



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:15 PM BST

PDB ID : 3J7Z
EMDB ID: : EMD-6057
Title : Structure of the E. coli 50S subunit with ErmCL nascent chain
Authors : Arenz, S.; Meydan, S.; Starosta, A.L.; Berninghausen, O.; Beckmann, R.;
Vazquez-Laslop, N.; Wilson, D.N.
Deposited on : 2014-08-27
Resolution : 3.90 Å(reported)
Based on PDB ID : 4KIX

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

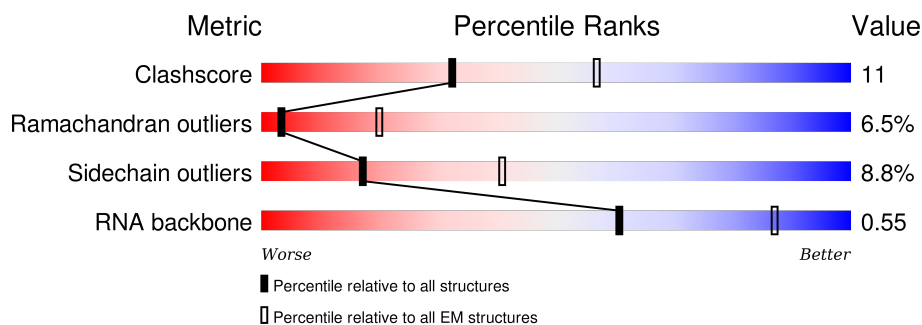
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.


























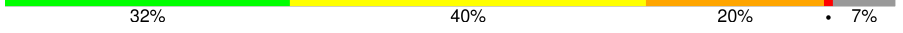

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	57	75% 19% . .
2	1	55	58% 25% 7% 9%
3	2	46	78% 20% .
4	3	65	77% 17% 5% .
5	4	38	55% 39% . .
6	5	165	25% 38% 18% 8% 10%
7	6	121	17% 6% . 75%
8	7	3	100%

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Mol	Chain	Length	Quality of chain
9	A	2903	
10	B	118	
11	C	273	
12	D	209	
13	E	201	
14	F	179	
15	G	177	
16	H	149	
17	I	142	
18	J	142	
19	K	123	
20	L	144	
21	M	136	
22	N	127	
23	O	117	
24	P	115	
25	Q	118	
26	R	103	
27	S	110	
28	T	100	
29	U	104	
30	V	94	
31	W	85	
32	X	78	
33	Y	63	

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Mol	Chain	Length	Quality of chain
34	Z	59	<div><div></div><div>54%</div><div>34%</div><div>8%</div><div></div></div>
35	a	19	<div><div></div><div>32%</div><div>5%</div><div>63%</div><div></div></div>

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 90700 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 7 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 8 is a RNA chain called P-tRNA CCA-end.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	3	Total	C	N	O	P	0	0
			58	28	11	17	2		

- Molecule 9 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	2854	Total	C	N	O	P	0	0
			61274	27334	11279	19807	2854		

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 13 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 17 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 18 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 19 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 20 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 21 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 22 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 23 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 24 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 25 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 26 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 27 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 28 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 29 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 30 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 32 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 33 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

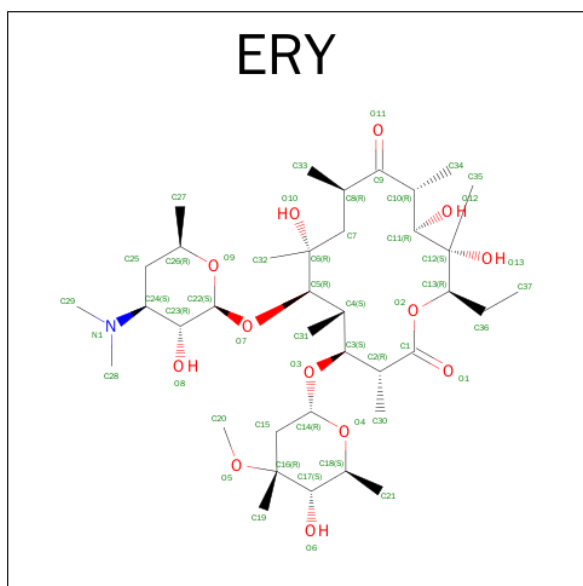
- Molecule 34 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 35 is a protein called ErmCL nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	a	7	Total	C	N	O	0	3
			36	27	4	5		

- Molecule 36 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $\text{C}_{37}\text{H}_{67}\text{NO}_{13}$).

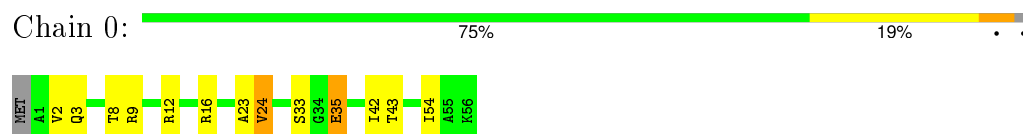


Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	N	O	0
			51	37	1	13	

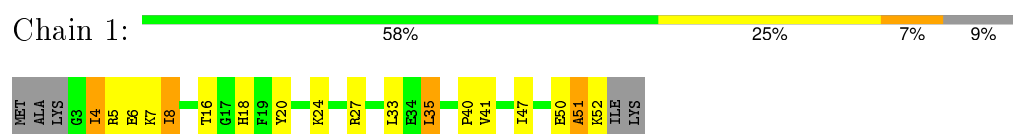
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

