



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:04 PM UTC

PDB ID : 1YJW / pdb_00001yjl
Title : Crystal Structure Of Quinupristin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-15
Resolution : 2.90 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
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

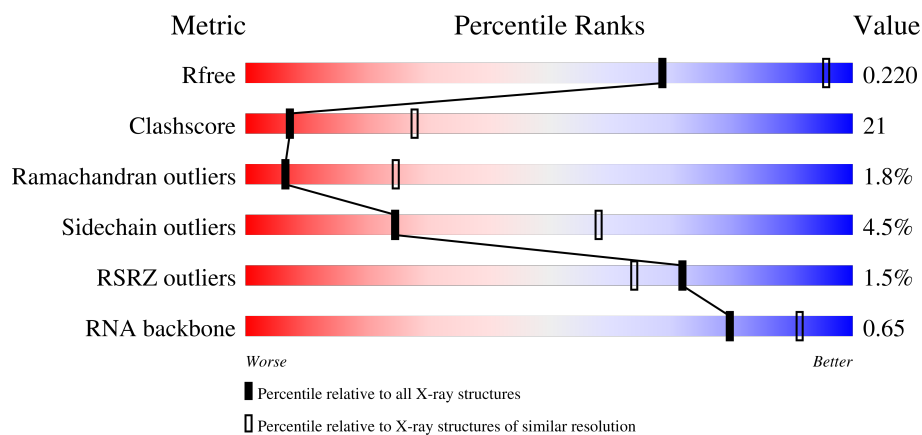
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	0	2922	4% 53% 36% 5% • 6%
2	1	57	60% 39% •
3	2	50	4% 42% 50% 8%
4	3	92	55% 42% •

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Mol	Chain	Length	Quality of chain
5	4	8	
6	9	122	
7	A	240	
8	B	338	
9	C	246	
10	D	177	
11	E	178	
12	F	120	
13	G	348	
14	H	177	
15	I	162	
16	J	145	
17	K	132	
18	L	165	
19	M	195	
20	N	187	
21	O	116	
22	P	149	
23	Q	96	
24	R	155	
25	S	85	
26	T	120	
27	U	66	
28	V	71	
29	W	154	

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Mol	Chain	Length	Quality of chain
30	X	92	
31	Y	241	
32	Z	83	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CL	O	3189	-	-	X	-
36	CL	N	201	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10873	19053	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	2099	A	G	conflict	GB 55229667

- Molecule 2 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 3 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 4 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 5 is a protein called QUINUPRISTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

- Molecule 6 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	conflict	UNP P12735

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 12 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 13 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	conflict	UNP P15825

- Molecule 14 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 15 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 16 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 17 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 18 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 19 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	UNP P60618

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 21 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 22 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 23 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	Q	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	T	119	Total	C	N	O	S	0	0	0
			950	568	180	202				

- Molecule 27 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 30 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 31 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	Y	142	Total	C	N	O	0	0	0
			1130	686	228	216			

- Molecule 32 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	-	expression tag	UNP P60619

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	109	Total	Mg	0	0
			109	109		
33	3	1	Total	Mg	0	0
			1	1		
33	4	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	74	Total Na 74 74	0	0
35	9	2	Total Na 2 2	0	0
35	A	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	3	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	1	1	Total 1	Cd 1	0	0
37	3	1	Total 1	Cd 1	0	0
37	O	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5842	Total 5842	O 5842	0	0
38	1	60	Total 60	O 60	0	0
38	2	49	Total 49	O 49	0	0
38	3	69	Total 69	O 69	0	0
38	4	2	Total 2	O 2	0	0
38	9	143	Total 143	O 143	0	0
38	A	123	Total 123	O 123	0	0
38	B	146	Total 146	O 146	0	0
38	C	185	Total 185	O 185	0	0
38	D	49	Total 49	O 49	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	E	42	Total 42	O 42	0	0
38	F	26	Total 26	O 26	0	0
38	G	20	Total 20	O 20	0	0
38	H	69	Total 69	O 69	0	0
38	I	9	Total 9	O 9	0	0
38	J	55	Total 55	O 55	0	0
38	K	59	Total 59	O 59	0	0
38	L	82	Total 82	O 82	0	0
38	M	129	Total 129	O 129	0	0
38	N	60	Total 60	O 60	0	0
38	O	42	Total 42	O 42	0	0
38	P	72	Total 72	O 72	0	0
38	Q	48	Total 48	O 48	0	0
38	R	85	Total 85	O 85	0	0
38	S	30	Total 30	O 30	0	0
38	T	39	Total 39	O 39	0	0
38	U	29	Total 29	O 29	0	0
38	V	13	Total 13	O 13	0	0
38	W	69	Total 69	O 69	0	0
38	X	26	Total 26	O 26	0	0
38	Y	101	Total 101	O 101	0	0

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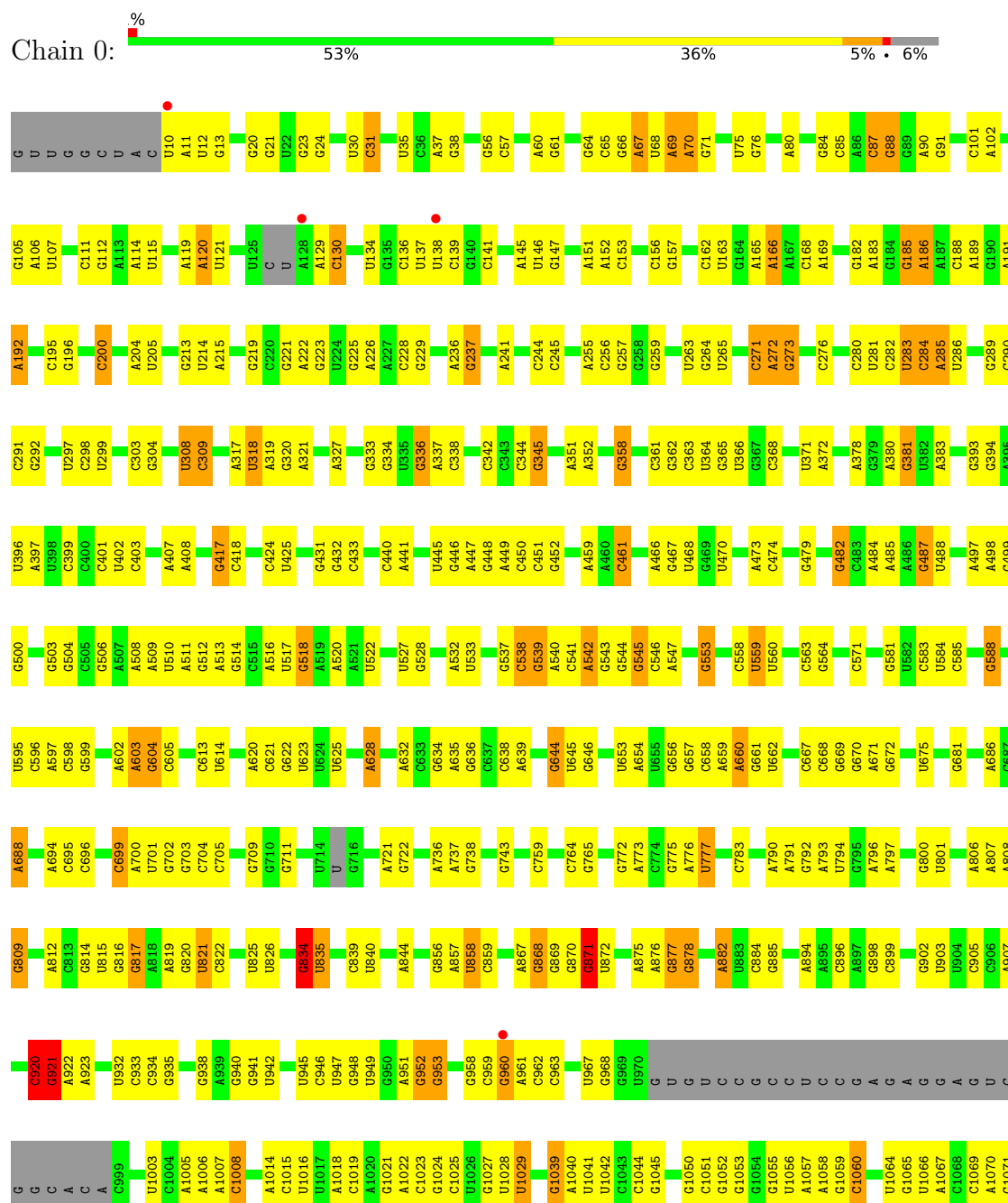
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	Z	37	Total	O	0	0
			37	37		

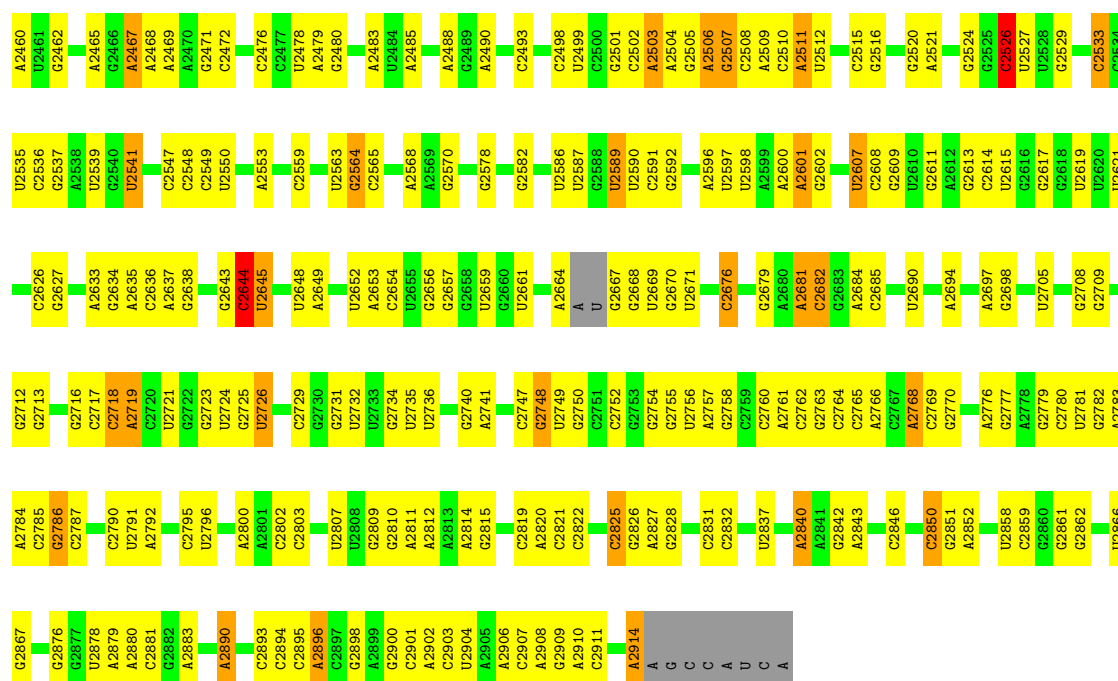
3 Residue-property plots

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: 23S RIBOSOMAL RNA

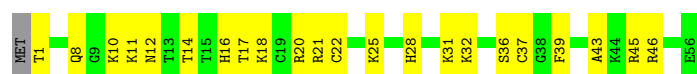


G2365	G2272	C	G	U2034	G1824	C1734	U1635	C1534	G1438	C1243	A1171	G1072
A2369	C2273	C	G	C2035	U1825	C1735	G1636	G1535	C1439	U1244	G1172	A1073
U2370	A2274	A	U	C2036	C1826	A1736	C1637	C1536	U1440	C1245	A1173	G1074
A2371	G2275	G	C	C2037	A1829	U1741	U1638	C1537	A1442	U1246	G1174	A1081
G2372	U2276	A	C	A2038	C1830	A1742	A1641	G1543	U1446	C1250	G1175	A1086
U2373	U2277	C	C	A2039	C1834	G1743	A1642	U1544	U1446	C1251	G1176	G1087
A2377	C2281	A	G	C2040	U1835	G1744	C1643	C1545	C1460	G1260	A1177	A1088
U2378	U2282	A	G	G2044	C1838	U1748	A1653	A1559	C1461	U1261	G1178	G1089
G2379	A2283	A	U	G2050	U1839	U1749	A1654	U	C1462	G1266	G1179	A1097
A2380	U2297	U	U	G1951	A1840	G1750	G1655	C1561	U1461	U1267	A1181	A1098
C2381	C2298	G	C	A2054	C1841	C1751	A1656	C1562	U1462	C1268	C1182	G1099
U2382	A2299	A	C	A2055	C1844	G1752	A1657	G1563	C1366	C1269	C1183	A1099
G2383	G2300	A	G	U2064	A1845	A1753	A1658	C1564	A1372	U1278	C1184	C1102
A2384	A2301	U	G	C2065	U1849	U1755	A1659	U1572	A1375	C1273	U1185	U1109
G2385	A2302	U	A	A2081	C1853	U1761	A1667	A1571	G1376	G1277	C1186	G1110
U2387	A2303	C	U	G2072	C1854	C1762	U1668	A1573	C1377	A1279	A1187	U1109
C2388	C2309	U	A	A2074	C1855	C1763	G1669	C1574	C1477	U1279	G1188	G1111
G2392	G2312	C	G	C2081	C1856	U1766	A1670	A1580	U1478	A1287	A1189	G1112
A2401	C2313	C	G	U1964	C1862	A1767	C1674	U1581	C1479	G1386	A1192	U1116
A2402	G2314	G	G	C1965	G1863	C1768	U1677	C1584	C1483	U1288	A1193	A1118
C2411	C2315	U	G	C1966	G1863	C1769	U1678	C1585	G1484	C1289	G1197	U1119
G2412	G2316	C	G	U1967	G1868	U1770	A1678	U1586	U1488	G1290	U1200	U1120
A2413	C2317	G	G	C1975	C1872	C1772	C1679	U1587	U1489	A1291	C1201	G1122
U2414	U2320	U	U	A1968	C1873	G1773	C1682	U1596	G1490	U1306	A1202	A1123
A2415	A2321	G	C	G1970	U1874	U1773	A1682	A1597	C1394	G1295	G1203	C1129
U2419	G2324	A	U	G1971	U1874	A1778	C1683	U1598	U1493	U1299	U1205	U1130
G2420	U2325	C	U	U1972	G1877	A1779	A1684	U1599	A1494	G1299	U1206	G1131
U2421	C2326	G	C	A1974	C1878	U1784	A1685	C1600	C1495	U1304	A1207	A1132
C2422	G2327	C	A	C1975	U1879	U1784	C1692	U1603	A1496	C1305	C1208	G1137
U2423	C2329	G	G	U1977	C1882	G1785	A1701	A1604	G1497	A1406	C1209	G1138
A2424	U2330	U	A	A1978	U1883	C1786	U1702	G1605	U1500	U1407	G1210	U1139
G2425	C2335	G	G	G1979	G1884	U1788	U1702	U1599	A1501	U1408	G1211	C1140
U2426	G2337	U	G	U1980	C1903	C1789	A1710	U1600	A1502	G1409	C1212	U1139
C2427	C2338	C	C	U1986	U1904	U1791	A1711	A1603	U1503	U1413	C1213	A1150
G2431	A	C	C	A1987	U1905	U1791	A1712	G1604	A1504	A1414	G1214	G1151
A2433	C	C	C	G2000	A1909	A1797	C1714	G1605	U1506	G1415	G1216	A1154
A2434	G2251	A	G	C2001	A1910	C1798	C1715	G1614	C1513	U1418	G1217	G1155
U2435	A2252	A	C	C2002	A1910	G1799	A1715	A1615	C1514	G1419	G1226	C1156
U2441	G2253	G	G	U2003	A1919	A1804	A1717	A1616	A1515	A1328	C1227	C1157
G2442	C2254	U	C	U2004	G1925	G1805	G1718	C1617	C1421	G1331	C1228	G1158
C2443	C2255	A	U	G2005	G1926	G1806	G1719	G1618	U1422	C1332	C1229	G1159
U2444	G2257	G	G	U2008	G1927	C1810	U1722	C1620	A1518	U1333	G1232	G1160
G2445	A2258	C	C	U2008	A1927	A1811	G1723	A1624	U1524	C1334	A1233	A1161
U2446	C2265	A	G	A2011	C1928	C1811	U1724	U1625	G1525	C1335	A1234	G1162
G2447	G2266	G	G	U2012	G1929	G1819	C1725	A1626	A1526	G1340	G1235	U1164
C2453	C2267	C	C	C2013	A1931	G1820	G1730	G1627	A1527	A1341	A1236	U1165
G2454	C2268	C	C	G2013	C1935	A1821	C1731	G1627	A1528	C1342	U1237	G1166
A2455	G2269	A	A	U2032	C1936	G1822	A1732	C1633	G1529	C1343	C1238	G1167
U2456	C2271	C	C	G2033	C1936	G1823	A1733	G1634	A1533	A1348	U1169	U1170



• Molecule 2: 50S ribosomal protein L37e

Chain 1: 60% 39%



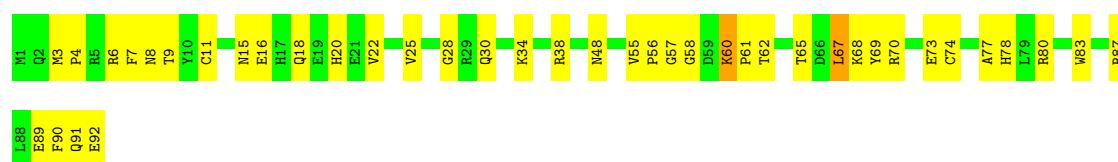
• Molecule 3: 50S ribosomal protein L39e

Chain 2: 4% 42% 50% 8%



• Molecule 4: 50S ribosomal protein L44e

Chain 3: 55% 42%

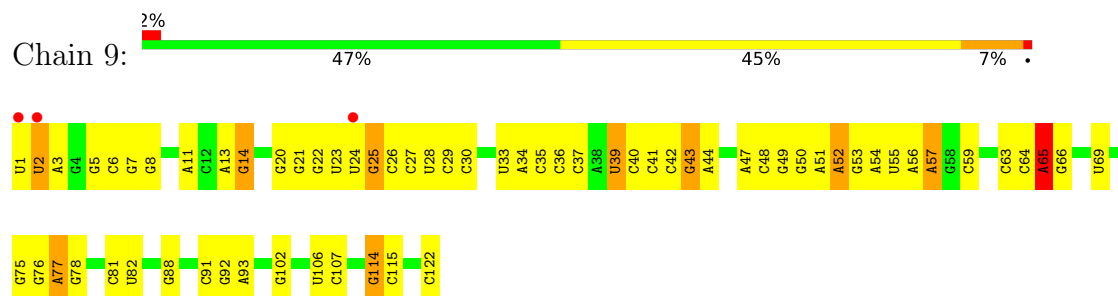


• Molecule 5: QUINUPRISTIN

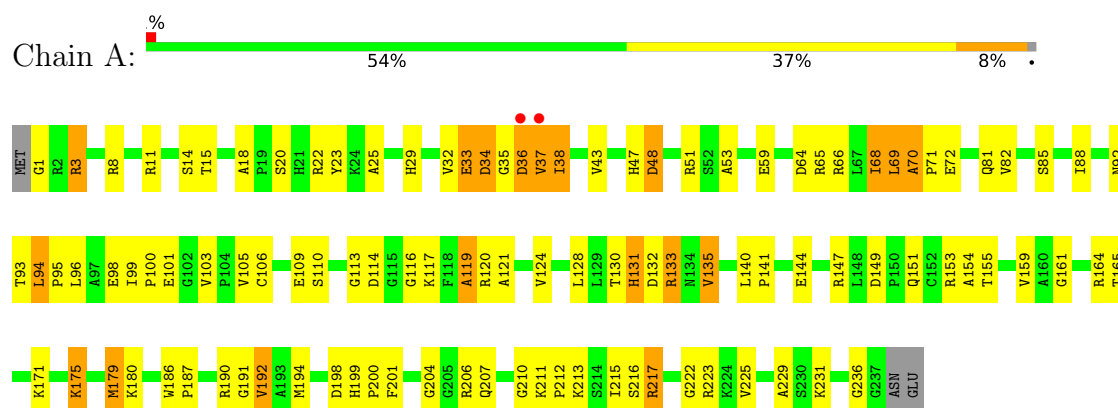
Chain 4: 38% 62%



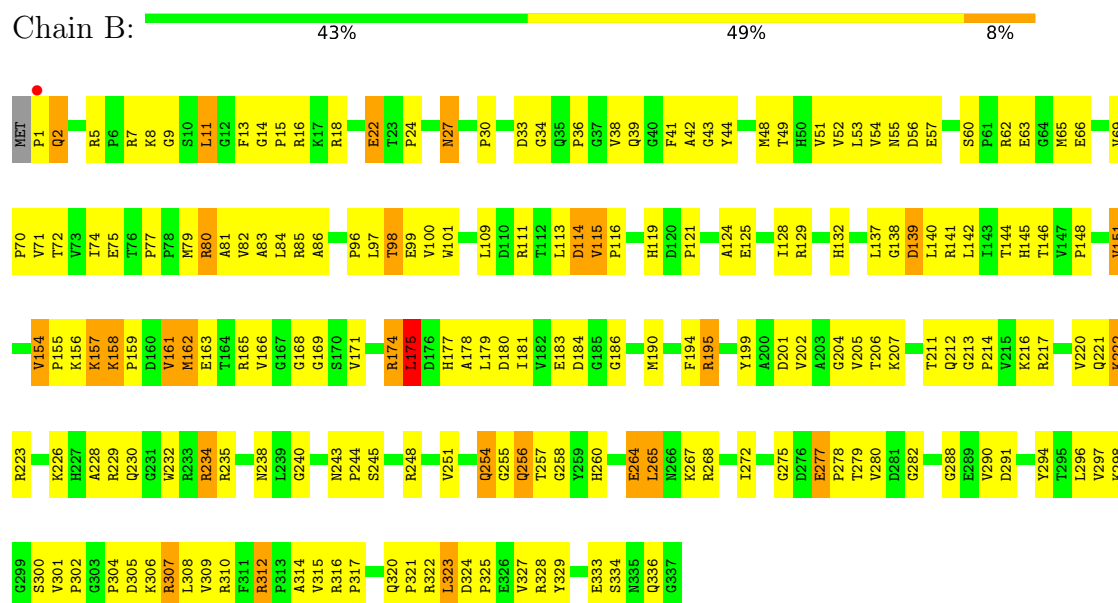
- Molecule 6: 5S RIBOSOMAL RNA



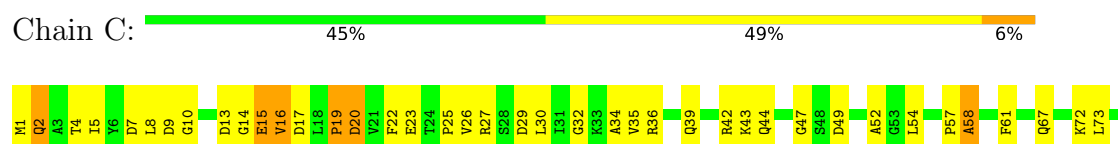
- Molecule 7: 50S ribosomal protein L2

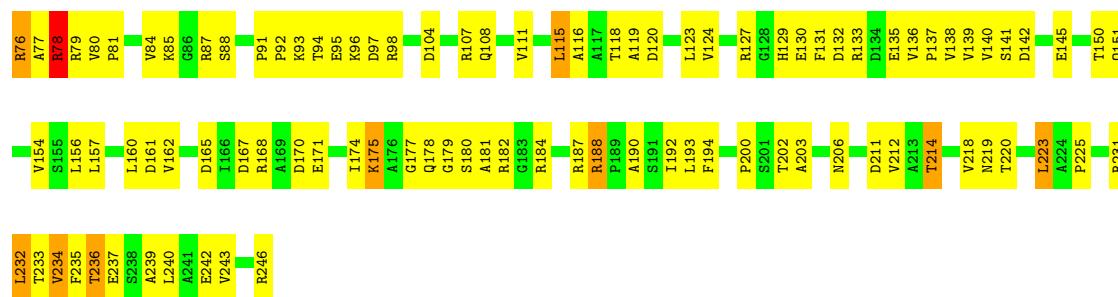


- Molecule 8: 50S ribosomal protein L3

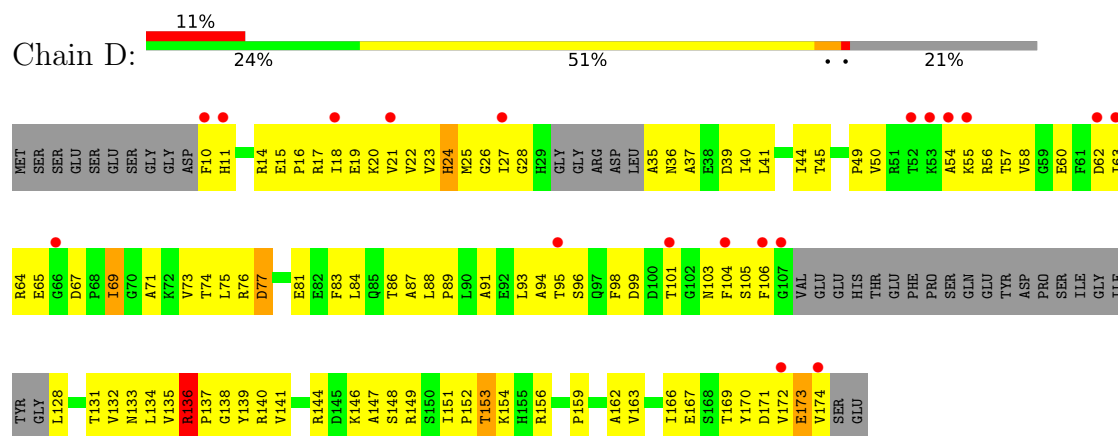


- Molecule 9: 50S ribosomal protein L4

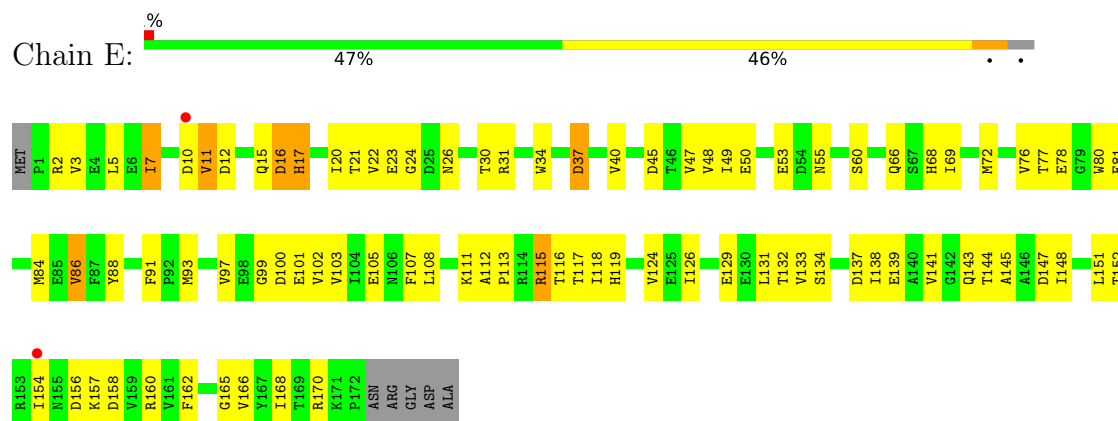




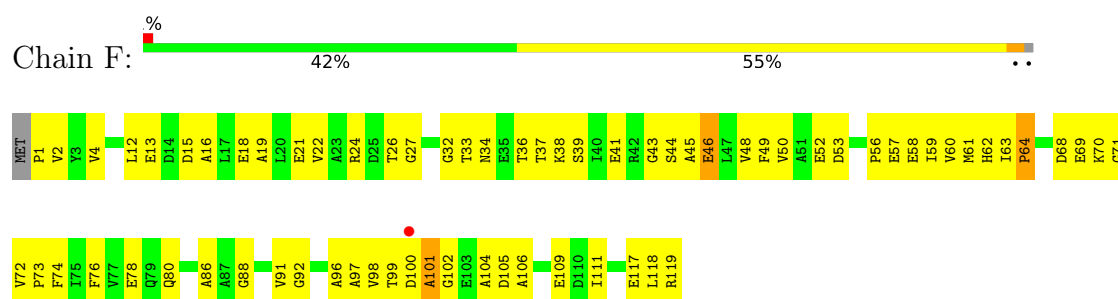
• Molecule 10: 50S ribosomal protein L5



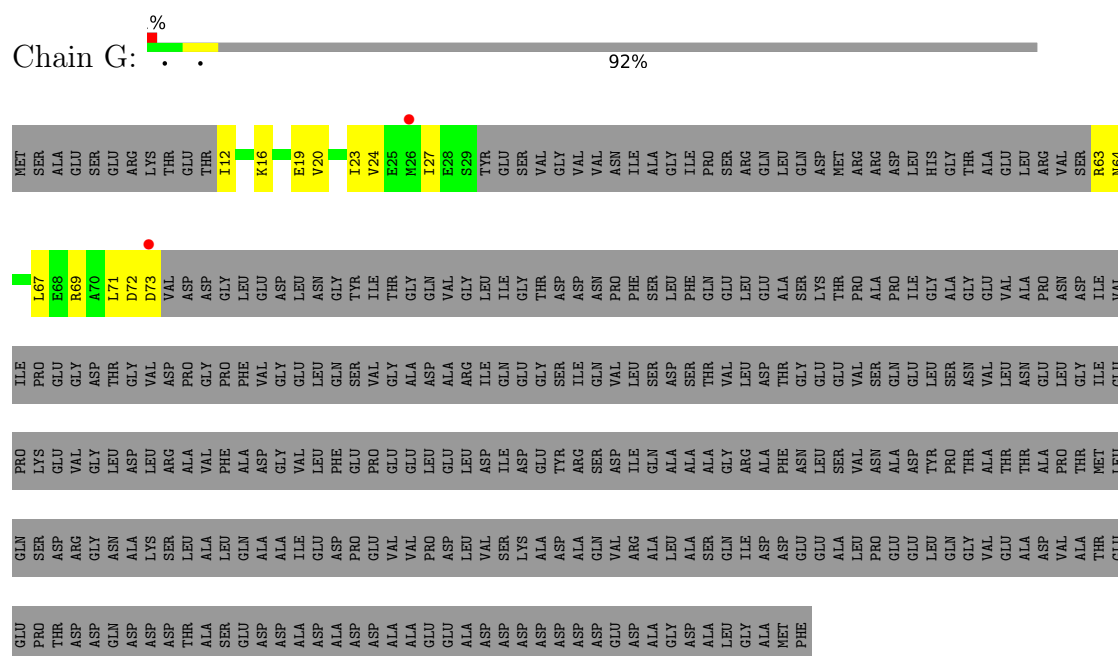
• Molecule 11: 50S ribosomal protein L6



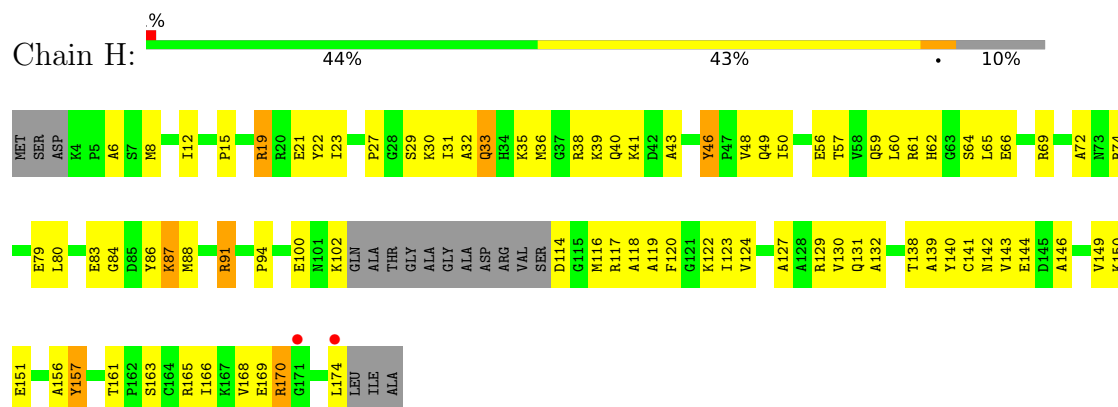
• Molecule 12: 50S ribosomal protein L7Ae



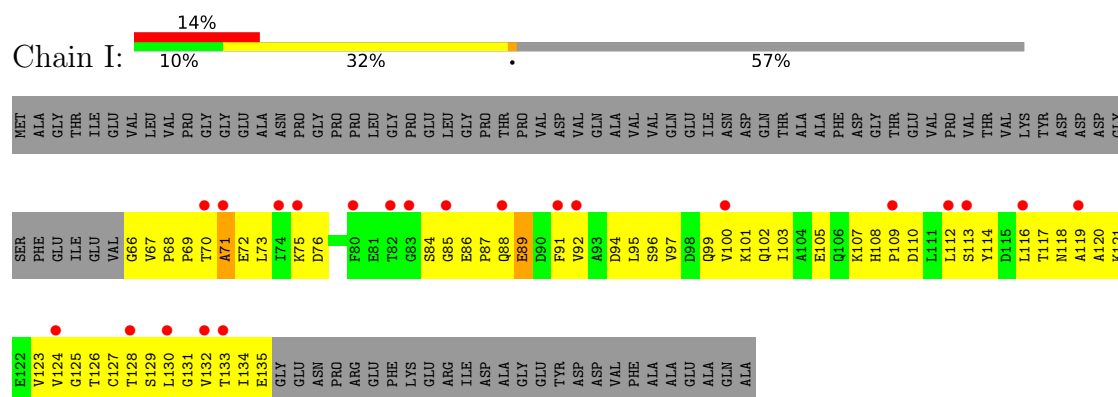
• Molecule 13: 50S ribosomal protein L10



- Molecule 14: 50S ribosomal protein L10e

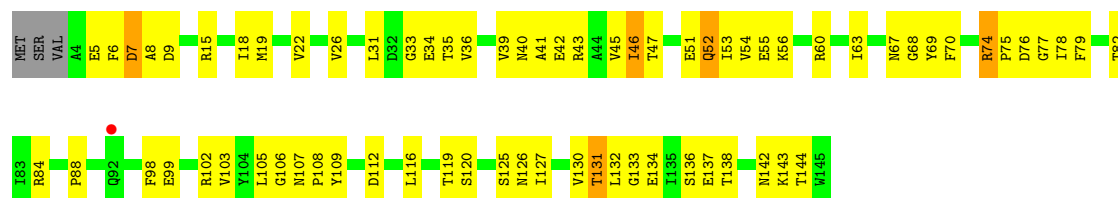


- Molecule 15: 50S ribosomal protein L11



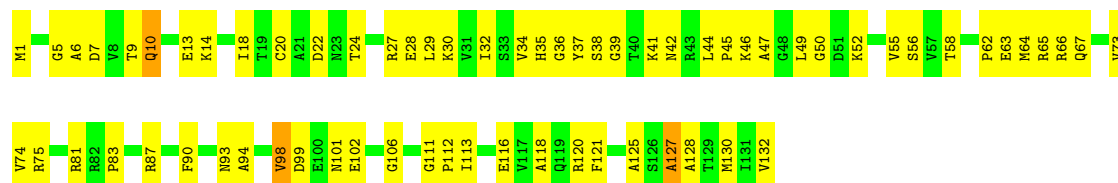
- Molecule 16: 50S ribosomal protein L13





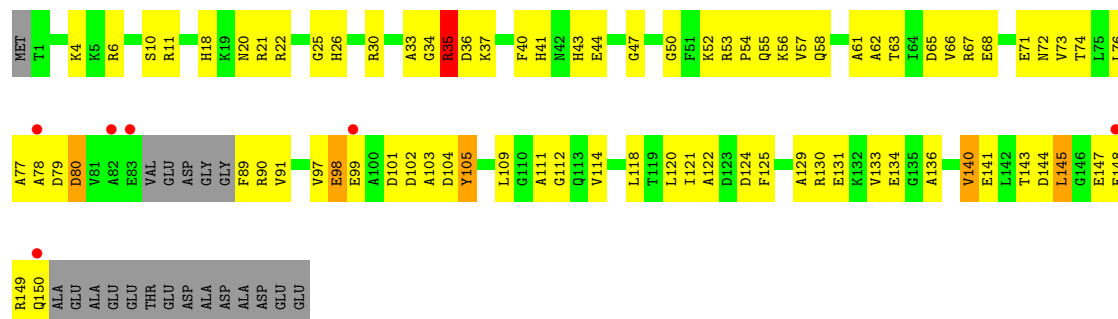
• Molecule 17: 50S ribosomal protein L14

Chain K: 49% 48% .



• Molecule 18: 50S ribosomal protein L15

Chain L: 4% 39% 45% . . 12%



• Molecule 19: 50S ribosomal protein L15e

Chain M: 60% 37% . .

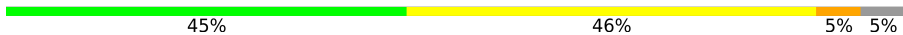


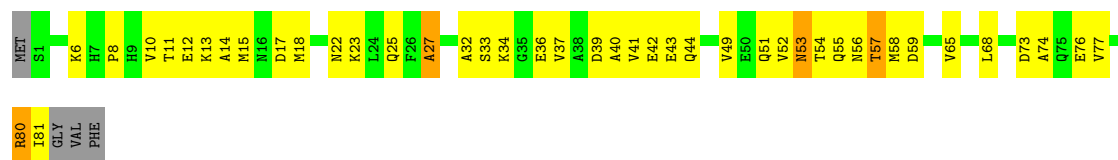
• Molecule 20: 50S ribosomal protein L18

Chain N: 3% 38% 53% 7% . .



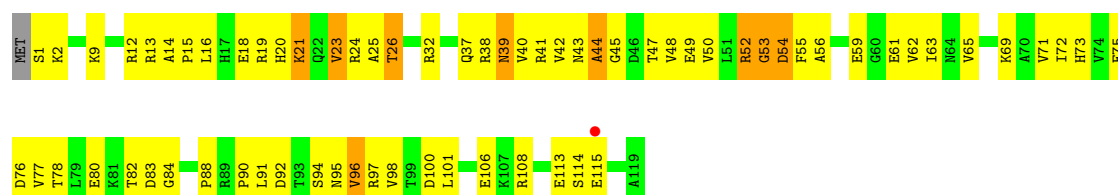
- Molecule 25: 50S ribosomal protein L23

Chain S:  45% 46% 5% 5%

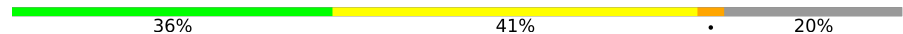


- Molecule 26: 50S ribosomal protein L24

Chain T:  42% 49% 8% .



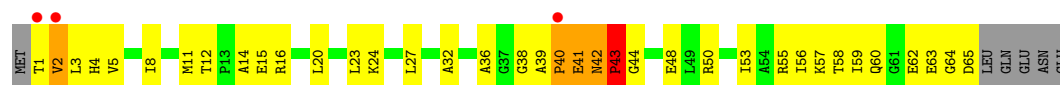
- Molecule 27: 50S ribosomal protein L24e

Chain U:  36% 41% . 20%

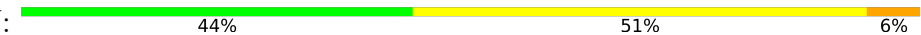


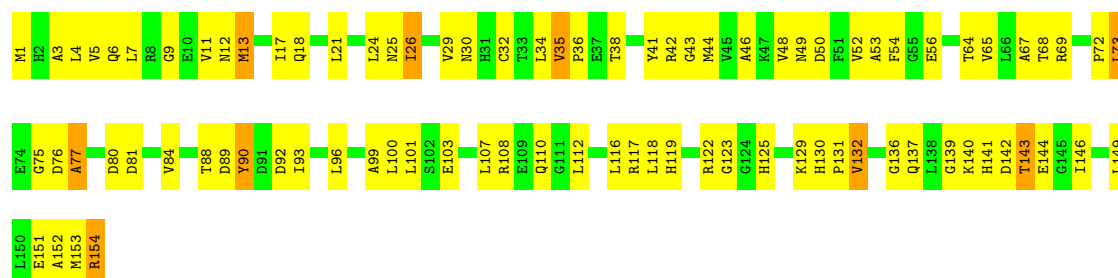
- Molecule 28: 50S ribosomal protein L29

Chain V:  4% 39% 45% 6% . 8%

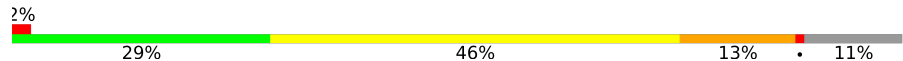


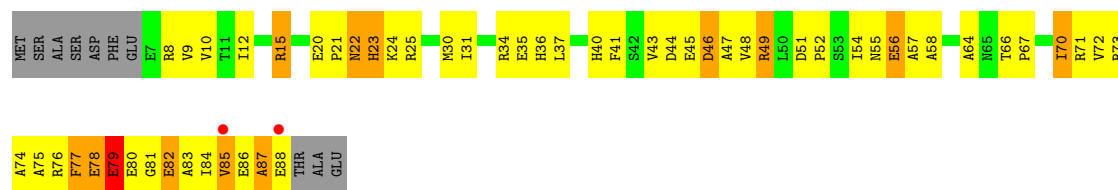
- Molecule 29: 50S ribosomal protein L30

Chain W:  44% 51% 6%

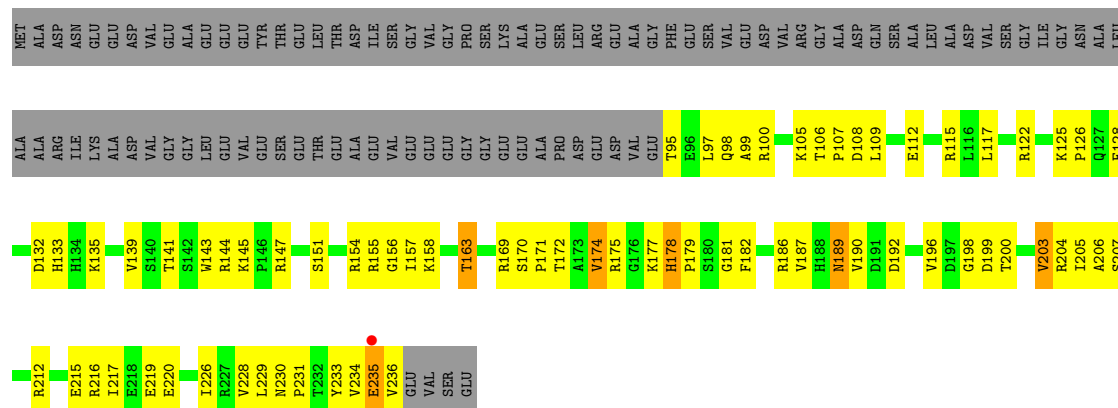
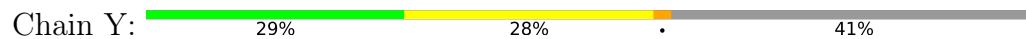


- Molecule 30: 50S ribosomal protein L31e

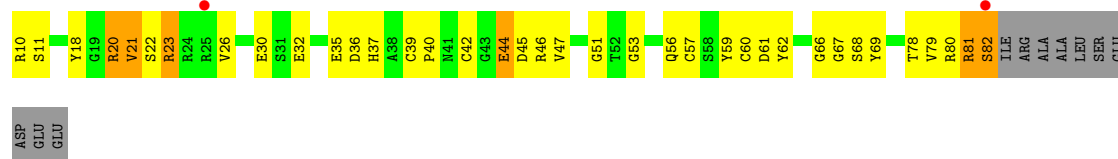
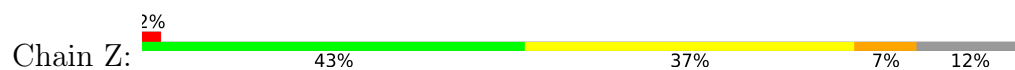
Chain X:  2% 29% 46% 13% . 11%



• Molecule 31: 50S ribosomal protein L32e



• Molecule 32: 50S ribosomal protein L37Ae



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.69Å 299.78Å 573.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.90 29.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.8 (29.98-2.90) 83.7 (29.98-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.171 , 0.223 0.171 , 0.220	Depositor DCC
R_{free} test set	3279 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99111	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: MHW, K, DBB, 1MA, MG, MHU, CL, OMU, CD, 004, UR3, PSU, NA, MHV, OMG, MHT

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	0	0.38	0/65957	0.60	22/102867 (0.0%)
2	1	0.44	0/438	0.93	1/578 (0.2%)
3	2	0.41	0/401	0.82	1/529 (0.2%)
4	3	0.42	0/771	0.86	2/1024 (0.2%)
5	4	1.72	0/13	1.80	0/15
6	9	0.37	0/2904	0.60	2/4526 (0.0%)
7	A	0.43	0/1786	1.02	11/2408 (0.5%)
8	B	0.42	0/2690	1.03	20/3652 (0.5%)
9	C	0.47	0/1884	1.01	9/2551 (0.4%)
10	D	0.37	0/1111	0.89	3/1498 (0.2%)
11	E	0.41	0/1382	0.89	2/1880 (0.1%)
12	F	0.40	0/901	0.89	2/1224 (0.2%)
13	G	0.37	0/241	0.80	0/324
14	H	0.41	0/1302	0.96	5/1743 (0.3%)
15	I	0.38	0/526	0.96	2/716 (0.3%)
16	J	0.43	0/1136	0.94	3/1530 (0.2%)
17	K	0.43	0/1001	1.00	3/1347 (0.2%)
18	L	0.39	0/1130	0.94	3/1509 (0.2%)
19	M	0.42	0/1582	0.89	2/2117 (0.1%)
20	N	0.39	0/1474	1.07	12/1999 (0.6%)
21	O	0.43	0/874	0.94	3/1181 (0.3%)
22	P	0.42	0/1147	0.88	1/1528 (0.1%)
23	Q	0.45	0/749	1.01	5/1005 (0.5%)
24	R	0.46	0/1172	0.96	5/1578 (0.3%)
25	S	0.41	0/648	0.87	2/875 (0.2%)
26	T	0.41	0/958	0.94	3/1289 (0.2%)
27	U	0.40	0/417	0.97	3/562 (0.5%)
28	V	0.38	0/502	0.99	2/675 (0.3%)
29	W	0.50	0/1219	0.99	5/1655 (0.3%)
30	X	0.43	0/664	0.99	2/895 (0.2%)
31	Y	0.44	0/1146	0.94	3/1536 (0.2%)
32	Z	0.41	0/589	0.97	1/787 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	0/98715	0.72	140/147603 (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
1	0	0	20
6	9	0	1
29	W	0	1
All	All	0	22

There are no bond length outliers.

