



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:10 AM UTC

PDB ID : 1K73 / pdb_00001k73
Title : Co-crystal Structure of Anisomycin Bound to the 50S Ribosomal Subunit
Authors : Hansen, J.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.
Deposited on : 2001-10-18
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

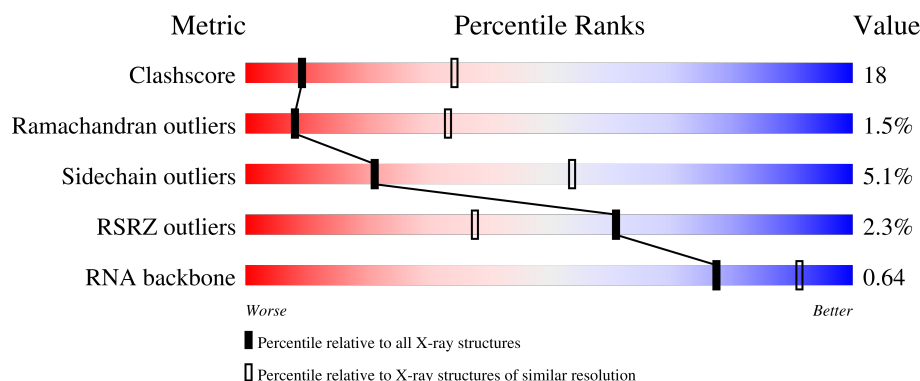
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

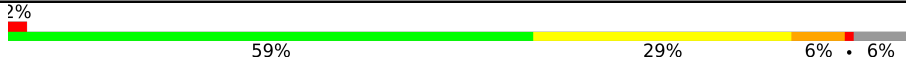
The reported resolution of this entry is 3.01 Å.

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.



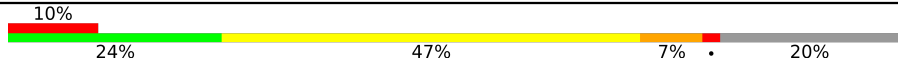
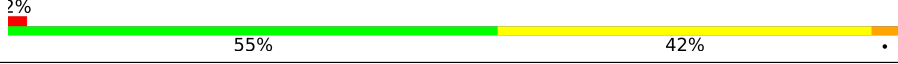
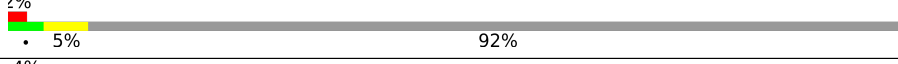
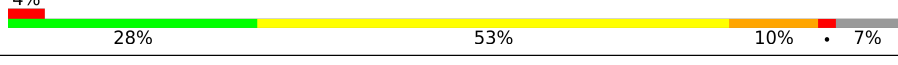
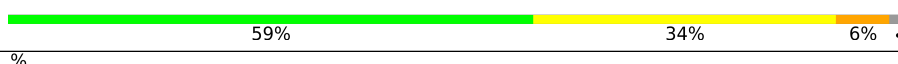
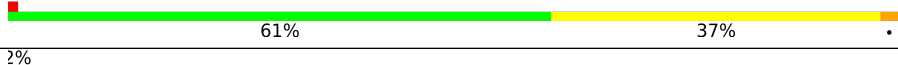
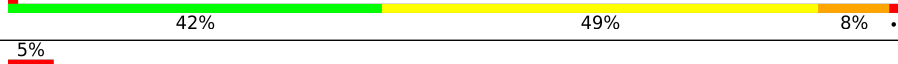
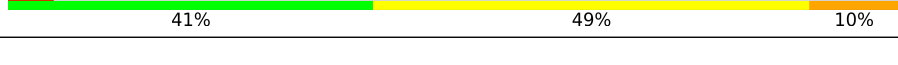
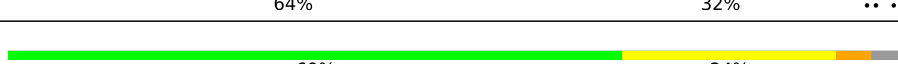
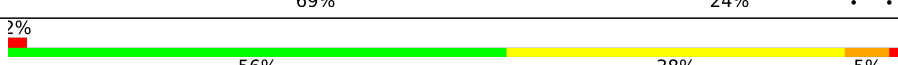
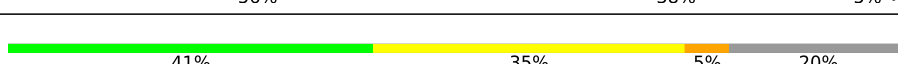
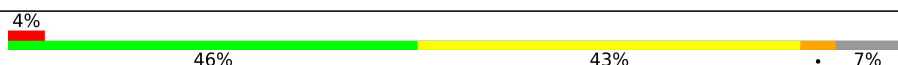
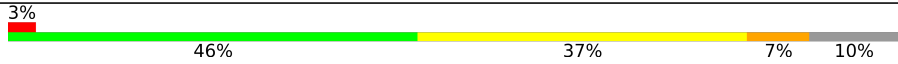
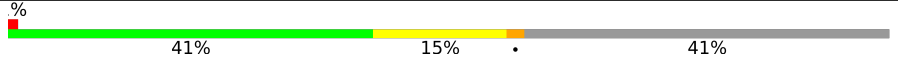
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)
RNA backbone	3983	1139 (3.24-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	2922	
2	B	122	
3	C	239	
4	D	337	
5	E	246	

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Mol	Chain	Length	Quality of chain
6	F	176	
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98548 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	conflict	? 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O		0	0	0
			1114	668	222	224				

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O		0	0	0
			864	529	161	174				

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O		0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	conflict	UNP P14119

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O			
			734	450	141	143	0	0	0

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O			
			949	568	180	201		0	0

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S		
			1195	737	209	243	6	0	0

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

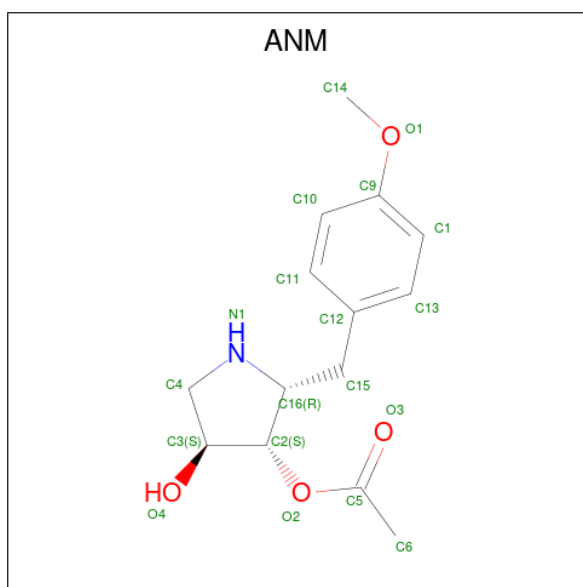
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	deletion	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is ANISOMYCIN (CCD ID: ANM) (formula: C₁₄H₁₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			19	14	1	4		

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	109	Total	Mg	0	0
			109	109		
32	B	1	Total	Mg	0	0
			1	1		
32	C	2	Total	Mg	0	0
			2	2		
32	D	1	Total	Mg	0	0
			1	1		
32	L	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	4	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	71	Total Na 71 71	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	0	0
34	T	1	Total Na 1 1	0	0
34	U	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	9	Total Cl 9 9	0	0
35	C	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	3	Total Cl 3 3	0	0
35	M	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	P	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	Z	1	Total 1	Cl 1	0	0
35	4	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cd 1	0	0
36	V	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	2	1	Total 1	Cd 1	0	0
36	4	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	5924	Total 5924	O 5924	0	0
37	B	143	Total 143	O 143	0	0
37	C	127	Total 127	O 127	0	0
37	D	146	Total 146	O 146	0	0
37	E	164	Total 164	O 164	0	0

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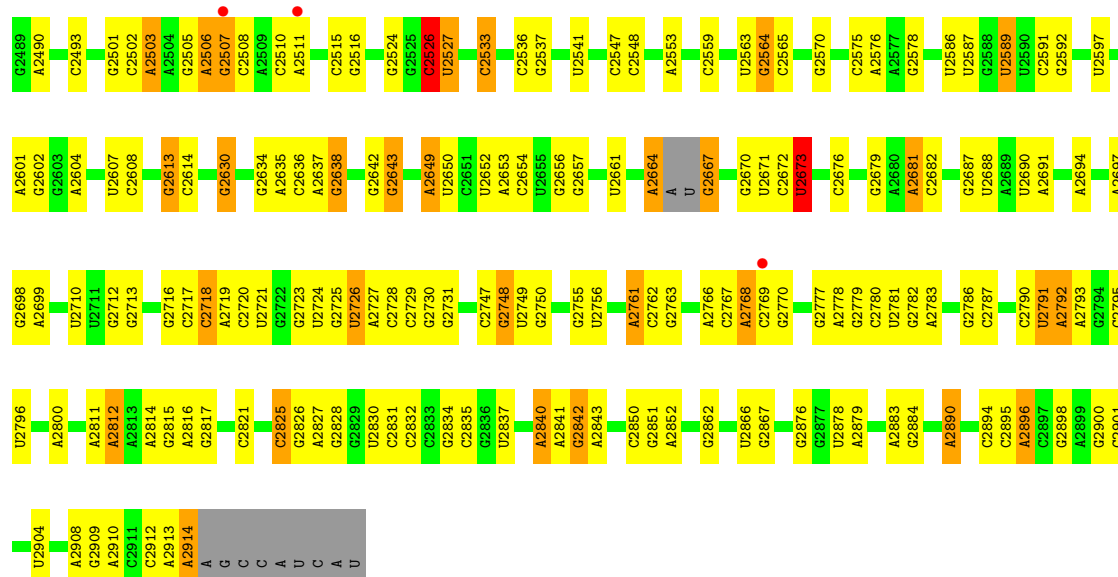
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	F	54	Total 54	O 54	0	0
37	G	42	Total 42	O 42	0	0
37	H	28	Total 28	O 28	0	0
37	I	22	Total 22	O 22	0	0
37	J	79	Total 79	O 79	0	0
37	K	56	Total 56	O 56	0	0
37	L	62	Total 62	O 62	0	0
37	M	81	Total 81	O 81	0	0
37	N	126	Total 126	O 126	0	0
37	O	66	Total 66	O 66	0	0
37	P	44	Total 44	O 44	0	0
37	Q	65	Total 65	O 65	0	0
37	R	54	Total 54	O 54	0	0
37	S	86	Total 86	O 86	0	0
37	T	35	Total 35	O 35	0	0
37	U	41	Total 41	O 41	0	0
37	V	25	Total 25	O 25	0	0
37	W	15	Total 15	O 15	0	0
37	X	67	Total 67	O 67	0	0
37	Y	29	Total 29	O 29	0	0
37	Z	92	Total 92	O 92	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	1	38	Total 38	O 38	0	0
37	2	56	Total 56	O 56	0	0
37	3	40	Total 40	O 40	0	0
37	4	72	Total 72	O 72	0	0

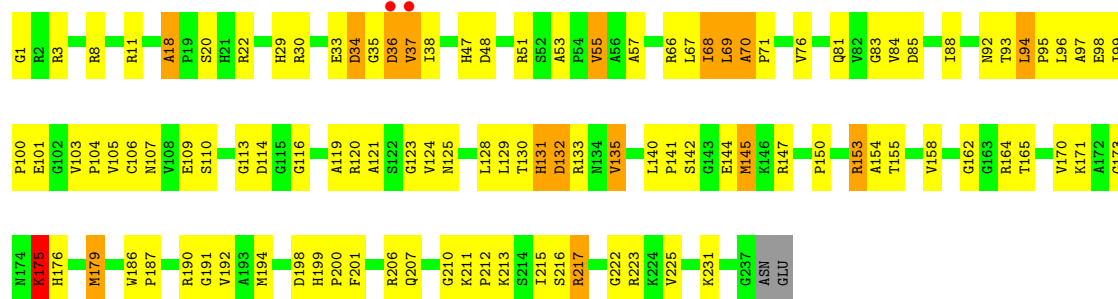
C2388	U2389	U2297	A	A	G2060	A1927	C1816	A1701	G1595	G1474	G1351	A1232	A1161	G1053
A2401	A2402	A2300	A	A	G2063	C1940	G1819	U1702	U1596	C1474	G1351	A1233	G1162	G1094
C2403	A2302	A2301	C	U	A2064	A1942	G1820	G1706	A1597	C1477	C1353	G1235	U1164	U1056
A2408	U2308	U2064	A	A	U2064	C1943	U1825	G1707	A1598	U1478	U1359	U1237	A1166	A1057
C2412	C2309	G2068	C	G	G2072	G1947	C1826	A1710	G1604	A1482	C1360	C1238	G1167	G1059
A2413	G2310	G2073	C	U	G2073	G1948	A1829	A1711	G1605	C1483	A1372	G1240	U1169	C1080
A2414	C2311	A2074	G	A	A2074	G1951	C1830	A1712	A1607	A1485	A1375	G1241	U1170	G1072
A2415	U2312	C2313	U	G	C2073	U	U1834	C1714	G1613	G1497	G1376	C1245	A1171	G1076
G2416	G2314	A2074	C	A	A2074	A	U1835	C1715	G1614	U1500	C1377	U1244	A1172	A1079
C2417	C2315	A2081	G	A	A2081	C	A1839	A1716	A1615	A1501	U1380	C1246	A1174	C1090
U2419	G2316	G2082	U	C	G2082	C	A1840	U1722	C1617	A1502	U1384	A1246	G1175	A1081
G2420	C2317	A2083	G	A	A2083	U	U1846	G1723	U1625	U1503	C1384	U1249	A1177	C1094
U2421	U2320	C2087	C	U	C2087	G	A1845	U1724	A1626	A1504	A1393	C1251	U1180	C1085
U2422	A2321	C2088	A	A	C2088	A	U1847	C1725	G1627	U1505	C1394	U1266	A1181	A1086
A2425	G2322	A2089	C	C	A2089	C	G1848	G1730	A1630	A1515	G1398	C1267	C1182	G1087
G2426	G2323	G2090	C	A	G2090	C	U1849	A1731	C1633	C1516	A1399	C1268	C1183	A1088
C2427	C2324	G2091	C	C	G2091	C	G1851	A1732	C1634	U1517	U1407	U1270	U1185	U1096
G2428	C2325	G2092	A	G	G2092	G1964	G1852	A1733	G1634	G1523	U1408	C1273	A1186	A1097
U2430	U2326	G2093	G	A	G2093	C1965	U1853	C1735	U1635	U1524	G1409	U1279	U1187	A1098
A2434	C2327	A2096	U	U	A2096	U1966	C1854	A1736	G1636	U1525	A1414	C1279	A1188	G1099
U2435	U2330	A2096	A	A	A2096	G1971	G1855	A1737	A1637	A1526	A1415	U1298	A1189	U1109
C2443	C2335	A2101	C	C	A2101	U1972	U1857	C1738	A1641	A1527	G1416	G1289	A1191	G1110
U2444	G2338	G2102	C	C	G2102	A1973	C1862	U1741	A1642	A1528	G1417	G1290	A1192	A1114
U2445	A	C2104	C	C	C2104	G1974	U1874	A1742	C1643	G1529	U1418	U1298	A1193	U1115
G2456	C	G2110	C	C	G2110	A1978	G1868	G1751	A1653	C1536	U1422	U1298	A1194	U1116
U2457	A	G2111	U	C	G2111	G1979	U1874	G1752	G1655	U1543	C1423	U1299	A1195	A1117
G2462	G2344	A2112	A	A	A2112	A1981	G1877	U1766	A1656	U1544	A1424	U1304	G1197	A1118
C2463	A2345	G2113	G	G	G2113	C1982	G1878	A1767	A1657	U1544	G1436	C1305	U1198	G1119
C2464	C2346	G2128	G	G	G2128	U1996	G1879	C1768	A1688	G1546	U1430	C1306	A1199	U1120
A2465	A2353	G2136	G	G	G2136	A1997	U1879	C1769	U1666	G1555	C1437	U1309	A1200	G1121
G2466	C2354	A	C	A	A	G2001	C1882	U1770	A1667	G1555	U1437	U1310	C1201	A1122
A2467	A2355	C	C	C	C	C2002	U1887	C1772	U1668	U1559	G1441	G1312	G1204	A1123
A2468	A2356	A	A	A	A	U2003	U1902	G1773	A1669	U	A1442	A1313	U1205	C1127
G2469	C2357	C	C	C	C	U2004	U1903	A1778	G1679	U1561	A1443	U1314	A1207	U1128
A2470	U2358	G	G	G	G	G2005	A1904	A1779	C1680	C1562	G1444	U1314	G1208	U1130
C2471	C2359	A	A	A	A	U2008	U1909	C1787	G1681	G1563	G1445	G1325	A1132	A1133
U2472	C2360	C	C	C	C	U2009	A1910	U1788	A1682	C1564	U1446	A1328	A1134	G1134
C2476	A2361	G	G	G	G	A2010	A1919	G1789	G1683	C1574	U1447	A1329	G1213	G1137
A2479	A2362	U	U	U	U	A2011	A1920	C1798	A1684	A1580	C1450	A1330	A1215	U1138
G2482	A2363	C	C	C	C	U2012	A1921	A1804	A1685	U1586	C1451	U1333	G1216	U1139
A2483	G2365	A	A	A	A	G2013	U1922	G1805	G1688	U1587	A1458	C1334	U1217	C1140
U2484	A2369	C	C	C	C	A2019	A1923	G1809	G1688	G1592	C1462	C1335	U1218	G1151
A2485	G2383	G	G	G	G	G2033	G1923	U1809	G1692	G1592	A1463	G1340	U1219	G1151
A2486	C2487	U	U	U	U	U2034	A1924	G1809	C1699	G1594	A1470	A1341	G1229	G1160
A2488	U2387	C	C	C	C	G2044	G1926	A1815	C1700	C1594		C1342		



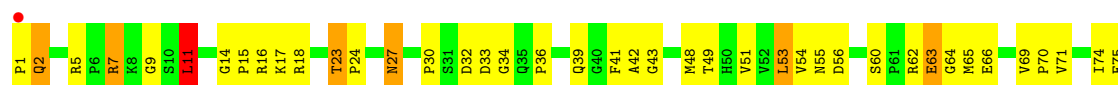
• Molecule 2: 5S rRNA



• Molecule 3: RIBOSOMAL PROTEIN L2



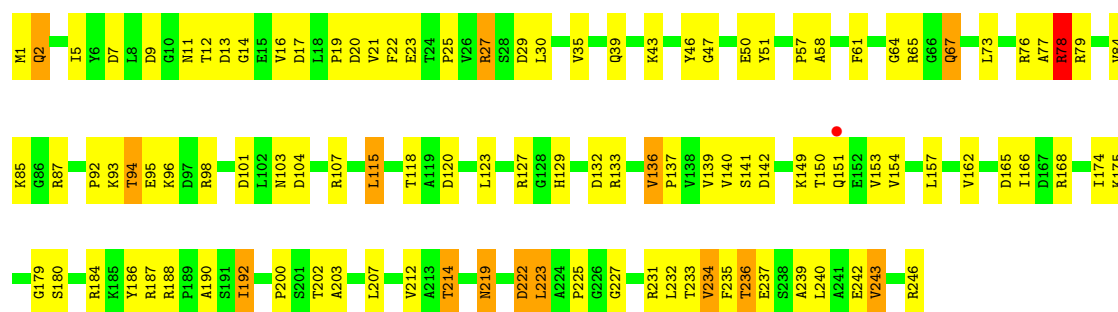
• Molecule 4: RIBOSOMAL PROTEIN L3





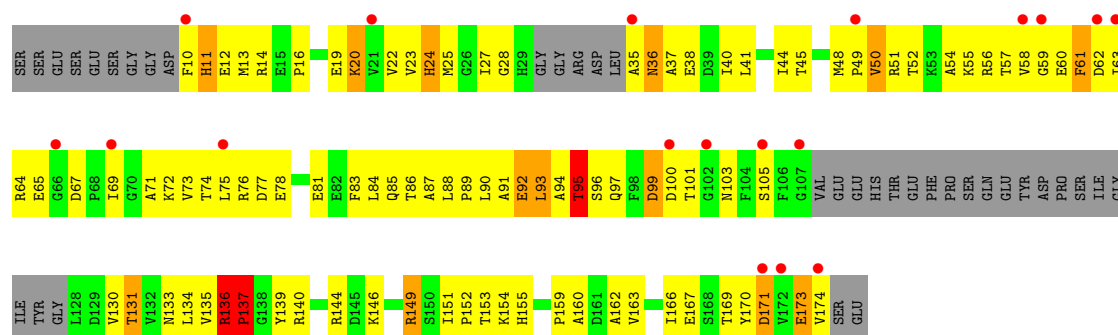
• Molecule 5: RIBOSOMAL PROTEIN L4

Chain E: 56% 38% 6%



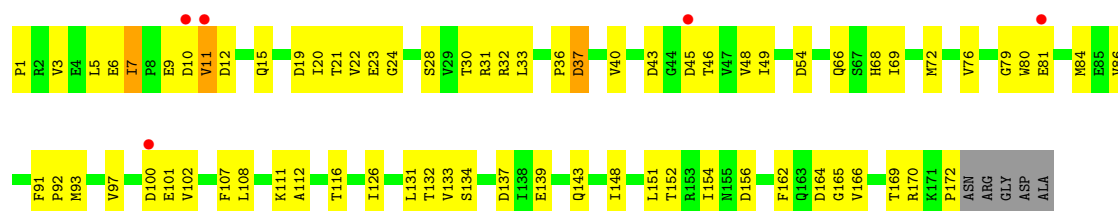
• Molecule 6: RIBOSOMAL PROTEIN L5

Chain F: 10% 24% 47% 7% 20%

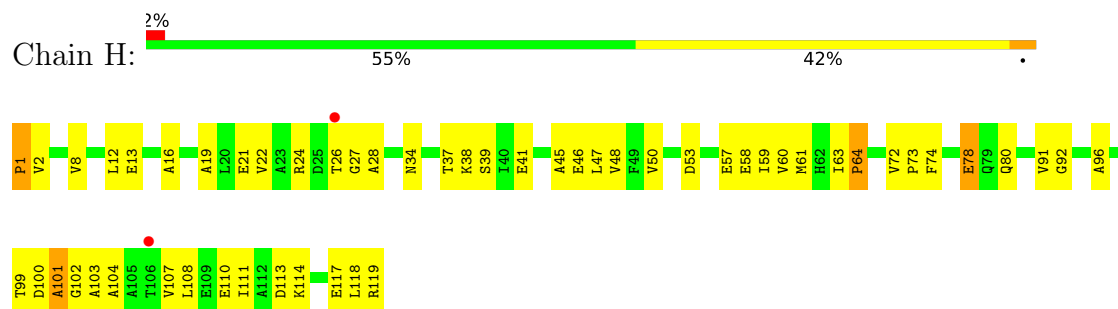


• Molecule 7: RIBOSOMAL PROTEIN L6

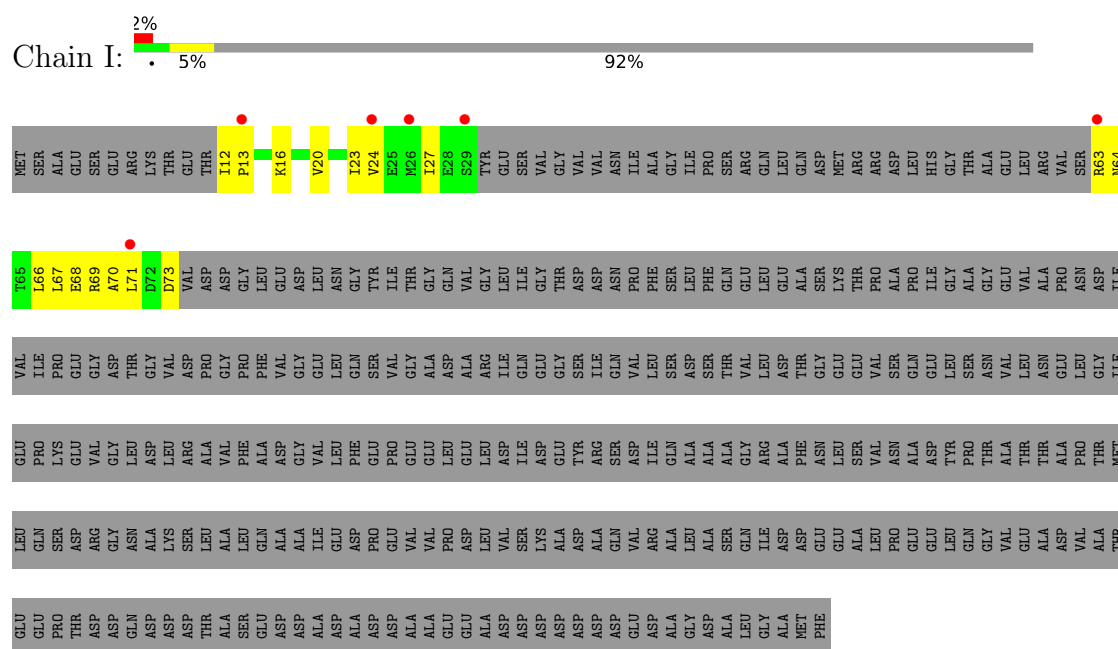
Chain G: 3% 56% 39%



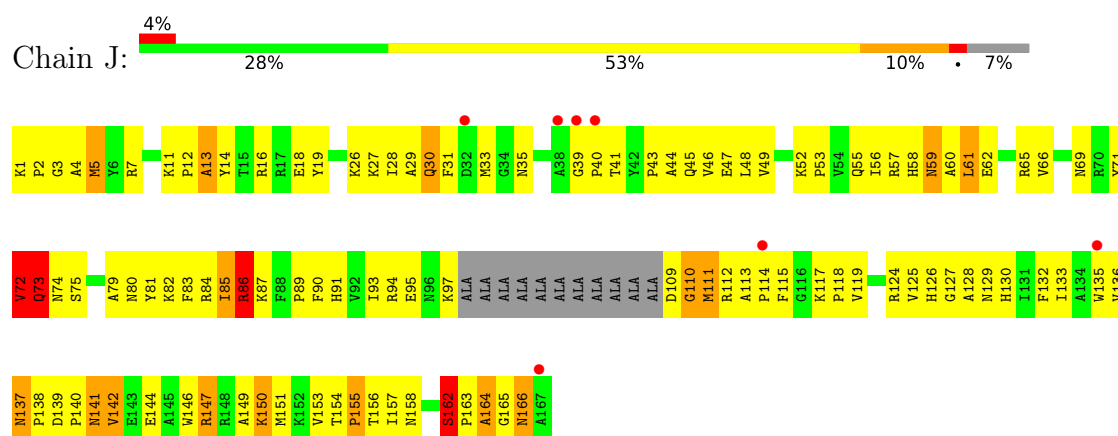
- Molecule 8: RIBOSOMAL PROTEIN L7AE



- Molecule 9: RIBOSOMAL PROTEIN L10

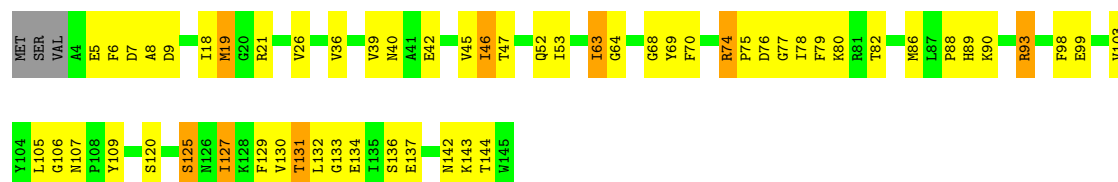


- Molecule 10: RIBOSOMAL PROTEIN L10E

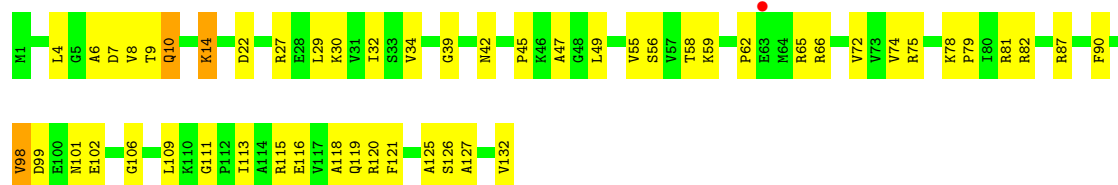


- Molecule 11: RIBOSOMAL PROTEIN L13

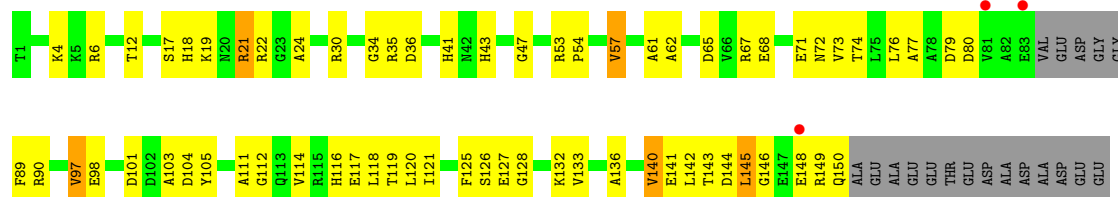




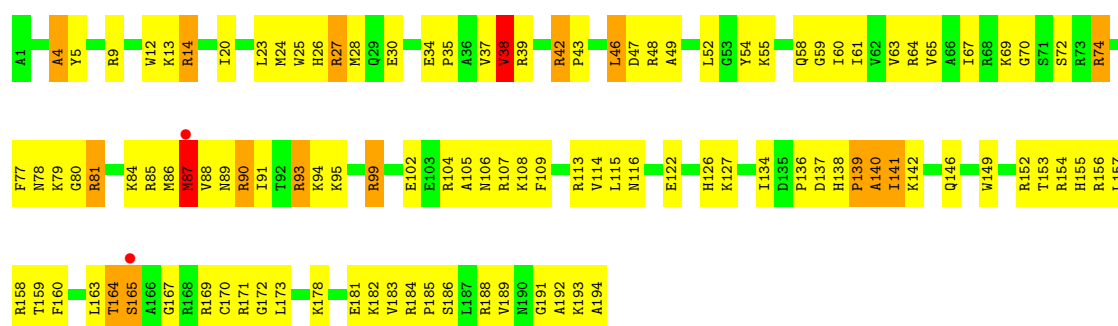
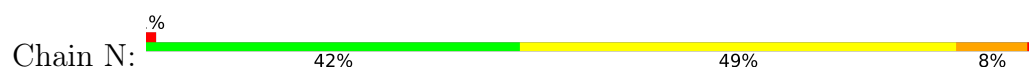
• Molecule 12: RIBOSOMAL PROTEIN L14



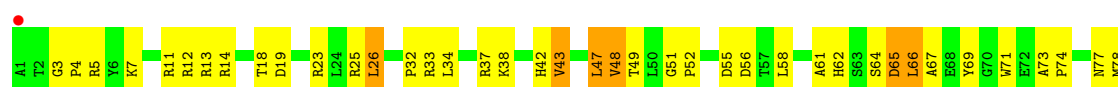
• Molecule 13: RIBOSOMAL PROTEIN L15

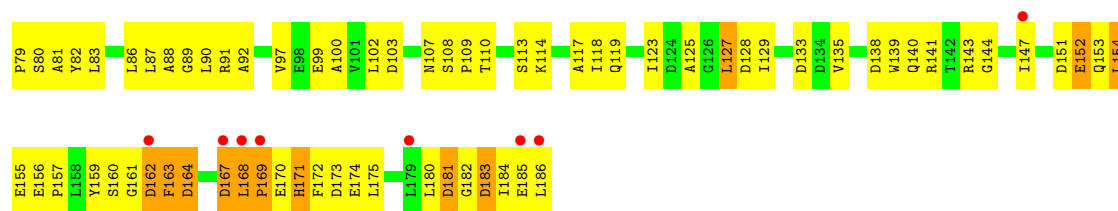


• Molecule 14: RIBOSOMAL PROTEIN L15E



• Molecule 15: RIBOSOMAL PROTEIN L18

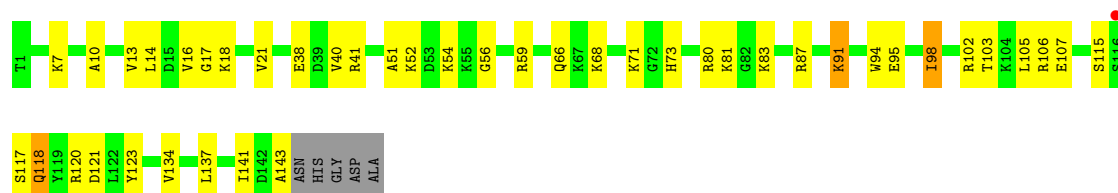




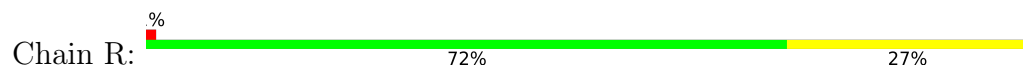
• Molecule 16: RIBOSOMAL PROTEIN L18E



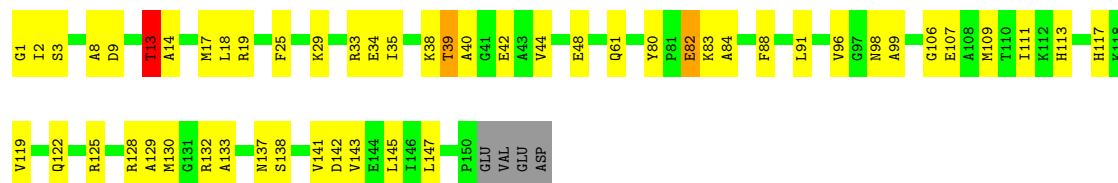
• Molecule 17: RIBOSOMAL PROTEIN L19E



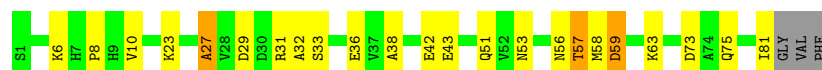
• Molecule 18: RIBOSOMAL PROTEIN L21E



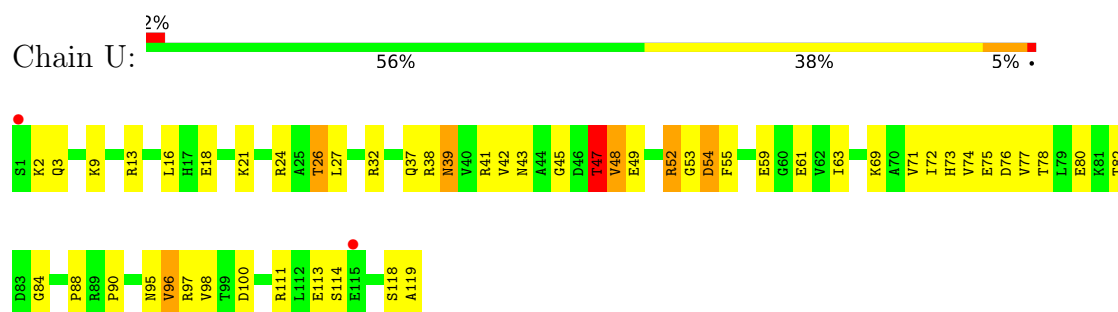
• Molecule 19: RIBOSOMAL PROTEIN L22



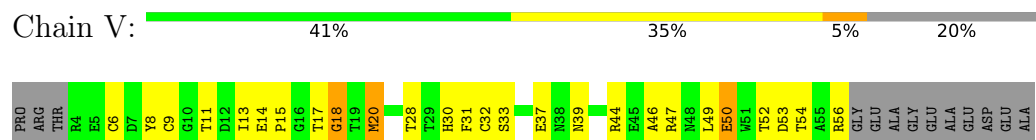
• Molecule 20: RIBOSOMAL PROTEIN L23



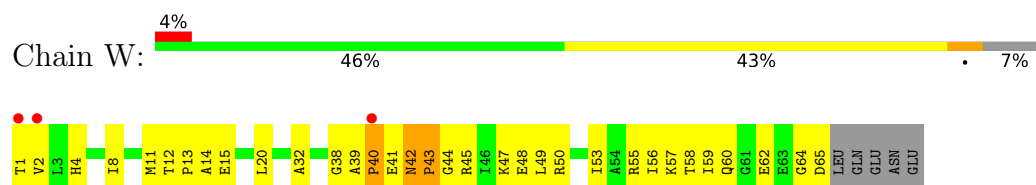
• Molecule 21: RIBOSOMAL PROTEIN L24



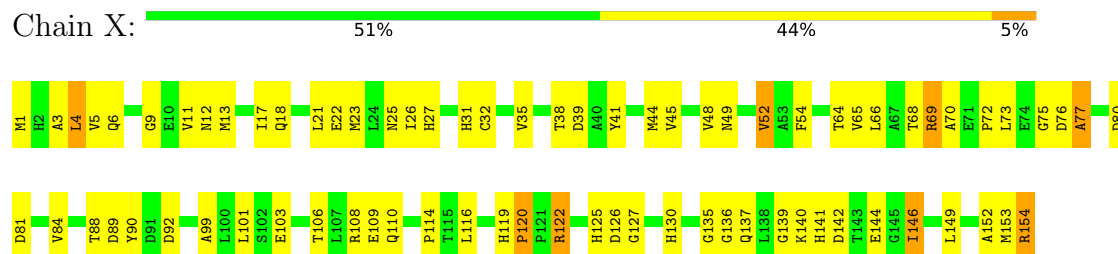
• Molecule 22: RIBOSOMAL PROTEIN L24E



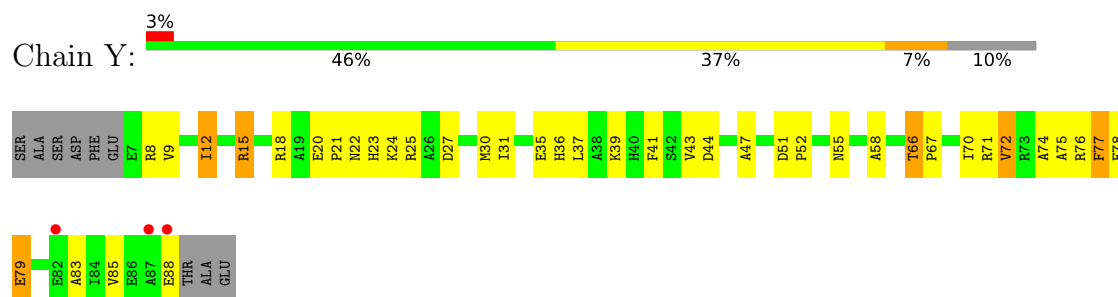
• Molecule 23: RIBOSOMAL PROTEIN L29



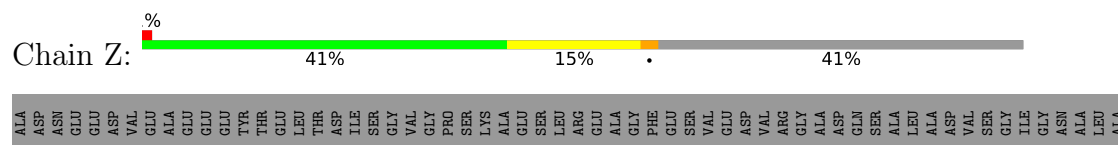
• Molecule 24: RIBOSOMAL PROTEIN L30

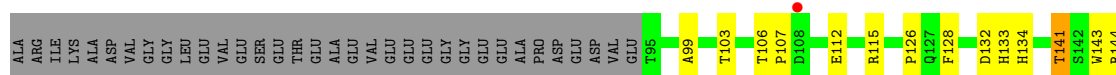


• Molecule 25: RIBOSOMAL PROTEIN L31E

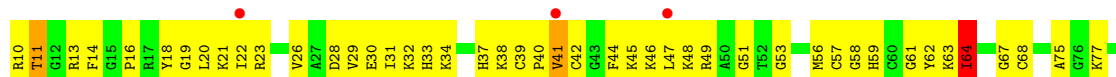


• Molecule 26: RIBOSOMAL PROTEIN L32E

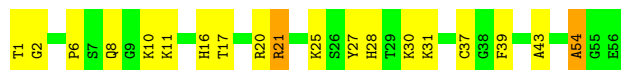




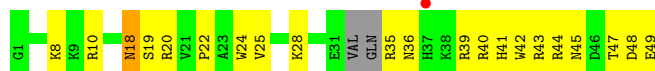
• Molecule 27: RIBOSOMAL PROTEIN L37Ae



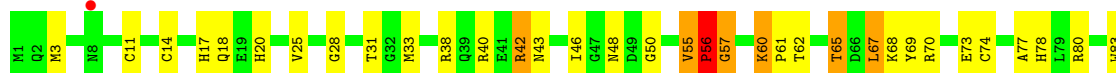
• Molecule 28: RIBOSOMAL PROTEIN L37E



• Molecule 29: RIBOSOMAL PROTEIN L39E



• Molecule 30: RIBOSOMAL PROTEIN L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.25Å 300.75Å 574.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.01 20.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	90.9 (20.00-3.01) 90.8 (20.00-3.01)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.246 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	98548	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: CD, NA, ANM, MG, K, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.57	12/66076 (0.0%)	0.77	61/103052 (0.1%)
2	B	0.55	1/2905 (0.0%)	0.83	6/4528 (0.1%)
3	C	0.68	1/1787 (0.1%)	1.11	7/2409 (0.3%)
4	D	0.68	0/2689	1.10	17/3652 (0.5%)
5	E	0.72	0/1883	1.12	10/2551 (0.4%)
6	F	0.54	0/1111	0.98	6/1498 (0.4%)
7	G	0.64	0/1382	0.97	5/1880 (0.3%)
8	H	0.64	0/896	0.97	2/1219 (0.2%)
9	I	0.55	0/241	0.83	0/324
10	J	0.77	2/1246 (0.2%)	1.33	16/1686 (0.9%)
11	K	0.72	2/1135 (0.2%)	1.02	3/1530 (0.2%)
12	L	0.64	0/1003	1.14	4/1351 (0.3%)
13	M	0.62	0/1126	1.13	6/1504 (0.4%)
14	N	0.74	1/1633 (0.1%)	1.18	13/2180 (0.6%)
15	O	0.65	0/1473	1.17	16/1999 (0.8%)
16	P	0.72	0/873	1.07	4/1181 (0.3%)
17	Q	0.61	0/1143	0.98	2/1521 (0.1%)
18	R	0.72	0/748	1.21	6/1005 (0.6%)
19	S	0.75	0/1172	1.13	6/1578 (0.4%)
20	T	0.62	0/648	0.98	3/875 (0.3%)
21	U	0.60	0/957	1.08	6/1289 (0.5%)
22	V	0.69	1/417 (0.2%)	1.03	2/562 (0.4%)
23	W	0.61	0/502	1.01	2/675 (0.3%)
24	X	0.76	0/1218	1.12	6/1655 (0.4%)
25	Y	0.71	0/664	1.06	3/895 (0.3%)
26	Z	0.67	0/1146	1.07	1/1536 (0.1%)
27	1	0.73	0/575	1.11	2/763 (0.3%)
28	2	0.72	0/437	1.09	3/578 (0.5%)
29	3	0.70	1/398 (0.3%)	0.84	0/527
30	4	0.64	0/771	1.06	5/1024 (0.5%)
All	All	0.60	21/98255 (0.0%)	0.87	223/147027 (0.2%)