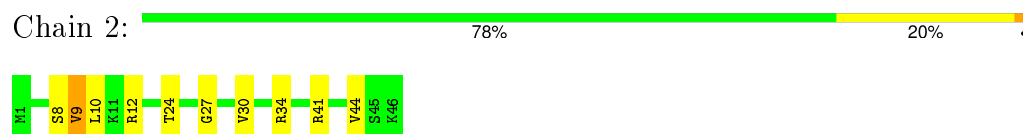
- Molecule 1: 50S ribosomal protein L32



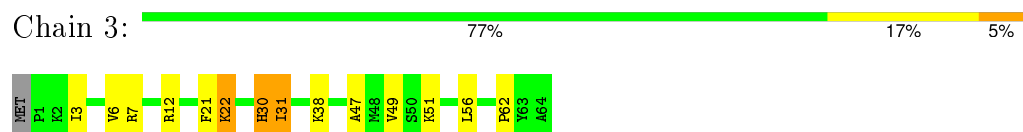
- Molecule 2: 50S ribosomal protein L33



- Molecule 3: 50S ribosomal protein L34



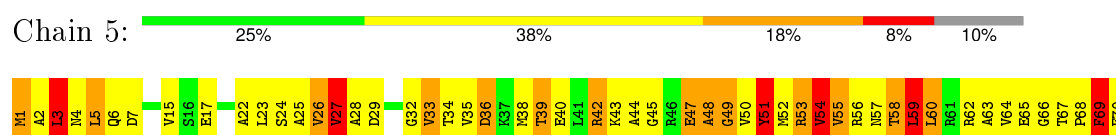
- Molecule 4: 50S ribosomal protein L35

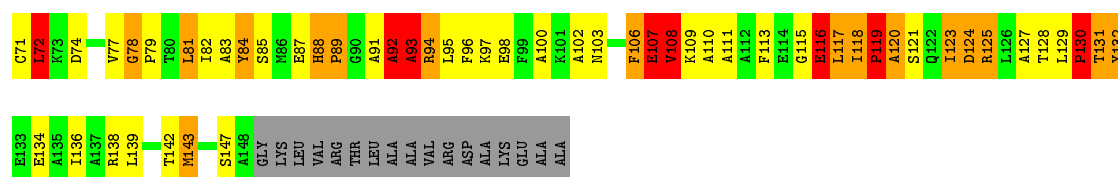


- Molecule 5: 50S ribosomal protein L36

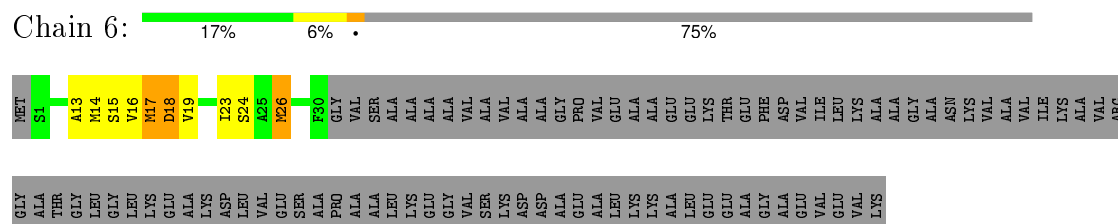


- Molecule 6: 50S ribosomal protein L10





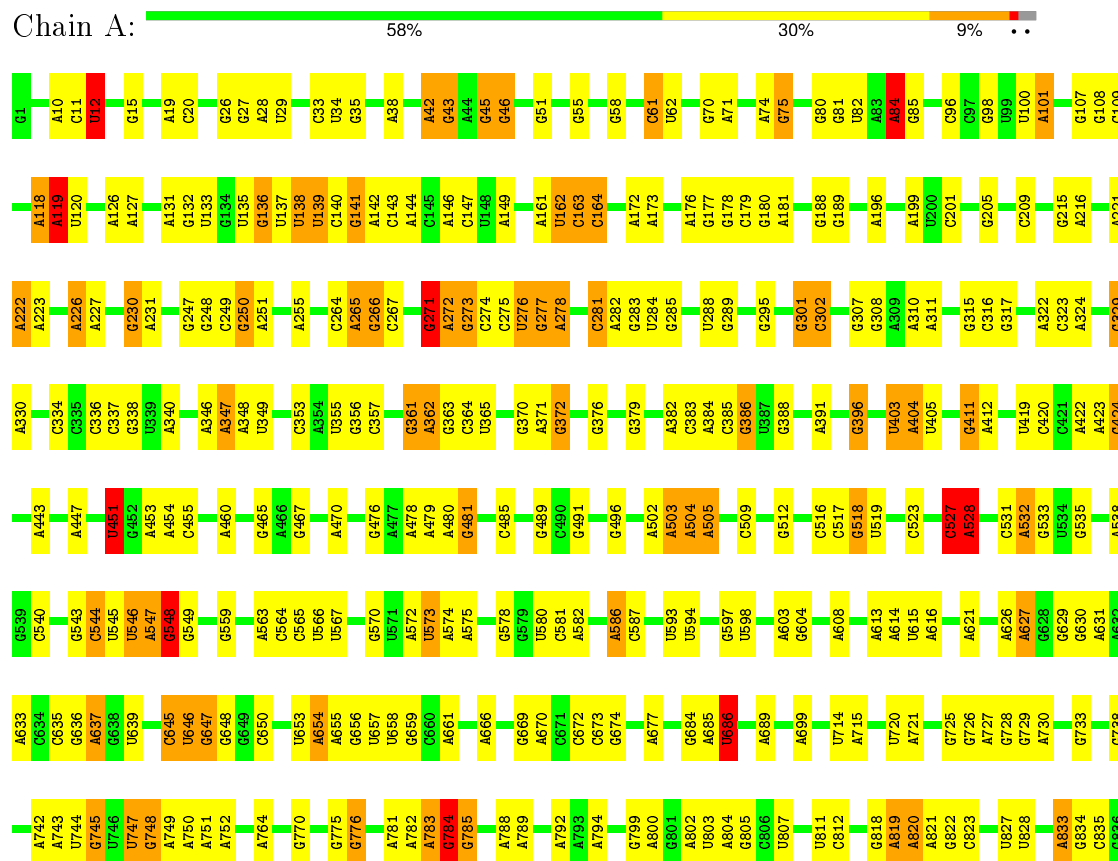
- Molecule 7: 50S ribosomal protein L7/L12



