	G
27	X	2625	U
27	X	2633	A
27	X	2639	A
27	X	2642	G
27	X	2650	G
27	X	2664	G
27	X	2666	U
27	X	2668	U
27	X	2670	C
27	X	2677	U
27	X	2688	G
27	X	2691	C
27	X	2692	A
27	X	2693	U
27	X	2694	G
27	X	2698	G
27	X	2706	U
27	X	2707	G
27	X	2711	G
27	X	2713	A
27	X	2724	G
27	X	2728	A
27	X	2732	C
27	X	2737	A
27	X	2738	A
27	X	2744	A
27	X	2745	A
27	X	2756	A
27	X	2757	G
27	X	2758	A
27	X	2759	U
27	X	2760	G
27	X	2761	A
27	X	2769	C
27	X	2771	C
27	X	2782	G
27	X	2793	G
27	X	2795	A
27	X	2796	A
27	X	2798	A

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Mol	Chain	Res	Type
27	X	2807	U
27	X	2808	U
27	X	2809	A
27	X	2811	G
27	X	2814	G
27	X	2825	A
27	X	2832	G
27	X	2846	G
27	X	2847	G
27	X	2849	C
27	X	2851	G
27	X	2855	C
27	X	2858	A
27	X	2861	A
27	X	2866	A
27	X	2868	G
28	Y	14	C
28	Y	15	A
28	Y	17	A
28	Y	22	U
28	Y	26	G
28	Y	28	A
28	Y	29	C
28	Y	37	C
28	Y	39	C
28	Y	40	C
28	Y	43	G
28	Y	44	C
28	Y	46	G
28	Y	47	A
28	Y	49	C
28	Y	52	G
28	Y	54	U
28	Y	56	G
28	Y	59	A
28	Y	69	G
28	Y	75	A
28	Y	86	A
28	Y	99	G
28	Y	102	A
28	Y	108	G
28	Y	111	C

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Mol	Chain	Res	Type
28	Y	112	A
28	Y	115	G
28	Y	123	U

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	X	38	G
27	X	50	G
27	X	537	C
27	X	538	A
27	X	542	A
27	X	557	U
27	X	760	U
27	X	788	G
27	X	789	G
27	X	956	A
27	X	1019	U
27	X	1053	G
27	X	1059	A
27	X	1096	A
27	X	1141	U
27	X	1182	U
27	X	1250	A
27	X	1313	U
27	X	1391	A
27	X	1441	A
27	X	1496	G
27	X	1607	A
27	X	1625	A
27	X	1664	G
27	X	1810	U
27	X	1919	A
27	X	1923	U
27	X	1975	G
27	X	2204	A
27	X	2299	A
27	X	2312	A
27	X	2363	G
27	X	2404	A
27	X	2409	A
27	X	2452	U

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Mol	Chain	Res	Type
27	X	2705	A
27	X	2736	U
27	X	2756	A
27	X	2824	C
27	X	2846	G
28	Y	58	G