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	A	1	58
2	B	1	2
All	All	2	60

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2486	A	O3'-P	32.86	2.10	1.61
1	A	2487	C	P-OP2	8.44	1.65	1.49
10	J	5	MET	SD-CE	-7.38	1.61	1.79
3	C	145	MET	SD-CE	6.95	1.97	1.79
11	K	19	MET	SD-CE	-6.57	1.63	1.79
22	V	20	MET	SD-CE	6.46	1.95	1.79
1	A	2487	C	O5'-C5'	6.31	1.51	1.42
1	A	2486	A	C4'-C3'	-5.95	1.43	1.52
1	A	2488	A	P-OP2	-5.86	1.37	1.49
1	A	2487	C	P-O5'	-5.75	1.51	1.59
14	N	38	VAL	CA-CB	5.64	1.61	1.54
2	B	3003	A	O5'-C5'	-5.46	1.34	1.42
10	J	60	ALA	CA-CB	-5.39	1.44	1.53
1	A	1206	U	C3'-O3'	5.36	1.50	1.42
1	A	2487	C	C4'-O4'	5.36	1.53	1.45
1	A	2486	A	C4'-O4'	5.34	1.53	1.45
1	A	2487	C	C5'-C4'	5.34	1.59	1.51
1	A	2487	C	O3'-P	-5.25	1.53	1.61
29	3	47	THR	CA-CB	5.15	1.60	1.53
1	A	2486	A	C3'-C2'	-5.12	1.45	1.52
11	K	63	ILE	CA-CB	-5.05	1.49	1.54

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-14.98	63.06	108.00
10	J	74	ASN	N-CA-C	-14.97	92.69	114.39
1	A	1563	G	C2'-C3'-O3'	13.94	130.40	109.50
2	B	3024	U	C2'-C3'-O3'	13.26	129.39	109.50
10	J	141	ASN	N-CA-C	-12.86	97.57	113.38
1	A	1164	U	OP2-P-O3'	-12.68	69.95	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1979	G	C2'-C3'-O3'	12.63	128.45	109.50
1	A	2486	A	O3'-P-O5'	-12.11	85.83	104.00
14	N	141	ILE	N-CA-C	-11.86	102.30	111.90
15	O	135	VAL	N-CA-C	-10.03	103.38	113.10
1	A	2486	A	C5'-C4'-C3'	9.90	130.85	116.00
1	A	2487	C	O4'-C4'-C3'	-9.88	94.12	104.00
1	A	1942	A	C5'-C4'-C3'	9.76	130.63	116.00
3	C	222	GLY	N-CA-C	-9.17	103.06	113.79
30	4	55	VAL	CA-C-N	8.58	130.56	119.84
30	4	55	VAL	C-N-CA	8.58	130.56	119.84
1	A	1563	G	C4'-C3'-O3'	8.51	122.17	109.40
21	U	52	ARG	N-CA-C	8.49	124.47	113.18
6	F	136	ARG	CA-C-N	8.41	130.35	119.84
6	F	136	ARG	C-N-CA	8.41	130.35	119.84
14	N	139	PRO	N-CA-C	-8.31	99.45	111.33
15	O	153	GLN	N-CA-C	-8.25	104.23	112.97
2	B	3024	U	C4'-C3'-O3'	8.16	121.64	109.40
18	R	17	LYS	N-CA-C	-8.09	99.55	109.83
15	O	169	PRO	N-CA-C	-8.07	103.37	114.27
4	D	157	LYS	N-CA-C	-8.00	104.12	114.04
7	G	11	VAL	N-CA-C	7.90	121.45	109.20
1	A	2486	A	O4'-C4'-C3'	7.68	111.68	104.00
11	K	68	GLY	N-CA-C	7.52	121.58	112.48
19	S	137	ASN	N-CA-C	7.52	121.59	110.46
15	O	133	ASP	N-CA-C	7.45	120.34	111.33
10	J	1	LYS	CA-C-N	7.44	127.36	119.85
10	J	1	LYS	C-N-CA	7.44	127.36	119.85
13	M	57	VAL	N-CA-C	-7.32	105.69	112.43
10	J	147	ARG	N-CA-C	-7.29	103.33	111.71
2	B	3039	U	N1-C1'-C2'	7.28	122.92	112.00
1	A	1165	G	O5'-P-OP1	-7.20	86.40	108.00
18	R	47	VAL	CA-C-N	7.19	126.45	118.97
18	R	47	VAL	C-N-CA	7.19	126.45	118.97
1	A	834	G	C2'-C3'-O3'	-7.04	103.14	113.70
5	E	78	ARG	N-CA-C	7.03	118.86	108.60
12	L	111	GLY	CA-C-N	6.93	126.87	120.21
12	L	111	GLY	C-N-CA	6.93	126.87	120.21
6	F	100	ASP	N-CA-C	-6.79	105.00	113.28
10	J	155	PRO	N-CA-C	6.78	121.57	111.41
3	C	70	ALA	N-CA-C	6.77	118.18	109.65
1	A	1120	U	C5'-C4'-C3'	-6.73	105.91	116.00
13	M	47	GLY	N-CA-C	6.66	118.91	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	75	GLY	N-CA-C	6.66	120.39	112.33
26	Z	143	TRP	N-CA-C	6.65	119.93	109.96
1	A	2486	A	C3'-C2'-C1'	6.64	107.94	101.30
10	J	137	ASN	N-CA-C	-6.52	101.62	110.36
23	W	42	ASN	CA-C-N	6.48	127.94	119.84
23	W	42	ASN	C-N-CA	6.48	127.94	119.84
5	E	175	LYS	N-CA-C	6.47	118.65	110.24
21	U	3	GLN	CA-C-N	6.45	127.91	119.84
21	U	3	GLN	C-N-CA	6.45	127.91	119.84
14	N	89	ASN	N-CA-C	6.44	117.96	111.07
10	J	156	THR	N-CA-C	-6.43	100.96	110.48
19	S	122	GLN	N-CA-C	-6.42	98.72	108.67
4	D	222	LYS	N-CA-C	-6.40	100.50	110.42
1	A	2096	A	C4'-C3'-O3'	-6.39	103.41	113.00
25	Y	22	ASN	N-CA-C	6.35	119.02	111.33
1	A	1819	G	C5'-C4'-C3'	6.32	125.48	116.00
2	B	3039	U	C4'-C3'-O3'	-6.31	103.53	113.00
1	A	2487	C	N1-C1'-C2'	6.30	121.45	112.00
20	T	57	THR	N-CA-C	6.29	119.04	110.55
1	A	1450	C	C2'-C3'-O3'	-6.28	104.27	113.70
15	O	13	ARG	N-CA-C	-6.27	104.69	112.90
14	N	42	ARG	CA-C-N	6.22	126.43	119.90
14	N	42	ARG	C-N-CA	6.22	126.43	119.90
7	G	37	ASP	N-CA-C	6.15	120.12	112.24
5	E	179	GLY	N-CA-C	-6.15	105.18	113.24
18	R	68	GLY	N-CA-C	-6.14	100.92	111.47
13	M	145	LEU	N-CA-C	-6.11	104.73	111.82
27	1	64	ILE	N-CA-C	6.09	118.64	109.20
21	U	54	ASP	N-CA-C	-6.07	105.14	112.54
1	A	1592	G	N9-C1'-C2'	6.01	121.02	112.00
22	V	18	GLY	N-CA-C	6.01	121.70	112.81
1	A	1504	A	N9-C1'-C2'	5.99	120.99	112.00
20	T	27	ALA	N-CA-C	-5.95	99.03	108.73
10	J	7	ARG	N-CA-C	5.94	119.78	112.54
28	2	21	ARG	N-CA-C	5.92	118.62	111.40
30	4	67	LEU	N-CA-C	5.91	119.18	109.85
16	P	43	VAL	N-CA-C	5.90	117.08	108.53
5	E	64	GLY	N-CA-C	5.89	119.89	113.58
1	A	129	A	C2'-C3'-O3'	5.86	122.49	113.70
1	A	1504	A	C1'-O4'-C4'	-5.86	104.04	109.90
15	O	51	GLY	CA-C-N	5.86	125.72	119.28
15	O	51	GLY	C-N-CA	5.86	125.72	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	60	LYS	N-CA-C	-5.84	102.23	110.29
16	P	2	LYS	N-CA-C	-5.83	101.85	110.48
19	S	13	THR	N-CA-C	5.83	118.27	109.23
14	N	27	ARG	N-CA-C	5.83	118.14	111.02
21	U	47	THR	N-CA-C	-5.82	100.70	109.95
1	A	206	G	C5'-C4'-C3'	-5.80	107.30	116.00
12	L	8	VAL	N-CA-C	5.78	116.81	108.48
14	N	70	GLY	N-CA-C	5.78	120.27	112.17
17	Q	118	GLN	N-CA-C	-5.76	104.92	111.14
20	T	59	ASP	N-CA-C	-5.73	106.27	113.72
1	A	874	A	C4'-C3'-O3'	-5.73	104.40	113.00
1	A	2664	A	N9-C1'-C2'	5.73	120.60	112.00
11	K	89	HIS	N-CA-C	5.73	119.74	112.87
13	M	43	HIS	N-CA-C	-5.73	99.67	109.24
3	C	135	VAL	N-CA-C	5.72	116.99	108.46
24	X	69	ARG	N-CA-C	5.72	119.85	112.41
1	A	924	G	C3'-C2'-O2'	5.71	119.27	110.70
14	N	14	ARG	CA-C-N	5.71	125.42	119.82
14	N	14	ARG	C-N-CA	5.71	125.42	119.82
1	A	2466	G	C4'-C3'-O3'	-5.70	104.44	113.00
4	D	323	LEU	N-CA-C	5.70	117.90	110.43
5	E	219	ASN	N-CA-C	5.70	117.89	109.69
1	A	1205	U	C3'-C2'-O2'	5.69	119.23	110.70
1	A	2488	A	O5'-C5'-C4'	-5.69	102.97	111.50
4	D	265	LEU	N-CA-C	5.68	118.21	110.55
3	C	198	ASP	N-CA-C	5.67	120.26	113.23
3	C	213	LYS	N-CA-C	5.66	119.44	112.54
19	S	34	GLU	N-CA-C	5.64	117.51	111.36
19	S	3	SER	N-CA-C	-5.62	100.82	109.52
5	E	9	ASP	N-CA-C	-5.61	106.42	113.72
15	O	171	HIS	N-CA-C	-5.60	105.27	111.71
1	A	2291	A	N9-C1'-C2'	5.59	120.39	112.00
1	A	1738	C	C5'-C4'-C3'	5.59	124.39	116.00
1	A	1330	A	C2'-C3'-O3'	-5.59	105.32	113.70
25	Y	79	GLU	N-CA-C	5.59	119.94	113.18
6	F	151	ILE	CA-C-N	5.58	125.51	119.76
6	F	151	ILE	C-N-CA	5.58	125.51	119.76
7	G	48	VAL	N-CA-C	5.58	115.92	108.11
15	O	3	GLY	CA-C-N	5.58	125.42	119.28
15	O	3	GLY	C-N-CA	5.58	125.42	119.28
1	A	921	G	N9-C1'-C2'	5.57	120.36	112.00
1	A	922	A	C4'-C3'-O3'	-5.54	104.69	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2096	A	N9-C1'-C2'	5.53	120.30	112.00
19	S	141	VAL	N-CA-C	5.51	116.42	108.48
1	A	2338	G	C2'-C3'-O3'	5.51	121.96	113.70
15	O	117	ALA	N-CA-C	-5.50	105.36	111.36
14	N	87	MET	N-CA-C	5.50	117.83	110.35
28	2	43	ALA	N-CA-C	-5.48	105.39	111.36
14	N	90	ARG	N-CA-C	5.45	119.92	113.16
12	L	14	LYS	N-CA-C	-5.45	101.98	110.10
15	O	168	LEU	N-CA-C	5.44	120.50	108.64
15	O	102	LEU	N-CA-C	5.43	117.58	109.59
4	D	242	TRP	N-CA-C	-5.42	105.28	111.07
1	A	2313	C	O4'-C4'-C3'	-5.41	98.59	104.00
4	D	175	LEU	N-CA-C	-5.41	105.28	111.07
6	F	137	PRO	N-CA-C	5.40	123.60	112.47
10	J	13	ALA	N-CA-C	-5.40	101.86	109.96
1	A	2486	A	OP1-P-O3'	-5.39	91.82	108.00
16	P	82	SER	N-CA-C	-5.38	103.79	110.41
4	D	154	VAL	CA-C-N	5.38	125.45	119.32
4	D	154	VAL	C-N-CA	5.38	125.45	119.32
1	A	2487	C	OP1-P-O3'	-5.38	91.87	108.00
1	A	835	U	C4'-C3'-O3'	-5.38	104.94	113.00
4	D	49	THR	N-CA-C	-5.37	101.13	108.38
1	A	457	U	C3'-C2'-O2'	5.37	118.75	110.70
21	U	78	THR	N-CA-C	5.36	116.79	109.18
4	D	111	ARG	N-CA-C	-5.36	106.74	113.28
8	H	118	LEU	N-CA-C	-5.35	106.83	113.19
8	H	8	VAL	N-CA-C	5.34	112.42	107.56
15	O	48	VAL	N-CA-C	5.34	116.27	108.53
2	B	3065	A	N9-C1'-C2'	5.33	120.00	112.00
4	D	114	ASP	N-CA-C	-5.33	99.29	108.56
1	A	2667	G	O5'-C5'-C4'	5.32	119.48	111.50
10	J	86	ARG	N-CA-C	5.32	119.62	113.18
1	A	1006	A	N9-C1'-C2'	5.32	119.98	112.00
10	J	162	SER	CA-C-N	-5.32	113.19	119.84
10	J	162	SER	C-N-CA	-5.32	113.19	119.84
5	E	186	TYR	N-CA-C	5.30	118.64	110.42
3	C	175	LYS	N-CA-C	-5.30	105.40	111.07
1	A	920	C	C2'-C3'-O3'	-5.29	105.76	113.70
1	A	2835	C	C4'-C3'-O3'	-5.29	105.07	113.00
15	O	42	HIS	N-CA-C	5.28	116.68	109.18
1	A	471	G	N9-C1'-C2'	5.28	119.92	112.00
1	A	2316	G	C5'-C4'-C3'	-5.26	107.31	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	50	GLU	N-CA-C	5.26	118.80	112.38
13	M	12	THR	N-CA-C	5.26	119.68	113.16
5	E	20	ASP	N-CA-C	5.24	117.40	111.11
4	D	11	LEU	N-CA-C	-5.23	106.48	112.92
18	R	49	ASN	N-CA-C	5.23	118.18	110.59
13	M	97	VAL	N-CA-C	5.22	116.42	109.37
1	A	1839	A	N9-C1'-C2'	5.21	119.81	112.00
2	B	3024	U	C4'-C3'-C2'	5.18	107.78	102.60
28	2	54	ALA	N-CA-C	5.18	117.60	111.33
5	E	192	ILE	N-CA-C	5.18	116.25	109.21
17	Q	56	GLY	N-CA-C	-5.17	102.98	110.90
1	A	2291	A	C4'-C3'-O3'	-5.16	105.26	113.00
11	K	9	ASP	N-CA-C	-5.16	106.49	112.89
1	A	1164	U	O3'-P-O5'	5.16	111.73	104.00
4	D	48	MET	N-CA-C	5.16	117.65	109.50
30	4	43	ASN	N-CA-C	5.14	119.40	113.18
1	A	2526	C	N1-C1'-C2'	5.14	119.71	112.00
1	A	2673	U	N1-C1'-C2'	5.14	119.71	112.00
14	N	74	ARG	N-CA-C	5.14	117.86	109.59
1	A	1359	U	N1-C1'-C2'	5.12	119.68	112.00
15	O	66	LEU	N-CA-C	-5.11	105.35	112.45
1	A	459	A	N9-C1'-C2'	5.10	119.65	112.00
27	1	18	TYR	N-CA-C	5.09	121.65	110.80
1	A	2470	A	C4'-C3'-O3'	-5.09	105.37	113.00
4	D	151	VAL	CA-C-N	5.09	124.26	118.97
4	D	151	VAL	C-N-CA	5.09	124.26	118.97
3	C	18	ALA	N-CA-C	-5.06	103.70	110.07
10	J	73	GLN	N-CA-C	-5.06	104.28	110.65
16	P	69	VAL	N-CA-C	5.06	115.77	108.48
24	X	9	GLY	N-CA-C	5.05	120.24	112.51
1	A	407	A	O4'-C4'-C3'	-5.05	98.95	104.00
25	Y	12	ILE	N-CA-C	5.05	112.86	107.76
1	A	2726	U	N1-C1'-C2'	5.05	119.58	112.00
7	G	112	ALA	CA-C-N	5.05	124.96	119.76
7	G	112	ALA	C-N-CA	5.05	124.96	119.76
10	J	111	MET	N-CA-C	-5.05	106.81	113.17
24	X	144	GLU	N-CA-C	-5.05	105.87	112.23
4	D	23	THR	CA-C-N	5.05	125.32	119.92
4	D	23	THR	C-N-CA	5.05	125.32	119.92
24	X	25	ASN	CA-C-N	-5.04	116.57	123.12
24	X	25	ASN	C-N-CA	-5.04	116.57	123.12
1	A	2425	A	O4'-C4'-C3'	-5.04	98.96	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	51	TYR	N-CA-C	5.04	119.11	112.92
1	A	2479	A	C3'-C2'-O2'	5.02	118.22	110.70
1	A	1559	A	C2'-C3'-O3'	5.01	121.22	113.70
14	N	4	ALA	N-CA-C	-5.01	105.90	111.36
18	R	20	ASP	N-CA-C	-5.01	106.76	112.92
1	A	2313	C	C5'-C4'-C3'	5.00	123.50	116.00
10	J	110	GLY	N-CA-C	-5.00	101.32	113.18

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1038	G	Sidechain
1	A	1039	G	Sidechain
1	A	1055	G	Sidechain
1	A	1122	U	Sidechain
1	A	1192	A	Sidechain
1	A	1206	U	Sidechain
1	A	1340	G	Sidechain
1	A	1376	G	Sidechain
1	A	1417	G	Sidechain
1	A	1430	G	Sidechain
1	A	1447	U	Sidechain
1	A	1458	A	Sidechain
1	A	1501	A	Sidechain
1	A	1524	U	Sidechain
1	A	1688	G	Sidechain
1	A	174	A	Sidechain
1	A	1809	G	Sidechain
1	A	1829	A	Sidechain
1	A	1835	U	Sidechain
1	A	1845	A	Sidechain
1	A	1848	G	Sidechain
1	A	1877	G	Sidechain
1	A	1878	G	Sidechain
1	A	1972	U	Sidechain
1	A	2073	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2308	U	Sidechain
1	A	2312	G	Sidechain
1	A	2313	C	Sidechain
1	A	2412	G	Sidechain
1	A	246	G	Sidechain
1	A	2465	A	Sidechain
1	A	2493	C	Sidechain
1	A	2503	A	Sidechain
1	A	2506	A	Sidechain
1	A	2526	C	Sidechain
1	A	2564	G	Sidechain
1	A	2607	U	Sidechain
1	A	2630	G	Sidechain
1	A	2643	G	Sidechain
1	A	2673	U	Sidechain
1	A	2793	A	Sidechain
1	A	2840	A	Sidechain
1	A	2842	G	Sidechain
1	A	321	A	Sidechain
1	A	333	G	Sidechain
1	A	396	U	Sidechain
1	A	458	G	Sidechain
1	A	462	A	Sidechain
1	A	482	G	Sidechain
1	A	486	A	Sidechain
1	A	487	G	Sidechain
1	A	518	G	Sidechain
1	A	755	G	Sidechain
1	A	781	C	Sidechain
1	A	867	A	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	903	U	Sidechain
2	B	3039	U	Sidechain
2	B	3065	A	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	A	59017	0	29807	900	0
2	B	2600	0	1326	84	0
3	C	1754	0	1763	127	0
4	D	2624	0	2533	181	0
5	E	1858	0	1816	113	0
6	F	1094	0	1085	142	0
7	G	1357	0	1266	80	0
8	H	885	0	854	65	0
9	I	240	0	231	24	0
10	J	1215	0	1215	160	0
11	K	1119	0	1098	63	0
12	L	993	0	1027	56	0
13	M	1114	0	1072	63	0
14	N	1605	0	1676	154	0
15	O	1444	0	1401	124	0
16	P	864	0	873	30	0
17	Q	1133	0	1127	47	0
18	R	734	0	728	16	0
19	S	1149	0	1122	57	0
20	T	641	0	605	25	0
21	U	949	0	923	54	0
22	V	410	0	364	33	0
23	W	499	0	511	30	0
24	X	1195	0	1137	95	0
25	Y	654	0	653	46	0
26	Z	1130	0	1133	57	0
27	1	563	0	597	57	0
28	2	430	0	426	23	0
29	3	393	0	406	28	0
30	4	755	0	730	37	0
31	A	19	0	19	1	0
32	4	1	0	0	0	0
32	A	109	0	0	0	0
32	B	1	0	0	0	0
32	C	2	0	0	0	0
32	D	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	0	0
35	A	9	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	2	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	38	0	0	13	0
37	2	56	0	0	1	0
37	3	40	0	0	6	0
37	4	72	0	0	9	0
37	A	5924	0	0	183	0
37	B	143	0	0	15	0
37	C	127	0	0	23	0
37	D	146	0	0	25	0
37	E	164	0	0	28	0
37	F	54	0	0	21	0
37	G	42	0	0	11	0
37	H	28	0	0	9	0
37	I	22	0	0	6	0
37	J	79	0	0	23	0
37	K	56	0	0	5	0
37	L	62	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	M	81	0	0	18	0
37	N	126	0	0	21	0
37	O	66	0	0	17	0
37	P	44	0	0	5	0
37	Q	65	0	0	3	0
37	R	54	0	0	2	0
37	S	86	0	0	10	0
37	T	35	0	0	5	0
37	U	41	0	0	4	0
37	V	25	0	0	6	0
37	W	15	0	0	2	0
37	X	67	0	0	8	0
37	Y	29	0	0	4	0
37	Z	92	0	0	16	0
All	All	98548	0	59524	2713	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 18.