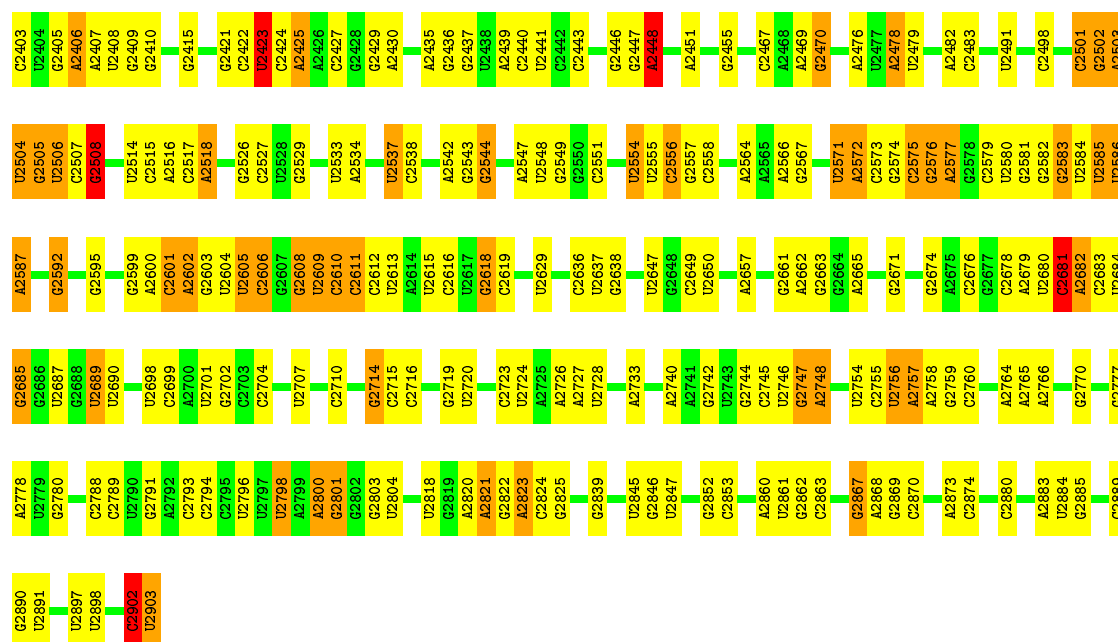
- Molecule 8: P-tRNA CCA-end



- Molecule 9: 23S rRNA



A2311	U2210	U2139	C2055	U1965	A1819	U1747	A1618	A1509	C1398	G1309	U1199	G1124	A1046	C837
U2312	A2211	G2141	G2056	U1966	U1820	C1748	G1622	G1510	A1403	G1310	U1203	G1125	G1047	C838
C2313	A2212	A2142	A2057	C1967	G1824	G1750	G1622	G1514	C1404	U1312	A1204	A1129	G1051	U839
A2314	U2213	C2143	A2059	C1967	G1824	G1750	G1622	A1515	C1404	U1312	G1206	U1130	C1052	C841
G2318	C2214	C2144	A2060	A1960	A1829	G1753	A1754	U1523	C1414	G1317	C1207	U1132	C1053	A845
G2319	A2225	C2145	G2061	U1963	G1830	A1754	C1638	G1524	U1415	U1317	U1219	A1134	A1057	U846
U2320	C2226	A2147	A2062	U1963	G1831	A1757	C1639	G1524	G1417	U1317	U1219	A1134	U1058	U847
U2321	A2227	C2148	C2063	A1966	G1832	A1758	C1639	C1533	A1418	A1322	G1223	A1135	U1059	A959
U2322	G2228	U2149	C2064	C1967	G1833	A1759	C1639	U1534	A1419	A1323	U1224	G1136	U1060	A960
G2323	U2229	C2150	A2069	G1968	C1837	C1760	G1644	A1535	A1419	G1324	U1224	U1141	U1061	A961
U2324	G2230	U2151	G2070	A1969	C1838	C1761	G1645	C1536	A1420	U1324	U1224	G1139	U1062	A962
G2325	U2231	C2152	A2071	A1970	G1839	A1762	G1646	G1537	C1428	A1327	C1229	C1140	G1063	A965
C2326	C2232	C2153	C2072	U1971	G1840	C1764	U1647	G1538	G1429	U1328	U1232	U1142	U1064	A966
A2327	G2238	A2154	C2073	G1972	C1843	C1764	U1648	U1542	G1430	U1329	G1232	U1142	U1065	A967
U2328	U2239	U2155	U2074	U1979	C1844	C1764	G1649	U1543	G1435	C1330	C1233	G1149	U1066	A971
G2329	G2240	G2157	U2075	G1980	G1847	C1771	A1652	G1543	G1436	A1336	G1238	C1150	A1067	A972
G2330	A2241	A	C2091	U1983	A1848	A1772	G1653	A1553	C1437	G1337	G1239	A1151	G1068	A973
C2331	U2244	C	U2092	C1983	A1848	A1772	G1653	A1553	C1437	G1337	U1240	G1152	A1069	A974
U2332	C	C	C2093	C	G1857	C1774	A1654	C1565	A1439	U1339	U1240	C1153	G1071	A975
U2333	U2244	C	A2094	U1991	A1858	U1775	A1655	A1566	U1440	U1340	A1247	G1154	C1072	A878
U2334	U2244	C	C	U1992	U1864	G1776	G1659	G1567	G1441	G1341	U1248	A1155	A1074	A979
A2335	G2250	G	C2103	U1993	U1864	U1777	U1662	G1568	U1442	A1342	U1249	A1156	G1075	A980
A2336	G2251	A	C2104	U1993	U1864	U1777	U1662	G1568	U1442	A1342	U1249	A1156	G1075	A981
G2337	G2252	C	C2105	C1996	G1867	U1778	U1662	G1568	U1443	G1343	G1250	G1157	A1077	A982
G2341	U2259	U	U2106	C1997	C1868	U1779	U1662	A1570	G1444	U1344	G1251	G1160	C1076	A983
U2342	U2260	C	C2107	A1998	G1869	U1782	C1670	A1571	G1445	C1349	G1252	C1161	U1078	A984
U2343	U2261	U	A2108	U2011	A1870	A1784	G1674	U1578	C1446	C1350	A1253	A1169	C1079	A985
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A2346	A2267	A	C2110	A2015	A1872	A1785	G1674	U1578	C1446	C1350	A1253	A1169	A1080	A987
U2347	A2268	U	U	U2016	A1873	A1786	A1677	G1581	U1458	U1352	A1262	C1170	U1083	A988
U2348	U2268	U	U	U2017	G1884	A1789	A1677	C1582	U1459	A1353	U1263	C1171	A1084	A989
A2352	G2271	C	A	G2018	C1905	C1790	G1681	U1584	G1465	G1355	A1265	U1174	A1086	A994
G2353	A2274	C	G	A2019	G1906	A1791	G1681	U1584	U1466	G1355	A1265	U1174	A1086	A995
C2354	G2275	A	G	A2020	G1906	A1791	G1681	U1584	U1466	G1355	A1265	U1174	A1086	A996
G2355	C2276	C	A	C2021	G1906	A1791	G1681	U1584	U1466	G1355	A1265	U1174	A1086	A996
U2356	U2277	C	U	C2022	A1913	C1914	U1795	G1587	U1469	U1358	U1267	G1177	A1089	A999
A2357	A2278	U	A	C2023	U1915	U1797	U1795	G1587	U1469	U1358	U1267	G1177	A1089	A999
G2358	G2279	G	G	G2024	U1915	U1797	U1795	G1587	U1469	U1358	U1267	G1177	A1089	A999
U2359	U2280	U	U	A2030	U1915	U1797	U1795	G1587	U1469	U1358	U1267	G1177	A1089	A999
A2360	G2281	C	U	G2031	A1927	C1800	G1703	C1691	U1474	G1368	A1272	U1181	U1094	A910
U2361	C2282	G	G	A2032	A1928	A1801	G1703	C1691	U1474	G1368	A1272	U1181	U1094	A911
G2362	A2283	U	U	C2033	G1929	A1802	G1703	C1691	U1474	G1368	A1272	U1181	U1094	A912
U2363	U2284	G	G	A2034	G1930	A1803	U1714	U1594	G1478	U1379	U1273	U1183	A1096	A913
G2364	G2285	A	A	G2035	G1930	A1803	U1714	U1594	G1478	U1379	U1273	U1183	A1096	A914
U2365	C2286	U	U	G2036	G1930	A1803	U1714	U1594	G1478	U1379	U1273	U1183	A1096	A915
A2366	A2287	U	U	A2037	G1935	A1805	U1722	C1606	U1485	G1384	A1284	G1186	A1098	A916
U2367	G2288	C	C	G2038	A1936	A1805	U1722	C1606	U1485	G1384	A1284	G1186	A1098	A916
A2368	U2289	U	U	U2039	A1937	A1805	U1722	C1606	U1485	G1384	A1284	G1186	A1098	A916
G2369	G2290	U	U	G2040	A1938	A1805	U1722	C1606	U1485	G1384	A1284	G1186	A1098	A916
U2370	A2291	U	U	C2043	U1939	U1811	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
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U2372	C2293	U	U	A2045	G1943	G1813	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
G2373	U2294	U	U	C2046	U1944	G1814	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2374	G2295	U	U	G2047	U1945	G1815	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
A2375	A2296	U	U	C2048	U1946	G1816	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2376	U2297	U	U	G2049	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
G2377	G2298	U	U	A2050	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2378	A2299	U	U	C2053	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
A2379	U2299	U	U	G2054	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2380	C2299	U	U	A2055	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
G2381	U2300	U	U	C2056	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2382	A2301	U	U	G2057	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
A2383	U2302	U	U	C2058	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2384	G2303	U	U	A2059	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
G2385	U2304	U	U	C2059	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
A2386	A2305	U	U	G2060	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2387	U2306	U	U	C2061	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
A2388	G2307	U	U	A2062	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2389	U2308	U	U	C2063	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
G2390	A2309	U	U	G2064	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2391	U2310	U	U	A2065	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
A2392	G2311	U	U	C2066	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2393	U2312	U	U	A2067	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
G2394	A2313	U	U	G2068	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2395	U2314	U	U	C2069	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
A2396	G2315	U	U	A2070	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2397	A2316	U	U	C2071	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
G2398	U2317	U	U	G2072	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2399	A2318	U	U	A2073	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
A2400	G2319	U	U	C2074	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2401	U2320	U	U	A2075	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
G2402	A2321	U	U	G2076	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2403	U2322	U	U	A2077	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
A2404	G2323	U	U	C2078	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2405	U2324	U	U	A2079	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
G2406	A2325	U	U	G2079	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2407	U2326	U	U	A2080	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
A2408	G2327	U	U	C2080	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
U2409	U2328	U	U	A2081	U1946	G1817	C1730	C1610	U1487	A1387	A1284	G1186	A1098	A916
G2410	A2329	U	U	G2082	U1946	G1817	C1730	C1610	U1487	A1387				