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 71 ligands modelled in this entry, 70 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
30	ERY	X	2902	-	53,53,53	0.88	1 (1%)	82,82,82	1.31	8 (9%)

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
30	ERY	X	2902	-	-	4/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	X	2902	ERY	O2-C13	2.17	1.50	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	X	2902	ERY	O8-C23-C22	-2.56	103.96	110.08
30	X	2902	ERY	C2-C3-C4	-2.42	105.94	112.91
30	X	2902	ERY	C30-C2-C1	-2.31	103.83	108.97
30	X	2902	ERY	C16-C15-C14	-2.21	111.25	114.99
30	X	2902	ERY	C13-O2-C1	-2.20	114.36	118.20
30	X	2902	ERY	O10-C6-C7	2.18	113.80	108.34
30	X	2902	ERY	C34-C10-C11	-2.06	111.69	114.30
30	X	2902	ERY	O3-C3-C2	2.02	114.56	111.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

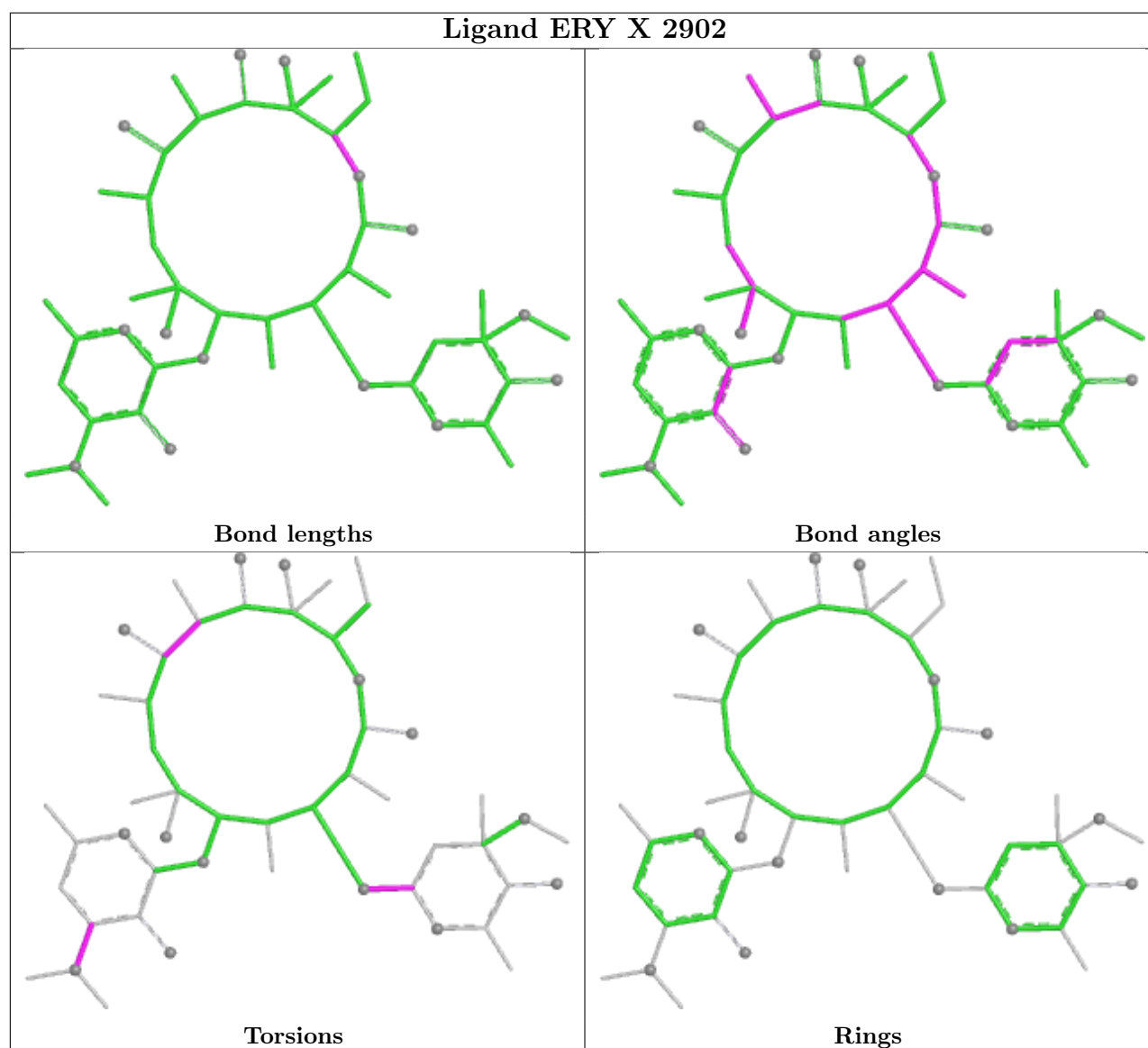
Mol	Chain	Res	Type	Atoms
30	X	2902	ERY	C15-C14-O3-C3
30	X	2902	ERY	O4-C14-O3-C3
30	X	2902	ERY	C25-C24-N1-C28
30	X	2902	ERY	C34-C10-C9-O11

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	2902	ERY	9	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	260/275 (94%)	0.68	31 (11%) 9 6	48, 104, 163, 221	0
2	B	205/211 (97%)	0.10	8 (3%) 43 22	27, 50, 107, 233	0
3	C	194/205 (94%)	0.34	16 (8%) 17 11	39, 102, 180, 292	0
4	D	177/180 (98%)	0.56	16 (9%) 15 9	114, 175, 232, 282	0
5	E	171/185 (92%)	0.20	8 (4%) 36 18	57, 131, 192, 243	0
6	G	142/174 (81%)	0.60	16 (11%) 10 6	38, 77, 160, 339	0
7	H	134/134 (100%)	0.01	2 (1%) 72 43	33, 45, 87, 135	0
8	I	134/156 (85%)	0.90	21 (15%) 5 4	55, 126, 192, 315	0
9	J	136/141 (96%)	0.59	13 (9%) 13 8	56, 94, 163, 214	0
10	K	113/116 (97%)	-0.07	3 (2%) 56 30	27, 32, 67, 100	0
11	L	104/114 (91%)	0.84	10 (9%) 13 8	130, 161, 200, 243	0