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	135	VAL	N-CA-C	-10.39	103.02	113.10
7	A	222	GLY	N-CA-C	-8.49	104.38	114.48
26	T	54	ASP	N-CA-C	-8.11	102.83	112.89
8	B	213	GLY	CA-C-N	8.09	127.38	118.97
8	B	213	GLY	C-N-CA	8.09	127.38	118.97
8	B	151	VAL	CA-C-N	7.35	127.21	119.05
8	B	151	VAL	C-N-CA	7.35	127.21	119.05
7	A	70	ALA	N-CA-C	7.35	118.91	109.65
19	M	89	THR	N-CA-C	7.24	118.81	111.07
8	B	157	LYS	N-CA-C	-7.19	105.12	114.04
23	Q	17	LYS	N-CA-C	-7.17	100.19	110.08
8	B	80	ARG	N-CA-C	7.02	118.96	107.23
18	L	145	LEU	N-CA-C	-6.98	103.60	111.07
1	0	920	C	C2'-C3'-O3'	-6.92	103.33	113.70
15	I	89	GLU	N-CA-C	-6.85	105.45	113.88
8	B	323	LEU	N-CA-C	6.84	119.39	110.43
20	N	48	VAL	N-CA-C	6.80	117.69	108.17
20	N	169	PRO	N-CA-C	-6.76	105.71	114.03
29	W	143	THR	N-CA-C	-6.73	105.03	113.18
20	N	42	HIS	N-CA-C	6.69	118.68	109.18
7	A	133	ARG	N-CA-C	-6.60	105.19	113.18
14	H	163	SER	N-CA-C	-6.56	99.89	110.32
30	X	22	ASN	N-CA-C	6.55	118.97	111.11
28	V	42	ASN	CA-C-N	6.51	127.98	119.84
28	V	42	ASN	C-N-CA	6.51	127.98	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	60	LYS	N-CA-C	-6.44	100.72	110.39
1	0	1942	A	C5'-C4'-C3'	6.41	125.61	116.00
8	B	115	VAL	CA-C-N	6.38	126.72	119.83
8	B	115	VAL	C-N-CA	6.38	126.72	119.83
9	C	78	ARG	N-CA-C	6.37	117.53	108.74
8	B	175	LEU	N-CA-C	-6.32	104.09	110.97
24	R	141	VAL	N-CA-C	6.29	117.53	108.48
7	A	175	LYS	N-CA-C	-6.27	104.37	111.14
1	0	2291	A	N9-C1'-C2'	6.26	121.39	112.00
20	N	14	ARG	N-CA-C	-6.25	104.39	111.14
10	D	136	ARG	CA-C-N	6.24	127.64	119.84
10	D	136	ARG	C-N-CA	6.24	127.64	119.84
12	F	62	HIS	N-CA-C	6.23	119.05	111.82
1	0	2726	U	N1-C1'-C2'	6.22	121.33	112.00
9	C	188	ARG	N-CA-C	6.21	113.81	108.22
12	F	118	LEU	N-CA-C	-6.20	105.78	113.15
29	W	25	ASN	N-CA-C	6.19	120.07	111.90
9	C	175	LYS	N-CA-C	6.18	118.28	110.24
8	B	265	LEU	N-CA-C	6.17	118.88	110.55
4	3	67	LEU	N-CA-C	6.16	119.69	110.14
6	9	39	U	N1-C1'-C2'	6.12	121.18	112.00
8	B	154	VAL	CA-C-N	6.12	126.29	119.32
8	B	154	VAL	C-N-CA	6.12	126.29	119.32
18	L	98	GLU	N-CA-C	-6.07	102.71	110.53
1	0	1979	G	C4'-C3'-O3'	-6.04	103.93	113.00
14	H	161	THR	N-CA-C	6.03	121.09	113.25
6	9	39	U	C4'-C3'-O3'	-5.92	104.12	113.00
27	U	50	GLU	N-CA-C	5.89	119.29	111.75
7	A	110	SER	N-CA-C	-5.89	102.55	111.56
8	B	222	LYS	N-CA-C	-5.89	100.69	110.17
20	N	152	GLU	N-CA-C	-5.89	104.99	111.82
19	M	74	LYS	N-CA-C	5.86	119.26	109.95
7	A	135	VAL	N-CA-C	5.83	116.88	108.48
1	0	1819	G	C5'-C4'-C3'	5.79	124.69	116.00
1	0	2644	C	C2'-C3'-O3'	5.74	118.10	109.50
7	A	198	ASP	N-CA-C	5.73	120.00	112.89
9	C	167	ASP	N-CA-C	-5.73	105.55	112.54
20	N	153	GLN	N-CA-C	-5.72	103.57	111.81
21	O	24	ALA	N-CA-C	-5.71	106.85	113.88
8	B	161	VAL	N-CA-C	5.71	115.88	107.15
9	C	177	GLY	N-CA-C	5.69	117.36	111.95
25	S	27	ALA	N-CA-C	-5.67	97.95	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	114	ASP	N-CA-C	-5.66	103.52	110.65
17	K	127	ALA	N-CA-C	-5.65	105.33	114.09
1	0	1120	U	C5'-C4'-C3'	-5.64	107.54	116.00
25	S	57	THR	N-CA-C	5.64	118.45	110.50
1	0	2526	C	N1-C1'-C2'	5.63	120.45	112.00
10	D	151	ILE	N-CA-C	5.63	113.47	108.63
20	N	117	ALA	N-CA-C	-5.62	105.07	111.14
20	N	51	GLY	CA-C-N	5.61	126.85	119.84
20	N	51	GLY	C-N-CA	5.61	126.85	119.84
31	Y	143	TRP	N-CA-C	5.59	118.28	109.96
21	O	4	ASN	CA-C-N	5.58	125.11	119.19
21	O	4	ASN	C-N-CA	5.58	125.11	119.19
24	R	34	GLU	N-CA-C	5.54	118.25	111.82
27	U	16	GLY	N-CA-C	-5.52	106.58	115.08
14	H	46	TYR	CA-C-N	5.50	126.71	119.84
14	H	46	TYR	C-N-CA	5.50	126.71	119.84
1	0	1504	A	N9-C1'-C2'	5.47	120.21	112.00
8	B	158	LYS	CA-C-N	5.44	125.44	119.89
8	B	158	LYS	C-N-CA	5.44	125.44	119.89
23	Q	68	GLY	N-CA-C	-5.43	102.13	111.47
1	0	1450	C	C4'-C3'-O3'	5.43	121.14	113.00
26	T	78	THR	N-CA-C	5.42	118.10	109.81
1	0	834	G	C2'-C3'-O3'	-5.42	105.57	113.70
24	R	122	GLN	N-CA-C	-5.40	97.70	107.75
1	0	921	G	N9-C1'-C2'	5.39	120.09	112.00
16	J	67	ASN	N-CA-C	-5.39	105.40	111.28
7	A	48	ASP	CA-C-N	5.38	125.02	119.05
7	A	48	ASP	C-N-CA	5.38	125.02	119.05
11	E	37	ASP	N-CA-C	5.37	119.42	112.86
11	E	11	VAL	N-CA-C	5.37	117.53	109.20
23	Q	47	VAL	CA-C-N	5.36	126.55	119.84
23	Q	47	VAL	C-N-CA	5.36	126.55	119.84
27	U	53	ASP	N-CA-C	-5.36	105.44	111.28
1	0	2291	A	C4'-C3'-O3'	-5.34	104.99	113.00
29	W	144	GLU	N-CA-C	-5.34	106.90	113.41
1	0	1979	G	N9-C1'-C2'	5.33	119.99	112.00
8	B	111	ARG	N-CA-C	-5.32	106.74	113.18
15	I	116	LEU	N-CA-C	-5.32	105.59	111.71
8	B	22	GLU	N-CA-C	-5.32	106.63	113.01
2	1	43	ALA	N-CA-C	-5.30	105.50	111.28
23	Q	47	VAL	N-CA-C	5.29	112.78	107.55
29	W	50	ASP	N-CA-C	5.28	119.57	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	178	HIS	N-CA-C	-5.28	102.94	109.64
16	J	68	GLY	N-CA-C	5.24	118.82	112.48
16	J	112	ASP	N-CA-C	-5.24	101.92	110.20
9	C	20	ASP	N-CA-C	5.17	116.91	111.28
31	Y	117	LEU	N-CA-C	-5.16	105.34	110.97
20	N	176	ARG	N-CA-C	-5.16	104.92	111.11
1	0	1504	A	C1'-O4'-C4'	-5.16	104.74	109.90
20	N	20	TYR	N-CA-C	5.14	116.89	111.28
7	A	25	ALA	N-CA-C	5.14	117.78	108.69
1	0	871	G	C5'-C4'-O4'	-5.13	102.10	109.80
1	0	2644	C	O4'-C4'-C3'	-5.13	100.97	106.10
1	0	2313	C	C5'-C4'-C3'	5.13	123.69	116.00
9	C	23	GLU	N-CA-C	-5.12	107.07	113.72
9	C	179	GLY	N-CA-C	-5.11	106.55	113.24
18	L	63	THR	N-CA-C	5.11	118.33	110.42
1	0	2301	A	N9-C1'-C2'	5.10	119.64	112.00
29	W	123	GLY	N-CA-C	-5.10	108.58	115.21
17	K	111	GLY	CA-C-N	5.09	126.20	119.84
17	K	111	GLY	C-N-CA	5.09	126.20	119.84
22	P	70	ALA	N-CA-C	-5.09	105.74	111.28
24	R	142	ASP	N-CA-C	-5.08	101.82	109.85
26	T	52	ARG	N-CA-C	5.08	121.61	110.80
3	2	24	TRP	N-CA-C	5.04	117.67	111.82
24	R	3	SER	N-CA-C	-5.04	101.63	109.24
32	Z	18	TYR	N-CA-C	5.04	121.53	110.80
7	A	68	ILE	N-CA-C	5.03	115.95	108.46
1	0	1261	A	N9-C1'-C2'	5.02	119.53	112.00
30	X	79	GLU	N-CA-C	5.01	119.11	113.15
14	H	166	ILE	N-CA-C	-5.00	100.05	107.51
1	0	1634	G	N9-C1'-C2'	5.00	119.50	112.00
9	C	219	ASN	N-CA-C	5.00	116.89	109.69

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1377	C	Sidechain
1	0	1430	G	Sidechain
1	0	1653	A	Sidechain
1	0	1829	A	Sidechain
1	0	1863	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2607	U	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	792	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	952	G	Sidechain
6	9	65	A	Sidechain
29	W	90	TYR	Sidechain

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	0	59020	0	29811	1132	0
2	1	431	0	426	29	0
3	2	396	0	413	33	0
4	3	755	0	728	39	0
5	4	73	0	64	1	0
6	9	2599	0	1325	72	0
7	A	1753	0	1766	124	0
8	B	2625	0	2533	208	0
9	C	1859	0	1816	147	0
10	D	1094	0	1085	116	0
11	E	1357	0	1266	87	0
12	F	890	0	843	63	0
13	G	240	0	231	19	0
14	H	1282	0	1292	96	0
15	I	519	0	500	65	0
16	J	1120	0	1098	78	0
17	K	992	0	1031	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	1118	0	1076	92	0
19	M	1558	0	1566	86	0
20	N	1445	0	1401	150	0
21	O	865	0	873	54	0
22	P	1136	0	1123	59	0
23	Q	735	0	729	45	0
24	R	1149	0	1122	67	0
25	S	641	0	605	40	0
26	T	950	0	923	73	0
27	U	410	0	364	36	0
28	V	499	0	511	45	0
29	W	1196	0	1137	120	0
30	X	654	0	653	63	0
31	Y	1130	0	1133	73	0
32	Z	578	0	539	29	0
33	0	109	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	74	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	2	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	M	1	0	0	0	0
36	N	1	0	0	2	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5842	0	0	196	0
38	1	60	0	0	8	0
38	2	49	0	0	6	0
38	3	69	0	0	12	0
38	4	2	0	0	0	0
38	9	143	0	0	9	0
38	A	123	0	0	20	0
38	B	146	0	0	19	0
38	C	185	0	0	37	0
38	D	49	0	0	22	0
38	E	42	0	0	12	0
38	F	26	0	0	5	0
38	G	20	0	0	2	0
38	H	69	0	0	16	0
38	I	9	0	0	4	0
38	J	55	0	0	4	0
38	K	59	0	0	10	0
38	L	82	0	0	22	0
38	M	129	0	0	12	0
38	N	60	0	0	11	0
38	O	42	0	0	7	0
38	P	72	0	0	5	0
38	Q	48	0	0	6	0
38	R	85	0	0	7	0
38	S	30	0	0	5	0
38	T	39	0	0	9	0
38	U	29	0	0	3	0
38	V	13	0	0	3	0
38	W	69	0	0	12	0
38	X	26	0	0	6	0
38	Y	101	0	0	16	0
38	Z	37	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	99111	0	59983	3112	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 21.