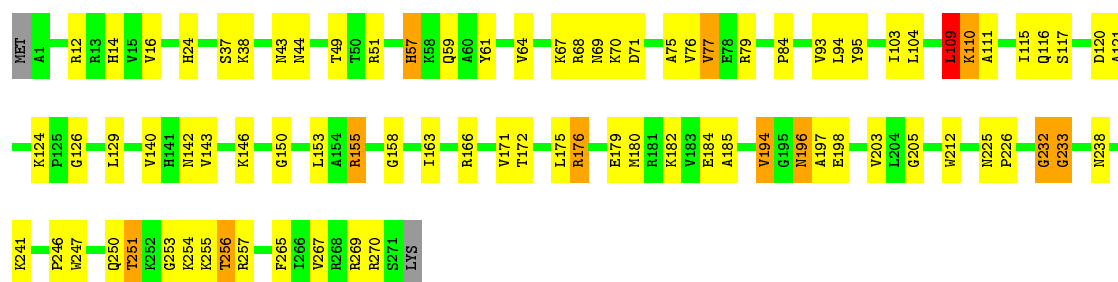
- Molecule 10: 5S rRNA

Chain B: 68% 25% 8%



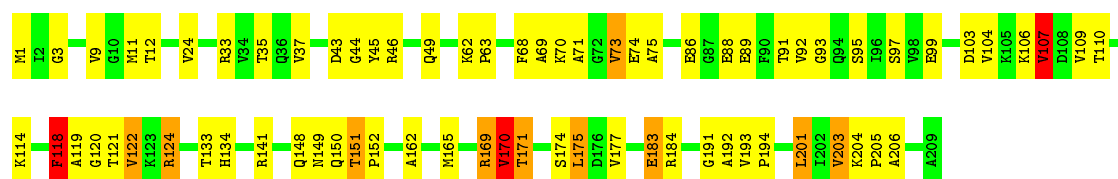
- Molecule 11: 50S ribosomal protein L2

Chain C: 68% 27% 5%

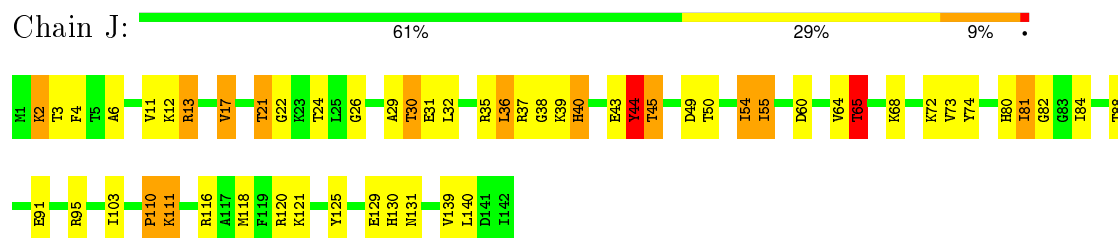


- Molecule 12: 50S ribosomal protein L3

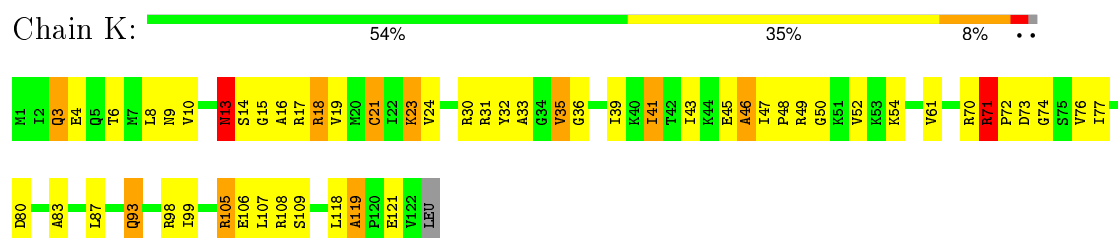
Chain D: 66% 28% 5%



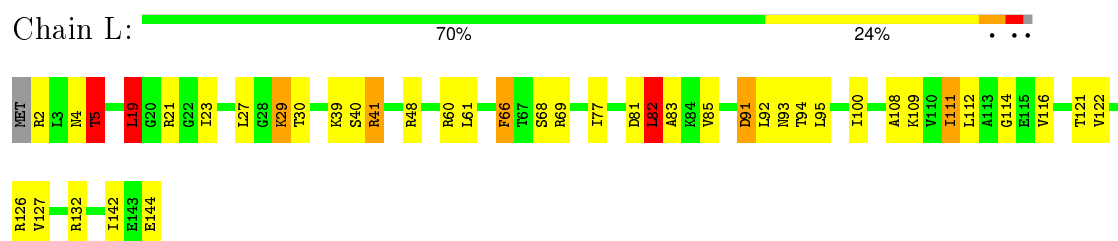
- Molecule 13: 50S ribosomal protein L4



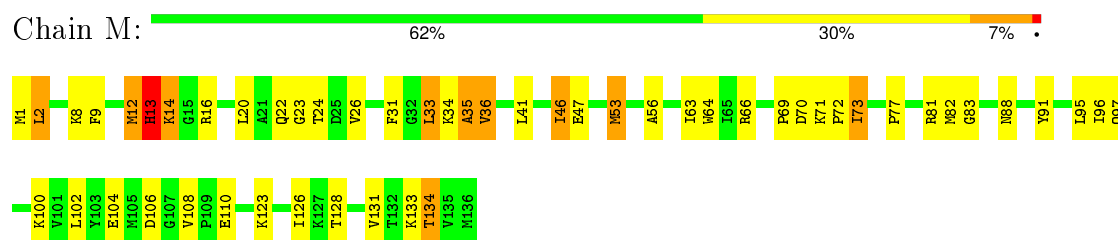
- Molecule 19: 50S ribosomal protein L14



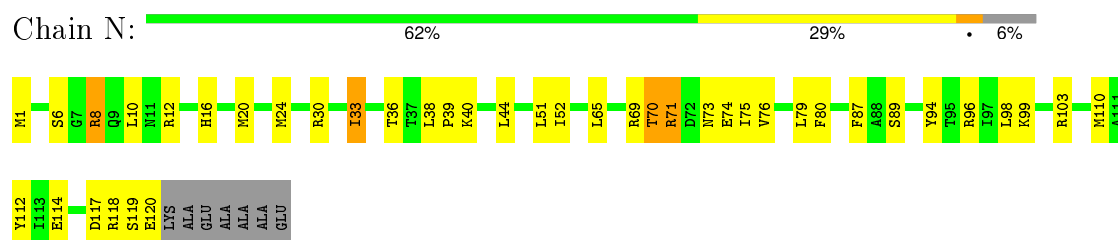
- Molecule 20: 50S ribosomal protein L15



- Molecule 21: 50S ribosomal protein L16

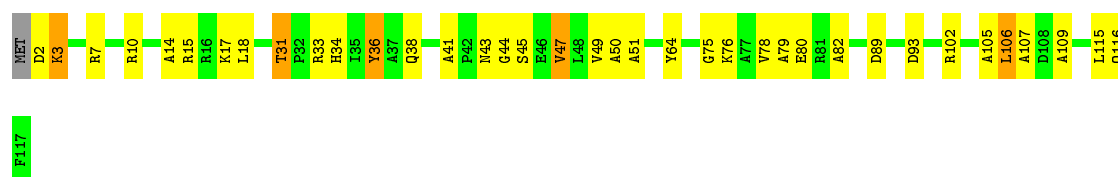


- Molecule 22: 50S ribosomal protein L17



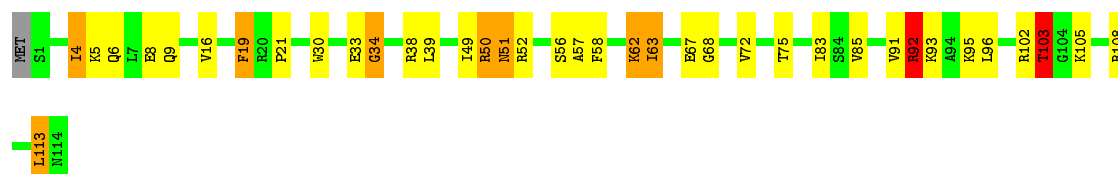
- Molecule 23: 50S ribosomal protein L18





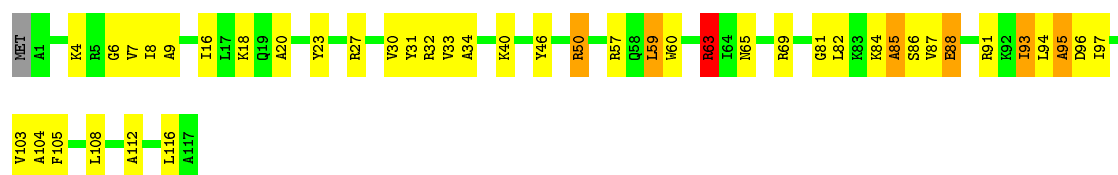
- Molecule 24: 50S ribosomal protein L19

Chain P: 66% 24% 7% ..



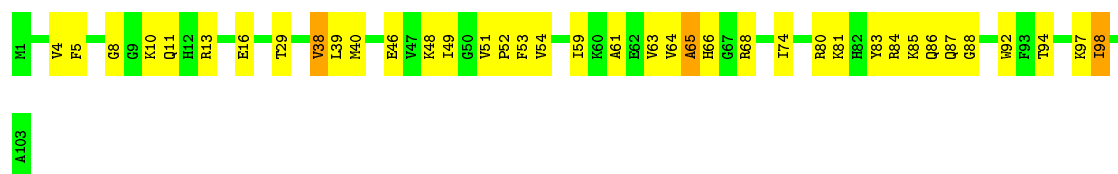
- Molecule 25: 50S ribosomal protein L20

Chain Q: 63% 31% 5% ..



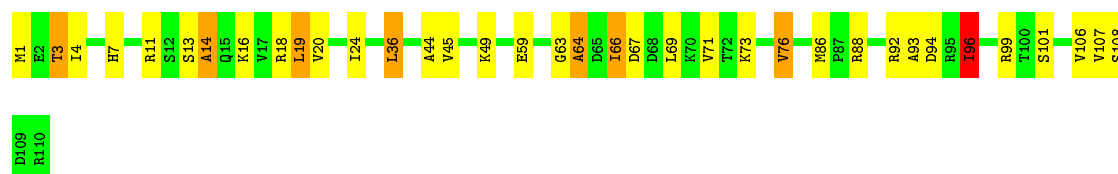
- Molecule 26: 50S ribosomal protein L21

Chain R: 63% 34% .



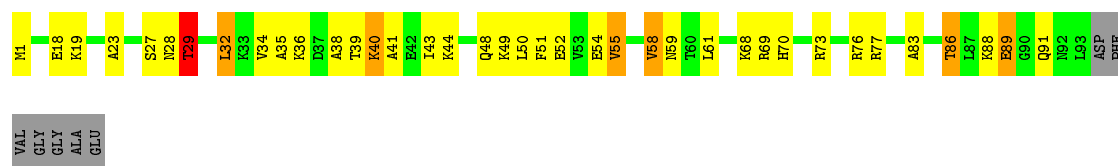
- Molecule 27: 50S ribosomal protein L22

Chain S: 67% 25% 6% .



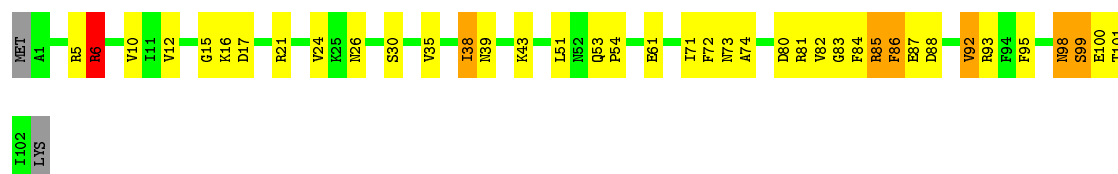
- Molecule 28: 50S ribosomal protein L23

Chain T: 55% 31% 6% • 7%



- Molecule 29: 50S ribosomal protein L24

Chain U: 61% 31% 6% ..



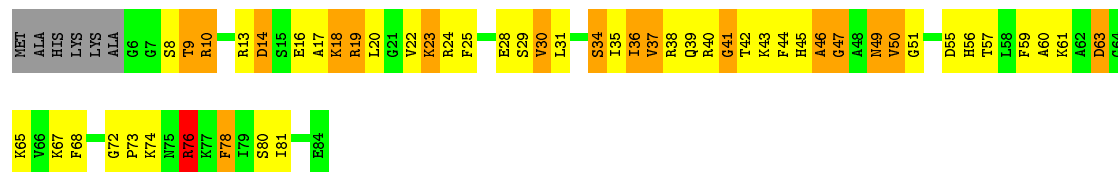
- Molecule 30: 50S ribosomal protein L25

Chain V: 79% 19% .



- Molecule 31: 50S ribosomal protein L27

Chain W: 32% 40% 20% 7% .



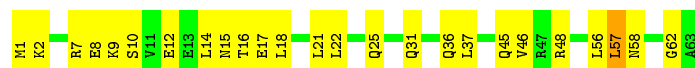
- Molecule 32: 50S ribosomal protein L28

Chain X: 71% 22% 5% ..