12	M	108/165 (65%)	0.14	3 (2%) 55 30	30, 43, 95, 242	0
13	N	117/118 (99%)	0.28	4 (3%) 48 26	41, 76, 133, 232	0
14	O	94/100 (94%)	0.38	6 (6%) 25 15	52, 94, 178, 204	0
15	P	130/137 (94%)	0.04	3 (2%) 61 34	33, 51, 147, 188	0
16	Q	93/95 (97%)	0.11	3 (3%) 50 27	49, 94, 162, 192	0
17	R	110/115 (95%)	0.66	8 (7%) 21 13	65, 100, 189, 259	0
18	S	175/237 (73%)	0.36	11 (6%) 26 15	93, 144, 224, 285	0
19	T	74/91 (81%)	0.63	7 (9%) 14 8	72, 112, 158, 228	0
20	U	72/81 (88%)	0.91	10 (13%) 6 5	75, 119, 185, 238	0
21	V	65/67 (97%)	-0.06	0 100 100	76, 115, 164, 208	0
22	W	55/55 (100%)	-0.02	3 (5%) 30 16	72, 91, 128, 190	0
23	Z	56/60 (93%)	0.23	2 (3%) 46 24	32, 40, 80, 152	0
24	1	53/55 (96%)	1.22	12 (22%) 2 2	102, 129, 217, 266	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	46/47 (97%)	0.57	5 (10%) 10 7	38, 67, 122, 169	0
26	3	59/65 (90%)	1.16	13 (22%) 2 2	80, 100, 172, 278	0
27	X	2680/2880 (93%)	0.27	111 (4%) 41 21	26, 76, 186, 299	0
28	Y	122/124 (98%)	0.70	10 (8%) 17 11	74, 153, 190, 332	0
All	All	5879/6383 (92%)	0.36	355 (6%) 27 15	26, 89, 188, 339	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	I	54	SER	14.5
19	T	16	SER	11.8
6	G	129	HIS	10.2
9	J	21	ASP	9.1
1	A	236	GLY	8.3
8	I	36	GLY	8.2
6	G	34	PRO	8.0
28	Y	2	C	7.9
12	M	29	PRO	7.7
14	O	23	GLU	7.6
1	A	54	ILE	7.6
9	J	84	MET	7.4
27	X	1104	G	6.9
4	D	42	SER	6.7
1	A	220	HIS	6.6
1	A	85	ASP	6.6
27	X	1082	G	6.5
17	R	93	ARG	6.4
1	A	237	GLU	6.3
28	Y	111	C	6.1
2	B	135	HIS	6.0
27	X	731	A	5.5
18	S	23	ALA	5.4
6	G	163	PRO	5.4
20	U	47	HIS	5.4
3	C	43	ALA	5.3
3	C	44	SER	5.3
8	I	11	GLY	5.2
18	S	32	PHE	5.2
27	X	871	U	5.1
25	2	43	THR	5.1
6	G	110	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
6	G	162	LYS	5.0
15	P	123	ARG	5.0
26	3	14	ILE	5.0
9	J	12	LYS	5.0
26	3	55	TRP	4.9
17	R	83	LEU	4.9
12	M	28	ARG	4.8