All (3112) 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)
6:9:6:C:H5''	20:N:37:ARG:NH1	1.59	1.16
1:0:156:C:H5''	19:M:171:ARG:HD3	1.25	1.15
6:9:6:C:H5''	20:N:37:ARG:HH12	0.97	1.14
29:W:5:VAL:HG11	29:W:153:MET:HE1	1.30	1.10
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.07
1:0:871:G:H5'	1:0:871:G:H8	1.10	1.06
24:R:18:LEU:HB2	24:R:143:VAL:HG12	1.34	1.05
9:C:236:THR:HG22	9:C:239:ALA:H	1.18	1.04
10:D:154:LYS:H	10:D:154:LYS:HD2	1.18	1.03
1:0:871:G:H5'	1:0:871:G:C8	1.94	1.02
28:V:12:THR:HG22	28:V:15:GLU:HG3	1.39	1.01
14:H:59:GLN:HE21	14:H:129:ARG:HE	1.08	1.00
9:C:127:ARG:NH2	9:C:225:PRO:HG2	1.76	1.00
14:H:174:LEU:HA	38:H:369:HOH:O	1.59	0.99
1:0:870:G:H2'	1:0:871:G:H5''	1.41	0.99
8:B:264:GLU:HG2	8:B:267:LYS:HE2	1.41	0.98
1:0:796:A:HO2'	32:Z:10:ARG:N	1.60	0.98
1:0:381:G:H5''	38:O:4902:HOH:O	1.67	0.95
1:0:1119:G:H2'	16:J:52:GLN:NE2	1.80	0.95
15:I:127:CYS:HB3	15:I:132:VAL:HB	1.45	0.95
29:W:149:LEU:HG	29:W:153:MET:HE2	1.46	0.95
31:Y:187:VAL:HG23	31:Y:192:ASP:HB2	1.47	0.95
1:0:21:G:H5'	24:R:2:ILE:HA	1.49	0.94
29:W:6:GLN:HB2	29:W:26:ILE:HD12	1.49	0.94
22:P:59:ARG:NH2	22:P:66:GLN:HE22	1.66	0.93
17:K:10:GLN:H	17:K:10:GLN:NE2	1.66	0.93
10:D:134:LEU:HD11	10:D:166:ILE:HD11	1.46	0.93
30:X:72:VAL:HG22	30:X:85:VAL:HG12	1.50	0.93
30:X:37:LEU:HD13	30:X:85:VAL:HG21	1.47	0.92
1:0:1116:U:HO2'	1:0:1118:A:H2	0.92	0.92
1:0:56:G:H5''	28:V:50:ARG:HH12	1.34	0.92
1:0:1474:C:H6	1:0:1474:C:H5'	1.35	0.92
19:M:164:THR:HG22	19:M:167:GLY:H	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:25:MET:HE2	10:D:41:LEU:HG	1.51	0.91
29:W:4:LEU:HD22	29:W:52:VAL:HG21	1.53	0.91
16:J:76:ASP:HA	38:J:4028:HOH:O	1.71	0.91
7:A:35:GLY:O	7:A:36:ASP:HB3	1.70	0.90
29:W:88:THR:HB	38:W:4041:HOH:O	1.69	0.90
1:0:1116:U:H3	1:0:1246:A:H62	1.18	0.90
1:0:2717:C:H2'	1:0:2718:C:H5''	1.53	0.90
32:Z:46:ARG:HD2	32:Z:59:TYR:HB2	1.52	0.90
1:0:1119:G:H2'	16:J:52:GLN:HE22	1.32	0.90
1:0:1242:A:H5'	16:J:82:THR:HG23	1.54	0.90
1:0:2756:U:H3	1:0:2896:A:H2	1.17	0.90
17:K:10:GLN:H	17:K:10:GLN:HE21	0.91	0.90
6:9:14:G:H5'	6:9:14:G:H8	1.36	0.90
17:K:10:GLN:HE21	17:K:10:GLN:N	1.70	0.89
1:0:1751:G:H2'	1:0:1752:G:H5''	1.54	0.89
17:K:74:VAL:HG11	17:K:113:ILE:HG12	1.53	0.89
1:0:545:G:H5'	1:0:545:G:H8	1.39	0.88
6:9:76:G:H3'	6:9:77:A:H5''	1.54	0.88
29:W:72:PRO:HG2	29:W:77:ALA:HB3	1.53	0.88
1:0:870:G:C2'	1:0:871:G:H5''	2.03	0.88
1:0:2586:U:H3	1:0:2592:G:H22	1.16	0.88
14:H:102:LYS:HD3	14:H:122:LYS:HD3	1.56	0.88
9:C:115:LEU:HD21	9:C:243:VAL:HG13	1.56	0.88
26:T:71:VAL:HG11	26:T:90:PRO:HB3	1.56	0.88
29:W:21:LEU:HD13	29:W:26:ILE:HD11	1.56	0.88
20:N:47:LEU:HD11	20:N:127:LEU:HD21	1.54	0.88
21:O:42:GLU:HB2	38:O:4021:HOH:O	1.73	0.88
1:0:2717:C:C2'	1:0:2718:C:H5''	2.04	0.87
14:H:59:GLN:NE2	14:H:129:ARG:HE	1.71	0.87
16:J:74:ARG:HB3	16:J:74:ARG:HH11	1.37	0.87
1:0:1160:G:C5'	1:0:1161:A:H5'	2.05	0.87
8:B:320:GLN:NE2	8:B:321:PRO:HD2	1.89	0.87
22:P:115:SER:H	22:P:118:GLN:NE2	1.73	0.87
1:0:542:A:H5'	1:0:542:A:H8	1.38	0.86
8:B:62:ARG:HA	8:B:65:MET:HE3	1.56	0.86
27:U:9:CYS:HA	27:U:52:THR:HG23	1.57	0.86
38:O:9537:HOH:O	17:K:39:GLY:HA2	1.74	0.86
1:0:200:C:H2'	38:O:4592:HOH:O	1.76	0.86
9:C:1:MET:HG2	9:C:2:GLN:H	1.41	0.86
1:0:962:C:H1'	20:N:5:ARG:HH12	1.38	0.85
1:0:1160:G:H5'	1:0:1161:A:C5'	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:41:HIS:H	3:2:45:ASN:HD22	1.23	0.85
1:0:877:G:H5'	1:0:878:G:OP1	1.76	0.85
16:J:19:MET:HE3	16:J:132:LEU:HD11	1.59	0.85
19:M:99:ARG:HD2	19:M:167:GLY:HA2	1.58	0.85
9:C:236:THR:HA	38:C:522:HOH:O	1.76	0.85
29:W:4:LEU:HD23	29:W:54:PHE:HB3	1.56	0.84
14:H:30:LYS:H	14:H:62:HIS:HD2	1.21	0.84
1:0:1701:A:H4'	1:0:1702:U:H5''	1.59	0.84
9:C:236:THR:HG22	9:C:239:ALA:N	1.90	0.84
14:H:12:ILE:HD12	14:H:57:THR:HG22	1.57	0.84
17:K:81:ARG:HB2	17:K:87:ARG:NH1	1.92	0.84
26:T:9:LYS:HE3	26:T:13:ARG:NH1	1.92	0.84
8:B:201:ASP:HB2	8:B:312:ARG:HD2	1.60	0.84
1:0:2291:A:C8	1:0:2309:C:H5'	2.12	0.84
7:A:191:GLY:HA2	7:A:194:MET:HE2	1.59	0.84
29:W:88:THR:HG22	29:W:89:ASP:H	1.42	0.84
7:A:135:VAL:HG21	7:A:147:ARG:HG2	1.57	0.83
14:H:12:ILE:HG23	14:H:129:ARG:NE	1.91	0.83
14:H:88:MET:HA	14:H:139:ALA:HA	1.59	0.83
17:K:98:VAL:HG13	17:K:102:GLU:HA	1.61	0.83
9:C:236:THR:H	9:C:239:ALA:HB3	1.44	0.83
1:0:558:C:C2'	1:0:559:U:H5''	2.08	0.83
7:A:194:MET:HE3	7:A:199:HIS:HB2	1.60	0.83
20:N:48:VAL:CG1	20:N:55:ASP:HB3	2.08	0.83
17:K:98:VAL:CG1	17:K:102:GLU:HA	2.09	0.82
19:M:102:GLU:OE1	19:M:164:THR:HG21	1.79	0.82
12:F:53:ASP:OD1	12:F:80:GLN:HB2	1.80	0.82
18:L:79:ASP:HB3	38:L:358:HOH:O	1.78	0.82
1:0:1679:C:H5'	38:0:7104:HOH:O	1.79	0.82
1:0:1684:A:H1'	3:2:43:ARG:HH22	1.44	0.82
6:9:28:U:H5''	20:N:40:ASN:ND2	1.95	0.82
1:0:21:G:C5'	24:R:2:ILE:HA	2.10	0.81
1:0:1559:A:H1'	38:0:7360:HOH:O	1.78	0.81
38:0:8709:HOH:O	10:D:99:ASP:HA	1.79	0.81
8:B:217:ARG:HG3	8:B:257:THR:HG22	1.62	0.81
1:0:1878:G:H1'	38:0:8000:HOH:O	1.80	0.81
1:0:506:G:H22	1:0:509:A:C5'	1.93	0.81
1:0:282:C:H1'	1:0:368:C:N4	1.95	0.81
6:9:29:C:H2'	6:9:30:C:H5'	1.62	0.81
1:0:962:C:H1'	20:N:5:ARG:NH1	1.94	0.81
9:C:162:VAL:HG12	9:C:192:ILE:HD11	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:6:C:C5'	20:N:37:ARG:NH1	2.44	0.81
28:V:12:THR:HG23	28:V:14:ALA:H	1.45	0.80
11:E:97:VAL:HG12	38:E:4024:HOH:O	1.81	0.80
20:N:37:ARG:HH21	20:N:105:GLY:CA	1.94	0.80
1:0:1162:G:H1'	15:I:112:LEU:HD11	1.61	0.80
9:C:2:GLN:HB3	38:C:417:HOH:O	1.81	0.80
1:0:1184:C:H1'	38:0:6617:HOH:O	1.82	0.80
38:0:6579:HOH:O	13:G:12:ILE:HA	1.81	0.80
18:L:35:ARG:HH12	18:L:43:HIS:HB3	1.46	0.80
1:0:2533:C:H5'	1:0:2533:C:H6	1.44	0.80
29:W:13:MET:HE2	29:W:18:GLN:HA	1.64	0.80
1:0:544:G:H2'	1:0:545:G:H5''	1.62	0.80
1:0:1835:U:H5	1:0:1840:A:N7	1.80	0.80
4:3:60:LYS:HG3	4:3:61:PRO:HD2	1.65	0.79
8:B:275:GLY:O	8:B:291:ASP:HA	1.82	0.79
29:W:52:VAL:HG22	29:W:53:ALA:H	1.47	0.79
1:0:157:G:H4'	19:M:95:LYS:HE2	1.64	0.79
17:K:81:ARG:HB2	17:K:87:ARG:HH11	1.47	0.79
17:K:63:GLU:HB2	38:K:4034:HOH:O	1.83	0.79
1:0:2716:G:H5''	8:B:206:THR:HG21	1.63	0.79
20:N:164:ASP:OD1	20:N:167:ASP:HA	1.84	0.79
7:A:100:PRO:HG2	7:A:103:VAL:HG21	1.64	0.78
10:D:57:THR:HG23	10:D:63:ILE:HA	1.64	0.78
10:D:28:GLY:HA2	10:D:69:ILE:HG23	1.63	0.78
23:Q:75:ILE:HD13	23:Q:84:ILE:HD11	1.66	0.78
24:R:18:LEU:HB2	24:R:143:VAL:CG1	2.14	0.78
14:H:49:GLN:HG3	14:H:140:TYR:CE2	2.19	0.78
28:V:56:ILE:O	28:V:60:GLN:HG3	1.84	0.78
1:0:2890:A:H1'	27:U:56:ARG:NH2	1.98	0.78
22:P:59:ARG:HH22	22:P:66:GLN:HE22	1.28	0.78
1:0:1666:C:H2'	1:0:1667:A:H5'	1.66	0.78
1:0:1118:A:H8	1:0:1118:A:H3'	1.48	0.78
16:J:75:PRO:HG2	16:J:105:LEU:HD21	1.65	0.78
28:V:1:THR:HG23	28:V:2:VAL:H	1.49	0.78
1:0:470:U:O2'	2:1:16:HIS:HD2	1.66	0.77
8:B:162:MET:HE1	8:B:308:LEU:HD21	1.66	0.77
12:F:46:GLU:OE1	12:F:100:ASP:HA	1.85	0.77
20:N:80:SER:HB2	38:N:4032:HOH:O	1.84	0.77
1:0:1244:U:OP1	16:J:18:ILE:HD13	1.85	0.77
22:P:13:VAL:HG21	22:P:41:ARG:HG2	1.66	0.77
15:I:117:THR:HG22	15:I:121:LYS:HE3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:506:G:H22	1:0:509:A:H5'	1.50	0.77
29:W:13:MET:HE3	29:W:17:ILE:HG22	1.65	0.77
1:0:1209:C:H2'	1:0:1210:G:H8	1.48	0.77
1:0:31:C:H2'	38:0:4091:HOH:O	1.84	0.77
8:B:248:ARG:O	8:B:251:VAL:HG22	1.85	0.77
30:X:71:ARG:HD3	38:X:4023:HOH:O	1.83	0.77
9:C:242:GLU:HG3	38:C:581:HOH:O	1.83	0.76
1:0:2908:A:H2'	1:0:2909:G:O4'	1.84	0.76
6:9:56:A:H2'	6:9:57:A:H5''	1.66	0.76
15:I:97:VAL:HG12	15:I:101:LYS:HE3	1.68	0.76
14:H:12:ILE:HG23	14:H:129:ARG:CZ	2.15	0.76
1:0:1163:G:H5'	15:I:110:ASP:O	1.85	0.76
1:0:1834:C:H2'	1:0:1840:A:N6	2.00	0.76
12:F:27:GLY:HA3	12:F:101:ALA:O	1.85	0.76
30:X:76:ARG:HH11	30:X:76:ARG:HG3	1.50	0.76
14:H:30:LYS:H	14:H:62:HIS:CD2	2.04	0.76
29:W:64:THR:O	29:W:68:THR:HG22	1.86	0.76
1:0:559:U:H6	1:0:559:U:H5'	1.49	0.76
1:0:1834:C:H2'	1:0:1840:A:H62	1.51	0.76
29:W:21:LEU:HD21	29:W:48:VAL:HG11	1.68	0.76
1:0:1701:A:H5'	38:0:7068:HOH:O	1.85	0.76
1:0:2780:C:H1'	11:E:143:GLN:HE21	1.51	0.76
8:B:140:LEU:HD23	38:B:559:HOH:O	1.86	0.76
8:B:320:GLN:HE21	8:B:321:PRO:HD2	1.47	0.76
17:K:30:LYS:O	17:K:55:VAL:HG13	1.86	0.76
1:0:182:G:H5'	38:0:4531:HOH:O	1.86	0.75
1:0:1293:U:H5'	31:Y:154:ARG:HH21	1.48	0.75
19:M:24:GLN:NE2	19:M:27:ARG:HH11	1.84	0.75
1:0:1118:A:H3'	1:0:1118:A:C8	2.21	0.75
7:A:81:GLN:HB2	7:A:92:ASN:ND2	2.02	0.75
1:0:56:G:H5''	28:V:50:ARG:NH1	2.00	0.75
8:B:86:ALA:HA	38:B:559:HOH:O	1.85	0.75
12:F:96:ALA:HA	38:F:4009:HOH:O	1.86	0.75
29:W:21:LEU:HD21	29:W:48:VAL:CG1	2.15	0.75
8:B:18:ARG:HG3	8:B:256:GLN:HG3	1.67	0.75
1:0:545:G:H5'	1:0:545:G:C8	2.21	0.75
29:W:13:MET:HE2	29:W:18:GLN:CA	2.17	0.75
6:9:14:G:H5'	6:9:14:G:C8	2.20	0.75
19:M:164:THR:HG22	19:M:167:GLY:N	2.01	0.75
1:0:383:A:H4'	38:0:4914:HOH:O	1.86	0.75
20:N:113:SER:HB2	38:N:4044:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:107:ASN:C	16:J:107:ASN:HD22	1.95	0.75
1:O:1474:C:H5'	1:O:1474:C:C6	2.22	0.74
7:A:36:ASP:OD2	7:A:85:SER:HB2	1.87	0.74
8:B:27:ASN:HD22	8:B:27:ASN:H	1.34	0.74
8:B:321:PRO:HA	38:B:578:HOH:O	1.88	0.74
14:H:49:GLN:OE1	14:H:169:GLU:HG3	1.87	0.74
28:V:8:ILE:HA	28:V:11:MET:HE3	1.68	0.74
2:1:25:LYS:HD2	3:2:49:GLU:H	1.52	0.74
16:J:74:ARG:HH11	16:J:74:ARG:CB	1.99	0.74
31:Y:187:VAL:HG23	31:Y:192:ASP:CB	2.17	0.74
1:O:10:U:H3'	38:O:5221:HOH:O	1.85	0.74
1:O:1741:U:H5'	1:O:1742:A:OP1	1.87	0.74
10:D:99:ASP:HB3	10:D:103:ASN:H	1.52	0.74
17:K:14:LYS:HB2	17:K:45:PRO:HG2	1.69	0.74
27:U:20:MET:HE2	27:U:30:HIS:NE2	2.02	0.74
1:O:2364:A:H5''	23:Q:15:LYS:HD3	1.70	0.74
4:3:25:VAL:HG22	4:3:68:LYS:HG3	1.68	0.74
6:9:48:C:H4'	20:N:141:ARG:NH2	2.03	0.74
9:C:236:THR:HG21	38:C:525:HOH:O	1.88	0.74
20:N:48:VAL:HG11	20:N:55:ASP:HB3	1.70	0.74
16:J:39:VAL:HG13	16:J:106:GLY:O	1.88	0.73
6:9:92:G:H2'	6:9:93:A:C8	2.22	0.73
12:F:91:VAL:HG12	12:F:92:GLY:N	2.00	0.73
23:Q:25:PRO:HB2	38:Q:223:HOH:O	1.88	0.73
1:O:711:G:H1'	38:O:5573:HOH:O	1.87	0.73
1:O:1667:A:H5'	1:O:1667:A:H8	1.54	0.73
1:O:2748:G:H2'	38:O:8252:HOH:O	1.89	0.73
1:O:2768:A:H2'	1:O:2769:C:O4'	1.87	0.73
29:W:151:GLU:O	29:W:154:ARG:HB3	1.88	0.73
18:L:143:THR:HG21	38:L:371:HOH:O	1.87	0.73
18:L:148:GLU:HA	38:L:376:HOH:O	1.88	0.73
24:R:119:VAL:HG21	24:R:142:ASP:CG	2.13	0.73
1:O:544:G:C2'	1:O:545:G:H5''	2.18	0.73
8:B:162:MET:HE2	8:B:310:ARG:HD3	1.70	0.73
28:V:42:ASN:HB3	38:V:4008:HOH:O	1.88	0.73
1:O:1130:U:H5'	38:O:6544:HOH:O	1.89	0.73
1:O:1884:G:O6	7:A:190:ARG:HD2	1.87	0.73
1:O:558:C:H2'	1:O:559:U:H5''	1.69	0.73
15:I:96:SER:H	15:I:99:GLN:NE2	1.87	0.73
28:V:12:THR:HG22	28:V:15:GLU:CG	2.19	0.73
14:H:62:HIS:HA	14:H:65:LEU:HD23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:75:ILE:CD1	23:Q:84:ILE:HD11	2.18	0.72
1:O:1603:A:H5'	1:O:1605:G:O4'	1.89	0.72
16:J:107:ASN:ND2	16:J:109:TYR:H	1.85	0.72
20:N:47:LEU:HD13	20:N:97:VAL:HG11	1.69	0.72
28:V:39:ALA:N	28:V:40:PRO:HD2	2.05	0.72
24:R:132:ARG:HG2	24:R:133:ALA:N	2.05	0.72
14:H:6:ALA:HA	14:H:61:ARG:HH12	1.53	0.72
20:N:169:PRO:O	20:N:172:PHE:HB3	1.88	0.72
22:P:143:ALA:HA	38:P:272:HOH:O	1.88	0.72
1:O:1165:G:H4'	1:O:1174:A:O2'	1.89	0.72
14:H:6:ALA:HA	14:H:61:ARG:NH1	2.04	0.72
29:W:132:VAL:HG21	29:W:140:LYS:O	1.89	0.72
8:B:179:LEU:O	8:B:183:GLU:HG2	1.89	0.72
10:D:25:MET:SD	10:D:40:ILE:HD11	2.30	0.72
12:F:58:GLU:OE1	19:M:27:ARG:NH2	2.23	0.72
29:W:52:VAL:HG22	29:W:53:ALA:N	2.05	0.72
29:W:88:THR:HG23	29:W:110:GLN:NE2	2.04	0.72
10:D:135:VAL:HG21	10:D:139:TYR:CD1	2.24	0.72
27:U:47:ARG:HG3	38:U:8826:HOH:O	1.90	0.72
1:O:1450:C:H4'	1:O:1451:C:OP2	1.88	0.71
6:9:48:C:H4'	20:N:141:ARG:HH21	1.55	0.71
1:O:821:U:H2'	1:O:822:C:H6	1.54	0.71
31:Y:174:VAL:HG12	31:Y:177:LYS:HD2	1.71	0.71
1:O:694:A:H2'	1:O:695:C:H5'	1.72	0.71
6:9:54:A:O2'	6:9:55:U:H5'	1.90	0.71
6:9:114:G:O6	20:N:11:ARG:HD3	1.91	0.71
14:H:165:ARG:HD3	38:H:319:HOH:O	1.89	0.71
1:O:2270:G:H4'	7:A:223:ARG:HH12	1.55	0.71
8:B:36:PRO:HA	8:B:168:GLY:HA3	1.73	0.71
8:B:190:MET:HE2	8:B:194:PHE:CD1	2.25	0.71
22:P:103:THR:O	22:P:107:GLU:HG3	1.91	0.71
1:O:2812:A:H2	1:O:2814:A:H62	1.37	0.71
8:B:212:GLN:HB2	8:B:257:THR:HG21	1.70	0.71
9:C:145:GLU:HG3	38:C:525:HOH:O	1.88	0.71
21:O:32:ARG:O	21:O:32:ARG:HD3	1.90	0.71
3:2:22:PRO:HG2	3:2:25:VAL:HG23	1.73	0.71
20:N:164:ASP:CG	20:N:167:ASP:HA	2.16	0.71
1:O:1819:G:H2'	1:O:1820:G:H4'	1.72	0.71
1:O:2320:U:H4'	1:O:2321:A:O4'	1.90	0.71
9:C:142:ASP:OD1	9:C:237:GLU:HB3	1.91	0.71
1:O:156:C:H5''	19:M:171:ARG:CD	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:32:ALA:HB3	14:H:69:ARG:HH12	1.54	0.71
1:0:960:G:H4'	38:0:6208:HOH:O	1.90	0.70
9:C:233:THR:HG22	9:C:234:VAL:H	1.56	0.70
10:D:146:LYS:NZ	20:N:107:ASN:HD21	1.89	0.70
20:N:38:LYS:HE2	20:N:107:ASN:ND2	2.05	0.70
1:0:1206:U:H5'	1:0:1206:U:H6	1.56	0.70
29:W:137:GLN:HE21	29:W:141:HIS:HE1	1.38	0.70
29:W:6:GLN:HB2	29:W:26:ILE:CD1	2.20	0.70
1:0:259:G:H21	19:M:58:GLN:NE2	1.88	0.70
12:F:2:VAL:HG22	12:F:57:GLU:OE1	1.92	0.70
14:H:59:GLN:HE21	14:H:129:ARG:NE	1.88	0.70
19:M:65:VAL:HG21	19:M:105:ALA:HB2	1.74	0.70
24:R:39:THR:HB	24:R:42:GLU:HG3	1.72	0.70
1:0:814:G:H4'	38:0:5765:HOH:O	1.90	0.70
1:0:1377:C:H5'	1:0:1377:C:H6	1.56	0.70
20:N:61:ALA:HB3	20:N:88:ALA:HB2	1.72	0.70
1:0:2578:G:H5'	1:0:2578:G:H8	1.55	0.70
8:B:55:ASN:HB3	8:B:63:GLU:HA	1.74	0.70
18:L:133:VAL:HA	38:L:375:HOH:O	1.91	0.70
1:0:2637:A:H5'	38:0:9419:HOH:O	1.91	0.70
25:S:51:GLN:HE21	25:S:53:ASN:HD21	1.40	0.70
30:X:72:VAL:HG22	30:X:85:VAL:CG1	2.19	0.70
12:F:63:ILE:HB	12:F:64:PRO:HD3	1.72	0.70
16:J:19:MET:HE2	16:J:79:PHE:HA	1.74	0.70
25:S:42:GLU:HG2	25:S:49:VAL:HG23	1.74	0.70
27:U:14:GLU:O	27:U:17:THR:HB	1.92	0.70
30:X:78:GLU:HG2	30:X:79:GLU:H	1.56	0.70
22:P:59:ARG:HH22	22:P:66:GLN:NE2	1.89	0.69
7:A:88:ILE:HD13	7:A:100:PRO:HD3	1.72	0.69
9:C:1:MET:HG2	9:C:2:GLN:N	2.07	0.69
10:D:35:ALA:C	10:D:37:ALA:H	1.99	0.69
24:R:99:ALA:HB1	24:R:109:MET:CE	2.22	0.69
1:0:558:C:H2'	1:0:559:U:C5'	2.21	0.69
38:0:4849:HOH:O	26:T:53:GLY:HA3	1.92	0.69
7:A:68:ILE:HD11	38:A:443:HOH:O	1.92	0.69
17:K:29:LEU:HB3	17:K:55:VAL:HG11	1.73	0.69
1:0:558:C:O2'	1:0:559:U:H5''	1.92	0.69
1:0:2783:A:H3'	38:0:9678:HOH:O	1.93	0.69
8:B:41:PHE:CD1	8:B:79:MET:HE2	2.27	0.69
29:W:88:THR:HG23	29:W:110:GLN:HE21	1.58	0.69
30:X:43:VAL:HG11	30:X:82:GLU:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1187:U:H2'	38:0:6627:HOH:O	1.92	0.69
9:C:246:ARG:HD2	38:C:584:HOH:O	1.93	0.69
1:0:57:C:H5''	38:0:4173:HOH:O	1.93	0.68
32:Z:26:VAL:O	32:Z:30:GLU:HG3	1.93	0.68
7:A:94:LEU:HG	7:A:99:ILE:HD11	1.75	0.68
15:I:101:LYS:O	15:I:105:GLU:HG3	1.94	0.68
18:L:35:ARG:HB2	18:L:35:ARG:NH1	2.08	0.68
1:0:2506:A:O2'	1:0:2507:G:H8	1.75	0.68
7:A:200:PRO:HD3	38:A:513:HOH:O	1.92	0.68
1:0:2426:G:H1'	38:0:8683:HOH:O	1.92	0.68
12:F:61:MET:HB3	19:M:19:GLN:OE1	1.93	0.68
11:E:145:ALA:HB1	11:E:168:ILE:HD11	1.76	0.68
15:I:88:GLN:HA	15:I:91:PHE:CE2	2.28	0.68
7:A:199:HIS:HD2	7:A:201:PHE:H	1.42	0.68
32:Z:37:HIS:HB2	32:Z:47:VAL:HB	1.75	0.68
1:0:214:U:H5'	38:0:4638:HOH:O	1.92	0.68
1:0:236:A:H4'	1:0:237:G:H5'	1.75	0.68
1:0:399:C:H5'	19:M:179:GLY:O	1.93	0.68
8:B:304:PRO:HD2	8:B:307:ARG:HD2	1.76	0.68
15:I:118:ASN:HA	15:I:121:LYS:HD2	1.75	0.68
17:K:74:VAL:CG1	17:K:113:ILE:HG12	2.22	0.68
27:U:17:THR:HG22	27:U:18:GLY:N	2.07	0.68
32:Z:57:CYS:SG	32:Z:59:TYR:HB3	2.32	0.68
1:0:447:A:P	26:T:1:SER:HB2	2.34	0.68
38:0:4764:HOH:O	19:M:58:GLN:HG3	1.93	0.68
7:A:51:ARG:HB2	38:A:435:HOH:O	1.94	0.68
8:B:162:MET:CE	8:B:308:LEU:HD21	2.23	0.68
15:I:87:PRO:C	15:I:89:GLU:H	2.02	0.68
24:R:8:ALA:HB1	24:R:13:THR:HG21	1.74	0.68
7:A:88:ILE:O	7:A:88:ILE:HG22	1.92	0.68
17:K:13:GLU:OE2	17:K:44:LEU:HB2	1.93	0.68
29:W:88:THR:HG22	29:W:89:ASP:N	2.08	0.68
1:0:450:C:OP1	9:C:184:ARG:NH2	2.24	0.68
1:0:1189:A:H1'	1:0:1209:C:O4'	1.94	0.68
8:B:141:ARG:HD2	8:B:163:GLU:OE2	1.94	0.68
10:D:154:LYS:HD2	10:D:154:LYS:N	2.02	0.68
1:0:21:G:H5''	24:R:1:GLY:O	1.95	0.67
9:C:61:PHE:HB3	38:C:459:HOH:O	1.93	0.67
29:W:84:VAL:HG12	38:W:4041:HOH:O	1.93	0.67
1:0:1157:C:H2'	1:0:1158:G:H8	1.56	0.67
1:0:2533:C:H5'	1:0:2533:C:C6	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:65:GLU:HA	38:D:225:HOH:O	1.93	0.67
24:R:96:VAL:HG13	24:R:106:GLY:HA3	1.75	0.67
1:0:1417:G:O2'	3:2:11:LEU:HD22	1.94	0.67
11:E:137:ASP:OD1	11:E:139:GLU:HB2	1.94	0.67
18:L:136:ALA:HB3	38:L:375:HOH:O	1.94	0.67
9:C:132:ASP:HB3	38:C:516:HOH:O	1.93	0.67
10:D:84:LEU:HA	10:D:87:ALA:HB3	1.74	0.67
18:L:67:ARG:O	18:L:71:GLU:HG3	1.95	0.67
1:0:1160:G:O2'	1:0:1190:G:H1'	1.95	0.67
1:0:2036:C:O4'	17:K:44:LEU:HG	1.94	0.67
7:A:161:GLY:O	32:Z:68:SER:HB2	1.95	0.67
2:1:21:ARG:HD2	2:1:37:CYS:SG	2.35	0.67
10:D:159:PRO:O	10:D:163:VAL:HG23	1.94	0.67
1:0:1654:U:H2'	7:A:47:HIS:HD2	1.59	0.67
1:0:2635:A:O2'	1:0:2636:C:H5'	1.95	0.67
4:3:70:ARG:HG2	4:3:77:ALA:HB2	1.77	0.67
8:B:140:LEU:HA	38:B:559:HOH:O	1.94	0.67
13:G:71:LEU:C	13:G:73:ASP:H	2.01	0.67
16:J:107:ASN:HD21	16:J:109:TYR:HB2	1.60	0.67
1:0:111:C:O2'	2:1:20:ARG:HG2	1.94	0.67
1:0:2524:G:H21	1:0:2526:C:N4	1.92	0.67
8:B:62:ARG:CA	8:B:65:MET:HE3	2.25	0.67
8:B:139:ASP:HB2	8:B:165:ARG:HE	1.60	0.67
10:D:146:LYS:NZ	20:N:107:ASN:ND2	2.43	0.67
17:K:34:VAL:HG22	17:K:47:ALA:HB2	1.77	0.67
19:M:99:ARG:CD	19:M:167:GLY:HA2	2.24	0.67
17:K:132:VAL:HG11	27:U:22:VAL:HG22	1.76	0.67
19:M:78:LYS:HE2	38:M:358:HOH:O	1.95	0.67
29:W:80:ASP:O	29:W:84:VAL:HG23	1.95	0.67
1:0:338:C:H4'	9:C:174:ILE:CD1	2.25	0.66
1:0:542:A:H5'	1:0:542:A:C8	2.27	0.66
1:0:1189:A:H1'	1:0:1209:C:C1'	2.25	0.66
1:0:1790:C:H2'	1:0:1791:U:H6	1.60	0.66
7:A:211:LYS:HB3	7:A:212:PRO:HD2	1.76	0.66
9:C:233:THR:HG22	9:C:234:VAL:N	2.10	0.66
24:R:39:THR:HG23	24:R:107:GLU:O	1.95	0.66
1:0:871:G:H8	1:0:871:G:C5'	1.99	0.66
7:A:64:ASP:OD1	7:A:66:ARG:HD2	1.95	0.66
31:Y:235:GLU:CD	31:Y:235:GLU:H	2.02	0.66
16:J:6:PHE:HB3	16:J:109:TYR:OH	1.94	0.66
1:0:21:G:H4'	24:R:2:ILE:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1593:C:OP1	22:P:117:SER:HB3	1.96	0.66
8:B:62:ARG:HA	8:B:65:MET:CE	2.23	0.66
9:C:180:SER:HB2	38:C:534:HOH:O	1.94	0.66
11:E:132:THR:HB	38:E:4031:HOH:O	1.95	0.66
14:H:23:ILE:HG23	14:H:123:ILE:HD11	1.77	0.66
17:K:28:GLU:HG2	17:K:58:THR:HB	1.78	0.66
28:V:64:GLY:O	28:V:65:ASP:HB2	1.96	0.66
31:Y:151:SER:HB3	31:Y:154:ARG:HB3	1.78	0.66
1:O:2508:C:H2'	38:O:9086:HOH:O	1.95	0.66
1:O:657:G:OP1	9:C:27:ARG:NH2	2.28	0.66
1:O:1666:C:O2'	1:O:1667:A:H5''	1.95	0.66
21:O:21:SER:OG	21:O:106:PRO:HB2	1.94	0.66
29:W:129:LYS:HG2	38:W:4056:HOH:O	1.96	0.66
1:O:1121:G:H4'	38:O:6523:HOH:O	1.94	0.66
9:C:139:VAL:HG13	38:C:580:HOH:O	1.95	0.66
10:D:64:ARG:HB3	10:D:67:ASP:OD2	1.95	0.66
1:O:1007:A:H2'	14:H:22:TYR:CZ	2.31	0.66
20:N:34:LEU:HA	20:N:47:LEU:HD23	1.77	0.66
20:N:120:GLU:HG3	20:N:136:LEU:HD13	1.76	0.66
23:Q:26:PRO:O	23:Q:30:VAL:HG23	1.95	0.66
3:2:22:PRO:HG2	3:2:25:VAL:CG2	2.25	0.66
20:N:37:ARG:HD3	36:N:201:CL:CL	2.32	0.66
22:P:65:ARG:HD3	22:P:69:ARG:NH1	2.10	0.66
24:R:4:TYR:CE1	24:R:17:MET:HE2	2.31	0.66
1:O:1372:A:H3'	38:O:6994:HOH:O	1.95	0.66
1:O:1615:A:H4'	38:O:7429:HOH:O	1.95	0.66
14:H:49:GLN:HB2	14:H:170:ARG:HD2	1.77	0.66
17:K:22:ASP:HB2	38:K:4013:HOH:O	1.96	0.66
4:3:62:THR:HB	38:3:248:HOH:O	1.95	0.65
7:A:199:HIS:CD2	7:A:201:PHE:H	2.14	0.65
7:A:200:PRO:HG2	7:A:225:VAL:HG21	1.78	0.65
12:F:26:THR:HG21	12:F:102:GLY:C	2.21	0.65
30:X:30:MET:HE1	30:X:58:ALA:HB3	1.78	0.65
1:O:447:A:OP1	26:T:2:LYS:HG2	1.97	0.65
1:O:1053:G:OP1	14:H:15:PRO:HG3	1.96	0.65
1:O:2414:A:H2'	1:O:2415:A:C8	2.29	0.65
15:I:120:ALA:O	15:I:124:VAL:HG23	1.96	0.65
20:N:78:MET:HB2	20:N:79:PRO:HD3	1.78	0.65
22:P:134:VAL:O	22:P:137:LEU:HB3	1.95	0.65
1:O:513:A:N3	38:O:5181:HOH:O	2.29	0.65
3:2:49:GLU:HB2	38:2:145:HOH:O	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:541:C:C2'	1:0:542:A:H5''	2.26	0.65
2:1:46:ARG:HA	38:1:246:HOH:O	1.96	0.65
9:C:5:ILE:HD11	9:C:16:VAL:CG2	2.27	0.65
28:V:55:ARG:O	28:V:59:ILE:HG12	1.95	0.65
1:0:645:U:OP2	18:L:4:LYS:HE2	1.96	0.65
7:A:121:ALA:O	7:A:124:VAL:HG22	1.96	0.65
21:O:47:ARG:HH11	21:O:47:ARG:HG3	1.61	0.65
24:R:18:LEU:HD12	24:R:143:VAL:HG11	1.78	0.65
27:U:52:THR:HG22	27:U:54:THR:H	1.61	0.65
1:0:2850:C:H6	1:0:2850:C:H5'	1.62	0.65
10:D:23:VAL:HG21	10:D:45:THR:HG21	1.77	0.65
27:U:9:CYS:SG	27:U:11:THR:HG23	2.36	0.65
1:0:447:A:OP2	26:T:1:SER:HB2	1.97	0.65
38:O:6613:HOH:O	15:I:87:PRO:HD3	1.96	0.65
10:D:35:ALA:HB1	38:D:218:HOH:O	1.95	0.65
23:Q:66:LYS:HB2	23:Q:70:ALA:O	1.97	0.65
25:S:77:VAL:O	25:S:80:ARG:HG2	1.97	0.65
7:A:109:GLU:HG2	7:A:116:GLY:H	1.61	0.65
7:A:194:MET:HE3	7:A:199:HIS:CB	2.25	0.65
11:E:118:ILE:HG23	11:E:144:THR:HG21	1.79	0.65
16:J:103:VAL:HG12	38:J:4028:HOH:O	1.97	0.65
18:L:22:ARG:HG2	38:L:329:HOH:O	1.96	0.65
1:0:272:A:H5'	1:0:273:G:OP2	1.96	0.65
7:A:66:ARG:HH11	7:A:66:ARG:HB2	1.61	0.65
21:O:10:LEU:HD13	21:O:99:GLU:HG3	1.79	0.65
38:O:7889:HOH:O	2:1:1:THR:HB	1.96	0.65
11:E:22:VAL:O	11:E:76:VAL:HG11	1.97	0.65
1:0:281:U:H2'	1:0:282:C:O4'	1.97	0.64
17:K:74:VAL:HG13	17:K:113:ILE:HG23	1.79	0.64
18:L:35:ARG:HB2	18:L:35:ARG:HH11	1.61	0.64
1:0:2769:C:C2'	1:0:2770:G:H5'	2.27	0.64
11:E:37:ASP:OD1	16:J:125:SER:HB3	1.97	0.64
26:T:24:ARG:HH21	26:T:39:ASN:HD22	1.44	0.64
14:H:146:ALA:O	14:H:149:VAL:HG12	1.98	0.64
4:3:87:ARG:HD2	4:3:89:GLU:OE2	1.98	0.64
14:H:12:ILE:O	14:H:12:ILE:HG22	1.96	0.64
20:N:67:ALA:HA	20:N:71:TRP:HB3	1.80	0.64
20:N:139:TRP:HA	20:N:139:TRP:CE3	2.31	0.64
28:V:39:ALA:C	28:V:41:GLU:H	2.05	0.64
29:W:137:GLN:HE21	29:W:141:HIS:CE1	2.15	0.64
17:K:75:ARG:CZ	38:K:4039:HOH:O	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:709:G:O2'	21:O:25:VAL:HG12	1.97	0.64
11:E:100:ASP:HB2	38:E:4025:HOH:O	1.96	0.64
11:E:20:ILE:HD11	11:E:40:VAL:HG11	1.80	0.64
16:J:54:VAL:HG11	16:J:138:THR:HG21	1.80	0.64
19:M:64:ARG:HD2	38:M:325:HOH:O	1.97	0.64
8:B:7:ARG:NH1	8:B:11:LEU:HD22	2.13	0.64
8:B:314:ALA:HB3	8:B:317:PRO:HG3	1.80	0.64
12:F:34:ASN:HA	19:M:4:ALA:HB2	1.78	0.64
20:N:132:ASN:O	20:N:135:VAL:HG12	1.98	0.64
1:O:259:G:H21	19:M:58:GLN:HE22	1.45	0.64
7:A:217:ARG:HG2	7:A:229:ALA:HB2	1.80	0.64
11:E:81:GLU:HG2	11:E:134:SER:HB3	1.79	0.64
14:H:100:GLU:HB3	14:H:124:VAL:HG11	1.78	0.64
1:O:1116:U:O2'	1:O:1118:A:H2	1.73	0.63
1:O:1119:G:N2	1:O:1246:A:C2	2.64	0.63
1:O:2524:G:H21	1:O:2526:C:H41	1.44	0.63
1:O:2807:U:P	8:B:27:ASN:HD21	2.21	0.63
6:9:20:G:H3'	38:9:323:HOH:O	1.98	0.63
8:B:162:MET:HG3	8:B:310:ARG:HD3	1.80	0.63
29:W:90:TYR:N	29:W:90:TYR:CD1	2.65	0.63
22:P:20:ARG:NH1	22:P:54:LYS:HD3	2.13	0.63
25:S:11:THR:H	25:S:14:ALA:HB3	1.64	0.63
27:U:46:ALA:HB1	27:U:52:THR:HG21	1.80	0.63
30:X:37:LEU:CD1	30:X:85:VAL:HG21	2.27	0.63
30:X:71:ARG:HB3	30:X:88:GLU:OE1	1.99	0.63
1:O:280:C:H2'	1:O:281:U:O4'	1.99	0.63
10:D:25:MET:HE2	10:D:41:LEU:CG	2.27	0.63
11:E:133:VAL:HG12	11:E:141:VAL:HG13	1.80	0.63
16:J:42:GLU:O	16:J:131:THR:HG23	1.99	0.63
18:L:72:ASN:HB2	38:L:351:HOH:O	1.98	0.63
20:N:47:LEU:HD12	20:N:92:ALA:HB1	1.78	0.63
26:T:9:LYS:HE3	26:T:13:ARG:CZ	2.27	0.63
29:W:4:LEU:CD2	29:W:54:PHE:HB3	2.25	0.63
29:W:13:MET:HE3	29:W:17:ILE:CG2	2.27	0.63
30:X:76:ARG:O	30:X:77:PHE:HB3	1.97	0.63
7:A:211:LYS:HB2	38:A:504:HOH:O	1.97	0.63
18:L:121:ILE:HG12	18:L:141:GLU:HB2	1.79	0.63
20:N:139:TRP:HA	20:N:139:TRP:HE3	1.63	0.63
23:Q:18:PRO:O	23:Q:21:ARG:HB2	1.98	0.63
30:X:21:PRO:HG2	30:X:24:LYS:HD3	1.81	0.63
8:B:5:ARG:NH1	8:B:8:LYS:HE2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:588:G:O6	29:W:154:ARG:NH1	2.32	0.63
1:O:1164:U:OP1	15:I:69:PRO:HA	1.98	0.63
1:O:2598:U:H5''	17:K:36:GLY:HA2	1.80	0.63
11:E:2:ARG:HH21	11:E:48:VAL:HG21	1.62	0.63
1:O:1751:G:C2'	1:O:1752:G:H5''	2.29	0.63
14:H:114:ASP:HB2	38:H:346:HOH:O	1.98	0.63
26:T:43:ASN:ND2	26:T:108:ARG:CZ	2.62	0.63
1:O:603:A:H5''	1:O:604:G:OP1	1.98	0.63
1:O:1641:A:H2'	1:O:1642:A:H5'	1.81	0.63
1:O:338:C:H4'	9:C:174:ILE:HD11	1.81	0.62
1:O:1819:G:H5'	38:O:7788:HOH:O	1.98	0.62
1:O:2112:A:H2'	1:O:2113:G:C8	2.34	0.62
7:A:29:HIS:CB	7:A:153:ARG:HH12	2.10	0.62
12:F:38:LYS:NZ	19:M:3:SER:HA	2.13	0.62
14:H:49:GLN:HB3	14:H:170:ARG:HG3	1.80	0.62
20:N:154:LEU:C	20:N:156:GLU:H	2.05	0.62
25:S:53:ASN:HD22	25:S:53:ASN:N	1.96	0.62
29:W:81:ASP:OD1	29:W:92:ASP:HB2	1.99	0.62
1:O:2547:C:OP2	8:B:5:ARG:NH1	2.32	0.62
1:O:541:C:H2'	1:O:542:A:C5'	2.29	0.62
10:D:25:MET:CE	10:D:37:ALA:HB1	2.29	0.62
14:H:30:LYS:N	14:H:62:HIS:HD2	1.94	0.62
16:J:39:VAL:HG11	16:J:107:ASN:HB2	1.80	0.62
1:O:2276:U:H5'	38:O:4469:HOH:O	1.99	0.62
1:O:2894:C:O2'	1:O:2895:C:H5'	1.99	0.62
15:I:119:ALA:O	15:I:123:VAL:HG23	2.00	0.62
1:O:1348:A:H3'	38:O:6915:HOH:O	1.99	0.62
1:O:1666:C:C2'	1:O:1667:A:H5'	2.30	0.62
38:3:235:HOH:O	19:M:84:LYS:HE2	1.98	0.62
7:A:96:LEU:HD22	7:A:128:LEU:HD13	1.80	0.62
8:B:264:GLU:HG2	8:B:267:LYS:CE	2.22	0.62
1:O:138:U:OP2	1:O:139:C:H5	1.83	0.62
6:9:56:A:C2'	6:9:57:A:H5''	2.29	0.62
10:D:104:PHE:CE2	10:D:132:VAL:HB	2.35	0.62
15:I:129:SER:O	15:I:130:LEU:HD23	2.00	0.62
16:J:46:ILE:HD11	16:J:53:ILE:CG2	2.29	0.62
20:N:58:LEU:N	20:N:58:LEU:HD12	2.15	0.62
22:P:98:ILE:HD12	22:P:102:ARG:NE	2.14	0.62
6:9:35:C:H5''	38:9:348:HOH:O	1.99	0.62
8:B:162:MET:CE	8:B:310:ARG:HD3	2.29	0.62
12:F:91:VAL:HG12	12:F:92:GLY:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:99:GLU:HA	38:J:4030:HOH:O	1.98	0.62
16:J:130:VAL:HG12	16:J:131:THR:N	2.12	0.62
14:H:57:THR:HA	14:H:130:VAL:O	2.00	0.62
14:H:61:ARG:HH11	14:H:61:ARG:HG3	1.63	0.62
20:N:73:ALA:HB1	20:N:74:PRO:CD	2.30	0.62
25:S:33:SER:OG	25:S:36:GLU:HG3	2.00	0.62
1:O:1242:A:H5'	16:J:82:THR:CG2	2.28	0.62
1:O:2862:G:H4'	8:B:336:GLN:O	2.00	0.62
8:B:145:HIS:HD2	8:B:146:THR:O	1.83	0.62
9:C:140:VAL:HB	38:C:522:HOH:O	2.00	0.62
11:E:21:THR:HG23	11:E:30:THR:OG1	1.99	0.62
28:V:44:GLY:O	28:V:48:GLU:HG2	1.99	0.62
29:W:4:LEU:HD22	29:W:52:VAL:CG2	2.26	0.62
1:O:1328:A:OP1	31:Y:169:ARG:HD2	2.00	0.62
1:O:2766:A:H5'	38:O:9658:HOH:O	1.99	0.62
7:A:191:GLY:HA2	7:A:194:MET:CE	2.29	0.62
7:A:211:LYS:HD3	38:A:505:HOH:O	1.99	0.62
19:M:125:ARG:NH1	38:M:390:HOH:O	2.32	0.62
1:O:2420:G:O2'	1:O:2421:G:H5'	1.99	0.61
4:3:74:CYS:N	38:3:258:HOH:O	2.31	0.61
21:O:73:ASP:HA	21:O:92:VAL:O	2.00	0.61
1:O:1717:A:H5''	22:P:54:LYS:HB2	1.82	0.61
17:K:62:PRO:HG3	17:K:65:ARG:HH21	1.65	0.61
18:L:143:THR:HG22	18:L:144:ASP:N	2.15	0.61
22:P:14:LEU:HD13	22:P:51:ALA:HB2	1.80	0.61
22:P:20:ARG:HH12	22:P:54:LYS:HD3	1.64	0.61
11:E:84:MET:HE1	11:E:148:ILE:HD12	1.82	0.61
28:V:57:LYS:HA	28:V:60:GLN:HE21	1.65	0.61
6:9:14:G:O2'	20:N:1:ALA:HB2	2.01	0.61
25:S:33:SER:O	25:S:37:VAL:HG23	2.00	0.61
1:O:541:C:H2'	1:O:542:A:H5''	1.82	0.61
1:O:1234:U:N3	8:B:244:PRO:HB3	2.15	0.61
26:T:69:LYS:O	26:T:71:VAL:HG23	2.00	0.61
1:O:621:C:H5'	31:Y:132:ASP:OD2	2.01	0.61
1:O:2756:U:N3	1:O:2896:A:H2	1.96	0.61
38:O:7475:HOH:O	7:A:165:THR:HG23	2.00	0.61
1:O:2453:G:H3'	38:O:8942:HOH:O	2.01	0.61
4:3:55:VAL:HB	4:3:56:PRO:HD2	1.83	0.61
8:B:202:VAL:HG11	8:B:301:VAL:HG13	1.81	0.61
10:D:25:MET:HE1	10:D:37:ALA:HB1	1.82	0.61
11:E:11:VAL:HG12	11:E:12:ASP:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:53:ARG:NH2	18:L:57:VAL:HG12	2.16	0.61
19:M:30:GLU:O	19:M:34:GLU:HG3	2.01	0.61
29:W:21:LEU:HB3	29:W:26:ILE:HG12	1.83	0.61
9:C:150:THR:HA	9:C:203:ALA:O	2.00	0.61
18:L:61:ALA:HA	38:L:365:HOH:O	2.01	0.61
18:L:143:THR:HG22	18:L:145:LEU:H	1.66	0.61
1:0:602:A:O2'	1:0:605:C:H4'	2.00	0.61
1:0:1919:A:H4'	38:0:8068:HOH:O	1.99	0.61
1:0:2472:C:O2'	1:0:2634:G:H4'	2.00	0.61
9:C:188:ARG:HD3	38:C:558:HOH:O	2.00	0.61
14:H:49:GLN:HG3	14:H:140:TYR:CD2	2.35	0.61
26:T:55:PHE:CD2	26:T:77:VAL:HG13	2.35	0.61
29:W:6:GLN:HG2	29:W:29:VAL:HA	1.82	0.61
1:0:1701:A:H4'	1:0:1702:U:C5'	2.30	0.61
1:0:2036:C:C1'	17:K:44:LEU:HG	2.30	0.61
8:B:294:TYR:HE2	38:B:629:HOH:O	1.82	0.61
9:C:78:ARG:HH11	9:C:78:ARG:HG3	1.66	0.61
29:W:65:VAL:CG1	29:W:116:LEU:HD13	2.30	0.61
1:0:1544:U:H2'	1:0:1545:C:H6	1.66	0.60
1:0:2004:U:H4'	38:0:8178:HOH:O	2.00	0.60
38:0:7680:HOH:O	8:B:254:GLN:HG3	2.00	0.60
38:0:9805:HOH:O	27:U:56:ARG:HD3	2.01	0.60
2:1:25:LYS:HE2	38:2:147:HOH:O	2.00	0.60
1:0:308:U:C4	1:0:342:C:H1'	2.36	0.60
1:0:660:A:H4'	1:0:661:G:O5'	2.01	0.60
1:0:794:U:H3	1:0:819:A:H61	1.49	0.60
8:B:80:ARG:HD3	38:B:572:HOH:O	2.02	0.60
8:B:154:VAL:HG12	8:B:156:LYS:HG2	1.83	0.60
8:B:195:ARG:HG2	8:B:323:LEU:HD22	1.82	0.60
13:G:27:ILE:HD13	13:G:71:LEU:HD23	1.82	0.60
24:R:99:ALA:HB1	24:R:109:MET:HE3	1.83	0.60
24:R:111:ILE:HG23	24:R:145:LEU:HD11	1.83	0.60
1:0:1972:U:H2'	1:0:1973:A:H5'	1.83	0.60
8:B:74:ILE:HG13	38:B:539:HOH:O	2.00	0.60
15:I:84:SER:HB3	15:I:92:VAL:CG2	2.32	0.60
16:J:133:GLY:O	16:J:137:GLU:HG3	2.00	0.60
1:0:2445:U:H2'	1:0:2446:G:C8	2.37	0.60
6:9:13:A:O2'	6:9:14:G:H5''	2.01	0.60
16:J:26:VAL:HG13	16:J:36:VAL:HG11	1.82	0.60
8:B:66:GLU:OE1	8:B:328:ARG:HD2	2.00	0.60
11:E:3:VAL:HG22	11:E:49:ILE:HB	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:23:ILE:HG23	14:H:123:ILE:CD1	2.31	0.60
24:R:47:LEU:HB2	24:R:89:LEU:HD21	1.83	0.60
26:T:43:ASN:HD22	26:T:108:ARG:NH2	1.98	0.60
26:T:73:HIS:HD2	26:T:88:PRO:HG3	1.66	0.60
1:0:470:U:O2'	2:1:16:HIS:CD2	2.53	0.60
1:0:544:G:C3'	1:0:545:G:H5''	2.32	0.60
1:0:1205:U:H2'	1:0:1206:U:C5'	2.31	0.60
16:J:45:VAL:HG23	16:J:130:VAL:O	2.00	0.60
19:M:164:THR:HG23	19:M:165:GLY:N	2.15	0.60
1:0:1130:U:H2'	1:0:1131:G:O4'	2.01	0.60
8:B:217:ARG:HG3	8:B:257:THR:CG2	2.30	0.60
15:I:108:HIS:N	15:I:109:PRO:HD2	2.16	0.60
16:J:75:PRO:HG2	16:J:105:LEU:CD2	2.32	0.60
26:T:52:ARG:HB2	26:T:95:ASN:HB3	1.82	0.60
11:E:107:PHE:CE2	11:E:108:LEU:HD13	2.37	0.60
19:M:15:PRO:HA	19:M:20:LEU:HD23	1.84	0.60
22:P:8:ARG:HG3	38:P:208:HOH:O	2.02	0.60
1:0:1058:A:H2'	1:0:1060:C:H5''	1.84	0.60
4:3:65:THR:HG23	4:3:67:LEU:HG	1.84	0.60
8:B:312:ARG:HD3	8:B:315:VAL:HG13	1.82	0.60
20:N:15:GLU:OE1	20:N:17:ARG:HD2	2.02	0.60
30:X:30:MET:HE3	30:X:55:ASN:OD1	2.02	0.60
31:Y:189:ASN:ND2	31:Y:192:ASP:H	2.00	0.60
1:0:1400:C:H4'	30:X:56:GLU:HG2	1.83	0.60
1:0:1768:C:H2'	1:0:1769:C:O4'	2.02	0.60
1:0:2248:C:H3'	38:0:8518:HOH:O	2.01	0.60
26:T:24:ARG:HH21	26:T:39:ASN:ND2	1.99	0.60
31:Y:105:LYS:HE2	31:Y:198:GLY:O	2.02	0.60
1:0:2112:A:H2'	1:0:2113:G:H8	1.67	0.59
7:A:36:ASP:O	7:A:38:ILE:N	2.34	0.59
17:K:34:VAL:HG21	17:K:46:LYS:O	2.02	0.59
19:M:133:LEU:O	19:M:134:ILE:HD13	2.01	0.59
20:N:64:SER:C	20:N:66:LEU:H	2.10	0.59
23:Q:94:GLN:O	23:Q:95:GLU:HB2	2.02	0.59
29:W:125:HIS:HE1	38:W:4003:HOH:O	1.85	0.59
1:0:2382:A:H5'	38:0:8765:HOH:O	2.01	0.59
38:9:357:HOH:O	20:N:147:ILE:HD12	2.01	0.59
13:G:23:ILE:O	13:G:27:ILE:HG13	2.02	0.59
28:V:12:THR:CG2	28:V:15:GLU:HG3	2.23	0.59
1:0:820:G:C5	7:A:171:LYS:HB2	2.38	0.59
20:N:179:LEU:HA	20:N:184:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:71:VAL:HG11	26:T:90:PRO:CB	2.30	0.59
30:X:43:VAL:HG22	30:X:76:ARG:NH1	2.17	0.59
1:O:1379:A:H1'	38:O:7015:HOH:O	2.01	0.59
1:O:2679:G:H2'	1:O:2681:A:OP2	2.03	0.59
29:W:13:MET:CE	29:W:17:ILE:HG22	2.30	0.59
1:O:2827:A:H2'	1:O:2828:G:O4'	2.02	0.59
6:9:28:U:H5''	20:N:40:ASN:HD21	1.66	0.59
8:B:57:GLU:O	8:B:63:GLU:HB3	2.03	0.59
16:J:107:ASN:HD22	16:J:109:TYR:H	1.50	0.59
18:L:30:ARG:NH2	38:L:332:HOH:O	2.35	0.59
20:N:37:ARG:CZ	38:N:4040:HOH:O	2.49	0.59
1:O:90:A:H2'	1:O:91:G:O4'	2.03	0.59
7:A:43:VAL:HG21	7:A:59:GLU:HG3	1.84	0.59
13:G:16:LYS:O	13:G:20:VAL:HG23	2.02	0.59
18:L:114:VAL:HG11	38:L:375:HOH:O	2.02	0.59
21:O:38:ARG:NH1	38:O:4017:HOH:O	2.35	0.59
22:P:80:ARG:HG2	22:P:87:ARG:CZ	2.33	0.59
26:T:41:ARG:HG2	26:T:41:ARG:HH11	1.66	0.59
1:O:407:A:H5'	38:O:4968:HOH:O	2.03	0.59
1:O:583:C:H2'	1:O:584:U:C6	2.38	0.59
8:B:85:ARG:NH1	38:B:546:HOH:O	2.35	0.59
9:C:236:THR:O	9:C:237:GLU:C	2.45	0.59
20:N:47:LEU:HD12	20:N:92:ALA:CB	2.32	0.59
20:N:73:ALA:HB1	20:N:74:PRO:HD2	1.85	0.59
30:X:25:ARG:HD3	30:X:64:ALA:O	2.03	0.59
31:Y:189:ASN:C	31:Y:189:ASN:HD22	2.09	0.59
1:O:2521:A:OP2	14:H:6:ALA:HB3	2.02	0.59
7:A:37:VAL:HG22	38:A:431:HOH:O	2.02	0.59
12:F:91:VAL:CG1	12:F:92:GLY:N	2.66	0.59
26:T:43:ASN:HD22	26:T:108:ARG:CZ	2.16	0.59
28:V:5:VAL:HG23	38:V:4002:HOH:O	2.02	0.59
1:O:2851:G:O2'	1:O:2852:A:H5'	2.03	0.59
12:F:69:GLU:O	12:F:70:LYS:HG2	2.03	0.59
14:H:168:VAL:HG13	38:H:324:HOH:O	2.02	0.59
18:L:35:ARG:NH1	18:L:43:HIS:HB3	2.17	0.59
1:O:1377:C:H5'	1:O:1377:C:C6	2.38	0.59
1:O:1477:C:H5'	1:O:1868:G:C5'	2.33	0.59
8:B:125:GLU:O	8:B:129:ARG:HG3	2.01	0.59
9:C:107:ARG:NE	38:C:504:HOH:O	2.23	0.59
14:H:72:ALA:HB2	14:H:156:ALA:HB2	1.85	0.59
18:L:62:ALA:HB2	18:L:103:ALA:CB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:134:ILE:HG23	19:M:141:ILE:HD13	1.84	0.59
21:O:41:ALA:HA	38:O:4020:HOH:O	2.02	0.59
31:Y:235:GLU:CD	31:Y:235:GLU:N	2.60	0.59
1:O:1835:U:C5	1:O:1840:A:N7	2.68	0.58
1:O:2559:C:H4'	38:O:9699:HOH:O	2.02	0.58
20:N:38:LYS:HD2	20:N:114:LYS:HE3	1.83	0.58
30:X:76:ARG:HG3	30:X:76:ARG:NH1	2.18	0.58
18:L:144:ASP:HA	18:L:147:GLU:HG3	1.84	0.58
19:M:80:GLY:O	19:M:81:ARG:HD2	2.02	0.58
27:U:4:ARG:N	38:U:8801:HOH:O	2.35	0.58
29:W:35:VAL:HG23	29:W:41:TYR:CD2	2.38	0.58
1:O:512:G:O3'	1:O:513:A:H8	1.86	0.58
1:O:547:A:H3'	38:O:5256:HOH:O	2.02	0.58
9:C:246:ARG:HB3	9:C:246:ARG:NH1	2.18	0.58
20:N:86:LEU:O	20:N:90:LEU:HG	2.03	0.58
22:P:135:ALA:HB1	22:P:139:ARG:HH12	1.67	0.58
24:R:39:THR:HB	24:R:42:GLU:CG	2.33	0.58
31:Y:141:THR:HG23	38:Y:449:HOH:O	2.01	0.58
1:O:1213:C:O2'	1:O:1214:G:H5'	2.03	0.58
11:E:10:ASP:HA	38:E:4004:HOH:O	2.03	0.58
22:P:7:LYS:HD3	22:P:21:VAL:CG2	2.33	0.58
31:Y:234:VAL:HG12	31:Y:235:GLU:N	2.18	0.58
1:O:1189:A:H1'	1:O:1209:C:H1'	1.86	0.58
1:O:1191:A:H2'	1:O:1193:A:H5'	1.86	0.58
1:O:2831:C:H2'	1:O:2832:C:H5'	1.84	0.58
1:O:2852:A:H5''	38:O:9773:HOH:O	2.03	0.58
10:D:44:ILE:HG23	10:D:45:THR:HG23	1.85	0.58
1:O:138:U:H5''	1:O:139:C:OP2	2.04	0.58
1:O:396:U:O2'	1:O:418:C:H4'	2.04	0.58
1:O:506:G:H22	1:O:509:A:H5''	1.66	0.58
1:O:603:A:H1'	1:O:605:C:C2	2.38	0.58
1:O:1157:C:H2'	1:O:1158:G:C8	2.36	0.58
1:O:2073:G:OP2	1:O:2490:A:H5'	2.04	0.58
1:O:2721:U:H4'	17:K:87:ARG:HG3	1.86	0.58
1:O:2904:U:H4'	30:X:8:ARG:NH1	2.19	0.58
8:B:217:ARG:CG	8:B:257:THR:HG22	2.32	0.58
8:B:238:ASN:HD22	8:B:240:GLY:H	1.52	0.58
10:D:91:ALA:HB1	38:D:233:HOH:O	2.03	0.58
10:D:163:VAL:HA	38:D:247:HOH:O	2.03	0.58
14:H:31:ILE:HA	14:H:66:GLU:OE1	2.04	0.58
1:O:656:G:OP2	21:O:37:ARG:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1097:A:H5''	29:W:125:HIS:NE2	2.19	0.58
1:O:1596:U:H2'	1:O:1598:A:OP2	2.03	0.58
38:O:8081:HOH:O	7:A:213:LYS:HB2	2.04	0.58
7:A:33:GLU:O	7:A:34:ASP:HB2	2.04	0.58
8:B:74:ILE:HD13	8:B:309:VAL:HG21	1.86	0.58
17:K:125:ALA:C	17:K:127:ALA:H	2.10	0.58
28:V:1:THR:HG23	28:V:2:VAL:N	2.19	0.58
1:O:962:C:H5''	38:O:6215:HOH:O	2.03	0.58
1:O:1060:C:H6	1:O:1060:C:H5'	1.68	0.58
1:O:1118:A:H62	1:O:1244:U:H3	1.51	0.58
1:O:1790:C:H2'	1:O:1791:U:C6	2.37	0.58
1:O:1862:C:H1'	38:O:7955:HOH:O	2.03	0.58
24:R:23:MET:HE3	24:R:28:SER:OG	2.03	0.58
38:O:4090:HOH:O	26:T:9:LYS:HB2	2.04	0.58
10:D:41:LEU:HA	10:D:44:ILE:HG22	1.86	0.58
15:I:134:ILE:HG22	15:I:135:GLU:N	2.18	0.58
18:L:41:HIS:H	18:L:41:HIS:CD2	2.20	0.58
18:L:130:ARG:HA	38:L:374:HOH:O	2.04	0.58
20:N:86:LEU:HD12	20:N:125:ALA:HB2	1.85	0.58
1:O:281:U:H3'	38:O:4801:HOH:O	2.04	0.58
1:O:1375:A:C2'	1:O:1376:G:H5'	2.34	0.58
12:F:16:ALA:HA	12:F:111:ILE:HD13	1.86	0.58
31:Y:187:VAL:HB	38:Y:478:HOH:O	2.02	0.58
1:O:407:A:H3'	38:O:4970:HOH:O	2.04	0.57
1:O:1182:C:H1'	1:O:1192:A:H8	1.69	0.57
1:O:1189:A:H3'	38:O:6620:HOH:O	2.03	0.57
1:O:1266:U:H4'	31:Y:115:ARG:HH21	1.69	0.57
1:O:2755:G:H1'	38:O:9634:HOH:O	2.03	0.57
2:1:25:LYS:O	2:1:25:LYS:HG2	2.04	0.57
9:C:5:ILE:HD11	9:C:16:VAL:HG23	1.85	0.57
10:D:58:VAL:CG1	10:D:60:GLU:HG2	2.34	0.57
29:W:88:THR:HG23	29:W:110:GLN:HB3	1.84	0.57
1:O:482:G:H4'	1:O:508:A:N1	2.19	0.57
1:O:1667:A:H2'	1:O:1668:U:C6	2.39	0.57
1:O:2434:A:O3'	4:3:28:GLY:HA3	2.04	0.57
1:O:517:U:H2'	1:O:518:G:H5'	1.86	0.57
1:O:1015:C:H2'	1:O:1016:U:C6	2.39	0.57
1:O:2135:A:O2'	1:O:2136:G:H5'	2.03	0.57
1:O:2361:A:H5'	1:O:2361:A:H8	1.69	0.57
1:O:2812:A:H2	1:O:2814:A:N6	2.01	0.57
38:O:9100:HOH:O	14:H:61:ARG:HG3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:50:VAL:O	10:D:71:ALA:HA	2.04	0.57
10:D:146:LYS:HZ3	20:N:107:ASN:HD21	1.52	0.57
20:N:154:LEU:HD11	20:N:157:PRO:HA	1.86	0.57
23:Q:28:ARG:HG2	38:Q:223:HOH:O	2.03	0.57
26:T:16:LEU:HA	26:T:19:ARG:HG3	1.86	0.57
31:Y:234:VAL:HG12	31:Y:235:GLU:H	1.69	0.57
1:0:1878:G:C1'	38:0:8000:HOH:O	2.45	0.57
14:H:12:ILE:HD12	14:H:57:THR:CG2	2.33	0.57
22:P:18:LYS:HE2	38:P:208:HOH:O	2.04	0.57
29:W:21:LEU:HD22	29:W:26:ILE:CD1	2.34	0.57
1:0:12:U:H2'	1:0:13:G:H5'	1.86	0.57
1:0:2243:C:H5''	38:0:8513:HOH:O	2.03	0.57
1:0:2270:G:H4'	7:A:223:ARG:NH1	2.18	0.57
9:C:19:PRO:HG2	9:C:22:PHE:CD1	2.39	0.57
31:Y:95:THR:N	31:Y:236:VAL:O	2.36	0.57
31:Y:220:GLU:HG3	38:Y:493:HOH:O	2.02	0.57
1:0:2055:A:H4'	24:R:132:ARG:NH2	2.19	0.57
1:0:2064:U:H5'	1:0:2652:U:H4'	1.86	0.57
12:F:50:VAL:HG13	12:F:60:VAL:HG11	1.87	0.57
22:P:7:LYS:HD3	22:P:21:VAL:HG22	1.86	0.57
30:X:47:ALA:HB1	30:X:82:GLU:HB3	1.86	0.57
1:0:669:G:O2'	1:0:670:G:H5'	2.05	0.57
1:0:958:G:H2'	1:0:959:C:C6	2.38	0.57
1:0:1504:A:H5'	38:0:7284:HOH:O	2.03	0.57
1:0:1741:U:O2'	1:0:2723:G:H4'	2.05	0.57
1:0:2365:G:H4'	23:Q:45:PRO:O	2.03	0.57
38:0:6882:HOH:O	31:Y:186:ARG:HD2	2.02	0.57
8:B:119:HIS:O	8:B:121:PRO:HD3	2.05	0.57
15:I:117:THR:O	15:I:121:LYS:HG3	2.04	0.57
16:J:52:GLN:HG3	16:J:53:ILE:N	2.19	0.57
20:N:151:ASP:O	20:N:154:LEU:HB2	2.05	0.57
1:0:1120:U:H5'	1:0:1121:G:OP2	2.04	0.57
3:2:20:ARG:HG3	3:2:21:VAL:H	1.70	0.57
10:D:49:PRO:HA	10:D:73:VAL:HG22	1.87	0.57
13:G:23:ILE:HD13	13:G:67:LEU:HD23	1.86	0.57
22:P:135:ALA:HB1	22:P:139:ARG:NH1	2.19	0.57
31:Y:106:THR:HG23	31:Y:107:PRO:HD2	1.85	0.57
1:0:2276:U:H2'	1:0:2277:U:C6	2.39	0.57
1:0:2548:C:OP2	8:B:5:ARG:NH2	2.38	0.57
3:2:41:HIS:HD2	3:2:44:ARG:H	1.53	0.57
4:3:73:GLU:HB3	38:3:258:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:132:HIS:HB2	8:B:137:LEU:HD22	1.87	0.57
18:L:80:ASP:HB2	18:L:90:ARG:O	2.04	0.57
19:M:24:GLN:HE21	19:M:27:ARG:HH11	1.52	0.57
30:X:51:ASP:OD2	30:X:52:PRO:HD2	2.05	0.57
1:0:585:C:H5''	38:0:5306:HOH:O	2.05	0.57
1:0:899:C:H5'	38:0:6055:HOH:O	2.04	0.57
1:0:1205:U:H2'	1:0:1206:U:H5'	1.86	0.57
1:0:1209:C:H2'	1:0:1210:G:C8	2.36	0.57
1:0:2718:C:H6	1:0:2718:C:H5'	1.70	0.57
9:C:98:ARG:NH1	38:C:493:HOH:O	2.36	0.57
24:R:33:ARG:HD2	38:R:331:HOH:O	2.04	0.57
7:A:48:ASP:HB3	38:A:435:HOH:O	2.04	0.56
10:D:88:LEU:HB2	10:D:89:PRO:HD3	1.86	0.56
12:F:38:LYS:HZ3	19:M:3:SER:HA	1.70	0.56
1:0:583:C:H2'	1:0:584:U:H6	1.69	0.56
1:0:775:G:OP1	2:1:16:HIS:HE1	1.89	0.56
1:0:1766:U:O2	1:0:1778:A:H5'	2.06	0.56
1:0:2846:C:H4'	8:B:156:LYS:HB3	1.86	0.56
1:0:2909:G:H2'	1:0:2910:A:H8	1.70	0.56
7:A:105:VAL:CG1	7:A:154:ALA:HB1	2.35	0.56
8:B:305:ASP:O	8:B:306:LYS:HB2	2.05	0.56
15:I:67:VAL:HG13	15:I:68:PRO:HD2	1.86	0.56
21:O:53:GLN:HG2	21:O:56:GLU:OE1	2.06	0.56
1:0:2667:G:H1'	1:0:2914:A:N3	2.21	0.56
1:0:2769:C:H2'	1:0:2770:G:H5'	1.87	0.56
1:0:2780:C:C1'	11:E:143:GLN:HE21	2.17	0.56
4:3:3:MET:HG3	4:3:4:PRO:HD2	1.86	0.56
4:3:3:MET:O	4:3:90:PHE:HA	2.04	0.56
7:A:94:LEU:HG	7:A:99:ILE:CD1	2.35	0.56
8:B:71:VAL:HG11	8:B:296:LEU:HB3	1.86	0.56
9:C:236:THR:O	9:C:239:ALA:N	2.39	0.56
14:H:66:GLU:HA	38:H:327:HOH:O	2.06	0.56
20:N:35:VAL:HG13	38:N:4040:HOH:O	2.04	0.56
22:P:59:ARG:NH2	22:P:66:GLN:NE2	2.45	0.56
24:R:104:PHE:CB	24:R:109:MET:HE2	2.35	0.56
29:W:149:LEU:CG	29:W:153:MET:HE2	2.29	0.56
1:0:292:G:H2'	1:0:358:G:N2	2.20	0.56
1:0:681:G:N3	1:0:681:G:H5'	2.20	0.56
1:0:945:U:O2'	29:W:43:GLY:HA3	2.04	0.56
1:0:2812:A:H1'	38:0:5225:HOH:O	2.05	0.56
15:I:100:VAL:HG11	15:I:124:VAL:CG2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:124:VAL:HG13	15:I:134:ILE:HD11	1.88	0.56
17:K:87:ARG:NE	38:K:4043:HOH:O	2.39	0.56
1:0:1183:C:N4	1:0:1184:C:H41	2.03	0.56
15:I:124:VAL:O	15:I:124:VAL:HG12	2.04	0.56
16:J:22:VAL:O	16:J:26:VAL:HG23	2.05	0.56
20:N:24:LEU:HD13	23:Q:26:PRO:HB3	1.87	0.56
20:N:49:THR:HG22	20:N:56:ASP:HB2	1.87	0.56
29:W:54:PHE:CZ	29:W:140:LYS:HB2	2.40	0.56
1:0:644:G:H5'	1:0:644:G:N3	2.20	0.56
1:0:871:G:C8	1:0:871:G:C5'	2.80	0.56
1:0:2401:A:H5'	38:0:8818:HOH:O	2.06	0.56
1:0:2565:C:H4'	38:0:9210:HOH:O	2.05	0.56
9:C:156:LEU:O	9:C:160:LEU:HG	2.05	0.56
10:D:146:LYS:HZ1	20:N:107:ASN:ND2	2.04	0.56
18:L:55:GLN:HA	18:L:58:GLN:HE21	1.70	0.56
20:N:163:PHE:O	20:N:164:ASP:O	2.23	0.56
32:Z:22:SER:O	32:Z:26:VAL:HG23	2.05	0.56
1:0:1165:G:H4'	1:0:1174:A:HO2'	1.68	0.56
3:2:36:ASN:HB3	3:2:39:ARG:HG3	1.88	0.56
7:A:65:ARG:C	7:A:66:ARG:HG3	2.31	0.56
9:C:119:ALA:HA	9:C:136:VAL:O	2.05	0.56
11:E:116:THR:HG22	11:E:151:LEU:HD22	1.88	0.56
1:0:870:G:H2'	1:0:871:G:C5'	2.27	0.56
1:0:1398:G:H2'	1:0:1399:A:C8	2.41	0.56
1:0:1461:U:H2'	1:0:1462:C:C6	2.41	0.56
1:0:1701:A:H5''	1:0:1702:U:H3'	1.86	0.56
1:0:1972:U:H2'	1:0:1973:A:C5'	2.36	0.56
1:0:2505:G:O2'	1:0:2506:A:H5'	2.05	0.56
7:A:128:LEU:HG	38:A:450:HOH:O	2.05	0.56
8:B:54:VAL:HB	38:B:536:HOH:O	2.05	0.56
8:B:154:VAL:CG1	8:B:156:LYS:HG2	2.36	0.56
11:E:2:ARG:HE	11:E:48:VAL:HG13	1.69	0.56
11:E:69:ILE:HA	11:E:72:MET:CE	2.36	0.56
18:L:26:HIS:HB2	38:L:327:HOH:O	2.06	0.56
1:0:1677:U:OP2	3:2:8:LYS:NZ	2.38	0.56
4:3:15:ASN:ND2	38:3:208:HOH:O	2.39	0.56
7:A:109:GLU:HG2	7:A:116:GLY:N	2.21	0.56
8:B:7:ARG:HG2	8:B:7:ARG:HH11	1.70	0.56
10:D:35:ALA:C	10:D:37:ALA:N	2.64	0.56
12:F:13:GLU:OE2	12:F:78:GLU:HG2	2.06	0.56
24:R:39:THR:HG22	24:R:42:GLU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:39:ALA:N	28:V:40:PRO:CD	2.69	0.56
29:W:26:ILE:O	29:W:26:ILE:HG13	2.06	0.56
1:0:1180:U:H2'	1:0:1181:A:C8	2.41	0.56
1:0:2769:C:H2'	1:0:2770:G:O4'	2.06	0.56
7:A:51:ARG:NH1	7:A:120:ARG:O	2.39	0.56
14:H:43:ALA:HB1	14:H:140:TYR:CE2	2.41	0.56
15:I:105:GLU:HA	15:I:108:HIS:NE2	2.20	0.56
19:M:78:LYS:HD3	38:M:357:HOH:O	2.06	0.56
23:Q:11:ARG:HD3	38:Q:213:HOH:O	2.06	0.56
27:U:11:THR:HG22	27:U:53:ASP:OD2	2.06	0.56
1:0:24:G:N2	1:0:518:G:H1'	2.21	0.55
1:0:272:A:H3'	38:0:4792:HOH:O	2.05	0.55
1:0:797:A:C4'	32:Z:10:ARG:N	2.69	0.55
1:0:1029:U:O2'	1:0:1273:C:OP1	2.23	0.55
1:0:2488:A:H1'	38:0:9047:HOH:O	2.05	0.55
1:0:2563:U:H2'	1:0:2565:C:O5'	2.06	0.55
6:9:34:A:H2'	6:9:35:C:O4'	2.06	0.55
6:9:56:A:O2'	10:D:14:ARG:HD3	2.06	0.55
8:B:314:ALA:CB	8:B:317:PRO:HG3	2.36	0.55
11:E:7:ILE:HD11	11:E:11:VAL:C	2.31	0.55
15:I:97:VAL:CG1	15:I:101:LYS:HE3	2.35	0.55
29:W:34:LEU:HD12	29:W:100:LEU:HD13	1.88	0.55
1:0:1434:A:H2'	1:0:1436:C:C5	2.41	0.55
1:0:2256:G:O2'	1:0:2257:G:H5'	2.05	0.55
8:B:27:ASN:HD22	8:B:27:ASN:N	1.98	0.55
9:C:88:SER:O	9:C:91:PRO:HD3	2.06	0.55
29:W:88:THR:HG22	29:W:90:TYR:HD1	1.70	0.55
1:0:188:C:H5''	19:M:163:LEU:HD21	1.88	0.55
1:0:2507:G:H2'	1:0:2510:C:H42	1.71	0.55
6:9:33:U:H2'	38:9:343:HOH:O	2.06	0.55
16:J:130:VAL:CG1	16:J:131:THR:N	2.69	0.55
1:0:671:A:O2'	1:0:672:G:H2'	2.07	0.55
1:0:1116:U:H3	1:0:1246:A:N6	1.95	0.55
1:0:1787:C:H4'	1:0:2883:A:O4'	2.05	0.55
1:0:2681:A:H4'	1:0:2682:C:H5'	1.88	0.55
1:0:2779:G:H21	11:E:143:GLN:NE2	2.03	0.55
38:0:7406:HOH:O	22:P:117:SER:HB2	2.06	0.55
8:B:265:LEU:HD21	8:B:316:ARG:HD3	1.88	0.55
11:E:68:HIS:O	11:E:72:MET:HG3	2.07	0.55
24:R:44:VAL:HG13	24:R:89:LEU:HD22	1.89	0.55
25:S:57:THR:HG22	25:S:59:ASP:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:38:GLY:C	28:V:40:PRO:HD2	2.31	0.55
30:X:47:ALA:HB1	30:X:82:GLU:CB	2.37	0.55
31:Y:155:ARG:NH1	38:Y:463:HOH:O	2.37	0.55
1:0:656:G:H5'	21:O:3:THR:HB	1.88	0.55
1:0:1380:U:H5'	38:0:7016:HOH:O	2.05	0.55
1:0:2502:C:C2'	1:0:2503:A:H5'	2.36	0.55
1:0:2904:U:H4'	30:X:8:ARG:HH12	1.71	0.55
3:2:40:ARG:HG3	3:2:45:ASN:HB2	1.88	0.55
6:9:1:U:H4'	6:9:3:A:OP1	2.06	0.55
17:K:18:ILE:HG22	17:K:93:ASN:HB2	1.88	0.55
20:N:110:THR:HB	20:N:113:SER:OG	2.05	0.55
1:0:380:A:OP2	19:M:9:ARG:HD2	2.07	0.55
1:0:1730:G:H5''	1:0:1731:C:C6	2.42	0.55
1:0:1845:A:OP2	7:A:190:ARG:NH1	2.39	0.55
9:C:7:ASP:C	9:C:9:ASP:H	2.15	0.55
14:H:168:VAL:CG1	38:H:324:HOH:O	2.54	0.55
31:Y:112:GLU:CD	31:Y:115:ARG:NH1	2.64	0.55
6:9:39:U:H1'	6:9:44:A:H61	1.71	0.55
17:K:98:VAL:HG11	17:K:102:GLU:HA	1.88	0.55
25:S:6:LYS:HB2	25:S:27:ALA:O	2.06	0.55
25:S:43:GLU:HB3	38:S:4013:HOH:O	2.06	0.55
1:0:488:U:H2'	38:0:5153:HOH:O	2.07	0.55
1:0:1165:G:H1'	1:0:1174:A:H1'	1.88	0.55
6:9:75:G:H1	6:9:106:U:H3	1.55	0.55
10:D:37:ALA:O	10:D:40:ILE:HG12	2.07	0.55
11:E:2:ARG:HE	11:E:48:VAL:CG1	2.20	0.55
19:M:122:GLN:OE1	19:M:127:LYS:HE2	2.07	0.55
26:T:50:VAL:HG12	26:T:56:ALA:HA	1.88	0.55
28:V:16:ARG:NH2	28:V:63:GLU:HG3	2.22	0.55
1:0:703:G:O2'	1:0:704:C:H5'	2.07	0.55
1:0:814:G:H2'	1:0:815:U:C6	2.41	0.55
1:0:1528:A:H2'	1:0:1529:G:O4'	2.06	0.55
1:0:1926:G:H2'	1:0:1927:A:C8	2.42	0.55
3:2:40:ARG:HG3	3:2:45:ASN:CB	2.37	0.55
10:D:54:ALA:HB2	10:D:69:ILE:HD12	1.88	0.55
12:F:21:GLU:O	12:F:24:ARG:HG2	2.06	0.55
20:N:49:THR:HG22	20:N:58:LEU:HD11	1.89	0.55
23:Q:64:GLU:HG3	23:Q:74:ASP:OD2	2.06	0.55
24:R:145:LEU:HD12	24:R:146:ILE:H	1.72	0.55
1:0:2504:A:H4'	14:H:74:ARG:HH11	1.72	0.55
2:1:1:THR:HA	38:1:204:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:200:PRO:HB3	9:C:212:VAL:HG23	1.88	0.55
12:F:56:PRO:CG	19:M:44:THR:HA	2.37	0.55
22:P:13:VAL:HG13	22:P:14:LEU:N	2.22	0.55
27:U:17:THR:CG2	27:U:18:GLY:N	2.70	0.55
29:W:90:TYR:CE2	29:W:99:ALA:HB2	2.42	0.55
29:W:110:GLN:NE2	29:W:110:GLN:HA	2.22	0.55
30:X:70:ILE:HG23	30:X:70:ILE:O	2.07	0.55
1:0:136:C:H2'	1:0:137:U:O4'	2.08	0.54
1:0:1741:U:HO2'	1:0:2723:G:H4'	1.71	0.54
20:N:176:ARG:O	20:N:180:LEU:HD13	2.07	0.54
27:U:14:GLU:OE1	27:U:15:PRO:HD2	2.07	0.54
28:V:12:THR:HG23	28:V:14:ALA:N	2.18	0.54
1:0:284:C:H4'	1:0:285:A:O5'	2.08	0.54
1:0:308:U:H5'	1:0:309:C:OP1	2.07	0.54
1:0:595:U:H2'	1:0:596:C:H6	1.72	0.54
1:0:1056:U:H2'	1:0:1057:A:O4'	2.07	0.54
1:0:1291:A:H2	38:0:6777:HOH:O	1.89	0.54
8:B:43:GLY:O	8:B:308:LEU:HD12	2.06	0.54
9:C:162:VAL:HG13	9:C:232:LEU:HD21	1.87	0.54
1:0:1537:C:H1'	38:0:7336:HOH:O	2.07	0.54
1:0:1544:U:H2'	1:0:1545:C:C6	2.42	0.54
12:F:46:GLU:O	12:F:73:PRO:HD2	2.06	0.54