- Molecule 33: 50S ribosomal protein L29

Chain Y: 60% 38% .



- Molecule 34: 50S ribosomal protein L30

Chain Z: 54% 34% 8% ..



● Molecule 35: ErmCL nascent chain



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	269163	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	defocus groups	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	125085	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ERY

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 > 2$	RMSZ	# $ Z > 2$
1	0	0.54	0/450	0.70	0/599
10	B	0.66	0/2828	1.10	2/4410 (0.0%)
11	C	0.54	0/2121	0.79	3/2852 (0.1%)
12	D	0.57	0/1586	0.77	1/2134 (0.0%)
13	E	0.53	0/1571	0.76	2/2113 (0.1%)
14	F	0.50	0/1434	0.71	1/1926 (0.1%)
15	G	0.55	0/1343	0.73	0/1816
16	H	0.53	0/389	0.73	0/523
17	I	0.62	0/1046	0.84	1/1410 (0.1%)
18	J	0.63	1/1152 (0.1%)	0.78	0/1551
19	K	0.65	1/947 (0.1%)	0.77	0/1268
2	1	0.53	0/416	0.74	0/554
20	L	0.56	0/1054	0.79	2/1403 (0.1%)
21	M	0.61	0/1093	0.77	0/1460
22	N	0.51	0/973	0.68	0/1301
23	O	0.46	0/902	0.70	0/1209
24	P	0.52	0/929	0.78	1/1242 (0.1%)
25	Q	0.62	0/960	0.71	1/1278 (0.1%)
26	R	0.61	1/829 (0.1%)	0.76	0/1107
27	S	0.54	0/864	0.73	0/1156
28	T	0.55	0/744	0.85	1/994 (0.1%)
29	U	0.56	0/787	0.78	0/1051
3	2	0.53	0/380	0.70	0/498
30	V	0.48	0/766	0.67	1/1025 (0.1%)
31	W	0.69	0/603	1.00	1/797 (0.1%)
32	X	0.50	0/635	0.79	1/848 (0.1%)
33	Y	0.46	0/510	0.75	0/677
34	Z	0.54	0/453	0.84	1/605 (0.2%)
35	a	0.86	0/32	1.43	1/40 (2.5%)
4	3	0.53	0/513	0.75	0/676
5	4	0.59	0/303	0.84	0/397
6	5	0.74	0/1131	1.32	26/1524 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
7	6	0.59	0/227	0.65	0/304
8	7	0.16	0/64	0.54	0/97
9	A	0.80	15/68626 (0.0%)	1.22	301/107056 (0.3%)
All	All	0.74	18/98661 (0.0%)	1.12	347/147901 (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
11	C	0	1
12	D	0	1
18	J	0	1
19	K	0	1
6	5	0	1
All	All	0	5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	984	A	N9-C4	-8.36	1.32	1.37
9	A	528	A	N9-C4	-6.60	1.33	1.37
9	A	1142	A	N9-C4	-6.51	1.33	1.37
9	A	783	A	N9-C4	-6.27	1.34	1.37
9	A	1569	A	N9-C4	-6.16	1.34	1.37
9	A	783	A	N3-C4	-5.96	1.31	1.34
9	A	2606	C	N1-C6	-5.84	1.33	1.37
9	A	1073	A	C5-C6	5.82	1.46	1.41
9	A	2508	G	O3'-P	-5.60	1.54	1.61
18	J	44	TYR	CD2-CE2	-5.59	1.30	1.39
9	A	528	A	N3-C4	-5.47	1.31	1.34
26	R	86	GLN	CB-CG	5.41	1.67	1.52
9	A	1142	A	C5-C6	-5.32	1.36	1.41
9	A	2478	A	N9-C4	-5.29	1.34	1.37
9	A	2053	G	C6-O6	5.26	1.28	1.24
9	A	783	A	N7-C5	-5.24	1.36	1.39
19	K	21	CYS	CB-SG	-5.23	1.73	1.81
9	A	783	A	C5-C6	-5.02	1.36	1.41