24	1	14	SER	4.8
4	D	121	ALA	4.8
24	1	22	TYR	4.7
8	I	63	ARG	4.7
2	B	136	ARG	4.6
25	2	1	MET	4.5
17	R	78	ALA	4.4
6	G	105	GLY	4.4
6	G	164	GLN	4.3
11	L	52	ALA	4.3
5	E	68	THR	4.2
25	2	46	ASP	4.2
1	A	241	GLY	4.2
18	S	22	VAL	4.2
11	L	40	ALA	4.1
24	1	47	HIS	4.1
26	3	54	GLU	4.1
27	X	304	A	4.1
6	G	107	GLN	4.0
1	A	22	SER	4.0
24	1	3	LYS	4.0
12	M	34	ARG	4.0
8	I	42	GLY	3.9
27	X	2370	G	3.9
20	U	26	ALA	3.9
27	X	1574	A	3.9
27	X	2444	C	3.9
27	X	1080	A	3.9
5	E	65	HIS	3.8
27	X	1068	A	3.8
15	P	19	LYS	3.8
2	B	138	PRO	3.8
20	U	52	ARG	3.7
3	C	166	TRP	3.7
27	X	1830	C	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	249	PRO	3.7
27	X	225	G	3.7
27	X	1588	A	3.7
24	1	24	THR	3.6
9	J	27	TYR	3.6
6	G	161	GLN	3.6
26	3	31	HIS	3.6
17	R	102	LYS	3.6
8	I	97	ARG	3.6
27	X	416	U	3.5
17	R	77	HIS	3.5
18	S	86	VAL	3.5
18	S	92	VAL	3.5
1	A	84	TYR	3.5
8	I	45	LYS	3.5
6	G	67	ARG	3.5
2	B	203	LYS	3.4
27	X	2189	A	3.4
27	X	1067	G	3.4
10	K	3	HIS	3.4
3	C	164	VAL	3.3
7	H	40	GLY	3.3
27	X	1569	A	3.3
18	S	21	ALA	3.3
9	J	82	THR	3.3
6	G	165	VAL	3.3
8	I	31	GLY	3.3
27	X	774	A	3.3
3	C	19	LEU	3.3
27	X	1089	C	3.3
2	B	137	ARG	3.3
3	C	193	LEU	3.3
5	E	123	PHE	3.2
16	Q	62	ARG	3.2
27	X	728	G	3.2
11	L	104	ALA	3.2
8	I	53	ARG	3.2
13	N	88	ILE	3.2
14	O	11	GLN	3.2
8	I	47	ALA	3.1
19	T	59	LEU	3.1
5	E	37	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
27	X	483	A	3.1
4	D	41	GLY	3.1
27	X	2287	G	3.1
27	X	248	A	3.1
3	C	41	GLY	3.1
4	D	84	PRO	3.0
27	X	1073	G	3.0
27	X	305	A	3.0
27	X	542	A	3.0
4	D	39	GLY	3.0
13	N	100	ALA	3.0
15	P	37	LYS	3.0
24	1	35	LEU	3.0
7	H	8	LEU	3.0
1	A	24	LEU	3.0
4	D	43	SER	3.0
4	D	85	VAL	3.0
27	X	1467	U	3.0
8	I	48	PHE	2.9
6	G	97	ASP	2.9
26	3	11	LYS	2.9
27	X	1086	C	2.9
27	X	2477	C	2.9
8	I	56	LEU	2.9
9	J	72	ASP	2.9
20	U	16	ASN	2.9
27	X	1099	A	2.9
8	I	100	ARG	2.9