14:H:102:LYS:HG3	38:H:341:HOH:O	2.06	0.54
1:0:947:U:H2'	1:0:948:G:H8	1.71	0.54
1:0:1187:U:O2'	1:0:1189:A:H2	1.91	0.54
1:0:1535:G:H2'	1:0:1536:C:C6	2.43	0.54
19:M:57:LYS:NZ	19:M:144:ASP:OD2	2.38	0.54
24:R:111:ILE:HG23	24:R:145:LEU:CD1	2.37	0.54
31:Y:99:ALA:HB2	31:Y:233:TYR:CE2	2.43	0.54
1:0:2717:C:H2'	1:0:2718:C:C5'	2.33	0.54
7:A:164:ARG:NE	38:A:456:HOH:O	2.39	0.54
23:Q:53:HIS:ND1	23:Q:55:ARG:HB2	2.23	0.54
29:W:76:ASP:O	29:W:77:ALA:C	2.49	0.54
31:Y:163:THR:HG23	38:Y:469:HOH:O	2.06	0.54
1:0:484:A:N1	1:0:506:G:H4'	2.22	0.54
1:0:2411:C:H4'	38:0:8845:HOH:O	2.06	0.54
1:0:2634:G:OP2	7:A:204:GLY:N	2.38	0.54
9:C:78:ARG:HG3	9:C:78:ARG:NH1	2.23	0.54
9:C:129:HIS:CE1	9:C:231:ARG:HA	2.43	0.54
10:D:10:PHE:CG	10:D:11:HIS:N	2.75	0.54
10:D:174:VAL:HG12	38:D:249:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:97:ARG:HD2	38:P:252:HOH:O	2.08	0.54
28:V:4:HIS:HB3	38:V:4003:HOH:O	2.08	0.54
29:W:21:LEU:HD21	29:W:48:VAL:HG13	1.90	0.54
29:W:34:LEU:CD1	29:W:100:LEU:HD13	2.38	0.54
29:W:65:VAL:HA	29:W:68:THR:CG2	2.38	0.54
1:O:1714:C:O2'	1:O:1715:C:H5'	2.08	0.54
1:O:2795:C:O2'	1:O:2796:U:H5'	2.07	0.54
8:B:254:GLN:HG2	8:B:255:GLY:N	2.22	0.54
10:D:135:VAL:HG22	10:D:136:ARG:N	2.23	0.54
15:I:130:LEU:HA	38:I:4002:HOH:O	2.06	0.54
27:U:9:CYS:HA	27:U:52:THR:CG2	2.33	0.54
27:U:52:THR:CG2	27:U:54:THR:HB	2.37	0.54
31:Y:212:ARG:HD2	38:Y:402:HOH:O	2.08	0.54
1:O:1942:A:H3'	38:O:8079:HOH:O	2.07	0.54
1:O:2256:G:C2'	1:O:2257:G:H5'	2.38	0.54
1:O:2787:C:H5	38:O:9680:HOH:O	1.90	0.54
8:B:238:ASN:ND2	8:B:240:GLY:H	2.05	0.54
10:D:65:GLU:HG3	38:D:225:HOH:O	2.07	0.54
18:L:145:LEU:HD23	18:L:145:LEU:C	2.32	0.54
20:N:151:ASP:CG	20:N:165:ALA:O	2.51	0.54
1:O:1151:G:OP1	13:G:63:ARG:NH1	2.41	0.54
18:L:43:HIS:O	18:L:44:GLU:C	2.51	0.54
24:R:25:PHE:CE2	24:R:29:LYS:HE2	2.43	0.54
25:S:57:THR:C	25:S:59:ASP:H	2.16	0.54
1:O:447:A:O2'	1:O:448:G:H5'	2.08	0.54
1:O:553:G:H5'	38:O:5266:HOH:O	2.07	0.54
1:O:2111:G:H1'	38:O:5678:HOH:O	2.08	0.54
38:O:4824:HOH:O	26:T:38:ARG:NH1	2.41	0.54
7:A:82:VAL:HG13	7:A:93:THR:HB	1.88	0.54
8:B:55:ASN:CB	8:B:63:GLU:HA	2.37	0.54
14:H:50:ILE:HD12	14:H:149:VAL:HG11	1.90	0.54
15:I:94:ASP:OD1	15:I:133:THR:HB	2.08	0.54
20:N:170:GLU:O	20:N:174:GLU:HG3	2.08	0.54
28:V:58:THR:O	28:V:62:GLU:HG3	2.08	0.54
1:O:461:C:N3	1:O:479:G:H5'	2.23	0.53
1:O:1118:A:C8	1:O:1118:A:C3'	2.85	0.53
8:B:223:ARG:HG3	8:B:232:TRP:O	2.08	0.53
9:C:34:ALA:HB3	9:C:220:THR:HG21	1.90	0.53
11:E:80:TRP:O	11:E:134:SER:HA	2.07	0.53
17:K:55:VAL:HG12	17:K:56:SER:N	2.22	0.53
22:P:10:ALA:HA	22:P:13:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:3:ALA:O	29:W:54:PHE:HA	2.08	0.53
1:0:907:A:H4'	1:0:1328:A:C2	2.43	0.53
1:0:1166:A:H1'	1:0:1192:A:C2	2.42	0.53
1:0:2717:C:O2'	1:0:2718:C:H5''	2.07	0.53
38:0:9708:HOH:O	8:B:27:ASN:HB3	2.08	0.53
10:D:40:ILE:HG13	10:D:41:LEU:N	2.22	0.53
12:F:19:ALA:O	12:F:22:VAL:HG22	2.08	0.53
32:Z:36:ASP:HB3	32:Z:45:ASP:HB3	1.88	0.53
1:0:553:G:O4'	1:0:1325:G:H5'	2.06	0.53
1:0:902:G:N7	18:L:18:HIS:HD2	2.06	0.53
1:0:920:C:H5''	1:0:921:G:O5'	2.08	0.53
1:0:1086:A:C6	29:W:11:VAL:HG11	2.44	0.53
1:0:2670:G:O2'	1:0:2671:U:H5'	2.08	0.53
1:0:2840:A:OP1	8:B:211:THR:HG23	2.08	0.53
38:0:9659:HOH:O	8:B:298:LYS:HD3	2.09	0.53
6:9:56:A:C3'	6:9:57:A:H5''	2.37	0.53
8:B:2:GLN:HA	38:B:506:HOH:O	2.07	0.53
10:D:94:ALA:HA	10:D:174:VAL:O	2.08	0.53
24:R:82:GLU:HG3	24:R:83:LYS:N	2.22	0.53
29:W:107:LEU:O	29:W:112:LEU:HB2	2.07	0.53
1:0:1242:A:OP2	16:J:60:ARG:NH2	2.41	0.53
1:0:1393:A:H2'	1:0:1394:C:C6	2.44	0.53
1:0:1735:C:OP2	8:B:234:ARG:HG3	2.09	0.53
1:0:1973:A:H2'	1:0:1974:G:O4'	2.09	0.53
1:0:2044:G:OP1	30:X:23:HIS:HE1	1.91	0.53
1:0:2784:A:H1'	11:E:60:SER:OG	2.07	0.53
6:9:64:C:C2'	6:9:65:A:H5'	2.38	0.53
8:B:41:PHE:CZ	8:B:79:MET:HG3	2.44	0.53
8:B:139:ASP:HB2	8:B:165:ARG:NE	2.23	0.53
8:B:199:TYR:CE2	8:B:268:ARG:HB2	2.43	0.53
11:E:158:ASP:OD1	11:E:160:ARG:HB2	2.08	0.53
20:N:154:LEU:O	20:N:155:GLU:HB3	2.07	0.53
26:T:49:GLU:OE2	26:T:97:ARG:NH1	2.42	0.53
31:Y:99:ALA:HB2	31:Y:233:TYR:CZ	2.43	0.53
1:0:192:A:H5'	38:0:4570:HOH:O	2.08	0.53
1:0:1595:G:O2'	1:0:1596:U:H5'	2.07	0.53
1:0:2478:U:H2'	1:0:2479:A:C8	2.44	0.53
8:B:51:VAL:CG2	8:B:327:VAL:HG13	2.38	0.53
20:N:37:ARG:HG3	20:N:37:ARG:HH11	1.74	0.53
31:Y:145:LYS:O	31:Y:147:ARG:HG2	2.09	0.53
32:Z:11:SER:HB3	32:Z:23:ARG:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1120:U:H5''	1:0:1120:U:C6	2.43	0.53
1:0:1173:A:H4'	1:0:1174:A:C8	2.44	0.53
1:0:1419:U:H2'	1:0:1685:A:C2	2.44	0.53
1:0:2589:U:H2'	1:0:2590:U:C6	2.44	0.53
6:9:28:U:H2'	6:9:29:C:C6	2.44	0.53
8:B:51:VAL:HG23	8:B:329:TYR:O	2.09	0.53
10:D:154:LYS:H	10:D:154:LYS:CD	1.97	0.53
12:F:57:GLU:O	12:F:61:MET:HG3	2.09	0.53
17:K:74:VAL:HG12	17:K:75:ARG:HG3	1.91	0.53
19:M:61:ILE:CG2	19:M:62:VAL:N	2.72	0.53
29:W:4:LEU:O	29:W:32:CYS:HA	2.09	0.53
29:W:143:THR:N	38:W:4064:HOH:O	2.42	0.53
1:0:1375:A:O2'	1:0:1376:G:H5'	2.09	0.53
1:0:1973:A:H5'	1:0:1973:A:H8	1.74	0.53
1:0:2050:G:H5''	24:R:80:TYR:O	2.09	0.53
1:0:2769:C:H2'	1:0:2770:G:C5'	2.39	0.53
38:0:5169:HOH:O	26:T:82:THR:HA	2.09	0.53
4:3:70:ARG:NH1	4:3:77:ALA:HB2	2.24	0.53
7:A:65:ARG:O	7:A:66:ARG:HG3	2.09	0.53
8:B:16:ARG:NH1	38:B:516:HOH:O	2.41	0.53
8:B:144:THR:HB	38:B:561:HOH:O	2.09	0.53
9:C:214:THR:HG21	38:C:565:HOH:O	2.08	0.53
11:E:24:GLY:HA3	11:E:76:VAL:HB	1.91	0.53
11:E:53:GLU:HB3	11:E:55:ASN:ND2	2.24	0.53
16:J:46:ILE:HD11	16:J:53:ILE:HG23	1.91	0.53
16:J:107:ASN:C	16:J:107:ASN:ND2	2.63	0.53
19:M:61:ILE:HA	38:M:330:HOH:O	2.08	0.53
20:N:89:GLY:O	20:N:92:ALA:HB3	2.08	0.53
1:0:1014:A:H2'	1:0:1015:C:H5'	1.91	0.53
1:0:1634:G:H2'	1:0:1635:U:C6	2.44	0.53
1:0:2441:U:H4'	18:L:53:ARG:HD2	1.91	0.53
9:C:27:ARG:HG2	9:C:30:LEU:HD12	1.91	0.53
9:C:115:LEU:HD13	9:C:223:LEU:HD21	1.90	0.53
10:D:63:ILE:HG13	10:D:64:ARG:N	2.24	0.53
12:F:91:VAL:CG1	12:F:92:GLY:H	2.21	0.53
17:K:7:ASP:OD2	17:K:81:ARG:NH2	2.42	0.53
18:L:66:VAL:HG23	18:L:67:ARG:N	2.22	0.53
18:L:104:ASP:O	18:L:105:TYR:HB3	2.08	0.53
20:N:37:ARG:HH21	20:N:105:GLY:HA2	1.72	0.53
1:0:282:C:H2'	1:0:283:U:O4'	2.09	0.53
1:0:1525:G:H5'	1:0:1526:A:OP2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2326:C:H4'	1:0:2412:G:H4'	1.91	0.53
1:0:2564:G:OP2	1:0:2565:C:H5''	2.09	0.53
6:9:29:C:C2'	6:9:30:C:H5'	2.36	0.53
6:9:69:U:OP1	20:N:4:PRO:HG3	2.09	0.53
8:B:56:ASP:OD1	8:B:322:ARG:HB3	2.08	0.53
8:B:139:ASP:CB	8:B:165:ARG:HE	2.22	0.53
10:D:144:ARG:O	10:D:148:SER:HB3	2.08	0.53
12:F:39:SER:HB3	12:F:45:ALA:HB2	1.91	0.53
16:J:46:ILE:HD11	16:J:53:ILE:HG21	1.90	0.53
20:N:49:THR:CG2	20:N:58:LEU:HD11	2.39	0.53
20:N:171:HIS:CE1	38:N:4031:HOH:O	2.62	0.53
21:O:50:ARG:HD2	21:O:51:TYR:CE1	2.43	0.53
25:S:57:THR:HG22	25:S:59:ASP:N	2.23	0.53
1:0:289:G:O2'	1:0:290:C:H5'	2.09	0.53
1:0:558:C:C2'	1:0:559:U:C5'	2.82	0.53
1:0:812:A:H1'	38:0:5764:HOH:O	2.08	0.53
1:0:1132:A:N6	1:0:1229:C:H2'	2.24	0.53
38:0:4840:HOH:O	9:C:188:ARG:HD2	2.08	0.53
10:D:166:ILE:HB	38:D:247:HOH:O	2.08	0.53
13:G:63:ARG:O	13:G:67:LEU:HG	2.09	0.53
13:G:71:LEU:O	13:G:73:ASP:N	2.42	0.53
25:S:52:VAL:C	25:S:53:ASN:HD22	2.17	0.53
29:W:52:VAL:CG2	29:W:53:ALA:H	2.20	0.53
1:0:244:C:OP2	12:F:38:LYS:HE3	2.09	0.52
1:0:2598:U:O2	1:0:2600:A:H8	1.92	0.52
1:0:2831:C:C2'	1:0:2832:C:H5'	2.39	0.52
4:3:56:PRO:N	38:3:245:HOH:O	2.42	0.52
6:9:8:G:H4'	23:Q:27:GLN:NE2	2.24	0.52
8:B:84:LEU:HD23	8:B:142:LEU:HD23	1.89	0.52
11:E:84:MET:HG2	11:E:168:ILE:HA	1.90	0.52
1:0:1160:G:HO2'	1:0:1190:G:H1'	1.74	0.52
1:0:1495:C:H1'	1:0:1573:A:H1'	1.92	0.52
1:0:1734:C:OP1	8:B:234:ARG:HD3	2.09	0.52
1:0:2601:A:N1	17:K:38:SER:HB2	2.24	0.52
4:3:83:TRP:HA	38:3:265:HOH:O	2.09	0.52
7:A:33:GLU:OE1	7:A:33:GLU:N	2.41	0.52
9:C:107:ARG:NH2	38:C:504:HOH:O	2.41	0.52
10:D:35:ALA:HB2	38:D:216:HOH:O	2.10	0.52
10:D:95:THR:OG1	10:D:174:VAL:HG22	2.10	0.52
11:E:93:MET:HE1	11:E:165:GLY:N	2.24	0.52
15:I:133:THR:HG22	15:I:134:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:62:PRO:HG3	17:K:65:ARG:NH2	2.23	0.52
29:W:48:VAL:O	29:W:48:VAL:HG12	2.09	0.52
29:W:142:ASP:HB2	38:W:4066:HOH:O	2.09	0.52
1:0:538:C:H5''	1:0:539:G:C8	2.44	0.52
1:0:1634:G:H3'	38:0:7450:HOH:O	2.08	0.52
1:0:1946:C:H1'	38:0:8090:HOH:O	2.08	0.52
6:9:39:U:H1'	6:9:44:A:N6	2.24	0.52
10:D:10:PHE:CD1	10:D:11:HIS:N	2.77	0.52
10:D:76:ARG:O	10:D:77:ASP:HB2	2.08	0.52
19:M:134:ILE:O	19:M:136:PRO:HD3	2.09	0.52
29:W:88:THR:HG21	29:W:96:LEU:HD13	1.90	0.52
1:0:255:A:H2'	1:0:256:C:O4'	2.09	0.52
1:0:816:G:C6	1:0:817:G:N1	2.77	0.52
1:0:947:U:H2'	1:0:948:G:C8	2.44	0.52
1:0:1118:A:H8	1:0:1119:G:H5''	1.73	0.52
1:0:1805:G:H2'	1:0:1806:G:H8	1.73	0.52
1:0:2781:U:H2'	1:0:2782:G:H5'	1.91	0.52
1:0:2802:C:H2'	1:0:2803:C:C6	2.44	0.52
8:B:177:HIS:O	8:B:181:ILE:HG13	2.09	0.52
9:C:127:ARG:HG2	9:C:127:ARG:HH11	1.73	0.52
9:C:214:THR:HG23	38:C:582:HOH:O	2.09	0.52
10:D:18:ILE:HD13	10:D:84:LEU:CD1	2.40	0.52
12:F:50:VAL:CG1	12:F:60:VAL:HG11	2.39	0.52
18:L:149:ARG:O	18:L:150:GLN:HB2	2.08	0.52
27:U:52:THR:HG22	27:U:54:THR:N	2.24	0.52
1:0:60:A:H5'	3:2:19:SER:OG	2.09	0.52
1:0:120:A:H2'	1:0:120:A:N3	2.25	0.52
1:0:1304:U:H2'	1:0:1305:C:C6	2.44	0.52
1:0:2740:G:H2'	1:0:2741:A:O4'	2.08	0.52
7:A:179:MET:HG2	7:A:186:TRP:CG	2.45	0.52
11:E:116:THR:CG2	11:E:151:LEU:HD22	2.39	0.52
12:F:105:ASP:O	12:F:109:GLU:HB2	2.09	0.52
20:N:167:ASP:O	20:N:168:LEU:HD23	2.10	0.52
28:V:39:ALA:O	28:V:41:GLU:N	2.42	0.52
30:X:30:MET:CE	30:X:55:ASN:HA	2.39	0.52
1:0:1087:G:H4'	1:0:1088:A:OP1	2.09	0.52
8:B:307:ARG:HH11	8:B:307:ARG:HB2	1.75	0.52
9:C:7:ASP:OD2	9:C:9:ASP:HB2	2.09	0.52
14:H:141:CYS:HB2	38:H:331:HOH:O	2.08	0.52
1:0:88:G:H8	1:0:88:G:H5'	1.75	0.52
1:0:474:C:O3'	9:C:73:LEU:HD21	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1015:C:H2'	1:O:1016:U:H6	1.74	0.52
38:O:6211:HOH:O	20:N:4:PRO:HD2	2.10	0.52
21:O:57:THR:O	21:O:111:VAL:HG23	2.10	0.52
1:O:317:A:H5''	26:T:52:ARG:HD2	1.92	0.52
1:O:790:A:H2'	1:O:791:A:O4'	2.10	0.52
1:O:1730:G:H5''	1:O:1731:C:H6	1.74	0.52
1:O:2781:U:H1'	11:E:139:GLU:OE2	2.10	0.52
8:B:248:ARG:NH2	38:B:611:HOH:O	2.42	0.52
8:B:260:HIS:HE1	38:B:618:HOH:O	1.91	0.52
11:E:69:ILE:HA	11:E:72:MET:HE2	1.90	0.52
15:I:87:PRO:CB	15:I:129:SER:C	2.83	0.52
15:I:88:GLN:NE2	15:I:128:THR:HG21	2.25	0.52
16:J:107:ASN:ND2	16:J:109:TYR:N	2.57	0.52
19:M:99:ARG:HD2	19:M:167:GLY:CA	2.37	0.52
20:N:61:ALA:CB	20:N:88:ALA:HB2	2.39	0.52
28:V:64:GLY:O	28:V:65:ASP:CB	2.57	0.52
29:W:13:MET:HE2	29:W:18:GLN:N	2.24	0.52
29:W:89:ASP:HB2	29:W:90:TYR:CE1	2.44	0.52
1:O:236:A:H4'	1:O:237:G:OP1	2.09	0.52
1:O:581:G:H5'	38:O:5301:HOH:O	2.09	0.52
3:2:48:ASP:O	3:2:49:GLU:HB2	2.09	0.52
8:B:205:VAL:O	8:B:307:ARG:NE	2.43	0.52
11:E:137:ASP:O	11:E:141:VAL:HG23	2.10	0.52
14:H:86:TYR:C	14:H:86:TYR:CD1	2.88	0.52
15:I:67:VAL:CG1	15:I:68:PRO:HD2	2.40	0.52
16:J:107:ASN:HD22	16:J:108:PRO:N	2.06	0.52
20:N:47:LEU:CD1	20:N:97:VAL:HG11	2.39	0.52
21:O:115:ARG:NH1	38:O:4041:HOH:O	2.41	0.52
26:T:1:SER:HA	38:T:4001:HOH:O	2.08	0.52
26:T:43:ASN:C	26:T:45:GLY:H	2.18	0.52
1:O:1287:A:O4'	29:W:117:ARG:HD3	2.09	0.52
1:O:1947:G:N2	1:O:1966:U:C2	2.78	0.52
1:O:1979:G:H2'	38:O:8127:HOH:O	2.09	0.52
6:9:51:A:H5'	20:N:160:SER:HB3	1.90	0.52
8:B:195:ARG:HD2	8:B:324:ASP:OD1	2.10	0.52
9:C:10:GLY:HA2	9:C:160:LEU:HD21	1.91	0.52
10:D:58:VAL:HG12	10:D:60:GLU:HG2	1.92	0.52
10:D:64:ARG:CD	10:D:67:ASP:HB3	2.40	0.52
10:D:128:LEU:O	10:D:128:LEU:HD23	2.10	0.52
16:J:19:MET:CE	16:J:132:LEU:HD11	2.35	0.52
16:J:131:THR:HG22	16:J:133:GLY:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:43:VAL:HG13	20:N:118:ILE:HD11	1.92	0.52
25:S:25:GLN:HG2	25:S:65:VAL:HG22	1.92	0.52
26:T:18:GLU:O	26:T:21:LYS:HG3	2.09	0.52
29:W:56:GLU:O	29:W:143:THR:HG23	2.10	0.52
30:X:49:ARG:HG2	30:X:84:ILE:HG23	1.92	0.52
31:Y:189:ASN:HA	31:Y:217:ILE:HD11	1.90	0.52
32:Z:60:CYS:O	32:Z:61:ASP:HB2	2.09	0.52
1:O:485:A:N3	1:O:487:G:H5''	2.25	0.51
1:O:1446:U:H2'	25:S:55:GLN:NE2	2.25	0.51
1:O:2600:A:H2'	1:O:2601:A:O4'	2.11	0.51
1:O:2768:A:O2'	1:O:2769:C:H5'	2.10	0.51
1:O:2785:C:H4'	1:O:2786:G:OP2	2.11	0.51
7:A:105:VAL:HG11	7:A:154:ALA:HB1	1.91	0.51
7:A:192:VAL:HB	38:A:481:HOH:O	2.10	0.51
8:B:96:PRO:HG3	38:B:546:HOH:O	2.10	0.51
8:B:109:LEU:HG	8:B:113:LEU:HD12	1.93	0.51
16:J:126:ASN:ND2	38:J:4050:HOH:O	2.42	0.51
30:X:66:THR:HG23	30:X:67:PRO:HD2	1.92	0.51
1:O:2840:A:H3'	38:O:9746:HOH:O	2.10	0.51
12:F:36:THR:HG23	12:F:97:ALA:HB2	1.91	0.51
14:H:117:ARG:O	14:H:118:ALA:C	2.53	0.51
19:M:72:ALA:HB2	19:M:93:ARG:HG2	1.93	0.51
21:O:25:VAL:HG23	21:O:26:TRP:N	2.24	0.51
21:O:59:VAL:CG2	21:O:111:VAL:HG21	2.39	0.51
22:P:116:SER:O	22:P:119:TYR:HB3	2.09	0.51
32:Z:56:GLN:HA	32:Z:62:TYR:O	2.10	0.51
1:O:37:A:H2'	1:O:38:G:C8	2.45	0.51
1:O:195:C:H5''	38:M:420:HOH:O	2.09	0.51
1:O:814:G:H2'	1:O:815:U:H6	1.74	0.51
1:O:1391:G:H2'	1:O:1392:A:H5'	1.92	0.51
1:O:2570:G:H5''	38:O:9222:HOH:O	2.09	0.51
1:O:2724:U:H2'	1:O:2725:G:O4'	2.09	0.51
9:C:19:PRO:HG2	9:C:22:PHE:CE1	2.45	0.51
19:M:27:ARG:NH2	19:M:44:THR:HG23	2.25	0.51
26:T:80:GLU:HG2	38:T:4027:HOH:O	2.10	0.51
30:X:74:ALA:HB2	30:X:85:VAL:HG13	1.92	0.51
1:O:1335:C:OP2	31:Y:207:SER:HB3	2.11	0.51
1:O:1641:A:C2'	1:O:1642:A:H5'	2.40	0.51
1:O:2769:C:O2'	1:O:2770:G:H5'	2.11	0.51
1:O:2781:U:C2'	1:O:2782:G:H5'	2.40	0.51
8:B:41:PHE:CE1	8:B:79:MET:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:118:ALA:HA	17:K:125:ALA:HB2	1.92	0.51
18:L:57:VAL:HG12	18:L:57:VAL:O	2.11	0.51
18:L:77:ALA:HB3	38:L:356:HOH:O	2.11	0.51
1:O:2634:G:H3'	38:O:9414:HOH:O	2.10	0.51
38:O:6579:HOH:O	13:G:12:ILE:HG23	2.10	0.51
2:1:45:ARG:HD2	38:1:244:HOH:O	2.11	0.51
10:D:22:VAL:HG22	10:D:74:THR:HG22	1.92	0.51
11:E:126:ILE:HB	11:E:131:LEU:HD23	1.92	0.51
12:F:43:GLY:C	12:F:45:ALA:H	2.18	0.51
13:G:20:VAL:O	13:G:24:VAL:HG23	2.10	0.51
17:K:75:ARG:O	17:K:93:ASN:HA	2.10	0.51
25:S:22:ASN:ND2	25:S:68:LEU:HB2	2.25	0.51
26:T:106:GLU:HG3	38:T:4035:HOH:O	2.10	0.51
29:W:38:THR:HG22	38:W:4020:HOH:O	2.10	0.51
1:O:285:A:C2	1:O:368:C:H4'	2.46	0.51
1:O:960:G:H3'	1:O:960:G:N3	2.25	0.51
1:O:2719:A:C2	8:B:70:PRO:HG3	2.46	0.51
38:O:9658:HOH:O	8:B:267:LYS:HD3	2.11	0.51
9:C:47:GLY:HA2	9:C:92:PRO:HB2	1.92	0.51
9:C:235:PHE:HE2	9:C:243:VAL:HG21	1.76	0.51
11:E:34:TRP:HB3	38:E:4012:HOH:O	2.10	0.51
12:F:32:GLY:N	38:F:4009:HOH:O	2.43	0.51
20:N:23:ARG:NH1	38:N:4013:HOH:O	2.42	0.51
26:T:49:GLU:HB3	26:T:59:GLU:HG3	1.92	0.51
26:T:113:GLU:O	26:T:114:SER:C	2.53	0.51
28:V:42:ASN:N	28:V:43:PRO:HD3	2.25	0.51
32:Z:53:GLY:HA2	32:Z:67:GLY:O	2.11	0.51
1:O:451:C:O2'	1:O:452:G:H5'	2.11	0.51
1:O:820:G:O2'	1:O:856:G:H4'	2.11	0.51
1:O:1024:G:H4'	29:W:41:TYR:OH	2.10	0.51
1:O:1226:G:O2'	1:O:1227:C:H5'	2.10	0.51
1:O:1634:G:H2'	1:O:1635:U:H6	1.76	0.51
1:O:1786:C:OP1	22:P:74:GLN:HG2	2.11	0.51
1:O:2081:A:H4'	16:J:69:TYR:CE1	2.46	0.51
1:O:2325:U:O2'	1:O:2411:C:H1'	2.09	0.51
8:B:258:GLY:H	8:B:260:HIS:CE1	2.28	0.51
12:F:15:ASP:O	12:F:18:GLU:HB2	2.10	0.51
14:H:61:ARG:NH1	14:H:61:ARG:HG3	2.26	0.51
15:I:96:SER:H	15:I:99:GLN:CD	2.18	0.51
15:I:105:GLU:HA	15:I:108:HIS:CE1	2.46	0.51
21:O:47:ARG:HG3	21:O:47:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:29:VAL:O	29:W:30:ASN:HB2	2.10	0.51
1:0:168:C:O5'	1:0:168:C:H6	1.93	0.51
1:0:721:A:H5''	21:O:51:TYR:CE2	2.46	0.51
1:0:1667:A:H5'	1:0:1667:A:C8	2.41	0.51
1:0:2326:C:H4'	1:0:2412:G:C4'	2.40	0.51
7:A:94:LEU:HD12	7:A:98:GLU:HB2	1.92	0.51
10:D:101:THR:O	10:D:101:THR:HG22	2.11	0.51
30:X:25:ARG:NH1	38:X:4012:HOH:O	2.44	0.51
1:0:877:G:C5'	1:0:878:G:OP1	2.56	0.51
1:0:1112:G:H1	1:0:1251:C:H42	1.56	0.51
38:0:7612:HOH:O	22:P:81:LYS:HG2	2.10	0.51
8:B:137:LEU:HD21	8:B:140:LEU:HD21	1.92	0.51
9:C:79:ARG:O	9:C:87:ARG:HG2	2.11	0.51
14:H:102:LYS:HD3	14:H:122:LYS:CD	2.35	0.51
15:I:91:PHE:HD2	15:I:131:GLY:HA2	1.75	0.51
23:Q:75:ILE:HA	38:Q:238:HOH:O	2.10	0.51
28:V:38:GLY:O	28:V:41:GLU:HG3	2.11	0.51
29:W:21:LEU:HB3	29:W:26:ILE:CG1	2.41	0.51
1:0:814:G:H1'	38:0:5767:HOH:O	2.09	0.51
1:0:1654:U:H2'	7:A:47:HIS:CD2	2.44	0.51
1:0:1666:C:O2'	1:0:1667:A:C5'	2.59	0.51
1:0:2812:A:C2	1:0:2814:A:N6	2.76	0.51
10:D:40:ILE:HG23	38:D:219:HOH:O	2.10	0.51
10:D:135:VAL:HG22	10:D:136:ARG:H	1.76	0.51
11:E:105:GLU:HG2	11:E:113:PRO:HB3	1.93	0.51
27:U:25:ASP:OD2	27:U:26:GLY:N	2.44	0.51
1:0:1003:U:H4'	14:H:91:ARG:O	2.10	0.50
38:0:8286:HOH:O	24:R:139:PRO:HD2	2.11	0.50
7:A:100:PRO:HG2	7:A:103:VAL:CG2	2.37	0.50
10:D:140:ARG:O	10:D:144:ARG:HG2	2.11	0.50
15:I:113:SER:HB2	15:I:118:ASN:HB2	1.93	0.50
20:N:49:THR:CG2	20:N:56:ASP:HB2	2.41	0.50
1:0:282:C:O2'	1:0:283:U:H5'	2.12	0.50
1:0:2005:G:H3'	1:0:2005:G:OP2	2.11	0.50
1:0:2361:A:H5''	38:0:8725:HOH:O	2.09	0.50
1:0:2387:U:H2'	1:0:2388:C:C6	2.46	0.50
1:0:2453:G:H4'	18:L:50:GLY:C	2.36	0.50
1:0:2467:A:O2'	1:0:2468:A:H2'	2.12	0.50
1:0:2582:G:O3'	17:K:41:LYS:HA	2.11	0.50
38:0:8978:HOH:O	18:L:37:LYS:HE2	2.11	0.50
8:B:81:ALA:O	8:B:186:GLY:HA3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:73:VAL:HG23	18:L:74:THR:N	2.26	0.50
18:L:97:VAL:HG12	18:L:98:GLU:O	2.10	0.50
1:0:69:A:H5'	1:0:69:A:C8	2.46	0.50
1:0:449:A:N7	9:C:43:LYS:HG2	2.26	0.50
1:0:527:U:H2'	1:0:528:G:C8	2.46	0.50
1:0:1279:U:O2	1:0:1279:U:H2'	2.12	0.50
1:0:1441:G:O2'	1:0:1442:A:H5'	2.11	0.50
1:0:1594:C:OP2	22:P:120:ARG:HD2	2.11	0.50
1:0:1761:U:H5''	22:P:83:LYS:HA	1.93	0.50
1:0:2114:C:O2'	1:0:2115:U:H5'	2.11	0.50
1:0:2424:U:H1'	23:Q:7:LEU:HD12	1.94	0.50
1:0:2506:A:O2'	1:0:2507:G:C8	2.62	0.50
8:B:55:ASN:CG	8:B:63:GLU:HA	2.36	0.50
11:E:77:THR:OG1	11:E:78:GLU:N	2.44	0.50
12:F:117:GLU:C	12:F:119:ARG:H	2.18	0.50
23:Q:21:ARG:HG2	23:Q:22:GLY:H	1.76	0.50
26:T:82:THR:C	26:T:84:GLY:H	2.20	0.50
32:Z:42:CYS:SG	32:Z:44:GLU:HB2	2.51	0.50
1:0:61:G:OP1	3:2:17:GLN:HG2	2.11	0.50
1:0:383:A:H5'	38:0:4994:HOH:O	2.11	0.50
1:0:545:G:H8	1:0:545:G:C5'	2.19	0.50
1:0:941:G:O2'	1:0:942:U:H5'	2.11	0.50
1:0:2252:A:C5	1:0:2253:G:H1'	2.47	0.50
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.93	0.50
7:A:105:VAL:HG12	7:A:106:CYS:N	2.25	0.50
8:B:199:TYR:HE2	8:B:268:ARG:HB2	1.76	0.50
9:C:7:ASP:O	9:C:9:ASP:N	2.43	0.50
15:I:87:PRO:C	15:I:89:GLU:N	2.68	0.50
17:K:75:ARG:HH21	17:K:94:ALA:CB	2.25	0.50
26:T:26:THR:HA	26:T:39:ASN:HB3	1.93	0.50
30:X:30:MET:HE1	30:X:55:ASN:HA	1.94	0.50
31:Y:109:LEU:HA	38:Y:417:HOH:O	2.11	0.50
1:0:764:C:H2'	1:0:765:G:O4'	2.11	0.50
1:0:1421:C:H2'	1:0:1422:U:H6	1.76	0.50
17:K:81:ARG:HH11	17:K:81:ARG:HG2	1.76	0.50
18:L:73:VAL:HG11	18:L:118:LEU:HD21	1.93	0.50
20:N:37:ARG:CD	36:N:201:CL:CL	2.96	0.50
29:W:65:VAL:HG12	29:W:116:LEU:HD13	1.93	0.50
1:0:290:C:O2'	1:0:291:C:H5'	2.12	0.50
1:0:1684:A:O2'	1:0:1685:A:H5''	2.11	0.50
1:0:1711:A:O2'	1:0:1712:A:H5'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2694:A:H4'	11:E:91:PHE:HE1	1.76	0.50
1:0:2880:A:H2'	1:0:2881:C:H5'	1.92	0.50
8:B:48:MET:HG2	8:B:72:THR:HA	1.94	0.50
11:E:103:VAL:HG22	11:E:115:ARG:HB3	1.94	0.50
15:I:87:PRO:HB3	15:I:129:SER:C	2.36	0.50
24:R:39:THR:HB	24:R:42:GLU:CD	2.36	0.50
1:0:522:U:O2'	1:0:1366:C:H5'	2.11	0.50
1:0:2072:G:C6	1:0:2533:C:H1'	2.47	0.50
1:0:2419:U:H5''	1:0:2420:G:H5'	1.94	0.50
6:9:88:G:OP1	29:W:130:HIS:NE2	2.41	0.50
9:C:200:PRO:HB3	9:C:212:VAL:CG2	2.41	0.50
22:P:115:SER:O	22:P:116:SER:C	2.54	0.50
1:0:466:A:H2'	1:0:467:G:O4'	2.12	0.50
1:0:1527:A:H1'	1:0:1528:A:C8	2.46	0.50
1:0:1853:C:OP1	7:A:231:LYS:HG3	2.11	0.50
1:0:2300:A:H4'	1:0:2301:A:O5'	2.12	0.50
19:M:46:LEU:O	19:M:50:ARG:HG3	2.12	0.50
20:N:43:VAL:O	20:N:84:THR:HG21	2.12	0.50
25:S:81:ILE:HG12	38:S:4028:HOH:O	2.12	0.50
1:0:64:G:H2'	1:0:65:C:O4'	2.12	0.50
1:0:517:U:C2'	1:0:518:G:H5'	2.42	0.50
1:0:1543:G:N1	1:0:1641:A:OP2	2.36	0.50
1:0:1855:G:H8	7:A:144:GLU:OE2	1.94	0.50
1:0:2671:U:H5''	8:B:161:VAL:O	2.12	0.50
1:0:2878:U:H2'	1:0:2879:A:O4'	2.12	0.50
7:A:66:ARG:HH11	7:A:66:ARG:CB	2.24	0.50
12:F:99:THR:HG23	12:F:99:THR:O	2.12	0.50
15:I:134:ILE:HG22	15:I:135:GLU:H	1.77	0.50
17:K:28:GLU:OE2	17:K:58:THR:HG21	2.12	0.50
19:M:169:ARG:NH1	38:M:413:HOH:O	2.43	0.50
24:R:113:HIS:O	24:R:145:LEU:HD12	2.12	0.50
26:T:47:THR:HB	26:T:100:ASP:HB3	1.94	0.50
29:W:35:VAL:HG22	29:W:36:PRO:O	2.12	0.50
1:0:195:C:H2'	1:0:196:G:H5'	1.94	0.49
1:0:653:U:H5''	38:O:4017:HOH:O	2.11	0.49
1:0:1102:C:H5	38:O:6483:HOH:O	1.94	0.49
1:0:1201:C:H5''	38:O:6630:HOH:O	2.12	0.49
1:0:1333:U:H2'	1:0:1334:C:C6	2.46	0.49
38:9:357:HOH:O	20:N:147:ILE:HB	2.12	0.49
8:B:14:GLY:HA2	8:B:15:PRO:C	2.37	0.49
10:D:58:VAL:HB	10:D:62:ASP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:11:VAL:CG1	11:E:12:ASP:N	2.75	0.49
15:I:84:SER:HB3	15:I:92:VAL:HG21	1.94	0.49
18:L:73:VAL:HG23	18:L:74:THR:H	1.77	0.49
26:T:40:VAL:HG22	26:T:41:ARG:N	2.27	0.49
1:0:119:A:H2'	1:0:120:A:H5''	1.94	0.49
1:0:571:C:O5'	1:0:571:C:H6	1.94	0.49
1:0:596:C:H2'	1:0:597:A:H8	1.77	0.49
1:0:598:C:H2'	1:0:599:G:H8	1.76	0.49
1:0:656:G:H3'	21:O:37:ARG:HH12	1.77	0.49
1:0:790:A:H1'	1:0:1710:A:H2'	1.94	0.49
1:0:821:U:H2'	1:0:822:C:C6	2.41	0.49
1:0:1762:C:H2'	1:0:1763:C:H6	1.77	0.49
1:0:2371:G:H5'	38:0:8744:HOH:O	2.11	0.49
9:C:246:ARG:HB3	9:C:246:ARG:HH11	1.77	0.49
13:G:64:ASN:HD22	13:G:64:ASN:N	2.10	0.49
19:M:65:VAL:CG2	19:M:105:ALA:HB2	2.41	0.49
1:0:559:U:H2'	1:0:560:U:O4'	2.12	0.49
1:0:702:G:O2'	1:0:703:G:H5'	2.12	0.49
1:0:1118:A:C8	1:0:1119:G:H5''	2.46	0.49
1:0:1307:A:H2'	1:0:1308:A:C8	2.46	0.49
1:0:1942:A:O2'	1:0:1943:C:H5'	2.11	0.49
2:1:22:CYS:HA	38:1:242:HOH:O	2.11	0.49
18:L:89:PHE:N	38:L:357:HOH:O	2.44	0.49
18:L:133:VAL:HB	38:L:374:HOH:O	2.12	0.49
19:M:47:ASP:CG	19:M:48:LYS:N	2.71	0.49
31:Y:126:PRO:HG2	31:Y:128:PHE:CE1	2.47	0.49
1:0:595:U:H2'	1:0:596:C:C6	2.47	0.49
1:0:1778:A:H2'	1:0:1779:A:H5'	1.95	0.49
9:C:107:ARG:O	9:C:111:VAL:HG23	2.11	0.49
14:H:80:LEU:O	14:H:84:GLY:HA3	2.13	0.49
14:H:91:ARG:HH11	14:H:138:THR:CB	2.24	0.49
16:J:79:PHE:HB3	16:J:103:VAL:HG11	1.94	0.49
26:T:38:ARG:HG3	26:T:38:ARG:HH11	1.77	0.49
1:0:189:A:OP1	19:M:171:ARG:NH2	2.45	0.49
1:0:820:G:C6	7:A:171:LYS:HB2	2.48	0.49
1:0:1069:C:H2'	1:0:1070:A:O4'	2.13	0.49
1:0:1715:C:H1'	22:P:57:ASN:HD21	1.77	0.49
1:0:2265:U:H2'	1:0:2266:A:C8	2.48	0.49
1:0:2668:G:H2'	1:0:2669:U:C6	2.48	0.49
8:B:75:GLU:C	8:B:77:PRO:HD3	2.37	0.49
14:H:94:PRO:HA	14:H:127:ALA:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:95:LEU:HA	15:I:99:GLN:OE1	2.12	0.49
20:N:34:LEU:HD13	20:N:47:LEU:HD21	1.95	0.49
21:O:14:LEU:HD23	21:O:102:ILE:HD11	1.93	0.49
28:V:1:THR:O	28:V:3:LEU:N	2.45	0.49
29:W:122:ARG:NH2	29:W:154:ARG:OXT	2.43	0.49
1:0:67:A:H5''	1:0:69:A:C8	2.48	0.49
1:0:1039:G:H2'	1:0:1040:A:O4'	2.12	0.49
1:0:1181:A:H2'	1:0:1182:C:H5'	1.94	0.49
1:0:1375:A:H2'	1:0:1376:G:H5'	1.92	0.49
1:0:2533:C:H6	1:0:2533:C:C5'	2.22	0.49
1:0:2764:C:H2'	1:0:2765:C:H6	1.76	0.49
8:B:329:TYR:CE2	27:U:15:PRO:HG2	2.48	0.49
10:D:93:LEU:HD23	38:D:233:HOH:O	2.12	0.49
20:N:73:ALA:N	38:N:4031:HOH:O	2.45	0.49
23:Q:32:GLU:HA	23:Q:71:TYR:OH	2.12	0.49
27:U:20:MET:HE2	27:U:30:HIS:CE1	2.48	0.49
1:0:130:C:H2'	38:0:4389:HOH:O	2.12	0.49
1:0:903:U:OP2	18:L:11:ARG:NH1	2.44	0.49
1:0:1316:G:H1'	1:0:1340:G:N2	2.28	0.49
1:0:1416:G:H2'	1:0:1417:G:H5'	1.93	0.49
1:0:1593:C:C6	22:P:120:ARG:HD3	2.47	0.49
1:0:1633:C:H5''	1:0:1634:G:OP1	2.13	0.49
1:0:1783:A:O2'	1:0:1784:U:H5'	2.12	0.49
1:0:1825:U:O2'	1:0:1826:C:H5'	2.13	0.49
1:0:2526:C:O2'	1:0:2527:U:H5'	2.13	0.49
7:A:18:ALA:O	7:A:20:SER:N	2.42	0.49
9:C:151:GLN:O	9:C:154:VAL:HB	2.13	0.49
10:D:128:LEU:HD23	10:D:128:LEU:C	2.37	0.49
12:F:100:ASP:O	12:F:101:ALA:O	2.31	0.49
17:K:24:THR:HB	17:K:64:MET:HE2	1.94	0.49
19:M:181:GLU:OE1	19:M:181:GLU:N	2.37	0.49
20:N:5:ARG:HG3	23:Q:18:PRO:HB3	1.94	0.49
30:X:78:GLU:HG2	30:X:79:GLU:N	2.27	0.49
1:0:694:A:C2'	1:0:695:C:H5'	2.41	0.49
1:0:834:G:H3'	1:0:835:U:H4'	1.95	0.49
1:0:1200:A:H1'	38:0:6635:HOH:O	2.13	0.49
1:0:1236:A:C8	16:J:63:ILE:HD11	2.48	0.49
1:0:1497:G:H4'	1:0:1627:G:O2'	2.13	0.49
1:0:1559:A:OP2	1:0:1559:A:H8	1.95	0.49
1:0:2837:U:H1'	8:B:307:ARG:HH12	1.77	0.49
1:0:2896:A:H5''	38:0:9810:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:2:GLN:HB3	38:C:415:HOH:O	2.13	0.49
9:C:237:GLU:HB2	38:C:523:HOH:O	2.13	0.49
11:E:84:MET:HE1	11:E:148:ILE:CD1	2.43	0.49
18:L:125:PHE:CZ	18:L:140:VAL:HG13	2.47	0.49
20:N:143:ARG:HA	20:N:172:PHE:CD2	2.48	0.49
26:T:71:VAL:CG1	26:T:90:PRO:HB3	2.36	0.49
29:W:88:THR:CG2	29:W:89:ASP:H	2.20	0.49
1:O:1119:G:H22	1:O:1246:A:H2	1.55	0.49
1:O:1185:U:H2'	1:O:1186:C:C6	2.48	0.49
1:O:1771:U:H5'	32:Z:20:ARG:HH21	1.76	0.49
1:O:2312:G:H2'	1:O:2313:C:H5'	1.94	0.49
1:O:2468:A:H61	4:3:48:ASN:HD21	1.60	0.49
1:O:2636:C:H3'	38:O:9419:HOH:O	2.12	0.49
7:A:153:ARG:HB2	7:A:153:ARG:NH1	2.28	0.49
7:A:180:LYS:NZ	38:A:469:HOH:O	2.45	0.49
8:B:243:ASN:HA	8:B:244:PRO:C	2.38	0.49
10:D:138:GLY:N	38:D:245:HOH:O	2.36	0.49
19:M:49:ALA:C	19:M:54:TYR:HB3	2.38	0.49
19:M:60:VAL:C	19:M:61:ILE:HD12	2.37	0.49
22:P:114:LEU:HA	22:P:118:GLN:NE2	2.28	0.49
24:R:39:THR:O	24:R:40:ALA:C	2.55	0.49
1:O:635:A:H2'	1:O:636:G:H5''	1.94	0.49
1:O:654:A:OP2	21:O:38:ARG:HD3	2.12	0.49
1:O:705:C:O2	1:O:705:C:H2'	2.13	0.49
1:O:1299:G:O6	18:L:6:ARG:HD3	2.13	0.49
7:A:36:ASP:C	7:A:38:ILE:H	2.20	0.49
7:A:153:ARG:CB	7:A:153:ARG:HH11	2.26	0.49
15:I:87:PRO:HD3	38:I:4009:HOH:O	2.13	0.49
29:W:38:THR:O	29:W:42:ARG:HB2	2.13	0.49
31:Y:107:PRO:HB3	31:Y:182:PHE:CD2	2.48	0.49
1:O:130:C:H5'	38:O:4351:HOH:O	2.13	0.48
1:O:226:A:H1'	1:O:393:G:C5	2.48	0.48
1:O:932:U:H2'	1:O:933:C:C6	2.47	0.48
1:O:1811:A:C2	1:O:2752:C:H1'	2.48	0.48
1:O:2578:G:H5'	1:O:2578:G:C8	2.43	0.48
1:O:2896:A:OP1	30:X:15:ARG:NH1	2.46	0.48
38:O:7955:HOH:O	7:A:11:ARG:HA	2.12	0.48
4:3:65:THR:HB	4:3:83:TRP:H	1.77	0.48
9:C:157:LEU:HD11	9:C:194:PHE:HZ	1.78	0.48
11:E:20:ILE:CD1	11:E:40:VAL:HG11	2.42	0.48
15:I:134:ILE:C	15:I:135:GLU:HG3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:121:PHE:HB3	38:K:4051:HOH:O	2.12	0.48
18:L:20:ASN:O	18:L:22:ARG:N	2.46	0.48
20:N:37:ARG:HE	20:N:105:GLY:HA3	1.78	0.48
24:R:59:PHE:HZ	24:R:81:PRO:HG3	1.77	0.48
30:X:66:THR:CG2	30:X:67:PRO:HD2	2.44	0.48
32:Z:10:ARG:HA	38:Z:218:HOH:O	2.11	0.48
1:0:396:U:H1'	38:0:4950:HOH:O	2.12	0.48
1:0:808:A:C5	1:0:809:G:H1'	2.48	0.48
1:0:1666:C:C2'	1:0:1667:A:C5'	2.91	0.48
38:0:6469:HOH:O	29:W:119:HIS:HE1	1.96	0.48
13:G:19:GLU:O	13:G:23:ILE:HG13	2.14	0.48
14:H:12:ILE:HG12	14:H:59:GLN:HG2	1.94	0.48
16:J:75:PRO:HD3	16:J:136:SER:OG	2.13	0.48
17:K:30:LYS:C	17:K:55:VAL:HG13	2.37	0.48
20:N:64:SER:O	20:N:66:LEU:N	2.46	0.48
22:P:98:ILE:O	22:P:98:ILE:HD13	2.13	0.48
30:X:22:ASN:C	30:X:24:LYS:H	2.21	0.48
1:0:777:U:O2'	2:1:11:LYS:HG2	2.13	0.48
1:0:1762:C:H4'	38:0:7768:HOH:O	2.13	0.48
1:0:2598:U:O2	1:0:2600:A:C8	2.66	0.48
7:A:186:TRP:CG	7:A:187:PRO:HA	2.48	0.48
8:B:171:VAL:O	8:B:175:LEU:HB2	2.12	0.48
8:B:255:GLY:O	8:B:257:THR:HG23	2.14	0.48
14:H:41:LYS:HD3	14:H:46:TYR:OH	2.12	0.48
18:L:6:ARG:NH2	38:L:308:HOH:O	2.45	0.48
18:L:62:ALA:HB2	18:L:103:ALA:HB2	1.95	0.48
19:M:164:THR:CG2	19:M:167:GLY:H	2.15	0.48
21:O:14:LEU:CD2	21:O:102:ILE:HD11	2.42	0.48
1:0:87:C:H2'	3:2:28:LYS:O	2.13	0.48
1:0:776:A:OP1	2:1:28:HIS:HE1	1.96	0.48
1:0:1277:C:OP2	21:O:19:ARG:NH1	2.47	0.48
1:0:1874:U:OP1	7:A:51:ARG:HD2	2.12	0.48
1:0:1909:A:N1	1:0:2128:G:H1'	2.27	0.48
1:0:2359:G:H3'	38:0:8727:HOH:O	2.12	0.48
3:2:41:HIS:HB3	3:2:44:ARG:HB2	1.96	0.48
4:3:56:PRO:HA	38:3:245:HOH:O	2.13	0.48
9:C:132:ASP:CB	38:C:516:HOH:O	2.58	0.48
14:H:57:THR:HG23	14:H:131:GLN:HA	1.94	0.48
14:H:59:GLN:NE2	14:H:129:ARG:NE	2.52	0.48
19:M:26:GLN:O	19:M:29:GLN:HB2	2.14	0.48
1:0:1278:A:H4'	1:0:1279:U:C4	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2314:G:C2'	1:0:2315:C:H5'	2.42	0.48
1:0:2659:U:H5''	38:0:9492:HOH:O	2.13	0.48
1:0:2909:G:H2'	1:0:2910:A:C8	2.47	0.48
11:E:5:LEU:HD21	11:E:66:GLN:HG3	1.95	0.48
15:I:73:LEU:HD12	15:I:107:LYS:NZ	2.29	0.48
19:M:98:GLN:HB2	19:M:129:HIS:NE2	2.28	0.48
21:O:44:ASN:OD1	21:O:65:LEU:HB2	2.13	0.48
29:W:11:VAL:O	29:W:12:ASN:HB2	2.13	0.48
30:X:46:ASP:OD2	30:X:46:ASP:N	2.45	0.48
1:0:84:G:O2'	1:0:85:C:H5'	2.13	0.48
1:0:228:C:H2'	1:0:229:G:H5'	1.94	0.48
1:0:722:G:H22	1:0:938:G:P	2.37	0.48
1:0:1787:C:OP1	22:P:68:LYS:HE2	2.13	0.48
1:0:2754:G:O2'	1:0:2755:G:H5'	2.14	0.48
9:C:151:GLN:HB3	38:C:527:HOH:O	2.13	0.48
10:D:81:GLU:C	10:D:83:PHE:H	2.22	0.48
19:M:54:TYR:HB2	19:M:132:ILE:HD13	1.95	0.48
20:N:37:ARG:HH21	20:N:105:GLY:N	2.12	0.48
20:N:116:PHE:HB3	20:N:136:LEU:HD23	1.95	0.48
22:P:142:ASP:O	22:P:143:ALA:O	2.30	0.48
1:0:541:C:H2'	1:0:542:A:H5'	1.94	0.48
1:0:1007:A:H2'	14:H:22:TYR:OH	2.14	0.48
1:0:1051:C:H2'	1:0:1052:G:O4'	2.14	0.48
8:B:83:ALA:HB2	8:B:101:TRP:CD2	2.49	0.48
12:F:4:VAL:HG13	12:F:76:PHE:CE1	2.48	0.48
17:K:99:ASP:OD1	17:K:101:ASN:N	2.47	0.48
18:L:129:ALA:O	18:L:133:VAL:HG23	2.14	0.48
23:Q:93:ARG:HG3	23:Q:93:ARG:HH11	1.79	0.48
24:R:104:PHE:HB3	24:R:109:MET:HE2	1.96	0.48
1:0:101:C:H2'	1:0:102:A:C8	2.49	0.48
1:0:351:A:O2'	1:0:352:A:H5'	2.13	0.48
1:0:553:G:H3'	38:0:5272:HOH:O	2.14	0.48
1:0:596:C:H2'	1:0:597:A:C8	2.48	0.48
1:0:1636:G:O2'	1:0:1637:A:H5'	2.14	0.48
1:0:1638:U:H5'	38:0:7453:HOH:O	2.14	0.48
1:0:2291:A:N9	1:0:2309:C:H5'	2.29	0.48
4:3:34:LYS:HE2	38:3:222:HOH:O	2.13	0.48
9:C:26:VAL:HG21	9:C:123:LEU:HD11	1.96	0.48
15:I:100:VAL:HG11	15:I:124:VAL:HG22	1.96	0.48
17:K:35:HIS:HB2	17:K:52:LYS:O	2.14	0.48
19:M:184:ARG:HG3	19:M:185:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:105:G:O2'	1:0:106:A:H5'	2.14	0.48
1:0:1018:A:H4'	23:Q:59:GLN:NE2	2.29	0.48
1:0:1041:U:H2'	1:0:1042:U:H5'	1.96	0.48
1:0:1477:C:H5'	1:0:1868:G:H5'	1.96	0.48
1:0:1524:U:OP1	1:0:1524:U:H4'	2.14	0.48
1:0:1882:C:OP1	7:A:192:VAL:HG23	2.14	0.48
1:0:2281:C:H2'	1:0:2282:U:H5'	1.95	0.48
1:0:2456:A:H5'	38:0:8945:HOH:O	2.14	0.48
10:D:67:ASP:O	10:D:69:ILE:HG13	2.13	0.48
11:E:34:TRP:HA	38:E:4013:HOH:O	2.13	0.48
13:G:67:LEU:O	13:G:71:LEU:HG	2.13	0.48
21:O:88:LYS:HB3	38:O:4026:HOH:O	2.13	0.48
24:R:82:GLU:HG3	24:R:83:LYS:H	1.79	0.48
24:R:132:ARG:NH2	38:R:379:HOH:O	2.46	0.48
27:U:6:CYS:C	27:U:8:TYR:H	2.22	0.48
30:X:71:ARG:HD2	38:X:4026:HOH:O	2.13	0.48
31:Y:97:LEU:C	31:Y:98:GLN:HG2	2.39	0.48
31:Y:115:ARG:NE	38:Y:423:HOH:O	2.47	0.48
32:Z:32:GLU:HA	32:Z:35:GLU:HG3	1.96	0.48
1:0:667:C:H2'	1:0:668:C:H6	1.79	0.48
1:0:1150:A:C2	13:G:20:VAL:HG21	2.49	0.48
1:0:1470:A:OP1	19:M:93:ARG:HD2	2.14	0.48
1:0:2617:G:H4'	38:0:9356:HOH:O	2.14	0.48
38:0:6451:HOH:O	29:W:9:GLY:HA3	2.13	0.48
8:B:27:ASN:H	8:B:27:ASN:ND2	2.06	0.48
8:B:268:ARG:NH2	8:B:325:PRO:HG3	2.29	0.48
9:C:27:ARG:NH1	9:C:29:ASP:OD1	2.43	0.48
9:C:136:VAL:HA	9:C:137:PRO:C	2.38	0.48
11:E:118:ILE:HD13	11:E:124:VAL:HG23	1.95	0.48
15:I:118:ASN:HA	15:I:121:LYS:CD	2.43	0.48
17:K:37:TYR:HD2	38:K:4016:HOH:O	1.97	0.48
19:M:9:ARG:HG3	38:M:338:HOH:O	2.14	0.48
20:N:184:ILE:HG23	20:N:184:ILE:O	2.14	0.48
21:O:105:ASN:HD21	21:O:109:SER:H	1.62	0.48
26:T:92:ASP:OD1	26:T:94:SER:HB3	2.14	0.48
31:Y:133:HIS:HD2	38:Y:440:HOH:O	1.96	0.48
31:Y:144:ARG:CZ	38:Y:451:HOH:O	2.62	0.48
1:0:68:U:O2'	1:0:69:A:H5''	2.14	0.47
1:0:134:U:C2	1:0:145:A:C2	3.02	0.47
1:0:533:U:H3'	38:0:5227:HOH:O	2.14	0.47
1:0:644:G:H1'	38:0:5437:HOH:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:825:U:H5''	1:0:826:U:OP1	2.14	0.47
1:0:1008:C:H5''	14:H:19:ARG:HH12	1.78	0.47
1:0:1406:A:H5'	1:0:1407:A:C8	2.48	0.47
1:0:2729:C:H4'	1:0:2893:C:O2	2.14	0.47
1:0:2735:U:H2'	1:0:2736:U:C6	2.48	0.47
1:0:2825:C:H4'	1:0:2826:G:O5'	2.14	0.47
8:B:80:ARG:O	8:B:82:VAL:HG23	2.14	0.47
18:L:34:GLY:C	18:L:36:ASP:H	2.22	0.47
18:L:125:PHE:CE1	18:L:140:VAL:HG13	2.49	0.47
20:N:158:LEU:C	20:N:159:TYR:HD1	2.22	0.47
27:U:52:THR:HG22	27:U:54:THR:HB	1.95	0.47
1:0:69:A:H5'	1:0:69:A:H8	1.78	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.47
1:0:1581:A:H61	1:0:1614:G:H1'	1.78	0.47
1:0:1948:G:H2'	1:0:1949:G:O4'	2.14	0.47
1:0:2002:C:H2'	1:0:2003:U:H5'	1.95	0.47
1:0:2100:A:H5'	38:0:8417:HOH:O	2.14	0.47
8:B:212:GLN:OE1	8:B:216:LYS:HD3	2.13	0.47
8:B:301:VAL:HG13	8:B:302:PRO:HD2	1.96	0.47
9:C:104:ASP:O	9:C:108:GLN:HG3	2.14	0.47
12:F:37:THR:O	12:F:41:GLU:HG3	2.14	0.47
12:F:78:GLU:HG3	38:F:4017:HOH:O	2.14	0.47
16:J:6:PHE:O	16:J:8:ALA:N	2.47	0.47
20:N:48:VAL:HG12	20:N:55:ASP:HB3	1.90	0.47
23:Q:23:THR:HG22	23:Q:24:SER:N	2.29	0.47
28:V:12:THR:HB	28:V:15:GLU:OE2	2.14	0.47
29:W:69:ARG:HD2	29:W:117:ARG:O	2.14	0.47
31:Y:144:ARG:NE	38:Y:451:HOH:O	2.46	0.47
31:Y:187:VAL:CG1	31:Y:205:ILE:HA	2.43	0.47
38:0:7682:HOH:O	8:B:214:PRO:HD2	2.14	0.47
6:9:3:A:H2'	38:9:330:HOH:O	2.14	0.47
6:9:34:A:O5'	6:9:34:A:H8	1.96	0.47
8:B:1:PRO:O	8:B:2:GLN:HB2	2.13	0.47
8:B:36:PRO:HG3	8:B:169:GLY:H	1.77	0.47
15:I:108:HIS:N	15:I:109:PRO:CD	2.77	0.47
17:K:32:ILE:HD11	17:K:56:SER:HB3	1.96	0.47
17:K:87:ARG:HB2	27:U:19:THR:HG23	1.95	0.47
20:N:7:LYS:HE3	23:Q:21:ARG:O	2.15	0.47
20:N:82:TYR:C	20:N:82:TYR:CD2	2.92	0.47
21:O:32:ARG:HD3	21:O:32:ARG:C	2.39	0.47
29:W:6:GLN:CB	29:W:26:ILE:HD12	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1173:A:H2	38:0:6634:HOH:O	1.96	0.47
1:0:1427:A:H61	1:0:1440:U:H1'	1.80	0.47
1:0:1840:A:H4'	1:0:1841:C:O5'	2.14	0.47
1:0:2241:C:O2'	1:0:2242:U:H5'	2.14	0.47
1:0:2388:C:H2'	1:0:2389:U:O4'	2.14	0.47
6:9:76:G:C3'	6:9:77:A:H5''	2.35	0.47
8:B:30:PRO:HB2	8:B:39:GLN:NE2	2.28	0.47
9:C:246:ARG:NH2	38:C:583:HOH:O	2.42	0.47
18:L:143:THR:CG2	18:L:144:ASP:N	2.77	0.47
20:N:67:ALA:HA	20:N:71:TRP:CB	2.44	0.47
1:0:213:G:N2	1:0:225:G:H2'	2.30	0.47
1:0:363:C:O2'	1:0:364:U:H5'	2.15	0.47
1:0:1044:C:H5''	38:0:6098:HOH:O	2.15	0.47
1:0:1154:A:H2'	1:0:1155:G:C8	2.49	0.47
1:0:1735:C:O2'	1:0:1736:A:H5'	2.13	0.47
1:0:2353:A:O2'	20:N:7:LYS:HB3	2.14	0.47
1:0:2520:G:H5'	14:H:64:SER:OG	2.15	0.47
2:1:21:ARG:HD2	2:1:39:PHE:HB2	1.97	0.47
7:A:8:ARG:HG2	38:A:413:HOH:O	2.13	0.47
8:B:175:LEU:C	8:B:175:LEU:CD2	2.88	0.47
10:D:81:GLU:C	10:D:83:PHE:N	2.72	0.47
11:E:16:ASP:O	11:E:17:HIS:HB2	2.14	0.47
14:H:142:ASN:O	14:H:144:GLU:N	2.47	0.47
20:N:37:ARG:NH2	20:N:105:GLY:CA	2.70	0.47
21:O:26:TRP:HA	21:O:26:TRP:CE3	2.49	0.47
24:R:114:VAL:HA	24:R:144:GLU:O	2.14	0.47
28:V:1:THR:O	28:V:2:VAL:C	2.56	0.47
29:W:139:GLY:O	29:W:141:HIS:CD2	2.67	0.47
1:0:2780:C:H2'	1:0:2781:U:C6	2.50	0.47
38:0:8077:HOH:O	7:A:236:GLY:HA3	2.14	0.47
9:C:233:THR:CG2	9:C:234:VAL:H	2.26	0.47
10:D:64:ARG:HD3	10:D:67:ASP:HB3	1.96	0.47
14:H:12:ILE:HG12	14:H:59:GLN:CG	2.45	0.47
16:J:39:VAL:CG1	16:J:107:ASN:HB2	2.45	0.47
27:U:13:ILE:HG12	27:U:32:CYS:HB3	1.96	0.47
30:X:80:GLU:O	30:X:80:GLU:HG2	2.14	0.47
1:0:101:C:H2'	1:0:102:A:H8	1.80	0.47
1:0:563:C:H2'	1:0:564:G:O4'	2.15	0.47
1:0:625:U:H5''	1:0:1044:C:N4	2.29	0.47
1:0:657:G:H2'	1:0:658:C:C6	2.50	0.47
1:0:946:C:O2'	1:0:947:U:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1116:U:O2'	1:0:1118:A:C2	2.56	0.47
1:0:1416:G:C2'	1:0:1417:G:H5'	2.44	0.47
1:0:1819:G:H2'	1:0:1820:G:C4'	2.40	0.47
1:0:2281:C:C2'	1:0:2282:U:H5'	2.45	0.47
1:0:2365:G:P	23:Q:15:LYS:HG3	2.54	0.47
1:0:2607:U:H4'	38:0:9306:HOH:O	2.14	0.47
3:2:31:ARG:NH1	38:2:127:HOH:O	2.48	0.47
3:2:35:ARG:HB2	38:2:132:HOH:O	2.15	0.47
4:3:30:GLN:NE2	38:3:218:HOH:O	2.43	0.47
6:9:91:C:H2'	6:9:92:G:O4'	2.15	0.47
8:B:52:VAL:O	8:B:53:LEU:HD12	2.15	0.47
10:D:23:VAL:HG21	10:D:45:THR:CG2	2.43	0.47
10:D:36:ASN:C	38:D:222:HOH:O	2.57	0.47
11:E:81:GLU:HG2	11:E:134:SER:CB	2.44	0.47
16:J:39:VAL:HG12	16:J:40:ASN:ND2	2.29	0.47
16:J:54:VAL:CG1	16:J:138:THR:HG21	2.45	0.47
17:K:106:GLY:HA3	38:K:4013:HOH:O	2.14	0.47
19:M:15:PRO:HA	19:M:20:LEU:CD2	2.45	0.47
19:M:61:ILE:HG22	19:M:62:VAL:N	2.28	0.47
20:N:11:ARG:HG3	20:N:14:ARG:NH1	2.29	0.47
20:N:94:GLU:HG3	20:N:186:LEU:HD12	1.96	0.47
20:N:100:ALA:O	20:N:129:ILE:HG23	2.15	0.47
26:T:42:VAL:CG1	26:T:62:VAL:HG21	2.44	0.47
28:V:39:ALA:C	28:V:41:GLU:N	2.72	0.47
29:W:140:LYS:C	29:W:141:HIS:HD2	2.23	0.47
30:X:43:VAL:HG12	30:X:44:ASP:N	2.30	0.47
31:Y:108:ASP:OD1	31:Y:108:ASP:N	2.48	0.47
1:0:876:A:H2'	1:0:876:A:N3	2.29	0.47
1:0:949:U:H4'	23:Q:95:GLU:HA	1.97	0.47
1:0:1236:A:C2'	1:0:1237:U:H5'	2.45	0.47
1:0:2064:U:H5'	1:0:2652:U:O3'	2.15	0.47
1:0:2114:C:OP1	7:A:1:GLY:HA2	2.15	0.47
1:0:2597:U:H2'	1:0:2598:U:H5'	1.96	0.47
1:0:2656:G:O2'	1:0:2657:G:H5'	2.15	0.47
7:A:164:ARG:CZ	38:A:456:HOH:O	2.62	0.47
8:B:304:PRO:HD2	8:B:307:ARG:CD	2.43	0.47
9:C:127:ARG:HG2	9:C:127:ARG:NH1	2.30	0.47
18:L:78:ALA:N	38:L:356:HOH:O	2.48	0.47
21:O:96:VAL:HG13	21:O:100:GLN:OE1	2.14	0.47
22:P:16:VAL:CG1	22:P:20:ARG:CZ	2.93	0.47
1:0:598:C:H2'	1:0:599:G:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:960:G:N3	1:0:960:G:C2'	2.77	0.47
1:0:1205:U:H2'	1:0:1206:U:H5''	1.97	0.47
1:0:2324:G:N2	1:0:2377:U:H1'	2.30	0.47
7:A:153:ARG:HB2	7:A:153:ARG:HH11	1.80	0.47
7:A:211:LYS:CB	38:A:504:HOH:O	2.60	0.47
8:B:24:PRO:CG	8:B:204:GLY:HA2	2.45	0.47
8:B:132:HIS:HB2	8:B:137:LEU:CD2	2.45	0.47
10:D:91:ALA:HB2	10:D:106:PHE:CD2	2.50	0.47
11:E:31:ARG:HH12	11:E:68:HIS:CE1	2.33	0.47
17:K:65:ARG:HD3	38:K:4032:HOH:O	2.15	0.47
18:L:65:ASP:HA	18:L:109:LEU:O	2.14	0.47
18:L:68:GLU:HB2	38:L:350:HOH:O	2.15	0.47
19:M:146:ASP:O	19:M:147:LEU:HD23	2.15	0.47
19:M:164:THR:HB	38:M:409:HOH:O	2.13	0.47
25:S:57:THR:HG22	25:S:58:MET:N	2.29	0.47
28:V:1:THR:O	28:V:4:HIS:CE1	2.68	0.47
1:0:327:A:N3	9:C:206:ASN:ND2	2.63	0.47
1:0:704:C:H2'	1:0:705:C:H6	1.80	0.47
1:0:2541:U:H5'	1:0:2611:G:O6	2.15	0.47
1:0:2596:A:H2	36:0:3189:CL:CL	2.35	0.47
1:0:2900:G:H2'	1:0:2901:C:O4'	2.15	0.47
2:1:1:THR:HG21	38:1:207:HOH:O	2.15	0.47
8:B:124:ALA:O	8:B:128:ILE:HG13	2.14	0.47
10:D:86:THR:HG23	38:D:231:HOH:O	2.14	0.47
12:F:70:LYS:C	12:F:72:VAL:H	2.22	0.47
14:H:48:VAL:HA	14:H:170:ARG:O	2.15	0.47
16:J:41:ALA:O	16:J:132:LEU:HD12	2.15	0.47
17:K:49:LEU:HA	17:K:73:VAL:HG12	1.97	0.47
20:N:72:GLU:HB3	20:N:171:HIS:HE1	1.80	0.47
20:N:154:LEU:CD1	20:N:157:PRO:HA	2.44	0.47
26:T:44:ALA:HA	26:T:62:VAL:HG12	1.95	0.47
1:0:23:G:H1'	1:0:520:A:N6	2.30	0.46
1:0:65:C:O2'	1:0:66:G:H5'	2.15	0.46
1:0:558:C:H2'	1:0:559:U:H5'	1.93	0.46
1:0:1064:U:H2'	1:0:1065:G:C8	2.50	0.46
1:0:1603:A:C5'	1:0:1605:G:H5'	2.45	0.46
1:0:2314:G:O2'	1:0:2315:C:H5'	2.15	0.46
2:1:45:ARG:HB3	38:1:244:HOH:O	2.14	0.46
3:2:20:ARG:CG	3:2:21:VAL:N	2.79	0.46
7:A:94:LEU:HD23	7:A:94:LEU:N	2.29	0.46
8:B:83:ALA:HA	8:B:100:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:84:LEU:HB3	8:B:100:VAL:HB	1.98	0.46
10:D:141:VAL:HG13	10:D:144:ARG:HH21	1.80	0.46
11:E:81:GLU:HA	11:E:133:VAL:O	2.15	0.46
12:F:56:PRO:HG2	19:M:44:THR:HA	1.97	0.46
12:F:58:GLU:HA	12:F:61:MET:HE2	1.97	0.46
14:H:32:ALA:C	14:H:33:GLN:HG3	2.38	0.46
16:J:51:GLU:O	16:J:55:GLU:HG3	2.15	0.46
17:K:49:LEU:HD23	17:K:50:GLY:N	2.30	0.46
1:O:152:A:O2'	1:O:153:C:H5'	2.15	0.46
1:O:806:A:H2'	1:O:807:A:O4'	2.15	0.46
1:O:870:G:OP2	7:A:3:ARG:HD3	2.15	0.46
1:O:1625:U:H4'	38:O:7442:HOH:O	2.15	0.46
1:O:2039:A:H4'	1:O:2760:C:O2'	2.16	0.46
1:O:2501:G:H1'	38:O:9075:HOH:O	2.16	0.46
1:O:2644:C:O2'	1:O:2645:U:OP1	2.29	0.46
4:3:55:VAL:HB	4:3:56:PRO:CD	2.45	0.46
9:C:133:ARG:NE	9:C:138:VAL:HG22	2.30	0.46
10:D:152:PRO:O	10:D:156:ARG:HG2	2.15	0.46
17:K:64:MET:HA	17:K:67:GLN:HE21	1.81	0.46
18:L:55:GLN:HA	18:L:58:GLN:NE2	2.30	0.46
20:N:47:LEU:HD23	20:N:47:LEU:HA	1.71	0.46
21:O:26:TRP:HB2	38:O:4009:HOH:O	2.14	0.46
28:V:1:THR:CG2	28:V:2:VAL:H	2.19	0.46
29:W:69:ARG:NH2	38:W:4068:HOH:O	2.45	0.46
30:X:54:ILE:O	30:X:57:ALA:HB3	2.15	0.46
1:O:553:G:P	31:Y:204:ARG:HH22	2.38	0.46
1:O:1168:C:H5	38:O:6595:HOH:O	1.98	0.46
1:O:1333:U:H2'	1:O:1334:C:H6	1.80	0.46
1:O:2656:G:C2'	1:O:2657:G:H5'	2.45	0.46
7:A:37:VAL:HG13	38:A:432:HOH:O	2.14	0.46
8:B:77:PRO:HG2	8:B:151:VAL:CG2	2.45	0.46
8:B:109:LEU:CG	8:B:113:LEU:HD12	2.46	0.46
9:C:95:GLU:CD	9:C:95:GLU:H	2.23	0.46
9:C:140:VAL:HG12	9:C:141:SER:N	2.30	0.46
10:D:167:GLU:HA	10:D:171:ASP:OD1	2.15	0.46
11:E:170:ARG:NH2	38:E:4042:HOH:O	2.48	0.46
14:H:151:GLU:HG3	38:H:359:HOH:O	2.15	0.46
17:K:5:GLY:O	17:K:83:PRO:HD3	2.16	0.46
17:K:66:ARG:HG2	17:K:66:ARG:HH11	1.81	0.46
21:O:26:TRP:HA	21:O:26:TRP:HE3	1.79	0.46
29:W:80:ASP:HB2	38:W:4039:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:22:ASN:O	30:X:25:ARG:HG3	2.15	0.46
31:Y:177:LYS:HD3	31:Y:181:GLY:O	2.15	0.46
1:0:31:C:H4'	38:0:4090:HOH:O	2.16	0.46
1:0:106:A:H2'	1:0:107:U:O4'	2.15	0.46
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.46
1:0:1515:A:H2'	1:0:1516:U:C6	2.50	0.46
1:0:1762:C:H2'	1:0:1763:C:C6	2.51	0.46
1:0:2505:G:H8	38:0:9080:HOH:O	1.99	0.46
1:0:2820:A:H2'	1:0:2821:C:C6	2.50	0.46
6:9:56:A:H1'	10:D:14:ARG:HG2	1.97	0.46
7:A:140:LEU:HB3	7:A:141:PRO:HD2	1.96	0.46
8:B:24:PRO:HD3	38:B:526:HOH:O	2.14	0.46
8:B:60:SER:C	8:B:62:ARG:H	2.24	0.46
11:E:145:ALA:HB1	11:E:168:ILE:CD1	2.44	0.46
15:I:133:THR:HG22	15:I:134:ILE:H	1.79	0.46
20:N:179:LEU:HA	20:N:184:ILE:CD1	2.44	0.46
31:Y:205:ILE:HB	31:Y:230:ASN:HD21	1.80	0.46
32:Z:51:GLY:HA3	38:Z:226:HOH:O	2.15	0.46
1:0:336:G:O6	26:T:54:ASP:N	2.48	0.46
1:0:541:C:C2'	1:0:542:A:C5'	2.92	0.46
1:0:1483:C:O2'	1:0:1484:G:H5'	2.14	0.46
1:0:2256:G:H2'	1:0:2257:G:C5'	2.46	0.46
17:K:64:MET:HA	17:K:67:GLN:NE2	2.31	0.46
17:K:130:MET:SD	27:U:25:ASP:O	2.73	0.46
19:M:61:ILE:HD12	19:M:61:ILE:N	2.30	0.46
29:W:67:ALA:HB2	29:W:93:ILE:HD13	1.98	0.46
30:X:80:GLU:N	38:X:4025:HOH:O	2.48	0.46
31:Y:196:VAL:CG1	31:Y:226:ILE:HD13	2.45	0.46
31:Y:216:ARG:CD	38:Y:489:HOH:O	2.63	0.46
1:0:121:U:OP2	3:2:10:ARG:NH2	2.48	0.46
1:0:1158:G:O2'	1:0:1159:G:H5'	2.15	0.46
1:0:1185:U:H5'	38:0:6617:HOH:O	2.14	0.46
1:0:1422:U:H4'	38:0:7110:HOH:O	2.14	0.46
1:0:1976:G:H5''	38:0:8114:HOH:O	2.15	0.46
1:0:2455:A:H2'	1:0:2456:A:O4'	2.16	0.46
1:0:2509:A:H2'	1:0:2510:C:O4'	2.15	0.46
38:0:5833:HOH:O	8:B:229:ARG:HD2	2.14	0.46
4:3:11:CYS:HB2	4:3:20:HIS:CE1	2.50	0.46
9:C:120:ASP:O	9:C:124:VAL:HG23	2.16	0.46
10:D:41:LEU:HA	10:D:44:ILE:CG2	2.45	0.46
11:E:84:MET:HE2	11:E:133:VAL:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:50:VAL:HG21	12:F:63:ILE:HG21	1.97	0.46
14:H:69:ARG:HB3	38:H:327:HOH:O	2.14	0.46
19:M:31:TRP:CD1	19:M:64:ARG:NH1	2.84	0.46
20:N:115:VAL:HG22	38:N:4044:HOH:O	2.15	0.46
29:W:4:LEU:HD23	29:W:54:PHE:CB	2.39	0.46
1:0:622:G:O2'	1:0:623:U:H5'	2.16	0.46
1:0:737:A:H2'	1:0:738:G:O4'	2.15	0.46
1:0:1614:G:H2'	38:0:7383:HOH:O	2.14	0.46
1:0:1619:G:H2'	1:0:1620:C:O4'	2.16	0.46
1:0:2549:C:H2'	1:0:2550:U:O4'	2.16	0.46
1:0:2708:G:H2'	1:0:2709:G:O4'	2.16	0.46
38:0:5243:HOH:O	31:Y:135:LYS:HE3	2.16	0.46
38:0:9604:HOH:O	22:P:58:SER:HB3	2.15	0.46
9:C:200:PRO:HA	38:C:552:HOH:O	2.16	0.46
11:E:15:GLN:HG3	11:E:20:ILE:HG12	1.98	0.46
14:H:50:ILE:HD12	14:H:149:VAL:CG1	2.45	0.46
15:I:102:GLN:HA	15:I:105:GLU:OE2	2.15	0.46
26:T:61:GLU:N	38:T:4021:HOH:O	2.40	0.46
1:0:894:A:C2	9:C:87:ARG:NH2	2.84	0.46
1:0:1471:A:H2'	1:0:1472:C:C6	2.49	0.46
1:0:2004:U:H2'	1:0:2004:U:O2	2.15	0.46
6:9:64:C:H2'	6:9:65:A:H5'	1.97	0.46
8:B:114:ASP:O	8:B:115:VAL:C	2.59	0.46
11:E:84:MET:HE2	11:E:133:VAL:HG23	1.98	0.46
14:H:157:TYR:CD1	14:H:157:TYR:C	2.93	0.46
20:N:154:LEU:C	20:N:156:GLU:N	2.74	0.46
26:T:25:ALA:O	26:T:39:ASN:CB	2.64	0.46
26:T:61:GLU:HG3	38:T:4018:HOH:O	2.15	0.46
28:V:24:LYS:O	28:V:27:LEU:HB3	2.16	0.46
29:W:1:MET:HB2	29:W:103:GLU:HG2	1.97	0.46
1:0:417:G:P	38:0:4977:HOH:O	2.73	0.46
1:0:545:G:H2'	1:0:546:C:O4'	2.16	0.46
1:0:699:C:C2	1:0:743:G:N2	2.84	0.46
1:0:962:C:C1'	20:N:5:ARG:NH1	2.73	0.46
1:0:1120:U:H5''	1:0:1120:U:H6	1.81	0.46
1:0:1450:C:O2'	1:0:1493:A:H2'	2.15	0.46
1:0:1878:G:O2'	1:0:1879:U:OP2	2.34	0.46
1:0:2002:C:C2'	1:0:2003:U:H5'	2.45	0.46
1:0:2421:G:H3'	1:0:2422:U:C5'	2.46	0.46
1:0:2831:C:H2'	1:0:2832:C:C5'	2.45	0.46
38:9:312:HOH:O	23:Q:27:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:80:ARG:HA	8:B:186:GLY:O	2.16	0.46
17:K:1:MET:HE3	17:K:120:ARG:CZ	2.46	0.46
25:S:32:ALA:HA	25:S:36:GLU:OE1	2.16	0.46
31:Y:216:ARG:HD3	38:Y:489:HOH:O	2.15	0.46
1:0:37:A:H2'	1:0:38:G:H8	1.80	0.46
1:0:661:G:C5	1:0:686:A:C2	3.04	0.46
1:0:675:U:O2'	9:C:42:ARG:NH1	2.49	0.46
1:0:960:G:H8	38:0:6207:HOH:O	1.98	0.46
1:0:1804:A:H2'	1:0:1805:G:C8	2.51	0.46
1:0:1878:G:H5''	38:0:7982:HOH:O	2.16	0.46
1:0:2717:C:OP1	8:B:207:LYS:HG3	2.16	0.46
38:9:440:HOH:O	20:N:65:ASP:HB3	2.14	0.46
7:A:101:GLU:OE2	7:A:131:HIS:HB2	2.16	0.46
7:A:130:THR:N	38:A:450:HOH:O	2.48	0.46
10:D:128:LEU:HB2	38:D:235:HOH:O	2.15	0.46
23:Q:4:ASN:ND2	38:Q:205:HOH:O	2.49	0.46
26:T:32:ARG:NH1	26:T:38:ARG:HH12	2.14	0.46
30:X:31:ILE:O	30:X:35:GLU:HG3	2.16	0.46
31:Y:122:ARG:NH2	38:Y:427:HOH:O	2.49	0.46
1:0:700:A:C2	18:L:71:GLU:HG2	2.51	0.45
1:0:1071:G:H4'	31:Y:154:ARG:HH22	1.80	0.45
1:0:1161:A:O5'	1:0:1161:A:H8	1.98	0.45
9:C:84:VAL:O	9:C:85:LYS:HB2	2.15	0.45
29:W:88:THR:HG22	29:W:90:TYR:CD1	2.51	0.45
1:0:130:C:H1'	38:0:4353:HOH:O	2.16	0.45
1:0:169:A:H1'	4:3:48:ASN:ND2	2.32	0.45
1:0:245:C:H2'	38:0:4738:HOH:O	2.16	0.45
1:0:407:A:H2'	1:0:408:A:C8	2.51	0.45
1:0:932:U:H2'	1:0:933:C:H6	1.81	0.45
1:0:1603:A:H5'	1:0:1605:G:C4'	2.46	0.45
1:0:2335:C:H2'	1:0:2336:G:C8	2.51	0.45
1:0:2802:C:H2'	1:0:2803:C:H6	1.81	0.45
3:2:41:HIS:CD2	3:2:44:ARG:H	2.33	0.45
6:9:5:G:O2'	6:9:6:C:H5'	2.17	0.45
7:A:132:ASP:OD1	7:A:133:ARG:N	2.49	0.45
9:C:133:ARG:HH11	9:C:133:ARG:HG3	1.81	0.45
9:C:180:SER:C	9:C:182:ARG:H	2.24	0.45
10:D:23:VAL:HG23	10:D:23:VAL:O	2.16	0.45
18:L:91:VAL:CG1	18:L:120:LEU:HD23	2.47	0.45
18:L:122:ALA:HB3	18:L:125:PHE:CZ	2.52	0.45
19:M:134:ILE:CG2	19:M:141:ILE:HD13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:73:HIS:HD2	26:T:88:PRO:CG	2.27	0.45
28:V:1:THR:C	28:V:3:LEU:N	2.73	0.45
1:O:1055:G:H1'	14:H:116:MET:HE1	1.98	0.45
8:B:280:VAL:CG1	8:B:334:SER:HA	2.46	0.45
11:E:86:VAL:CG1	11:E:129:GLU:HA	2.46	0.45
15:I:66:GLY:O	15:I:67:VAL:C	2.58	0.45
22:P:98:ILE:HD12	22:P:102:ARG:CZ	2.46	0.45
31:Y:112:GLU:HA	31:Y:112:GLU:OE1	2.17	0.45
31:Y:132:ASP:OD1	31:Y:135:LYS:HD2	2.16	0.45