All (347) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1073	A	N1-C6-N6	-20.00	106.60	118.60
9	A	1073	A	C5-C6-N6	14.06	134.95	123.70
9	A	2053	G	N1-C6-O6	13.89	128.23	119.90
9	A	984	A	C2-N3-C4	-12.15	104.53	110.60
9	A	961	C	O5'-P-OP2	-11.75	95.12	105.70
9	A	2053	G	C6-C5-N7	-11.60	123.44	130.40
9	A	1073	A	C6-C5-N7	11.45	140.32	132.30
9	A	2053	G	C5-C6-N1	-11.39	105.80	111.50
9	A	1073	A	C4-C5-N7	-11.28	105.06	110.70
9	A	783	A	C5-N7-C8	-10.82	98.49	103.90
9	A	974	G	C6-C5-N7	-10.52	124.09	130.40
9	A	2053	G	C4-C5-C6	10.22	124.93	118.80
9	A	974	G	C4-C5-N7	9.91	114.76	110.80
9	A	783	A	N7-C8-N9	9.65	118.63	113.80
6	5	92	ALA	C-N-CA	9.60	145.71	121.70
9	A	1534	U	C2-N1-C1'	9.34	128.91	117.70
9	A	1073	A	C5-N7-C8	9.30	108.55	103.90
9	A	528	A	C2-N3-C4	-9.13	106.03	110.60
6	5	93	ALA	C-N-CA	9.06	144.35	121.70
9	A	1950	G	N1-C6-O6	8.81	125.19	119.90
9	A	465	G	C8-N9-C4	-8.69	102.92	106.40
9	A	1533	C	N1-C2-O2	8.66	124.09	118.90
9	A	783	A	C8-N9-C4	-8.64	102.35	105.80
9	A	1073	A	N9-C4-C5	8.61	109.24	105.80
9	A	2074	U	O5'-P-OP2	-8.55	98.00	105.70
9	A	2534	A	N1-C6-N6	8.53	123.72	118.60
9	A	1936	A	C2-N3-C4	-8.52	106.34	110.60
9	A	974	G	C4-N9-C1'	8.44	137.47	126.50
9	A	2572	A	N1-C6-N6	8.41	123.65	118.60
9	A	1533	C	C2-N1-C1'	8.40	128.04	118.80
9	A	1142	A	C2-N3-C4	-8.35	106.42	110.60
6	5	27	VAL	CG1-CB-CG2	8.20	124.02	110.90
9	A	586	A	O5'-P-OP1	-8.12	98.39	105.70
12	D	151	THR	C-N-CD	8.00	145.20	128.40
9	A	1533	C	C6-N1-C2	-7.99	117.10	120.30
9	A	783	A	C4-C5-N7	7.82	114.61	110.70
9	A	984	A	N3-C4-C5	7.76	132.23	126.80
9	A	1478	G	N1-C6-O6	7.75	124.55	119.90
9	A	1795	C	C6-N1-C2	-7.73	117.21	120.30
6	5	51	TYR	C-N-CA	7.70	140.95	121.70
9	A	2053	G	C4-N9-C1'	7.68	136.48	126.50
9	A	2606	C	C5-C6-N1	-7.68	117.16	121.00
9	A	783	A	N1-C6-N6	7.66	123.19	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2053	G	C2-N3-C4	-7.65	108.07	111.90
6	5	49	GLY	C-N-CA	7.64	140.81	121.70
9	A	974	G	C8-N9-C1'	-7.63	117.09	127.00
6	5	123	ILE	CG1-CB-CG2	7.61	128.13	111.40
9	A	465	G	N3-C4-C5	-7.60	124.80	128.60
6	5	119	PRO	C-N-CA	7.58	140.64	121.70
31	W	76	ARG	NE-CZ-NH2	7.54	124.07	120.30
9	A	783	A	C6-C5-N7	-7.53	127.03	132.30
35	a	84	ILE	CB-CA-C	-7.52	96.55	111.60
9	A	776	G	C5-C6-O6	7.49	133.10	128.60
9	A	1839	G	N1-C6-O6	7.44	124.36	119.90
9	A	2508	G	P-O3'-C3'	-7.43	110.78	119.70
6	5	72	LEU	C-N-CA	7.37	140.14	121.70
13	E	44	ARG	NE-CZ-NH2	7.35	123.98	120.30
9	A	2146	C	N3-C4-C5	-7.35	118.96	121.90
9	A	1533	C	N3-C2-O2	-7.33	116.77	121.90
9	A	2053	G	N1-C2-N3	7.33	128.30	123.90
9	A	974	G	C5-N7-C8	-7.29	100.65	104.30
6	5	81	LEU	CB-CG-CD2	7.28	123.37	111.00
9	A	2250	G	C6-C5-N7	-7.28	126.03	130.40
9	A	1073	A	O5'-P-OP2	7.27	119.42	110.70
9	A	1142	A	N1-C6-N6	7.26	122.96	118.60
9	A	1534	U	C6-N1-C1'	-7.26	111.04	121.20
9	A	1950	G	C6-C5-N7	-7.23	126.06	130.40
9	A	2501	C	C2-N1-C1'	-7.20	110.88	118.80
9	A	2447	G	O5'-P-OP1	-7.19	99.22	105.70
6	5	28	ALA	C-N-CA	7.12	139.50	121.70
9	A	776	G	C5-C6-N1	-7.12	107.94	111.50
9	A	2053	G	C8-N9-C1'	-7.10	117.77	127.00
6	5	47	GLU	C-N-CA	7.02	139.25	121.70
6	5	54	VAL	CG1-CB-CG2	6.99	122.09	110.90
9	A	2423	U	P-O3'-C3'	6.99	128.09	119.70
9	A	2250	G	N1-C6-O6	6.96	124.08	119.90
9	A	1935	G	O5'-P-OP2	-6.94	99.45	105.70
9	A	984	A	N3-C4-N9	-6.92	121.86	127.40
9	A	1284	A	O5'-P-OP2	-6.91	99.48	105.70
9	A	802	A	N1-C6-N6	-6.91	114.45	118.60
9	A	2448	A	N1-C6-N6	6.88	122.73	118.60
9	A	783	A	C2-N3-C4	-6.87	107.17	110.60
9	A	1839	G	C6-C5-N7	-6.84	126.30	130.40
9	A	1654	A	O5'-P-OP1	-6.82	99.56	105.70
9	A	1378	A	P-O3'-C3'	6.82	127.88	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	12	U	N3-C2-O2	-6.81	117.44	122.20
9	A	2681	C	C6-N1-C2	6.79	123.02	120.30
9	A	1311	G	C8-N9-C4	-6.76	103.70	106.40
9	A	503	A	C8-N9-C4	-6.75	103.10	105.80
9	A	974	G	N9-C4-C5	-6.75	102.70	105.40
9	A	974	G	N3-C4-N9	6.74	130.05	126.00
9	A	974	G	N1-C6-O6	6.74	123.94	119.90
9	A	974	G	C5-C6-O6	-6.71	124.57	128.60
9	A	1192	G	C8-N9-C4	6.70	109.08	106.40
20	L	19	LEU	CA-CB-CG	6.70	130.70	115.30
9	A	974	G	N7-C8-N9	6.65	116.43	113.10
14	F	94	ARG	NE-CZ-NH1	6.61	123.60	120.30
11	C	233	GLY	N-CA-C	-6.59	96.62	113.10
9	A	2823	A	C8-N9-C4	-6.58	103.17	105.80
9	A	2508	G	O3'-P-O5'	6.56	116.47	104.00
9	A	2689	U	C5-C4-O4	6.56	129.83	125.90
9	A	528	A	N1-C6-N6	6.55	122.53	118.60
9	A	1263	U	N3-C4-C5	-6.50	110.70	114.60
9	A	984	A	N1-C6-N6	6.49	122.50	118.60
9	A	1815	A	N9-C4-C5	6.48	108.39	105.80
6	5	147	SER	C-N-CA	6.47	137.88	121.70
6	5	84	TYR	C-N-CA	6.46	137.86	121.70
6	5	40	GLU	C-N-CA	6.43	137.78	121.70
9	A	2146	C	C2-N3-C4	6.41	123.11	119.90
9	A	2447	G	N1-C6-O6	6.41	123.75	119.90
9	A	820	A	O5'-P-OP1	-6.40	99.94	105.70
6	5	50	VAL	C-N-CA	6.38	137.65	121.70
9	A	2551	C	OP2-P-O3'	6.37	119.21	105.20
9	A	670	A	O4'-C1'-N9	-6.36	103.11	108.20
9	A	404	A	P-O3'-C3'	6.36	127.33	119.70
9	A	2142	A	OP2-P-O3'	6.34	119.14	105.20
9	A	2267	A	C8-N9-C4	-6.33	103.27	105.80
13	E	44	ARG	NE-CZ-NH1	-6.32	117.14	120.30
9	A	2754	U	N3-C4-O4	6.31	123.82	119.40
9	A	1142	A	N3-C4-C5	6.30	131.21	126.80
9	A	748	G	O4'-C1'-N9	6.28	113.23	108.20
6	5	108	VAL	CG1-CB-CG2	6.27	120.94	110.90
9	A	2770	G	N1-C6-O6	-6.26	116.15	119.90
6	5	60	LEU	CB-CG-CD1	6.22	121.58	111.00
6	5	39	THR	C-N-CA	6.22	137.24	121.70
9	A	1839	G	C5-C6-O6	-6.19	124.89	128.60
9	A	2250	G	C4-C5-N7	6.18	113.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1003	G	O5'-P-OP2	-6.18	100.14	105.70
9	A	1125	G	N1-C6-O6	6.18	123.61	119.90
9	A	567	U	N1-C2-O2	-6.17	118.48	122.80
9	A	1142	A	C5-N7-C8	-6.17	100.81	103.90
9	A	2592	G	O5'-P-OP2	-6.16	100.16	105.70
9	A	2606	C	C6-N1-C2	6.16	122.76	120.30
9	A	1950	G	C5-C6-O6	-6.15	124.91	128.60
11	C	109	LEU	CA-CB-CG	6.15	129.45	115.30
9	A	548	G	C8-N9-C4	-6.13	103.95	106.40
9	A	2250	G	C5-N7-C8	-6.12	101.24	104.30
9	A	1142	A	C4-C5-N7	6.12	113.76	110.70
9	A	784	G	O4'-C1'-N9	-6.08	103.34	108.20
9	A	2241	A	C8-N9-C4	-6.07	103.37	105.80
9	A	784	G	P-O3'-C3'	6.06	126.97	119.70
9	A	379	G	N1-C6-O6	6.05	123.53	119.90
9	A	2606	C	N1-C1'-C2'	-6.05	105.35	112.00
6	5	59	LEU	C-N-CA	6.04	136.81	121.70
9	A	1025	G	P-O3'-C3'	6.02	126.92	119.70
20	L	82	LEU	CA-CB-CG	6.01	129.13	115.30
9	A	1328	A	O5'-P-OP2	-5.99	100.31	105.70
9	A	1069	A	OP2-P-O3'	5.98	118.36	105.20
9	A	1073	A	N7-C8-N9	-5.98	110.81	113.80
9	A	2534	A	C4-C5-N7	5.97	113.69	110.70
6	5	53	ARG	C-N-CA	5.96	136.60	121.70
9	A	528	A	C5-C6-N1	-5.93	114.73	117.70
9	A	1779	U	N3-C4-O4	-5.93	115.25	119.40
9	A	2448	A	C6-C5-N7	-5.93	128.15	132.30
9	A	2747	G	OP2-P-O3'	5.93	118.24	105.20
9	A	119	A	O5'-P-OP2	-5.91	100.38	105.70
9	A	2554	U	O5'-P-OP1	-5.91	100.38	105.70
9	A	1428	C	O5'-P-OP1	-5.91	100.39	105.70
9	A	2447	G	C5-C6-O6	-5.89	125.06	128.60
9	A	866	A	N1-C6-N6	5.89	122.13	118.60
9	A	1094	U	N3-C4-C5	-5.89	111.07	114.60
9	A	1069	A	C8-N9-C4	-5.88	103.45	105.80
9	A	527	C	P-O3'-C3'	5.88	126.75	119.70
9	A	2043	C	C6-N1-C2	-5.87	117.95	120.30
9	A	964	C	O5'-P-OP2	-5.86	100.42	105.70
9	A	1509	A	O4'-C1'-N9	5.85	112.88	108.20
9	A	1837	C	O5'-P-OP1	-5.85	100.44	105.70
9	A	1670	C	N1-C2-O2	-5.84	115.39	118.90
9	A	1645	G	N3-C4-C5	-5.80	125.70	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1815	A	C8-N9-C4	-5.80	103.48	105.80
9	A	2715	C	C6-N1-C2	5.80	122.62	120.30
9	A	516	C	O5'-P-OP1	-5.79	100.49	105.70
9	A	1066	U	N3-C2-O2	-5.74	118.18	122.20
6	5	117	LEU	C-N-CA	5.73	136.02	121.70
9	A	1247	A	P-O3'-C3'	5.73	126.57	119.70
9	A	1263	U	C6-N1-C2	-5.73	117.56	121.00
9	A	2534	A	C5-N7-C8	-5.72	101.04	103.90
9	A	1979	U	C6-N1-C2	-5.72	117.57	121.00
9	A	209	C	C6-N1-C2	5.71	122.58	120.30
9	A	1789	A	O5'-P-OP1	-5.71	100.56	105.70
9	A	2508	G	C6-C5-N7	-5.68	126.99	130.40
9	A	2719	G	C5-C6-N1	-5.67	108.66	111.50
9	A	1606	C	C2-N3-C4	-5.66	117.07	119.90
9	A	2719	G	N1-C6-O6	5.65	123.29	119.90
9	A	1358	G	C8-N9-C4	-5.63	104.15	106.40
9	A	271	G	OP1-P-O3'	5.63	117.58	105.20