18	S	33	ALA	2.9
27	X	2270	U	2.9
24	1	4	ASP	2.9
1	A	44	ASN	2.9
1	A	91	ARG	2.9
1	A	23	GLY	2.9
1	A	87	ASN	2.9
2	B	142	GLY	2.8
28	Y	16	U	2.8
27	X	1803	G	2.8
27	X	1912	G	2.8
11	L	34	SER	2.8
27	X	341	A	2.8
27	X	2289	A	2.8

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Mol	Chain	Res	Type	RSRZ
6	G	103	TYR	2.8
4	D	94	GLU	2.8
11	L	53	ALA	2.8
27	X	2170	C	2.8
28	Y	58	G	2.8
28	Y	68	A	2.8
3	C	57	LYS	2.8
11	L	12	ARG	2.8
5	E	64	LEU	2.8
14	O	5	ILE	2.8
26	3	45	GLY	2.8
1	A	219	PRO	2.7
13	N	91	ASN	2.7
8	I	39	SER	2.7
20	U	28	GLY	2.7
25	2	6	GLN	2.7
27	X	1069	G	2.7
4	D	169	LEU	2.7
27	X	434	C	2.7
27	X	1190	C	2.7
6	G	66	HIS	2.7
6	G	68	PRO	2.7
9	J	14	PHE	2.7
4	D	40	LEU	2.7
17	R	64	ASN	2.6
17	R	26	SER	2.6
8	I	74	VAL	2.6
14	O	36	LYS	2.6
27	X	661	C	2.6
8	I	64	GLY	2.6
23	Z	38	GLY	2.6
3	C	189	ASP	2.6
27	X	955	G	2.6
27	X	1432	G	2.6
1	A	263	ARG	2.6
27	X	537	C	2.6
11	L	89	PHE	2.6
27	X	1429	A	2.6
24	1	27	ASN	2.5
1	A	238	GLY	2.5
18	S	167	THR	2.5
27	X	1094	C	2.5

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Mol	Chain	Res	Type	RSRZ
28	Y	29	C	2.5
13	N	48	ARG	2.5
27	X	1602	G	2.5
27	X	1111	C	2.5
20	U	48	LYS	2.5
26	3	44	LYS	2.5
27	X	1059	A	2.5
27	X	1923	U	2.5
8	I	88	PHE	2.5
1	A	239	ARG	2.5
10	K	93	GLY	2.5
6	G	74	MET	2.5
18	S	116	VAL	2.5
4	D	99	PHE	2.4
9	J	78	LYS	2.4
24	1	13	GLU	2.4
27	X	1060	C	2.4
27	X	435	A	2.4
27	X	1055	A	2.4
27	X	1084	A	2.4
9	J	140	GLU	2.4
27	X	2090	U	2.4
27	X	1074	G	2.4
16	Q	15	LYS	2.4
3	C	42	THR	2.4
4	D	122	PHE	2.4
27	X	346	C	2.4
27	X	2193	C	2.4
27	X	2585	C	2.4
22	W	1	MET	2.4
1	A	46	ARG	2.4
5	E	111	HIS	2.3
20	U	46	LEU	2.3
27	X	2381	A	2.3
27	X	2478	C	2.3
3	C	62	LYS	2.3
24	1	11	LYS	2.3
27	X	1100	G	2.3
23	Z	56	GLN	2.3
25	2	40	HIS	2.3
27	X	727	U	2.3
19	T	15	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