1:O:2895:C:H2'	38:O:9813:HOH:O	2.17	0.45
38:O:4093:HOH:O	26:T:9:LYS:CD	2.64	0.45
6:9:6:C:O2'	20:N:33:ARG:NH2	2.46	0.45
8:B:38:VAL:HA	8:B:166:VAL:HG22	1.99	0.45
8:B:82:VAL:HG12	8:B:101:TRP:CE3	2.51	0.45
9:C:111:VAL:HB	38:C:506:HOH:O	2.15	0.45
14:H:149:VAL:HG13	38:H:358:HOH:O	2.16	0.45
20:N:42:HIS:CG	20:N:62:HIS:HE1	2.35	0.45
20:N:151:ASP:OD1	20:N:154:LEU:HD13	2.16	0.45
25:S:73:ASP:OD1	25:S:76:GLU:HG3	2.17	0.45
1:O:166:A:N7	18:L:25:GLY:HA2	2.31	0.45
1:O:264:G:H1'	1:O:265:U:H5	1.81	0.45
1:O:1450:C:C4'	1:O:1451:C:OP2	2.62	0.45
1:O:1496:A:H5'	1:O:1572:A:H1'	1.98	0.45
1:O:1733:A:H4'	8:B:212:GLN:HA	1.99	0.45
1:O:2053:G:H4'	24:R:136:TRP:CE2	2.52	0.45
1:O:2335:C:H2'	1:O:2336:G:H8	1.81	0.45
1:O:2421:G:H3'	1:O:2422:U:H5''	1.97	0.45
2:1:36:SER:O	2:1:46:ARG:HD3	2.16	0.45
8:B:305:ASP:O	8:B:306:LYS:CB	2.64	0.45
9:C:14:GLY:O	9:C:15:GLU:HB3	2.16	0.45
11:E:93:MET:HE1	11:E:165:GLY:H	1.81	0.45
20:N:11:ARG:O	20:N:15:GLU:HG3	2.15	0.45
20:N:144:GLY:O	20:N:147:ILE:CG2	2.65	0.45
21:O:11:ILE:HD13	21:O:34:GLU:HG3	1.98	0.45
24:R:96:VAL:O	24:R:99:ALA:HB3	2.16	0.45
29:W:117:ARG:HB3	29:W:117:ARG:HH11	1.82	0.45
31:Y:112:GLU:OE2	31:Y:115:ARG:NH1	2.50	0.45
1:O:60:A:O2'	1:O:61:G:H5'	2.17	0.45
1:O:285:A:H2'	1:O:286:U:O4'	2.17	0.45
1:O:777:U:HO2'	2:1:11:LYS:HG2	1.81	0.45
1:O:839:C:O2'	5:4:9:MHT:H7	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:907:A:H4'	1:0:1328:A:N1	2.31	0.45
1:0:962:C:H2'	1:0:963:C:H5'	1.99	0.45
1:0:1139:U:H2'	1:0:1140:C:C6	2.52	0.45
1:0:1942:A:H4'	38:0:8081:HOH:O	2.16	0.45
1:0:2001:G:O2'	1:0:2002:C:H5'	2.16	0.45
1:0:2104:C:O2	1:0:2485:A:N1	2.49	0.45
1:0:2353:A:H4'	1:0:2354:A:O5'	2.16	0.45
38:0:6697:HOH:O	16:J:46:ILE:HA	2.16	0.45
7:A:165:THR:O	7:A:165:THR:HG22	2.16	0.45
8:B:329:TYR:HE2	27:U:15:PRO:HG2	1.82	0.45
16:J:127:ILE:HG22	36:J:202:CL:CL	2.54	0.45
1:0:146:U:O2'	1:0:147:G:H5'	2.17	0.45
1:0:281:U:O2'	1:0:282:C:H5'	2.17	0.45
1:0:297:U:H2'	1:0:298:C:C6	2.51	0.45
1:0:821:U:H5''	38:0:5786:HOH:O	2.15	0.45
1:0:858:U:H2'	1:0:859:C:H6	1.82	0.45
1:0:958:G:H2'	1:0:959:C:H6	1.82	0.45
1:0:1186:C:H42	1:0:1190:G:H22	1.63	0.45
1:0:1625:U:H5''	38:0:7441:HOH:O	2.16	0.45
1:0:1872:C:H2'	7:A:23:TYR:HD1	1.82	0.45
1:0:2266:A:OP2	19:M:90:ARG:NH2	2.50	0.45
1:0:2478:U:H2'	1:0:2479:A:H8	1.82	0.45
1:0:2498:C:O2'	1:0:2499:U:H5'	2.16	0.45
1:0:2511:A:H5'	1:0:2511:A:H8	1.82	0.45
1:0:2515:C:H2'	1:0:2516:G:O4'	2.16	0.45
1:0:2690:U:O2'	11:E:111:LYS:HE3	2.17	0.45
1:0:2910:A:H5''	38:0:9822:HOH:O	2.17	0.45
8:B:24:PRO:HG2	8:B:204:GLY:HA2	1.98	0.45
9:C:57:PRO:HD2	9:C:73:LEU:HD22	1.98	0.45
9:C:165:ASP:O	9:C:168:ARG:HB3	2.17	0.45
10:D:21:VAL:HA	10:D:131:THR:O	2.17	0.45
16:J:74:ARG:NH1	16:J:76:ASP:HB2	2.32	0.45
18:L:91:VAL:HB	38:L:358:HOH:O	2.16	0.45
19:M:18:GLY:O	19:M:21:ALA:HB3	2.16	0.45
20:N:38:LYS:HE2	20:N:107:ASN:HD21	1.80	0.45
20:N:72:GLU:O	20:N:72:GLU:HG2	2.17	0.45
24:R:18:LEU:HD22	24:R:21:ARG:NE	2.32	0.45
24:R:114:VAL:HG13	24:R:114:VAL:O	2.17	0.45
29:W:154:ARG:C	38:W:4068:HOH:O	2.59	0.45
1:0:1183:C:H41	1:0:1192:A:H5'	1.81	0.45
1:0:1903:U:O2'	1:0:1904:A:C8	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:214:PRO:C	8:B:220:VAL:HG22	2.42	0.45
9:C:29:ASP:HB2	21:O:3:THR:HG22	1.98	0.45
20:N:72:GLU:H	20:N:171:HIS:CE1	2.34	0.45
20:N:144:GLY:O	20:N:147:ILE:HG22	2.16	0.45
22:P:40:VAL:O	22:P:44:VAL:HG23	2.17	0.45
26:T:24:ARG:NH2	26:T:39:ASN:HD22	2.14	0.45
26:T:75:GLU:O	26:T:76:ASP:HB2	2.16	0.45
29:W:21:LEU:HD22	29:W:26:ILE:HD13	1.98	0.45
30:X:20:GLU:OE1	30:X:21:PRO:HD2	2.17	0.45
30:X:45:GLU:HG3	38:X:4017:HOH:O	2.16	0.45
30:X:73:ARG:HB2	30:X:88:GLU:OE2	2.17	0.45
1:0:1261:A:H4'	38:0:6453:HOH:O	2.17	0.45
1:0:1414:A:H2'	1:0:1415:G:O4'	2.17	0.45
1:0:1588:G:C6	1:0:1589:G:N1	2.84	0.45
1:0:1624:A:H5'	1:0:1626:A:O4'	2.16	0.45
1:0:2032:U:O2'	1:0:2033:G:H5''	2.16	0.45
1:0:2054:A:C2	24:R:128:ARG:NH2	2.85	0.45
1:0:2361:A:H2'	1:0:2362:A:O4'	2.17	0.45
2:1:28:HIS:HB3	2:1:31:LYS:HB2	1.99	0.45
6:9:30:C:OP1	10:D:137:PRO:O	2.34	0.45
7:A:29:HIS:HB3	7:A:153:ARG:HH12	1.82	0.45
9:C:133:ARG:HD2	38:C:518:HOH:O	2.15	0.45
10:D:173:GLU:O	10:D:174:VAL:C	2.59	0.45
11:E:11:VAL:HG13	11:E:23:GLU:O	2.16	0.45
12:F:1:PRO:H3	12:F:4:VAL:CG2	2.30	0.45
17:K:75:ARG:HE	17:K:94:ALA:HB3	1.82	0.45
20:N:12:ARG:HH21	20:N:17:ARG:HD3	1.80	0.45
21:O:96:VAL:HG12	21:O:97:SER:N	2.31	0.45
26:T:38:ARG:NH1	26:T:38:ARG:HG3	2.31	0.45
1:0:363:C:H2'	1:0:364:U:C6	2.52	0.45
1:0:657:G:H2'	1:0:658:C:H6	1.81	0.45
1:0:902:G:N7	18:L:18:HIS:CD2	2.85	0.45
1:0:1268:C:H2'	1:0:1269:G:H8	1.82	0.45
1:0:1500:U:P	22:P:41:ARG:HH22	2.40	0.45
1:0:2782:G:O6	1:0:2790:C:H5''	2.16	0.45
2:1:25:LYS:HD2	3:2:49:GLU:N	2.25	0.45
8:B:297:VAL:HB	38:B:539:HOH:O	2.17	0.45
9:C:235:PHE:CE2	9:C:243:VAL:HG21	2.52	0.45
12:F:43:GLY:O	12:F:45:ALA:N	2.46	0.45
12:F:50:VAL:CG2	12:F:63:ILE:HG21	2.47	0.45
29:W:154:ARG:HB3	29:W:154:ARG:HE	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1028:U:H1'	38:0:6270:HOH:O	2.17	0.44
1:0:1175:G:H1'	1:0:1193:A:H2'	1.99	0.44
1:0:1659:A:H2'	1:0:1660:G:O4'	2.16	0.44
1:0:1761:U:H4'	22:P:82:GLY:O	2.18	0.44
1:0:1940:C:H4'	38:0:8079:HOH:O	2.16	0.44
1:0:2054:A:N3	24:R:128:ARG:NH2	2.65	0.44
1:0:2256:G:H2'	1:0:2257:G:H5'	1.98	0.44
1:0:2614:C:O2'	1:0:2615:U:H5'	2.17	0.44
9:C:54:LEU:HD23	9:C:79:ARG:HG3	1.99	0.44
12:F:48:VAL:CG2	12:F:74:PHE:HB3	2.47	0.44
24:R:32:ALA:O	24:R:33:ARG:C	2.61	0.44
25:S:13:LYS:HE2	38:S:4005:HOH:O	2.17	0.44
26:T:55:PHE:CG	26:T:77:VAL:HG13	2.51	0.44
30:X:75:ALA:O	30:X:83:ALA:HA	2.17	0.44
1:0:24:G:H22	1:0:518:G:H1'	1.82	0.44
1:0:1930:A:H2'	1:0:1931:A:C8	2.52	0.44
1:0:1940:C:H1'	38:0:8074:HOH:O	2.17	0.44
1:0:2781:U:H2'	1:0:2782:G:C5'	2.47	0.44
1:0:2821:C:H4'	8:B:116:PRO:HB3	1.99	0.44
8:B:84:LEU:HD23	8:B:142:LEU:CD2	2.46	0.44
8:B:98:THR:HG22	8:B:99:GLU:H	1.81	0.44
9:C:246:ARG:NE	38:C:583:HOH:O	2.39	0.44
18:L:56:LYS:HA	38:L:302:HOH:O	2.16	0.44
18:L:124:ASP:OD1	18:L:149:ARG:NH2	2.50	0.44
20:N:86:LEU:HD21	20:N:180:LEU:CD1	2.47	0.44
20:N:119:GLN:O	20:N:123:ILE:HG13	2.17	0.44
29:W:7:LEU:CD1	29:W:53:ALA:HB2	2.48	0.44
1:0:1490:G:H4'	1:0:1533:A:OP1	2.17	0.44
1:0:1909:A:H2'	1:0:1910:A:C8	2.53	0.44
1:0:2712:G:O2'	1:0:2713:G:H5'	2.18	0.44
1:0:2911:C:H3'	38:0:9823:HOH:O	2.16	0.44
3:2:19:SER:O	3:2:36:ASN:ND2	2.51	0.44
8:B:7:ARG:CD	8:B:9:GLY:O	2.65	0.44
8:B:217:ARG:CD	8:B:257:THR:HG22	2.47	0.44
8:B:240:GLY:HA3	38:B:608:HOH:O	2.17	0.44
9:C:131:PHE:CD2	9:C:232:LEU:HD22	2.52	0.44
9:C:246:ARG:NH1	38:C:584:HOH:O	2.49	0.44
11:E:26:ASN:HB3	11:E:76:VAL:C	2.43	0.44
11:E:126:ILE:HB	11:E:131:LEU:CD2	2.48	0.44
18:L:10:SER:O	18:L:11:ARG:HB3	2.18	0.44
19:M:125:ARG:HD3	38:M:390:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:29:LYS:HD3	38:R:332:HOH:O	2.17	0.44
24:R:33:ARG:NH2	38:R:332:HOH:O	2.50	0.44
28:V:42:ASN:O	28:V:44:GLY:N	2.50	0.44
32:Z:20:ARG:O	32:Z:21:VAL:C	2.60	0.44
1:0:499:G:O2'	1:0:500:G:H5'	2.16	0.44
1:0:2344:G:H2'	1:0:2344:G:N3	2.33	0.44
6:9:52:A:H2'	6:9:53:G:O4'	2.18	0.44
6:9:114:G:H2'	6:9:115:C:C6	2.53	0.44
9:C:72:LYS:HG2	9:C:77:ALA:HA	1.98	0.44
38:C:542:HOH:O	26:T:2:LYS:HE2	2.17	0.44
18:L:67:ARG:HB2	18:L:112:GLY:HA3	1.99	0.44
20:N:23:ARG:NH2	20:N:55:ASP:OD1	2.50	0.44
22:P:138:GLU:O	22:P:139:ARG:C	2.60	0.44
25:S:15:MET:O	25:S:18:MET:HB3	2.18	0.44
29:W:46:ALA:O	29:W:49:ASN:HB2	2.17	0.44
30:X:10:VAL:HG11	30:X:36:HIS:HE1	1.82	0.44
31:Y:133:HIS:HA	31:Y:139:VAL:HG12	1.98	0.44
1:0:380:A:H2'	38:0:4901:HOH:O	2.15	0.44
1:0:401:C:H2'	1:0:402:U:C6	2.53	0.44
1:0:1019:C:H5'	38:0:6251:HOH:O	2.16	0.44
1:0:1137:G:H1'	38:0:6562:HOH:O	2.17	0.44
1:0:1250:C:O2'	1:0:1251:C:H5'	2.17	0.44
1:0:1478:U:H2'	1:0:1479:G:H8	1.82	0.44
1:0:2038:A:H5''	8:B:222:LYS:HG3	1.99	0.44
1:0:2055:A:H4'	24:R:132:ARG:HH21	1.82	0.44
38:0:7957:HOH:O	7:A:11:ARG:HG2	2.18	0.44
6:9:42:C:H5'	6:9:43:G:OP2	2.17	0.44
8:B:41:PHE:HA	8:B:79:MET:HE2	1.99	0.44
8:B:42:ALA:HB3	8:B:79:MET:SD	2.57	0.44
8:B:142:LEU:HD21	8:B:178:ALA:HB1	2.00	0.44
8:B:336:GLN:NE2	38:B:643:HOH:O	2.49	0.44
10:D:27:ILE:HB	10:D:69:ILE:O	2.17	0.44
10:D:56:ARG:N	38:D:225:HOH:O	2.50	0.44
10:D:86:THR:C	10:D:89:PRO:HD2	2.42	0.44
11:E:162:PHE:N	11:E:162:PHE:CD1	2.85	0.44
12:F:106:ALA:HB3	38:F:4024:HOH:O	2.18	0.44
14:H:114:ASP:N	38:H:344:HOH:O	2.50	0.44
14:H:157:TYR:C	14:H:157:TYR:HD1	2.25	0.44
16:J:19:MET:CE	16:J:132:LEU:HD21	2.47	0.44
17:K:99:ASP:OD1	17:K:99:ASP:C	2.61	0.44
22:P:83:LYS:HG3	22:P:84:ALA:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:142:ASP:C	22:P:143:ALA:O	2.61	0.44
26:T:71:VAL:HG12	26:T:72:ILE:N	2.32	0.44
29:W:26:ILE:O	29:W:26:ILE:CG1	2.64	0.44
1:O:797:A:H5'	32:Z:10:ARG:N	2.32	0.44
1:O:1025:C:P	29:W:108:ARG:NH1	2.91	0.44
1:O:1421:C:O2'	1:O:1422:U:H5'	2.17	0.44
1:O:1517:C:O2'	1:O:1518:A:H5'	2.18	0.44
1:O:1730:G:C5'	1:O:1731:C:C6	3.01	0.44
1:O:2064:U:H4'	1:O:2653:A:OP1	2.17	0.44
1:O:2637:A:H5'	38:O:9422:HOH:O	2.16	0.44
7:A:38:ILE:HD13	7:A:38:ILE:HA	1.85	0.44
7:A:53:ALA:HB3	38:A:435:HOH:O	2.17	0.44
8:B:115:VAL:HA	8:B:116:PRO:HD3	1.75	0.44
8:B:221:GLN:HE22	17:K:42:ASN:ND2	2.16	0.44
9:C:39:GLN:O	9:C:43:LYS:HD3	2.18	0.44
10:D:140:ARG:N	38:D:240:HOH:O	2.49	0.44
10:D:153:THR:O	10:D:156:ARG:HB2	2.17	0.44
11:E:154:ILE:HD11	11:E:157:LYS:HE2	1.99	0.44
17:K:112:PRO:C	17:K:113:ILE:HG13	2.42	0.44
18:L:54:PRO:HG2	18:L:57:VAL:CG2	2.47	0.44
20:N:170:GLU:HA	20:N:173:ASP:OD2	2.18	0.44
24:R:31:ILE:O	24:R:32:ALA:C	2.58	0.44
24:R:100:ASP:C	24:R:102:GLN:H	2.26	0.44
28:V:20:LEU:HD11	28:V:53:ILE:HG23	1.99	0.44
30:X:36:HIS:CE1	30:X:40:HIS:CD2	3.06	0.44
31:Y:219:GLU:HG3	31:Y:220:GLU:N	2.32	0.44
1:O:185:G:H4'	1:O:186:A:OP1	2.17	0.44
1:O:271:C:H41	1:O:378:A:H2	1.63	0.44
1:O:1181:A:C2'	1:O:1182:C:H5'	2.47	0.44
1:O:1234:U:C4	8:B:244:PRO:HB3	2.53	0.44
1:O:2268:C:H2'	1:O:2269:C:C6	2.53	0.44
1:O:2858:U:H2'	1:O:2859:C:C6	2.52	0.44
6:9:106:U:O5'	6:9:106:U:H6	2.01	0.44
10:D:15:GLU:HA	10:D:16:PRO:HD3	1.88	0.44
10:D:41:LEU:CA	10:D:44:ILE:HG22	2.46	0.44
15:I:91:PHE:HA	15:I:131:GLY:CA	2.48	0.44
17:K:27:ARG:HD2	38:K:4015:HOH:O	2.18	0.44
19:M:76:ARG:HG2	19:M:76:ARG:HH11	1.81	0.44
25:S:57:THR:CG2	25:S:58:MET:N	2.80	0.44
27:U:9:CYS:CA	27:U:52:THR:HG23	2.36	0.44
29:W:4:LEU:HD23	29:W:4:LEU:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:163:U:O3'	1:0:896:C:H4'	2.17	0.44
1:0:545:G:C8	1:0:545:G:C5'	2.99	0.44
1:0:559:U:H6	1:0:559:U:C5'	2.27	0.44
1:0:658:C:O2'	1:0:662:U:OP1	2.32	0.44
1:0:1180:U:H4'	15:I:86:GLU:HG2	2.00	0.44
1:0:1437:A:O2'	1:0:1438:G:H5'	2.18	0.44
1:0:1584:C:O2'	1:0:1585:C:H5'	2.17	0.44
1:0:1754:A:H2'	1:0:1755:A:O4'	2.18	0.44
1:0:2072:G:H3'	1:0:2073:G:C5'	2.48	0.44
1:0:2506:A:N6	1:0:2511:A:O2'	2.48	0.44
3:2:35:ARG:HG2	38:2:133:HOH:O	2.17	0.44
4:3:55:VAL:C	38:3:245:HOH:O	2.61	0.44
4:3:69:TYR:HB2	4:3:78:HIS:CE1	2.53	0.44
6:9:11:A:P	23:Q:19:ARG:HH21	2.40	0.44
8:B:69:VAL:HA	8:B:70:PRO:HD3	1.84	0.44
9:C:133:ARG:HE	9:C:138:VAL:HG22	1.83	0.44
10:D:140:ARG:HH11	10:D:140:ARG:HG3	1.82	0.44
12:F:49:PHE:HE1	12:F:98:VAL:HG23	1.83	0.44
13:G:63:ARG:N	38:G:4014:HOH:O	2.50	0.44
17:K:62:PRO:CG	17:K:65:ARG:HH21	2.31	0.44
20:N:143:ARG:NH1	20:N:173:ASP:OD1	2.50	0.44
25:S:39:ASP:O	25:S:40:ALA:C	2.61	0.44
26:T:96:VAL:HG13	26:T:97:ARG:N	2.33	0.44
31:Y:187:VAL:CG2	31:Y:192:ASP:HB2	2.33	0.44
1:0:736:A:H2'	1:0:737:A:O4'	2.18	0.44
1:0:858:U:H2'	1:0:859:C:C6	2.52	0.44
1:0:1386:G:O2'	1:0:1387:G:H5'	2.18	0.44
1:0:1513:C:O2'	1:0:1514:C:H5'	2.17	0.44
1:0:2819:C:O4'	8:B:96:PRO:HB2	2.18	0.44
4:3:16:GLU:HG3	4:3:18:GLN:HE21	1.82	0.44
4:3:20:HIS:HA	4:3:70:ARG:O	2.18	0.44
7:A:70:ALA:HA	7:A:71:PRO:HD3	1.80	0.44
10:D:167:GLU:C	10:D:169:THR:H	2.26	0.44
13:G:71:LEU:C	13:G:73:ASP:N	2.65	0.44
15:I:69:PRO:C	15:I:107:LYS:HZ1	2.26	0.44
20:N:110:THR:HB	20:N:113:SER:HG	1.82	0.44
21:O:80:ASP:OD1	21:O:81:PHE:N	2.50	0.44
30:X:41:PHE:CZ	30:X:74:ALA:HB3	2.53	0.44
31:Y:100:ARG:NH1	31:Y:215:GLU:HA	2.33	0.44
31:Y:171:PRO:O	31:Y:172:THR:C	2.61	0.44
1:0:35:U:H5'	9:C:47:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:485:A:O2'	1:0:487:G:H5'	2.18	0.43
1:0:844:A:C6	1:0:882:A:C5	3.06	0.43
1:0:952:G:N3	1:0:2302:A:H2'	2.33	0.43
1:0:1056:U:O4'	14:H:8:MET:HE3	2.18	0.43
1:0:1415:G:H5'	2:1:12:ASN:O	2.18	0.43
1:0:1573:A:H2'	1:0:1574:C:O4'	2.18	0.43
1:0:2433:A:H2'	1:0:2434:A:C8	2.52	0.43
1:0:2524:G:N2	1:0:2526:C:H41	2.12	0.43
1:0:2866:U:H4'	1:0:2867:G:H5'	2.00	0.43
7:A:223:ARG:HG3	38:A:514:HOH:O	2.17	0.43
9:C:218:VAL:N	38:C:583:HOH:O	2.50	0.43
10:D:166:ILE:HD12	38:D:247:HOH:O	2.17	0.43
15:I:70:THR:C	15:I:72:GLU:N	2.74	0.43
17:K:41:LYS:O	17:K:42:ASN:HB2	2.18	0.43
19:M:47:ASP:CG	19:M:48:LYS:H	2.25	0.43
19:M:59:GLY:HA3	19:M:141:ILE:CD1	2.47	0.43
25:S:76:GLU:HB3	38:S:4029:HOH:O	2.18	0.43
26:T:9:LYS:CE	26:T:13:ARG:NH1	2.73	0.43
28:V:4:HIS:O	28:V:8:ILE:HG13	2.18	0.43
31:Y:182:PHE:HD2	31:Y:200:THR:O	2.01	0.43
32:Z:10:ARG:HG3	32:Z:11:SER:N	2.33	0.43
1:0:688:A:N7	18:L:65:ASP:OD2	2.51	0.43
1:0:1119:G:H8	16:J:52:GLN:HE22	1.66	0.43
1:0:1174:A:C5	1:0:1201:C:H4'	2.52	0.43
1:0:2274:A:H1'	19:M:86:GLN:NE2	2.33	0.43
1:0:2809:G:H2'	1:0:2810:G:O4'	2.18	0.43
2:1:10:LYS:HG3	38:1:212:HOH:O	2.18	0.43
7:A:32:VAL:O	7:A:33:GLU:C	2.61	0.43
8:B:54:VAL:O	8:B:55:ASN:C	2.60	0.43
9:C:44:GLN:HA	38:C:439:HOH:O	2.18	0.43
10:D:64:ARG:HD3	10:D:67:ASP:CB	2.48	0.43
12:F:33:THR:HG21	12:F:59:ILE:O	2.17	0.43
14:H:38:ARG:C	14:H:40:GLN:H	2.26	0.43
14:H:83:GLU:HA	38:H:330:HOH:O	2.18	0.43
19:M:34:GLU:HB3	19:M:38:GLU:HG3	1.99	0.43
21:O:82:SER:O	21:O:83:GLY:C	2.60	0.43
24:R:9:ASP:O	24:R:13:THR:HG22	2.17	0.43
25:S:14:ALA:HA	25:S:25:GLN:NE2	2.33	0.43
26:T:25:ALA:O	26:T:39:ASN:HB2	2.18	0.43
1:0:256:C:H2'	1:0:257:G:O4'	2.18	0.43
1:0:445:U:H2'	1:0:446:G:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1207:A:N6	38:0:6642:HOH:O	2.51	0.43
1:0:1839:A:H5'	1:0:2643:G:H4'	2.00	0.43
1:0:2091:G:O3'	8:B:235:ARG:HD3	2.17	0.43
1:0:2460:A:H5''	4:3:58:GLY:O	2.18	0.43
38:0:8248:HOH:O	8:B:216:LYS:HA	2.18	0.43
4:3:56:PRO:CA	38:3:245:HOH:O	2.66	0.43
8:B:180:ASP:O	8:B:181:ILE:C	2.61	0.43
9:C:168:ARG:NH2	9:C:190:ALA:O	2.51	0.43
10:D:39:ASP:HB2	38:D:219:HOH:O	2.18	0.43
14:H:27:PRO:HD3	14:H:123:ILE:HG22	2.01	0.43
16:J:84:ARG:HB2	16:J:98:PHE:CE1	2.53	0.43
21:O:9:SER:O	21:O:10:LEU:C	2.61	0.43
21:O:35:LYS:HB3	21:O:36:PRO:HD2	2.00	0.43
22:P:22:TRP:CH2	22:P:24:ASN:HA	2.53	0.43
1:0:299:U:H5'	38:0:5026:HOH:O	2.19	0.43
1:0:667:C:H2'	1:0:668:C:C6	2.54	0.43
1:0:793:A:H5''	22:P:83:LYS:HG2	1.99	0.43
1:0:1098:A:H2'	1:0:1099:G:O4'	2.17	0.43
1:0:1119:G:N2	1:0:1246:A:H2	2.13	0.43
1:0:1119:G:H8	16:J:52:GLN:NE2	2.16	0.43
1:0:1211:G:H2'	1:0:1212:C:H6	1.83	0.43
1:0:1517:C:O2	1:0:1670:A:C2	2.71	0.43
1:0:1674:C:P	25:S:34:LYS:HG3	2.59	0.43
1:0:1718:G:O2'	1:0:1719:G:H5'	2.19	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.53	0.43
1:0:2443:C:H1'	18:L:56:LYS:HE3	2.00	0.43
1:0:2521:A:P	14:H:6:ALA:HB3	2.59	0.43
2:1:10:LYS:NZ	38:1:211:HOH:O	2.51	0.43
4:3:22:VAL:HG11	4:3:67:LEU:HD13	2.00	0.43
6:9:106:U:O2'	6:9:107:C:H5'	2.19	0.43
7:A:149:ASP:OD1	7:A:151:GLN:HB2	2.17	0.43
7:A:215:ILE:HG13	7:A:216:SER:N	2.33	0.43
8:B:190:MET:HG2	8:B:272:ILE:CG2	2.48	0.43
9:C:130:GLU:OE1	9:C:130:GLU:HA	2.17	0.43
9:C:133:ARG:NH2	38:C:517:HOH:O	2.50	0.43
12:F:68:ASP:C	12:F:70:LYS:H	2.26	0.43
16:J:39:VAL:HG11	16:J:107:ASN:CB	2.47	0.43
16:J:45:VAL:HG22	16:J:46:ILE:N	2.33	0.43
19:M:184:ARG:CG	19:M:185:PRO:HA	2.49	0.43
24:R:46:TYR:O	24:R:49:ALA:HB3	2.17	0.43
29:W:5:VAL:O	29:W:52:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:24:LEU:HD21	29:W:44:MET:SD	2.58	0.43
29:W:122:ARG:HG3	29:W:152:ALA:O	2.18	0.43
1:0:165:A:H5'	18:L:33:ALA:HB2	2.01	0.43
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.43
1:0:613:C:H2'	1:0:614:U:H6	1.83	0.43
1:0:922:A:N7	1:0:2281:C:H5'	2.34	0.43
1:0:1478:U:H2'	1:0:1479:G:C8	2.53	0.43
1:0:1617:C:C4	1:0:1643:C:H4'	2.53	0.43
1:0:2299:G:C6	1:0:2300:A:C6	3.07	0.43
1:0:2609:G:N2	8:B:238:ASN:HD21	2.17	0.43
1:0:2861:G:H4'	8:B:282:GLY:N	2.34	0.43
1:0:2906:A:H5'	1:0:2907:C:O4'	2.18	0.43
8:B:84:LEU:O	8:B:99:GLU:HA	2.18	0.43
9:C:175:LYS:HD3	9:C:184:ARG:O	2.19	0.43
16:J:108:PRO:HG2	16:J:109:TYR:CD1	2.54	0.43
19:M:99:ARG:NH1	38:M:375:HOH:O	2.49	0.43
20:N:163:PHE:O	20:N:164:ASP:OD1	2.36	0.43
23:Q:35:ASP:N	23:Q:35:ASP:OD1	2.51	0.43
25:S:8:PRO:HD2	28:V:32:ALA:HA	2.00	0.43
30:X:34:ARG:NH1	30:X:48:VAL:O	2.40	0.43
32:Z:79:VAL:O	32:Z:80:ARG:C	2.61	0.43
1:0:10:U:O4	1:0:532:A:OP2	2.36	0.43
1:0:69:A:C2'	1:0:70:A:OP2	2.67	0.43
1:0:204:A:C2'	1:0:205:U:H5'	2.49	0.43
1:0:1052:G:H2'	1:0:1052:G:N3	2.33	0.43
1:0:1102:C:H4'	38:0:6484:HOH:O	2.18	0.43
1:0:1123:A:C2	1:0:1129:C:H4'	2.54	0.43
1:0:1641:A:H2'	1:0:1642:A:C5'	2.46	0.43
1:0:1735:C:H5'	8:B:235:ARG:NH2	2.34	0.43
6:9:3:A:H2	6:9:21:G:N3	2.17	0.43
7:A:20:SER:C	7:A:22:ARG:H	2.24	0.43
7:A:36:ASP:C	7:A:38:ILE:N	2.74	0.43
10:D:24:HIS:CE1	10:D:26:GLY:H	2.37	0.43
10:D:173:GLU:OE1	10:D:174:VAL:HG23	2.19	0.43
11:E:107:PHE:CZ	11:E:152:THR:HB	2.53	0.43
11:E:137:ASP:OD1	11:E:137:ASP:C	2.61	0.43
12:F:48:VAL:HG12	12:F:97:ALA:CB	2.48	0.43
15:I:99:GLN:O	15:I:103:ILE:HG13	2.18	0.43
17:K:6:ALA:HB3	17:K:116:GLU:HG2	2.01	0.43
24:R:84:ALA:O	24:R:88:PHE:HD1	2.01	0.43
25:S:80:ARG:NH1	38:S:4029:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:20:GLU:CD	30:X:21:PRO:HD2	2.44	0.43
30:X:78:GLU:CG	30:X:79:GLU:H	2.28	0.43
31:Y:133:HIS:HA	31:Y:139:VAL:CG1	2.48	0.43
32:Z:81:ARG:O	32:Z:82:SER:C	2.62	0.43
1:0:297:U:H2'	1:0:298:C:H6	1.82	0.43
1:0:659:A:N7	21:O:63:LYS:NZ	2.64	0.43
1:0:1023:C:H2'	1:0:1024:G:O4'	2.18	0.43
1:0:1066:U:H2'	1:0:1067:A:C8	2.54	0.43
1:0:1421:C:H2'	1:0:1422:U:C6	2.52	0.43
1:0:1427:A:H61	1:0:1440:U:C1'	2.30	0.43
1:0:1477:C:H5'	1:0:1868:G:H5''	2.01	0.43
1:0:1845:A:O3'	7:A:187:PRO:HB2	2.19	0.43
1:0:2731:G:H2'	1:0:2732:U:O4'	2.18	0.43
1:0:2761:A:C4	1:0:2763:G:C8	3.07	0.43
7:A:95:PRO:HA	7:A:153:ARG:HA	1.99	0.43
7:A:164:ARG:HA	32:Z:69:TYR:CE1	2.54	0.43
8:B:157:LYS:O	8:B:159:PRO:HD3	2.18	0.43
9:C:57:PRO:O	9:C:58:ALA:C	2.61	0.43
9:C:194:PHE:HA	9:C:234:VAL:HG13	2.01	0.43
11:E:47:VAL:HG11	11:E:69:ILE:HD13	2.00	0.43
18:L:147:GLU:C	38:L:381:HOH:O	2.61	0.43
23:Q:93:ARG:HG3	23:Q:93:ARG:NH1	2.33	0.43
25:S:11:THR:O	25:S:15:MET:HG2	2.18	0.43
25:S:18:MET:HG3	25:S:74:ALA:HB1	2.00	0.43
1:0:396:U:OP2	4:3:38:ARG:HD2	2.19	0.43
1:0:1506:U:H6	1:0:1506:U:H5'	1.83	0.43
1:0:1603:A:H5''	1:0:1604:G:H3'	2.00	0.43
1:0:1925:G:O2'	1:0:1926:G:H5'	2.19	0.43
6:9:59:C:H4'	38:9:364:HOH:O	2.19	0.43
9:C:233:THR:CG2	9:C:234:VAL:N	2.78	0.43
11:E:2:ARG:HG3	11:E:50:GLU:HB3	2.00	0.43
17:K:125:ALA:C	17:K:127:ALA:N	2.77	0.43
19:M:107:ARG:NH1	38:M:378:HOH:O	2.49	0.43
20:N:108:SER:HA	20:N:109:PRO:HD3	1.82	0.43
25:S:10:VAL:HG11	28:V:36:ALA:HA	2.00	0.43
1:0:468:U:H3'	38:0:5101:HOH:O	2.18	0.43
1:0:968:G:H1'	14:H:35:LYS:HD2	2.00	0.43
1:0:1213:C:C2'	1:0:1214:G:H5'	2.49	0.43
1:0:1571:G:H1'	1:0:1627:G:N2	2.34	0.43
1:0:1600:G:H4'	38:0:7411:HOH:O	2.17	0.43
1:0:2039:A:H2'	1:0:2040:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:8:G:H4'	23:Q:27:GLN:HE21	1.84	0.43
7:A:119:ALA:C	7:A:120:ARG:HG2	2.43	0.43
8:B:13:PHE:O	8:B:16:ARG:HD2	2.19	0.43
8:B:22:GLU:HA	8:B:205:VAL:HG21	2.01	0.43
8:B:278:PRO:HD3	8:B:294:TYR:CE2	2.54	0.43
10:D:14:ARG:NH1	38:D:209:HOH:O	2.50	0.43
12:F:56:PRO:HG2	19:M:43:PRO:O	2.18	0.43
14:H:69:ARG:HD3	38:H:327:HOH:O	2.19	0.43
15:I:126:THR:HG22	15:I:126:THR:O	2.19	0.43
18:L:101:ASP:C	18:L:103:ALA:H	2.27	0.43
26:T:37:GLN:HB3	38:T:4017:HOH:O	2.19	0.43
1:0:213:G:O2'	1:0:214:U:OP2	2.37	0.43
1:0:361:C:H2'	1:0:362:G:O4'	2.19	0.43
1:0:1314:U:H5''	1:0:1316:G:O4'	2.18	0.43
1:0:2120:U:H2'	1:0:2121:G:O4'	2.19	0.43
1:0:2712:G:H5'	38:0:9537:HOH:O	2.18	0.43
1:0:2764:C:H2'	1:0:2765:C:C6	2.53	0.43
1:0:2898:G:H4'	8:B:288:GLY:HA2	2.00	0.43
6:9:29:C:H2'	6:9:30:C:C5'	2.43	0.43
7:A:105:VAL:HG13	7:A:155:THR:O	2.18	0.43
7:A:149:ASP:C	7:A:151:GLN:H	2.26	0.43
9:C:97:ASP:OD2	9:C:97:ASP:C	2.62	0.43
10:D:20:LYS:HA	10:D:75:LEU:O	2.19	0.43
12:F:46:GLU:N	38:F:4011:HOH:O	2.52	0.43
14:H:6:ALA:CA	14:H:61:ARG:HH12	2.26	0.43
14:H:49:GLN:HB3	14:H:170:ARG:CG	2.48	0.43
14:H:49:GLN:CB	14:H:170:ARG:HG3	2.46	0.43
26:T:14:ALA:HA	26:T:15:PRO:HD3	1.93	0.43
26:T:71:VAL:HG13	26:T:91:LEU:O	2.19	0.43
27:U:17:THR:HG22	27:U:18:GLY:H	1.84	0.43
30:X:76:ARG:O	30:X:77:PHE:CB	2.64	0.43
1:0:1289:C:O2'	1:0:1290:G:H5'	2.19	0.42
1:0:1427:A:N6	1:0:1440:U:H1'	2.34	0.42
1:0:1702:U:H1'	38:0:7352:HOH:O	2.20	0.42
1:0:1849:G:H1'	1:0:2011:A:N1	2.34	0.42
1:0:1929:G:H1'	38:0:8072:HOH:O	2.18	0.42
1:0:2402:A:H1'	38:0:8828:HOH:O	2.19	0.42
38:0:6158:HOH:O	21:O:39:THR:HB	2.18	0.42
6:9:3:A:OP2	6:9:25:G:N2	2.52	0.42
8:B:222:LYS:O	8:B:223:ARG:C	2.62	0.42
9:C:115:LEU:HD21	9:C:243:VAL:CG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:132:THR:HG23	11:E:132:THR:O	2.19	0.42
12:F:60:VAL:O	12:F:61:MET:C	2.62	0.42
14:H:36:MET:HE1	14:H:88:MET:HE3	2.00	0.42
15:I:95:LEU:O	15:I:134:ILE:HG23	2.18	0.42
17:K:98:VAL:HG13	17:K:102:GLU:CA	2.40	0.42
20:N:114:LYS:O	20:N:117:ALA:HB3	2.19	0.42
21:O:14:LEU:HG	21:O:102:ILE:HD11	2.00	0.42
21:O:25:VAL:HG23	21:O:26:TRP:CE3	2.54	0.42
27:U:23:HIS:HB2	27:U:27:ALA:HB3	2.00	0.42
29:W:1:MET:HE3	29:W:101:LEU:HD23	1.99	0.42
29:W:69:ARG:HG3	29:W:118:LEU:HD23	2.01	0.42
30:X:15:ARG:HB3	30:X:15:ARG:HH11	1.84	0.42
1:O:111:C:H2'	1:O:112:G:O4'	2.19	0.42
1:O:960:G:N3	1:O:960:G:H2'	2.33	0.42
1:O:2039:A:OP2	8:B:234:ARG:NH2	2.52	0.42
1:O:2815:G:C5	16:J:102:ARG:HG2	2.54	0.42
6:9:26:C:O2'	6:9:27:C:H5'	2.19	0.42
6:9:44:A:O4'	10:D:76:ARG:NE	2.48	0.42
8:B:178:ALA:O	8:B:179:LEU:C	2.62	0.42
9:C:16:VAL:HG21	9:C:237:GLU:OE1	2.19	0.42
9:C:35:VAL:HG23	9:C:220:THR:HG22	2.01	0.42
9:C:170:ASP:C	9:C:171:GLU:HG3	2.44	0.42
12:F:86:ALA:C	12:F:88:GLY:N	2.76	0.42
14:H:79:GLU:C	14:H:80:LEU:HD23	2.44	0.42
14:H:119:ALA:O	14:H:120:PHE:C	2.62	0.42
15:I:71:ALA:O	15:I:75:LYS:HG3	2.19	0.42
16:J:15:ARG:NH1	16:J:43:ARG:NH1	2.67	0.42
16:J:31:LEU:C	16:J:33:GLY:H	2.25	0.42
19:M:46:LEU:HD22	19:M:50:ARG:HD2	2.00	0.42
20:N:48:VAL:HG11	20:N:55:ASP:CB	2.46	0.42
21:O:105:ASN:HD21	21:O:109:SER:N	2.16	0.42
26:T:65:VAL:HG22	26:T:72:ILE:HG22	2.01	0.42
28:V:12:THR:HG22	28:V:15:GLU:H	1.83	0.42
30:X:86:GLU:C	30:X:87:ALA:O	2.62	0.42
31:Y:229:LEU:O	31:Y:231:PRO:HD3	2.19	0.42
1:O:87:C:C2	3:2:30:ASP:OD2	2.72	0.42
1:O:221:G:H2'	1:O:222:A:C8	2.53	0.42
1:O:553:G:P	31:Y:204:ARG:NH2	2.92	0.42
1:O:634:G:O2'	1:O:1358:A:OP1	2.37	0.42
1:O:953:G:H2'	38:O:6189:HOH:O	2.19	0.42
1:O:1123:A:C6	1:O:1238:C:H5'	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:5339:HOH:O	31:Y:158:LYS:HD3	2.18	0.42
4:3:91:GLN:O	4:3:92:GLU:HB2	2.20	0.42
7:A:66:ARG:CB	7:A:66:ARG:NH1	2.83	0.42
8:B:63:GLU:O	8:B:63:GLU:HG3	2.19	0.42
9:C:49:ASP:HB3	9:C:52:ALA:HB2	2.00	0.42
10:D:19:GLU:HG3	38:D:210:HOH:O	2.19	0.42
10:D:25:MET:HE1	10:D:37:ALA:O	2.19	0.42
11:E:31:ARG:NH1	38:E:4034:HOH:O	2.52	0.42
18:L:35:ARG:O	18:L:40:PHE:HA	2.19	0.42
18:L:66:VAL:CG2	18:L:67:ARG:N	2.83	0.42
21:O:79:VAL:O	21:O:80:ASP:HB2	2.19	0.42
26:T:63:ILE:HD11	26:T:75:GLU:HB2	2.01	0.42
29:W:21:LEU:HD22	29:W:26:ILE:HD11	2.00	0.42
29:W:48:VAL:HG12	29:W:52:VAL:CG1	2.50	0.42
1:O:162:C:H2'	1:O:163:U:H5'	2.02	0.42
1:O:503:G:H2'	1:O:504:G:H8	1.83	0.42
1:O:694:A:H4'	1:O:2441:U:OP1	2.20	0.42
1:O:1772:C:H5'	1:O:1773:G:C5	2.55	0.42
1:O:1805:G:H2'	1:O:1806:G:C8	2.53	0.42
1:O:2090:G:H2'	1:O:2091:G:C8	2.54	0.42
1:O:2445:U:H2'	1:O:2446:G:H8	1.79	0.42
1:O:2653:A:H2'	1:O:2654:C:C6	2.55	0.42
1:O:2676:C:H4'	16:J:70:PHE:CE1	2.54	0.42
1:O:2842:G:H2'	1:O:2843:A:H5'	2.01	0.42
4:3:69:TYR:CZ	4:3:80:ARG:HD2	2.55	0.42
8:B:278:PRO:HD3	8:B:294:TYR:CZ	2.53	0.42
8:B:320:GLN:NE2	8:B:321:PRO:CD	2.72	0.42
10:D:55:LYS:O	10:D:56:ARG:HB2	2.19	0.42
14:H:169:GLU:C	38:H:368:HOH:O	2.62	0.42
20:N:64:SER:C	20:N:66:LEU:N	2.74	0.42
20:N:154:LEU:HG	20:N:155:GLU:N	2.34	0.42
29:W:48:VAL:CG1	29:W:48:VAL:O	2.67	0.42
31:Y:108:ASP:OD1	31:Y:199:ASP:HB3	2.19	0.42
1:O:20:G:H21	24:R:117:HIS:HD2	1.66	0.42
1:O:303:C:H2'	1:O:304:G:O4'	2.20	0.42
1:O:541:C:O2'	1:O:542:A:H5''	2.20	0.42
1:O:1041:U:H4'	1:O:1295:G:H5'	2.01	0.42
1:O:1163:G:N2	38:I:4004:HOH:O	2.49	0.42
1:O:1935:C:H2'	1:O:1936:C:H6	1.84	0.42
1:O:2502:C:H2'	1:O:2503:A:H5'	2.01	0.42
8:B:223:ARG:O	8:B:228:ALA:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:87:PRO:O	15:I:89:GLU:HG3	2.19	0.42
17:K:65:ARG:O	17:K:66:ARG:HB2	2.19	0.42
18:L:130:ARG:O	18:L:131:GLU:C	2.61	0.42
20:N:132:ASN:O	20:N:133:ASP:C	2.62	0.42
21:O:25:VAL:CG2	21:O:26:TRP:N	2.81	0.42
21:O:89:ILE:C	21:O:91:GLN:H	2.28	0.42
22:P:91:LYS:O	22:P:95:GLU:HG3	2.20	0.42
24:R:59:PHE:O	24:R:63:ASN:HB3	2.19	0.42
27:U:14:GLU:HA	27:U:15:PRO:HD2	1.94	0.42
29:W:122:ARG:HG3	29:W:122:ARG:HH11	1.84	0.42
31:Y:205:ILE:O	31:Y:206:ALA:C	2.63	0.42
1:0:318:U:O2'	1:0:338:C:H2'	2.19	0.42
1:0:396:U:C1'	38:0:4950:HOH:O	2.66	0.42
1:0:1183:C:O2	1:0:1183:C:H2'	2.19	0.42
1:0:1874:U:P	7:A:51:ARG:HD2	2.59	0.42
7:A:69:LEU:HD11	7:A:159:VAL:HG13	2.01	0.42
7:A:109:GLU:CD	7:A:113:GLY:H	2.28	0.42
8:B:277:GLU:N	8:B:278:PRO:CD	2.83	0.42
15:I:85:GLY:C	15:I:86:GLU:HG3	2.45	0.42
16:J:34:GLU:HA	16:J:34:GLU:OE1	2.19	0.42
16:J:52:GLN:HG3	16:J:53:ILE:H	1.83	0.42
17:K:28:GLU:HG2	17:K:58:THR:CB	2.47	0.42
18:L:134:GLU:C	18:L:136:ALA:H	2.27	0.42
24:R:4:TYR:N	38:R:308:HOH:O	2.53	0.42
29:W:65:VAL:HG11	29:W:116:LEU:HD13	2.02	0.42
29:W:119:HIS:O	29:W:153:MET:HB3	2.19	0.42
1:0:431:G:O2'	1:0:432:G:H5'	2.20	0.42
1:0:1268:C:O2'	31:Y:169:ARG:HB2	2.20	0.42
1:0:1666:C:H2'	1:0:1667:A:H8	1.84	0.42
1:0:1798:C:H1'	22:P:66:GLN:OE1	2.20	0.42
1:0:2115:U:H2'	1:0:2116:U:C6	2.54	0.42
1:0:2820:A:OP1	8:B:98:THR:HG23	2.18	0.42
1:0:2822:C:O2'	1:0:2827:A:H4'	2.19	0.42
2:1:8:GLN:HE22	2:1:11:LYS:NZ	2.18	0.42
3:2:21:VAL:O	3:2:22:PRO:C	2.63	0.42
6:9:55:U:H4'	6:9:56:A:C8	2.55	0.42
7:A:72:GLU:HG3	32:Z:66:GLY:HA2	2.02	0.42
7:A:223:ARG:O	7:A:223:ARG:HG2	2.20	0.42
9:C:16:VAL:HG12	9:C:17:ASP:N	2.35	0.42
10:D:54:ALA:HB2	10:D:69:ILE:CD1	2.48	0.42
10:D:172:VAL:HG12	10:D:173:GLU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:29:SER:HA	14:H:62:HIS:CD2	2.55	0.42
14:H:146:ALA:O	14:H:150:LYS:HG3	2.19	0.42
18:L:34:GLY:C	18:L:36:ASP:N	2.78	0.42
20:N:74:PRO:HG2	20:N:159:TYR:CZ	2.55	0.42
21:O:96:VAL:CG1	21:O:97:SER:N	2.83	0.42
23:Q:24:SER:HB3	23:Q:28:ARG:HH21	1.83	0.42
24:R:29:LYS:CD	38:R:335:HOH:O	2.68	0.42
26:T:41:ARG:HG2	26:T:41:ARG:NH1	2.33	0.42
30:X:9:VAL:HG22	30:X:88:GLU:OE2	2.20	0.42
31:Y:125:LYS:HB2	31:Y:126:PRO:HD2	2.01	0.42
1:O:474:C:O3'	9:C:73:LEU:CD2	2.67	0.42
1:O:951:A:H5''	23:Q:42:LYS:HD3	2.02	0.42
1:O:963:C:O2	1:O:1005:A:N1	2.53	0.42
1:O:1186:C:H5''	38:O:6619:HOH:O	2.20	0.42
1:O:1201:C:H2'	1:O:1202:A:H5'	2.02	0.42
1:O:1334:C:H2'	1:O:1335:C:H6	1.84	0.42
1:O:1743:G:H2'	1:O:1744:G:O4'	2.19	0.42
1:O:2087:C:O2'	1:O:2088:C:H5'	2.20	0.42
1:O:2251:G:H2'	1:O:2252:A:C8	2.54	0.42
2:1:17:THR:O	2:1:18:LYS:C	2.62	0.42
8:B:175:LEU:C	8:B:175:LEU:HD23	2.44	0.42
10:D:23:VAL:CG2	10:D:73:VAL:HB	2.49	0.42
11:E:101:GLU:HB2	11:E:116:THR:O	2.19	0.42
20:N:143:ARG:NH1	20:N:173:ASP:OD2	2.52	0.42
23:Q:16:ASN:HB2	38:Q:215:HOH:O	2.19	0.42
24:R:145:LEU:HD12	24:R:146:ILE:N	2.34	0.42
30:X:81:GLY:O	30:X:82:GLU:HB3	2.20	0.42
31:Y:178:HIS:O	31:Y:179:PRO:C	2.63	0.42
1:O:69:A:H2'	1:O:70:A:OP2	2.19	0.42
1:O:934:C:H2'	1:O:935:G:C8	2.54	0.42
1:O:962:C:C2'	1:O:963:C:H5'	2.50	0.42
1:O:1181:A:H2'	1:O:1182:C:C5'	2.49	0.42
1:O:1268:C:O2'	1:O:1269:G:H5'	2.20	0.42
1:O:1377:C:H2'	1:O:1723:G:O6	2.20	0.42
1:O:1903:U:O2'	1:O:1904:A:N7	2.51	0.42
1:O:2133:U:H4'	1:O:2134:G:C5'	2.49	0.42
1:O:2237:G:H1'	38:O:8506:HOH:O	2.19	0.42
4:3:6:ARG:O	4:3:7:PHE:HB3	2.20	0.42
4:3:69:TYR:O	4:3:77:ALA:HA	2.20	0.42
6:9:27:C:H2'	6:9:28:U:O4'	2.20	0.42
6:9:57:A:C8	10:D:141:VAL:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:226:LYS:O	8:B:230:GLN:HG2	2.20	0.42
10:D:96:SER:C	10:D:98:PHE:H	2.27	0.42
10:D:170:TYR:O	10:D:171:ASP:HB3	2.20	0.42
11:E:101:GLU:HB3	11:E:117:THR:HA	2.01	0.42
11:E:119:HIS:HE1	11:E:147:ASP:OD2	2.02	0.42
12:F:52:GLU:OE1	12:F:78:GLU:OE1	2.38	0.42
18:L:72:ASN:O	18:L:76:LEU:HG	2.20	0.42
20:N:151:ASP:HB3	38:N:4054:HOH:O	2.19	0.42
24:R:61:GLN:HE21	24:R:61:GLN:HB2	1.63	0.42
26:T:73:HIS:CD2	26:T:88:PRO:CG	3.03	0.42
29:W:73:LEU:HD12	29:W:73:LEU:HA	1.73	0.42
30:X:25:ARG:HG2	38:X:4011:HOH:O	2.20	0.42
31:Y:170:SER:OG	31:Y:175:ARG:HG3	2.19	0.42
1:O:183:A:H1'	19:M:161:ARG:NH1	2.35	0.42
1:O:432:G:O2'	1:O:433:C:H5'	2.20	0.42
1:O:967:U:O2	14:H:35:LYS:HE3	2.19	0.42
1:O:1018:A:H4'	23:Q:59:GLN:HE22	1.85	0.42
1:O:1169:U:H3	1:O:1177:A:H61	1.68	0.42
1:O:1422:U:H2'	1:O:1423:C:C6	2.54	0.42
1:O:1838:U:O4'	1:O:2644:C:C2	2.73	0.42
1:O:1943:C:O4'	7:A:212:PRO:HA	2.20	0.42
1:O:2096:A:C8	1:O:2539:U:C2	3.07	0.42
1:O:2353:A:H1'	23:Q:21:ARG:HH12	1.85	0.42
1:O:2846:C:OP1	8:B:158:LYS:HD3	2.19	0.42
3:2:49:GLU:CD	38:2:145:HOH:O	2.62	0.42
4:3:11:CYS:HB2	4:3:20:HIS:NE2	2.34	0.42
30:X:30:MET:CE	30:X:58:ALA:HB3	2.48	0.42
1:O:333:G:O2'	1:O:334:G:H5'	2.20	0.41
1:O:424:C:H2'	1:O:425:U:C6	2.55	0.41
1:O:1163:G:H2'	1:O:1164:U:C5	2.54	0.41
1:O:1797:A:H2'	1:O:1799:G:O5'	2.20	0.41
1:O:2134:G:N2	1:O:2242:U:C2	2.89	0.41
1:O:2443:C:O3'	18:L:56:LYS:HE3	2.20	0.41
1:O:2456:A:H1'	38:O:8946:HOH:O	2.20	0.41
6:9:47:A:C2	6:9:48:C:C2	3.07	0.41
7:A:192:VAL:HG12	7:A:207:GLN:HB3	2.01	0.41
8:B:145:HIS:CD2	8:B:146:THR:O	2.68	0.41
9:C:32:GLY:O	9:C:36:ARG:HB2	2.20	0.41
9:C:140:VAL:CG1	9:C:141:SER:N	2.82	0.41
10:D:99:ASP:CB	10:D:103:ASN:HB2	2.50	0.41
14:H:56:GLU:HA	14:H:132:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:46:ILE:O	16:J:46:ILE:CG1	2.67	0.41
17:K:113:ILE:HD12	17:K:128:ALA:CB	2.49	0.41
19:M:57:LYS:HG2	19:M:58:GLN:H	1.85	0.41
20:N:21:HIS:HB3	38:N:4011:HOH:O	2.19	0.41
23:Q:16:ASN:HD22	23:Q:16:ASN:HA	1.60	0.41
24:R:40:ALA:O	24:R:44:VAL:HG23	2.19	0.41
26:T:43:ASN:C	26:T:45:GLY:N	2.78	0.41
1:O:80:A:H5''	26:T:41:ARG:CZ	2.50	0.41
1:O:628:1MA:HM13	1:O:2535:U:OP1	2.20	0.41
1:O:1021:G:O2'	1:O:1022:A:H5'	2.19	0.41
1:O:1050:G:C6	1:O:1051:C:C4	3.08	0.41
1:O:1968:A:H2'	1:O:1969:A:C8	2.55	0.41
1:O:2303:A:H4'	38:O:8645:HOH:O	2.20	0.41
36:O:3189:CL:CL	38:K:4017:HOH:O	2.59	0.41
3:2:36:ASN:HB3	3:2:39:ARG:NE	2.34	0.41
8:B:221:GLN:HE22	17:K:42:ASN:HD22	1.68	0.41
9:C:236:THR:CG2	9:C:239:ALA:H	2.08	0.41
12:F:58:GLU:CD	19:M:27:ARG:HH22	2.28	0.41
20:N:83:LEU:HD13	20:N:175:LEU:HD23	2.02	0.41
23:Q:32:GLU:O	23:Q:93:ARG:NH2	2.53	0.41
24:R:43:ALA:O	24:R:47:LEU:HG	2.20	0.41
29:W:13:MET:HE1	29:W:21:LEU:HD12	2.01	0.41
1:O:440:C:H2'	1:O:441:A:C8	2.55	0.41
1:O:638:C:H2'	1:O:639:A:C8	2.56	0.41
1:O:876:A:N3	1:O:876:A:C2'	2.84	0.41
1:O:1197:G:H1'	1:O:1203:G:N2	2.35	0.41
1:O:1948:G:N2	1:O:1965:C:H1'	2.34	0.41
1:O:2064:U:H2'	1:O:2065:C:H6	1.84	0.41
1:O:2379:G:H5'	1:O:2381:C:O4'	2.21	0.41
1:O:2511:A:H2'	1:O:2512:U:O4'	2.20	0.41
6:9:2:U:OP2	6:9:3:A:H5'	2.21	0.41
6:9:78:G:HO2'	6:9:102:G:H1	1.68	0.41
7:A:217:ARG:HH11	7:A:217:ARG:CG	2.33	0.41
8:B:294:TYR:CD1	8:B:294:TYR:C	2.98	0.41
9:C:27:ARG:NH2	21:O:4:ASN:ND2	2.68	0.41
9:C:93:LYS:O	9:C:98:ARG:NH2	2.52	0.41
10:D:40:ILE:O	10:D:44:ILE:HG22	2.20	0.41
12:F:21:GLU:O	12:F:24:ARG:CG	2.67	0.41
14:H:43:ALA:O	14:H:170:ARG:NH1	2.53	0.41
16:J:56:LYS:HE2	16:J:60:ARG:NH2	2.35	0.41
19:M:59:GLY:C	19:M:141:ILE:HD11	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:62:HIS:HB3	20:N:65:ASP:OD1	2.21	0.41
21:O:4:ASN:HA	21:O:5:PRO:HD3	1.84	0.41
21:O:33:LEU:HA	21:O:40:HIS:NE2	2.36	0.41
23:Q:17:LYS:O	23:Q:18:PRO:C	2.61	0.41
29:W:117:ARG:CB	29:W:117:ARG:NH1	2.83	0.41
1:O:30:U:OP2	9:C:181:ALA:HB2	2.19	0.41
1:O:394:G:H1	19:M:181:GLU:CD	2.28	0.41
1:O:903:U:O4	18:L:18:HIS:HB2	2.20	0.41
1:O:1206:U:H2'	1:O:1207:A:O4'	2.20	0.41
1:O:1472:C:O5'	1:O:1472:C:H6	2.03	0.41
38:O:4093:HOH:O	26:T:9:LYS:HD3	2.19	0.41
6:9:81:C:O2'	6:9:82:U:H5'	2.20	0.41
8:B:5:ARG:HH11	8:B:8:LYS:HE2	1.83	0.41
8:B:154:VAL:HA	8:B:155:PRO:HD3	1.81	0.41
10:D:159:PRO:O	10:D:162:ALA:HB3	2.21	0.41
11:E:7:ILE:HG22	11:E:45:ASP:O	2.20	0.41
14:H:91:ARG:NH1	14:H:138:THR:OG1	2.53	0.41
16:J:116:LEU:HB2	16:J:119:THR:HG21	2.02	0.41
16:J:131:THR:HG22	16:J:134:GLU:H	1.84	0.41
17:K:20:CYS:HB2	17:K:29:LEU:HG	2.02	0.41
18:L:145:LEU:C	18:L:147:GLU:N	2.79	0.41
20:N:32:PRO:HD2	20:N:99:GLU:O	2.20	0.41
20:N:79:PRO:HG3	20:N:143:ARG:C	2.44	0.41
20:N:114:LYS:O	20:N:118:ILE:HG13	2.21	0.41
20:N:155:GLU:O	20:N:156:GLU:HG3	2.20	0.41
22:P:59:ARG:HG2	22:P:59:ARG:HH11	1.85	0.41
24:R:104:PHE:HB2	24:R:109:MET:HE2	2.01	0.41
25:S:37:VAL:O	25:S:41:VAL:HG23	2.20	0.41
25:S:73:ASP:O	25:S:77:VAL:HG23	2.20	0.41
26:T:39:ASN:ND2	38:T:4017:HOH:O	2.54	0.41
29:W:21:LEU:CD1	29:W:26:ILE:HD11	2.40	0.41
1:O:320:G:H2'	1:O:321:A:C8	2.55	0.41
1:O:646:G:H5''	9:C:96:LYS:HD2	2.03	0.41
1:O:820:G:H5'	1:O:821:U:H5'	2.02	0.41
1:O:1041:U:C2'	1:O:1042:U:H5'	2.51	0.41
1:O:1112:G:H1	1:O:1251:C:N4	2.18	0.41
1:O:2697:A:H2'	1:O:2698:G:O4'	2.19	0.41
1:O:2866:U:C4	27:U:50:GLU:HB3	2.55	0.41
6:9:20:G:O2'	6:9:21:G:H5'	2.20	0.41
9:C:13:ASP:OD1	9:C:13:ASP:O	2.39	0.41
9:C:218:VAL:HG12	38:C:583:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:117:GLU:C	12:F:119:ARG:N	2.78	0.41
13:G:69:ARG:NH1	38:G:4016:HOH:O	2.53	0.41
14:H:41:LYS:O	14:H:87:LYS:HE2	2.20	0.41
15:I:88:GLN:HE21	15:I:128:THR:HG21	1.85	0.41
20:N:152:GLU:C	20:N:154:LEU:H	2.29	0.41
20:N:163:PHE:CZ	20:N:171:HIS:ND1	2.88	0.41
26:T:82:THR:C	26:T:84:GLY:N	2.79	0.41
31:Y:203:VAL:HG12	31:Y:228:VAL:HG22	2.00	0.41
1:0:11:A:H5'	1:0:12:U:OP2	2.20	0.41
1:0:595:U:O2'	1:0:596:C:H5'	2.21	0.41
1:0:1216:G:O2'	1:0:1217:G:H5'	2.21	0.41
1:0:1819:G:H2'	1:0:1820:G:C5'	2.51	0.41
1:0:1972:U:C2'	1:0:1973:A:C5'	2.99	0.41
1:0:2271:G:N3	1:0:2271:G:H2'	2.35	0.41
1:0:2392:C:H4'	38:0:8782:HOH:O	2.19	0.41
1:0:2471:G:N3	1:0:2633:A:H2	2.19	0.41
1:0:2568:A:H8	1:0:2568:A:O5'	2.03	0.41
7:A:210:GLY:HA3	38:A:490:HOH:O	2.19	0.41
9:C:7:ASP:C	9:C:9:ASP:N	2.78	0.41
9:C:211:ASP:HB3	38:C:575:HOH:O	2.21	0.41
11:E:88:TYR:CD1	11:E:88:TYR:C	2.98	0.41
11:E:166:VAL:HG12	38:E:4041:HOH:O	2.20	0.41
16:J:19:MET:HE1	16:J:78:ILE:HG22	2.03	0.41
16:J:88:PRO:HA	36:J:203:CL:CL	2.58	0.41
17:K:9:THR:O	17:K:10:GLN:C	2.63	0.41
17:K:55:VAL:CG1	17:K:56:SER:N	2.83	0.41
22:P:18:LYS:O	22:P:21:VAL:HG13	2.20	0.41
29:W:131:PRO:HB2	38:W:4057:HOH:O	2.21	0.41
31:Y:190:VAL:HG23	38:Y:482:HOH:O	2.20	0.41
1:0:75:U:H2'	1:0:76:G:C8	2.55	0.41
1:0:215:A:OP1	18:L:52:LYS:NZ	2.46	0.41
1:0:283:U:C5	1:0:284:C:N3	2.88	0.41
1:0:291:C:H2'	1:0:292:G:O4'	2.21	0.41
1:0:440:C:O2'	1:0:441:A:H5'	2.19	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.55	0.41
1:0:783:C:OP1	7:A:180:LYS:HE3	2.21	0.41
1:0:940:G:C5	1:0:1027:G:C2	3.09	0.41
1:0:1166:A:H61	1:0:1180:U:H3	1.69	0.41
1:0:2000:G:O2'	1:0:2001:G:H5'	2.21	0.41
1:0:2297:U:H1'	38:0:8672:HOH:O	2.19	0.41
1:0:2502:C:H2'	1:0:2503:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:28:HIS:CD2	2:1:31:LYS:HG3	2.55	0.41
3:2:16:ASN:C	3:2:18:ASN:N	2.78	0.41
8:B:280:VAL:HG13	8:B:333:GLU:O	2.19	0.41
9:C:139:VAL:CG1	38:C:580:HOH:O	2.62	0.41
12:F:119:ARG:HD3	12:F:119:ARG:C	2.45	0.41
15:I:70:THR:O	15:I:72:GLU:N	2.53	0.41
20:N:81:ALA:O	20:N:82:TYR:C	2.63	0.41
20:N:147:ILE:O	20:N:150:TYR:HB3	2.20	0.41
21:O:11:ILE:O	21:O:15:LYS:HG3	2.20	0.41
22:P:11:ALA:HB2	22:P:18:LYS:HA	2.03	0.41
22:P:24:ASN:HA	22:P:25:PRO:HD3	1.90	0.41
23:Q:50:GLY:HA3	23:Q:87:THR:OG1	2.21	0.41
28:V:12:THR:CG2	28:V:15:GLU:H	2.34	0.41
28:V:42:ASN:N	28:V:43:PRO:CD	2.83	0.41
1:0:241:A:C2	1:0:378:A:H4'	2.56	0.41
1:0:948:G:C6	1:0:949:U:C4	3.08	0.41
1:0:1181:A:H5'	15:I:89:GLU:OE2	2.19	0.41
1:0:1477:C:H4'	1:0:1868:G:OP1	2.20	0.41
1:0:1882:C:H5''	7:A:192:VAL:HG21	2.03	0.41
1:0:1926:G:H2'	1:0:1927:A:H8	1.84	0.41
1:0:2661:U:H3	1:0:2812:A:H62	1.67	0.41
6:9:49:G:O2'	6:9:50:G:H5'	2.21	0.41
6:9:63:C:O2'	6:9:64:C:H5'	2.21	0.41
8:B:195:ARG:NE	8:B:323:LEU:HD13	2.36	0.41
10:D:17:ARG:NH2	38:D:240:HOH:O	2.52	0.41
10:D:147:ALA:HA	20:N:15:GLU:O	2.21	0.41
14:H:117:ARG:HB3	38:H:347:HOH:O	2.20	0.41
16:J:142:ASN:O	16:J:144:THR:N	2.54	0.41
20:N:37:ARG:HH11	20:N:37:ARG:CG	2.31	0.41
20:N:115:VAL:HG13	38:N:4043:HOH:O	2.20	0.41
26:T:98:VAL:HG11	26:T:101:LEU:HD23	2.01	0.41
29:W:65:VAL:HA	29:W:68:THR:HG22	2.02	0.41
32:Z:10:ARG:CG	32:Z:11:SER:H	2.33	0.41
1:0:473:A:O2'	1:0:474:C:H5'	2.21	0.41
1:0:539:G:H2'	1:0:540:A:C8	2.56	0.41
1:0:542:A:H2'	1:0:543:G:O4'	2.21	0.41
1:0:772:G:H2'	1:0:773:A:O4'	2.20	0.41
1:0:1501:A:H4'	38:O:7280:HOH:O	2.20	0.41
1:0:1787:C:O2'	1:0:1788:U:H5'	2.21	0.41
1:0:1829:A:H2'	1:0:1830:C:H5'	2.03	0.41
1:0:1883:U:C2'	1:0:1884:G:H5'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1904:A:H2'	1:0:1905:U:O4'	2.20	0.41
1:0:2329:C:O2'	1:0:2330:U:H5'	2.21	0.41
1:0:2384:U:H5''	38:0:5594:HOH:O	2.21	0.41
1:0:2388:C:H5'	23:Q:83:THR:O	2.20	0.41
1:0:2626:C:H2'	1:0:2627:G:C8	2.56	0.41
1:0:2694:A:H4'	11:E:91:PHE:CE1	2.55	0.41
1:0:2851:G:H2'	1:0:2902:A:H61	1.85	0.41
2:1:28:HIS:O	2:1:32:LYS:N	2.47	0.41
4:3:8:ASN:O	4:3:9:THR:HB	2.19	0.41
7:A:206:ARG:NH1	38:A:498:HOH:O	2.54	0.41
8:B:13:PHE:CD1	8:B:13:PHE:N	2.89	0.41
8:B:41:PHE:HA	8:B:79:MET:CE	2.51	0.41
8:B:162:MET:HG3	8:B:310:ARG:NH1	2.36	0.41
8:B:279:THR:OG1	8:B:290:VAL:O	2.35	0.41
9:C:20:ASP:HB2	38:C:420:HOH:O	2.20	0.41
11:E:72:MET:HA	38:E:4032:HOH:O	2.21	0.41
11:E:99:GLY:N	38:E:4024:HOH:O	2.53	0.41
14:H:60:LEU:O	14:H:65:LEU:HD21	2.21	0.41
20:N:33:ARG:HD2	20:N:103:ASP:OD2	2.20	0.41
21:O:89:ILE:C	21:O:91:GLN:N	2.77	0.41
24:R:61:GLN:CD	38:R:335:HOH:O	2.63	0.41
26:T:12:ARG:NH1	38:T:4007:HOH:O	2.50	0.41
26:T:20:HIS:O	26:T:23:VAL:HG23	2.21	0.41
26:T:45:GLY:C	38:T:4018:HOH:O	2.63	0.41
30:X:43:VAL:HG12	30:X:47:ALA:HB3	2.03	0.41
31:Y:156:GLY:O	31:Y:157:ILE:C	2.64	0.41
31:Y:204:ARG:HA	31:Y:230:ASN:OD1	2.20	0.41
1:0:137:U:OP1	1:0:259:G:O2'	2.39	0.41
1:0:344:C:H2'	1:0:345:G:O4'	2.21	0.41
1:0:1355:A:H5''	38:Y:453:HOH:O	2.21	0.41
1:0:1748:U:C5	1:0:1749:U:C4	3.09	0.41
1:0:1761:U:H2'	1:0:1762:C:C6	2.55	0.41
1:0:1951:G:N2	38:0:8099:HOH:O	2.54	0.41
1:0:1996:U:O2'	1:0:1997:A:H5'	2.20	0.41
1:0:2644:C:O2'	1:0:2645:U:H5'	2.21	0.41
8:B:138:GLY:O	8:B:139:ASP:C	2.63	0.41
9:C:25:PRO:HG2	38:C:422:HOH:O	2.21	0.41
9:C:80:VAL:HA	9:C:81:PRO:HD3	1.88	0.41
11:E:107:PHE:CD2	11:E:108:LEU:HD13	2.56	0.41
11:E:154:ILE:HG23	11:E:154:ILE:O	2.20	0.41
12:F:38:LYS:HZ1	19:M:3:SER:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:45:VAL:HA	16:J:130:VAL:O	2.21	0.41
17:K:22:ASP:C	17:K:22:ASP:OD1	2.63	0.41
18:L:148:GLU:HG3	38:L:377:HOH:O	2.20	0.41
19:M:106:SER:HB2	19:M:114:VAL:CG2	2.51	0.41
25:S:44:GLN:OE1	25:S:44:GLN:HA	2.21	0.41
29:W:21:LEU:CD2	29:W:48:VAL:HG11	2.46	0.41
1:0:800:G:H2'	1:0:801:U:C6	2.57	0.40
1:0:1074:G:H4'	1:0:1260:G:C6	2.56	0.40
1:0:1174:A:H5'	38:0:6594:HOH:O	2.21	0.40
1:0:1235:G:OP2	1:0:2550:U:H4'	2.21	0.40
1:0:1363:G:OP1	9:C:76:ARG:NH2	2.54	0.40
1:0:1413:A:H2'	1:0:1414:A:O4'	2.20	0.40
1:0:1771:U:O2'	1:0:1773:G:N7	2.51	0.40
1:0:1783:A:C2'	1:0:1784:U:H5'	2.51	0.40
1:0:2338:G:H1'	10:D:105:SER:OG	2.20	0.40
1:0:2431:C:H5'	18:L:47:GLY:HA2	2.02	0.40
1:0:2507:G:H2'	1:0:2510:C:N4	2.36	0.40
1:0:2591:C:H2'	1:0:2592:G:O4'	2.21	0.40
1:0:2734:G:O2'	1:0:2735:U:H5'	2.20	0.40
7:A:20:SER:C	7:A:22:ARG:N	2.79	0.40
9:C:178:GLN:C	9:C:180:SER:N	2.76	0.40
14:H:87:LYS:O	14:H:140:TYR:HD1	2.04	0.40
15:I:127:CYS:CB	15:I:132:VAL:HB	2.34	0.40
16:J:77:GLY:O	16:J:78:ILE:C	2.62	0.40
20:N:58:LEU:N	20:N:58:LEU:CD1	2.83	0.40
20:N:166:ALA:O	20:N:167:ASP:HB2	2.21	0.40
22:P:141:ILE:O	22:P:143:ALA:N	2.49	0.40
25:S:34:LYS:HG2	25:S:54:THR:HG23	2.03	0.40
27:U:28:THR:HB	38:U:8814:HOH:O	2.20	0.40
30:X:76:ARG:NH1	30:X:76:ARG:CG	2.83	0.40
30:X:87:ALA:C	30:X:88:GLU:HG3	2.47	0.40
32:Z:39:CYS:HA	32:Z:40:PRO:HD3	1.92	0.40
1:0:222:A:H2'	1:0:223:G:O4'	2.20	0.40
1:0:263:U:O4'	12:F:59:ILE:HD13	2.21	0.40
1:0:694:A:H2'	1:0:695:C:C5'	2.45	0.40
1:0:1058:A:H2'	1:0:1060:C:C5'	2.51	0.40
1:0:1586:G:O2'	1:0:1587:U:H5'	2.20	0.40
1:0:1657:A:H2'	1:0:1658:A:C8	2.56	0.40
1:0:1674:C:OP2	25:S:34:LYS:HE3	2.22	0.40
1:0:1702:U:H5'	38:0:7620:HOH:O	2.20	0.40
1:0:1733:A:C2	1:0:1734:C:H1'	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1822:A:O2'	1:0:1823:G:H5'	2.21	0.40
1:0:1883:U:O2'	1:0:1884:G:H5'	2.21	0.40
1:0:2385:G:H2'	1:0:2386:U:C6	2.57	0.40
1:0:2684:A:H2'	1:0:2685:C:C6	2.56	0.40
6:9:1:U:C4'	6:9:3:A:OP1	2.70	0.40
6:9:81:C:C2'	6:9:82:U:H5'	2.50	0.40
7:A:190:ARG:NH2	7:A:207:GLN:OE1	2.54	0.40
9:C:4:THR:HB	9:C:135:GLU:OE1	2.21	0.40
9:C:138:VAL:O	9:C:234:VAL:HA	2.21	0.40
11:E:138:ILE:HG23	11:E:139:GLU:N	2.35	0.40
11:E:139:GLU:CD	38:E:4034:HOH:O	2.64	0.40
15:I:114:TYR:CD1	15:I:114:TYR:N	2.89	0.40
16:J:9:ASP:H	16:J:35:THR:HB	1.86	0.40
16:J:39:VAL:HG12	16:J:40:ASN:CG	2.47	0.40
18:L:35:ARG:C	18:L:35:ARG:HD3	2.47	0.40
18:L:144:ASP:CA	18:L:147:GLU:HG3	2.51	0.40
23:Q:46:SER:O	23:Q:48:PRO:HD3	2.22	0.40
24:R:119:VAL:HG12	24:R:119:VAL:O	2.21	0.40
27:U:52:THR:HG21	27:U:54:THR:HB	2.02	0.40
32:Z:78:THR:O	32:Z:79:VAL:C	2.64	0.40
1:0:276:C:H6	1:0:276:C:O5'	2.04	0.40
1:0:365:G:C6	1:0:366:U:C4	3.10	0.40
1:0:821:U:H1'	38:0:5789:HOH:O	2.21	0.40
1:0:1164:U:H3	1:0:1192:A:H2	1.69	0.40
1:0:1197:G:N2	38:0:6630:HOH:O	2.52	0.40
1:0:1268:C:H2'	1:0:1269:G:C8	2.57	0.40
1:0:1306:U:OP1	9:C:184:ARG:HD2	2.21	0.40
1:0:1342:C:C2'	1:0:1343:C:H5'	2.52	0.40
1:0:1810:C:H1'	27:U:42:LEU:HD22	2.04	0.40
1:0:1976:G:H1'	1:0:2005:G:N2	2.37	0.40
1:0:2255:A:O2'	1:0:2256:G:H5'	2.21	0.40
1:0:2705:U:O4'	11:E:112:ALA:HB2	2.21	0.40
1:0:2757:A:H2'	1:0:2758:G:O4'	2.20	0.40
3:2:40:ARG:HH11	3:2:40:ARG:HG2	1.85	0.40
6:9:2:U:OP2	6:9:2:U:H4'	2.22	0.40
7:A:14:SER:O	7:A:15:THR:C	2.64	0.40
7:A:105:VAL:HG11	7:A:154:ALA:CB	2.51	0.40
8:B:41:PHE:HB3	8:B:190:MET:CE	2.50	0.40
8:B:44:TYR:OH	8:B:148:PRO:HG3	2.22	0.40
9:C:116:ALA:C	9:C:118:THR:N	2.77	0.40
18:L:54:PRO:HG2	18:L:57:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:91:VAL:HG13	18:L:120:LEU:HD23	2.04	0.40
18:L:134:GLU:C	18:L:136:ALA:N	2.79	0.40
21:O:100:GLN:O	21:O:101:ALA:C	2.64	0.40
22:P:59:ARG:HD3	38:P:226:HOH:O	2.20	0.40
24:R:18:LEU:HD12	24:R:143:VAL:CG1	2.47	0.40
25:S:53:ASN:N	25:S:53:ASN:ND2	2.67	0.40
27:U:6:CYS:HA	27:U:13:ILE:HD11	2.03	0.40
28:V:23:LEU:O	28:V:24:LYS:C	2.63	0.40
29:W:75:GLY:HA3	38:W:4031:HOH:O	2.21	0.40
1:O:402:U:H2'	1:O:403:C:C6	2.56	0.40
1:O:459:A:H4'	38:O:5069:HOH:O	2.21	0.40
38:O:8830:HOH:O	23:Q:50:GLY:HA2	2.21	0.40
3:2:8:LYS:NZ	25:S:56:ASN:O	2.50	0.40
6:9:36:C:H2'	6:9:37:C:O4'	2.22	0.40
7:A:105:VAL:CG1	7:A:106:CYS:N	2.84	0.40
8:B:36:PRO:HB3	8:B:174:ARG:HA	2.03	0.40
8:B:265:LEU:CD2	8:B:316:ARG:HD3	2.50	0.40
9:C:180:SER:C	9:C:182:ARG:N	2.79	0.40
9:C:193:LEU:HA	9:C:211:ASP:O	2.21	0.40
10:D:135:VAL:HG23	38:D:239:HOH:O	2.21	0.40
13:G:64:ASN:N	13:G:64:ASN:ND2	2.70	0.40
20:N:71:TRP:CE3	20:N:175:LEU:CD2	3.05	0.40
29:W:130:HIS:O	29:W:136:GLY:HA3	2.21	0.40
31:Y:186:ARG:HH11	31:Y:186:ARG:HG2	1.86	0.40
1:O:962:C:H2'	1:O:963:C:C5'	2.52	0.40
1:O:1500:U:OP2	22:P:41:ARG:NH2	2.55	0.40
1:O:2435:U:OP1	4:3:28:GLY:HA3	2.22	0.40
1:O:2529:G:H5'	38:O:9120:HOH:O	2.22	0.40
1:O:2776:A:H2'	1:O:2777:G:O4'	2.21	0.40
6:9:28:U:H5''	20:N:40:ASN:HD22	1.81	0.40
7:A:114:ASP:HB2	7:A:117:LYS:HE2	2.02	0.40
8:B:51:VAL:HG21	8:B:327:VAL:HG13	2.02	0.40
9:C:78:ARG:HD3	38:C:472:HOH:O	2.22	0.40
9:C:160:LEU:O	9:C:161:ASP:HB2	2.22	0.40
9:C:170:ASP:O	9:C:171:GLU:HG3	2.22	0.40
10:D:25:MET:HE2	10:D:41:LEU:CD1	2.52	0.40
15:I:125:GLY:C	38:I:4004:HOH:O	2.65	0.40
17:K:75:ARG:HG2	17:K:90:PHE:CD2	2.56	0.40
18:L:65:ASP:CG	18:L:111:ALA:HB3	2.47	0.40
19:M:24:GLN:HE22	19:M:27:ARG:HH11	1.67	0.40
23:Q:34:ASP:O	23:Q:37:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:100:ASP:C	24:R:102:GLN:N	2.80	0.40
25:S:17:ASP:HB3	25:S:23:LYS:HB2	2.03	0.40
30:X:43:VAL:CG2	30:X:76:ARG:NH1	2.83	0.40
32:Z:57:CYS:C	32:Z:59:TYR:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
3	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
4	3	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	11	36
5	4	2/8 (25%)	2 (100%)	0	0	100	100
7	A	235/240 (98%)	203 (86%)	28 (12%)	4 (2%)	7	26
8	B	335/338 (99%)	294 (88%)	36 (11%)	5 (2%)	8	28
9	C	244/246 (99%)	218 (89%)	21 (9%)	5 (2%)	6	22
10	D	134/177 (76%)	92 (69%)	39 (29%)	3 (2%)	5	20
11	E	170/178 (96%)	158 (93%)	11 (6%)	1 (1%)	21	51
12	F	117/120 (98%)	100 (86%)	12 (10%)	5 (4%)	2	8
13	G	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	2	9
14	H	156/177 (88%)	139 (89%)	14 (9%)	3 (2%)	6	23
15	I	68/162 (42%)	50 (74%)	16 (24%)	2 (3%)	3	15
16	J	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	5	21
17	K	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
18	L	141/165 (86%)	113 (80%)	24 (17%)	4 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	M	192/195 (98%)	175 (91%)	17 (9%)	0	100	100
20	N	184/187 (98%)	154 (84%)	21 (11%)	9 (5%)	1	6
21	O	113/116 (97%)	100 (88%)	12 (11%)	1 (1%)	14	41
22	P	141/149 (95%)	127 (90%)	14 (10%)	0	100	100
23	Q	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	11	36
24	R	148/155 (96%)	133 (90%)	14 (10%)	1 (1%)	18	48
25	S	79/85 (93%)	68 (86%)	11 (14%)	0	100	100
26	T	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	4	17
27	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
28	V	63/71 (89%)	53 (84%)	6 (10%)	4 (6%)	1	3
29	W	152/154 (99%)	138 (91%)	13 (9%)	1 (1%)	18	48
30	X	80/92 (87%)	66 (82%)	9 (11%)	5 (6%)	1	3
31	Y	140/241 (58%)	133 (95%)	7 (5%)	0	100	100
32	Z	71/83 (86%)	54 (76%)	14 (20%)	3 (4%)	2	9
All	All	3707/4445 (83%)	3245 (88%)	397 (11%)	65 (2%)	6	25