All (2713) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:G:H5'	1:A:1161:A:H5'	1.24	1.18
5:E:236:THR:HG22	5:E:239:ALA:H	1.04	1.14
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.64	1.12
1:A:1134:G:H4'	10:J:151:MET:HE1	1.26	1.11
6:F:25:MET:HE2	6:F:41:LEU:HG	1.31	1.10
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.29	1.10
1:A:2486:A:O3'	1:A:2487:C:P	2.10	1.09
14:N:164:THR:HG22	14:N:167:GLY:H	1.18	1.07
11:K:19:MET:HE3	11:K:132:LEU:HD11	1.37	1.06
1:A:1242:A:H5'	11:K:82:THR:HG23	1.35	1.06
5:E:5:ILE:HD11	5:E:16:VAL:HG23	1.39	1.05
1:A:156:C:H5''	14:N:171:ARG:HD3	1.38	1.03
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.36	1.03
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.41	1.02
2:B:3006:C:H5''	15:O:37:ARG:NH1	1.75	1.02
5:E:127:ARG:NH2	5:E:225:PRO:HG2	1.74	1.02
12:L:10:GLN:NE2	12:L:10:GLN:H	1.58	1.01
6:F:134:LEU:HD11	6:F:166:ILE:HD11	1.40	1.01
10:J:86:ARG:HH11	10:J:133:ILE:HG13	0.85	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:G:H4'	37:A:7421:HOH:O	1.58	1.00
1:A:2717:C:H2'	1:A:2718:C:H5''	1.43	1.00
10:J:45:GLN:HB3	10:J:163:PRO:HD2	1.39	1.00
2:B:3023:U:H4'	2:B:3024:U:OP2	1.58	1.00
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.41	1.00
24:X:88:THR:HB	37:X:6679:HOH:O	1.63	0.99
2:B:3076:G:H3'	2:B:3077:A:H5''	1.45	0.99
10:J:26:LYS:HD2	10:J:28:ILE:HD12	1.42	0.98
10:J:162:SER:HB2	10:J:163:PRO:HD3	1.43	0.98
17:Q:115:SER:H	17:Q:118:GLN:HE21	0.99	0.98
1:A:1474:C:H6	1:A:1474:C:H5'	1.30	0.96
4:D:86:ALA:HA	37:D:8579:HOH:O	1.63	0.96
1:A:871:G:H5'	1:A:871:G:C8	2.00	0.96
1:A:871:G:H5'	1:A:871:G:H8	1.30	0.96
10:J:86:ARG:HH11	10:J:133:ILE:CG1	1.79	0.96
27:1:10:ARG:HA	37:1:8415:HOH:O	1.64	0.95
1:A:856:G:H2'	37:A:5405:HOH:O	1.65	0.95
1:A:1751:G:H2'	1:A:1752:G:H5''	1.47	0.95
24:X:88:THR:HG22	24:X:89:ASP:H	1.29	0.95
3:C:191:GLY:HA2	3:C:194:MET:HE2	1.48	0.95
26:Z:200:THR:HG22	26:Z:201:GLU:HG3	1.48	0.95
12:L:29:LEU:HB3	12:L:55:VAL:HG11	1.45	0.94
15:O:47:LEU:HD11	15:O:127:LEU:HD21	1.48	0.94
2:B:3006:C:H5''	15:O:37:ARG:HH12	1.32	0.94
4:D:162:MET:HE1	4:D:308:LEU:HD21	1.49	0.94
5:E:78:ARG:HG3	5:E:78:ARG:HH11	1.33	0.94
2:B:3056:A:H2'	2:B:3057:A:H5''	1.49	0.94
1:A:870:G:H2'	1:A:871:G:H5''	1.49	0.94
1:A:1835:U:H5	1:A:1840:A:N7	1.66	0.94
4:D:264:GLU:HG2	4:D:267:LYS:HE2	1.50	0.93
37:A:4836:HOH:O	14:N:14:ARG:HG2	1.68	0.93
27:1:38:LYS:HE2	27:1:45:LYS:HE2	1.49	0.92
4:D:140:LEU:HA	37:D:8579:HOH:O	1.68	0.92
24:X:149:LEU:HG	24:X:153:MET:HE2	1.48	0.92
4:D:212:GLN:HB2	4:D:257:THR:HG21	1.50	0.92
14:N:52:LEU:HD11	37:N:8615:HOH:O	1.69	0.92
6:F:154:LYS:H	6:F:154:LYS:HD2	1.33	0.92
10:J:165:GLY:HA3	37:J:8399:HOH:O	1.70	0.92
1:A:21:G:H5'	19:S:2:ILE:HA	1.53	0.91
3:C:211:LYS:HB3	3:C:212:PRO:HD2	1.52	0.91
1:A:542:A:H5'	1:A:542:A:H8	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:137:GLN:HE21	24:X:141:HIS:HE1	1.16	0.89
12:L:10:GLN:H	12:L:10:GLN:HE21	0.92	0.89
12:L:10:GLN:HE21	12:L:10:GLN:N	1.70	0.89
13:M:68:GLU:HA	37:M:8545:HOH:O	1.72	0.89
4:D:238:ASN:HD22	4:D:240:GLY:H	1.20	0.89
20:T:57:THR:HG22	20:T:59:ASP:H	1.36	0.89
6:F:105:SER:HB2	6:F:131:THR:HG23	1.52	0.89
27:1:46:LYS:HD3	27:1:59:HIS:HB2	1.54	0.89
5:E:2:GLN:HB3	37:E:8335:HOH:O	1.73	0.89
5:E:115:LEU:HD13	5:E:223:LEU:HD21	1.53	0.88
11:K:76:ASP:HA	37:K:5907:HOH:O	1.74	0.88
5:E:236:THR:HG22	5:E:239:ALA:N	1.88	0.88
10:J:29:ALA:HB3	10:J:65:ARG:HH12	1.36	0.88
37:A:3703:HOH:O	14:N:157:LEU:HD11	1.74	0.88
1:A:2717:C:C2'	1:A:2718:C:H5''	2.02	0.88
12:L:81:ARG:HB2	12:L:87:ARG:HH11	1.37	0.88
14:N:24:MET:HE3	14:N:28:MET:HE3	1.54	0.87
4:D:321:PRO:HA	37:D:8658:HOH:O	1.74	0.87
13:M:79:ASP:HB3	37:M:8560:HOH:O	1.75	0.87
15:O:83:LEU:HD13	15:O:175:LEU:HD23	1.56	0.87
37:A:4437:HOH:O	14:N:146:GLN:HG2	1.74	0.87
1:A:1372:A:H3'	37:A:7178:HOH:O	1.73	0.87
1:A:381:G:H5''	37:A:4291:HOH:O	1.73	0.87
10:J:55:GLN:HE21	10:J:124:ARG:HE	1.22	0.87
4:D:7:ARG:HG2	4:D:7:ARG:HH11	1.38	0.86
10:J:27:LYS:H	10:J:58:HIS:HD2	1.23	0.86
1:A:962:C:H1'	15:O:5:ARG:NH1	1.90	0.86
1:A:645:U:OP2	13:M:4:LYS:HE2	1.74	0.86
5:E:132:ASP:HB3	37:E:8362:HOH:O	1.76	0.86
1:A:2506:A:HO2'	1:A:2507:G:H8	0.86	0.85
1:A:2812:A:H2	1:A:2814:A:H62	1.23	0.85
24:X:4:LEU:HD22	24:X:52:VAL:HG21	1.58	0.85
29:3:39:ARG:HG2	37:3:3143:HOH:O	1.76	0.85
4:D:62:ARG:HA	4:D:65:MET:HE3	1.57	0.85
1:A:1701:A:H5'	37:A:6265:HOH:O	1.77	0.84
27:1:38:LYS:HG2	27:1:45:LYS:HG2	1.57	0.84
1:A:1184:C:H1'	37:A:7458:HOH:O	1.76	0.84
10:J:139:ASP:N	10:J:140:PRO:HD3	1.92	0.84
1:A:1116:U:H3	1:A:1246:A:H62	1.23	0.84
1:A:1667:A:H5'	1:A:1667:A:H8	1.41	0.84
15:O:49:THR:HG22	15:O:56:ASP:HB2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:C:H5'	1:A:1474:C:C6	2.12	0.84
15:O:7:LYS:HE3	18:R:21:ARG:O	1.77	0.84
17:Q:115:SER:H	17:Q:118:GLN:NE2	1.76	0.84
27:1:58:GLY:HA3	37:1:8439:HOH:O	1.78	0.84
10:J:150:LYS:HE2	37:J:8385:HOH:O	1.77	0.84
23:W:42:ASN:HB3	37:W:7247:HOH:O	1.77	0.84
1:A:214:U:H5'	37:A:6122:HOH:O	1.76	0.84
15:O:144:GLY:O	15:O:147:ILE:HG22	1.77	0.83
1:A:1134:G:C4'	10:J:151:MET:HE1	2.09	0.83
15:O:87:LEU:HD12	15:O:186:LEU:HD21	1.59	0.83
29:3:41:HIS:H	29:3:45:ASN:HD22	1.24	0.83
2:B:3024:U:O2'	2:B:3025:G:H4'	1.77	0.83
6:F:20:LYS:HA	6:F:75:LEU:O	1.78	0.83
14:N:102:GLU:OE1	14:N:164:THR:HG21	1.77	0.83
6:F:64:ARG:HG2	6:F:67:ASP:HB3	1.60	0.83
4:D:201:ASP:HB2	4:D:312:ARG:HD2	1.60	0.82
10:J:162:SER:HB2	10:J:163:PRO:CD	2.08	0.82
14:N:35:PRO:HG2	14:N:38:VAL:HG23	1.58	0.82
37:A:3762:HOH:O	14:N:189:VAL:HG21	1.79	0.82
3:C:199:HIS:HD2	3:C:201:PHE:H	1.25	0.82
24:X:6:GLN:HB2	24:X:26:ILE:HD12	1.60	0.82
10:J:2:PRO:HB2	37:J:8368:HOH:O	1.80	0.82
1:A:506:G:H22	1:A:509:A:C5'	1.92	0.81
13:M:133:VAL:HA	37:M:8575:HOH:O	1.79	0.81
24:X:88:THR:HG23	24:X:110:GLN:NE2	1.95	0.81
37:A:6277:HOH:O	6:F:99:ASP:HA	1.79	0.81
7:G:97:VAL:HG12	37:G:4191:HOH:O	1.79	0.81
37:A:5197:HOH:O	12:L:39:GLY:HA2	1.80	0.81
19:S:8:ALA:HB1	19:S:13:THR:HG21	1.62	0.81
10:J:142:VAL:HG13	37:J:8383:HOH:O	1.80	0.81
25:Y:78:GLU:HG2	25:Y:79:GLU:H	1.46	0.81
27:1:40:PRO:HD3	27:1:47:LEU:HD11	1.61	0.81
24:X:88:THR:HG22	24:X:89:ASP:N	1.96	0.81
19:S:9:ASP:O	19:S:13:THR:HB	1.81	0.81
1:A:2274:A:N3	14:N:86:MET:HE1	1.96	0.80
2:B:3023:U:H3'	37:B:8479:HOH:O	1.81	0.80
35:K:8501:CL:CL	37:K:4038:HOH:O	2.36	0.80
5:E:140:VAL:HB	37:E:8446:HOH:O	1.81	0.80
1:A:545:G:H5'	1:A:545:G:H8	1.44	0.80
1:A:1116:U:O2'	1:A:1118:A:H2	1.64	0.80
1:A:1329:A:H2	37:A:4655:HOH:O	1.65	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:62:THR:HB	37:4:8551:HOH:O	1.80	0.80
1:A:871:G:H8	1:A:871:G:C5'	1.95	0.80
8:H:96:ALA:HA	37:H:3111:HOH:O	1.79	0.80
1:A:560:C:H42	1:A:597:A:H61	1.26	0.80
14:N:172:GLY:O	14:N:183:VAL:HG11	1.80	0.80
1:A:1603:A:H5'	1:A:1605:G:O4'	1.82	0.80
15:O:164:ASP:CG	15:O:167:ASP:HA	2.07	0.80
14:N:35:PRO:CG	14:N:38:VAL:HG23	2.11	0.80
25:Y:30:MET:HE1	25:Y:58:ALA:HB3	1.62	0.79
1:A:559:U:H6	1:A:559:U:H5'	1.48	0.79
24:X:68:THR:HG23	24:X:69:ARG:HG2	1.62	0.79
1:A:346:U:H4'	37:A:6826:HOH:O	1.82	0.79
1:A:1164:U:H3	1:A:1192:A:H2	1.28	0.79
1:A:1209:C:H4'	37:A:5257:HOH:O	1.82	0.79
4:D:41:PHE:CD1	4:D:79:MET:HE2	2.16	0.79
6:F:27:ILE:HG22	6:F:28:GLY:H	1.47	0.79
12:L:74:VAL:HG11	12:L:113:ILE:HG12	1.63	0.79
30:4:70:ARG:HG2	30:4:77:ALA:HB2	1.63	0.79
37:A:3660:HOH:O	14:N:79:LYS:HD3	1.81	0.79
14:N:164:THR:HG23	14:N:165:SER:N	1.96	0.79
3:C:35:GLY:O	3:C:36:ASP:HB3	1.81	0.79
2:B:3001:U:O3'	2:B:3003:A:H5''	1.83	0.79
1:A:1160:G:H5'	1:A:1161:A:C5'	2.11	0.78
14:N:164:THR:HG22	14:N:167:GLY:N	1.96	0.78
3:C:100:PRO:HG2	3:C:103:VAL:HG21	1.64	0.78
1:A:1165:G:H4'	1:A:1174:A:O2'	1.83	0.78
5:E:236:THR:HG21	37:E:8373:HOH:O	1.83	0.78
1:A:1166:A:H1'	1:A:1192:A:C2	2.18	0.78
1:A:2716:G:H5''	4:D:206:THR:HG21	1.66	0.78
4:D:190:MET:HE2	4:D:194:PHE:CD1	2.18	0.78
23:W:1:THR:HG23	23:W:2:VAL:H	1.48	0.78
4:D:18:ARG:HG3	4:D:256:GLN:HG3	1.64	0.78
6:F:146:LYS:NZ	15:O:107:ASN:HD21	1.81	0.78
27:1:49:ARG:HD2	37:1:8429:HOH:O	1.82	0.78
26:Z:212:ARG:HD2	37:Z:8598:HOH:O	1.83	0.78
1:A:544:G:H2'	1:A:545:G:H5''	1.65	0.78
14:N:87:MET:HB3	30:4:46:ILE:HG21	1.63	0.78
26:Z:187:VAL:HG23	26:Z:192:ASP:HB2	1.66	0.78
1:A:870:G:C2'	1:A:871:G:H5''	2.14	0.77
7:G:100:ASP:HB2	37:G:2789:HOH:O	1.84	0.77
8:H:91:VAL:HG12	8:H:92:GLY:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:U:HO2'	1:A:1118:A:H2	0.82	0.77
37:A:6856:HOH:O	14:N:178:LYS:HB2	1.84	0.77
12:L:14:LYS:HB2	12:L:45:PRO:HG2	1.66	0.77
4:D:162:MET:HE2	4:D:310:ARG:HD3	1.65	0.77
17:Q:115:SER:OG	17:Q:118:GLN:HG3	1.83	0.77
1:A:1160:G:C5'	1:A:1161:A:H5'	2.11	0.77
1:A:2890:A:H1'	22:V:56:ARG:NH2	1.99	0.77
15:O:48:VAL:CG1	15:O:55:ASP:HB3	2.15	0.77
2:B:3025:G:H3'	2:B:3026:C:H5'	1.66	0.77
37:A:6754:HOH:O	15:O:4:PRO:HD2	1.85	0.77
2:B:3023:U:H6	2:B:3023:U:H5''	1.50	0.77
17:Q:59:ARG:NH2	17:Q:66:GLN:HE22	1.83	0.77
3:C:88:ILE:HD13	3:C:100:PRO:HD3	1.67	0.76
14:N:139:PRO:O	14:N:140:ALA:HB3	1.85	0.76
1:A:2506:A:O2'	1:A:2507:G:H8	1.66	0.76
24:X:122:ARG:HH21	24:X:154:ARG:HD2	1.50	0.76
1:A:284:C:H4'	1:A:285:A:O5'	1.84	0.76
20:T:57:THR:HG22	20:T:59:ASP:N	1.99	0.76
10:J:26:LYS:HG2	10:J:28:ILE:H	1.49	0.76
12:L:81:ARG:HB2	12:L:87:ARG:NH1	1.99	0.76
1:A:288:A:H61	1:A:364:C:H42	1.34	0.76
7:G:15:GLN:HG3	7:G:20:ILE:HG12	1.65	0.76
1:A:541:C:H2'	1:A:542:A:H5''	1.67	0.76
24:X:21:LEU:HD22	24:X:26:ILE:HD11	1.67	0.76
1:A:1701:A:H4'	1:A:1702:U:H5''	1.66	0.76
7:G:20:ILE:HD11	7:G:40:VAL:HG11	1.68	0.76
6:F:88:LEU:HB2	6:F:89:PRO:HD3	1.69	0.75
16:P:42:GLU:HB2	37:P:2176:HOH:O	1.83	0.75
1:A:1625:U:H4'	37:A:4639:HOH:O	1.86	0.75
5:E:139:VAL:HG13	37:E:8443:HOH:O	1.85	0.75
19:S:17:MET:HE1	19:S:19:ARG:NH2	2.00	0.75
5:E:5:ILE:HD11	5:E:16:VAL:CG2	2.14	0.75
21:U:61:GLU:HG3	37:U:3851:HOH:O	1.84	0.75
1:A:1450:C:H4'	1:A:1451:C:OP2	1.87	0.75
4:D:221:GLN:HE22	12:L:42:ASN:HD22	1.32	0.75
9:I:23:ILE:HD13	9:I:67:LEU:HD23	1.67	0.75
15:O:113:SER:HB2	37:O:8559:HOH:O	1.85	0.75
16:P:47:ARG:HH11	16:P:47:ARG:HG3	1.51	0.75
1:A:289:G:H22	1:A:363:A:H2	1.35	0.75
1:A:1170:U:O2'	1:A:1172:G:N7	2.19	0.74
2:B:3025:G:H3'	2:B:3026:C:C5'	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:55:GLN:NE2	10:J:124:ARG:HE	1.84	0.74
24:X:122:ARG:HG2	24:X:122:ARG:HH11	1.51	0.74
5:E:236:THR:H	5:E:239:ALA:HB3	1.53	0.74
25:Y:71:ARG:HB3	25:Y:88:GLU:OE1	1.87	0.74
1:A:31:C:H2'	37:A:7687:HOH:O	1.86	0.74
1:A:506:G:H22	1:A:509:A:H5'	1.51	0.74
12:L:74:VAL:HG13	12:L:113:ILE:HG23	1.69	0.74
22:V:14:GLU:O	22:V:17:THR:HB	1.88	0.74
24:X:88:THR:HG23	24:X:110:GLN:HE21	1.51	0.74
1:A:541:C:C2'	1:A:542:A:H5''	2.17	0.74
5:E:78:ARG:HG3	5:E:78:ARG:NH1	2.02	0.74
1:A:2468:A:H61	30:4:48:ASN:HD21	1.32	0.74
14:N:94:LYS:HE3	37:N:8583:HOH:O	1.87	0.74
17:Q:115:SER:N	17:Q:118:GLN:HE21	1.83	0.74
1:A:2768:A:H2'	1:A:2769:C:O4'	1.87	0.73
37:A:4925:HOH:O	2:B:3103:A:H4'	1.88	0.73
15:O:164:ASP:OD2	15:O:167:ASP:HA	1.87	0.73
2:B:3014:G:H5'	2:B:3014:G:H8	1.53	0.73
26:Z:187:VAL:HG23	26:Z:192:ASP:CB	2.19	0.73
1:A:2710:U:H1'	37:A:7619:HOH:O	1.89	0.73
1:A:1666:C:O2'	1:A:1667:A:H5''	1.89	0.73
3:C:36:ASP:OD2	3:C:85:ASP:HB2	1.88	0.73
14:N:138:HIS:ND1	14:N:139:PRO:O	2.21	0.73
15:O:80:SER:HB2	37:O:8535:HOH:O	1.87	0.73
23:W:12:THR:HG22	23:W:15:GLU:CG	2.16	0.73
7:G:84:MET:HE2	7:G:133:VAL:CG2	2.17	0.73
10:J:137:ASN:O	10:J:139:ASP:N	2.21	0.73
3:C:105:VAL:HG11	3:C:154:ALA:HB1	1.71	0.73
1:A:2533:C:H6	1:A:2533:C:H5'	1.54	0.73
8:H:91:VAL:HG12	8:H:92:GLY:N	2.04	0.73
14:N:152:ARG:HG3	37:N:8555:HOH:O	1.89	0.73
1:A:299:U:H5'	37:A:7326:HOH:O	1.89	0.72
2:B:3056:A:C2'	2:B:3057:A:H5''	2.19	0.72
1:A:711:G:H1'	37:A:7082:HOH:O	1.89	0.72
37:A:4809:HOH:O	11:K:47:THR:HB	1.88	0.72
37:A:5774:HOH:O	14:N:170:CYS:SG	2.46	0.72
9:I:12:ILE:N	9:I:13:PRO:HD3	2.04	0.72
1:A:871:G:C8	1:A:871:G:C5'	2.72	0.72
37:A:7415:HOH:O	21:U:9:LYS:HB2	1.87	0.72
2:B:3039:U:H1'	2:B:3044:A:H61	1.54	0.72
10:J:46:VAL:HG12	10:J:146:TRP:HZ3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:242:GLU:HG3	37:E:8381:HOH:O	1.89	0.72
10:J:33:MET:HB2	10:J:83:PHE:HB3	1.72	0.72
14:N:87:MET:HB3	30:4:46:ILE:HD13	1.71	0.72
1:A:272:A:H3'	37:A:7523:HOH:O	1.89	0.72
5:E:236:THR:CG2	5:E:239:ALA:H	1.94	0.72
13:M:67:ARG:O	13:M:71:GLU:HG3	1.88	0.72
24:X:65:VAL:HA	24:X:68:THR:HG22	1.72	0.72
10:J:4:ALA:HB3	37:J:8368:HOH:O	1.90	0.72
10:J:41:THR:HA	37:J:8397:HOH:O	1.88	0.72
11:K:45:VAL:HG23	11:K:130:VAL:O	1.89	0.72
1:A:877:G:H5'	1:A:878:G:OP1	1.89	0.72
1:A:1119:G:N2	1:A:1246:A:C2	2.57	0.72
19:S:99:ALA:CB	19:S:109:MET:HE1	2.16	0.72
30:4:25:VAL:HG22	30:4:68:LYS:HG3	1.72	0.72
1:A:2586:U:H3	1:A:2592:G:H22	1.35	0.71
1:A:1666:C:H2'	1:A:1667:A:H5'	1.71	0.71
6:F:95:THR:O	6:F:97:GLN:N	2.19	0.71
1:A:2426:G:H1'	37:A:6073:HOH:O	1.88	0.71
16:P:14:LEU:HD23	16:P:102:ILE:HD11	1.72	0.71
3:C:131:HIS:O	3:C:132:ASP:HB2	1.89	0.71
4:D:179:LEU:O	4:D:183:GLU:HG2	1.90	0.71
8:H:50:VAL:HG13	8:H:60:VAL:HG11	1.73	0.71
10:J:47:GLU:HB3	10:J:133:ILE:CD1	2.19	0.71
15:O:23:ARG:HD3	37:O:8547:HOH:O	1.91	0.71
3:C:191:GLY:HA2	3:C:194:MET:CE	2.20	0.71
7:G:81:GLU:HG2	7:G:134:SER:HB3	1.71	0.71
23:W:39:ALA:N	23:W:40:PRO:HD2	2.06	0.71
1:A:1118:A:C8	1:A:1118:A:H3'	2.25	0.71
20:T:51:GLN:HE21	20:T:53:ASN:HD21	1.38	0.71
27:1:37:HIS:HB2	27:1:47:LEU:HB2	1.72	0.71
1:A:2420:G:O2'	1:A:2421:G:H5'	1.90	0.71
5:E:115:LEU:O	5:E:118:THR:HB	1.89	0.71
7:G:6:GLU:HA	7:G:46:THR:HG22	1.73	0.71
1:A:1191:A:H3'	1:A:1192:A:H5''	1.73	0.71
13:M:114:VAL:HG11	37:M:8575:HOH:O	1.90	0.71
13:M:143:THR:HG22	13:M:144:ASP:N	2.04	0.71
30:4:70:ARG:HD3	37:4:8540:HOH:O	1.90	0.71
1:A:183:A:H5'	14:N:157:LEU:HD12	1.72	0.71
1:A:282:C:H1'	1:A:368:C:N4	2.05	0.71
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.73	0.71
1:A:2812:A:N7	37:A:7510:HOH:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:26:LYS:HD2	10:J:28:ILE:CD1	2.19	0.70
19:S:39:THR:HB	19:S:42:GLU:HG3	1.72	0.70
26:Z:216:ARG:HD3	37:Z:8566:HOH:O	1.89	0.70
1:A:1118:A:H3'	1:A:1118:A:H8	1.56	0.70
1:A:447:A:OP1	21:U:2:LYS:HG2	1.90	0.70
1:A:1080:C:H4'	1:A:1081:A:OP1	1.91	0.70
6:F:135:VAL:HG22	6:F:136:ARG:H	1.56	0.70
3:C:199:HIS:CD2	3:C:201:PHE:H	2.08	0.70
4:D:162:MET:HE2	4:D:310:ARG:CD	2.21	0.70
5:E:104:ASP:HA	5:E:107:ARG:HH12	1.55	0.70
24:X:4:LEU:HD22	24:X:52:VAL:CG2	2.22	0.70
1:A:1119:G:H22	1:A:1246:A:H2	1.37	0.70
6:F:19:GLU:O	6:F:20:LYS:HG2	1.92	0.70
6:F:64:ARG:CG	6:F:67:ASP:HB3	2.21	0.70
14:N:106:ASN:HD22	14:N:114:VAL:HG23	1.55	0.70
4:D:254:GLN:HG3	37:D:8530:HOH:O	1.92	0.70
10:J:140:PRO:HB3	37:J:8383:HOH:O	1.92	0.70
11:K:74:ARG:HB3	11:K:74:ARG:HH11	1.55	0.70
1:A:236:A:H4'	1:A:237:G:H5'	1.74	0.69
1:A:962:C:H1'	15:O:5:ARG:HH12	1.55	0.69
1:A:1244:U:OP1	11:K:18:ILE:HD13	1.92	0.69
1:A:1751:G:C2'	1:A:1752:G:H5''	2.21	0.69
11:K:107:ASN:ND2	11:K:109:TYR:H	1.89	0.69
1:A:470:U:O2'	28:2:16:HIS:HD2	1.74	0.69
24:X:72:PRO:HG2	24:X:77:ALA:HB3	1.73	0.69
1:A:657:G:OP1	5:E:27:ARG:NH2	2.22	0.69
6:F:35:ALA:N	37:F:5576:HOH:O	2.24	0.69
10:J:71:TYR:C	10:J:73:GLN:H	2.00	0.69
19:S:17:MET:SD	37:S:8547:HOH:O	2.50	0.69
1:A:2064:U:H5'	1:A:2652:U:O3'	1.93	0.69
2:B:3029:C:H2'	2:B:3030:C:H5'	1.74	0.69
14:N:61:ILE:HG13	37:N:8623:HOH:O	1.91	0.69
1:A:282:C:O2'	1:A:283:U:H5'	1.92	0.69
3:C:153:ARG:HB2	3:C:153:ARG:HH11	1.56	0.69
4:D:62:ARG:HA	4:D:65:MET:CE	2.22	0.69
7:G:84:MET:HE1	7:G:148:ILE:HD12	1.74	0.69
10:J:49:VAL:O	10:J:157:ILE:HG23	1.92	0.69
21:U:9:LYS:HE3	21:U:13:ARG:NH1	2.08	0.69
24:X:21:LEU:HD22	24:X:26:ILE:CD1	2.22	0.69
13:M:148:GLU:HA	37:M:8574:HOH:O	1.91	0.69
1:A:485:A:N3	1:A:487:G:H5''	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:A:H5'	1:A:542:A:C8	2.25	0.69
1:A:1377:C:H6	1:A:1377:C:H5'	1.58	0.69
2:B:3006:C:C5'	15:O:37:ARG:NH1	2.55	0.69
4:D:82:VAL:O	4:D:82:VAL:HG12	1.92	0.69
1:A:536:A:H3'	37:A:5022:HOH:O	1.92	0.69
1:A:2840:A:OP1	4:D:211:THR:HG23	1.92	0.69
10:J:14:TYR:H	10:J:91:HIS:CE1	2.10	0.69
10:J:47:GLU:HB3	10:J:133:ILE:HD13	1.74	0.69
14:N:80:GLY:O	14:N:81:ARG:HD3	1.93	0.69
25:Y:72:VAL:HG22	25:Y:85:VAL:HG12	1.74	0.69
3:C:192:VAL:HB	37:C:8595:HOH:O	1.91	0.69
7:G:166:VAL:HG12	37:G:3134:HOH:O	1.92	0.69
24:X:154:ARG:C	37:X:4276:HOH:O	2.35	0.69
25:Y:25:ARG:HD2	37:Y:3861:HOH:O	1.92	0.69
29:3:18:ASN:HD21	29:3:40:ARG:H	1.41	0.69
3:C:69:LEU:HD21	3:C:120:ARG:HB3	1.75	0.69
3:C:121:ALA:O	3:C:124:VAL:HG22	1.92	0.69
7:G:23:GLU:HG2	7:G:28:SER:HB3	1.75	0.69
10:J:46:VAL:O	10:J:146:TRP:HH2	1.76	0.69
14:N:60:ILE:C	14:N:61:ILE:HD12	2.18	0.69
14:N:139:PRO:O	14:N:140:ALA:CB	2.41	0.69
25:Y:76:ARG:HH11	25:Y:76:ARG:HG3	1.58	0.69
1:A:1353:C:P	37:A:4651:HOH:O	2.52	0.68
15:O:86:LEU:HD12	15:O:125:ALA:HB2	1.75	0.68
7:G:84:MET:HE1	7:G:148:ILE:CD1	2.23	0.68
1:A:2291:A:C8	1:A:2309:C:H5'	2.28	0.68
2:B:3003:A:H2'	37:B:8422:HOH:O	1.93	0.68
10:J:53:PRO:HG3	10:J:127:GLY:H	1.59	0.68
10:J:139:ASP:H	10:J:140:PRO:HD3	1.58	0.68
14:N:113:ARG:NH2	14:N:156:ARG:HG2	2.09	0.68
19:S:39:THR:HG23	19:S:107:GLU:O	1.94	0.68
1:A:182:G:H5'	37:A:5131:HOH:O	1.93	0.68
1:A:2597:U:OP2	37:A:3804:HOH:O	2.11	0.68
37:E:8356:HOH:O	16:P:3:THR:HG21	1.93	0.68
14:N:87:MET:HE3	37:N:8593:HOH:O	1.92	0.68
22:V:13:ILE:HG12	22:V:32:CYS:HB3	1.73	0.68
1:A:2851:G:O2'	1:A:2852:A:H5'	1.93	0.68
12:L:62:PRO:HG3	12:L:65:ARG:HH21	1.58	0.68
26:Z:235:GLU:H	26:Z:235:GLU:CD	2.01	0.68
1:A:450:C:OP1	5:E:184:ARG:NH2	2.20	0.68
2:B:3006:C:OP1	15:O:37:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:22:ASP:HB2	37:L:5264:HOH:O	1.93	0.68
24:X:149:LEU:CG	24:X:153:MET:HE2	2.22	0.68
21:U:32:ARG:NH1	21:U:38:ARG:HH12	1.92	0.68
24:X:137:GLN:HE21	24:X:141:HIS:CE1	2.05	0.68
10:J:162:SER:CB	10:J:163:PRO:HD3	2.22	0.68
14:N:87:MET:CB	30:4:46:ILE:HG21	2.22	0.68
30:4:65:THR:HG23	30:4:67:LEU:HG	1.75	0.68
1:A:21:G:C5'	19:S:2:ILE:HA	2.23	0.68
1:A:1835:U:C5	1:A:1840:A:N7	2.56	0.68
26:Z:189:ASN:HA	26:Z:217:ILE:HD11	1.74	0.68
5:E:236:THR:HA	37:E:8446:HOH:O	1.94	0.68
10:J:3:GLY:HA2	10:J:57:ARG:HH12	1.58	0.68
3:C:190:ARG:NH2	3:C:207:GLN:OE1	2.27	0.67
7:G:11:VAL:HG12	7:G:12:ASP:N	2.09	0.67
14:N:34:GLU:HB3	14:N:35:PRO:HD2	1.76	0.67
6:F:37:ALA:O	6:F:40:ILE:HG12	1.95	0.67
11:K:93:ARG:HB3	11:K:93:ARG:HH11	1.56	0.67
14:N:35:PRO:O	37:N:8537:HOH:O	2.11	0.67
1:A:281:U:H2'	1:A:282:C:O4'	1.94	0.67
1:A:2054:A:N3	19:S:128:ARG:NH2	2.42	0.67
1:A:2637:A:H5'	37:A:9264:HOH:O	1.94	0.67
2:B:3023:U:H5''	2:B:3023:U:C6	2.30	0.67
22:V:20:MET:HE2	22:V:30:HIS:NE2	2.09	0.67
4:D:62:ARG:CA	4:D:65:MET:HE3	2.25	0.67
5:E:162:VAL:HG12	5:E:192:ILE:HD11	1.75	0.67
2:B:3014:G:H5'	2:B:3014:G:C8	2.29	0.67
1:A:338:C:H4'	5:E:174:ILE:CD1	2.24	0.67
5:E:214:THR:HG21	37:E:8400:HOH:O	1.94	0.67
10:J:59:ASN:HD22	10:J:59:ASN:N	1.92	0.67
14:N:64:ARG:HD2	37:N:8586:HOH:O	1.94	0.67
1:A:1058:A:H2'	1:A:1060:C:H5''	1.74	0.67
6:F:57:THR:HG23	6:F:63:ILE:HG22	1.76	0.67
7:G:7:ILE:HD11	7:G:11:VAL:C	2.20	0.67
7:G:93:MET:HE1	7:G:165:GLY:N	2.09	0.67
15:O:71:TRP:CE3	15:O:175:LEU:HD22	2.30	0.67
1:A:338:C:H5''	37:E:8416:HOH:O	1.94	0.67
1:A:1730:G:H5'	1:A:1731:C:C5	2.30	0.67
11:K:107:ASN:HD21	11:K:109:TYR:HB2	1.60	0.67
1:A:902:G:N7	13:M:18:HIS:HD2	1.93	0.67
1:A:2346:C:O2'	6:F:52:THR:HG21	1.95	0.67
8:H:53:ASP:OD1	8:H:80:GLN:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:258:GLY:H	4:D:260:HIS:CE1	2.12	0.66
19:S:18:LEU:HB2	19:S:143:VAL:HG12	1.77	0.66
1:A:2346:C:O5'	1:A:2346:C:H6	1.78	0.66
6:F:23:VAL:HG23	6:F:23:VAL:O	1.96	0.66
1:A:2064:U:H4'	1:A:2653:A:OP1	1.95	0.66
14:N:38:VAL:C	14:N:63:VAL:HG13	2.20	0.66
16:P:32:ARG:O	16:P:32:ARG:HD3	1.94	0.66
21:U:47:THR:HB	21:U:100:ASP:HB3	1.77	0.66
23:W:8:ILE:HA	23:W:11:MET:HE3	1.77	0.66
1:A:1973:A:H5'	1:A:1973:A:H8	1.60	0.66
1:A:2635:A:O2'	1:A:2636:C:H5'	1.96	0.66
8:H:63:ILE:HB	8:H:64:PRO:HD3	1.75	0.66
10:J:28:ILE:HA	10:J:62:GLU:OE1	1.95	0.66
14:N:74:ARG:HH11	14:N:74:ARG:HG3	1.61	0.66
19:S:39:THR:HG22	19:S:42:GLU:H	1.60	0.66
30:4:60:LYS:HG3	30:4:61:PRO:HD2	1.76	0.66
1:A:2908:A:H2'	1:A:2909:G:O4'	1.95	0.66
3:C:210:GLY:HA3	37:C:8589:HOH:O	1.95	0.66
1:A:1209:C:H2'	1:A:1210:G:H8	1.59	0.66
1:A:2676:C:H4'	11:K:70:PHE:CE1	2.31	0.66
11:K:19:MET:HE2	11:K:79:PHE:HA	1.76	0.66
13:M:53:ARG:NH2	13:M:57:VAL:HG12	2.09	0.66
6:F:95:THR:C	6:F:97:GLN:H	2.04	0.66
8:H:50:VAL:HG21	8:H:63:ILE:HG21	1.77	0.66
27:1:61:GLY:HA3	37:1:8427:HOH:O	1.96	0.66
1:A:506:G:H22	1:A:509:A:H5''	1.60	0.66
1:A:2748:G:H2'	37:A:7535:HOH:O	1.95	0.66
13:M:143:THR:HG22	13:M:145:LEU:H	1.60	0.66
26:Z:141:THR:HG23	37:Z:8586:HOH:O	1.96	0.66
26:Z:186:ARG:HG2	26:Z:186:ARG:HH11	1.60	0.66
1:A:31:C:H4'	37:A:7415:HOH:O	1.95	0.66
1:A:396:U:H1'	37:A:7627:HOH:O	1.96	0.66
1:A:1351:G:OP1	5:E:96:LYS:NZ	2.27	0.66
1:A:2487:C:OP2	37:A:6225:HOH:O	2.13	0.66
1:A:2578:G:H5'	1:A:2578:G:H8	1.61	0.66
1:A:2827:A:H2'	1:A:2828:G:O4'	1.95	0.66
3:C:33:GLU:O	3:C:34:ASP:HB2	1.95	0.66
3:C:105:VAL:CG1	3:C:154:ALA:HB1	2.24	0.66
4:D:145:HIS:HD2	4:D:146:THR:O	1.79	0.66
6:F:38:GLU:HB3	6:F:49:PRO:HG2	1.78	0.66
10:J:84:ARG:NH2	10:J:135:TRP:HH2	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:18:LEU:HD12	19:S:143:VAL:HG11	1.76	0.66
25:Y:15:ARG:HB3	25:Y:15:ARG:HH11	1.60	0.66
1:A:1120:U:C6	1:A:1120:U:H5''	2.31	0.65
1:A:1441:G:O2'	1:A:1442:A:H5'	1.96	0.65
1:A:1819:G:H2'	1:A:1820:G:H4'	1.77	0.65
3:C:81:GLN:HB2	3:C:92:ASN:ND2	2.10	0.65
5:E:12:THR:HB	37:E:8436:HOH:O	1.95	0.65
6:F:55:LYS:HA	37:F:6752:HOH:O	1.96	0.65
11:K:19:MET:HE3	11:K:132:LEU:CD1	2.21	0.65
14:N:30:GLU:O	14:N:34:GLU:HG3	1.96	0.65
19:S:111:ILE:HG23	19:S:145:LEU:HD11	1.78	0.65
26:Z:133:HIS:HD2	37:Z:8579:HOH:O	1.77	0.65
29:3:41:HIS:N	29:3:45:ASN:HD22	1.90	0.65
1:A:1679:C:H5'	37:A:9314:HOH:O	1.97	0.65
3:C:194:MET:HE3	3:C:199:HIS:HB2	1.76	0.65
6:F:146:LYS:HZ3	15:O:107:ASN:HD21	1.41	0.65
8:H:58:GLU:HG3	8:H:61:MET:HE2	1.78	0.65
12:L:34:VAL:HG22	12:L:47:ALA:HB2	1.78	0.65
1:A:111:C:O2'	28:2:20:ARG:HG2	1.97	0.65
4:D:238:ASN:HD22	4:D:240:GLY:N	1.93	0.65
10:J:139:ASP:HA	37:J:8374:HOH:O	1.95	0.65
10:J:150:LYS:HB2	10:J:157:ILE:HD12	1.78	0.65
11:K:99:GLU:HA	37:K:7377:HOH:O	1.96	0.65
1:A:1119:G:H8	11:K:52:GLN:HE22	1.42	0.65
1:A:1741:U:H5'	1:A:1742:A:OP1	1.96	0.65
1:A:2878:U:H2'	1:A:2879:A:O4'	1.96	0.65
14:N:104:ARG:O	14:N:108:LYS:HE2	1.95	0.65
4:D:195:ARG:HG2	4:D:323:LEU:HD22	1.76	0.65
24:X:26:ILE:HG13	24:X:26:ILE:O	1.96	0.65
1:A:2780:C:H1'	7:G:143:GLN:HE21	1.61	0.65
4:D:71:VAL:HG11	4:D:296:LEU:HB3	1.79	0.65
24:X:13:MET:HE2	24:X:18:GLN:CA	2.27	0.65
1:A:1667:A:H5'	1:A:1667:A:C8	2.29	0.65
1:A:1684:A:H1'	29:3:43:ARG:HH22	1.62	0.65
7:G:101:GLU:HB2	7:G:116:THR:O	1.96	0.65
8:H:99:THR:HA	37:H:3461:HOH:O	1.97	0.65
1:A:1328:A:OP1	26:Z:169:ARG:HD2	1.95	0.65
3:C:55:VAL:HG22	3:C:68:ILE:O	1.97	0.65
6:F:97:GLN:HG2	6:F:97:GLN:O	1.97	0.65
4:D:175:LEU:HD23	4:D:175:LEU:C	2.21	0.65
8:H:58:GLU:OE1	14:N:27:ARG:NH2	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:107:ASN:C	11:K:107:ASN:HD22	2.05	0.65
1:A:20:G:H21	19:S:117:HIS:HD2	1.46	0.64
3:C:194:MET:HE3	3:C:199:HIS:CB	2.27	0.64
5:E:1:MET:HG2	5:E:2:GLN:H	1.60	0.64
14:N:48:ARG:NH2	37:N:8562:HOH:O	2.30	0.64
17:Q:10:ALA:HA	17:Q:13:VAL:HG12	1.78	0.64
24:X:4:LEU:O	24:X:32:CYS:HA	1.97	0.64
26:Z:200:THR:HG22	26:Z:201:GLU:CG	2.26	0.64
27:1:53:GLY:HA2	27:1:67:GLY:O	1.97	0.64
1:A:259:G:H21	14:N:58:GLN:NE2	1.96	0.64
1:A:1771:U:H4'	27:1:20:LEU:HD21	1.77	0.64
1:A:2414:A:H2'	1:A:2415:A:C8	2.31	0.64
4:D:51:VAL:HG23	4:D:329:TYR:O	1.98	0.64
11:K:133:GLY:O	11:K:137:GLU:HG3	1.97	0.64
16:P:87:THR:O	16:P:91:GLN:HG3	1.98	0.64
23:W:49:LEU:O	23:W:53:ILE:HG13	1.97	0.64
1:A:1594:C:OP2	17:Q:120:ARG:HD2	1.97	0.64
1:A:1834:C:H2'	1:A:1840:A:N6	2.11	0.64
23:W:39:ALA:C	23:W:41:GLU:H	2.06	0.64
37:A:3821:HOH:O	10:J:11:LYS:HE2	1.97	0.64
6:F:99:ASP:HB2	6:F:103:ASN:HB2	1.80	0.64
10:J:35:ASN:ND2	10:J:80:ASN:HA	2.12	0.64
15:O:183:ASP:OD2	15:O:186:LEU:HD12	1.96	0.64
1:A:2505:G:O2'	1:A:2506:A:H5'	1.98	0.64
37:B:8466:HOH:O	15:O:147:ILE:HB	1.98	0.64
4:D:314:ALA:HB3	4:D:317:PRO:HG3	1.80	0.64
10:J:58:HIS:HA	10:J:61:LEU:HD23	1.78	0.64
13:M:136:ALA:HB3	37:M:8575:HOH:O	1.97	0.64
23:W:58:THR:O	23:W:62:GLU:HG3	1.98	0.64
8:H:50:VAL:CG1	8:H:60:VAL:HG11	2.27	0.64
22:V:14:GLU:OE1	22:V:15:PRO:HD2	1.97	0.64
24:X:13:MET:HE2	24:X:18:GLN:HA	1.80	0.64
29:3:41:HIS:H	29:3:45:ASN:ND2	1.96	0.64
2:B:3013:A:O2'	2:B:3014:G:H5''	1.98	0.64
4:D:305:ASP:O	4:D:306:LYS:HB2	1.98	0.64
23:W:64:GLY:O	23:W:65:ASP:HB2	1.96	0.64
1:A:2301:A:H5''	1:A:2302:A:H5'	1.80	0.64
1:A:2783:A:H3'	37:A:5208:HOH:O	1.97	0.64
9:I:12:ILE:N	9:I:13:PRO:CD	2.61	0.64
21:U:9:LYS:HE3	21:U:13:ARG:HH11	1.63	0.64
1:A:2508:C:H2'	37:A:6736:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:PRO:HA	4:D:168:GLY:HA3	1.80	0.64
10:J:27:LYS:N	10:J:58:HIS:HD2	1.92	0.64
26:Z:187:VAL:CG2	26:Z:192:ASP:HB2	2.27	0.64
1:A:1505:U:H6	1:A:1505:U:H5'	1.62	0.63
1:A:2718:C:H6	1:A:2718:C:H5'	1.64	0.63
5:E:142:ASP:OD1	5:E:237:GLU:HB3	1.99	0.63
7:G:132:THR:HB	37:G:2227:HOH:O	1.98	0.63
15:O:78:MET:HB2	15:O:79:PRO:HD3	1.80	0.63
2:B:3039:U:H1'	2:B:3044:A:N6	2.13	0.63
10:J:141:ASN:HA	37:J:8370:HOH:O	1.99	0.63
1:A:603:A:H5''	1:A:604:G:OP1	1.98	0.63
2:B:3048:C:H4'	15:O:141:ARG:HH21	1.63	0.63
3:C:101:GLU:OE2	3:C:131:HIS:HB2	1.99	0.63
10:J:85:ILE:HB	10:J:132:PHE:CE2	2.33	0.63
10:J:140:PRO:O	37:J:8370:HOH:O	2.15	0.63
16:P:14:LEU:CD2	16:P:102:ILE:HD11	2.27	0.63
24:X:5:VAL:HG11	24:X:153:MET:HE1	1.79	0.63
1:A:1120:U:H5''	1:A:1120:U:H6	1.64	0.63
1:A:1130:U:H5'	37:A:7671:HOH:O	1.98	0.63
4:D:36:PRO:HA	4:D:168:GLY:CA	2.28	0.63
5:E:16:VAL:HG12	5:E:17:ASP:N	2.13	0.63
15:O:151:ASP:O	15:O:154:LEU:HB2	1.99	0.63
1:A:182:G:O3'	14:N:157:LEU:HD13	1.99	0.63
7:G:79:GLY:HA3	37:G:7046:HOH:O	1.99	0.63
14:N:164:THR:CG2	14:N:165:SER:N	2.60	0.63
22:V:9:CYS:HA	22:V:52:THR:HG23	1.79	0.63
24:X:21:LEU:HB3	24:X:26:ILE:HG12	1.81	0.63
1:A:541:C:H2'	1:A:542:A:C5'	2.28	0.63
1:A:545:G:H5'	1:A:545:G:C8	2.30	0.63
9:I:12:ILE:HA	37:I:4499:HOH:O	1.99	0.63
12:L:55:VAL:HG12	12:L:56:SER:N	2.14	0.63
1:A:558:C:C2'	1:A:559:U:H5''	2.29	0.63
1:A:200:U:H2'	37:A:3427:HOH:O	1.97	0.62
1:A:431:G:P	14:N:48:ARG:HH12	2.21	0.62
1:A:1766:U:O2	1:A:1778:A:H5'	1.99	0.62
1:A:2638:G:H1'	37:A:7759:HOH:O	1.99	0.62
6:F:69:ILE:HG22	6:F:69:ILE:O	1.98	0.62
15:O:159:TYR:HB3	15:O:162:ASP:HB2	1.81	0.62
1:A:1086:A:C6	24:X:11:VAL:HG11	2.33	0.62
1:A:1118:A:H62	1:A:1244:U:H3	1.46	0.62
3:C:76:VAL:HG23	27:1:63:LYS:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:LEU:HA	6:F:44:ILE:HG22	1.81	0.62
10:J:127:GLY:O	10:J:128:ALA:HB3	1.99	0.62
29:3:22:PRO:HB2	29:3:24:TRP:CD1	2.35	0.62
1:A:263:U:O4'	8:H:59:ILE:HD13	1.99	0.62
1:A:553:G:P	26:Z:204:ARG:HH22	2.22	0.62
1:A:1185:U:H2'	1:A:1186:C:C6	2.34	0.62
3:C:105:VAL:HG12	3:C:106:CYS:N	2.15	0.62
6:F:36:ASN:HA	37:F:7500:HOH:O	1.99	0.62
10:J:130:HIS:CD2	10:J:133:ILE:HD11	2.34	0.62
10:J:136:VAL:HG23	37:J:8346:HOH:O	1.99	0.62
14:N:87:MET:HB2	14:N:91:ILE:HD11	1.81	0.62
1:A:1634:G:H3'	37:A:3871:HOH:O	1.97	0.62
1:A:2526:C:O2'	1:A:2527:U:H5'	1.99	0.62
11:K:130:VAL:HG12	11:K:131:THR:N	2.14	0.62
19:S:106:GLY:HA2	19:S:109:MET:HE3	1.81	0.62
28:2:25:LYS:HE2	37:3:7213:HOH:O	1.98	0.62
6:F:44:ILE:HG23	6:F:45:THR:HG23	1.81	0.62
12:L:62:PRO:HG3	12:L:65:ARG:NH2	2.15	0.62
1:A:2756:U:H3	1:A:2896:A:H2	1.44	0.62
3:C:37:VAL:HG22	37:C:8598:HOH:O	2.00	0.62
6:F:166:ILE:HD12	37:F:6326:HOH:O	1.99	0.62
11:K:131:THR:HG22	11:K:133:GLY:N	2.14	0.62
15:O:61:ALA:HB3	15:O:88:ALA:HB2	1.82	0.62
1:A:1242:A:C5'	11:K:82:THR:HG23	2.22	0.62
1:A:2672:C:H1'	37:D:8635:HOH:O	1.99	0.62
19:S:44:VAL:O	19:S:48:GLU:HG3	1.99	0.62
27:1:38:LYS:HE2	27:1:45:LYS:CE	2.25	0.62
4:D:307:ARG:HH11	4:D:307:ARG:CG	2.12	0.62
4:D:307:ARG:HH11	4:D:307:ARG:HB2	1.62	0.62
5:E:162:VAL:HG13	5:E:232:LEU:HD21	1.82	0.62
26:Z:165:GLU:HB3	37:Z:8591:HOH:O	1.98	0.62
1:A:1116:U:O2'	1:A:1118:A:C2	2.45	0.62
1:A:2638:G:H5'	37:A:4903:HOH:O	2.00	0.62
25:Y:41:PHE:O	25:Y:43:VAL:HG23	1.99	0.62
1:A:1636:G:O2'	1:A:1637:A:H5'	1.99	0.61
1:A:2570:G:H5''	37:A:4887:HOH:O	1.99	0.61
14:N:63:VAL:HG21	14:N:109:PHE:CE1	2.35	0.61
1:A:1641:A:H2'	1:A:1642:A:H5'	1.81	0.61
1:A:1919:A:H4'	37:A:4823:HOH:O	2.00	0.61
1:A:449:A:N7	5:E:43:LYS:HG2	2.15	0.61
1:A:2717:C:H2'	1:A:2718:C:C5'	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3035:C:H5''	37:B:8456:HOH:O	2.00	0.61
11:K:131:THR:HG22	11:K:134:GLU:H	1.63	0.61
24:X:88:THR:CG2	24:X:89:ASP:H	2.09	0.61
27:1:39:CYS:HA	27:1:47:LEU:HD11	1.82	0.61
3:C:96:LEU:HD22	3:C:128:LEU:HD13	1.80	0.61
13:M:145:LEU:O	13:M:148:GLU:HG3	2.00	0.61
1:A:1187:U:O2'	1:A:1189:A:H2	1.84	0.61
3:C:223:ARG:HG3	37:C:8604:HOH:O	1.99	0.61
26:Z:220:GLU:HG2	37:Z:8546:HOH:O	2.00	0.61
1:A:447:A:O2'	1:A:448:G:H5'	2.01	0.61
1:A:2690:U:O2'	7:G:111:LYS:HE3	2.01	0.61
7:G:15:GLN:NE2	7:G:40:VAL:O	2.33	0.61
15:O:48:VAL:HG11	15:O:55:ASP:HB3	1.82	0.61
1:A:544:G:C2'	1:A:545:G:H5''	2.29	0.61
1:A:2533:C:H5'	1:A:2533:C:C6	2.35	0.61
17:Q:18:LYS:O	17:Q:21:VAL:HG22	2.00	0.61
24:X:122:ARG:NH2	24:X:154:ARG:HD2	2.13	0.61
4:D:195:ARG:HD2	4:D:324:ASP:OD1	2.00	0.61
6:F:136:ARG:HD2	6:F:155:HIS:O	2.00	0.61
10:J:3:GLY:HA2	10:J:57:ARG:NH1	2.16	0.61
14:N:104:ARG:O	14:N:108:LYS:HG2	2.01	0.61
24:X:21:LEU:HD21	24:X:48:VAL:HG11	1.82	0.61
1:A:2630:G:O6	3:C:206:ARG:NH2	2.33	0.61
37:A:7679:HOH:O	14:N:154:ARG:HB2	2.01	0.61
3:C:171:LYS:NZ	37:C:8524:HOH:O	2.31	0.61
6:F:99:ASP:CB	6:F:103:ASN:H	2.14	0.61
6:F:101:THR:HG22	37:F:7400:HOH:O	2.01	0.61
23:W:44:GLY:O	23:W:48:GLU:HG2	2.01	0.61
2:B:3069:U:OP1	15:O:4:PRO:HG3	2.01	0.60
10:J:166:ASN:N	10:J:166:ASN:HD22	1.98	0.60
24:X:81:ASP:OD1	24:X:92:ASP:HB2	2.00	0.60
29:3:35:ARG:HB2	37:3:2691:HOH:O	1.99	0.60
1:A:417:G:P	37:A:7409:HOH:O	2.58	0.60
1:A:1086:A:N6	24:X:11:VAL:HG11	2.16	0.60
5:E:237:GLU:HB2	37:E:8426:HOH:O	2.00	0.60
15:O:170:GLU:O	15:O:174:GLU:HG3	2.02	0.60
5:E:233:THR:HG22	5:E:234:VAL:N	2.15	0.60
13:M:133:VAL:HB	37:M:8559:HOH:O	2.01	0.60
15:O:155:GLU:O	15:O:156:GLU:HG3	2.01	0.60
17:Q:16:VAL:HG12	17:Q:17:GLY:N	2.16	0.60
23:W:4:HIS:HB3	37:W:6622:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:7:ARG:NH1	4:D:11:LEU:HD22	2.17	0.60
6:F:174:VAL:HG13	37:F:6555:HOH:O	2.01	0.60
7:G:23:GLU:HG2	7:G:28:SER:CB	2.32	0.60
1:A:558:C:H5'	37:A:5234:HOH:O	2.01	0.60
3:C:95:PRO:HG2	3:C:98:GLU:HG2	1.83	0.60
8:H:110:GLU:HG2	37:H:6926:HOH:O	2.02	0.60
12:L:81:ARG:HD3	12:L:87:ARG:NH1	2.16	0.60
20:T:57:THR:CG2	20:T:58:MET:N	2.64	0.60
21:U:71:VAL:HG11	21:U:90:PRO:CB	2.24	0.60
25:Y:21:PRO:HG2	25:Y:24:LYS:HD3	1.83	0.60
6:F:23:VAL:HG22	6:F:73:VAL:HB	1.82	0.60
11:K:19:MET:HE1	11:K:78:ILE:HG22	1.84	0.60
15:O:89:GLY:O	15:O:92:ALA:HB3	2.01	0.60
1:A:2587:U:H2'	1:A:2589:U:H5''	1.82	0.60
1:A:2694:A:H4'	7:G:91:PHE:CE1	2.36	0.60
1:A:2779:G:H21	7:G:143:GLN:NE2	1.99	0.60
5:E:79:ARG:O	5:E:87:ARG:HG2	2.02	0.60
7:G:84:MET:HE2	7:G:133:VAL:HG21	1.82	0.60
12:L:75:ARG:CZ	37:L:4172:HOH:O	2.49	0.60
1:A:2310:G:OP2	10:J:114:PRO:HD2	2.02	0.60
4:D:204:GLY:HA3	37:D:8654:HOH:O	1.99	0.60
6:F:105:SER:CB	6:F:131:THR:HG23	2.28	0.60
10:J:45:GLN:HE21	10:J:135:TRP:HE1	1.50	0.60
10:J:59:ASN:HD22	10:J:59:ASN:H	1.48	0.60
37:A:7446:HOH:O	4:D:211:THR:HG21	2.01	0.60
4:D:329:TYR:CE2	22:V:15:PRO:HG2	2.37	0.60
6:F:86:THR:O	6:F:90:LEU:HG	2.02	0.60
6:F:91:ALA:HB1	37:F:5198:HOH:O	2.01	0.60
15:O:47:LEU:HD13	15:O:97:VAL:HG11	1.84	0.60
26:Z:155:ARG:NH1	37:Z:8555:HOH:O	2.33	0.60
1:A:168:C:O2'	1:A:169:A:H5'	2.02	0.60
2:B:3003:A:N6	2:B:3022:G:H1'	2.16	0.60
7:G:43:ASP:HA	37:G:5864:HOH:O	2.01	0.60
10:J:118:PRO:HD2	37:J:8342:HOH:O	2.01	0.60
15:O:12:ARG:HD3	15:O:18:THR:OG1	2.02	0.60
26:Z:189:ASN:HD22	26:Z:189:ASN:C	2.09	0.60
1:A:1008:C:H5''	10:J:16:ARG:HH12	1.66	0.59
8:H:19:ALA:O	8:H:22:VAL:HG22	2.02	0.59
8:H:101:ALA:HB2	8:H:108:LEU:HD22	1.84	0.59
10:J:44:ALA:HA	10:J:163:PRO:O	2.02	0.59
10:J:136:VAL:HG22	10:J:137:ASN:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:G:H1'	37:A:4948:HOH:O	2.01	0.59
3:C:211:LYS:NZ	37:C:8623:HOH:O	2.35	0.59
5:E:180:SER:HB2	37:E:8440:HOH:O	2.01	0.59
10:J:69:ASN:O	10:J:72:VAL:HG12	2.02	0.59
25:Y:78:GLU:CG	25:Y:79:GLU:H	2.14	0.59
1:A:1701:A:H5''	1:A:1702:U:H3'	1.84	0.59
1:A:2769:C:H2'	1:A:2770:G:O4'	2.02	0.59
20:T:43:GLU:HB3	37:T:8344:HOH:O	2.02	0.59
1:A:558:C:O2'	1:A:559:U:H5''	2.02	0.59
2:B:3076:G:C3'	2:B:3077:A:H5''	2.26	0.59
4:D:103:ASP:HB2	37:D:8592:HOH:O	2.01	0.59
15:O:184:ILE:HG22	15:O:185:GLU:HG3	1.84	0.59
12:L:74:VAL:CG1	12:L:113:ILE:HG12	2.30	0.59
27:1:29:VAL:O	27:1:33:HIS:HB2	2.02	0.59
4:D:51:VAL:CG2	4:D:327:VAL:HG13	2.32	0.59
7:G:7:ILE:HD11	7:G:11:VAL:O	2.01	0.59
13:M:143:THR:CG2	13:M:144:ASP:N	2.65	0.59
14:N:74:ARG:HG3	14:N:74:ARG:NH1	2.18	0.59
1:A:65:C:O2'	1:A:66:G:H5'	2.03	0.59
1:A:272:A:H5'	1:A:273:G:OP2	2.02	0.59
37:A:7577:HOH:O	27:1:31:ILE:HG13	2.01	0.59
5:E:27:ARG:HG3	5:E:29:ASP:OD1	2.02	0.59
37:L:408:HOH:O	22:V:37:GLU:HB3	2.03	0.59
1:A:184:G:H5''	14:N:153:THR:HG22	1.84	0.59
37:A:4516:HOH:O	10:J:151:MET:HE2	2.02	0.59
1:A:1701:A:H4'	1:A:1702:U:C5'	2.32	0.59
1:A:1878:G:H1'	37:A:6102:HOH:O	2.02	0.59
1:A:2676:C:H4'	11:K:70:PHE:HE1	1.67	0.59
1:A:703:G:O2'	1:A:704:C:H5'	2.02	0.59
4:D:7:ARG:HG2	4:D:7:ARG:NH1	2.12	0.59
4:D:140:LEU:HD23	37:D:8579:HOH:O	2.02	0.59
15:O:71:TRP:HE3	15:O:175:LEU:HD22	1.68	0.59
25:Y:31:ILE:O	25:Y:35:GLU:HG3	2.03	0.59
1:A:2419:U:H5''	1:A:2420:G:H5'	1.85	0.58
24:X:38:THR:HG22	37:X:3580:HOH:O	2.03	0.58
1:A:2768:A:O2'	1:A:2769:C:H5'	2.02	0.58
8:H:39:SER:HB3	8:H:45:ALA:HB2	1.83	0.58
8:H:58:GLU:CD	14:N:27:ARG:HH22	2.11	0.58
10:J:27:LYS:H	10:J:58:HIS:CD2	2.12	0.58
15:O:169:PRO:O	15:O:172:PHE:HB3	2.03	0.58
24:X:122:ARG:HH22	24:X:154:ARG:C	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:73:GLU:HB3	37:4:8561:HOH:O	2.03	0.58
1:A:1134:G:C5'	10:J:151:MET:HE1	2.33	0.58
1:A:1189:A:H1'	1:A:1209:C:C1'	2.33	0.58
3:C:125:ASN:HB3	3:C:158:VAL:HG12	1.84	0.58
8:H:46:GLU:O	8:H:73:PRO:HD2	2.03	0.58
1:A:656:G:OP2	16:P:37:ARG:HD2	2.03	0.58
1:A:777:U:O2'	28:2:11:LYS:HG2	2.04	0.58
7:G:107:PHE:CE2	7:G:108:LEU:HD13	2.38	0.58
24:X:41:TYR:HA	24:X:44:MET:HE3	1.86	0.58
25:Y:75:ALA:O	25:Y:83:ALA:HA	2.03	0.58
1:A:2241:C:O2'	1:A:2242:U:H5'	2.03	0.58
6:F:11:HIS:C	6:F:13:MET:H	2.11	0.58
6:F:25:MET:CE	6:F:37:ALA:HB1	2.33	0.58
6:F:65:GLU:HG3	37:F:6752:HOH:O	2.02	0.58
10:J:75:SER:C	10:J:79:ALA:HB2	2.29	0.58
14:N:87:MET:CG	30:4:46:ILE:HG21	2.33	0.58
19:S:39:THR:HB	19:S:42:GLU:CG	2.32	0.58
24:X:21:LEU:HD21	24:X:48:VAL:CG1	2.33	0.58
1:A:470:U:O2'	28:2:16:HIS:CD2	2.55	0.58
2:B:3020:G:O2'	2:B:3021:G:H5'	2.04	0.58
10:J:56:ILE:HG22	10:J:61:LEU:HD22	1.84	0.58
11:K:103:VAL:HG12	37:K:5907:HOH:O	2.03	0.58
12:L:115:ARG:HG3	12:L:116:GLU:N	2.18	0.58
15:O:152:GLU:C	15:O:154:LEU:H	2.10	0.58
1:A:285:A:H2'	1:A:286:U:O4'	2.03	0.58
7:G:11:VAL:HG13	7:G:23:GLU:O	2.02	0.58
8:H:107:VAL:O	8:H:111:ILE:HG13	2.03	0.58
14:N:84:LYS:HE2	37:N:8577:HOH:O	2.03	0.58
15:O:90:LEU:HB2	15:O:186:LEU:HD22	1.84	0.58
24:X:26:ILE:O	24:X:26:ILE:CG1	2.51	0.58
27:1:28:ASP:O	27:1:31:ILE:HG22	2.03	0.58
1:A:1299:G:O6	13:M:6:ARG:HD3	2.04	0.58
3:C:88:ILE:HG22	3:C:88:ILE:O	2.02	0.58
4:D:138:GLY:O	4:D:139:ASP:O	2.21	0.58
4:D:154:VAL:HG12	4:D:156:LYS:HG2	1.86	0.58
27:1:62:TYR:CE2	27:1:64:ILE:HG23	2.38	0.58
1:A:138:U:H5''	1:A:139:C:OP2	2.04	0.58
1:A:1333:U:H2'	1:A:1334:C:C6	2.38	0.58
1:A:1595:G:O2'	1:A:1596:U:H5'	2.04	0.58
1:A:2363:G:O3'	18:R:11:ARG:NH1	2.37	0.58
6:F:22:VAL:HG22	6:F:74:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:13:MET:HE3	24:X:17:ILE:HG22	1.85	0.58
1:A:1205:U:H2'	1:A:1206:U:H5'	1.85	0.58
4:D:190:MET:HE2	4:D:194:PHE:HD1	1.68	0.58
6:F:44:ILE:HG12	6:F:83:PHE:HE1	1.68	0.58
6:F:54:ALA:HB2	6:F:69:ILE:HD12	1.86	0.58
10:J:31:PHE:HE2	10:J:87:LYS:O	1.86	0.58
19:S:33:ARG:NH1	37:S:8543:HOH:O	2.36	0.58
24:X:139:GLY:O	24:X:141:HIS:HD2	1.86	0.58
27:1:19:GLY:O	27:1:23:ARG:HG2	2.04	0.58
1:A:558:C:H2'	1:A:559:U:C5'	2.34	0.57
7:G:69:ILE:HA	7:G:72:MET:CE	2.34	0.57
6:F:135:VAL:HG21	6:F:139:TYR:CD1	2.39	0.57
10:J:46:VAL:HG12	10:J:146:TRP:CZ3	2.38	0.57
10:J:139:ASP:N	10:J:140:PRO:CD	2.66	0.57
1:A:1053:G:OP1	10:J:12:PRO:HG3	2.04	0.57
1:A:1523:G:H2'	1:A:1524:U:C6	2.39	0.57
3:C:1:GLY:N	37:C:8610:HOH:O	2.38	0.57
11:K:74:ARG:HH11	11:K:74:ARG:CB	2.16	0.57
14:N:61:ILE:HA	37:N:8623:HOH:O	2.04	0.57
15:O:64:SER:C	15:O:66:LEU:H	2.13	0.57
1:A:2004:U:H4'	37:A:5284:HOH:O	2.04	0.57
6:F:49:PRO:HG3	37:F:5828:HOH:O	2.04	0.57
8:H:2:VAL:HG22	8:H:57:GLU:OE1	2.04	0.57
8:H:101:ALA:HB2	8:H:108:LEU:CD2	2.34	0.57
15:O:49:THR:CG2	15:O:56:ASP:HB2	2.33	0.57
2:B:3049:G:H5''	37:B:8466:HOH:O	2.03	0.57
4:D:41:PHE:HB3	4:D:190:MET:HE1	1.85	0.57
6:F:135:VAL:HG22	6:F:136:ARG:N	2.19	0.57
10:J:45:GLN:HE21	10:J:135:TRP:NE1	2.03	0.57
13:M:53:ARG:HH22	13:M:57:VAL:HG12	1.68	0.57
14:N:37:VAL:HG21	14:N:108:LYS:CG	2.34	0.57
19:S:119:VAL:O	19:S:119:VAL:HG12	2.03	0.57
24:X:13:MET:CE	24:X:17:ILE:HG22	2.34	0.57
1:A:1377:C:H5'	1:A:1377:C:C6	2.39	0.57
1:A:1669:A:H2'	1:A:1670:G:C8	2.39	0.57
1:A:2073:G:OP2	1:A:2490:A:H5'	2.04	0.57
1:A:2265:U:H2'	1:A:2266:A:C8	2.40	0.57
4:D:125:GLU:O	4:D:129:ARG:HG3	2.03	0.57
4:D:141:ARG:HD2	4:D:163:GLU:OE2	2.04	0.57
6:F:154:LYS:H	6:F:154:LYS:CD	2.11	0.57
24:X:80:ASP:O	24:X:84:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:C:H5'	14:N:163:LEU:HD21	1.86	0.57
1:A:289:G:N2	1:A:363:A:H2	2.00	0.57
6:F:23:VAL:HG21	6:F:45:THR:HG21	1.85	0.57
12:L:32:ILE:HD11	12:L:56:SER:HB3	1.86	0.57
14:N:149:TRP:O	14:N:152:ARG:HG2	2.03	0.57
22:V:52:THR:CG2	22:V:54:THR:HB	2.35	0.57
25:Y:78:GLU:HG2	25:Y:79:GLU:N	2.18	0.57
1:A:1268:C:O2'	1:A:1269:G:H5'	2.04	0.57
7:G:31:ARG:NH1	7:G:68:HIS:CG	2.73	0.57
15:O:38:LYS:HD2	15:O:114:LYS:HE3	1.86	0.57
15:O:154:LEU:O	15:O:155:GLU:HB3	2.03	0.57
24:X:149:LEU:HG	24:X:153:MET:CE	2.28	0.57
37:A:9388:HOH:O	14:N:94:LYS:HE2	2.04	0.57
11:K:75:PRO:HG2	11:K:105:LEU:HD21	1.86	0.57
27:1:57:CYS:SG	27:1:59:HIS:HB3	2.45	0.57
4:D:307:ARG:HH11	4:D:307:ARG:CB	2.18	0.57
6:F:51:ARG:HD3	37:F:7636:HOH:O	2.05	0.57
7:G:93:MET:HE1	7:G:165:GLY:H	1.69	0.57
13:M:90:ARG:NH2	13:M:121:ILE:HD11	2.19	0.57
14:N:12:TRP:CE2	14:N:20:ILE:HD11	2.40	0.57
14:N:169:ARG:HD2	37:N:8590:HOH:O	2.05	0.57
15:O:11:ARG:HG3	15:O:14:ARG:NH1	2.20	0.57
24:X:38:THR:HG22	24:X:39:ASP:N	2.20	0.57
15:O:37:ARG:NE	37:O:8533:HOH:O	2.38	0.56
2:B:3044:A:O4'	6:F:76:ARG:NE	2.39	0.56
6:F:38:GLU:OE2	6:F:51:ARG:CZ	2.53	0.56
15:O:77:ASN:OD1	15:O:80:SER:HB2	2.06	0.56
23:W:39:ALA:N	23:W:40:PRO:CD	2.67	0.56
25:Y:18:ARG:NH1	37:Y:4132:HOH:O	2.35	0.56
29:3:24:TRP:CD1	37:3:6863:HOH:O	2.57	0.56
1:A:1166:A:H1'	1:A:1192:A:N1	2.19	0.56
1:A:1181:A:H2'	1:A:1182:C:O4'	2.04	0.56
1:A:2270:G:H4'	3:C:223:ARG:HH12	1.70	0.56
37:A:6176:HOH:O	29:3:44:ARG:HG2	2.05	0.56
3:C:175:LYS:HE2	37:C:8578:HOH:O	2.04	0.56
5:E:115:LEU:HD21	5:E:243:VAL:HG13	1.87	0.56
5:E:219:ASN:O	5:E:222:ASP:OD1	2.24	0.56
6:F:64:ARG:CD	6:F:67:ASP:HB3	2.36	0.56
11:K:26:VAL:HG13	11:K:36:VAL:HG11	1.85	0.56
12:L:82:ARG:NH2	12:L:115:ARG:HG2	2.20	0.56
14:N:87:MET:CB	30:4:46:ILE:HD13	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:A:H5'	1:A:69:A:C8	2.40	0.56
1:A:2694:A:H4'	7:G:91:PHE:HE1	1.70	0.56
37:A:3957:HOH:O	30:4:57:GLY:HA2	2.04	0.56
4:D:141:ARG:HG2	4:D:165:ARG:HA	1.87	0.56
11:K:74:ARG:O	11:K:78:ILE:HG12	2.05	0.56
14:N:77:PHE:HD2	37:N:8526:HOH:O	1.88	0.56
17:Q:13:VAL:HG21	17:Q:41:ARG:HG2	1.87	0.56
30:4:31:THR:HB	30:4:33:MET:HE3	1.88	0.56
1:A:2821:C:H4'	4:D:116:PRO:HB3	1.88	0.56
4:D:144:THR:HG22	4:D:145:HIS:N	2.20	0.56
5:E:118:THR:O	5:E:136:VAL:HG13	2.05	0.56
12:L:101:ASN:O	12:L:102:GLU:HB2	2.05	0.56
17:Q:143:ALA:HA	37:Q:167:HOH:O	2.05	0.56
24:X:31:HIS:HB3	37:X:5420:HOH:O	2.05	0.56
1:A:182:G:O3'	14:N:157:LEU:CD1	2.54	0.56
1:A:371:U:H2'	1:A:372:A:H8	1.70	0.56
1:A:1123:A:C6	1:A:1238:C:H5'	2.41	0.56
1:A:1159:G:H21	1:A:1189:A:H8	1.51	0.56
1:A:1234:U:N3	4:D:244:PRO:HB3	2.21	0.56
1:A:1667:A:H2'	1:A:1668:U:C6	2.41	0.56
3:C:94:LEU:HG	3:C:99:ILE:HD11	1.88	0.56
3:C:211:LYS:HB3	3:C:212:PRO:CD	2.30	0.56
7:G:20:ILE:CD1	7:G:40:VAL:HG11	2.34	0.56