27	X	2203	G	2.3
8	I	27	ASP	2.3
17	R	81	VAL	2.3
1	A	52	ARG	2.3
27	X	210	A	2.3
27	X	541	C	2.3
27	X	1083	C	2.3
28	Y	98	C	2.3
24	1	41	ASP	2.3
11	L	36	LYS	2.3
16	Q	56	MET	2.3
19	T	19	LYS	2.3
27	X	1749	G	2.3
27	X	2085	G	2.3
28	Y	50	U	2.3
28	Y	31	A	2.3
9	J	57	ARG	2.3
1	A	247	VAL	2.2
27	X	359	G	2.2
27	X	965	G	2.2
27	X	1133	G	2.2
27	X	1955	G	2.2
2	B	159	HIS	2.2
26	3	24	ALA	2.2
1	A	14	ARG	2.2
3	C	55	GLY	2.2
3	C	66	ASN	2.2
19	T	17	ASN	2.2
8	I	17	LYS	2.2
27	X	2198	U	2.2
27	X	1098	G	2.2
1	A	128	GLY	2.2
27	X	1096	A	2.2
27	X	2718	A	2.2
3	C	45	THR	2.2
4	D	154	ILE	2.2
11	L	33	ARG	2.2
27	X	1093	U	2.2
27	X	2086	U	2.2
27	X	2192	U	2.2
3	C	128	ALA	2.2
27	X	1061	A	2.2

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Mol	Chain	Res	Type	RSRZ
27	X	1599	G	2.2
27	X	2290	A	2.2
9	J	63	GLY	2.2
27	X	2008	C	2.2
1	A	248	THR	2.2
19	T	14	ARG	2.1
27	X	1469	U	2.1
8	I	62	LYS	2.1
22	W	33	GLU	2.1
18	S	4	THR	2.1
27	X	242	A	2.1
27	X	1250	A	2.1
4	D	79	LEU	2.1
27	X	2555	G	2.1
27	X	1103	C	2.1
27	X	1531	C	2.1
27	X	1593	C	2.1
9	J	91	VAL	2.1
20	U	24	ALA	2.1
20	U	65	ASN	2.1
26	3	56	ALA	2.1
1	A	186	HIS	2.1
27	X	116	A	2.1
27	X	671	A	2.1
1	A	250	TRP	2.1
9	J	106	GLU	2.1
27	X	841	G	2.1
27	X	1913	G	2.1
27	X	1801	C	2.1
27	X	2329	C	2.1
27	X	2735	C	2.1
5	E	63	ALA	2.1
27	X	1357	U	2.1
27	X	200	A	2.1
27	X	2045	A	2.1
26	3	52	LYS	2.1
1	A	198	ASN	2.1
14	O	27	GLY	2.1
27	X	726	G	2.1
27	X	2782	G	2.1
22	W	7	ARG	2.1
27	X	1030	U	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	138	VAL	2.1
11	L	39	TYR	2.0
20	U	75	TYR	2.0
3	C	20	PRO	2.0
27	X	1753	A	2.0
27	X	1087	C	2.0
27	X	1489	C	2.0
27	X	2567	G	2.0
27	X	2759	U	2.0
28	Y	42	U	2.0
4	D	86	GLY	2.0
24	1	21	TYR	2.0
1	A	244	ARG	2.0
26	3	7	HIS	2.0
19	T	61	ALA	2.0
26	3	62	LEU	2.0
5	E	139	GLN	2.0
8	I	79	GLN	2.0
27	X	247	A	2.0