9	A	2241	A	N9-C4-C5	5.62	108.05	105.80
9	A	1073	A	C4-N9-C1'	-5.62	116.19	126.30
9	A	1534	U	C5-C6-N1	5.62	125.51	122.70
9	A	2605	U	P-O3'-C3'	-5.62	112.96	119.70
9	A	1088	A	O4'-C1'-N9	-5.61	103.71	108.20
9	A	2053	G	N3-C2-N2	-5.57	116.00	119.90
9	A	1157	G	N1-C6-O6	5.57	123.24	119.90
9	A	1509	A	P-O3'-C3'	5.55	126.36	119.70
9	A	626	A	N1-C6-N6	5.55	121.93	118.60
9	A	2271	G	C5-C6-O6	-5.55	125.27	128.60
9	A	2544	G	C6-C5-N7	-5.55	127.07	130.40
9	A	1198	U	O5'-P-OP2	-5.55	100.71	105.70
9	A	532	A	C8-N9-C4	-5.55	103.58	105.80
9	A	1125	G	C6-C5-N7	-5.55	127.07	130.40
9	A	2282	G	C8-N9-C4	-5.53	104.19	106.40
9	A	2501	C	N3-C4-C5	5.53	124.11	121.90
9	A	1611	C	N1-C2-O2	-5.53	115.58	118.90
9	A	2326	C	C5-C4-N4	-5.52	116.33	120.20
9	A	2689	U	N3-C4-O4	-5.52	115.54	119.40
9	A	1192	G	N9-C4-C5	-5.51	103.19	105.40
9	A	2244	U	C5-C4-O4	-5.51	122.59	125.90
9	A	55	G	C5-C6-O6	-5.50	125.30	128.60
9	A	2353	G	N1-C6-O6	-5.50	116.60	119.90
9	A	1069	A	O4'-C1'-N9	5.50	112.60	108.20
9	A	1153	C	N1-C2-O2	-5.50	115.60	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	672	C	N1-C2-O2	5.49	122.20	118.90
9	A	29	U	OP2-P-O3'	5.49	117.28	105.20
9	A	1207	C	C6-N1-C2	-5.48	118.11	120.30
10	B	80	U	N1-C2-N3	5.48	118.19	114.90
9	A	2146	C	C6-N1-C2	-5.48	118.11	120.30
9	A	1027	A	O4'-C1'-N9	-5.47	103.83	108.20
9	A	2446	G	OP2-P-O3'	5.47	117.22	105.20
9	A	984	A	C5-C6-N1	-5.45	114.98	117.70
9	A	451	U	O4'-C1'-N1	5.45	112.56	108.20
9	A	989	G	O4'-C1'-N9	5.44	112.55	108.20
9	A	1073	A	C8-N9-C1'	5.43	137.47	127.70
9	A	598	U	OP2-P-O3'	5.42	117.12	105.20
9	A	1430	G	N1-C6-O6	5.42	123.15	119.90
9	A	1350	C	C6-N1-C2	5.41	122.46	120.30
9	A	1759	A	N1-C6-N6	5.39	121.84	118.60
9	A	2439	A	N1-C6-N6	5.38	121.83	118.60
9	A	2015	A	N1-C6-N6	-5.38	115.38	118.60
9	A	1229	C	C6-N1-C2	5.37	122.45	120.30
9	A	2250	G	C2-N3-C4	-5.37	109.21	111.90
9	A	1950	G	C8-N9-C1'	-5.37	120.02	127.00
9	A	1311	G	N7-C8-N9	5.36	115.78	113.10
9	A	2353	G	C2-N3-C4	5.36	114.58	111.90
9	A	1129	A	O5'-P-OP1	-5.36	100.88	105.70
9	A	548	G	N3-C4-C5	-5.35	125.92	128.60
9	A	250	G	O5'-P-OP2	-5.35	100.88	105.70
9	A	1420	A	O4'-C1'-N9	5.35	112.48	108.20
9	A	1565	C	C6-N1-C2	-5.34	118.16	120.30
9	A	2571	U	C2-N1-C1'	-5.34	111.29	117.70
9	A	1831	G	C8-N9-C4	-5.34	104.27	106.40
24	P	113	LEU	CA-CB-CG	5.33	127.57	115.30
9	A	2544	G	N1-C6-O6	5.33	123.10	119.90
9	A	677	A	OP1-P-O3'	5.33	116.92	105.20
9	A	733	G	C8-N9-C4	-5.33	104.27	106.40
9	A	1190	G	C5-N7-C8	-5.33	101.64	104.30
9	A	2271	G	N1-C6-O6	5.33	123.10	119.90
9	A	940	G	N1-C6-O6	5.33	123.09	119.90
9	A	2508	G	C4-N9-C1'	5.33	133.42	126.50
9	A	1533	C	C5-C6-N1	5.32	123.66	121.00
9	A	2355	G	C8-N9-C4	5.32	108.53	106.40
6	5	50	VAL	CG1-CB-CG2	5.31	119.40	110.90
9	A	837	C	N1-C2-O2	-5.31	115.71	118.90
6	5	131	THR	N-CA-C	-5.31	96.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2153	C	O4'-C1'-N1	5.31	112.45	108.20
9	A	776	G	C4-N9-C1'	5.30	133.39	126.50
9	A	1970	A	C8-N9-C4	-5.30	103.68	105.80
9	A	2015	A	N9-C4-C5	5.30	107.92	105.80
9	A	2250	G	N7-C8-N9	5.29	115.75	113.10
9	A	2470	G	OP2-P-O3'	5.29	116.84	105.20
9	A	2723	C	C6-N1-C2	-5.29	118.18	120.30
9	A	2508	G	O4'-C1'-N9	-5.29	103.97	108.20
9	A	84	A	N1-C6-N6	-5.29	115.43	118.60
9	A	518	G	O5'-P-OP1	-5.29	100.94	105.70
9	A	2071	A	OP2-P-O3'	5.29	116.83	105.20
9	A	2685	G	C5-C6-N1	-5.27	108.86	111.50
6	5	50	VAL	CA-CB-CG1	5.27	118.80	110.90
9	A	1131	G	OP1-P-O3'	5.27	116.80	105.20
9	A	1025	G	N3-C4-C5	-5.26	125.97	128.60
9	A	1458	U	P-O3'-C3'	5.25	126.00	119.70
9	A	2618	G	C5-C6-N1	-5.25	108.87	111.50
9	A	991	C	C6-N1-C2	-5.25	118.20	120.30
9	A	2368	C	C6-N1-C2	5.25	122.40	120.30
9	A	2501	C	C6-N1-C1'	5.24	127.09	120.80
25	Q	63	ARG	NE-CZ-NH2	-5.24	117.68	120.30
9	A	2518	A	N1-C6-N6	5.24	121.75	118.60
9	A	2508	G	C8-N9-C1'	-5.24	120.19	127.00
9	A	1684	G	N3-C4-C5	-5.24	125.98	128.60
34	Z	15	ARG	NE-CZ-NH1	5.24	122.92	120.30
32	X	29	LEU	CA-CB-CG	5.23	127.34	115.30
9	A	1264	A	O5'-P-OP1	-5.23	101.00	105.70
9	A	1355	G	C8-N9-C4	-5.22	104.31	106.40
9	A	2263	C	N3-C4-C5	-5.22	119.81	121.90
9	A	1025	G	C8-N9-C4	-5.21	104.31	106.40
9	A	1206	G	N3-C4-C5	-5.21	125.99	128.60
9	A	833	A	C8-N9-C4	-5.21	103.72	105.80
9	A	2825	G	N3-C4-N9	5.21	129.12	126.00
9	A	1936	A	N3-C4-C5	5.20	130.44	126.80
9	A	2534	A	C5-C6-N6	-5.20	119.54	123.70
9	A	1943	U	C5-C4-O4	5.20	129.02	125.90
9	A	699	A	N1-C6-N6	5.20	121.72	118.60
9	A	2537	U	C5-C4-O4	5.18	129.01	125.90
9	A	1446	C	C6-N1-C2	-5.18	118.23	120.30
9	A	2704	C	C6-N1-C2	5.18	122.37	120.30
9	A	748	G	C4-C5-N7	-5.18	108.73	110.80
9	A	2508	G	P-O5'-C5'	-5.17	112.62	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	119	A	P-O3'-C3'	5.17	125.90	119.70
9	A	465	G	C4-C5-C6	5.17	121.90	118.80
9	A	1395	A	O4'-C1'-N9	5.17	112.33	108.20
9	A	776	G	C4-C5-C6	5.16	121.90	118.80
9	A	1824	G	N9-C4-C5	5.16	107.47	105.40
6	5	130	PRO	CA-N-CD	-5.16	104.28	111.50
9	A	1355	G	N3-C2-N2	-5.16	116.29	119.90
9	A	454	A	O5'-P-OP2	-5.16	101.06	105.70
9	A	1928	A	N1-C6-N6	5.16	121.69	118.60
9	A	916	G	C6-C5-N7	-5.14	127.31	130.40
9	A	984	A	N1-C2-N3	5.14	131.87	129.30
9	A	2037	A	N9-C4-C5	5.14	107.85	105.80
9	A	1524	G	C8-N9-C4	-5.13	104.35	106.40
9	A	1238	G	O5'-P-OP2	-5.12	101.09	105.70
9	A	1639	C	C6-N1-C2	5.12	122.35	120.30
9	A	2198	A	O4'-C1'-N9	5.12	112.29	108.20
9	A	1452	G	C4-C5-N7	5.11	112.84	110.80
9	A	404	A	C8-N9-C4	-5.11	103.76	105.80
30	V	61	LEU	CA-CB-CG	5.11	127.05	115.30
9	A	1538	G	N3-C4-C5	5.11	131.15	128.60
9	A	1534	U	N1-C2-O2	5.10	126.37	122.80
9	A	2443	C	C6-N1-C2	-5.10	118.26	120.30
9	A	2422	C	N1-C2-O2	5.09	121.96	118.90
10	B	114	C	C5-C4-N4	-5.09	116.64	120.20
9	A	376	G	C6-C5-N7	-5.09	127.35	130.40
9	A	1122	G	N3-C4-N9	-5.08	122.95	126.00
17	I	79	LEU	CA-CB-CG	5.08	127.00	115.30
9	A	807	U	N3-C4-O4	5.08	122.96	119.40
9	A	1983	G	C5-C6-N1	-5.08	108.96	111.50
9	A	2537	U	N1-C2-N3	5.08	117.95	114.90
9	A	752	A	C2-N3-C4	-5.07	108.06	110.60
9	A	403	U	P-O3'-C3'	5.07	125.78	119.70
9	A	2455	G	O5'-P-OP2	-5.05	101.16	105.70
9	A	55	G	N1-C6-O6	5.05	122.93	119.90
9	A	467	G	N7-C8-N9	-5.04	110.58	113.10
9	A	1659	G	N3-C4-C5	5.04	131.12	128.60
9	A	686	U	C2-N1-C1'	-5.04	111.65	117.70
9	A	1779	U	C5-C6-N1	-5.04	120.18	122.70
9	A	2278	A	OP2-P-O3'	5.03	116.27	105.20
9	A	1533	C	C6-N1-C1'	-5.02	114.78	120.80
9	A	1979	U	C5-C6-N1	5.02	125.21	122.70
9	A	2396	G	N1-C6-O6	-5.02	116.89	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2551	C	O5'-P-OP1	-5.02	101.19	105.70
28	T	29	THR	N-CA-C	5.02	124.54	111.00
9	A	1314	C	C5-C4-N4	-5.01	116.69	120.20
9	A	1606	C	P-O3'-C3'	5.01	125.72	119.70
9	A	2017	U	N3-C4-O4	5.01	122.91	119.40
9	A	1314	C	C2-N1-C1'	5.01	124.31	118.80
9	A	2015	A	C5-C6-N6	5.01	127.71	123.70
9	A	2902	C	P-O3'-C3'	5.01	125.71	119.70
9	A	745	G	N3-C4-N9	5.00	129.00	126.00
11	C	155	ARG	CG-CD-NE	5.00	122.31	111.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	130	PRO	Peptide
11	C	233	GLY	Peptide
12	D	9	VAL	Peptide
18	J	110	PRO	Peptide
19	K	71	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	16	0
2	1	409	0	440	15	0
3	2	377	0	418	5	0
4	3	504	0	574	10	0
5	4	302	0	340	14	0
6	5	1117	0	1155	123	0
7	6	227	0	237	6	0
8	7	58	0	33	12	0
9	A	61274	0	30817	801	0
10	B	2529	0	1281	20	0
11	C	2082	0	2157	54	0
12	D	1565	0	1616	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	E	1552	0	1619	40	0
14	F	1410	0	1447	44	0
15	G	1323	0	1374	37	0
16	H	384	0	405	12	0
17	I	1032	0	1088	53	0
18	J	1129	0	1162	50	0
19	K	938	0	1012	40	0
20	L	1045	0	1117	37	0
21	M	1074	0	1157	29	0
22	N	960	0	1000	30	0
23	O	892	0	923	21	0
24	P	917	0	965	38	0
25	Q	947	0	1022	52	0
26	R	816	0	839	35	0
27	S	857	0	922	28	0
28	T	738	0	807	33	0
29	U	779	0	834	27	0
30	V	753	0	780	12	0
31	W	596	0	610	80	0
32	X	625	0	655	18	0
33	Y	509	0	543	13	0
34	Z	449	0	491	15	0
35	a	36	0	34	0	0
36	A	51	0	67	8	0
All	All	90700	0	60402	1640	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 11.