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	34	ASP
7	A	37	VAL
8	B	184	ASP
9	C	8	LEU
10	D	173	GLU
12	F	101	ALA
20	N	133	ASP
20	N	154	LEU
20	N	164	ASP
20	N	184	ILE
32	Z	20	ARG
32	Z	81	ARG
8	B	139	ASP
12	F	44	SER
13	G	72	ASP
14	H	143	VAL
16	J	143	LYS
18	L	21	ARG

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Mol	Chain	Res	Type
18	L	80	ASP
20	N	65	ASP
26	T	44	ALA
28	V	43	PRO
30	X	70	ILE
8	B	245	SER
9	C	58	ALA
12	F	71	GLY
16	J	7	ASP
20	N	183	ASP
23	Q	21	ARG
26	T	53	GLY
26	T	83	ASP
28	V	41	GLU
29	W	77	ALA
30	X	23	HIS
30	X	77	PHE
30	X	87	ALA
4	3	57	GLY
7	A	119	ALA
9	C	232	LEU
10	D	77	ASP
14	H	19	ARG
14	H	39	LYS
15	I	71	ALA
16	J	5	GLU
18	L	35	ARG
18	L	105	TYR
20	N	74	PRO
32	Z	21	VAL
9	C	15	GLU
11	E	17	HIS
12	F	104	ALA
15	I	76	ASP
20	N	139	TRP
21	O	90	ASP
28	V	40	PRO
30	X	78	GLU
28	V	2	VAL
8	B	34	GLY
24	R	106	GLY
8	B	2	GLN