27	X	984	A	2.0
1	A	28	ARG	2.0
10	K	17	ARG	2.0
26	3	26	LYS	2.0
1	A	240	THR	2.0
2	B	66	HIS	2.0
4	D	38	GLU	2.0
27	X	1023	U	2.0
14	O	46	VAL	2.0
18	S	30	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
29	MG	X	2916	1/1	0.46	0.76	41,41,41,41	0
29	MG	X	2915	1/1	0.54	0.51	63,63,63,63	0
29	MG	X	2943	1/1	0.56	0.45	42,42,42,42	0
29	MG	X	2935	1/1	0.59	0.47	34,34,34,34	0
29	MG	X	2919	1/1	0.62	0.24	62,62,62,62	0
29	MG	A	301	1/1	0.65	0.34	54,54,54,54	0
29	MG	X	2914	1/1	0.66	0.46	27,27,27,27	0
29	MG	X	2918	1/1	0.72	0.82	43,43,43,43	0
29	MG	K	202	1/1	0.73	0.37	27,27,27,27	0
29	MG	X	2910	1/1	0.74	0.35	56,56,56,56	0
29	MG	X	2904	1/1	0.75	0.52	32,32,32,32	0
29	MG	X	2926	1/1	0.75	0.84	44,44,44,44	0
29	MG	X	2965	1/1	0.79	0.83	43,43,43,43	0
29	MG	X	2956	1/1	0.80	0.25	27,27,27,27	0
29	MG	X	2942	1/1	0.80	0.33	46,46,46,46	0
29	MG	X	2950	1/1	0.81	0.51	32,32,32,32	0
29	MG	X	2952	1/1	0.81	0.29	29,29,29,29	0
29	MG	X	2908	1/1	0.81	0.36	32,32,32,32	0
29	MG	X	2925	1/1	0.81	0.54	31,31,31,31	0
29	MG	X	2958	1/1	0.82	0.24	44,44,44,44	0
29	MG	X	2941	1/1	0.83	0.25	38,38,38,38	0
29	MG	X	2960	1/1	0.83	0.37	61,61,61,61	0
29	MG	X	2920	1/1	0.83	0.29	52,52,52,52	0
29	MG	X	2944	1/1	0.84	0.29	35,35,35,35	0
29	MG	M	201	1/1	0.85	0.16	35,35,35,35	0
29	MG	X	2955	1/1	0.85	0.39	30,30,30,30	0
29	MG	X	2905	1/1	0.85	0.24	31,31,31,31	0
29	MG	X	2930	1/1	0.85	0.61	29,29,29,29	0
29	MG	X	2923	1/1	0.85	0.27	40,40,40,40	0
29	MG	X	2936	1/1	0.85	0.40	45,45,45,45	0
29	MG	X	2901	1/1	0.86	0.43	69,69,69,69	0
29	MG	X	2921	1/1	0.86	0.27	28,28,28,28	0
29	MG	X	2957	1/1	0.86	0.58	52,52,52,52	0
29	MG	X	2946	1/1	0.86	0.73	46,46,46,46	0
29	MG	X	2927	1/1	0.86	0.35	29,29,29,29	0
29	MG	B	301	1/1	0.86	0.23	34,34,34,34	0

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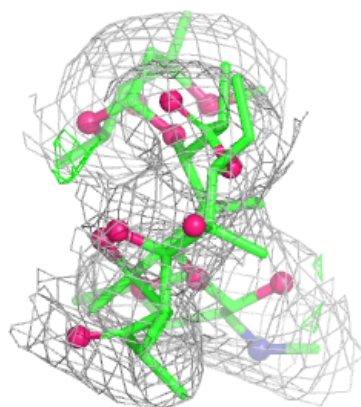