10:J:75:SER:HB3	10:J:79:ALA:HB1	1.86	0.56
17:Q:38:GLU:HA	17:Q:41:ARG:NH1	2.21	0.56
1:A:282:C:H1'	1:A:368:C:H42	1.68	0.56
1:A:1183:C:N4	37:A:4373:HOH:O	2.35	0.56
1:A:1528:A:H2'	1:A:1529:G:O4'	2.06	0.56
1:A:2866:U:H4'	1:A:2867:G:H5'	1.87	0.56
1:A:2890:A:H1'	22:V:56:ARG:HH21	1.71	0.56
14:N:37:VAL:HG13	14:N:63:VAL:HG11	1.88	0.56
14:N:59:GLY:HA3	14:N:141:ILE:HD12	1.88	0.56
1:A:1470:A:OP1	14:N:93:ARG:HD2	2.06	0.56
1:A:2472:C:O2'	1:A:2634:G:H4'	2.05	0.56
4:D:16:ARG:NH1	37:D:8615:HOH:O	2.39	0.56
27:1:30:GLU:O	27:1:33:HIS:HB3	2.06	0.56
2:B:3041:C:O4'	6:F:50:VAL:HG23	2.06	0.56
4:D:119:HIS:O	4:D:121:PRO:HD3	2.06	0.56
4:D:248:ARG:HG2	37:K:3517:HOH:O	2.04	0.56
6:F:146:LYS:NZ	15:O:107:ASN:ND2	2.53	0.56
12:L:109:LEU:HD13	12:L:113:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:U:OP2	30:4:38:ARG:NH1	2.38	0.56
1:A:2502:C:C2'	1:A:2503:A:H5'	2.36	0.56
3:C:170:VAL:HG22	27:1:22:ILE:HG23	1.87	0.56
14:N:114:VAL:HG21	14:N:159:THR:HG21	1.87	0.56
14:N:172:GLY:C	14:N:183:VAL:HG11	2.30	0.56
27:1:77:LYS:HA	27:1:80:MET:HE2	1.88	0.56
1:A:280:C:H2'	1:A:281:U:O4'	2.06	0.55
1:A:1474:C:H6	1:A:1474:C:C5'	2.13	0.55
1:A:2769:C:C2'	1:A:2770:G:H5'	2.37	0.55
4:D:2:GLN:HA	37:D:8620:HOH:O	2.05	0.55
4:D:314:ALA:CB	4:D:317:PRO:HG3	2.36	0.55
7:G:3:VAL:HG22	7:G:49:ILE:HB	1.88	0.55
1:A:1119:G:H8	11:K:52:GLN:NE2	2.04	0.55
37:B:8522:HOH:O	15:O:107:ASN:HB3	2.06	0.55
6:F:10:PHE:CG	6:F:11:HIS:N	2.74	0.55
9:I:64:ASN:HD22	9:I:64:ASN:N	2.03	0.55
10:J:144:GLU:OE1	10:J:144:GLU:HA	2.06	0.55
12:L:74:VAL:HG12	12:L:75:ARG:HG3	1.87	0.55
14:N:69:LYS:HG2	14:N:127:LYS:HG3	1.88	0.55
19:S:99:ALA:HB1	19:S:109:MET:CE	2.19	0.55
1:A:474:C:O3'	5:E:73:LEU:HD21	2.06	0.55
1:A:1559:A:H1'	37:A:5846:HOH:O	2.05	0.55
1:A:2506:A:O2'	1:A:2507:G:O5'	2.24	0.55
2:B:3028:U:H2'	2:B:3029:C:C6	2.41	0.55
1:A:1187:U:H2'	37:A:6880:HOH:O	2.05	0.55
3:C:94:LEU:N	3:C:94:LEU:HD23	2.21	0.55
4:D:297:VAL:HB	37:D:8604:HOH:O	2.07	0.55
10:J:35:ASN:HD21	10:J:80:ASN:HA	1.71	0.55
14:N:59:GLY:HA3	14:N:141:ILE:CD1	2.36	0.55
27:1:30:GLU:HA	27:1:33:HIS:CB	2.37	0.55
1:A:182:G:H4'	14:N:157:LEU:HD13	1.88	0.55
1:A:1213:C:O2'	1:A:1214:G:H5'	2.07	0.55
5:E:107:ARG:NH1	5:E:107:ARG:HB3	2.21	0.55
16:P:38:ARG:NH1	37:P:7674:HOH:O	2.39	0.55
17:Q:59:ARG:HH22	17:Q:66:GLN:HE22	1.54	0.55
25:Y:43:VAL:CG1	25:Y:47:ALA:HB3	2.36	0.55
1:A:1250:C:O2'	1:A:1251:C:H5'	2.06	0.55
1:A:2320:U:H4'	1:A:2321:A:O4'	2.07	0.55
1:A:2502:C:H4'	10:J:151:MET:HG2	1.89	0.55
2:B:3025:G:C3'	2:B:3026:C:H5'	2.34	0.55
3:C:36:ASP:HA	3:C:83:GLY:HA3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:14:GLY:HA2	4:D:15:PRO:C	2.31	0.55
5:E:129:HIS:CE1	5:E:231:ARG:HA	2.42	0.55
6:F:54:ALA:CB	6:F:69:ILE:HD12	2.36	0.55
7:G:15:GLN:HG2	7:G:19:ASP:O	2.07	0.55
14:N:37:VAL:HG21	14:N:108:LYS:HG3	1.89	0.55
14:N:55:LYS:HB2	14:N:60:ILE:CD1	2.37	0.55
21:U:9:LYS:CE	21:U:13:ARG:NH1	2.69	0.55
24:X:110:GLN:NE2	24:X:110:GLN:HA	2.22	0.55
25:Y:43:VAL:HG12	25:Y:44:ASP:N	2.21	0.55
26:Z:144:ARG:CZ	37:Z:8608:HOH:O	2.54	0.55
2:B:3023:U:H3'	2:B:3024:U:H5''	1.89	0.55
2:B:3023:U:H6	2:B:3023:U:C5'	2.20	0.55
3:C:211:LYS:HD3	37:C:8613:HOH:O	2.06	0.55
9:I:12:ILE:HG13	37:I:6833:HOH:O	2.05	0.55
13:M:57:VAL:HG12	13:M:57:VAL:O	2.06	0.55
23:W:12:THR:CG2	23:W:15:GLU:HG3	2.26	0.55
26:Z:189:ASN:ND2	26:Z:192:ASP:H	2.04	0.55
1:A:1209:C:H2'	1:A:1210:G:C8	2.40	0.55
1:A:2721:U:H4'	12:L:87:ARG:HG3	1.88	0.55
4:D:212:GLN:HB2	4:D:257:THR:CG2	2.32	0.55
8:H:50:VAL:CG2	8:H:63:ILE:HG21	2.35	0.55
13:M:104:ASP:HB3	37:M:8565:HOH:O	2.07	0.55
1:A:407:A:H5'	37:A:6005:HOH:O	2.07	0.55
1:A:1189:A:H1'	1:A:1209:C:O4'	2.07	0.55
1:A:1730:G:H5'	1:A:1731:C:C6	2.42	0.55
8:H:37:THR:O	8:H:41:GLU:HG3	2.07	0.55
8:H:117:GLU:C	8:H:119:ARG:H	2.15	0.55
10:J:83:PHE:HZ	10:J:146:TRP:HE1	1.51	0.55
1:A:281:U:H3'	37:A:7196:HOH:O	2.07	0.55
4:D:85:ARG:NH1	37:D:8635:HOH:O	2.40	0.55
4:D:264:GLU:HG2	4:D:267:LYS:CE	2.33	0.55
9:I:12:ILE:HG22	9:I:12:ILE:O	2.06	0.55
1:A:189:A:OP1	14:N:171:ARG:NH2	2.39	0.54
1:A:1778:A:H2'	1:A:1779:A:H5'	1.89	0.54
1:A:2862:G:H4'	4:D:336:GLN:O	2.06	0.54
2:B:3092:G:H2'	2:B:3093:A:C8	2.42	0.54
10:J:71:TYR:C	10:J:73:GLN:N	2.63	0.54
17:Q:71:LYS:HG3	17:Q:71:LYS:O	2.06	0.54
17:Q:80:ARG:HG2	17:Q:87:ARG:CZ	2.37	0.54
26:Z:99:ALA:HB2	26:Z:233:TYR:CZ	2.42	0.54
1:A:1189:A:H1'	1:A:1209:C:H1'	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:48:LEU:HG	10:J:157:ILE:HG21	1.89	0.54
13:M:149:ARG:O	13:M:150:GLN:HB2	2.08	0.54
1:A:738:G:H3'	37:A:7034:HOH:O	2.07	0.54
1:A:1137:G:H1'	37:A:3855:HOH:O	2.06	0.54
1:A:1168:C:H2'	1:A:1169:U:O4'	2.07	0.54
1:A:1197:G:N2	37:A:6216:HOH:O	2.40	0.54
1:A:2548:C:OP2	4:D:5:ARG:NH2	2.40	0.54
5:E:236:THR:O	5:E:237:GLU:C	2.49	0.54
7:G:81:GLU:HG2	7:G:134:SER:CB	2.38	0.54
10:J:81:TYR:CD1	10:J:81:TYR:C	2.85	0.54
19:S:111:ILE:HG23	19:S:145:LEU:CD1	2.37	0.54
24:X:141:HIS:HB2	24:X:146:ILE:HG12	1.88	0.54
1:A:2524:G:H21	1:A:2526:C:N4	2.05	0.54
2:B:3002:U:OP2	2:B:3003:A:H5'	2.08	0.54
37:B:8466:HOH:O	15:O:147:ILE:HD12	2.06	0.54
4:D:27:ASN:HB3	37:D:8627:HOH:O	2.07	0.54
4:D:168:GLY:N	4:D:174:ARG:HD3	2.22	0.54
17:Q:98:ILE:HD12	17:Q:102:ARG:NE	2.23	0.54
30:4:17:HIS:O	30:4:18:GLN:HG3	2.08	0.54
4:D:7:ARG:CD	4:D:9:GLY:O	2.56	0.54
7:G:172:PRO:HB3	37:G:6931:HOH:O	2.08	0.54
21:U:52:ARG:HB2	21:U:95:ASN:HB3	1.90	0.54
24:X:38:THR:HG22	24:X:39:ASP:H	1.73	0.54
1:A:542:A:H2'	1:A:543:G:O4'	2.07	0.54
1:A:1333:U:H2'	1:A:1334:C:H6	1.73	0.54
3:C:36:ASP:O	3:C:38:ILE:N	2.41	0.54
4:D:108:GLU:HB3	4:D:111:ARG:HD2	1.89	0.54
5:E:104:ASP:HA	5:E:107:ARG:NH1	2.20	0.54
1:A:2502:C:C4'	10:J:151:MET:HG2	2.38	0.54
5:E:16:VAL:HG12	5:E:17:ASP:H	1.70	0.54
6:F:11:HIS:O	6:F:12:GLU:HB3	2.07	0.54
6:F:93:LEU:HB3	6:F:97:GLN:OE1	2.08	0.54
8:H:100:ASP:HB3	37:H:5691:HOH:O	2.08	0.54
14:N:37:VAL:CG1	14:N:63:VAL:HG11	2.37	0.54
14:N:115:LEU:HD13	14:N:116:ASN:HB2	1.89	0.54
20:T:23:LYS:HE2	37:T:8331:HOH:O	2.08	0.54
21:U:24:ARG:HH21	21:U:39:ASN:HD22	1.54	0.54
1:A:317:A:H5''	21:U:52:ARG:HD2	1.89	0.54
1:A:951:A:C2'	1:A:952:G:H5'	2.37	0.54
3:C:53:ALA:HB3	37:C:8608:HOH:O	2.08	0.54
5:E:77:ALA:O	5:E:78:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:59:GLY:C	6:F:61:PHE:H	2.16	0.54
14:N:79:LYS:HD2	37:N:8556:HOH:O	2.08	0.54
14:N:164:THR:HB	37:N:8519:HOH:O	2.08	0.54
22:V:52:THR:HG22	22:V:54:THR:N	2.22	0.54
27:1:30:GLU:HA	27:1:33:HIS:HB3	1.89	0.54
1:A:2314:G:C2'	1:A:2315:C:H5'	2.38	0.54
37:A:4166:HOH:O	26:Z:186:ARG:HD2	2.08	0.54
37:A:5508:HOH:O	14:N:58:GLN:HG3	2.08	0.54
4:D:238:ASN:ND2	4:D:240:GLY:H	1.99	0.54
8:H:28:ALA:HB3	8:H:99:THR:O	2.07	0.54
10:J:14:TYR:N	10:J:91:HIS:CE1	2.76	0.54
12:L:106:GLY:HA3	37:L:5264:HOH:O	2.07	0.54
13:M:143:THR:CG2	13:M:144:ASP:H	2.21	0.54
15:O:159:TYR:HE2	15:O:163:PHE:HE2	1.56	0.54
17:Q:121:ASP:HB2	37:Q:197:HOH:O	2.08	0.54
23:W:39:ALA:O	23:W:41:GLU:N	2.41	0.54
1:A:2896:A:H5''	37:A:6080:HOH:O	2.07	0.54
4:D:66:GLU:OE1	4:D:328:ARG:HD2	2.07	0.54
4:D:74:ILE:HD13	4:D:309:VAL:HG21	1.89	0.54
5:E:127:ARG:CZ	5:E:225:PRO:HG2	2.36	0.54
7:G:31:ARG:HH12	7:G:68:HIS:CD2	2.26	0.54
10:J:39:GLY:O	10:J:41:THR:N	2.41	0.54
12:L:34:VAL:CG2	12:L:47:ALA:HB2	2.37	0.54
14:N:106:ASN:ND2	35:N:8518:CL:CL	2.78	0.54
14:N:157:LEU:HB3	14:N:160:PHE:HD1	1.72	0.54
26:Z:185:VAL:HG12	37:Z:8567:HOH:O	2.07	0.54
1:A:797:A:C4'	27:1:10:ARG:N	2.71	0.53
1:A:2274:A:H1'	14:N:86:MET:SD	2.48	0.53
37:A:3965:HOH:O	21:U:82:THR:HA	2.08	0.53
2:B:3092:G:H22	10:J:52:LYS:NZ	2.06	0.53
8:H:47:LEU:HB2	8:H:108:LEU:HD11	1.90	0.53
13:M:104:ASP:O	13:M:105:TYR:HB3	2.08	0.53
19:S:119:VAL:HG21	19:S:142:ASP:CG	2.33	0.53
23:W:55:ARG:O	23:W:59:ILE:HG12	2.08	0.53
26:Z:106:THR:HG23	26:Z:107:PRO:HD2	1.90	0.53
28:2:10:LYS:HG3	37:2:8433:HOH:O	2.07	0.53
1:A:328:U:O4'	5:E:202:THR:HG22	2.07	0.53
1:A:1130:U:H2'	1:A:1131:G:O4'	2.09	0.53
1:A:1735:C:O2'	1:A:1736:A:H5'	2.08	0.53
1:A:2326:U:H4'	1:A:2412:G:H4'	1.90	0.53
4:D:42:ALA:HB1	4:D:308:LEU:HD11	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:SER:C	4:D:62:ARG:H	2.17	0.53
5:E:246:ARG:HB3	5:E:246:ARG:NH1	2.23	0.53
10:J:86:ARG:HD3	10:J:130:HIS:HD2	1.73	0.53
15:O:37:ARG:NH2	37:O:8533:HOH:O	2.42	0.53
3:C:186:TRP:CG	3:C:187:PRO:HA	2.43	0.53
5:E:47:GLY:HA2	5:E:92:PRO:HB2	1.90	0.53
14:N:108:LYS:HE3	37:N:8613:HOH:O	2.08	0.53
29:3:22:PRO:HG2	29:3:25:VAL:HG23	1.91	0.53
1:A:119:A:H2'	1:A:120:A:H5''	1.89	0.53
1:A:2502:C:H2'	1:A:2503:A:H5'	1.90	0.53
4:D:55:ASN:HB3	4:D:63:GLU:HA	1.89	0.53
4:D:75:GLU:C	4:D:77:PRO:HD3	2.33	0.53
26:Z:112:GLU:CD	26:Z:115:ARG:NH1	2.66	0.53
1:A:113:A:OP2	1:A:114:A:H2'	2.08	0.53
1:A:1329:A:C2	37:A:4655:HOH:O	2.49	0.53
7:G:49:ILE:HD11	7:G:69:ILE:HD12	1.90	0.53
19:S:18:LEU:HD12	19:S:143:VAL:CG1	2.39	0.53
26:Z:107:PRO:HB3	26:Z:182:PHE:CD2	2.44	0.53
1:A:558:C:H2'	1:A:559:U:H5'	1.91	0.53
10:J:75:SER:O	10:J:79:ALA:HB2	2.09	0.53
10:J:166:ASN:N	10:J:166:ASN:ND2	2.56	0.53
22:V:46:ALA:HB1	22:V:52:THR:HG21	1.90	0.53
25:Y:12:ILE:HD12	25:Y:36:HIS:ND1	2.24	0.53
1:A:2415:A:C2	15:O:25:ARG:HB3	2.44	0.53
1:A:2435:U:H1'	37:A:5408:HOH:O	2.09	0.53
1:A:2649:A:H5'	1:A:2649:A:H8	1.74	0.53
2:B:3055:U:H4'	2:B:3056:A:C8	2.44	0.53
6:F:50:VAL:O	6:F:71:ALA:HA	2.09	0.53
10:J:132:PHE:O	10:J:133:ILE:HD13	2.08	0.53
11:K:45:VAL:HG21	11:K:129:PHE:CD1	2.44	0.53
24:X:13:MET:HE3	24:X:17:ILE:CG2	2.39	0.53
25:Y:74:ALA:CB	25:Y:85:VAL:HG22	2.39	0.53
1:A:281:U:O2'	1:A:282:C:H5'	2.09	0.53
1:A:1182:C:H1'	1:A:1192:A:H8	1.74	0.53
2:B:3042:C:H2'	37:B:8503:HOH:O	2.07	0.53
6:F:27:ILE:HG22	6:F:28:GLY:N	2.18	0.53
13:M:143:THR:HG22	13:M:144:ASP:H	1.74	0.53
14:N:185:PRO:HG2	14:N:189:VAL:HG11	1.90	0.53
22:V:52:THR:HG22	22:V:54:THR:HB	1.91	0.53
27:1:58:GLY:CA	37:1:8439:HOH:O	2.48	0.53
30:4:11:CYS:HB2	30:4:20:HIS:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2486:A:C2	31:A:9000:ANM:H1	2.44	0.53
1:A:2729:C:O2'	1:A:2730:G:H5'	2.09	0.53
37:A:7449:HOH:O	5:E:188:ARG:HD2	2.09	0.53
3:C:88:ILE:HD13	3:C:100:PRO:CD	2.39	0.53
3:C:129:LEU:CD1	3:C:145:MET:HE1	2.39	0.53
4:D:30:PRO:HB2	4:D:39:GLN:NE2	2.24	0.53
4:D:162:MET:HG3	4:D:310:ARG:CZ	2.39	0.53
6:F:58:VAL:HG12	6:F:59:GLY:N	2.23	0.53
12:L:30:LYS:O	12:L:55:VAL:HG13	2.08	0.53
13:M:73:VAL:HG23	13:M:74:THR:N	2.23	0.53
19:S:132:ARG:HG2	19:S:133:ALA:N	2.24	0.53
21:U:63:ILE:HD11	21:U:75:GLU:HB2	1.90	0.53
26:Z:144:ARG:NH1	37:Z:8573:HOH:O	2.39	0.53
26:Z:186:ARG:HG2	26:Z:186:ARG:NH1	2.23	0.53
1:A:283:U:H5''	1:A:284:C:P	2.49	0.53
1:A:567:U:H5''	37:X:5817:HOH:O	2.09	0.53
1:A:2815:G:N7	11:K:80:LYS:NZ	2.56	0.53
9:I:63:ARG:N	37:I:2569:HOH:O	2.42	0.53
13:M:101:ASP:C	13:M:103:ALA:H	2.17	0.53
1:A:88:G:H5'	1:A:88:G:H8	1.74	0.52
37:A:9108:HOH:O	5:E:103:ASN:HB3	2.09	0.52
4:D:305:ASP:O	4:D:306:LYS:CB	2.56	0.52
5:E:214:THR:HG23	37:E:8432:HOH:O	2.08	0.52
16:P:25:VAL:HG23	16:P:26:TRP:N	2.24	0.52
21:U:48:VAL:HG22	21:U:97:ARG:C	2.34	0.52
1:A:380:A:H5''	14:N:48:ARG:NH2	2.24	0.52
1:A:834:G:H4'	1:A:835:U:OP2	2.09	0.52
1:A:920:C:H5'	1:A:921:G:C4	2.44	0.52
1:A:1132:A:N6	1:A:1229:C:H2'	2.24	0.52
1:A:2359:G:H3'	37:A:5670:HOH:O	2.09	0.52
37:A:4041:HOH:O	4:D:27:ASN:HB2	2.07	0.52
3:C:153:ARG:HH11	3:C:153:ARG:CB	2.22	0.52
4:D:7:ARG:NH1	4:D:7:ARG:CG	2.70	0.52
6:F:170:TYR:O	6:F:171:ASP:HB3	2.08	0.52
11:K:107:ASN:HD22	11:K:109:TYR:H	1.56	0.52
15:O:47:LEU:HD12	15:O:92:ALA:HB1	1.91	0.52
16:P:7:LEU:HD22	37:P:5650:HOH:O	2.09	0.52
20:T:6:LYS:HB2	20:T:27:ALA:O	2.08	0.52
23:W:56:ILE:O	23:W:60:GLN:HG3	2.09	0.52
23:W:64:GLY:O	23:W:65:ASP:CB	2.57	0.52
24:X:106:THR:OG1	24:X:109:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:126:PRO:HG2	26:Z:128:PHE:CE1	2.44	0.52
1:A:710:G:OP1	16:P:24:ALA:HB3	2.09	0.52
1:A:1249:U:H2'	1:A:1250:C:C6	2.44	0.52
1:A:1527:A:H1'	1:A:1528:A:C8	2.44	0.52
1:A:2251:G:H2'	1:A:2252:A:C8	2.45	0.52
1:A:2486:A:C3'	1:A:2487:C:P	2.97	0.52
8:H:46:GLU:N	37:H:3461:HOH:O	2.42	0.52
18:R:66:LYS:HB2	18:R:70:ALA:O	2.10	0.52
28:2:28:HIS:CE1	28:2:31:LYS:HE2	2.45	0.52
28:2:28:HIS:CD2	28:2:31:LYS:HG3	2.44	0.52
1:A:1874:U:H2'	3:C:120:ARG:HG3	1.91	0.52
7:G:31:ARG:NH1	37:G:5919:HOH:O	2.41	0.52
9:I:12:ILE:HD12	37:I:692:HOH:O	2.08	0.52
15:O:154:LEU:HG	15:O:155:GLU:H	1.73	0.52
24:X:21:LEU:HD13	24:X:26:ILE:HD11	1.91	0.52
26:Z:172:THR:HG22	26:Z:173:ALA:N	2.25	0.52
29:3:22:PRO:HG2	29:3:25:VAL:CG2	2.39	0.52
1:A:1119:G:N2	1:A:1246:A:H2	2.04	0.52
1:A:1393:A:H2'	1:A:1394:C:C6	2.45	0.52
1:A:1657:A:H2'	1:A:1658:A:C8	2.44	0.52
1:A:1909:A:N1	1:A:2128:G:H1'	2.24	0.52
1:A:2050:G:H5''	19:S:80:TYR:O	2.10	0.52
3:C:200:PRO:HG2	3:C:225:VAL:HG21	1.92	0.52
13:M:73:VAL:HG23	13:M:74:THR:H	1.73	0.52
21:U:49:GLU:OE2	21:U:97:ARG:HD2	2.09	0.52
22:V:49:LEU:HD11	37:V:3805:HOH:O	2.10	0.52
30:4:48:ASN:ND2	30:4:50:GLY:H	2.07	0.52
1:A:283:U:H5	1:A:284:C:N4	2.07	0.52
1:A:1118:A:C8	1:A:1118:A:C3'	2.89	0.52
1:A:1192:A:O2'	1:A:1193:A:OP1	2.26	0.52
1:A:2094:G:H4'	4:D:245:SER:HB3	1.90	0.52
2:B:3055:U:H4'	2:B:3056:A:H8	1.74	0.52
8:H:99:THR:O	8:H:99:THR:HG23	2.09	0.52
10:J:147:ARG:HA	10:J:150:LYS:NZ	2.25	0.52
14:N:182:LYS:HB2	14:N:194:ALA:HB2	1.92	0.52
21:U:53:GLY:HA3	37:U:6384:HOH:O	2.08	0.52
1:A:1189:A:O2'	1:A:1208:C:H2'	2.09	0.52
1:A:1497:G:H4'	1:A:1627:G:O2'	2.10	0.52
3:C:179:MET:HG2	3:C:186:TRP:CB	2.40	0.52
4:D:55:ASN:HB3	4:D:64:GLY:H	1.75	0.52
15:O:157:PRO:HA	37:O:8526:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:111:ARG:HB3	21:U:119:ALA:HB2	1.92	0.52
24:X:38:THR:HB	37:X:5390:HOH:O	2.09	0.52
24:X:130:HIS:O	24:X:136:GLY:HA3	2.10	0.52
27:1:11:THR:OG1	27:1:23:ARG:HB2	2.09	0.52
1:A:204:A:C2'	1:A:205:U:H5'	2.40	0.52
1:A:960:G:H2'	1:A:960:G:N3	2.25	0.52
1:A:1205:U:H2'	1:A:1206:U:C5'	2.39	0.52
37:A:9550:HOH:O	4:D:267:LYS:HD3	2.08	0.52
4:D:279:THR:OG1	4:D:290:VAL:HB	2.09	0.52
5:E:246:ARG:NE	37:E:8419:HOH:O	2.43	0.52
1:A:482:G:H4'	1:A:508:A:N1	2.25	0.52
1:A:1787:C:OP1	17:Q:68:LYS:HE2	2.10	0.52
1:A:2730:G:O2'	1:A:2731:G:H5'	2.10	0.52
1:A:2780:C:H1'	7:G:143:GLN:NE2	2.24	0.52
1:A:1423:C:O2'	1:A:1424:A:H5'	2.10	0.52
1:A:1503:U:H2'	1:A:1504:A:O4'	2.10	0.52
1:A:2547:C:OP2	4:D:5:ARG:NH1	2.43	0.52
1:A:2837:U:H2'	37:A:6822:HOH:O	2.09	0.52
7:G:11:VAL:CG1	7:G:12:ASP:N	2.73	0.52
11:K:42:GLU:O	11:K:131:THR:HG23	2.10	0.52
24:X:125:HIS:CD2	24:X:127:GLY:H	2.27	0.52
3:C:192:VAL:O	3:C:192:VAL:CG1	2.58	0.51
4:D:248:ARG:O	4:D:251:VAL:CG1	2.58	0.51
6:F:57:THR:HG23	6:F:63:ILE:CB	2.40	0.51
10:J:47:GLU:CB	10:J:133:ILE:HD13	2.40	0.51
10:J:109:ASP:HB2	37:J:8349:HOH:O	2.10	0.51
15:O:34:LEU:HA	15:O:47:LEU:HD23	1.93	0.51
20:T:29:ASP:OD1	20:T:31:ARG:HG3	2.09	0.51
20:T:81:ILE:HG23	37:T:8337:HOH:O	2.09	0.51
24:X:21:LEU:HB3	24:X:26:ILE:CG1	2.40	0.51
1:A:204:A:H2'	1:A:205:U:H5'	1.90	0.51
1:A:2443:C:H3'	37:A:3455:HOH:O	2.10	0.51
1:A:2717:C:O2'	1:A:2718:C:H5''	2.09	0.51
37:A:6224:HOH:O	3:C:22:ARG:HG2	2.10	0.51
2:B:3064:C:H2'	2:B:3065:A:H5'	1.92	0.51
3:C:192:VAL:O	3:C:192:VAL:HG12	2.10	0.51
8:H:58:GLU:HA	8:H:61:MET:HG3	1.92	0.51
12:L:58:THR:HG22	12:L:59:LYS:HG3	1.93	0.51
13:M:53:ARG:NH2	13:M:57:VAL:CG1	2.74	0.51
19:S:132:ARG:CZ	37:S:8584:HOH:O	2.57	0.51
26:Z:107:PRO:HB3	26:Z:182:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:144:ARG:NH2	37:Z:8608:HOH:O	2.43	0.51
27:1:34:LYS:HE2	37:1:8426:HOH:O	2.10	0.51
1:A:814:G:H4'	37:A:3118:HOH:O	2.10	0.51
4:D:139:ASP:HB2	4:D:165:ARG:HE	1.75	0.51
5:E:39:GLN:O	5:E:43:LYS:HD3	2.10	0.51
6:F:140:ARG:O	6:F:144:ARG:HG2	2.09	0.51
19:S:39:THR:HB	19:S:42:GLU:CD	2.35	0.51
22:V:17:THR:HG22	22:V:18:GLY:N	2.26	0.51
28:2:8:GLN:HE22	28:2:11:LYS:NZ	2.08	0.51
1:A:69:A:H5'	1:A:69:A:H8	1.76	0.51
1:A:256:C:H2'	1:A:257:G:O4'	2.11	0.51
1:A:875:A:C2	3:C:194:MET:SD	3.04	0.51
1:A:1462:C:H2'	1:A:1463:A:C8	2.46	0.51
1:A:1477:C:H5'	1:A:1868:G:C5'	2.40	0.51
1:A:1862:C:H1'	37:A:7209:HOH:O	2.09	0.51
5:E:235:PHE:HE2	5:E:243:VAL:HG21	1.76	0.51
6:F:65:GLU:HA	37:F:6752:HOH:O	2.09	0.51
6:F:99:ASP:HB3	6:F:103:ASN:H	1.75	0.51
14:N:38:VAL:O	14:N:63:VAL:HG13	2.10	0.51
14:N:173:LEU:HD23	14:N:183:VAL:HG12	1.92	0.51
20:T:51:GLN:NE2	20:T:53:ASN:HD21	2.07	0.51
24:X:6:GLN:HB2	24:X:26:ILE:CD1	2.35	0.51
28:2:28:HIS:CD2	28:2:30:LYS:HB2	2.46	0.51
1:A:538:C:OP2	26:Z:134:HIS:HE1	1.93	0.51
1:A:820:G:C5	3:C:171:LYS:HB2	2.46	0.51
1:A:2256:G:H2'	1:A:2257:G:H5'	1.93	0.51
1:A:2300:A:H4'	1:A:2301:A:O5'	2.11	0.51
2:B:3049:G:O2'	2:B:3050:G:H5'	2.10	0.51
6:F:41:LEU:HA	6:F:44:ILE:CG2	2.40	0.51
6:F:94:ALA:HB3	6:F:174:VAL:HA	1.93	0.51
6:F:144:ARG:NH2	37:F:3839:HOH:O	2.39	0.51
10:J:129:ASN:HD22	10:J:129:ASN:N	2.08	0.51
13:M:77:ALA:HB3	37:M:8532:HOH:O	2.10	0.51
15:O:143:ARG:HA	15:O:172:PHE:CD2	2.45	0.51
15:O:180:LEU:O	15:O:181:ASP:HB3	2.10	0.51
25:Y:25:ARG:NH1	37:Y:3861:HOH:O	2.44	0.51
27:1:42:CYS:SG	27:1:44:PHE:HB2	2.50	0.51
30:4:91:GLN:O	30:4:92:GLU:HB2	2.10	0.51
1:A:56:G:H5''	23:W:50:ARG:NH1	2.26	0.51
2:B:3049:G:H2'	2:B:3050:G:O4'	2.10	0.51
3:C:192:VAL:O	3:C:207:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:16:ARG:NE	37:D:8554:HOH:O	2.16	0.51
5:E:107:ARG:NE	37:E:8450:HOH:O	2.25	0.51
6:F:57:THR:HG23	6:F:63:ILE:CG2	2.39	0.51
6:F:95:THR:C	6:F:97:GLN:N	2.66	0.51
6:F:99:ASP:O	6:F:159:PRO:HG3	2.10	0.51
8:H:113:ASP:O	8:H:117:GLU:HG3	2.11	0.51
12:L:10:GLN:NE2	12:L:10:GLN:N	2.42	0.51
12:L:125:ALA:C	12:L:127:ALA:H	2.18	0.51
1:A:1506:U:H6	1:A:1506:U:H5'	1.76	0.51
1:A:2787:C:H5	37:A:4603:HOH:O	1.92	0.51
2:B:3029:C:C2'	2:B:3030:C:H5'	2.41	0.51
3:C:105:VAL:HG11	3:C:154:ALA:CB	2.40	0.51
4:D:320:GLN:HG3	4:D:321:PRO:HD2	1.93	0.51
24:X:22:GLU:HG2	24:X:27:HIS:CD2	2.46	0.51
1:A:371:U:H2'	1:A:372:A:C8	2.44	0.51
1:A:661:G:C5	1:A:686:A:C2	2.98	0.51
1:A:1543:G:N1	1:A:1641:A:OP2	2.33	0.51
1:A:2281:C:C2'	1:A:2282:U:H5'	2.41	0.51
37:A:7449:HOH:O	5:E:188:ARG:CD	2.59	0.51
4:D:156:LYS:HZ1	4:D:160:ASP:CG	2.19	0.51
9:I:23:ILE:O	9:I:27:ILE:HG13	2.11	0.51
11:K:75:PRO:HG2	11:K:105:LEU:CD2	2.40	0.51
12:L:45:PRO:HB2	37:L:7169:HOH:O	2.11	0.51
26:Z:144:ARG:NE	37:Z:8608:HOH:O	2.43	0.51
1:A:1306:U:OP1	5:E:184:ARG:HD2	2.11	0.51
1:A:1733:A:H4'	4:D:212:GLN:HA	1.92	0.51
1:A:2604:A:H5'	37:A:5772:HOH:O	2.09	0.51
37:A:6112:HOH:O	29:3:20:ARG:HB3	2.11	0.51
3:C:192:VAL:HG13	37:C:8557:HOH:O	2.10	0.51
10:J:149:ALA:C	10:J:151:MET:H	2.17	0.51
14:N:52:LEU:HD13	14:N:116:ASN:HB3	1.93	0.51
37:A:9936:HOH:O	25:Y:23:HIS:HD2	1.93	0.51
5:E:46:TYR:CE2	5:E:98:ARG:NH1	2.79	0.51
14:N:146:GLN:NE2	37:N:8642:HOH:O	2.44	0.51
15:O:139:TRP:HA	15:O:139:TRP:CE3	2.45	0.51
20:T:33:SER:OG	20:T:36:GLU:HG3	2.11	0.51
24:X:65:VAL:HA	24:X:68:THR:CG2	2.40	0.51
1:A:324:G:O2'	1:A:325:U:H5'	2.11	0.50
1:A:681:G:H5'	1:A:681:G:N3	2.27	0.50
1:A:2503:A:OP1	10:J:147:ARG:NH2	2.41	0.50
12:L:34:VAL:HB	37:L:7169:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:25:VAL:HG23	16:P:26:TRP:H	1.76	0.50
18:R:64:GLU:HG3	18:R:74:ASP:OD2	2.11	0.50
26:Z:185:VAL:HA	37:Z:8561:HOH:O	2.10	0.50
1:A:121:U:OP2	29:3:10:ARG:NH2	2.40	0.50
1:A:175:G:H2'	14:N:192:ALA:HB3	1.91	0.50
1:A:538:C:H5''	1:A:539:G:C8	2.46	0.50
1:A:1116:U:H3	1:A:1246:A:N6	2.00	0.50
1:A:1189:A:H3'	37:A:7680:HOH:O	2.10	0.50
1:A:1484:G:H2'	37:A:9099:HOH:O	2.11	0.50
1:A:1524:U:H4'	1:A:1524:U:OP1	2.11	0.50
1:A:1972:U:H2'	1:A:1973:A:H5'	1.94	0.50
1:A:2081:A:H4'	11:K:69:TYR:CE1	2.46	0.50
1:A:2421:G:H3'	1:A:2422:U:H5''	1.93	0.50
3:C:100:PRO:HG2	3:C:103:VAL:CG2	2.38	0.50
4:D:162:MET:HG3	4:D:310:ARG:NH1	2.25	0.50
6:F:99:ASP:HB2	6:F:103:ASN:H	1.76	0.50
21:U:73:HIS:CD2	21:U:88:PRO:HG3	2.46	0.50
1:A:1173:A:H2'	37:A:4320:HOH:O	2.10	0.50
1:A:1384:C:H5'	25:Y:30:MET:HG2	1.94	0.50
1:A:1500:U:P	17:Q:41:ARG:HH22	2.33	0.50
1:A:2365:G:H4'	18:R:45:PRO:O	2.11	0.50
2:B:3002:U:OP2	2:B:3002:U:H4'	2.10	0.50
2:B:3006:C:C5'	15:O:37:ARG:HH12	2.13	0.50
3:C:93:THR:HG23	3:C:154:ALA:O	2.11	0.50
4:D:82:VAL:O	4:D:82:VAL:CG1	2.58	0.50
4:D:205:VAL:O	4:D:307:ARG:NE	2.44	0.50
10:J:46:VAL:O	10:J:146:TRP:CH2	2.60	0.50
15:O:67:ALA:C	15:O:69:TYR:N	2.70	0.50
26:Z:187:VAL:HG23	26:Z:192:ASP:HB3	1.92	0.50
1:A:1060:C:H6	1:A:1060:C:H5'	1.77	0.50
1:A:1191:A:N1	1:A:1206:U:O4	2.45	0.50
6:F:103:ASN:ND2	6:F:134:LEU:H	2.08	0.50
15:O:86:LEU:O	15:O:90:LEU:HG	2.11	0.50
17:Q:10:ALA:HA	17:Q:13:VAL:CG1	2.40	0.50
1:A:566:A:H2'	1:A:567:U:O4'	2.12	0.50
1:A:778:C:C4	1:A:779:U:C4	3.00	0.50
1:A:1166:A:H61	1:A:1180:U:H3	1.58	0.50
1:A:1441:G:H1'	37:A:7765:HOH:O	2.10	0.50
1:A:2064:U:H5'	1:A:2652:U:H4'	1.92	0.50
5:E:35:VAL:HG21	5:E:227:GLY:HA2	1.93	0.50
7:G:68:HIS:O	7:G:72:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:84:ARG:CZ	10:J:135:TRP:HH2	2.23	0.50
19:S:29:LYS:HD3	37:S:8532:HOH:O	2.11	0.50
1:A:383:A:H4'	37:A:5307:HOH:O	2.11	0.50
1:A:1118:A:H8	1:A:1119:G:H5''	1.75	0.50
1:A:1656:A:H2'	1:A:1657:A:O4'	2.11	0.50
4:D:56:ASP:OD1	4:D:322:ARG:HB3	2.11	0.50
8:H:58:GLU:HA	8:H:61:MET:HE2	1.93	0.50
13:M:120:LEU:HD12	13:M:133:VAL:HG21	1.94	0.50
25:Y:25:ARG:HG2	37:Y:5356:HOH:O	2.11	0.50
1:A:821:U:O2'	1:A:822:C:H5'	2.12	0.50
1:A:1666:C:C2'	1:A:1667:A:C5'	2.90	0.50
1:A:1996:U:O2'	1:A:1997:A:H5'	2.12	0.50
3:C:105:VAL:CG1	3:C:106:CYS:N	2.74	0.50
10:J:53:PRO:HA	10:J:125:VAL:O	2.12	0.50
24:X:108:ARG:HE	24:X:114:PRO:HG3	1.77	0.50
25:Y:66:THR:HG23	25:Y:67:PRO:HD2	1.94	0.50
1:A:2687:G:O2'	1:A:2688:U:H5'	2.11	0.50
37:A:9974:HOH:O	13:M:22:ARG:HG2	2.12	0.50
2:B:3030:C:OP1	6:F:137:PRO:O	2.29	0.50
5:E:7:ASP:OD1	5:E:11:ASN:O	2.29	0.50
6:F:27:ILE:HD11	6:F:37:ALA:CB	2.41	0.50
8:H:28:ALA:CB	8:H:99:THR:HG23	2.41	0.50
1:A:241:A:C2	1:A:378:A:H4'	2.47	0.50
1:A:1940:C:H4'	37:A:7336:HOH:O	2.10	0.50
1:A:2456:A:H5'	37:A:5674:HOH:O	2.11	0.50
9:I:69:ARG:NH1	37:I:3513:HOH:O	2.45	0.50
14:N:59:GLY:C	14:N:141:ILE:HD11	2.37	0.50
14:N:155:HIS:CE1	14:N:158:ARG:HE	2.30	0.50
1:A:57:C:H5''	37:A:6741:HOH:O	2.11	0.49
1:A:138:U:OP2	1:A:139:C:H5	1.95	0.49
1:A:920:C:H5''	1:A:921:G:O5'	2.12	0.49
1:A:1882:C:O2'	1:A:2012:U:OP2	2.28	0.49
4:D:24:PRO:CG	4:D:204:GLY:HA2	2.42	0.49
6:F:84:LEU:C	6:F:86:THR:H	2.19	0.49
6:F:149:ARG:NH1	37:F:3066:HOH:O	2.36	0.49
7:G:69:ILE:HA	7:G:72:MET:HE2	1.94	0.49
7:G:132:THR:O	7:G:132:THR:HG23	2.12	0.49
8:H:46:GLU:OE1	8:H:100:ASP:HA	2.11	0.49
15:O:154:LEU:HG	15:O:155:GLU:N	2.26	0.49
20:T:51:GLN:HE21	20:T:53:ASN:ND2	2.08	0.49
1:A:244:C:OP2	8:H:38:LYS:HE3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:C:H4'	5:E:246:ARG:NH2	2.27	0.49
1:A:1003:U:O2	10:J:90:PHE:CZ	2.65	0.49
1:A:2281:C:H2'	1:A:2282:U:H5'	1.95	0.49
1:A:2851:G:C2'	1:A:2852:A:H5'	2.42	0.49
12:L:29:LEU:HB3	12:L:55:VAL:CG1	2.30	0.49
15:O:167:ASP:O	15:O:168:LEU:HD23	2.12	0.49
16:P:96:VAL:HG13	16:P:100:GLN:HB2	1.94	0.49
21:U:48:VAL:HG22	21:U:97:ARG:O	2.12	0.49
1:A:136:C:H2'	1:A:137:U:O4'	2.10	0.49
1:A:157:G:H4'	14:N:95:LYS:HE3	1.94	0.49
1:A:396:U:H5'	30:4:42:ARG:NH1	2.27	0.49
1:A:1003:U:O2'	10:J:90:PHE:HE1	1.95	0.49
1:A:2256:G:H2'	1:A:2257:G:C5'	2.42	0.49
1:A:2898:G:H4'	4:D:288:GLY:HA2	1.93	0.49
6:F:163:VAL:HA	37:F:6326:HOH:O	2.12	0.49
8:H:47:LEU:HD22	8:H:108:LEU:CD1	2.42	0.49
21:U:41:ARG:NH1	21:U:42:VAL:O	2.45	0.49
22:V:47:ARG:HG3	37:V:4381:HOH:O	2.12	0.49
22:V:52:THR:HG22	22:V:54:THR:H	1.77	0.49
26:Z:187:VAL:HB	37:Z:8567:HOH:O	2.12	0.49
1:A:344:C:H2'	1:A:345:G:O4'	2.11	0.49
1:A:1180:U:H2'	1:A:1181:A:O4'	2.12	0.49
1:A:1972:U:H2'	1:A:1973:A:C5'	2.43	0.49
1:A:2748:G:H5'	37:A:7535:HOH:O	2.13	0.49
4:D:16:ARG:NH2	37:D:8554:HOH:O	2.41	0.49
5:E:27:ARG:HG2	5:E:30:LEU:HG	1.94	0.49
14:N:24:MET:HE3	14:N:28:MET:CE	2.35	0.49
15:O:138:ASP:O	15:O:140:GLN:N	2.44	0.49
24:X:13:MET:HE2	24:X:18:GLN:N	2.26	0.49
24:X:84:VAL:HG12	37:X:6679:HOH:O	2.12	0.49
25:Y:9:VAL:HG13	25:Y:88:GLU:OE2	2.12	0.49
25:Y:27:ASP:OD2	25:Y:27:ASP:N	2.45	0.49
26:Z:178:HIS:CG	26:Z:179:PRO:HD2	2.47	0.49
1:A:396:U:O2'	1:A:418:C:H4'	2.13	0.49
1:A:500:G:H21	19:S:98:ASN:HD21	1.59	0.49
1:A:644:G:N3	1:A:644:G:H5'	2.27	0.49
1:A:669:G:O2'	1:A:670:G:H5'	2.12	0.49
1:A:825:U:H5''	1:A:826:U:OP1	2.13	0.49
1:A:2837:U:H1'	4:D:307:ARG:HH12	1.78	0.49
4:D:207:LYS:HG2	4:D:304:PRO:HB3	1.94	0.49
8:H:91:VAL:CG1	8:H:92:GLY:H	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:65:ARG:HB3	37:J:8387:HOH:O	2.13	0.49
15:O:110:THR:HB	15:O:113:SER:OG	2.12	0.49
18:R:30:VAL:O	18:R:30:VAL:HG12	2.12	0.49
22:V:11:THR:HG22	22:V:53:ASP:OD2	2.12	0.49
25:Y:76:ARG:HG3	25:Y:76:ARG:NH1	2.25	0.49
1:A:338:C:H4'	5:E:174:ILE:HD12	1.93	0.49
1:A:775:G:OP1	28:2:16:HIS:HE1	1.95	0.49
1:A:1450:C:C4'	1:A:1451:C:OP2	2.60	0.49
1:A:2507:G:H2'	1:A:2510:C:H42	1.78	0.49
3:C:164:ARG:HB2	27:1:68:CYS:SG	2.52	0.49
4:D:79:MET:HE3	4:D:144:THR:HG21	1.95	0.49
14:N:81:ARG:O	14:N:86:MET:HE2	2.12	0.49
1:A:185:G:H4'	1:A:186:A:H4'	1.94	0.49
1:A:2724:U:H2'	1:A:2725:G:O4'	2.13	0.49
1:A:2791:U:H1'	1:A:2792:A:H5''	1.95	0.49
4:D:156:LYS:HE3	37:D:8631:HOH:O	2.11	0.49
4:D:248:ARG:NH2	37:D:8524:HOH:O	2.46	0.49
5:E:1:MET:HG2	5:E:2:GLN:N	2.26	0.49
7:G:22:VAL:O	7:G:28:SER:HA	2.13	0.49
8:H:48:VAL:CG2	8:H:74:PHE:HB3	2.42	0.49
10:J:84:ARG:CZ	10:J:135:TRP:CH2	2.96	0.49
13:M:72:ASN:HB2	37:M:8583:HOH:O	2.12	0.49
14:N:95:LYS:HG2	14:N:99:ARG:HB3	1.94	0.49
24:X:41:TYR:O	24:X:45:VAL:HG13	2.12	0.49
1:A:820:G:O2'	1:A:856:G:H4'	2.13	0.49
1:A:820:G:C6	3:C:171:LYS:HB2	2.48	0.49
1:A:1236:A:H2'	1:A:1237:U:O4'	2.13	0.49
1:A:1311:G:C2	1:A:1312:G:C8	3.01	0.49
1:A:2781:U:H1'	7:G:139:GLU:OE2	2.13	0.49
4:D:41:PHE:CE1	4:D:79:MET:HG3	2.47	0.49
15:O:161:GLY:O	15:O:162:ASP:C	2.55	0.49
16:P:39:THR:O	16:P:115:ARG:NH2	2.45	0.49
24:X:90:TYR:N	24:X:90:TYR:CD1	2.80	0.49
30:4:55:VAL:HB	30:4:56:PRO:HD2	1.95	0.49
1:A:558:C:C2'	1:A:559:U:C5'	2.91	0.49
1:A:1119:G:H2'	11:K:52:GLN:NE2	2.28	0.49
1:A:1205:U:O2'	1:A:1206:U:H5''	2.13	0.49
1:A:1741:U:O2'	1:A:2723:G:H4'	2.12	0.49
1:A:1819:G:H2'	1:A:1820:G:C4'	2.43	0.49
5:E:1:MET:HG2	5:E:2:GLN:NE2	2.28	0.49
6:F:62:ASP:HA	37:F:4233:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:101:ASN:O	12:L:102:GLU:CB	2.61	0.49
30:4:56:PRO:N	37:4:8550:HOH:O	2.45	0.49
1:A:183:A:C5'	14:N:157:LEU:HD12	2.41	0.49
1:A:240:C:H4'	14:N:146:GLN:NE2	2.28	0.49
1:A:489:A:C8	21:U:82:THR:HG22	2.48	0.49
1:A:2072:G:C6	1:A:2533:C:H1'	2.48	0.49
1:A:2326:U:H4'	1:A:2412:G:C4'	2.43	0.49
6:F:23:VAL:O	6:F:23:VAL:CG2	2.60	0.49
6:F:58:VAL:CG1	6:F:59:GLY:N	2.75	0.49
11:K:52:GLN:HG3	11:K:53:ILE:N	2.28	0.49
13:M:34:GLY:C	13:M:36:ASP:H	2.21	0.49
14:N:52:LEU:HD21	37:N:8615:HOH:O	2.13	0.49
19:S:25:PHE:CE2	19:S:29:LYS:HE2	2.48	0.49
20:T:81:ILE:HG12	37:T:8337:HOH:O	2.12	0.49
27:1:51:GLY:HA3	37:1:8417:HOH:O	2.13	0.49
4:D:217:ARG:HG3	4:D:257:THR:HG22	1.95	0.48
4:D:275:GLY:O	4:D:291:ASP:HA	2.13	0.48
11:K:93:ARG:HB3	11:K:93:ARG:NH1	2.26	0.48
12:L:98:VAL:HG22	12:L:102:GLU:C	2.37	0.48
19:S:14:ALA:HB3	19:S:147:LEU:HB2	1.95	0.48
19:S:29:LYS:HB3	37:S:8532:HOH:O	2.12	0.48
1:A:2004:U:O2	1:A:2004:U:H2'	2.12	0.48
4:D:185:GLY:HA2	37:D:8634:HOH:O	2.13	0.48
5:E:129:HIS:HD2	5:E:165:ASP:OD2	1.97	0.48
15:O:182:GLY:O	15:O:183:ASP:O	2.31	0.48
17:Q:103:THR:HA	17:Q:106:ARG:NH1	2.28	0.48
1:A:602:A:O2'	1:A:605:C:H4'	2.13	0.48
1:A:1266:U:H4'	26:Z:115:ARG:HH21	1.77	0.48
37:A:7012:HOH:O	3:C:211:LYS:HG2	2.12	0.48
4:D:168:GLY:O	4:D:169:GLY:O	2.31	0.48
5:E:95:GLU:H	5:E:95:GLU:CD	2.21	0.48
6:F:86:THR:C	6:F:89:PRO:HD2	2.37	0.48
7:G:21:THR:HG23	7:G:30:THR:OG1	2.13	0.48
11:K:45:VAL:HG22	11:K:46:ILE:N	2.27	0.48
14:N:67:ILE:CD1	14:N:104:ARG:HD2	2.43	0.48
17:Q:16:VAL:CG1	17:Q:17:GLY:N	2.75	0.48
18:R:11:ARG:HD3	37:R:5620:HOH:O	2.13	0.48
21:U:41:ARG:HG2	21:U:41:ARG:HH11	1.78	0.48
1:A:212:A:O4'	1:A:214:U:C6	2.67	0.48
1:A:2361:A:H5'	1:A:2361:A:H8	1.78	0.48
1:A:2649:A:H5'	1:A:2649:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2896:A:H2'	1:A:2896:A:N3	2.28	0.48
7:G:31:ARG:HH12	7:G:68:HIS:CG	2.31	0.48
10:J:110:GLY:N	37:J:8398:HOH:O	2.46	0.48
14:N:78:ASN:C	14:N:79:LYS:HG2	2.39	0.48
15:O:33:ARG:NH1	15:O:103:ASP:OD2	2.41	0.48
15:O:67:ALA:C	15:O:69:TYR:H	2.21	0.48
21:U:38:ARG:HH11	21:U:38:ARG:HG3	1.77	0.48
21:U:69:LYS:O	21:U:71:VAL:HG23	2.14	0.48
1:A:2361:A:H5''	37:A:9001:HOH:O	2.14	0.48
1:A:2777:G:O2'	1:A:2778:A:H5'	2.14	0.48
3:C:200:PRO:HD3	37:C:8519:HOH:O	2.13	0.48
5:E:76:ARG:HD3	37:E:8366:HOH:O	2.13	0.48
8:H:21:GLU:O	8:H:24:ARG:HG3	2.12	0.48
10:J:26:LYS:HG2	10:J:28:ILE:N	2.25	0.48
10:J:111:MET:O	10:J:114:PRO:HD3	2.13	0.48
11:K:39:VAL:HG12	11:K:40:ASN:ND2	2.28	0.48
11:K:142:ASN:O	11:K:144:THR:N	2.46	0.48
13:M:54:PRO:HG2	13:M:57:VAL:CG2	2.44	0.48
15:O:73:ALA:HB1	15:O:74:PRO:CD	2.43	0.48
15:O:143:ARG:NH1	15:O:173:ASP:OD2	2.38	0.48
20:T:53:ASN:ND2	37:T:8321:HOH:O	2.46	0.48
28:2:21:ARG:HD2	28:2:37:CYS:SG	2.54	0.48
1:A:638:C:H2'	1:A:639:A:C8	2.48	0.48
1:A:1056:U:H2'	1:A:1057:A:O4'	2.14	0.48
1:A:2830:U:H3'	37:A:5204:HOH:O	2.12	0.48
37:A:9525:HOH:O	17:Q:81:LYS:HG2	2.13	0.48
3:C:66:ARG:HB2	3:C:66:ARG:HH11	1.77	0.48
3:C:125:ASN:CB	3:C:158:VAL:HG12	2.44	0.48
9:I:71:LEU:C	9:I:73:ASP:H	2.20	0.48
21:U:45:GLY:C	37:U:3851:HOH:O	2.56	0.48
21:U:71:VAL:CG1	21:U:72:ILE:N	2.75	0.48
22:V:9:CYS:CA	22:V:52:THR:HG23	2.43	0.48
25:Y:9:VAL:HG22	25:Y:88:GLU:OE2	2.13	0.48
1:A:128:A:H3'	1:A:128:A:C8	2.48	0.48
1:A:514:G:H8	1:A:514:G:O5'	1.96	0.48
1:A:894:A:C2	5:E:87:ARG:NH2	2.82	0.48
1:A:1007:A:H2'	10:J:19:TYR:CZ	2.49	0.48
1:A:1669:A:H2'	1:A:1670:G:H8	1.78	0.48
1:A:2270:G:H4'	3:C:223:ARG:NH1	2.29	0.48
1:A:2563:U:H2'	1:A:2565:C:O5'	2.13	0.48
2:B:3023:U:C3'	2:B:3024:U:H5''	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:ASP:CB	6:F:103:ASN:HB2	2.43	0.48
13:M:97:VAL:HG12	13:M:98:GLU:O	2.14	0.48
17:Q:38:GLU:HA	17:Q:41:ARG:HH11	1.78	0.48
24:X:65:VAL:CA	24:X:68:THR:HG22	2.43	0.48
1:A:737:A:H2'	1:A:738:G:O4'	2.14	0.48
1:A:794:U:H3	1:A:819:A:H61	1.61	0.48
1:A:821:U:H2'	1:A:822:C:H6	1.78	0.48
37:A:7396:HOH:O	21:U:2:LYS:HE2	2.12	0.48
4:D:63:GLU:O	4:D:63:GLU:HG3	2.13	0.48
4:D:248:ARG:O	4:D:251:VAL:HG13	2.14	0.48
6:F:10:PHE:CD1	6:F:11:HIS:N	2.82	0.48
6:F:23:VAL:HG12	6:F:130:VAL:HG22	1.96	0.48
8:H:48:VAL:HG23	8:H:74:PHE:CB	2.44	0.48
9:I:63:ARG:O	9:I:67:LEU:HG	2.14	0.48
10:J:47:GLU:HG2	10:J:133:ILE:HD12	1.94	0.48
14:N:65:VAL:HG21	14:N:105:ALA:HB2	1.94	0.48
15:O:73:ALA:N	37:O:8566:HOH:O	2.46	0.48
15:O:163:PHE:HE1	15:O:171:HIS:HD1	1.62	0.48
1:A:152:A:O2'	1:A:153:C:H5'	2.14	0.48
1:A:278:A:H2'	1:A:279:C:O4'	2.14	0.48
1:A:816:G:H5'	1:A:1598:A:H4'	1.95	0.48
1:A:1855:G:H8	3:C:144:GLU:OE2	1.97	0.48
1:A:2428:G:N7	30:4:60:LYS:NZ	2.61	0.48
1:A:2720:C:O2	12:L:87:ARG:NH2	2.47	0.48
1:A:2782:G:O6	1:A:2790:C:H5'	2.13	0.48
4:D:74:ILE:HG13	37:D:8604:HOH:O	2.13	0.48
11:K:130:VAL:CG1	11:K:131:THR:N	2.76	0.48
15:O:62:HIS:HB3	15:O:65:ASP:OD1	2.13	0.48
19:S:82:GLU:HG3	19:S:83:LYS:N	2.28	0.48
24:X:139:GLY:O	24:X:141:HIS:CD2	2.66	0.48
26:Z:187:VAL:HG12	26:Z:205:ILE:HA	1.95	0.48
1:A:926:A:O2'	13:M:41:HIS:HD2	1.96	0.48
1:A:1218:U:H2'	1:A:1219:U:C6	2.48	0.48
2:B:3024:U:H4'	2:B:3025:G:OP1	2.13	0.48
4:D:41:PHE:CZ	4:D:79:MET:HG3	2.48	0.48
8:H:91:VAL:CG1	8:H:92:GLY:N	2.75	0.48
8:H:101:ALA:HA	37:H:5413:HOH:O	2.14	0.48
17:Q:91:LYS:O	17:Q:95:GLU:HG3	2.13	0.48
26:Z:187:VAL:O	26:Z:187:VAL:HG13	2.14	0.48
1:A:289:G:O2'	1:A:290:C:H5'	2.14	0.47
1:A:671:A:O2'	1:A:672:G:H2'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:G:O2'	1:A:942:U:H5'	2.13	0.47
1:A:1167:G:O2'	1:A:1168:C:H5'	2.14	0.47
1:A:1289:C:O2'	1:A:1290:G:H5'	2.14	0.47
3:C:105:VAL:HG13	3:C:155:THR:O	2.13	0.47
4:D:175:LEU:HD23	4:D:175:LEU:O	2.13	0.47
5:E:168:ARG:NH2	5:E:190:ALA:O	2.47	0.47
6:F:81:GLU:O	6:F:85:GLN:HG3	2.14	0.47
10:J:26:LYS:HD3	10:J:89:PRO:HG3	1.96	0.47
10:J:48:LEU:HD13	10:J:146:TRP:HB3	1.96	0.47
13:M:65:ASP:CG	13:M:111:ALA:HB3	2.39	0.47
21:U:80:GLU:OE2	21:U:84:GLY:HA2	2.14	0.47
1:A:1768:C:H2'	1:A:1769:C:O4'	2.14	0.47
1:A:2044:G:OP1	25:Y:23:HIS:HE1	1.96	0.47
1:A:2434:A:O3'	30:4:28:GLY:HA3	2.14	0.47
37:A:4539:HOH:O	5:E:50:GLU:HG2	2.13	0.47
3:C:194:MET:CE	3:C:199:HIS:HB2	2.44	0.47
4:D:24:PRO:HG2	4:D:204:GLY:HA2	1.96	0.47
27:1:11:THR:CG2	27:1:23:ARG:HB2	2.44	0.47
30:4:18:GLN:OE1	30:4:73:GLU:HB3	2.14	0.47
1:A:401:C:H5'	37:A:5774:HOH:O	2.13	0.47
1:A:797:A:H5'	27:1:10:ARG:HG2	1.96	0.47
1:A:1151:G:OP1	9:I:63:ARG:NH1	2.47	0.47
1:A:1200:A:H4'	37:A:7330:HOH:O	2.13	0.47
1:A:1328:A:C8	26:Z:169:ARG:HD3	2.49	0.47
37:A:5498:HOH:O	4:D:298:LYS:HD3	2.13	0.47
4:D:258:GLY:N	4:D:260:HIS:CE1	2.81	0.47
5:E:236:THR:C	37:E:8443:HOH:O	2.56	0.47
13:M:24:ALA:HB2	13:M:30:ARG:HD2	1.95	0.47
16:P:23:GLY:C	37:P:3062:HOH:O	2.57	0.47
20:T:56:ASN:O	29:3:8:LYS:HE2	2.14	0.47
22:V:31:PHE:CG	22:V:37:GLU:HG2	2.49	0.47
24:X:122:ARG:HH11	24:X:122:ARG:CG	2.23	0.47
27:1:59:HIS:HA	37:1:8441:HOH:O	2.14	0.47
1:A:88:G:N7	29:3:28:LYS:HD2	2.28	0.47
1:A:949:U:O2'	18:R:40:HIS:HE1	1.98	0.47
1:A:1517:U:C2	1:A:1670:G:N2	2.82	0.47
1:A:1804:A:H2'	1:A:1805:G:C8	2.48	0.47
1:A:2314:G:H2'	1:A:2315:C:H5'	1.96	0.47
1:A:2904:U:H4'	25:Y:8:ARG:NH1	2.28	0.47
4:D:223:ARG:HG3	4:D:232:TRP:O	2.14	0.47
4:D:243:ASN:HA	4:D:244:PRO:C	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:150:LYS:NZ	37:J:8381:HOH:O	2.46	0.47
14:N:134:ILE:O	14:N:136:PRO:HD3	2.14	0.47
14:N:186:SER:OG	14:N:189:VAL:HG12	2.14	0.47
21:U:71:VAL:HG12	21:U:72:ILE:N	2.29	0.47
29:3:18:ASN:ND2	29:3:40:ARG:H	2.09	0.47
1:A:401:C:C5'	37:A:5774:HOH:O	2.62	0.47
1:A:558:C:H2'	1:A:559:U:H5''	1.95	0.47
1:A:797:A:H4'	27:1:10:ARG:N	2.29	0.47
1:A:1185:U:H5'	37:A:7458:HOH:O	2.15	0.47
1:A:1299:G:H5'	37:A:4049:HOH:O	2.13	0.47
1:A:1535:G:H2'	1:A:1536:C:C6	2.49	0.47
1:A:1717:A:H5''	17:Q:54:LYS:HB2	1.97	0.47
4:D:125:GLU:OE2	4:D:129:ARG:NH1	2.47	0.47
4:D:221:GLN:HE22	12:L:42:ASN:ND2	2.04	0.47
7:G:7:ILE:HG22	7:G:45:ASP:O	2.15	0.47
10:J:97:LYS:HD3	10:J:117:LYS:HE2	1.96	0.47
12:L:27:ARG:HD2	37:L:4747:HOH:O	2.13	0.47
27:1:56:MET:HE2	27:1:63:LYS:CD	2.44	0.47
1:A:694:A:H2'	1:A:695:C:H5'	1.96	0.47
1:A:714:U:H3'	37:A:6928:HOH:O	2.14	0.47
1:A:1269:G:H2'	1:A:1270:U:C6	2.50	0.47
1:A:1525:G:H5'	1:A:1526:A:OP2	2.14	0.47
1:A:1562:C:O2	1:A:1562:C:H2'	2.14	0.47
1:A:1947:G:N2	1:A:1966:U:C2	2.82	0.47
1:A:2591:C:H2'	1:A:2592:G:O4'	2.15	0.47
1:A:2768:A:H5''	37:A:4396:HOH:O	2.15	0.47
2:B:3107:C:H5	37:B:8438:HOH:O	1.96	0.47
4:D:1:PRO:O	4:D:2:GLN:HB2	2.13	0.47
4:D:60:SER:C	4:D:62:ARG:N	2.71	0.47
8:H:99:THR:O	8:H:100:ASP:HB2	2.14	0.47
10:J:5:MET:HG3	37:J:8368:HOH:O	2.14	0.47
14:N:81:ARG:HG3	14:N:85:ARG:HB2	1.96	0.47
15:O:37:ARG:CZ	37:O:8533:HOH:O	2.63	0.47
15:O:182:GLY:N	37:O:8570:HOH:O	2.47	0.47
21:U:37:GLN:OE1	21:U:118:SER:HA	2.15	0.47
28:2:17:THR:N	28:2:27:TYR:O	2.41	0.47
1:A:1299:G:N2	37:A:4655:HOH:O	2.47	0.47
1:A:1422:U:H2'	1:A:1423:C:C6	2.50	0.47
1:A:1730:G:C5'	1:A:1731:C:C6	2.97	0.47
1:A:1789:G:O6	17:Q:73:HIS:HE1	1.98	0.47
1:A:2001:G:O2'	1:A:2002:C:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2866:U:C2	37:V:7349:HOH:O	2.55	0.47
5:E:76:ARG:HG2	5:E:78:ARG:NH1	2.29	0.47
8:H:16:ALA:HA	8:H:111:ILE:HD13	1.97	0.47
8:H:22:VAL:HG21	8:H:104:ALA:HB2	1.96	0.47
10:J:71:TYR:O	10:J:73:GLN:N	2.47	0.47
24:X:122:ARG:CZ	37:X:5817:HOH:O	2.63	0.47
29:3:48:ASP:O	29:3:49:GLU:HB2	2.15	0.47
30:4:3:MET:O	30:4:90:PHE:HA	2.15	0.47
1:A:426:G:H2'	1:A:427:C:O4'	2.15	0.47
1:A:1592:G:O2'	1:A:1593:C:O4'	2.27	0.47
1:A:1819:G:H2'	1:A:1820:G:C5'	2.45	0.47
1:A:1850:U:H2'	1:A:1851:G:H8	1.79	0.47
1:A:2842:G:H2'	1:A:2843:A:H5'	1.96	0.47
4:D:17:LYS:O	4:D:260:HIS:HD2	1.98	0.47
4:D:307:ARG:HH11	4:D:307:ARG:HG3	1.79	0.47
5:E:151:GLN:O	5:E:154:VAL:HB	2.15	0.47
7:G:5:LEU:HD21	7:G:66:GLN:HG3	1.96	0.47
8:H:34:ASN:HA	14:N:4:ALA:HB2	1.97	0.47
10:J:151:MET:HA	10:J:151:MET:HE3	1.97	0.47
14:N:122:GLU:HB2	14:N:126:HIS:O	2.15	0.47
15:O:91:ARG:HG3	15:O:186:LEU:HD23	1.97	0.47
18:R:32:GLU:HA	18:R:71:TYR:OH	2.15	0.47
20:T:32:ALA:HA	20:T:36:GLU:OE1	2.14	0.47
22:V:13:ILE:HG12	22:V:32:CYS:CB	2.42	0.47
27:1:33:HIS:HE1	27:1:49:ARG:NE	2.13	0.47
1:A:870:G:C3'	1:A:871:G:H5''	2.45	0.47
1:A:1028:U:H1'	37:A:3625:HOH:O	2.15	0.47
1:A:1139:U:H2'	1:A:1140:C:C6	2.49	0.47
1:A:2769:C:O2'	1:A:2770:G:H5'	2.14	0.47
2:B:3042:C:O2	6:F:76:ARG:NH1	2.48	0.47
2:B:3054:A:O2'	2:B:3055:U:H5'	2.15	0.47
10:J:47:GLU:CB	10:J:133:ILE:CD1	2.91	0.47
27:1:26:VAL:O	27:1:30:GLU:HG3	2.14	0.47
1:A:1014:A:H2'	1:A:1015:C:H5'	1.97	0.47
1:A:1120:U:H5'	1:A:1121:G:OP2	2.15	0.47
1:A:2634:G:O2'	1:A:2635:A:H5'	2.15	0.47
2:B:3020:G:H3'	37:B:8436:HOH:O	2.14	0.47
4:D:7:ARG:NH1	4:D:11:LEU:CD2	2.78	0.47
4:D:27:ASN:HD22	4:D:27:ASN:H	1.63	0.47
4:D:41:PHE:CD2	4:D:190:MET:HE3	2.50	0.47
4:D:162:MET:HE2	4:D:310:ARG:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:2:VAL:HG11	14:N:23:LEU:HD23	1.96	0.47
14:N:114:VAL:HB	14:N:159:THR:HG23	1.96	0.47
15:O:43:VAL:HG11	15:O:81:ALA:HA	1.97	0.47
1:A:283:U:H5''	1:A:284:C:OP2	2.16	0.46
1:A:553:G:O4'	1:A:1325:G:H5'	2.15	0.46
1:A:2464:C:H5''	1:A:2465:A:OP1	2.15	0.46
37:A:9209:HOH:O	3:C:11:ARG:HD3	2.14	0.46
2:B:3025:G:H2'	37:B:8462:HOH:O	2.15	0.46
13:M:73:VAL:HG11	13:M:118:LEU:HD21	1.95	0.46
19:S:129:ALA:O	19:S:130:MET:HB2	2.15	0.46
21:U:75:GLU:O	21:U:76:ASP:HB2	2.14	0.46
24:X:126:ASP:HB3	24:X:135:GLY:O	2.15	0.46
25:Y:51:ASP:OD2	25:Y:52:PRO:HD2	2.15	0.46
26:Z:189:ASN:HD22	26:Z:192:ASP:H	1.63	0.46
1:A:559:U:H5'	1:A:559:U:C6	2.38	0.46
1:A:1176:C:H1'	37:A:3908:HOH:O	2.15	0.46
1:A:1700:C:OP2	37:A:6015:HOH:O	2.21	0.46
1:A:2825:C:H4'	1:A:2826:G:O5'	2.15	0.46
1:A:2832:C:H5	37:A:7203:HOH:O	1.99	0.46
4:D:62:ARG:CB	4:D:65:MET:HE3	2.45	0.46
5:E:76:ARG:HD2	37:E:8429:HOH:O	2.14	0.46
5:E:150:THR:HA	5:E:203:ALA:O	2.16	0.46
6:F:93:LEU:HG	37:F:3862:HOH:O	2.14	0.46
15:O:47:LEU:CD1	15:O:97:VAL:HG11	2.44	0.46
15:O:58:LEU:HD12	15:O:58:LEU:N	2.31	0.46
19:S:18:LEU:HB2	19:S:143:VAL:CG1	2.45	0.46
20:T:8:PRO:HD2	23:W:32:ALA:HA	1.98	0.46
25:Y:43:VAL:CG1	25:Y:44:ASP:N	2.77	0.46
25:Y:76:ARG:O	25:Y:77:PHE:HB3	2.15	0.46
1:A:316:A:H5'	21:U:54:ASP:OD2	2.14	0.46
1:A:954:U:O2'	1:A:955:A:H5'	2.15	0.46
1:A:1593:C:OP1	17:Q:117:SER:HB3	2.15	0.46
1:A:1925:G:O2'	1:A:1926:G:H5'	2.16	0.46
37:A:7552:HOH:O	30:4:60:LYS:HG3	2.15	0.46
4:D:148:PRO:HD2	37:D:8580:HOH:O	2.16	0.46
5:E:120:ASP:C	5:E:120:ASP:OD1	2.58	0.46
6:F:23:VAL:HG21	6:F:45:THR:CG2	2.45	0.46
8:H:107:VAL:HG23	37:H:6617:HOH:O	2.15	0.46
12:L:55:VAL:HG12	12:L:56:SER:H	1.79	0.46
20:T:57:THR:C	20:T:59:ASP:H	2.24	0.46
25:Y:30:MET:HE3	25:Y:55:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:4382:HOH:O	3:C:11:ARG:CZ	2.64	0.46
2:B:3031:C:O2'	2:B:3032:G:H5'	2.15	0.46
3:C:36:ASP:O	3:C:37:VAL:C	2.59	0.46
3:C:164:ARG:NE	37:C:8590:HOH:O	2.48	0.46
4:D:41:PHE:HB3	4:D:190:MET:CE	2.45	0.46
4:D:82:VAL:HG12	4:D:101:TRP:CE3	2.51	0.46
5:E:246:ARG:NH1	37:E:8369:HOH:O	2.47	0.46
6:F:101:THR:HG22	6:F:101:THR:O	2.15	0.46
10:J:45:GLN:HG3	10:J:135:TRP:NE1	2.30	0.46
12:L:118:ALA:C	12:L:120:ARG:H	2.24	0.46
21:U:38:ARG:HG3	21:U:38:ARG:NH1	2.29	0.46
22:V:33:SER:O	22:V:37:GLU:HG3	2.14	0.46
24:X:5:VAL:O	24:X:52:VAL:HG22	2.15	0.46
29:3:36:ASN:HB3	29:3:39:ARG:NE	2.31	0.46
1:A:1613:C:H2'	1:A:1614:G:O4'	2.15	0.46
1:A:1943:C:O4'	3:C:212:PRO:HA	2.15	0.46
1:A:2276:U:H2'	1:A:2277:U:C6	2.50	0.46
1:A:2329:C:O2'	1:A:2330:U:H5'	2.16	0.46
1:A:2467:A:H2'	37:A:5434:HOH:O	2.16	0.46
1:A:2670:G:O2'	1:A:2671:U:H5'	2.15	0.46
1:A:2896:A:OP1	25:Y:15:ARG:NH1	2.49	0.46
2:B:3091:C:H2'	2:B:3092:G:O4'	2.15	0.46
5:E:118:THR:CG2	5:E:137:PRO:HB3	2.46	0.46
8:H:39:SER:CB	8:H:45:ALA:HB2	2.46	0.46
1:A:1667:A:H2'	1:A:1668:U:H6	1.79	0.46
1:A:2010:A:H2'	37:A:5939:HOH:O	2.16	0.46
1:A:2102:G:C2	1:A:2104:C:C4	3.04	0.46
2:B:3031:C:H2'	2:B:3032:G:O4'	2.16	0.46
3:C:132:ASP:OD1	3:C:133:ARG:N	2.48	0.46
6:F:41:LEU:CA	6:F:44:ILE:HG22	2.44	0.46
7:G:69:ILE:HA	7:G:72:MET:HE3	1.97	0.46
10:J:150:LYS:HG2	37:J:8385:HOH:O	2.15	0.46
19:S:18:LEU:HG	19:S:91:LEU:HD13	1.97	0.46
22:V:6:CYS:C	22:V:8:TYR:H	2.22	0.46
3:C:48:ASP:HB3	37:C:8608:HOH:O	2.16	0.46
6:F:166:ILE:O	6:F:169:THR:N	2.49	0.46
8:H:117:GLU:C	8:H:119:ARG:N	2.74	0.46
14:N:49:ALA:C	14:N:54:TYR:HB3	2.40	0.46
14:N:61:ILE:HD12	14:N:61:ILE:N	2.30	0.46
22:V:50:GLU:CD	37:V:7349:HOH:O	2.58	0.46