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Mol	Chain	Res	Type
10	D	69	ILE
7	A	192	VAL
9	C	19	PRO
20	N	130	PRO
12	F	64	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	46/47 (98%)	45 (98%)	1 (2%)	45	77
3	2	42/46 (91%)	42 (100%)	0	100	100
4	3	79/79 (100%)	79 (100%)	0	100	100
5	4	2/2 (100%)	2 (100%)	0	100	100
7	A	179/182 (98%)	169 (94%)	10 (6%)	19	50
8	B	282/283 (100%)	264 (94%)	18 (6%)	16	44
9	C	193/193 (100%)	179 (93%)	14 (7%)	13	38
10	D	117/148 (79%)	112 (96%)	5 (4%)	26	60
11	E	152/156 (97%)	146 (96%)	6 (4%)	28	63
12	F	93/94 (99%)	91 (98%)	2 (2%)	45	77
13	G	27/283 (10%)	27 (100%)	0	100	100
14	H	134/145 (92%)	128 (96%)	6 (4%)	24	58
15	I	58/130 (45%)	58 (100%)	0	100	100
16	J	118/121 (98%)	111 (94%)	7 (6%)	18	48
17	K	106/106 (100%)	104 (98%)	2 (2%)	50	79
18	L	113/127 (89%)	109 (96%)	4 (4%)	32	66
19	M	158/159 (99%)	151 (96%)	7 (4%)	25	59
20	N	149/150 (99%)	144 (97%)	5 (3%)	32	66
21	O	93/94 (99%)	90 (97%)	3 (3%)	34	68
22	P	113/117 (97%)	108 (96%)	5 (4%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	Q	79/80 (99%)	73 (92%)	6 (8%)	12	36
24	R	117/122 (96%)	113 (97%)	4 (3%)	32	66
25	S	71/74 (96%)	68 (96%)	3 (4%)	26	60
26	T	105/106 (99%)	98 (93%)	7 (7%)	15	43
27	U	44/52 (85%)	44 (100%)	0	100	100
28	V	51/57 (90%)	50 (98%)	1 (2%)	48	78
29	W	130/130 (100%)	123 (95%)	7 (5%)	20	51
30	X	66/74 (89%)	58 (88%)	8 (12%)	5	16
31	Y	120/196 (61%)	115 (96%)	5 (4%)	26	60
32	Z	60/68 (88%)	57 (95%)	3 (5%)	22	53
All	All	3097/3621 (86%)	2958 (96%)	139 (4%)	24	58