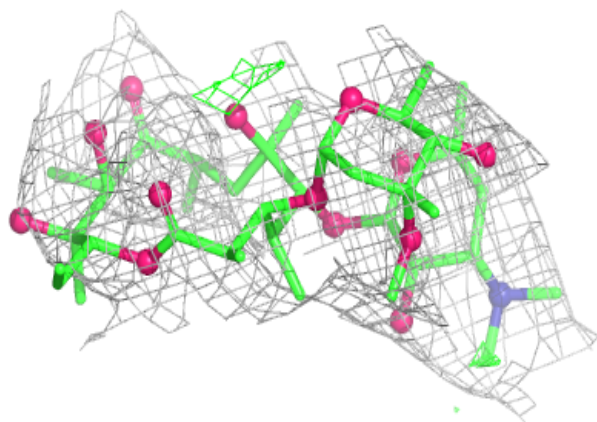
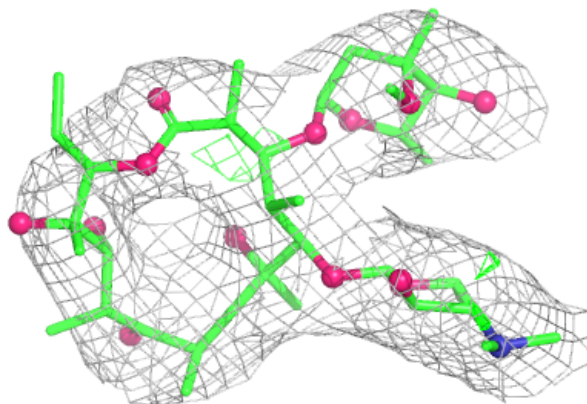
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	2962	1/1	0.87	0.08	69,69,69,69	0
29	MG	X	2949	1/1	0.88	0.41	42,42,42,42	0
29	MG	X	2903	1/1	0.88	0.72	30,30,30,30	0
29	MG	X	2911	1/1	0.88	0.56	56,56,56,56	0
29	MG	X	2938	1/1	0.88	0.40	31,31,31,31	0
29	MG	X	2913	1/1	0.88	0.65	43,43,43,43	0
29	MG	X	2954	1/1	0.89	0.43	45,45,45,45	0
29	MG	X	2940	1/1	0.89	0.25	36,36,36,36	0
29	MG	K	201	1/1	0.89	0.27	27,27,27,27	0
29	MG	X	2963	1/1	0.89	0.20	56,56,56,56	0
29	MG	X	2917	1/1	0.89	0.53	40,40,40,40	0
29	MG	X	2931	1/1	0.90	1.06	46,46,46,46	0
29	MG	M	202	1/1	0.91	0.15	35,35,35,35	0
29	MG	X	2959	1/1	0.91	0.41	41,41,41,41	0
29	MG	X	2906	1/1	0.91	0.67	28,28,28,28	0
29	MG	X	2947	1/1	0.92	0.19	34,34,34,34	0
29	MG	X	2922	1/1	0.92	0.18	29,29,29,29	0
29	MG	X	2928	1/1	0.92	0.25	55,55,55,55	0
29	MG	X	2951	1/1	0.92	0.72	32,32,32,32	0
29	MG	X	2932	1/1	0.92	0.26	37,37,37,37	0
29	MG	X	2939	1/1	0.93	0.29	50,50,50,50	0
29	MG	X	2909	1/1	0.93	0.41	28,28,28,28	0
29	MG	X	2945	1/1	0.94	0.28	38,38,38,38	0
29	MG	X	2953	1/1	0.94	0.48	56,56,56,56	0
29	MG	X	2937	1/1	0.94	0.61	44,44,44,44	0
29	MG	X	2961	1/1	0.95	0.85	56,56,56,56	0
29	MG	X	2933	1/1	0.95	0.93	36,36,36,36	0
29	MG	X	2934	1/1	0.95	0.50	29,29,29,29	0
29	MG	X	2964	1/1	0.95	0.27	28,28,28,28	0
29	MG	X	2907	1/1	0.95	0.39	28,28,28,28	0
30	ERY	X	2902	51/51	0.95	0.10	31,34,36,36	0
29	MG	X	2912	1/1	0.96	0.18	27,27,27,27	0
29	MG	X	2924	1/1	0.96	0.46	38,38,38,38	0
29	MG	X	2948	1/1	0.96	0.18	34,34,34,34	0
29	MG	X	2929	1/1	0.97	0.10	30,30,30,30	0

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

Electron density around ERY X 2902:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.