26:Z:115:ARG:NE	37:Z:8553:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:23:ARG:NH1	37:1:8404:HOH:O	2.48	0.46
29:3:19:SER:HB3	37:3:4479:HOH:O	2.16	0.46
1:A:1205:U:C2'	1:A:1206:U:H5''	2.46	0.46
1:A:2718:C:H5'	1:A:2718:C:C6	2.49	0.46
1:A:2795:C:O2'	1:A:2796:U:H5'	2.15	0.46
1:A:2831:C:H2'	1:A:2832:C:H5'	1.98	0.46
5:E:25:PRO:HG2	37:E:8324:HOH:O	2.15	0.46
6:F:23:VAL:CG2	6:F:73:VAL:HB	2.44	0.46
7:G:31:ARG:HH12	7:G:68:HIS:CE1	2.34	0.46
12:L:66:ARG:HG2	12:L:66:ARG:HH11	1.81	0.46
16:P:21:SER:OG	16:P:106:PRO:HB2	2.16	0.46
23:W:20:LEU:HD22	23:W:60:GLN:HE22	1.80	0.46
25:Y:70:ILE:O	25:Y:70:ILE:HG23	2.15	0.46
27:1:32:LYS:HE2	27:1:32:LYS:HB3	1.79	0.46
1:A:154:C:H2'	1:A:155:C:H6	1.81	0.46
1:A:440:C:H2'	1:A:441:A:C8	2.51	0.46
1:A:474:C:O3'	5:E:73:LEU:CD2	2.64	0.46
1:A:1151:G:OP1	9:I:16:LYS:NZ	2.46	0.46
1:A:1192:A:H3'	1:A:1193:A:H5'	1.96	0.46
1:A:1666:C:C2'	1:A:1667:A:H5'	2.43	0.46
4:D:279:THR:CG2	4:D:280:VAL:N	2.78	0.46
5:E:153:VAL:O	5:E:157:LEU:HG	2.16	0.46
6:F:153:THR:HG22	37:F:5234:HOH:O	2.16	0.46
7:G:84:MET:HE2	7:G:133:VAL:HG23	1.95	0.46
19:S:132:ARG:NH1	37:S:8584:HOH:O	2.47	0.46
1:A:793:A:H5''	17:Q:83:LYS:HG2	1.98	0.46
1:A:1418:U:OP1	29:3:42:TRP:HB3	2.16	0.46
1:A:2505:G:H8	37:A:5618:HOH:O	1.99	0.46
10:J:130:HIS:CG	10:J:133:ILE:HD11	2.50	0.46
11:K:107:ASN:ND2	11:K:107:ASN:C	2.69	0.46
12:L:78:LYS:HA	12:L:79:PRO:HD3	1.84	0.46
14:N:47:ASP:CG	14:N:48:ARG:N	2.74	0.46
1:A:249:G:O2'	1:A:250:C:H5'	2.16	0.45
1:A:584:U:H3'	37:A:6076:HOH:O	2.14	0.45
1:A:1044:C:H5''	37:A:9021:HOH:O	2.16	0.45
1:A:1730:G:H5'	1:A:1731:C:H5	1.79	0.45
37:A:4946:HOH:O	10:J:57:ARG:HG3	2.17	0.45
37:A:9312:HOH:O	27:1:16:PRO:HG3	2.15	0.45
2:B:3040:C:N4	6:F:51:ARG:HB2	2.30	0.45
3:C:130:THR:HG22	3:C:131:HIS:O	2.15	0.45
3:C:192:VAL:CG1	3:C:207:GLN:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:26:LYS:HD2	10:J:28:ILE:CG1	2.45	0.45
10:J:113:ALA:N	10:J:114:PRO:HD3	2.30	0.45
14:N:25:TRP:HE3	14:N:26:HIS:HD2	1.64	0.45
14:N:113:ARG:HH21	14:N:156:ARG:HG2	1.81	0.45
20:T:38:ALA:O	20:T:42:GLU:HG3	2.16	0.45
22:V:39:ASN:ND2	22:V:44:ARG:HH11	2.15	0.45
24:X:1:MET:HE3	24:X:101:LEU:HA	1.98	0.45
1:A:244:C:O5'	1:A:244:C:H6	1.99	0.45
1:A:432:G:O2'	1:A:433:C:H5'	2.16	0.45
1:A:1314:U:H2'	37:A:5855:HOH:O	2.15	0.45
1:A:1398:G:H2'	1:A:1399:A:C8	2.51	0.45
1:A:1593:C:OP1	17:Q:117:SER:CB	2.65	0.45
1:A:1711:A:O2'	1:A:1712:A:H5'	2.16	0.45
1:A:1878:G:C1'	37:A:6102:HOH:O	2.63	0.45
1:A:2083:A:N6	11:K:90:LYS:HE2	2.31	0.45
1:A:2653:A:H2'	1:A:2654:C:C6	2.51	0.45
1:A:2672:C:O2'	1:A:2673:U:H5'	2.16	0.45
6:F:94:ALA:HB3	6:F:174:VAL:CA	2.46	0.45
7:G:32:ARG:O	7:G:33:LEU:HD23	2.15	0.45
10:J:57:ARG:C	10:J:59:ASN:N	2.73	0.45
11:K:131:THR:CG2	11:K:133:GLY:H	2.29	0.45
14:N:122:GLU:OE2	14:N:127:LYS:HE2	2.16	0.45
15:O:82:TYR:C	15:O:82:TYR:CD2	2.94	0.45
21:U:96:VAL:HG13	21:U:97:ARG:N	2.31	0.45
22:V:47:ARG:CG	37:V:4381:HOH:O	2.64	0.45
26:Z:216:ARG:CD	37:Z:8566:HOH:O	2.56	0.45
1:A:226:A:H1'	1:A:393:G:C5	2.51	0.45
1:A:1641:A:C2'	1:A:1642:A:H5'	2.46	0.45
1:A:2256:G:C2'	1:A:2257:G:H5'	2.46	0.45
37:A:7707:HOH:O	5:E:94:THR:HG21	2.16	0.45
4:D:145:HIS:CD2	4:D:146:THR:O	2.65	0.45
4:D:175:LEU:C	4:D:175:LEU:CD2	2.89	0.45
6:F:86:THR:HG23	37:F:7477:HOH:O	2.17	0.45
8:H:57:GLU:O	8:H:61:MET:HG3	2.16	0.45
13:M:146:GLY:C	13:M:148:GLU:H	2.25	0.45
15:O:143:ARG:HH12	15:O:173:ASP:CG	2.22	0.45
18:R:40:HIS:CE1	18:R:94:GLN:HA	2.52	0.45
19:S:106:GLY:HA2	19:S:109:MET:CE	2.44	0.45
1:A:305:A:C5	1:A:329:A:C2	3.04	0.45
1:A:1168:C:H5	37:A:7490:HOH:O	1.98	0.45
1:A:1594:C:O2'	1:A:1607:A:H4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2769:C:H2'	1:A:2770:G:H5'	1.99	0.45
3:C:170:VAL:HG13	27:1:22:ILE:HG21	1.98	0.45
12:L:132:VAL:C	37:L:3160:HOH:O	2.58	0.45
13:M:6:ARG:NH2	37:M:8550:HOH:O	2.50	0.45
23:W:39:ALA:C	23:W:41:GLU:N	2.74	0.45
24:X:1:MET:HB2	24:X:103:GLU:HG2	1.97	0.45
1:A:943:A:C5	24:X:23:MET:HE2	2.52	0.45
1:A:2251:G:H4'	37:A:7399:HOH:O	2.17	0.45
1:A:2894:C:O2'	1:A:2895:C:H5'	2.15	0.45
5:E:233:THR:CG2	5:E:234:VAL:N	2.80	0.45
10:J:13:ALA:HA	10:J:91:HIS:CE1	2.52	0.45
13:M:112:GLY:O	13:M:132:LYS:NZ	2.44	0.45
15:O:5:ARG:HG3	18:R:18:PRO:CB	2.46	0.45
15:O:67:ALA:HA	15:O:71:TRP:H	1.81	0.45
15:O:87:LEU:CD1	15:O:186:LEU:HD21	2.40	0.45
17:Q:105:LEU:HD21	17:Q:137:LEU:HD21	1.98	0.45
26:Z:154:ARG:NH1	26:Z:155:ARG:HG3	2.31	0.45
1:A:764:C:C2'	1:A:765:G:H5'	2.46	0.45
1:A:962:C:C1'	15:O:5:ARG:NH1	2.72	0.45
1:A:1015:C:H2'	1:A:1016:U:C6	2.52	0.45
1:A:1850:U:H2'	1:A:1851:G:C8	2.50	0.45
1:A:2324:G:H4'	1:A:2418:G:O2'	2.16	0.45
4:D:144:THR:CG2	4:D:145:HIS:N	2.79	0.45
4:D:307:ARG:CG	4:D:307:ARG:NH1	2.78	0.45
5:E:93:LYS:O	5:E:98:ARG:NH2	2.50	0.45
6:F:173:GLU:O	6:F:174:VAL:C	2.60	0.45
8:H:28:ALA:HB3	8:H:99:THR:HG23	1.99	0.45
10:J:165:GLY:C	10:J:166:ASN:HD22	2.25	0.45
16:P:26:TRP:HA	16:P:26:TRP:CE3	2.52	0.45
25:Y:72:VAL:HG22	25:Y:85:VAL:CG1	2.46	0.45
28:2:2:GLY:O	28:2:6:PRO:HG2	2.17	0.45
30:4:40:ARG:HD2	37:4:8549:HOH:O	2.17	0.45
1:A:21:G:H4'	19:S:2:ILE:HG22	1.99	0.45
1:A:130:C:H5'	37:A:5189:HOH:O	2.16	0.45
1:A:333:G:O2'	1:A:334:G:H5'	2.17	0.45
1:A:603:A:H4'	1:A:604:G:O5'	2.16	0.45
1:A:1857:A:N6	1:A:2247:C:H1'	2.32	0.45
1:A:2011:A:P	37:A:5939:HOH:O	2.74	0.45
2:B:3088:G:OP1	24:X:130:HIS:NE2	2.47	0.45
4:D:195:ARG:NH1	4:D:324:ASP:OD1	2.48	0.45
6:F:55:LYS:O	6:F:56:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:36:PRO:HD3	11:K:127:ILE:HD12	1.99	0.45
11:K:80:LYS:HE2	11:K:98:PHE:CZ	2.52	0.45
11:K:131:THR:HB	11:K:134:GLU:HG3	1.97	0.45
14:N:35:PRO:HD2	14:N:38:VAL:CG2	2.46	0.45
15:O:154:LEU:O	15:O:155:GLU:CB	2.65	0.45
15:O:171:HIS:CE1	37:O:8566:HOH:O	2.69	0.45
17:Q:120:ARG:NH2	17:Q:123:TYR:CD2	2.85	0.45
22:V:44:ARG:HB3	37:V:3805:HOH:O	2.16	0.45
1:A:1375:A:C2'	1:A:1376:G:H5'	2.47	0.45
1:A:1500:U:OP2	17:Q:41:ARG:NH2	2.50	0.45
1:A:2361:A:H2'	1:A:2362:A:C8	2.51	0.45
1:A:2575:C:H2'	1:A:2576:A:O4'	2.17	0.45
1:A:2578:G:H5'	1:A:2578:G:C8	2.48	0.45
3:C:128:LEU:HG	37:C:8575:HOH:O	2.15	0.45
3:C:173:GLY:O	3:C:176:HIS:HB3	2.16	0.45
6:F:25:MET:HE1	6:F:37:ALA:O	2.17	0.45
6:F:59:GLY:C	6:F:61:PHE:N	2.74	0.45
13:M:61:ALA:HA	37:M:8565:HOH:O	2.17	0.45
14:N:42:ARG:HA	14:N:43:PRO:HD3	1.83	0.45
20:T:57:THR:HG22	20:T:58:MET:N	2.31	0.45
21:U:18:GLU:O	21:U:21:LYS:HG2	2.17	0.45
1:A:40:C:H6	1:A:40:C:O5'	2.00	0.45
1:A:213:G:HO2'	1:A:214:U:P	2.39	0.45
1:A:1887:U:OP1	27:1:21:LYS:HE3	2.16	0.45
2:B:3024:U:HO2'	2:B:3025:G:H4'	1.78	0.45
4:D:315:VAL:HG23	4:D:316:ARG:HG2	1.99	0.45
6:F:169:THR:O	6:F:170:TYR:HB2	2.17	0.45
7:G:11:VAL:HG12	7:G:12:ASP:H	1.81	0.45
8:H:22:VAL:CG2	8:H:104:ALA:HB2	2.46	0.45
9:I:12:ILE:O	9:I:13:PRO:C	2.58	0.45
9:I:71:LEU:C	9:I:73:ASP:N	2.75	0.45
13:M:17:SER:C	13:M:19:LYS:H	2.24	0.45
13:M:72:ASN:O	13:M:76:LEU:HG	2.17	0.45
13:M:143:THR:HG21	37:M:8540:HOH:O	2.16	0.45
14:N:46:LEU:HG	37:N:8621:HOH:O	2.17	0.45
17:Q:143:ALA:HA	37:Q:193:HOH:O	2.15	0.45
21:U:55:PHE:HB2	37:U:6384:HOH:O	2.16	0.45
30:4:65:THR:HB	30:4:83:TRP:H	1.81	0.45
1:A:23:G:C6	1:A:24:G:N1	2.85	0.45
1:A:95:A:H5''	1:A:97:G:O4'	2.17	0.45
1:A:154:C:P	14:N:188:ARG:HH12	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:G:O2'	1:A:214:U:OP2	2.31	0.45
1:A:816:G:C6	1:A:817:G:N1	2.85	0.45
1:A:818:A:O2'	27:1:13:ARG:HD3	2.16	0.45
1:A:2353:A:H4'	1:A:2354:A:O5'	2.16	0.45
3:C:140:LEU:HB3	3:C:141:PRO:HD2	1.99	0.45
4:D:43:GLY:O	4:D:308:LEU:HD12	2.16	0.45
5:E:129:HIS:HE1	5:E:231:ARG:HA	1.82	0.45
5:E:140:VAL:HG12	5:E:141:SER:N	2.32	0.45
7:G:126:ILE:HB	7:G:131:LEU:CD2	2.46	0.45
7:G:154:ILE:HG13	7:G:156:ASP:OD1	2.16	0.45
12:L:55:VAL:CG1	12:L:56:SER:N	2.80	0.45
13:M:125:PHE:CZ	13:M:140:VAL:HG13	2.52	0.45
14:N:138:HIS:C	14:N:139:PRO:O	2.54	0.45
16:P:32:ARG:NE	37:P:3360:HOH:O	2.49	0.45
16:P:96:VAL:HG12	16:P:97:SER:O	2.17	0.45
17:Q:103:THR:O	17:Q:107:GLU:HG3	2.16	0.45
19:S:119:VAL:O	19:S:119:VAL:CG1	2.64	0.45
21:U:49:GLU:HB3	21:U:59:GLU:CG	2.47	0.45
1:A:2755:G:H1'	37:A:4654:HOH:O	2.16	0.44
1:A:2812:A:C2	1:A:2814:A:N6	2.74	0.44
37:A:6985:HOH:O	18:R:9:GLY:HA2	2.16	0.44
37:C:8615:HOH:O	27:1:75:ALA:HB3	2.17	0.44
10:J:59:ASN:N	10:J:59:ASN:ND2	2.63	0.44
10:J:154:THR:HB	10:J:155:PRO:HD3	2.00	0.44
14:N:85:ARG:HA	14:N:87:MET:HE2	1.99	0.44
14:N:94:LYS:CE	37:N:8583:HOH:O	2.54	0.44
23:W:57:LYS:HA	23:W:60:GLN:HE21	1.82	0.44
24:X:48:VAL:CG1	24:X:48:VAL:O	2.64	0.44
29:3:49:GLU:CD	37:3:719:HOH:O	2.60	0.44
1:A:303:C:H2'	1:A:304:G:O4'	2.18	0.44
1:A:2271:G:H2'	1:A:2271:G:N3	2.32	0.44
1:A:2403:C:H3'	37:A:5187:HOH:O	2.17	0.44
1:A:2421:G:H3'	1:A:2422:U:C5'	2.47	0.44
3:C:29:HIS:CE1	3:C:107:ASN:ND2	2.85	0.44
3:C:179:MET:HA	3:C:179:MET:HE3	1.98	0.44
5:E:123:LEU:HD23	5:E:123:LEU:HA	1.86	0.44
10:J:26:LYS:HD3	10:J:89:PRO:CG	2.48	0.44
12:L:22:ASP:C	12:L:22:ASP:OD1	2.60	0.44
1:A:40:C:H4'	37:A:6987:HOH:O	2.17	0.44
1:A:1010:C:H4'	15:O:4:PRO:HB2	2.00	0.44
1:A:1052:G:N3	1:A:1052:G:H2'	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1730:G:C5'	1:A:1731:C:H6	2.29	0.44
1:A:2362:A:H2'	1:A:2363:G:C8	2.53	0.44
1:A:2415:A:H2'	1:A:2416:G:H5'	1.98	0.44
1:A:2781:U:H2'	1:A:2782:G:H5'	1.99	0.44
2:B:3078:G:O2'	2:B:3079:U:P	2.75	0.44
3:C:94:LEU:HG	3:C:99:ILE:CD1	2.46	0.44
4:D:162:MET:CE	4:D:308:LEU:HD21	2.33	0.44
4:D:280:VAL:CG1	4:D:334:SER:HA	2.47	0.44
12:L:99:ASP:OD1	12:L:101:ASN:N	2.50	0.44
13:M:90:ARG:NH1	13:M:119:THR:HG21	2.32	0.44
13:M:148:GLU:HB2	37:M:8589:HOH:O	2.16	0.44
14:N:35:PRO:HD2	14:N:38:VAL:HG21	1.99	0.44
1:A:1304:U:H2'	1:A:1305:C:C6	2.52	0.44
3:C:33:GLU:H	3:C:33:GLU:CD	2.25	0.44
6:F:64:ARG:O	6:F:67:ASP:OD2	2.35	0.44
6:F:92:GLU:O	6:F:93:LEU:O	2.35	0.44
7:G:11:VAL:HG11	7:G:22:VAL:HG13	1.99	0.44
10:J:62:GLU:O	10:J:66:VAL:HG23	2.18	0.44
24:X:90:TYR:CE2	24:X:99:ALA:HB2	2.53	0.44
1:A:656:G:H5'	16:P:3:THR:HG22	1.99	0.44
1:A:858:U:H2'	1:A:859:C:C6	2.52	0.44
1:A:1477:C:O2'	1:A:1478:U:H5'	2.17	0.44
1:A:2265:U:H2'	1:A:2266:A:H8	1.82	0.44
1:A:2420:G:H4'	37:A:4072:HOH:O	2.17	0.44
3:C:109:GLU:CD	3:C:113:GLY:H	2.25	0.44
4:D:87:TYR:OH	4:D:163:GLU:OE2	2.35	0.44
5:E:13:ASP:N	37:E:8436:HOH:O	2.51	0.44
19:S:35:ILE:O	19:S:38:LYS:HB2	2.17	0.44
21:U:24:ARG:HH21	21:U:39:ASN:ND2	2.15	0.44
21:U:27:LEU:HD23	21:U:98:VAL:HB	2.00	0.44
24:X:4:LEU:HD23	24:X:54:PHE:HB3	1.99	0.44
26:Z:126:PRO:HG2	26:Z:128:PHE:CZ	2.52	0.44
28:2:25:LYS:HD2	29:3:49:GLU:H	1.82	0.44
1:A:559:U:H2'	1:A:560:C:O4'	2.18	0.44
1:A:764:C:H2'	1:A:765:G:O4'	2.17	0.44
1:A:1634:G:H2'	1:A:1635:U:C6	2.52	0.44
1:A:2769:C:H2'	1:A:2770:G:C5'	2.47	0.44
2:B:3004:G:OP1	2:B:3059:C:O2'	2.34	0.44
6:F:81:GLU:C	6:F:83:PHE:N	2.74	0.44
10:J:113:ALA:N	10:J:114:PRO:CD	2.81	0.44
10:J:157:ILE:CG2	10:J:158:ASN:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:39:VAL:HG13	11:K:106:GLY:O	2.18	0.44
13:M:114:VAL:CG1	37:M:8575:HOH:O	2.59	0.44
14:N:114:VAL:HG21	14:N:159:THR:CG2	2.47	0.44
15:O:52:PRO:HD2	37:O:8529:HOH:O	2.18	0.44
16:P:47:ARG:HG3	16:P:47:ARG:NH1	2.23	0.44
17:Q:105:LEU:CD2	17:Q:137:LEU:HD21	2.48	0.44
1:A:771:G:OP2	14:N:79:LYS:HE3	2.18	0.44
1:A:876:A:N3	1:A:876:A:H2'	2.33	0.44
1:A:1098:A:H2'	1:A:1099:G:O4'	2.18	0.44
1:A:2088:C:H1'	1:A:2841:A:N1	2.32	0.44
1:A:2613:G:O2'	1:A:2614:C:H5'	2.18	0.44
2:B:3064:C:C2'	2:B:3065:A:H5'	2.48	0.44
11:K:75:PRO:HD3	11:K:136:SER:OG	2.17	0.44
12:L:4:LEU:HD22	12:L:116:GLU:HB3	2.00	0.44
18:R:25:PRO:HB2	37:R:4350:HOH:O	2.16	0.44
24:X:88:THR:HG23	24:X:110:GLN:HB3	1.99	0.44
1:A:1118:A:C8	1:A:1119:G:H5''	2.52	0.44
1:A:1684:A:O2'	1:A:1685:A:H5''	2.18	0.44
3:C:36:ASP:HB2	3:C:84:VAL:N	2.33	0.44
6:F:35:ALA:C	6:F:37:ALA:N	2.75	0.44
10:J:56:ILE:HG21	10:J:61:LEU:HD13	2.00	0.44
10:J:163:PRO:O	10:J:164:ALA:HB2	2.18	0.44
14:N:165:SER:HB3	37:N:8533:HOH:O	2.18	0.44
19:S:39:THR:O	19:S:40:ALA:C	2.60	0.44
23:W:42:ASN:O	23:W:44:GLY:N	2.50	0.44
24:X:3:ALA:O	24:X:54:PHE:HA	2.18	0.44
26:Z:106:THR:CG2	26:Z:107:PRO:HD2	2.48	0.44
1:A:338:C:H4'	5:E:174:ILE:HD11	1.99	0.44
1:A:1654:U:H2'	3:C:47:HIS:CD2	2.53	0.44
1:A:2089:A:O2'	1:A:2090:G:H5'	2.18	0.44
1:A:2316:G:H4'	37:A:6073:HOH:O	2.17	0.44
1:A:2656:G:O2'	1:A:2657:G:H5'	2.18	0.44
5:E:61:PHE:HB3	37:E:8439:HOH:O	2.17	0.44
6:F:63:ILE:C	37:F:5728:HOH:O	2.60	0.44
6:F:94:ALA:O	6:F:95:THR:O	2.35	0.44
10:J:55:GLN:HE21	10:J:124:ARG:NE	2.03	0.44
13:M:89:PHE:N	37:M:8573:HOH:O	2.51	0.44
15:O:32:PRO:HD2	15:O:99:GLU:O	2.18	0.44
15:O:139:TRP:HA	15:O:139:TRP:HE3	1.83	0.44
17:Q:14:LEU:HD13	17:Q:51:ALA:HB2	1.99	0.44
25:Y:15:ARG:HB3	25:Y:15:ARG:NH1	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:25:LYS:HD2	29:3:49:GLU:N	2.33	0.44
28:2:28:HIS:HD2	28:2:30:LYS:H	1.64	0.44
29:3:19:SER:O	29:3:36:ASN:ND2	2.51	0.44
1:A:42:C:H1'	37:A:4648:HOH:O	2.18	0.43
1:A:177:A:H2'	1:A:178:U:O4'	2.17	0.43
1:A:955:A:C2	1:A:1013:A:C4	3.06	0.43
1:A:960:G:N3	1:A:960:G:C2'	2.80	0.43
1:A:1847:A:OP1	3:C:175:LYS:HG3	2.18	0.43
1:A:2890:A:C1'	22:V:56:ARG:NH2	2.78	0.43
4:D:2:GLN:CD	37:D:8620:HOH:O	2.60	0.43
4:D:312:ARG:HD3	4:D:315:VAL:HG13	2.00	0.43
5:E:84:VAL:O	5:E:85:LYS:HB2	2.18	0.43
10:J:127:GLY:O	10:J:128:ALA:CB	2.62	0.43
12:L:49:LEU:HD21	12:L:74:VAL:O	2.18	0.43
15:O:73:ALA:HB1	15:O:74:PRO:HD2	1.98	0.43
15:O:184:ILE:HG22	15:O:185:GLU:N	2.31	0.43
17:Q:10:ALA:CA	17:Q:13:VAL:HG12	2.45	0.43
1:A:926:A:O2'	13:M:41:HIS:CD2	2.72	0.43
1:A:1015:C:H2'	1:A:1016:U:H6	1.82	0.43
1:A:1166:A:N3	1:A:1166:A:H2'	2.33	0.43
3:C:69:LEU:C	3:C:69:LEU:HD12	2.43	0.43
3:C:103:VAL:HA	3:C:104:PRO:HD3	1.88	0.43
5:E:166:ILE:CD1	5:E:207:LEU:HD13	2.49	0.43
6:F:167:GLU:OE2	6:F:173:GLU:HG2	2.17	0.43
10:J:55:GLN:HE22	10:J:91:HIS:CD2	2.35	0.43
10:J:86:ARG:NH1	10:J:130:HIS:CD2	2.86	0.43
14:N:137:ASP:HA	14:N:142:LYS:HE3	2.00	0.43
14:N:186:SER:O	14:N:189:VAL:HG12	2.17	0.43
17:Q:98:ILE:O	17:Q:98:ILE:HD13	2.18	0.43
20:T:29:ASP:OD1	20:T:31:ARG:NH1	2.52	0.43
24:X:76:ASP:O	24:X:77:ALA:C	2.61	0.43
26:Z:99:ALA:HB2	26:Z:233:TYR:CE2	2.53	0.43
1:A:795:G:N3	1:A:817:G:C2	2.86	0.43
1:A:958:G:O2'	1:A:959:C:H5'	2.18	0.43
1:A:1592:G:O2'	1:A:1593:C:O5'	2.37	0.43
1:A:1653:A:N6	37:A:4238:HOH:O	2.51	0.43
1:A:2323:G:H5'	37:A:7006:HOH:O	2.17	0.43
1:A:2515:C:H2'	1:A:2516:G:O4'	2.18	0.43
37:A:9072:HOH:O	4:D:214:PRO:HD2	2.17	0.43
2:B:3041:C:C6	6:F:50:VAL:HG21	2.53	0.43
5:E:200:PRO:HB3	5:E:212:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:52:LEU:HD13	14:N:116:ASN:CG	2.43	0.43
16:P:98:LEU:HD12	16:P:98:LEU:HA	1.85	0.43
21:U:43:ASN:C	21:U:45:GLY:H	2.26	0.43
27:1:13:ARG:NH1	37:1:8421:HOH:O	2.51	0.43
1:A:553:G:P	26:Z:204:ARG:NH2	2.90	0.43
1:A:1825:U:O2'	1:A:1826:C:H5'	2.18	0.43
1:A:1829:A:H2'	1:A:1830:C:H5'	2.01	0.43
1:A:1853:C:OP1	3:C:231:LYS:HG3	2.18	0.43
1:A:2912:C:H2'	1:A:2913:A:O4'	2.19	0.43
2:B:3039:U:H3'	2:B:3040:C:H5''	1.99	0.43
4:D:23:THR:HG23	4:D:162:MET:HE3	2.00	0.43
4:D:51:VAL:HG21	4:D:327:VAL:HG13	2.00	0.43
7:G:84:MET:HB2	7:G:131:LEU:HB2	2.00	0.43
10:J:43:PRO:HD2	10:J:137:ASN:HA	2.00	0.43
10:J:114:PRO:O	10:J:115:PHE:C	2.60	0.43
14:N:63:VAL:HG21	14:N:109:PHE:CZ	2.53	0.43
19:S:132:ARG:NH2	37:S:8584:HOH:O	2.51	0.43
4:D:254:GLN:HG2	4:D:255:GLY:N	2.32	0.43
6:F:25:MET:HE3	6:F:37:ALA:HB1	2.00	0.43
6:F:59:GLY:O	6:F:61:PHE:N	2.39	0.43
15:O:23:ARG:NH1	37:O:8547:HOH:O	2.51	0.43
15:O:90:LEU:CB	15:O:186:LEU:HD22	2.48	0.43
1:A:512:G:O3'	1:A:513:A:H8	2.01	0.43
1:A:929:A:H8	1:A:929:A:O5'	2.02	0.43
1:A:958:G:H2'	1:A:959:C:C6	2.53	0.43
1:A:1058:A:H2'	1:A:1060:C:C5'	2.47	0.43
1:A:1200:A:C4'	37:A:7330:HOH:O	2.66	0.43
1:A:1235:G:C1'	11:K:63:ILE:HG23	2.48	0.43
1:A:1545:C:H2'	1:A:1546:G:O4'	2.18	0.43
1:A:1654:U:H2'	3:C:47:HIS:HD2	1.82	0.43
2:B:3059:C:O5'	2:B:3059:C:H6	2.01	0.43
3:C:123:GLY:HA3	3:C:162:GLY:HA2	2.01	0.43
3:C:135:VAL:HG21	3:C:147:ARG:NH1	2.33	0.43
4:D:146:THR:O	4:D:159:PRO:HB3	2.18	0.43
6:F:49:PRO:HA	6:F:73:VAL:HG22	2.01	0.43
8:H:27:GLY:HA3	37:H:5413:HOH:O	2.18	0.43
16:P:26:TRP:HA	16:P:26:TRP:HE3	1.82	0.43
24:X:5:VAL:HG22	24:X:32:CYS:HB2	2.00	0.43
25:Y:15:ARG:HH11	25:Y:15:ARG:CB	2.29	0.43
25:Y:20:GLU:CD	25:Y:21:PRO:HD2	2.43	0.43
26:Z:154:ARG:HH12	26:Z:155:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:A:H1'	1:A:1921:A:C2	2.54	0.43
1:A:656:G:H5'	16:P:3:THR:CG2	2.49	0.43
1:A:710:G:P	16:P:24:ALA:HB3	2.59	0.43
1:A:1029:U:O2'	1:A:1273:C:OP1	2.33	0.43
1:A:1309:U:O2'	1:A:1310:U:H5'	2.19	0.43
1:A:1787:C:H4'	1:A:2883:A:O4'	2.18	0.43
1:A:1878:G:O2'	1:A:1879:U:C6	2.67	0.43
1:A:2064:U:H4'	1:A:2653:A:P	2.58	0.43
1:A:2506:A:H1'	37:A:6036:HOH:O	2.19	0.43
37:A:7130:HOH:O	28:2:1:THR:HB	2.18	0.43
2:B:3056:A:N1	6:F:13:MET:HE3	2.33	0.43
3:C:35:GLY:O	3:C:36:ASP:CB	2.59	0.43
3:C:135:VAL:N	37:C:8597:HOH:O	2.50	0.43
4:D:69:VAL:HA	4:D:70:PRO:HD3	1.87	0.43
4:D:307:ARG:HG3	4:D:307:ARG:NH1	2.33	0.43
5:E:127:ARG:HG2	5:E:127:ARG:HH11	1.83	0.43
7:G:80:TRP:O	7:G:134:SER:HA	2.18	0.43
8:H:21:GLU:HA	8:H:24:ARG:HE	1.83	0.43
10:J:112:ARG:O	10:J:113:ALA:C	2.62	0.43
13:M:62:ALA:HB2	13:M:103:ALA:CB	2.48	0.43
17:Q:94:TRP:CZ2	17:Q:98:ILE:HG13	2.54	0.43
19:S:96:VAL:HG13	19:S:106:GLY:HA3	2.00	0.43
25:Y:9:VAL:HG13	25:Y:88:GLU:OE1	2.19	0.43
27:1:81:LYS:O	27:1:82:ALA:C	2.62	0.43
1:A:2547:C:H2'	1:A:2548:C:H6	1.84	0.43
4:D:320:GLN:HG3	4:D:321:PRO:CD	2.48	0.43
5:E:139:VAL:CG1	37:E:8443:HOH:O	2.58	0.43
5:E:246:ARG:NH2	37:E:8419:HOH:O	2.52	0.43
7:G:37:ASP:OD1	11:K:125:SER:HB3	2.19	0.43
15:O:100:ALA:O	15:O:129:ILE:HG23	2.18	0.43
17:Q:115:SER:C	17:Q:117:SER:N	2.77	0.43
24:X:125:HIS:HD2	24:X:127:GLY:H	1.66	0.43
30:4:74:CYS:N	37:4:8561:HOH:O	2.51	0.43
1:A:349:U:O2'	1:A:350:C:H5'	2.19	0.43
1:A:639:A:H2'	1:A:640:G:C8	2.53	0.43
1:A:716:G:C2'	1:A:717:C:O5'	2.67	0.43
1:A:1815:A:H2'	1:A:1816:C:O4'	2.19	0.43
1:A:2408:A:H2	37:4:8517:HOH:O	2.01	0.43
1:A:2717:C:H5'	4:D:302:PRO:HA	2.00	0.43
1:A:2781:U:C2'	1:A:2782:G:H5'	2.49	0.43
4:D:32:ASP:HA	37:D:8573:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:241:PRO:HD2	37:D:8656:HOH:O	2.18	0.43
4:D:268:ARG:NH2	4:D:325:PRO:HG3	2.34	0.43
5:E:57:PRO:O	5:E:58:ALA:C	2.61	0.43
6:F:48:MET:HA	6:F:49:PRO:HD3	1.83	0.43
11:K:77:GLY:O	11:K:78:ILE:C	2.59	0.43
21:U:41:ARG:O	21:U:43:ASN:ND2	2.52	0.43
24:X:88:THR:CG2	24:X:110:GLN:NE2	2.76	0.43
27:1:13:ARG:NH1	27:1:14:PHE:CE2	2.87	0.43
29:3:18:ASN:HD22	29:3:18:ASN:HA	1.60	0.43
1:A:1205:U:C2'	1:A:1206:U:C5'	2.97	0.43
1:A:1279:U:H5''	37:A:9579:HOH:O	2.19	0.43
2:B:3051:A:H5'	15:O:160:SER:HB3	2.01	0.43
3:C:93:THR:C	3:C:94:LEU:HD23	2.44	0.43
3:C:165:THR:HG22	37:C:8621:HOH:O	2.18	0.43
6:F:76:ARG:O	6:F:77:ASP:HB2	2.19	0.43
6:F:77:ASP:HB3	6:F:78:GLU:H	1.58	0.43
10:J:59:ASN:H	10:J:59:ASN:ND2	2.15	0.43
10:J:150:LYS:HE2	37:J:8381:HOH:O	2.19	0.43
11:K:70:PHE:CD2	11:K:70:PHE:O	2.72	0.43
14:N:87:MET:H	14:N:87:MET:HG3	1.35	0.43
20:T:73:ASP:OD1	20:T:75:GLN:HB2	2.19	0.43
21:U:74:VAL:HB	21:U:77:VAL:HG21	2.01	0.43
24:X:54:PHE:CZ	24:X:140:LYS:HB2	2.54	0.43
24:X:66:LEU:O	24:X:70:ALA:CB	2.67	0.43
25:Y:43:VAL:HG22	25:Y:76:ARG:NH1	2.34	0.43
1:A:716:G:H2'	1:A:717:C:O5'	2.19	0.42
1:A:1706:G:C6	1:A:1707:G:N1	2.86	0.42
1:A:2090:G:H2'	1:A:2091:G:C8	2.53	0.42
1:A:2661:U:H3	1:A:2812:A:H62	1.67	0.42
3:C:57:ALA:HA	3:C:67:LEU:HD23	2.00	0.42
3:C:211:LYS:NZ	37:C:8574:HOH:O	2.52	0.42
5:E:133:ARG:HD2	37:E:8407:HOH:O	2.19	0.42
7:G:84:MET:HE1	7:G:148:ILE:HD13	2.01	0.42
9:I:27:ILE:HD12	9:I:70:ALA:HB1	2.01	0.42
12:L:9:THR:O	12:L:10:GLN:C	2.60	0.42
21:U:113:GLU:O	21:U:114:SER:C	2.62	0.42
24:X:122:ARG:HG2	24:X:152:ALA:O	2.18	0.42
1:A:29:C:O2'	1:A:30:U:H5'	2.19	0.42
1:A:37:A:H2'	1:A:38:G:C8	2.53	0.42
1:A:120:A:H2'	1:A:120:A:N3	2.33	0.42
1:A:245:C:H2'	1:A:246:G:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:G:H1'	37:A:6292:HOH:O	2.20	0.42
1:A:585:C:H6	37:A:6076:HOH:O	2.00	0.42
1:A:622:G:O2'	1:A:623:U:H5'	2.18	0.42
1:A:1164:U:C4'	1:A:1165:G:OP1	2.65	0.42
1:A:1574:C:H6	1:A:1574:C:O5'	2.02	0.42
1:A:1699:C:H4'	37:A:6423:HOH:O	2.19	0.42
1:A:2247:C:H5''	37:A:7334:HOH:O	2.19	0.42
1:A:2679:G:H2'	1:A:2681:A:OP2	2.19	0.42
1:A:2691:A:H8	1:A:2691:A:OP1	2.02	0.42
1:A:2779:G:O2'	1:A:2780:C:H5'	2.20	0.42
7:G:162:PHE:CD1	7:G:162:PHE:N	2.86	0.42
10:J:72:VAL:HG11	10:J:81:TYR:CZ	2.54	0.42
12:L:72:VAL:HG11	12:L:121:PHE:CD1	2.54	0.42
14:N:191:GLY:O	14:N:192:ALA:HB3	2.19	0.42
15:O:38:LYS:HE3	15:O:38:LYS:HB2	1.65	0.42
15:O:141:ARG:HB3	37:O:8569:HOH:O	2.19	0.42
18:R:31:GLU:CD	18:R:93:ARG:HH12	2.27	0.42
25:Y:9:VAL:HG13	25:Y:88:GLU:CD	2.43	0.42
27:1:48:LYS:NZ	37:1:8437:HOH:O	2.52	0.42
1:A:407:A:H2'	1:A:408:A:C8	2.55	0.42
1:A:907:A:H2'	1:A:908:A:H8	1.84	0.42
1:A:1615:A:H5'	37:A:4159:HOH:O	2.19	0.42
1:A:1714:C:O2'	1:A:1715:C:H5'	2.19	0.42
1:A:1772:C:H5'	1:A:1773:G:C5	2.54	0.42
1:A:2356:A:H2'	1:A:2357:G:O4'	2.19	0.42
1:A:2506:A:C1'	37:A:6036:HOH:O	2.67	0.42
1:A:2723:G:H1'	37:A:4814:HOH:O	2.18	0.42
1:A:2780:C:H2'	1:A:2781:U:C6	2.54	0.42
2:B:3026:C:P	37:B:8442:HOH:O	2.77	0.42
2:B:3076:G:C8	2:B:3077:A:H2'	2.54	0.42
3:C:81:GLN:CB	3:C:92:ASN:ND2	2.81	0.42
3:C:99:ILE:O	3:C:131:HIS:CE1	2.72	0.42
3:C:164:ARG:CZ	37:C:8590:HOH:O	2.66	0.42
6:F:19:GLU:O	6:F:133:ASN:HB3	2.19	0.42
6:F:24:HIS:HB2	6:F:72:LYS:CB	2.49	0.42
6:F:84:LEU:HA	6:F:87:ALA:HB3	2.02	0.42
6:F:167:GLU:C	6:F:169:THR:H	2.27	0.42
8:H:110:GLU:O	8:H:114:LYS:HG3	2.18	0.42
15:O:67:ALA:HA	15:O:71:TRP:HB3	2.01	0.42
23:W:38:GLY:C	23:W:40:PRO:HD2	2.44	0.42
24:X:4:LEU:CD2	24:X:52:VAL:HG21	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:41:VAL:HG12	27:1:42:CYS:N	2.33	0.42
28:2:37:CYS:SG	28:2:39:PHE:HB2	2.58	0.42
1:A:92:G:H4'	23:W:44:GLY:HA3	2.01	0.42
1:A:484:A:N1	1:A:506:G:H4'	2.34	0.42
1:A:951:A:O2'	1:A:952:G:H5'	2.20	0.42
1:A:1174:A:C5	1:A:1201:C:H4'	2.54	0.42
1:A:2251:G:H2'	1:A:2252:A:H8	1.85	0.42
1:A:2266:A:H2'	1:A:2267:G:C8	2.55	0.42
1:A:2445:U:H2'	1:A:2446:G:C8	2.54	0.42
1:A:2456:A:H2'	1:A:2457:U:C6	2.54	0.42
1:A:2697:A:H2'	1:A:2698:G:O4'	2.18	0.42
3:C:18:ALA:O	3:C:20:SER:N	2.47	0.42
4:D:55:ASN:HB3	4:D:64:GLY:N	2.34	0.42
4:D:132:HIS:CE1	4:D:171:VAL:HG21	2.54	0.42
5:E:14:GLY:N	37:E:8436:HOH:O	2.50	0.42
5:E:19:PRO:HG2	5:E:22:PHE:CD1	2.54	0.42
6:F:60:GLU:C	6:F:62:ASP:N	2.75	0.42
9:I:64:ASN:N	9:I:64:ASN:ND2	2.66	0.42
15:O:164:ASP:C	15:O:164:ASP:OD1	2.62	0.42
24:X:119:HIS:HD2	24:X:120:PRO:O	2.01	0.42
1:A:282:C:O2'	1:A:283:U:C5'	2.65	0.42
1:A:516:A:OP2	37:A:5625:HOH:O	2.21	0.42
1:A:625:U:H5''	1:A:1044:C:N4	2.34	0.42
1:A:1730:G:H4'	1:A:1731:C:O5'	2.19	0.42
1:A:2667:G:H1'	1:A:2914:A:N3	2.33	0.42
37:A:5693:HOH:O	12:L:87:ARG:CZ	2.67	0.42
37:A:6302:HOH:O	6:F:55:LYS:HB2	2.19	0.42
2:B:3025:G:N2	37:B:8510:HOH:O	2.52	0.42
3:C:70:ALA:HA	3:C:71:PRO:HD3	1.77	0.42
3:C:215:ILE:HG13	3:C:216:SER:N	2.35	0.42
10:J:14:TYR:N	10:J:91:HIS:HE1	2.17	0.42
13:M:126:SER:O	13:M:127:GLU:C	2.61	0.42
14:N:183:VAL:HG12	14:N:184:ARG:N	2.34	0.42
15:O:19:ASP:C	15:O:19:ASP:OD1	2.63	0.42
16:P:59:VAL:HG23	16:P:111:VAL:HG23	2.01	0.42
1:A:12:U:H2'	1:A:13:G:H5'	2.01	0.42
1:A:506:G:N2	1:A:509:A:H5''	2.33	0.42
1:A:1006:A:N1	1:A:2311:A:H1'	2.34	0.42
1:A:1041:U:H2'	1:A:1042:U:H5'	2.00	0.42
1:A:1072:G:OP2	26:Z:154:ARG:NH2	2.52	0.42
1:A:1076:G:C2	1:A:1084:C:C2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2011:A:H4'	1:A:2012:U:O5'	2.20	0.42
1:A:2092:G:H2'	1:A:2613:G:OP1	2.20	0.42
1:A:2559:C:H4'	37:A:7247:HOH:O	2.19	0.42
1:A:2712:G:O2'	1:A:2713:G:H5'	2.20	0.42
2:B:3003:A:H2	2:B:3021:G:N3	2.17	0.42
7:G:126:ILE:HB	7:G:131:LEU:HD23	2.00	0.42
11:K:6:PHE:O	11:K:8:ALA:N	2.53	0.42
15:O:64:SER:C	15:O:66:LEU:N	2.78	0.42
15:O:71:TRP:N	37:O:8538:HOH:O	2.52	0.42
17:Q:13:VAL:HG11	17:Q:40:VAL:CG1	2.49	0.42
1:A:1119:G:C8	11:K:52:GLN:NE2	2.86	0.42
1:A:1175:G:H1'	1:A:1193:A:H2'	2.02	0.42
1:A:1545:C:O2'	1:A:1546:G:H5'	2.20	0.42
1:A:2482:G:N2	1:A:2485:A:OP2	2.50	0.42
5:E:223:LEU:HD12	5:E:223:LEU:HA	1.89	0.42
7:G:11:VAL:CG1	7:G:12:ASP:H	2.33	0.42
7:G:91:PHE:HA	7:G:92:PRO:HD3	1.90	0.42
7:G:137:ASP:OD1	7:G:137:ASP:C	2.63	0.42
10:J:65:ARG:HD3	37:J:8387:HOH:O	2.18	0.42
10:J:141:ASN:CA	37:J:8370:HOH:O	2.63	0.42
10:J:157:ILE:HG22	10:J:158:ASN:N	2.34	0.42
11:K:74:ARG:C	11:K:76:ASP:N	2.78	0.42
22:V:17:THR:CG2	22:V:18:GLY:N	2.83	0.42
22:V:20:MET:CG	22:V:28:THR:HG23	2.50	0.42
1:A:1114:A:H2'	1:A:1115:U:H6	1.85	0.42
1:A:1172:G:H5'	37:A:7251:HOH:O	2.20	0.42
1:A:2505:G:C2'	1:A:2506:A:H5'	2.50	0.42
1:A:2642:G:H2'	1:A:2643:G:O4'	2.18	0.42
7:G:92:PRO:HB2	37:G:4917:HOH:O	2.20	0.42
7:G:116:THR:HG22	7:G:151:LEU:HD22	2.02	0.42
8:H:1:PRO:HB2	37:H:5897:HOH:O	2.20	0.42
15:O:163:PHE:HA	37:O:8519:HOH:O	2.20	0.42
26:Z:197:ASP:C	26:Z:197:ASP:OD1	2.62	0.42
27:1:38:LYS:HD3	37:1:8425:HOH:O	2.18	0.42
28:2:8:GLN:HE22	28:2:11:LYS:HZ1	1.67	0.42
1:A:331:A:C6	1:A:332:G:C4	3.07	0.42
1:A:380:A:OP2	14:N:9:ARG:HD2	2.19	0.42
1:A:621:C:H5'	26:Z:132:ASP:OD2	2.20	0.42
1:A:797:A:O4'	27:1:10:ARG:N	2.52	0.42
1:A:920:C:H4'	1:A:921:G:C2	2.54	0.42
1:A:1241:G:N3	11:K:86:MET:HE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:C:H2'	1:A:1269:G:H8	1.85	0.42
1:A:2363:G:O2'	18:R:11:ARG:HG3	2.20	0.42
1:A:2842:G:H2'	1:A:2843:A:C5'	2.49	0.42
2:B:3047:A:C2	2:B:3048:C:C2	3.06	0.42
4:D:53:LEU:HD11	4:D:327:VAL:HG22	2.02	0.42
4:D:177:HIS:O	4:D:181:ILE:HG13	2.20	0.42
6:F:35:ALA:HB1	37:F:3279:HOH:O	2.19	0.42
7:G:7:ILE:CG2	7:G:45:ASP:O	2.67	0.42
10:J:31:PHE:HA	10:J:85:ILE:CG2	2.50	0.42
10:J:46:VAL:C	10:J:146:TRP:CZ3	2.98	0.42
13:M:34:GLY:C	13:M:36:ASP:N	2.78	0.42
13:M:128:GLY:O	13:M:132:LYS:HG3	2.19	0.42
15:O:61:ALA:CB	15:O:88:ALA:HB2	2.47	0.42
15:O:108:SER:HA	15:O:109:PRO:HD3	1.80	0.42
24:X:122:ARG:HG2	24:X:122:ARG:NH1	2.27	0.42
1:A:134:U:C2	1:A:145:A:C2	3.08	0.42
1:A:291:C:H2'	1:A:292:G:O4'	2.20	0.42
1:A:314:G:N2	1:A:316:A:H3'	2.35	0.42
1:A:660:A:H4'	1:A:661:G:O5'	2.20	0.42
1:A:1096:U:O2'	1:A:1097:A:H5'	2.20	0.42
1:A:1298:U:H2'	1:A:1299:G:C8	2.55	0.42
1:A:1524:U:O2'	1:A:1525:G:P	2.78	0.42
1:A:1603:A:H5''	1:A:1605:G:H5'	2.01	0.42
1:A:1902:G:H2'	1:A:1903:U:O4'	2.20	0.42
1:A:1926:G:H2'	1:A:1927:A:C8	2.55	0.42
1:A:2087:C:O2'	1:A:2088:C:H5'	2.19	0.42
1:A:2241:C:H2'	1:A:2242:U:C6	2.55	0.42
1:A:2756:U:N3	1:A:2896:A:H2	2.13	0.42
3:C:81:GLN:HB2	3:C:92:ASN:HD22	1.84	0.42
3:C:109:GLU:HG2	3:C:116:GLY:N	2.34	0.42
4:D:329:TYR:HE2	22:V:15:PRO:HG2	1.83	0.42
5:E:16:VAL:CG1	5:E:17:ASP:N	2.81	0.42
6:F:160:ALA:C	6:F:162:ALA:N	2.78	0.42
6:F:173:GLU:HG3	6:F:174:VAL:N	2.35	0.42
7:G:24:GLY:HA3	7:G:76:VAL:HB	2.02	0.42
9:I:20:VAL:O	9:I:24:VAL:HG23	2.20	0.42
13:M:21:ARG:N	37:M:8533:HOH:O	2.53	0.42
13:M:121:ILE:HG12	13:M:141:GLU:HB2	2.01	0.42
16:P:14:LEU:HD23	16:P:102:ILE:CD1	2.48	0.42
1:A:1706:G:C6	1:A:1707:G:C6	3.08	0.41
1:A:2883:A:H2'	1:A:2884:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:12:ILE:HB	37:I:4714:HOH:O	2.18	0.41
9:I:64:ASN:O	9:I:68:GLU:HG3	2.20	0.41
9:I:67:LEU:O	9:I:71:LEU:HG	2.20	0.41
13:M:17:SER:C	13:M:19:LYS:N	2.77	0.41
19:S:39:THR:CB	19:S:42:GLU:HG3	2.44	0.41
1:A:10:U:H5'	37:A:6018:HOH:O	2.19	0.41
1:A:100:C:H4'	21:U:16:LEU:HB2	2.02	0.41
1:A:111:C:H2'	1:A:112:G:O4'	2.20	0.41
1:A:262:A:OP2	8:H:91:VAL:HG11	2.20	0.41
1:A:539:G:H2'	1:A:540:A:C8	2.54	0.41
1:A:593:A:OP2	37:A:4372:HOH:O	2.22	0.41
1:A:1079:A:N1	1:A:2068:G:O2'	2.50	0.41
1:A:1681:G:H5''	1:A:1682:A:H5'	2.02	0.41
1:A:1855:G:O6	3:C:142:SER:HB3	2.20	0.41
1:A:1923:G:H4'	30:4:31:THR:O	2.21	0.41
1:A:2112:A:H2'	1:A:2113:G:C8	2.55	0.41
2:B:3041:C:H4'	6:F:48:MET:HB2	2.02	0.41
3:C:8:ARG:NH1	37:C:8552:HOH:O	2.52	0.41
5:E:234:VAL:O	5:E:234:VAL:HG22	2.20	0.41
8:H:26:THR:HG21	8:H:103:ALA:CB	2.49	0.41
10:J:94:ARG:NH2	37:J:8333:HOH:O	2.52	0.41
11:K:63:ILE:HG22	11:K:64:GLY:N	2.34	0.41
12:L:90:PHE:CD1	12:L:90:PHE:N	2.88	0.41
18:R:25:PRO:HA	18:R:26:PRO:HD3	1.86	0.41
1:A:392:U:O2'	14:N:182:LYS:HE2	2.20	0.41
1:A:392:U:C5'	14:N:193:LYS:HB3	2.50	0.41
1:A:431:G:OP1	14:N:48:ARG:NH1	2.53	0.41
1:A:1123:A:C2	1:A:1129:C:H4'	2.55	0.41
1:A:1436:C:O2'	1:A:1437:A:H5'	2.20	0.41
1:A:1515:A:H2'	1:A:1516:C:C6	2.55	0.41
1:A:1555:G:H4'	1:A:1630:A:H2	1.86	0.41
1:A:1617:C:C4	1:A:1643:C:H4'	2.54	0.41
1:A:2383:G:H1'	37:A:6687:HOH:O	2.19	0.41
1:A:2387:U:H2'	1:A:2388:C:C6	2.55	0.41
1:A:2419:U:H5''	1:A:2420:G:C5'	2.49	0.41
2:B:3092:G:H22	10:J:52:LYS:HZ3	1.68	0.41
4:D:23:THR:CG2	4:D:162:MET:HE3	2.50	0.41
5:E:246:ARG:HB3	5:E:246:ARG:HH11	1.84	0.41
6:F:154:LYS:HD2	6:F:154:LYS:N	2.16	0.41
7:G:108:LEU:HD11	7:G:164:ASP:HB2	2.02	0.41
7:G:152:THR:HG21	7:G:165:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:35:ASN:ND2	10:J:79:ALA:O	2.53	0.41
10:J:58:HIS:CE1	10:J:59:ASN:ND2	2.88	0.41
15:O:37:ARG:HA	15:O:37:ARG:HD3	1.79	0.41
19:S:84:ALA:O	19:S:88:PHE:HD1	2.03	0.41
27:1:56:MET:HA	27:1:62:TYR:O	2.20	0.41
1:A:588:G:O6	24:X:154:ARG:NH1	2.54	0.41
1:A:2010:A:C2'	37:A:5939:HOH:O	2.68	0.41
1:A:2413:A:N7	15:O:109:PRO:HB3	2.35	0.41
37:A:9336:HOH:O	20:T:63:LYS:NZ	2.53	0.41
4:D:310:ARG:NH2	37:D:8557:HOH:O	2.53	0.41
6:F:44:ILE:HG12	6:F:83:PHE:CE1	2.53	0.41
9:I:66:LEU:O	9:I:69:ARG:HB3	2.20	0.41
10:J:95:GLU:HB3	10:J:119:VAL:HG11	2.02	0.41
10:J:163:PRO:HG2	37:J:8341:HOH:O	2.19	0.41
11:K:39:VAL:CG1	11:K:107:ASN:HB2	2.51	0.41
15:O:154:LEU:C	15:O:156:GLU:H	2.27	0.41
17:Q:134:VAL:O	17:Q:137:LEU:HB3	2.20	0.41
19:S:25:PHE:CE2	19:S:29:LYS:CE	3.03	0.41
20:T:58:MET:SD	29:3:8:LYS:HE3	2.59	0.41
21:U:32:ARG:NH1	21:U:38:ARG:NH1	2.62	0.41
28:2:25:LYS:HD2	29:3:48:ASP:HA	2.02	0.41
1:A:288:A:H2'	1:A:289:G:C8	2.56	0.41
1:A:321:A:H1'	37:A:7019:HOH:O	2.20	0.41
1:A:545:G:H2'	1:A:546:C:O4'	2.20	0.41
1:A:664:U:O4	1:A:681:G:H5''	2.20	0.41
1:A:2269:C:C2'	1:A:2270:G:H5'	2.50	0.41
3:C:212:PRO:HB2	37:C:8561:HOH:O	2.21	0.41
4:D:36:PRO:HA	4:D:168:GLY:HA2	1.98	0.41
4:D:76:THR:N	4:D:77:PRO:HD3	2.35	0.41
4:D:138:GLY:O	4:D:139:ASP:C	2.62	0.41
7:G:9:GLU:HG3	7:G:10:ASP:N	2.35	0.41
8:H:60:VAL:O	8:H:61:MET:C	2.64	0.41
37:L:7438:HOH:O	22:V:20:MET:HE1	2.20	0.41
14:N:37:VAL:HG21	14:N:108:LYS:HG2	2.02	0.41
14:N:87:MET:HB2	14:N:91:ILE:CD1	2.49	0.41
15:O:43:VAL:O	15:O:43:VAL:HG12	2.21	0.41
15:O:154:LEU:CG	15:O:155:GLU:H	2.30	0.41
16:P:77:ALA:HA	16:P:96:VAL:O	2.20	0.41
17:Q:115:SER:O	17:Q:117:SER:N	2.53	0.41
17:Q:141:ILE:C	17:Q:143:ALA:H	2.28	0.41
26:Z:189:ASN:C	26:Z:189:ASN:ND2	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:38:LYS:HG3	37:1:8430:HOH:O	2.19	0.41
1:A:39:G:N2	1:A:444:C:C2	2.89	0.41
1:A:105:G:O2'	1:A:106:A:H5'	2.19	0.41
1:A:245:C:C2'	1:A:246:G:H5'	2.51	0.41
1:A:327:A:OP1	5:E:149:LYS:NZ	2.35	0.41
1:A:2467:A:O2'	1:A:2468:A:H2'	2.20	0.41
1:A:2698:G:H2'	1:A:2699:A:C8	2.55	0.41
2:B:3025:G:H5''	2:B:3026:C:C6	2.56	0.41
3:C:100:PRO:O	3:C:103:VAL:HG23	2.20	0.41
4:D:23:THR:HA	4:D:24:PRO:HD3	1.90	0.41
10:J:75:SER:HB3	10:J:79:ALA:CB	2.49	0.41
10:J:149:ALA:C	10:J:151:MET:N	2.79	0.41
14:N:72:SER:HB2	14:N:93:ARG:HG2	2.02	0.41
15:O:73:ALA:HB2	15:O:163:PHE:CZ	2.56	0.41
17:Q:115:SER:C	17:Q:117:SER:H	2.29	0.41
1:A:282:C:H2'	1:A:283:U:O4'	2.20	0.41
1:A:1409:G:H5'	37:A:3705:HOH:O	2.20	0.41
1:A:2266:A:OP2	14:N:90:ARG:NH2	2.53	0.41
3:C:110:SER:N	3:C:114:ASP:OD2	2.53	0.41
4:D:80:ARG:HD3	37:D:8605:HOH:O	2.21	0.41
6:F:11:HIS:O	6:F:12:GLU:CB	2.68	0.41
7:G:20:ILE:O	7:G:30:THR:HA	2.20	0.41
10:J:48:LEU:CD1	10:J:157:ILE:HG21	2.49	0.41
10:J:150:LYS:HA	10:J:153:VAL:HG22	2.03	0.41
13:M:148:GLU:HG2	37:M:8553:HOH:O	2.20	0.41
14:N:67:ILE:HD11	14:N:104:ARG:HD2	2.01	0.41
17:Q:7:LYS:CD	17:Q:21:VAL:CG2	2.99	0.41
19:S:125:ARG:HG2	37:S:8542:HOH:O	2.20	0.41
24:X:64:THR:O	24:X:68:THR:HG22	2.20	0.41
24:X:154:ARG:HE	24:X:154:ARG:HB3	1.61	0.41
1:A:240:C:O2	1:A:240:C:H2'	2.20	0.41
1:A:394:G:H1	14:N:181:GLU:CD	2.29	0.41
1:A:1127:C:H2'	1:A:1128:U:H5'	2.02	0.41
1:A:1878:G:O2'	1:A:1879:U:OP2	2.38	0.41
1:A:2004:U:H2'	1:A:2005:G:OP1	2.20	0.41
3:C:217:ARG:CG	3:C:217:ARG:HH11	2.33	0.41
4:D:277:GLU:N	4:D:278:PRO:HD2	2.35	0.41
5:E:65:ARG:HG3	5:E:67:GLN:HB2	2.03	0.41
5:E:127:ARG:HG2	5:E:127:ARG:NH1	2.36	0.41
6:F:10:PHE:CE1	6:F:11:HIS:HB3	2.55	0.41
6:F:11:HIS:C	6:F:13:MET:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:30:GLN:H	10:J:65:ARG:NH1	2.19	0.41
14:N:107:ARG:NH1	37:N:8578:HOH:O	2.51	0.41
15:O:43:VAL:HG13	15:O:118:ILE:HD11	2.02	0.41
15:O:163:PHE:O	15:O:164:ASP:O	2.38	0.41
19:S:119:VAL:HG11	37:S:8585:HOH:O	2.20	0.41
1:A:21:G:H5''	19:S:1:GLY:O	2.21	0.41
1:A:79:G:H22	1:A:97:G:H1'	1.86	0.41
1:A:80:A:H5''	21:U:41:ARG:CZ	2.51	0.41
1:A:128:A:O2'	1:A:129:A:H5'	2.20	0.41
1:A:154:C:H2'	1:A:155:C:C6	2.56	0.41
1:A:646:G:H2'	1:A:647:U:C6	2.56	0.41
1:A:682:A:H2'	1:A:683:G:O4'	2.20	0.41
1:A:1191:A:C3'	1:A:1192:A:H5''	2.48	0.41
1:A:1909:A:H2'	1:A:1910:A:C8	2.56	0.41
1:A:2019:A:H5'	37:A:4511:HOH:O	2.20	0.41
1:A:2401:A:H5'	37:A:9481:HOH:O	2.20	0.41
1:A:2415:A:N3	15:O:26:LEU:HD13	2.36	0.41
1:A:2657:G:OP1	4:D:17:LYS:HB2	2.21	0.41
1:A:2766:A:O2'	1:A:2767:C:H5'	2.21	0.41
1:A:2791:U:H4'	1:A:2792:A:OP1	2.21	0.41
1:A:2909:G:H2'	1:A:2910:A:H8	1.86	0.41
37:A:6230:HOH:O	22:V:56:ARG:HD3	2.21	0.41
37:A:7217:HOH:O	14:N:13:LYS:HE2	2.21	0.41
2:B:3012:C:H5'	2:B:3070:U:O4'	2.20	0.41
3:C:30:ARG:HE	3:C:30:ARG:HB3	1.69	0.41
3:C:51:ARG:HB2	37:C:8608:HOH:O	2.20	0.41
4:D:92:TYR:CD1	4:D:92:TYR:N	2.89	0.41
4:D:132:HIS:HB2	4:D:137:LEU:HD22	2.03	0.41
5:E:21:VAL:C	5:E:23:GLU:H	2.29	0.41
6:F:99:ASP:HB2	6:F:103:ASN:CB	2.50	0.41
7:G:10:ASP:HA	37:G:3707:HOH:O	2.20	0.41
7:G:169:THR:HG22	7:G:170:ARG:HG3	2.03	0.41
8:H:26:THR:HB	8:H:102:GLY:HA3	2.02	0.41
10:J:126:HIS:O	10:J:127:GLY:C	2.64	0.41
12:L:30:LYS:C	12:L:55:VAL:HG13	2.46	0.41
13:M:73:VAL:HG21	13:M:116:HIS:CD2	2.56	0.41
15:O:119:GLN:O	15:O:123:ILE:HG13	2.21	0.41
19:S:113:HIS:O	19:S:145:LEU:HD12	2.21	0.41
21:U:48:VAL:HG23	21:U:98:VAL:HA	2.02	0.41
1:A:164:G:O3'	13:M:30:ARG:HB2	2.20	0.41
1:A:306:A:P	21:U:38:ARG:HH21	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:A:OP2	19:S:128:ARG:HD2	2.21	0.41
1:A:1109:U:O4	11:K:21:ARG:HA	2.20	0.41
1:A:1414:A:H2'	1:A:1415:G:O4'	2.20	0.41
1:A:1947:G:H2'	1:A:1948:G:C8	2.55	0.41
4:D:54:VAL:O	4:D:55:ASN:C	2.63	0.41
6:F:57:THR:HA	6:F:63:ILE:HA	2.02	0.41
8:H:72:VAL:HA	8:H:73:PRO:HD3	1.79	0.41
24:X:65:VAL:HG12	24:X:116:LEU:HD13	2.02	0.41
24:X:122:ARG:CG	24:X:122:ARG:NH1	2.83	0.41
24:X:137:GLN:O	24:X:137:GLN:HG3	2.21	0.41
27:1:30:GLU:HB3	27:1:34:LYS:HE3	2.03	0.41
30:4:69:TYR:HB2	30:4:78:HIS:CE1	2.56	0.41
30:4:73:GLU:HB2	37:4:8529:HOH:O	2.21	0.41
1:A:74:A:H2'	1:A:75:U:C6	2.56	0.40
1:A:128:A:C8	1:A:128:A:C3'	3.03	0.40
1:A:412:C:H2'	1:A:413:G:O4'	2.22	0.40
1:A:940:G:C5	1:A:1027:G:C2	3.09	0.40
1:A:1023:C:H2'	1:A:1024:G:O4'	2.21	0.40
1:A:1172:G:C5'	37:A:7251:HOH:O	2.69	0.40
1:A:1973:A:H5'	1:A:1973:A:C8	2.48	0.40
1:A:2297:U:H1'	37:A:5151:HOH:O	2.21	0.40
1:A:2834:G:OP1	25:Y:39:LYS:HE2	2.21	0.40
1:A:2900:G:H2'	1:A:2901:C:O4'	2.21	0.40
4:D:88:GLU:O	4:D:88:GLU:HG3	2.20	0.40
6:F:35:ALA:C	6:F:37:ALA:H	2.28	0.40
7:G:9:GLU:HA	37:G:5240:HOH:O	2.20	0.40
8:H:34:ASN:O	8:H:38:LYS:HG3	2.22	0.40
12:L:6:ALA:HB3	12:L:116:GLU:HG2	2.02	0.40
14:N:5:TYR:HE2	14:N:46:LEU:HD13	1.85	0.40
24:X:11:VAL:O	24:X:12:ASN:HB2	2.20	0.40
30:4:69:TYR:CZ	30:4:80:ARG:HD2	2.57	0.40
1:A:806:A:H2'	1:A:807:A:O4'	2.21	0.40
1:A:1477:C:H5'	1:A:1868:G:H5''	2.02	0.40
1:A:1980:U:O2	1:A:2008:U:H4'	2.22	0.40
1:A:2053:G:OP1	19:S:138:SER:OG	2.34	0.40
1:A:2289:G:H21	1:A:2291:A:H2	1.66	0.40
1:A:2501:G:H1'	37:A:4516:HOH:O	2.21	0.40
1:A:2761:A:C4	1:A:2763:G:C8	3.09	0.40
1:A:2909:G:O2'	1:A:2910:A:H5'	2.22	0.40
37:A:4809:HOH:O	11:K:47:THR:CB	2.60	0.40
4:D:53:LEU:HD21	4:D:270:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:46:VAL:CG1	10:J:146:TRP:HZ3	2.30	0.40
13:M:142:LEU:HD12	13:M:142:LEU:HA	1.94	0.40
14:N:39:ARG:HA	14:N:63:VAL:HG22	2.04	0.40
14:N:134:ILE:HG23	14:N:141:ILE:HD13	2.02	0.40
20:T:29:ASP:CG	20:T:31:ARG:NH1	2.79	0.40
21:U:55:PHE:CD2	21:U:77:VAL:HG13	2.56	0.40
23:W:12:THR:HG23	23:W:14:ALA:H	1.86	0.40
25:Y:74:ALA:HB1	25:Y:85:VAL:HG22	2.03	0.40
27:1:46:LYS:O	27:1:57:CYS:HA	2.21	0.40
1:A:68:U:O2'	1:A:69:A:H5''	2.20	0.40
1:A:420:U:H2'	1:A:421:C:C6	2.56	0.40
1:A:488:U:O2'	21:U:82:THR:HG21	2.21	0.40
1:A:612:U:H2'	1:A:613:C:C6	2.57	0.40
1:A:963:C:H2'	1:A:964:G:C8	2.57	0.40
1:A:1462:C:H2'	1:A:1463:A:H8	1.85	0.40
1:A:1482:A:O2'	1:A:1483:C:H5'	2.22	0.40
1:A:1666:C:O2'	1:A:1667:A:C5'	2.66	0.40
1:A:2727:A:H2'	1:A:2728:C:H5'	2.03	0.40
2:B:3031:C:H1'	37:B:8394:HOH:O	2.21	0.40
2:B:3056:A:H1'	6:F:14:ARG:HG2	2.04	0.40
2:B:3057:A:N6	37:B:8445:HOH:O	2.48	0.40
2:B:3057:A:O2'	6:F:152:PRO:HD2	2.22	0.40
3:C:97:ALA:HB2	3:C:150:PRO:HB2	2.02	0.40
6:F:67:ASP:O	6:F:69:ILE:HG13	2.20	0.40
15:O:141:ARG:N	37:O:8569:HOH:O	2.54	0.40
21:U:96:VAL:CG1	21:U:97:ARG:N	2.80	0.40
23:W:1:THR:HG23	23:W:2:VAL:N	2.27	0.40
23:W:12:THR:OG1	23:W:13:PRO:HD2	2.22	0.40
1:A:128:A:H3'	1:A:128:A:H8	1.87	0.40
1:A:516:A:P	37:A:5625:HOH:O	2.79	0.40
1:A:892:G:H5''	28:2:54:ALA:HB2	2.02	0.40
1:A:1335:C:OP2	26:Z:207:SER:CB	2.70	0.40
1:A:1559:A:C1'	37:A:5846:HOH:O	2.68	0.40
1:A:1586:G:O2'	1:A:1587:U:H5'	2.20	0.40
1:A:1845:A:OP2	3:C:190:ARG:NH1	2.53	0.40
1:A:2506:A:O2'	1:A:2507:G:P	2.80	0.40
1:A:2816:A:H5''	1:A:2817:G:H5'	2.04	0.40
2:B:3065:A:C2'	2:B:3066:G:OP2	2.69	0.40
3:C:36:ASP:CB	3:C:85:ASP:H	2.34	0.40
3:C:192:VAL:HG12	3:C:207:GLN:HB3	2.04	0.40
4:D:215:VAL:HA	4:D:220:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:19:GLU:HG3	37:F:6165:HOH:O	2.20	0.40
8:H:26:THR:HB	8:H:102:GLY:C	2.46	0.40
10:J:26:LYS:HA	10:J:58:HIS:CD2	2.56	0.40
14:N:55:LYS:O	14:N:60:ILE:HD12	2.21	0.40
14:N:182:LYS:HD2	14:N:193:LYS:HB2	2.02	0.40
15:O:80:SER:CB	37:O:8535:HOH:O	2.57	0.40
19:S:61:GLN:NE2	37:S:8540:HOH:O	2.54	0.40
21:U:26:THR:HA	21:U:39:ASN:HB3	2.02	0.40
24:X:66:LEU:HD23	24:X:66:LEU:HA	1.86	0.40
26:Z:184:GLU:OE1	26:Z:204:ARG:NH1	2.54	0.40
30:4:87:ARG:NH1	37:4:8527:HOH:O	2.54	0.40
1:A:88:G:H2'	1:A:89:G:C8	2.56	0.40
1:A:445:U:H2'	1:A:446:G:H8	1.86	0.40
1:A:449:A:C8	5:E:43:LYS:HG2	2.56	0.40
1:A:525:G:H2'	1:A:526:U:O4'	2.21	0.40
1:A:776:A:OP1	28:2:28:HIS:HE1	2.05	0.40
1:A:1114:A:H2'	1:A:1115:U:C6	2.57	0.40
1:A:1162:G:H2'	37:A:6565:HOH:O	2.22	0.40
1:A:1444:G:O2'	1:A:1445:G:H5'	2.21	0.40
1:A:2388:C:O2'	1:A:2389:U:H5'	2.22	0.40
1:A:2712:G:P	37:A:5197:HOH:O	2.80	0.40
1:A:2781:U:H2'	1:A:2782:G:C5'	2.51	0.40
5:E:133:ARG:NH2	37:E:8421:HOH:O	2.54	0.40
8:H:13:GLU:OE2	8:H:78:GLU:HG2	2.21	0.40
11:K:88:PRO:C	35:K:8502:CL:CL	3.01	0.40
16:P:113:VAL:O	16:P:114:ILE:HD13	2.22	0.40
19:S:39:THR:CG2	19:S:42:GLU:HG3	2.51	0.40
23:W:45:ARG:C	23:W:47:LYS:N	2.78	0.40
25:Y:74:ALA:HB2	25:Y:85:VAL:HG13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	235/239 (98%)	212 (90%)	19 (8%)	4 (2%)	7	30
4	D	335/337 (99%)	310 (92%)	18 (5%)	7 (2%)	5	25
5	E	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
6	F	134/176 (76%)	99 (74%)	24 (18%)	11 (8%)	0	3
7	G	170/177 (96%)	162 (95%)	8 (5%)	0	100	100
8	H	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	7	30
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	132 (87%)	15 (10%)	5 (3%)	3	16
11	K	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	5	25
12	L	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	8	33
13	M	141/164 (86%)	122 (86%)	17 (12%)	2 (1%)	9	34
14	N	192/194 (99%)	177 (92%)	12 (6%)	3 (2%)	7	32
15	O	184/186 (99%)	167 (91%)	10 (5%)	7 (4%)	2	13
16	P	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
17	Q	141/148 (95%)	137 (97%)	4 (3%)	0	100	100
18	R	93/95 (98%)	87 (94%)	6 (6%)	0	100	100
19	S	148/154 (96%)	142 (96%)	6 (4%)	0	100	100
20	T	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
21	U	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
22	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
23	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	17
24	X	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	9	36
25	Y	80/91 (88%)	70 (88%)	9 (11%)	1 (1%)	9	36
26	Z	140/240 (58%)	140 (100%)	0	0	100	100
27	1	71/73 (97%)	64 (90%)	5 (7%)	2 (3%)	4	19
28	2	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	87 (97%)	1 (1%)	2 (2%)	5	24
All	All	3633/4235 (86%)	3351 (92%)	227 (6%)	55 (2%)	8	33