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	14	THR
7	A	3	ARG
7	A	33	GLU
7	A	36	ASP
7	A	38	ILE
7	A	69	LEU
7	A	94	LEU
7	A	131	HIS
7	A	175	LYS
7	A	179	MET
7	A	217	ARG
8	B	11	LEU
8	B	27	ASN
8	B	33	ASP
8	B	49	THR
8	B	97	LEU
8	B	98	THR
8	B	162	MET
8	B	174	ARG
8	B	175	LEU
8	B	195	ARG
8	B	234	ARG
8	B	254	GLN

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Mol	Chain	Res	Type
8	B	256	GLN
8	B	264	GLU
8	B	277	GLU
8	B	300	SER
8	B	307	ARG
8	B	312	ARG
9	C	2	GLN
9	C	16	VAL
9	C	67	GLN
9	C	76	ARG
9	C	78	ARG
9	C	94	THR
9	C	115	LEU
9	C	187	ARG
9	C	202	THR
9	C	214	THR
9	C	223	LEU
9	C	234	VAL
9	C	236	THR
9	C	240	LEU
10	D	24	HIS
10	D	133	ASN
10	D	136	ARG
10	D	149	ARG
10	D	153	THR
11	E	7	ILE
11	E	16	ASP
11	E	86	VAL
11	E	102	VAL
11	E	115	ARG
11	E	156	ASP
12	F	12	LEU
12	F	46	GLU
14	H	21	GLU
14	H	33	GLN
14	H	87	LYS
14	H	91	ARG
14	H	157	TYR
14	H	170	ARG
16	J	7	ASP
16	J	46	ILE
16	J	47	THR

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Mol	Chain	Res	Type
16	J	52	GLN
16	J	74	ARG
16	J	120	SER
16	J	131	THR
17	K	10	GLN
17	K	98	VAL
18	L	35	ARG
18	L	99	GLU
18	L	102	ASP
18	L	140	VAL
19	M	41	GLU
19	M	46	LEU
19	M	93	ARG
19	M	99	ARG
19	M	115	LEU
19	M	164	THR
19	M	186	SER
20	N	101	VAL
20	N	127	LEU
20	N	138	ASP
20	N	139	TRP
20	N	152	GLU
21	O	67	SER
21	O	97	SER
21	O	98	LEU
22	P	16	VAL
22	P	21	VAL
22	P	52	LYS
22	P	94	TRP
22	P	98	ILE
23	Q	11	ARG
23	Q	16	ASN
23	Q	30	VAL
23	Q	54	PRO
23	Q	55	ARG
23	Q	95	GLU
24	R	13	THR
24	R	39	THR
24	R	82	GLU
24	R	128	ARG
25	S	12	GLU
25	S	53	ASN

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Mol	Chain	Res	Type
25	S	80	ARG
26	T	21	LYS
26	T	23	VAL
26	T	26	THR
26	T	39	ASN
26	T	48	VAL
26	T	96	VAL
26	T	115	GLU
28	V	43	PRO
29	W	13	MET
29	W	26	ILE
29	W	35	VAL
29	W	73	LEU
29	W	132	VAL
29	W	146	ILE
29	W	154	ARG
30	X	12	ILE
30	X	15	ARG
30	X	46	ASP
30	X	49	ARG
30	X	56	GLU
30	X	79	GLU
30	X	82	GLU
30	X	85	VAL
31	Y	163	THR
31	Y	174	VAL
31	Y	189	ASN
31	Y	203	VAL
31	Y	235	GLU
32	Z	23	ARG
32	Z	44	GLU
32	Z	82	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	8	GLN
2	1	16	HIS
2	1	28	HIS
3	2	16	ASN
3	2	18	ASN
3	2	37	HIS

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Mol	Chain	Res	Type
3	2	41	HIS
3	2	45	ASN
4	3	2	GLN
4	3	15	ASN
4	3	30	GLN
4	3	48	ASN
7	A	5	GLN
7	A	47	HIS
7	A	92	ASN
7	A	199	HIS
8	B	27	ASN
8	B	94	GLN
8	B	106	HIS
8	B	145	HIS
8	B	221	GLN
8	B	238	ASN
8	B	243	ASN
8	B	260	HIS
8	B	320	GLN
8	B	332	ASN
9	C	67	GLN
9	C	129	HIS
9	C	163	HIS
9	C	206	ASN
10	D	47	GLN
10	D	97	GLN
10	D	133	ASN
11	E	55	ASN
11	E	90	HIS
11	E	106	ASN
11	E	119	HIS
11	E	143	GLN
12	F	80	GLN
13	G	64	ASN
14	H	33	GLN
14	H	34	HIS
14	H	40	GLN
14	H	59	GLN
14	H	62	HIS
14	H	73	ASN
15	I	88	GLN
15	I	108	HIS

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Mol	Chain	Res	Type
16	J	52	GLN
16	J	107	ASN
16	J	126	ASN
17	K	10	GLN
18	L	18	HIS
18	L	41	HIS
18	L	42	ASN
18	L	58	GLN
18	L	116	HIS
19	M	24	GLN
19	M	28	GLN
19	M	58	GLN
19	M	143	ASN
19	M	170	ASN
20	N	22	GLN
20	N	40	ASN
20	N	93	GLN
20	N	107	ASN
21	O	53	GLN
21	O	110	HIS
22	P	50	GLN
22	P	66	GLN
22	P	88	GLN
22	P	118	GLN
23	Q	16	ASN
23	Q	40	HIS
23	Q	49	ASN
23	Q	59	GLN
24	R	61	GLN
24	R	94	ASN
24	R	98	ASN
24	R	113	HIS
24	R	117	HIS
25	S	25	GLN
25	S	53	ASN
25	S	55	GLN
26	T	39	ASN
26	T	43	ASN
26	T	73	HIS
27	U	39	ASN
27	U	48	ASN
28	V	60	GLN

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Mol	Chain	Res	Type
29	W	6	GLN
29	W	87	HIS
29	W	110	GLN
29	W	119	HIS
29	W	125	HIS
29	W	141	HIS
30	X	22	ASN
30	X	23	HIS
30	X	36	HIS
31	Y	129	ASN
31	Y	133	HIS
31	Y	134	HIS
31	Y	149	GLN
31	Y	189	ASN
32	Z	50	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	247 (8%)	23 (0%)
6	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	263 (9%)	24 (0%)

All (263) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G

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Mol	Chain	Res	Type
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	C
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	319	A
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	516	A
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G

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Mol	Chain	Res	Type
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	882	A
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U

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Mol	Chain	Res	Type
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1234	U
1	0	1238	C
1	0	1239	G
1	0	1242	A
1	0	1279	U
1	0	1289	C
1	0	1331	G
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1409	G
1	0	1451	C
1	0	1474	C
1	0	1488	U
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1562	C
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G

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Mol	Chain	Res	Type
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1968	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A

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Mol	Chain	Res	Type
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2320	U
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	2465	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2638	G
1	0	2645	U
1	0	2648	U
1	0	2649	A
1	0	2664	A
1	0	2676	C
1	0	2681	A

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Mol	Chain	Res	Type
1	0	2682	C
1	0	2718	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2840	A
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
6	9	2	U
6	9	7	G
6	9	14	G
6	9	22	G
6	9	23	U
6	9	24	U
6	9	25	G
6	9	40	C
6	9	41	C
6	9	43	G
6	9	52	A
6	9	57	A
6	9	66	G
6	9	77	A
6	9	114	G
6	9	122	C

All (24) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	0	129	A
1	0	318	U
1	0	603	A
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1232	A
1	0	1237	U
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1474	C
1	0	1856	C
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2644	C
1	0	2718	C
1	0	2791	U
6	9	65	A

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	PSU	0	2621	1	18,21,22	1.52	2 (11%)	21,30,33	1.36	3 (14%)
1	1MA	0	628	35,1	21,25,26	0.75	1 (4%)	30,37,40	0.75	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UR3	0	2619	1	19,22,23	0.46	0	26,32,35	0.69	1 (3%)
5	MHU	4	5	5	14,15,16	3.04	10 (71%)	18,19,21	1.72	5 (27%)
5	DBB	4	3	5	4,5,6	1.09	0	1,5,7	0.09	0
5	MHW	4	1	33,5	9,9,10	2.77	4 (44%)	10,11,13	1.70	3 (30%)
5	MHV	4	6	5	7,9,10	2.07	2 (28%)	8,11,13	1.57	2 (25%)
1	OMG	0	2588	1	23,26,27	0.29	0	32,38,41	0.36	0
1	OMU	0	2587	35,1	19,22,23	0.22	0	25,31,34	0.43	0
5	004	4	7	5	9,10,11	3.17	4 (44%)	9,12,14	1.83	3 (33%)

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
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	35,1	-	2/7/25/26	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
5	MHU	4	5	5	-	0/9/12/14	0/1/1/1
5	DBB	4	3	5	-	0/3/4/6	-
5	MHW	4	1	33,5	-	0/2/2/4	0/1/1/1
5	MHV	4	6	5	-	0/1/12/14	0/1/1/1
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3
1	OMU	0	2587	35,1	-	0/9/27/28	0/2/2/2
5	004	4	7	5	-	0/4/6/8	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	7	004	CB-CA	7.46	1.60	1.52
5	4	1	MHW	CA-N	5.39	1.42	1.35
1	0	2621	PSU	C2-N1	4.84	1.43	1.36
5	4	5	MHU	CA-N	4.64	1.55	1.47
5	4	6	MHV	CB-CG	4.49	1.57	1.50
5	4	5	MHU	CD2-CE2	4.42	1.46	1.38
5	4	5	MHU	CE2-CZ	4.37	1.47	1.39
5	4	7	004	CD2-CG2	4.26	1.46	1.38
5	4	5	MHU	CB-CA	3.83	1.62	1.54
5	4	1	MHW	CB-CA	3.62	1.46	1.40
5	4	5	MHU	CD1-CG	3.55	1.45	1.38
5	4	5	MHU	CE1-CZ	3.48	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	1	MHW	CG2-CB	3.31	1.45	1.39
1	0	2621	PSU	C6-C5	3.24	1.38	1.35
5	4	1	MHW	CA-C	2.83	1.51	1.48
5	4	5	MHU	CE1-CD1	2.78	1.43	1.38
1	0	628	1MA	C6-N6	2.55	1.34	1.28
5	4	7	004	CG1-CB	2.42	1.42	1.39
5	4	6	MHV	CD2-CG	2.20	1.55	1.50
5	4	7	004	CD1-CG1	2.19	1.42	1.38
5	4	5	MHU	CM-N	2.09	1.52	1.46
5	4	5	MHU	O-C	2.08	1.27	1.20
5	4	5	MHU	CZ-NZ	2.04	1.42	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	7	004	CG2-CB-CA	3.97	126.81	120.64
5	4	1	MHW	CB-CA-C	3.80	122.91	120.09
5	4	5	MHU	CB-CA-N	3.75	116.00	110.48
1	0	2621	PSU	C6-C5-C4	3.36	120.44	118.17
5	4	5	MHU	O-C-CA	-3.24	116.43	124.77
1	0	2621	PSU	C6-N1-C2	-3.21	119.71	122.69
1	0	628	1MA	N1-C2-N3	2.84	129.37	126.00
5	4	6	MHV	CB-CA-N	-2.83	106.64	112.50
1	0	2621	PSU	O2-C2-N1	2.78	125.65	122.79
1	0	2619	UR3	C4-N3-C2	2.74	126.78	124.58
5	4	5	MHU	CG-CB-CA	2.57	117.18	113.51
5	4	5	MHU	CB-CA-C	-2.42	107.00	111.81
5	4	6	MHV	CD2-CE-N	-2.37	104.86	109.98
5	4	1	MHW	CG2-CB-CA	-2.12	116.71	119.79
5	4	7	004	CG1-CB-CA	-2.11	117.36	120.64
5	4	5	MHU	CM-N-CA	2.11	120.00	113.70
5	4	1	MHW	CE-N-CA	2.00	120.17	116.83
5	4	7	004	CD1-CG1-CB	2.00	123.04	120.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	628	1MA	1	0
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 232 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	0	2749/2922 (94%)	-0.60	22 (0%) 82 77	18, 42, 85, 147	0
2	1	56/57 (98%)	-0.73	0 100 100	23, 28, 34, 41	0
3	2	46/50 (92%)	0.16	2 (4%) 40 31	24, 56, 82, 96	0
4	3	92/92 (100%)	-0.20	0 100 100	30, 48, 61, 79	0
5	4	2/8 (25%)	0.16	0 100 100	49, 49, 49, 54	0
6	9	122/122 (100%)	-0.13	3 (2%) 58 48	36, 57, 84, 148	0
7	A	237/240 (98%)	-0.18	2 (0%) 82 77	21, 44, 80, 100	0
8	B	337/338 (99%)	-0.14	1 (0%) 90 87	23, 50, 76, 86	0
9	C	246/246 (100%)	-0.30	0 100 100	19, 39, 62, 72	0
10	D	140/177 (79%)	0.99	19 (13%) 7 5	47, 94, 117, 125	0
11	E	172/178 (96%)	0.10	2 (1%) 76 69	41, 61, 83, 88	0
12	F	119/120 (99%)	0.17	1 (0%) 82 77	41, 63, 88, 104	0
13	G	29/348 (8%)	0.64	2 (6%) 23 18	71, 87, 95, 96	0
14	H	160/177 (90%)	0.08	2 (1%) 75 67	36, 52, 88, 105	0
15	I	70/162 (43%)	1.69	22 (31%) 1 1	108, 118, 136, 138	0
16	J	142/145 (97%)	-0.20	1 (0%) 84 79	34, 46, 66, 86	0
17	K	132/132 (100%)	-0.25	0 100 100	26, 46, 65, 75	0
18	L	145/165 (87%)	0.13	6 (4%) 41 33	22, 60, 100, 114	0
19	M	194/195 (99%)	-0.44	0 100 100	25, 36, 52, 59	0
20	N	186/187 (99%)	0.20	6 (3%) 50 41	34, 58, 100, 110	0
21	O	115/116 (99%)	-0.17	0 100 100	33, 47, 66, 71	0
22	P	143/149 (95%)	-0.19	0 100 100	33, 49, 61, 73	0
23	Q	95/96 (98%)	-0.36	0 100 100	28, 39, 54, 66	0
24	R	150/155 (96%)	-0.51	0 100 100	28, 40, 58, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	S	81/85 (95%)	-0.21	0 100 100	37, 52, 71, 79	0
26	T	119/120 (99%)	-0.05	1 (0%) 82 77	35, 51, 80, 94	0
27	U	53/66 (80%)	-0.17	0 100 100	39, 51, 67, 78	0
28	V	65/71 (91%)	0.38	3 (4%) 37 29	46, 66, 105, 112	0
29	W	154/154 (100%)	-0.29	0 100 100	27, 42, 59, 71	0
30	X	82/92 (89%)	-0.03	2 (2%) 59 50	38, 55, 76, 96	0
31	Y	142/241 (58%)	-0.33	1 (0%) 84 79	24, 40, 62, 81	0
32	Z	73/83 (87%)	0.16	2 (2%) 56 47	39, 53, 69, 87	0
All	All	6648/7489 (88%)	-0.29	100 (1%) 72 64	18, 46, 91, 148	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	I	128	THR	4.8
28	V	1	THR	4.7
32	Z	82	SER	4.7
14	H	174	LEU	4.4
14	H	171	GLY	4.2
6	9	1	U	4.0
10	D	10	PHE	3.8
15	I	74	ILE	3.8
10	D	63	ILE	3.8
1	0	1177	A	3.8
10	D	174	VAL	3.7
7	A	37	VAL	3.5
15	I	71	ALA	3.5
28	V	2	VAL	3.4
15	I	132	VAL	3.4
15	I	91	PHE	3.4
30	X	88	GLU	3.4
20	N	154	LEU	3.3
15	I	83	GLY	3.3
28	V	40	PRO	3.2
10	D	107	GLY	3.2
15	I	80	PHE	3.2
1	0	1175	G	3.2
15	I	112	LEU	3.1
10	D	53	LYS	3.1
15	I	133	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	0	10	U	3.1
10	D	27	ILE	3.1
1	0	1176	C	3.0
15	I	88	GLN	2.9
7	A	36	ASP	2.9
18	L	82	ALA	2.9
1	0	1161	A	2.9
18	L	148	GLU	2.8
20	N	168	LEU	2.8
10	D	55	LYS	2.8
15	I	85	GLY	2.7
6	9	2	U	2.7
8	B	1	PRO	2.7
30	X	85	VAL	2.7
15	I	119	ALA	2.7
15	I	124	VAL	2.7
1	0	1172	G	2.6
20	N	158	LEU	2.6
10	D	18	ILE	2.6
18	L	99	GLU	2.6
15	I	113	SER	2.6
10	D	101	THR	2.5
10	D	172	VAL	2.5
15	I	92	VAL	2.5
15	I	82	THR	2.5
13	G	73	ASP	2.5
1	0	1193	A	2.5
1	0	1173	A	2.4
1	0	1192	A	2.4
1	0	1525	G	2.4
11	E	154	ILE	2.4
10	D	66	GLY	2.4
15	I	100	VAL	2.4
18	L	150	GLN	2.4
1	0	2344	G	2.4
10	D	54	ALA	2.4
10	D	11	HIS	2.4
1	0	1171	A	2.4
1	0	2345	A	2.4
10	D	104	PHE	2.4
10	D	21	VAL	2.3
1	0	138	U	2.3

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Mol	Chain	Res	Type	RSRZ
6	9	24	U	2.3
15	I	109	PRO	2.3
18	L	83	GLU	2.3
3	2	27	LEU	2.3
12	F	100	ASP	2.3
1	0	1524	U	2.3
1	0	1178	G	2.2
20	N	137	ALA	2.2
15	I	130	LEU	2.2
31	Y	235	GLU	2.2
10	D	62	ASP	2.2
15	I	70	THR	2.2
20	N	169	PRO	2.2
20	N	150	TYR	2.2
3	2	38	LYS	2.2
10	D	106	PHE	2.2
18	L	78	ALA	2.2
1	0	1169	U	2.2
10	D	52	THR	2.2
26	T	115	GLU	2.2
1	0	128	A	2.1
1	0	1182	C	2.1
15	I	116	LEU	2.1
1	0	960	G	2.1
10	D	95	THR	2.1
11	E	10	ASP	2.1
32	Z	25	ARG	2.1
15	I	75	LYS	2.0
1	0	1168	C	2.0
1	0	1190	G	2.0
13	G	26	MET	2.0
16	J	92	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	MHV	4	6	9/10	0.85	0.12	53,55,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DBB	4	3	6/7	0.88	0.14	51,51,52,53	0
5	MHW	4	1	9/10	0.93	0.11	46,47,49,50	0
5	MHU	4	5	15/16	0.94	0.12	56,59,62,63	0
5	004	4	7	10/11	0.95	0.10	45,48,49,51	0
1	PSU	0	2621	20/21	0.97	0.07	33,35,37,38	0
1	OMU	0	2587	21/22	0.97	0.07	29,32,37,38	0
1	OMG	0	2588	24/25	0.97	0.07	28,31,34,35	0
1	1MA	0	628	23/24	0.98	0.07	25,28,31,32	0
1	UR3	0	2619	21/22	0.98	0.06	30,35,39,42	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
35	NA	0	3183	1/1	0.53	0.27	81,81,81,81	0
35	NA	0	3137	1/1	0.62	0.25	81,81,81,81	0
35	NA	0	3173	1/1	0.76	0.24	53,53,53,53	0
35	NA	0	3175	1/1	0.77	0.14	54,54,54,54	0
33	MG	0	3087	1/1	0.80	0.23	75,75,75,75	0
35	NA	0	3140	1/1	0.83	0.09	47,47,47,47	0
33	MG	0	3050	1/1	0.83	0.09	72,72,72,72	0
33	MG	0	3089	1/1	0.85	0.12	47,47,47,47	0
35	NA	R	202	1/1	0.85	0.44	75,75,75,75	0
35	NA	0	3122	1/1	0.86	0.08	47,47,47,47	0
33	MG	0	3082	1/1	0.86	0.11	46,46,46,46	0
35	NA	9	203	1/1	0.86	0.31	85,85,85,85	0
35	NA	0	3174	1/1	0.86	0.20	75,75,75,75	0
33	MG	0	3105	1/1	0.87	0.18	47,47,47,47	0
33	MG	0	3063	1/1	0.87	0.14	37,37,37,37	0
35	NA	0	3182	1/1	0.88	0.09	40,40,40,40	0
36	CL	0	3192	1/1	0.88	0.17	88,88,88,88	0
35	NA	0	3120	1/1	0.89	0.15	36,36,36,36	0
35	NA	L	201	1/1	0.89	0.30	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	3176	1/1	0.89	0.19	60,60,60,60	0
35	NA	9	202	1/1	0.89	0.19	31,31,31,31	0
35	NA	0	3179	1/1	0.90	0.31	64,64,64,64	0
33	MG	0	3049	1/1	0.90	0.15	58,58,58,58	0
33	MG	0	3064	1/1	0.91	0.10	96,96,96,96	0
35	NA	0	3138	1/1	0.91	0.05	41,41,41,41	0
35	NA	0	3125	1/1	0.91	0.11	39,39,39,39	0
35	NA	0	3166	1/1	0.91	0.08	35,35,35,35	0
35	NA	0	3168	1/1	0.92	0.06	40,40,40,40	0
35	NA	0	3170	1/1	0.92	0.25	72,72,72,72	0
35	NA	0	3118	1/1	0.92	0.06	39,39,39,39	0
35	NA	0	3157	1/1	0.92	0.16	71,71,71,71	0
35	NA	0	3160	1/1	0.92	0.27	48,48,48,48	0
35	NA	R	201	1/1	0.92	0.07	33,33,33,33	0
35	NA	0	3165	1/1	0.92	0.25	60,60,60,60	0
35	NA	0	3121	1/1	0.92	0.10	50,50,50,50	0
33	MG	0	3046	1/1	0.93	0.07	52,52,52,52	0
35	NA	Q	101	1/1	0.93	0.07	33,33,33,33	0
35	NA	0	3159	1/1	0.93	0.18	49,49,49,49	0
33	MG	0	3047	1/1	0.93	0.09	62,62,62,62	0
33	MG	0	3041	1/1	0.93	0.09	38,38,38,38	0
35	NA	0	3142	1/1	0.94	0.08	26,26,26,26	0
35	NA	0	3147	1/1	0.94	0.10	44,44,44,44	0
33	MG	0	3098	1/1	0.94	0.07	48,48,48,48	0
35	NA	0	3181	1/1	0.94	0.09	46,46,46,46	0
33	MG	0	3088	1/1	0.94	0.07	48,48,48,48	0
33	MG	K	201	1/1	0.94	0.05	46,46,46,46	0
35	NA	0	3161	1/1	0.94	0.12	54,54,54,54	0
33	MG	T	201	1/1	0.94	0.05	45,45,45,45	0
35	NA	0	3132	1/1	0.94	0.10	39,39,39,39	0
34	K	0	3110	1/1	0.94	0.23	86,86,86,86	0
33	MG	0	3045	1/1	0.94	0.06	58,58,58,58	0
35	NA	0	3119	1/1	0.94	0.08	40,40,40,40	0
36	CL	0	3187	1/1	0.94	0.10	57,57,57,57	0
35	NA	0	3141	1/1	0.94	0.11	37,37,37,37	0
36	CL	J	203	1/1	0.94	0.07	63,63,63,63	0
33	MG	0	3081	1/1	0.95	0.06	41,41,41,41	0
35	NA	0	3143	1/1	0.95	0.11	47,47,47,47	0
33	MG	0	3107	1/1	0.95	0.06	49,49,49,49	0
35	NA	0	3148	1/1	0.95	0.04	29,29,29,29	0
35	NA	0	3151	1/1	0.95	0.06	30,30,30,30	0
35	NA	0	3154	1/1	0.95	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	3068	1/1	0.95	0.07	59,59,59,59	0
35	NA	0	3184	1/1	0.95	0.08	45,45,45,45	0
33	MG	0	3092	1/1	0.95	0.10	42,42,42,42	0
35	NA	0	3130	1/1	0.95	0.18	61,61,61,61	0
35	NA	C	301	1/1	0.95	0.05	32,32,32,32	0
33	MG	0	3094	1/1	0.95	0.14	73,73,73,73	0
35	NA	0	3134	1/1	0.95	0.15	72,72,72,72	0
34	K	0	3111	1/1	0.95	0.13	62,62,62,62	0
35	NA	0	3167	1/1	0.95	0.24	43,43,43,43	0
35	NA	0	3117	1/1	0.95	0.07	56,56,56,56	0
33	MG	0	3097	1/1	0.95	0.16	79,79,79,79	0
36	CL	0	3193	1/1	0.95	0.06	56,56,56,56	0
36	CL	0	3195	1/1	0.95	0.12	88,88,88,88	0
36	CL	J	202	1/1	0.95	0.07	55,55,55,55	0
33	MG	0	3077	1/1	0.95	0.14	58,58,58,58	0
36	CL	J	204	1/1	0.95	0.08	57,57,57,57	0
36	CL	L	202	1/1	0.95	0.09	46,46,46,46	0
36	CL	N	201	1/1	0.95	0.08	57,57,57,57	0
33	MG	0	3083	1/1	0.96	0.06	25,25,25,25	0
33	MG	0	3101	1/1	0.96	0.09	73,73,73,73	0
35	NA	0	3150	1/1	0.96	0.05	42,42,42,42	0
35	NA	0	3114	1/1	0.96	0.19	50,50,50,50	0
35	NA	0	3115	1/1	0.96	0.06	29,29,29,29	0
35	NA	S	101	1/1	0.96	0.05	10,10,10,10	0
33	MG	0	3090	1/1	0.96	0.04	41,41,41,41	0
33	MG	0	3106	1/1	0.96	0.06	42,42,42,42	0
33	MG	0	3085	1/1	0.96	0.07	41,41,41,41	0
36	CL	0	3194	1/1	0.96	0.06	58,58,58,58	0
33	MG	9	201	1/1	0.96	0.04	53,53,53,53	0
36	CL	3	103	1/1	0.96	0.05	53,53,53,53	0
35	NA	0	3164	1/1	0.96	0.15	75,75,75,75	0
33	MG	0	3043	1/1	0.96	0.09	35,35,35,35	0
35	NA	0	3185	1/1	0.96	0.19	38,38,38,38	0
33	MG	0	3056	1/1	0.96	0.06	42,42,42,42	0
35	NA	0	3146	1/1	0.96	0.03	26,26,26,26	0
36	CL	O	202	1/1	0.96	0.09	74,74,74,74	0
35	NA	0	3139	1/1	0.97	0.13	62,62,62,62	0
35	NA	0	3163	1/1	0.97	0.08	44,44,44,44	0
35	NA	A	302	1/1	0.97	0.10	38,38,38,38	0
33	MG	0	3084	1/1	0.97	0.07	49,49,49,49	0
35	NA	H	201	1/1	0.97	0.09	38,38,38,38	0
35	NA	J	201	1/1	0.97	0.04	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	3065	1/1	0.97	0.04	38,38,38,38	0
33	MG	0	3066	1/1	0.97	0.04	34,34,34,34	0
35	NA	0	3112	1/1	0.97	0.04	21,21,21,21	0
35	NA	0	3144	1/1	0.97	0.04	44,44,44,44	0
35	NA	0	3113	1/1	0.97	0.05	44,44,44,44	0
36	CL	0	3186	1/1	0.97	0.07	43,43,43,43	0
35	NA	0	3172	1/1	0.97	0.19	58,58,58,58	0
36	CL	0	3188	1/1	0.97	0.08	57,57,57,57	0
36	CL	0	3189	1/1	0.97	0.07	39,39,39,39	0
36	CL	0	3190	1/1	0.97	0.07	46,46,46,46	0
35	NA	0	3127	1/1	0.97	0.06	26,26,26,26	0
33	MG	0	3067	1/1	0.97	0.05	41,41,41,41	0
33	MG	0	3108	1/1	0.97	0.06	46,46,46,46	0
35	NA	0	3116	1/1	0.97	0.19	33,33,33,33	0
35	NA	0	3135	1/1	0.97	0.10	60,60,60,60	0
35	NA	0	3180	1/1	0.97	0.18	45,45,45,45	0
35	NA	0	3156	1/1	0.97	0.12	55,55,55,55	0
35	NA	0	3136	1/1	0.97	0.13	50,50,50,50	0
35	NA	0	3158	1/1	0.97	0.25	43,43,43,43	0
33	MG	0	3039	1/1	0.97	0.08	33,33,33,33	0
33	MG	0	3099	1/1	0.97	0.06	53,53,53,53	0
36	CL	R	203	1/1	0.97	0.08	43,43,43,43	0
36	CL	Y	302	1/1	0.97	0.08	30,30,30,30	0
35	NA	0	3152	1/1	0.98	0.14	34,34,34,34	0
35	NA	0	3153	1/1	0.98	0.08	43,43,43,43	0
35	NA	0	3124	1/1	0.98	0.06	48,48,48,48	0
35	NA	0	3155	1/1	0.98	0.08	39,39,39,39	0
33	MG	0	3048	1/1	0.98	0.04	48,48,48,48	0
35	NA	0	3126	1/1	0.98	0.05	28,28,28,28	0
33	MG	0	3034	1/1	0.98	0.05	29,29,29,29	0
35	NA	0	3129	1/1	0.98	0.05	25,25,25,25	0
35	NA	M	201	1/1	0.98	0.04	30,30,30,30	0
33	MG	0	3109	1/1	0.98	0.06	20,20,20,20	0
35	NA	0	3131	1/1	0.98	0.09	39,39,39,39	0
35	NA	0	3162	1/1	0.98	0.15	49,49,49,49	0
33	MG	0	3001	1/1	0.98	0.06	30,30,30,30	0
33	MG	0	3053	1/1	0.98	0.07	48,48,48,48	0
33	MG	0	3055	1/1	0.98	0.03	40,40,40,40	0
33	MG	0	3071	1/1	0.98	0.04	55,55,55,55	0
33	MG	0	3093	1/1	0.98	0.06	45,45,45,45	0
33	MG	0	3076	1/1	0.98	0.06	50,50,50,50	0
35	NA	0	3169	1/1	0.98	0.04	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	3095	1/1	0.98	0.05	49,49,49,49	0
33	MG	0	3012	1/1	0.98	0.07	25,25,25,25	0
33	MG	0	3080	1/1	0.98	0.03	65,65,65,65	0
33	MG	0	3059	1/1	0.98	0.07	44,44,44,44	0
36	CL	A	303	1/1	0.98	0.09	58,58,58,58	0
36	CL	B	402	1/1	0.98	0.09	40,40,40,40	0
33	MG	0	3060	1/1	0.98	0.03	27,27,27,27	0
33	MG	0	3102	1/1	0.98	0.03	23,23,23,23	0
33	MG	0	3103	1/1	0.98	0.05	60,60,60,60	0
33	MG	0	3104	1/1	0.98	0.05	40,40,40,40	0
33	MG	0	3061	1/1	0.98	0.04	52,52,52,52	0
35	NA	0	3149	1/1	0.98	0.03	35,35,35,35	0
33	MG	0	3042	1/1	0.98	0.06	31,31,31,31	0
35	NA	0	3123	1/1	0.98	0.04	27,27,27,27	0
37	CD	O	201	1/1	0.98	0.04	70,70,70,70	0
33	MG	Y	301	1/1	0.99	0.04	34,34,34,34	0
33	MG	0	3027	1/1	0.99	0.05	40,40,40,40	0
35	NA	0	3145	1/1	0.99	0.04	55,55,55,55	0
33	MG	0	3051	1/1	0.99	0.04	58,58,58,58	0
33	MG	0	3052	1/1	0.99	0.03	35,35,35,35	0
33	MG	0	3086	1/1	0.99	0.04	41,41,41,41	0
33	MG	0	3028	1/1	0.99	0.03	39,39,39,39	0
33	MG	0	3054	1/1	0.99	0.03	24,24,24,24	0
33	MG	0	3029	1/1	0.99	0.03	33,33,33,33	0
33	MG	0	3030	1/1	0.99	0.02	31,31,31,31	0
33	MG	0	3091	1/1	0.99	0.04	26,26,26,26	0
33	MG	0	3031	1/1	0.99	0.03	28,28,28,28	0
33	MG	0	3033	1/1	0.99	0.02	31,31,31,31	0
33	MG	0	3010	1/1	0.99	0.03	24,24,24,24	0
33	MG	0	3035	1/1	0.99	0.02	50,50,50,50	0
33	MG	0	3096	1/1	0.99	0.04	49,49,49,49	0
33	MG	0	3037	1/1	0.99	0.03	44,44,44,44	0
33	MG	0	3002	1/1	0.99	0.08	26,26,26,26	0
33	MG	0	3040	1/1	0.99	0.05	70,70,70,70	0
33	MG	0	3014	1/1	0.99	0.05	31,31,31,31	0
35	NA	0	3128	1/1	0.99	0.03	22,22,22,22	0
33	MG	0	3015	1/1	0.99	0.03	38,38,38,38	0
36	CL	0	3191	1/1	0.99	0.05	51,51,51,51	0
33	MG	0	3069	1/1	0.99	0.04	56,56,56,56	0
33	MG	0	3016	1/1	0.99	0.03	23,23,23,23	0
33	MG	0	3072	1/1	0.99	0.02	47,47,47,47	0
35	NA	0	3133	1/1	0.99	0.05	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	3075	1/1	0.99	0.04	38,38,38,38	0
33	MG	0	3017	1/1	0.99	0.05	26,26,26,26	0
35	NA	0	3171	1/1	0.99	0.12	65,65,65,65	0
33	MG	0	3018	1/1	0.99	0.02	34,34,34,34	0
33	MG	0	3079	1/1	0.99	0.07	42,42,42,42	0
33	MG	0	3021	1/1	0.99	0.04	32,32,32,32	0
33	MG	A	301	1/1	0.99	0.03	44,44,44,44	0
36	CL	M	202	1/1	0.99	0.04	31,31,31,31	0
33	MG	B	401	1/1	0.99	0.04	32,32,32,32	0
35	NA	0	3177	1/1	0.99	0.08	58,58,58,58	0
35	NA	0	3178	1/1	0.99	0.04	29,29,29,29	0
33	MG	0	3024	1/1	0.99	0.04	12,12,12,12	0
37	CD	1	101	1/1	0.99	0.03	56,56,56,56	0
37	CD	3	102	1/1	0.99	0.03	55,55,55,55	0
33	MG	0	3025	1/1	0.99	0.03	42,42,42,42	0
33	MG	0	3013	1/1	1.00	0.03	37,37,37,37	0
33	MG	0	3005	1/1	1.00	0.01	27,27,27,27	0
33	MG	0	3006	1/1	1.00	0.03	46,46,46,46	0
33	MG	0	3007	1/1	1.00	0.03	12,12,12,12	0
33	MG	0	3070	1/1	1.00	0.02	25,25,25,25	0
33	MG	0	3008	1/1	1.00	0.03	33,33,33,33	0
33	MG	0	3032	1/1	1.00	0.05	40,40,40,40	0
33	MG	0	3073	1/1	1.00	0.02	28,28,28,28	0
33	MG	0	3074	1/1	1.00	0.02	20,20,20,20	0
33	MG	0	3100	1/1	1.00	0.02	35,35,35,35	0
33	MG	0	3009	1/1	1.00	0.03	22,22,22,22	0
33	MG	0	3019	1/1	1.00	0.02	23,23,23,23	0
33	MG	0	3020	1/1	1.00	0.02	22,22,22,22	0
33	MG	0	3078	1/1	1.00	0.04	22,22,22,22	0
33	MG	0	3036	1/1	1.00	0.04	32,32,32,32	0
33	MG	0	3003	1/1	1.00	0.02	31,31,31,31	0
33	MG	0	3038	1/1	1.00	0.02	28,28,28,28	0
33	MG	0	3057	1/1	1.00	0.04	32,32,32,32	0
33	MG	0	3058	1/1	1.00	0.04	27,27,27,27	0
33	MG	3	101	1/1	1.00	0.05	40,40,40,40	0
33	MG	4	102	1/1	1.00	0.03	46,46,46,46	0
33	MG	0	3022	1/1	1.00	0.02	36,36,36,36	0
33	MG	0	3023	1/1	1.00	0.01	34,34,34,34	0
33	MG	0	3011	1/1	1.00	0.02	21,21,21,21	0
33	MG	0	3062	1/1	1.00	0.01	51,51,51,51	0
33	MG	0	3004	1/1	1.00	0.02	27,27,27,27	0
33	MG	0	3026	1/1	1.00	0.01	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	3044	1/1	1.00	0.06	37,37,37,37	0
37	CD	U	8701	1/1	1.00	0.02	60,60,60,60	0
37	CD	Z	101	1/1	1.00	0.03	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.