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	137	PRO
6	F	173	GLU
8	H	101	ALA
10	J	162	SER
13	M	80	ASP
15	O	154	LEU
15	O	164	ASP
15	O	183	ASP
23	W	43	PRO
3	C	34	ASP
3	C	37	VAL
3	C	132	ASP
4	D	34	GLY
4	D	169	GLY
6	F	11	HIS
6	F	20	LYS
10	J	164	ALA
11	K	5	GLU
11	K	7	ASP
11	K	143	LYS
15	O	162	ASP
15	O	181	ASP
30	4	57	GLY
4	D	107	SER
4	D	184	ASP
6	F	171	ASP
10	J	40	PRO
10	J	138	PRO
12	L	119	GLN
12	L	126	SER
14	N	140	ALA
15	O	167	ASP
24	X	77	ALA
25	Y	77	PHE
27	1	81	LYS
30	4	56	PRO
4	D	185	GLY
6	F	36	ASN
6	F	61	PHE
10	J	72	VAL

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Mol	Chain	Res	Type
13	M	21	ARG
8	H	64	PRO
15	O	65	ASP
3	C	119	ALA
6	F	96	SER
14	N	165	SER
23	W	40	PRO
24	X	49	ASN
4	D	2	GLN
27	1	41	VAL
6	F	16	PRO
14	N	88	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	168 (94%)	11 (6%)	17	47
4	D	282/282 (100%)	263 (93%)	19 (7%)	15	44
5	E	193/193 (100%)	177 (92%)	16 (8%)	10	35
6	F	117/147 (80%)	108 (92%)	9 (8%)	12	38
7	G	152/155 (98%)	147 (97%)	5 (3%)	33	65
8	H	92/92 (100%)	89 (97%)	3 (3%)	33	65
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	109 (89%)	13 (11%)	6	25
11	K	118/121 (98%)	111 (94%)	7 (6%)	18	49
12	L	106/106 (100%)	103 (97%)	3 (3%)	38	69
13	M	112/126 (89%)	109 (97%)	3 (3%)	39	70
14	N	166/166 (100%)	159 (96%)	7 (4%)	26	59
15	O	149/149 (100%)	142 (95%)	7 (5%)	23	56
16	P	93/93 (100%)	89 (96%)	4 (4%)	26	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	113/116 (97%)	110 (97%)	3 (3%)	39	70
18	R	79/79 (100%)	74 (94%)	5 (6%)	16	46
19	S	117/121 (97%)	114 (97%)	3 (3%)	40	71
20	T	71/73 (97%)	70 (99%)	1 (1%)	59	79
21	U	105/105 (100%)	100 (95%)	5 (5%)	23	56
22	V	44/52 (85%)	44 (100%)	0	100	100
23	W	51/56 (91%)	50 (98%)	1 (2%)	48	75
24	X	130/130 (100%)	121 (93%)	9 (7%)	14	43
25	Y	66/73 (90%)	63 (96%)	3 (4%)	24	57
26	Z	120/195 (62%)	111 (92%)	9 (8%)	12	39
27	1	56/56 (100%)	54 (96%)	2 (4%)	31	64
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	43	72
30	4	79/79 (100%)	75 (95%)	4 (5%)	21	54
All	All	3027/3441 (88%)	2874 (95%)	153 (5%)	21	54

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	ARG
3	C	36	ASP
3	C	55	VAL
3	C	68	ILE
3	C	69	LEU
3	C	94	LEU
3	C	131	HIS
3	C	153	ARG
3	C	175	LYS
3	C	179	MET
3	C	217	ARG
4	D	7	ARG
4	D	11	LEU
4	D	27	ASN
4	D	33	ASP
4	D	53	LEU
4	D	63	GLU
4	D	84	LEU

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Mol	Chain	Res	Type
4	D	97	LEU
4	D	98	THR
4	D	103	ASP
4	D	190	MET
4	D	195	ARG
4	D	245	SER
4	D	251	VAL
4	D	254	GLN
4	D	256	GLN
4	D	304	PRO
4	D	307	ARG
4	D	312	ARG
5	E	2	GLN
5	E	27	ARG
5	E	67	GLN
5	E	78	ARG
5	E	94	THR
5	E	101	ASP
5	E	115	LEU
5	E	136	VAL
5	E	187	ARG
5	E	214	THR
5	E	222	ASP
5	E	223	LEU
5	E	234	VAL
5	E	236	THR
5	E	240	LEU
5	E	243	VAL
6	F	24	HIS
6	F	50	VAL
6	F	92	GLU
6	F	95	THR
6	F	99	ASP
6	F	131	THR
6	F	136	ARG
6	F	137	PRO
6	F	149	ARG
7	G	1	PRO
7	G	7	ILE
7	G	54	ASP
7	G	86	VAL
7	G	102	VAL

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Mol	Chain	Res	Type
8	H	1	PRO
8	H	12	LEU
8	H	78	GLU
10	J	18	GLU
10	J	30	GLN
10	J	59	ASN
10	J	61	LEU
10	J	72	VAL
10	J	73	GLN
10	J	82	LYS
10	J	85	ILE
10	J	86	ARG
10	J	93	ILE
10	J	142	VAL
10	J	150	LYS
10	J	166	ASN
11	K	46	ILE
11	K	74	ARG
11	K	93	ARG
11	K	120	SER
11	K	125	SER
11	K	127	ILE
11	K	131	THR
12	L	7	ASP
12	L	10	GLN
12	L	98	VAL
13	M	35	ARG
13	M	117	GLU
13	M	140	VAL
14	N	38	VAL
14	N	46	LEU
14	N	81	ARG
14	N	87	MET
14	N	93	ARG
14	N	99	ARG
14	N	164	THR
15	O	26	LEU
15	O	43	VAL
15	O	47	LEU
15	O	127	LEU
15	O	128	ASP
15	O	152	GLU

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Mol	Chain	Res	Type
15	O	163	PHE
16	P	3	THR
16	P	28	ASP
16	P	98	LEU
16	P	111	VAL
17	Q	52	LYS
17	Q	91	LYS
17	Q	98	ILE
18	R	11	ARG
18	R	16	ASN
18	R	54	PRO
18	R	57	ASP
18	R	95	GLU
19	S	13	THR
19	S	39	THR
19	S	82	GLU
20	T	10	VAL
21	U	26	THR
21	U	39	ASN
21	U	47	THR
21	U	48	VAL
21	U	96	VAL
23	W	43	PRO
24	X	4	LEU
24	X	35	VAL
24	X	52	VAL
24	X	73	LEU
24	X	120	PRO
24	X	122	ARG
24	X	142	ASP
24	X	146	ILE
24	X	154	ARG
25	Y	15	ARG
25	Y	66	THR
25	Y	72	VAL
26	Z	103	THR
26	Z	141	THR
26	Z	154	ARG
26	Z	163	THR
26	Z	172	THR
26	Z	189	ASN
26	Z	200	THR

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Mol	Chain	Res	Type
26	Z	203	VAL
26	Z	235	GLU
27	1	11	THR
27	1	64	ILE
29	3	18	ASN
30	4	14	CYS
30	4	42	ARG
30	4	56	PRO
30	4	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	47	HIS
3	C	92	ASN
3	C	127	GLN
3	C	199	HIS
3	C	218	ASN
4	D	27	ASN
4	D	145	HIS
4	D	221	GLN
4	D	238	ASN
4	D	256	GLN
4	D	260	HIS
4	D	318	ASN
5	E	2	GLN
5	E	39	GLN
5	E	67	GLN
5	E	108	GLN
5	E	129	HIS
5	E	163	HIS
6	F	103	ASN
7	G	66	GLN
7	G	96	ASN
7	G	106	ASN
7	G	119	HIS
7	G	143	GLN
9	I	17	GLN
9	I	64	ASN
10	J	8	ASN
10	J	30	GLN
10	J	35	ASN

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Mol	Chain	Res	Type
10	J	45	GLN
10	J	55	GLN
10	J	58	HIS
10	J	59	ASN
10	J	74	ASN
10	J	91	HIS
10	J	129	ASN
10	J	130	HIS
10	J	137	ASN
10	J	166	ASN
11	K	25	GLN
11	K	29	GLN
11	K	52	GLN
11	K	107	ASN
11	K	126	ASN
12	L	10	GLN
13	M	18	HIS
13	M	41	HIS
13	M	42	ASN
13	M	58	GLN
13	M	116	HIS
14	N	26	HIS
14	N	58	GLN
14	N	89	ASN
14	N	106	ASN
14	N	176	GLN
15	O	21	HIS
15	O	22	GLN
15	O	107	ASN
15	O	140	GLN
15	O	153	GLN
17	Q	50	GLN
17	Q	66	GLN
17	Q	73	HIS
17	Q	118	GLN
18	R	16	ASN
18	R	40	HIS
18	R	67	GLN
19	S	22	GLN
19	S	61	GLN
19	S	94	ASN
19	S	98	ASN

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Mol	Chain	Res	Type
19	S	113	HIS
19	S	117	HIS
20	T	51	GLN
20	T	53	ASN
20	T	55	GLN
20	T	56	ASN
21	U	39	ASN
21	U	73	HIS
21	U	95	ASN
22	V	39	ASN
23	W	4	HIS
23	W	6	GLN
23	W	60	GLN
24	X	27	HIS
24	X	28	HIS
24	X	87	HIS
24	X	110	GLN
24	X	119	HIS
24	X	125	HIS
24	X	141	HIS
25	Y	23	HIS
26	Z	119	GLN
26	Z	133	HIS
26	Z	134	HIS
26	Z	149	GLN
26	Z	153	GLN
26	Z	189	ASN
27	1	33	HIS
27	1	70	GLN
28	2	8	GLN
28	2	16	HIS
28	2	28	HIS
29	3	16	ASN
29	3	17	GLN
29	3	18	ASN
29	3	37	HIS
29	3	41	HIS
29	3	45	ASN
30	4	30	GLN
30	4	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	244 (8%)	35 (1%)
2	B	121/122 (99%)	19 (15%)	7 (5%)
All	All	2868/3044 (94%)	263 (9%)	42 (1%)

All (263) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A
1	A	186	A
1	A	191	A
1	A	192	A
1	A	219	G
1	A	237	G
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	318	C
1	A	336	G
1	A	337	A
1	A	338	C
1	A	339	A

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Mol	Chain	Res	Type
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	461	C
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	620	A
1	A	632	A
1	A	644	G
1	A	645	U
1	A	660	A
1	A	688	A
1	A	701	U
1	A	717	C
1	A	759	C
1	A	777	U
1	A	809	G
1	A	821	U
1	A	835	U
1	A	840	U
1	A	857	A
1	A	858	U
1	A	868	G
1	A	869	G
1	A	871	G
1	A	872	U
1	A	875	A
1	A	877	G

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Mol	Chain	Res	Type
1	A	878	G
1	A	884	C
1	A	898	G
1	A	905	C
1	A	921	G
1	A	923	A
1	A	953	G
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	C
1	A	1029	U
1	A	1045	G
1	A	1059	G
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1161	A
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1216	G
1	A	1237	U
1	A	1238	C
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1342	C

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Mol	Chain	Res	Type
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1380	U
1	A	1407	A
1	A	1409	G
1	A	1451	C
1	A	1474	C
1	A	1485	A
1	A	1505	U
1	A	1506	U
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1710	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1857	A
1	A	1879	U
1	A	1904	A

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Mol	Chain	Res	Type
1	A	1919	A
1	A	1942	A
1	A	1943	C
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1980	U
1	A	1982	C
1	A	1996	U
1	A	2004	U
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2101	A
1	A	2102	G
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2291	A
1	A	2317	C
1	A	2321	A
1	A	2346	C
1	A	2354	A
1	A	2361	A
1	A	2362	A
1	A	2369	A
1	A	2422	U
1	A	2462	G
1	A	2469	A
1	A	2476	C
1	A	2483	A

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Mol	Chain	Res	Type
1	A	2507	G
1	A	2511	A
1	A	2526	C
1	A	2527	U
1	A	2533	C
1	A	2537	G
1	A	2541	U
1	A	2553	A
1	A	2564	G
1	A	2589	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2638	G
1	A	2649	A
1	A	2650	U
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2718	C
1	A	2719	A
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2812	A
1	A	2825	C
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A
1	A	2914	A
2	B	3002	U
2	B	3003	A

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Mol	Chain	Res	Type
2	B	3004	G
2	B	3011	A
2	B	3014	G
2	B	3022	G
2	B	3023	U
2	B	3024	U
2	B	3025	G
2	B	3026	C
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	129	A
1	A	284	C
1	A	338	C
1	A	603	A
1	A	644	G
1	A	699	C
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	1080	C
1	A	1164	U
1	A	1232	A
1	A	1237	U
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1506	U
1	A	1563	G

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Mol	Chain	Res	Type
1	A	1685	A
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2313	C
1	A	2361	A
1	A	2467	A
1	A	2526	C
1	A	2536	C
1	A	2649	A
1	A	2718	C
1	A	2761	A
1	A	2791	U
2	B	3002	U
2	B	3003	A
2	B	3023	U
2	B	3024	U
2	B	3043	G
2	B	3065	A
2	B	3103	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	ANM	A	9000	33	20,20,20	1.78	4 (20%)	24,27,27	1.71	7 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	ANM	A	9000	33	-	2/10/23/23	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9000	ANM	C1-C9	5.55	1.49	1.38
31	A	9000	ANM	C10-C9	2.92	1.44	1.38
31	A	9000	ANM	C11-C12	2.80	1.44	1.38
31	A	9000	ANM	O1-C9	2.60	1.42	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9000	ANM	C2-O2-C5	3.49	123.15	117.72
31	A	9000	ANM	C10-C9-C1	-3.29	115.37	120.16
31	A	9000	ANM	C13-C1-C9	2.78	122.91	119.73
31	A	9000	ANM	C12-C15-C16	-2.55	109.08	113.40
31	A	9000	ANM	O2-C5-O3	2.12	127.09	122.99
31	A	9000	ANM	C15-C16-N1	2.12	113.93	111.21
31	A	9000	ANM	C14-O1-C9	2.12	122.04	117.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

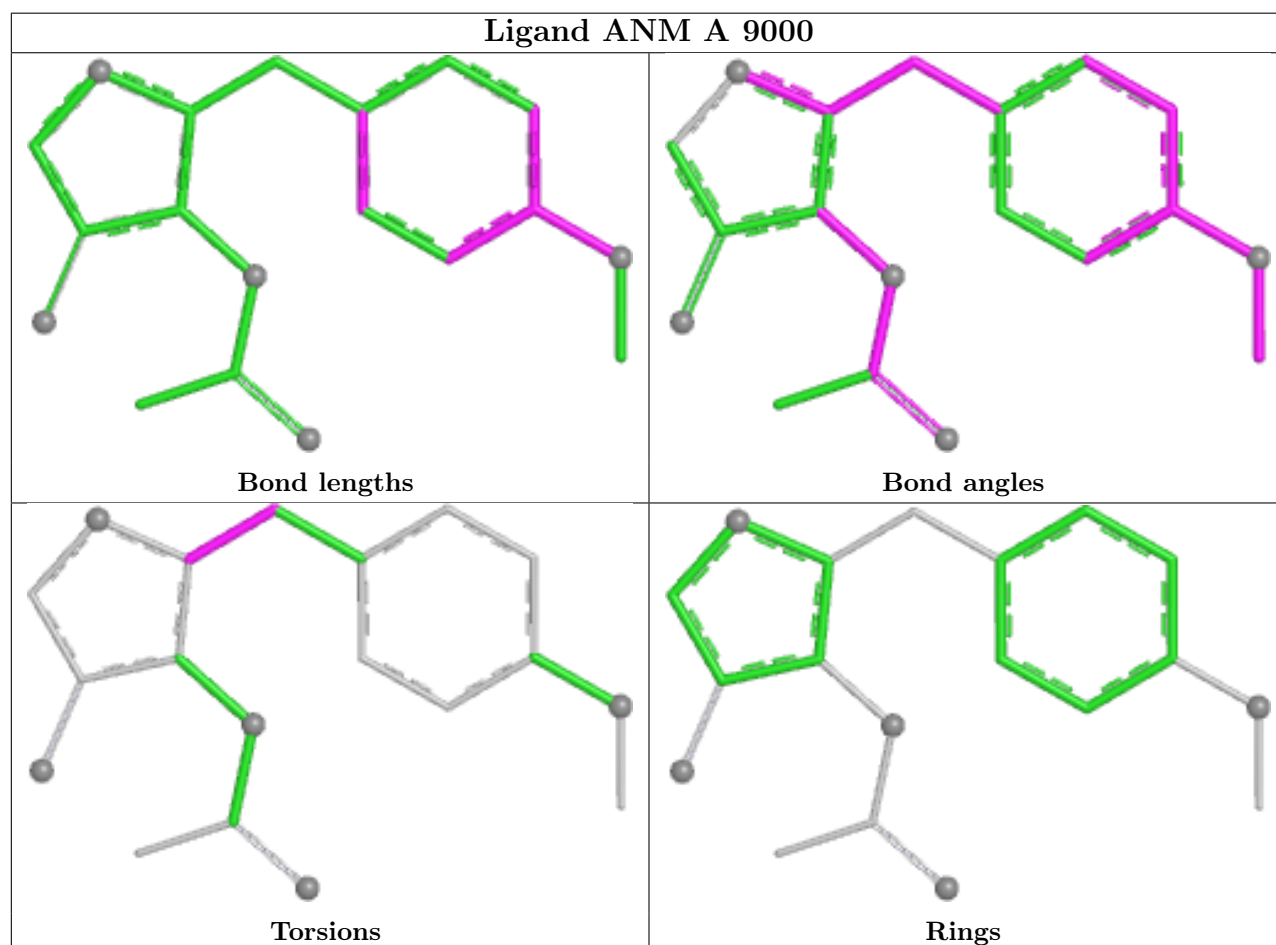
Mol	Chain	Res	Type	Atoms
31	A	9000	ANM	C12-C15-C16-C2
31	A	9000	ANM	C12-C15-C16-N1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9000	ANM	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2486:A	O3'	2487:C	P	2.10

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2754/2922 (94%)	-0.12	67 (2%) 59 36	20, 45, 89, 137	0
2	B	122/122 (100%)	0.48	7 (5%) 29 15	32, 61, 88, 146	0
3	C	237/239 (99%)	0.02	2 (0%) 82 64	27, 49, 83, 104	0
4	D	337/337 (100%)	0.09	1 (0%) 90 79	25, 54, 79, 88	0
5	E	246/246 (100%)	-0.00	1 (0%) 88 76	18, 44, 68, 79	0
6	F	140/176 (79%)	1.10	18 (12%) 7 4	51, 96, 114, 118	0
7	G	172/177 (97%)	0.46	5 (2%) 53 31	44, 66, 85, 91	0
8	H	119/119 (100%)	0.52	2 (1%) 69 46	50, 68, 93, 100	0
9	I	29/348 (8%)	1.34	6 (20%) 2 2	73, 88, 96, 100	0
10	J	156/167 (93%)	0.40	7 (4%) 38 20	34, 55, 84, 88	0
11	K	142/145 (97%)	0.03	0 100 100	34, 49, 70, 90	0
12	L	132/132 (100%)	0.06	1 (0%) 82 64	30, 50, 71, 78	0
13	M	145/164 (88%)	0.31	3 (2%) 63 40	23, 64, 101, 112	0
14	N	194/194 (100%)	0.04	2 (1%) 79 59	29, 43, 60, 72	0
15	O	186/186 (100%)	0.60	9 (4%) 35 18	40, 61, 101, 114	0
16	P	115/115 (100%)	0.23	0 100 100	38, 53, 69, 75	0
17	Q	143/148 (96%)	0.10	1 (0%) 84 66	35, 54, 68, 75	0
18	R	95/95 (100%)	-0.07	1 (1%) 78 57	33, 43, 58, 71	0
19	S	150/154 (97%)	-0.24	0 100 100	24, 43, 65, 71	0
20	T	81/84 (96%)	0.11	0 100 100	41, 58, 78, 81	0
21	U	119/119 (100%)	0.26	2 (1%) 69 46	37, 56, 79, 92	0
22	V	53/66 (80%)	0.29	0 100 100	40, 55, 72, 79	0
23	W	65/70 (92%)	0.48	3 (4%) 37 20	49, 71, 105, 112	0
24	X	154/154 (100%)	-0.08	0 100 100	34, 46, 65, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	82/91 (90%)	0.26	3 (3%) 45 25	42, 57, 82, 99	0
26	Z	142/240 (59%)	-0.06	2 (1%) 73 51	26, 44, 65, 83	0
27	1	73/73 (100%)	0.56	3 (4%) 41 22	45, 59, 75, 84	0
28	2	56/56 (100%)	-0.40	0 100 100	21, 34, 39, 41	0
29	3	46/48 (95%)	0.38	1 (2%) 62 39	35, 60, 85, 96	0
30	4	92/92 (100%)	0.19	1 (1%) 78 57	35, 55, 69, 80	0
All	All	6577/7279 (90%)	0.07	148 (2%) 61 38	18, 50, 90, 146	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1173	A	6.5
23	W	1	THR	6.4
2	B	3025	G	6.3
1	A	1175	G	5.4
1	A	1176	C	4.6
2	B	3001	U	4.4
6	F	10	PHE	4.4
7	G	10	ASP	4.3
1	A	1160	G	4.3
1	A	1177	A	4.0
1	A	10	U	4.0
2	B	3024	U	4.0
15	O	186	LEU	3.9
1	A	1190	G	3.8
1	A	1165	G	3.7
1	A	2345	A	3.7
1	A	138	U	3.6
18	R	95	GLU	3.6
1	A	1168	C	3.6
4	D	1	PRO	3.6
17	Q	116	SER	3.6
1	A	1204	C	3.5
1	A	1161	A	3.5
1	A	1193	A	3.4
1	A	1184	C	3.4
1	A	1964	U	3.4
15	O	168	LEU	3.4
1	A	1167	G	3.3
1	A	1172	G	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	37	VAL	3.3
7	G	45	ASP	3.3
3	C	36	ASP	3.3
2	B	3023	U	3.3
2	B	3002	U	3.3
1	A	1174	A	3.2
1	A	1192	A	3.2
1	A	1181	A	3.2
6	F	69	ILE	3.2
6	F	63	ILE	3.1
1	A	735	C	3.1
1	A	1195	G	3.1
1	A	1171	A	3.0
1	A	1162	G	3.0
10	J	167	ALA	3.0
10	J	135	TRP	3.0
25	Y	88	GLU	2.9
15	O	162	ASP	2.9
9	I	26	MET	2.9
1	A	1169	U	2.8
14	N	87	MET	2.8
23	W	40	PRO	2.8
6	F	62	ASP	2.7
10	J	32	ASP	2.7
1	A	1198	U	2.7
1	A	1199	A	2.7
1	A	1561	U	2.7
1	A	2256	G	2.7
1	A	1205	U	2.7
1	A	2257	G	2.7
14	N	165	SER	2.7
26	Z	235	GLU	2.6
1	A	2254	G	2.6
1	A	1188	A	2.6
13	M	83	GLU	2.6
10	J	40	PRO	2.6
1	A	2507	G	2.6
9	I	71	LEU	2.6
10	J	114	PRO	2.6
1	A	736	A	2.6
6	F	21	VAL	2.6
1	A	1191	A	2.5

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Mol	Chain	Res	Type	RSRZ
27	1	22	ILE	2.5
29	3	37	HIS	2.5
2	B	3022	G	2.5
23	W	2	VAL	2.5
15	O	1	ALA	2.5
6	F	35	ALA	2.5
6	F	66	GLY	2.5
1	A	1163	G	2.4
1	A	1206	U	2.4
12	L	63	GLU	2.4
1	A	1203	G	2.4
6	F	75	LEU	2.4
7	G	100	ASP	2.4
1	A	1166	A	2.4
15	O	169	PRO	2.4
6	F	59	GLY	2.4
26	Z	108	ASP	2.4
1	A	128	A	2.4
13	M	148	GLU	2.4
1	A	130	C	2.3
1	A	2769	C	2.3
6	F	100	ASP	2.3
6	F	107	GLY	2.3
15	O	185	GLU	2.3
21	U	115	GLU	2.3
9	I	29	SER	2.3
1	A	716	G	2.3
1	A	1197	G	2.3
1	A	1951	G	2.3
1	A	2250	G	2.3
1	A	2344	G	2.3
7	G	81	GLU	2.3
9	I	63	ARG	2.3
13	M	81	VAL	2.3
10	J	38	ALA	2.3
1	A	1201	C	2.3
2	B	3039	U	2.2
1	A	960	G	2.2
1	A	1524	U	2.2
1	A	285	A	2.2
1	A	574	C	2.2
7	G	11	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1185	U	2.2
1	A	2511	A	2.2
6	F	49	PRO	2.2
1	A	999	C	2.2
9	I	24	VAL	2.2
1	A	1170	U	2.2
6	F	171	ASP	2.2
1	A	806	A	2.2
6	F	102	GLY	2.1
1	A	1207	A	2.1
6	F	105	SER	2.1
9	I	13	PRO	2.1
21	U	1	SER	2.1
30	4	8	ASN	2.1
15	O	167	ASP	2.1
27	1	47	LEU	2.1
25	Y	82	GLU	2.1
1	A	1525	G	2.1
15	O	179	LEU	2.1
27	1	41	VAL	2.1
1	A	1194	A	2.1
8	H	106	THR	2.1
6	F	58	VAL	2.0
15	O	147	ILE	2.0
1	A	1189	A	2.0
1	A	1200	A	2.0
10	J	39	GLY	2.0
1	A	282	C	2.0
1	A	2335	C	2.0
1	A	1214	G	2.0
8	H	26	THR	2.0
25	Y	87	ALA	2.0
5	E	151	GLN	2.0
6	F	172	VAL	2.0
6	F	174	VAL	2.0

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

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

6.3 Carbohydrates [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
34	NA	A	8329	1/1	0.38	0.16	60,60,60,60	0
34	NA	A	8371	1/1	0.48	0.38	47,47,47,47	0
34	NA	S	8386	1/1	0.63	0.31	83,83,83,83	0
34	NA	A	8384	1/1	0.64	0.17	79,79,79,79	0
34	NA	A	8306	1/1	0.66	0.17	39,39,39,39	0
34	NA	A	8385	1/1	0.67	0.24	50,50,50,50	0
34	NA	A	8363	1/1	0.68	0.35	54,54,54,54	0
34	NA	B	8383	1/1	0.69	0.32	52,52,52,52	0
32	MG	A	8106	1/1	0.72	0.13	50,50,50,50	0
34	NA	A	8382	1/1	0.72	0.35	71,71,71,71	0
34	NA	A	8365	1/1	0.72	0.11	36,36,36,36	0
34	NA	B	8351	1/1	0.75	0.14	30,30,30,30	0
32	MG	A	8066	1/1	0.75	0.17	94,94,94,94	0
32	MG	A	8049	1/1	0.75	0.14	68,68,68,68	0
32	MG	A	8092	1/1	0.76	0.13	75,75,75,75	0
34	NA	A	8368	1/1	0.77	0.24	57,57,57,57	0
34	NA	A	8340	1/1	0.78	0.14	47,47,47,47	0
34	NA	A	8367	1/1	0.78	0.11	41,41,41,41	0
32	MG	A	8102	1/1	0.80	0.12	48,48,48,48	0
34	NA	A	8328	1/1	0.80	0.17	41,41,41,41	0
32	MG	A	8087	1/1	0.80	0.12	67,67,67,67	0
34	NA	T	8312	1/1	0.80	0.10	39,39,39,39	0
34	NA	A	8352	1/1	0.81	0.13	49,49,49,49	0
34	NA	A	8381	1/1	0.82	0.16	44,44,44,44	0
34	NA	A	8326	1/1	0.82	0.21	61,61,61,61	0
34	NA	A	8324	1/1	0.83	0.24	43,43,43,43	0
34	NA	A	8369	1/1	0.83	0.30	49,49,49,49	0
32	MG	A	8050	1/1	0.83	0.09	57,57,57,57	0
34	NA	A	8374	1/1	0.83	0.34	65,65,65,65	0
34	NA	A	8366	1/1	0.83	0.16	60,60,60,60	0
34	NA	A	8313	1/1	0.83	0.15	64,64,64,64	0
34	NA	A	8349	1/1	0.84	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	A	8377	1/1	0.84	0.25	61,61,61,61	0
34	NA	A	8302	1/1	0.84	0.14	44,44,44,44	0
32	MG	B	8095	1/1	0.84	0.23	75,75,75,75	0
34	NA	A	8372	1/1	0.84	0.29	60,60,60,60	0
34	NA	A	8301	1/1	0.85	0.08	16,16,16,16	0
34	NA	A	8359	1/1	0.85	0.20	53,53,53,53	0
34	NA	A	8362	1/1	0.85	0.28	66,66,66,66	0
32	MG	U	8073	1/1	0.86	0.07	52,52,52,52	0
34	NA	A	8333	1/1	0.86	0.13	38,38,38,38	0
32	MG	A	8090	1/1	0.86	0.27	55,55,55,55	0
32	MG	A	8045	1/1	0.86	0.10	49,49,49,49	0
32	MG	A	8094	1/1	0.86	0.16	65,65,65,65	0
35	CL	A	8522	1/1	0.86	0.29	85,85,85,85	0
34	NA	A	8379	1/1	0.87	0.16	44,44,44,44	0
34	NA	A	8341	1/1	0.87	0.06	36,36,36,36	0
34	NA	A	8323	1/1	0.87	0.13	33,33,33,33	0
34	NA	A	8332	1/1	0.87	0.19	42,42,42,42	0
34	NA	A	8358	1/1	0.87	0.31	86,86,86,86	0
35	CL	Z	8520	1/1	0.87	0.14	39,39,39,39	0
35	CL	A	8517	1/1	0.88	0.08	52,52,52,52	0
32	MG	A	8088	1/1	0.88	0.12	24,24,24,24	0
34	NA	A	8376	1/1	0.88	0.17	38,38,38,38	0
34	NA	A	8357	1/1	0.89	0.16	50,50,50,50	0
34	NA	A	8319	1/1	0.89	0.07	23,23,23,23	0
32	MG	A	8081	1/1	0.89	0.07	60,60,60,60	0
34	NA	A	8361	1/1	0.89	0.15	60,60,60,60	0
34	NA	A	8373	1/1	0.89	0.21	49,49,49,49	0
34	NA	R	8348	1/1	0.89	0.04	34,34,34,34	0
34	NA	S	8337	1/1	0.89	0.09	41,41,41,41	0
32	MG	A	8091	1/1	0.89	0.07	52,52,52,52	0
32	MG	A	8051	1/1	0.89	0.10	70,70,70,70	0
34	NA	A	8311	1/1	0.89	0.10	55,55,55,55	0
32	MG	A	8076	1/1	0.89	0.11	68,68,68,68	0
35	CL	N	8518	1/1	0.89	0.09	53,53,53,53	0
34	NA	A	8355	1/1	0.89	0.20	58,58,58,58	0
34	NA	A	8330	1/1	0.90	0.07	41,41,41,41	0
34	NA	A	8331	1/1	0.90	0.14	51,51,51,51	0
34	NA	A	8308	1/1	0.90	0.14	53,53,53,53	0
34	NA	J	8322	1/1	0.90	0.23	59,59,59,59	0
35	CL	C	8509	1/1	0.90	0.10	64,64,64,64	0
35	CL	M	8510	1/1	0.90	0.10	74,74,74,74	0
32	MG	A	8114	1/1	0.90	0.07	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	CL	O	8507	1/1	0.90	0.08	65,65,65,65	0
32	MG	A	8024	1/1	0.90	0.07	29,29,29,29	0
32	MG	A	8052	1/1	0.91	0.09	63,63,63,63	0
32	MG	C	8105	1/1	0.91	0.12	6,6,6,6	0
32	MG	A	8046	1/1	0.91	0.07	53,53,53,53	0
32	MG	A	8103	1/1	0.91	0.13	49,49,49,49	0
34	NA	A	8354	1/1	0.91	0.17	39,39,39,39	0
35	CL	K	8502	1/1	0.91	0.07	62,62,62,62	0
34	NA	A	8375	1/1	0.91	0.16	47,47,47,47	0
34	NA	A	8321	1/1	0.91	0.18	39,39,39,39	0
32	MG	A	8082	1/1	0.91	0.14	60,60,60,60	0
32	MG	A	8067	1/1	0.91	0.12	48,48,48,48	0
35	CL	4	8504	1/1	0.91	0.10	54,54,54,54	0
31	ANM	A	9000	19/19	0.92	0.14	27,35,41,42	0
32	MG	A	8041	1/1	0.92	0.09	43,43,43,43	0
32	MG	A	8093	1/1	0.92	0.05	37,37,37,37	0
32	MG	A	8042	1/1	0.92	0.08	41,41,41,41	0
34	NA	A	8360	1/1	0.92	0.21	53,53,53,53	0
32	MG	A	8099	1/1	0.92	0.08	47,47,47,47	0
32	MG	A	8101	1/1	0.92	0.13	55,55,55,55	0
35	CL	R	8511	1/1	0.92	0.11	63,63,63,63	0
32	MG	A	8064	1/1	0.92	0.15	20,20,20,20	0
35	CL	A	8505	1/1	0.92	0.19	85,85,85,85	0
34	NA	A	8364	1/1	0.93	0.16	43,43,43,43	0
35	CL	A	8503	1/1	0.93	0.08	60,60,60,60	0
34	NA	A	8350	1/1	0.93	0.14	45,45,45,45	0
35	CL	A	8512	1/1	0.93	0.11	22,22,22,22	0
35	CL	A	8514	1/1	0.93	0.11	67,67,67,67	0
32	MG	A	8104	1/1	0.93	0.06	42,42,42,42	0
34	NA	A	8314	1/1	0.93	0.06	13,13,13,13	0
34	NA	A	8316	1/1	0.93	0.20	52,52,52,52	0
34	NA	A	8318	1/1	0.93	0.13	40,40,40,40	0
34	NA	A	8305	1/1	0.93	0.07	34,34,34,34	0
32	MG	A	8116	1/1	0.93	0.06	46,46,46,46	0
34	NA	A	8335	1/1	0.93	0.15	52,52,52,52	0
33	K	A	8201	1/1	0.93	0.15	69,69,69,69	0
34	NA	A	8310	1/1	0.93	0.10	32,32,32,32	0
32	MG	A	8111	1/1	0.93	0.06	49,49,49,49	0
32	MG	A	8089	1/1	0.94	0.11	63,63,63,63	0
34	NA	A	8378	1/1	0.94	0.15	41,41,41,41	0
32	MG	A	8075	1/1	0.94	0.06	51,51,51,51	0
32	MG	A	8096	1/1	0.94	0.04	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8053	1/1	0.94	0.07	34,34,34,34	0
34	NA	A	8356	1/1	0.94	0.17	53,53,53,53	0
32	MG	A	8010	1/1	0.94	0.03	26,26,26,26	0
34	NA	A	8325	1/1	0.94	0.09	51,51,51,51	0
34	NA	A	8336	1/1	0.94	0.05	45,45,45,45	0
34	NA	E	8304	1/1	0.94	0.09	35,35,35,35	0
34	NA	A	8339	1/1	0.94	0.04	15,15,15,15	0
34	NA	K	8346	1/1	0.94	0.07	35,35,35,35	0
34	NA	A	8315	1/1	0.94	0.12	36,36,36,36	0
34	NA	A	8327	1/1	0.94	0.10	18,18,18,18	0
34	NA	A	8307	1/1	0.94	0.07	45,45,45,45	0
34	NA	A	8334	1/1	0.95	0.07	30,30,30,30	0
32	MG	A	8057	1/1	0.95	0.09	31,31,31,31	0
32	MG	A	8117	1/1	0.95	0.07	40,40,40,40	0
34	NA	A	8370	1/1	0.95	0.24	58,58,58,58	0
32	MG	A	8044	1/1	0.95	0.15	51,51,51,51	0
34	NA	A	8317	1/1	0.95	0.04	29,29,29,29	0
34	NA	C	8345	1/1	0.95	0.06	52,52,52,52	0
35	CL	D	8519	1/1	0.95	0.12	57,57,57,57	0
32	MG	A	8108	1/1	0.95	0.16	79,79,79,79	0
34	NA	A	8344	1/1	0.95	0.07	29,29,29,29	0
32	MG	A	8086	1/1	0.95	0.07	47,47,47,47	0
32	MG	Z	8109	1/1	0.95	0.07	41,41,41,41	0
35	CL	P	8508	1/1	0.95	0.08	85,85,85,85	0
32	MG	A	8112	1/1	0.95	0.12	45,45,45,45	0
34	NA	A	8353	1/1	0.95	0.05	27,27,27,27	0
32	MG	A	8098	1/1	0.95	0.16	18,18,18,18	0
34	NA	M	8380	1/1	0.96	0.16	48,48,48,48	0
32	MG	A	8047	1/1	0.96	0.08	55,55,55,55	0
32	MG	L	8069	1/1	0.96	0.05	55,55,55,55	0
34	NA	A	8303	1/1	0.96	0.17	62,62,62,62	0
32	MG	A	8070	1/1	0.96	0.09	33,33,33,33	0
34	NA	U	8343	1/1	0.96	0.04	24,24,24,24	0
32	MG	A	8085	1/1	0.96	0.07	63,63,63,63	0
33	K	A	8200	1/1	0.96	0.10	66,66,66,66	0
34	NA	A	8342	1/1	0.96	0.07	28,28,28,28	0
35	CL	A	8513	1/1	0.96	0.06	44,44,44,44	0
35	CL	S	8506	1/1	0.96	0.05	44,44,44,44	0
32	MG	A	8100	1/1	0.96	0.11	72,72,72,72	0
35	CL	A	8515	1/1	0.96	0.17	68,68,68,68	0
32	MG	A	8097	1/1	0.97	0.11	30,30,30,30	0
32	MG	A	8027	1/1	0.97	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	A	8320	1/1	0.97	0.08	31,31,31,31	0
35	CL	K	8501	1/1	0.97	0.04	58,58,58,58	0
35	CL	A	8516	1/1	0.97	0.06	45,45,45,45	0
35	CL	K	8521	1/1	0.97	0.05	44,44,44,44	0
32	MG	A	8022	1/1	0.97	0.05	53,53,53,53	0
36	CD	P	8405	1/1	0.97	0.04	82,82,82,82	0
32	MG	A	8072	1/1	0.98	0.05	60,60,60,60	0
32	MG	A	8008	1/1	0.98	0.05	37,37,37,37	0
32	MG	A	8048	1/1	0.98	0.04	39,39,39,39	0
32	MG	D	8055	1/1	0.98	0.04	34,34,34,34	0
32	MG	A	8059	1/1	0.98	0.04	32,32,32,32	0
34	NA	S	8338	1/1	0.98	0.04	38,38,38,38	0
32	MG	A	8062	1/1	0.98	0.05	64,64,64,64	0
32	MG	A	8023	1/1	0.98	0.04	33,33,33,33	0
32	MG	A	8110	1/1	0.98	0.05	20,20,20,20	0
32	MG	A	8001	1/1	0.98	0.04	16,16,16,16	0
32	MG	A	8016	1/1	0.98	0.04	46,46,46,46	0
32	MG	A	8113	1/1	0.98	0.08	25,25,25,25	0
32	MG	A	8068	1/1	0.98	0.03	57,57,57,57	0
32	MG	A	8115	1/1	0.98	0.04	41,41,41,41	0
32	MG	A	8040	1/1	0.98	0.10	49,49,49,49	0
34	NA	J	8309	1/1	0.98	0.03	18,18,18,18	0
36	CD	4	8404	1/1	0.98	0.02	62,62,62,62	0
34	NA	N	8347	1/1	0.99	0.06	12,12,12,12	0
32	MG	A	8083	1/1	0.99	0.04	35,35,35,35	0
32	MG	A	8084	1/1	0.99	0.06	49,49,49,49	0
32	MG	A	8009	1/1	0.99	0.06	37,37,37,37	0
32	MG	A	8005	1/1	0.99	0.03	49,49,49,49	0
32	MG	A	8012	1/1	0.99	0.05	29,29,29,29	0
32	MG	A	8028	1/1	0.99	0.03	41,41,41,41	0
32	MG	A	8030	1/1	0.99	0.03	19,19,19,19	0
32	MG	A	8032	1/1	0.99	0.07	30,30,30,30	0
32	MG	4	8078	1/1	0.99	0.04	45,45,45,45	0
32	MG	A	8056	1/1	0.99	0.05	37,37,37,37	0
32	MG	A	8033	1/1	0.99	0.03	27,27,27,27	0
32	MG	A	8035	1/1	0.99	0.06	38,38,38,38	0
32	MG	A	8060	1/1	0.99	0.03	29,29,29,29	0
32	MG	A	8061	1/1	0.99	0.04	22,22,22,22	0
32	MG	A	8037	1/1	0.99	0.05	34,34,34,34	0
32	MG	A	8063	1/1	0.99	0.08	78,78,78,78	0
32	MG	A	8038	1/1	0.99	0.03	16,16,16,16	0
32	MG	A	8039	1/1	0.99	0.04	47,47,47,47	0

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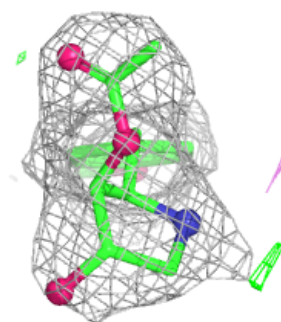
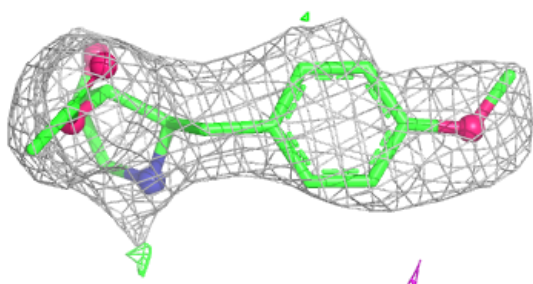
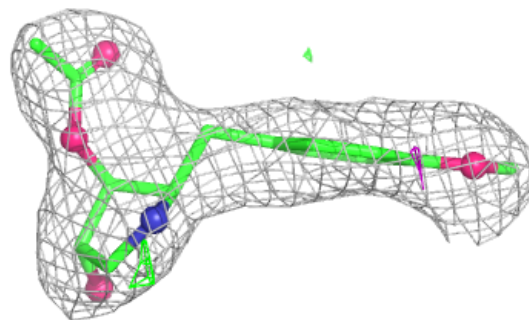
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8013	1/1	0.99	0.02	39,39,39,39	0
32	MG	A	8014	1/1	0.99	0.05	18,18,18,18	0
32	MG	A	8007	1/1	0.99	0.05	14,14,14,14	0
32	MG	A	8071	1/1	0.99	0.03	75,75,75,75	0
32	MG	A	8043	1/1	0.99	0.04	23,23,23,23	0
32	MG	A	8018	1/1	0.99	0.03	49,49,49,49	0
32	MG	A	8019	1/1	0.99	0.06	27,27,27,27	0
32	MG	A	8077	1/1	0.99	0.06	20,20,20,20	0
32	MG	A	8079	1/1	0.99	0.04	39,39,39,39	0
32	MG	A	8080	1/1	0.99	0.04	55,55,55,55	0
32	MG	A	8020	1/1	0.99	0.03	38,38,38,38	0
36	CD	V	8401	1/1	0.99	0.03	59,59,59,59	0
36	CD	1	8403	1/1	0.99	0.02	60,60,60,60	0
36	CD	2	8402	1/1	0.99	0.03	59,59,59,59	0
32	MG	A	8003	1/1	0.99	0.04	17,17,17,17	0
32	MG	A	8004	1/1	1.00	0.07	24,24,24,24	0
32	MG	A	8031	1/1	1.00	0.03	22,22,22,22	0
32	MG	A	8021	1/1	1.00	0.06	22,22,22,22	0
32	MG	A	8015	1/1	1.00	0.04	47,47,47,47	0
32	MG	C	8065	1/1	1.00	0.04	35,35,35,35	0
32	MG	A	8034	1/1	1.00	0.06	10,10,10,10	0
32	MG	A	8011	1/1	1.00	0.02	20,20,20,20	0
32	MG	A	8036	1/1	1.00	0.03	25,25,25,25	0
32	MG	A	8017	1/1	1.00	0.03	20,20,20,20	0
32	MG	A	8025	1/1	1.00	0.02	37,37,37,37	0
32	MG	A	8026	1/1	1.00	0.05	12,12,12,12	0
32	MG	A	8107	1/1	1.00	0.02	41,41,41,41	0
32	MG	A	8002	1/1	1.00	0.03	32,32,32,32	0
32	MG	A	8054	1/1	1.00	0.02	40,40,40,40	0
32	MG	A	8074	1/1	1.00	0.06	16,16,16,16	0
32	MG	A	8006	1/1	1.00	0.02	46,46,46,46	0
32	MG	A	8029	1/1	1.00	0.02	49,49,49,49	0
32	MG	A	8058	1/1	1.00	0.03	42,42,42,42	0

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

Electron density around ANM A 9000:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.