All (1640) 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)
9:A:912:C:OP1	21:M:8:LYS:NZ	1.79	1.15
9:A:2062:A:N6	36:A:9000:ERY:H273	1.64	1.13
9:A:2061:G:OP2	13:E:63:LYS:NZ	1.88	1.06
6:5:71:CYS:HB3	6:5:117:LEU:HD12	1.33	1.04
9:A:2579:C:H2'	9:A:2580:U:H5'	1.40	1.03
9:A:2579:C:C2'	9:A:2580:U:H5'	1.88	1.02
9:A:2574:G:C2'	9:A:2575:C:H5'	1.90	1.01
6:5:26:VAL:HG21	6:5:115:GLY:H	1.23	1.00
6:5:3:LEU:O	6:5:7:ASP:OD1	1.79	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2063:C:C5	9:A:2064:C:C5	2.50	1.00
9:A:2574:G:H2'	9:A:2575:C:H5'	1.46	0.98
8:7:74:C:O2	9:A:2252:G:N2	1.97	0.97
9:A:2063:C:H2'	9:A:2064:C:H5'	1.48	0.95
9:A:2582:G:C2	9:A:2583:G:C8	2.55	0.94
6:5:117:LEU:CD2	6:5:120:ALA:HA	1.97	0.94
9:A:2600:A:H2'	9:A:2601:C:H5'	1.48	0.94
6:5:71:CYS:HB3	6:5:117:LEU:CD1	1.98	0.92
9:A:1154:G:OP2	25:Q:57:ARG:NH1	2.03	0.92
9:A:2580:U:H2'	9:A:2581:G:H5'	1.52	0.91
6:5:71:CYS:CB	6:5:117:LEU:HD12	2.00	0.91
9:A:1248:G:OP2	13:E:44:ARG:NH1	2.03	0.91
10:B:43:C:O2	14:F:91:ARG:NH2	2.04	0.90
9:A:2279:G:N7	31:W:10:ARG:NH2	2.20	0.90
29:U:98:ASN:O	29:U:100:GLU:N	2.06	0.89
9:A:1336:A:OP2	28:T:68:LYS:NZ	2.06	0.88
9:A:2582:G:N3	9:A:2583:G:C8	2.41	0.88
9:A:2600:A:C2'	9:A:2601:C:H5'	2.04	0.88
6:5:71:CYS:CB	6:5:117:LEU:CD1	2.50	0.88
9:A:996:A:OP2	25:Q:91:ARG:NH2	2.07	0.88
6:5:24:SER:HB2	6:5:116:GLU:HG2	1.54	0.87
9:A:2505:G:O2'	9:A:2506:U:H5''	1.75	0.87
9:A:2599:G:O2'	9:A:2600:A:H5'	1.74	0.87
9:A:2062:A:H62	36:A:9000:ERY:H273	1.33	0.86
28:T:39:THR:O	28:T:41:ALA:N	2.09	0.86
9:A:1723:G:O6	9:A:1737:G:O2'	1.94	0.85
9:A:2061:G:OP2	13:E:63:LYS:CE	2.24	0.84
6:5:71:CYS:HA	6:5:117:LEU:HD13	1.60	0.84
9:A:2053:G:N2	9:A:2616:C:N3	2.24	0.84
9:A:1069:A:N3	9:A:1073:A:N6	2.26	0.84
6:5:33:VAL:N	6:5:36:ASP:OD2	2.12	0.82
6:5:77:VAL:C	6:5:79:PRO:HD2	2.00	0.82
6:5:71:CYS:HA	6:5:117:LEU:CD1	2.09	0.82
9:A:2603:G:O2'	9:A:2604:U:H5'	1.80	0.82
9:A:504:A:O2'	9:A:505:A:OP1	1.98	0.81
24:P:50:ARG:HB3	24:P:57:ALA:H	1.43	0.81
23:O:34:HIS:O	23:O:102:ARG:NH1	2.14	0.81
11:C:196:ASN:O	11:C:198:GLU:N	2.12	0.81
6:5:103:ASN:ND2	6:5:107:GLU:O	2.13	0.81
9:A:1782:U:O2	9:A:2608:G:O2'	1.97	0.80
9:A:2576:G:O2'	9:A:2577:A:O5'	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1012:U:OP2	25:Q:69:ARG:NH1	2.14	0.80
9:A:2576:G:H5'	9:A:2576:G:N3	1.97	0.79
9:A:2720:U:OP1	24:P:52:ARG:NH2	2.15	0.79
6:5:33:VAL:HG12	6:5:34:THR:H	1.48	0.79
9:A:2579:C:O2'	9:A:2580:U:H5'	1.82	0.79
6:5:43:LYS:NZ	6:5:98:GLU:OE1	2.16	0.79
9:A:2576:G:H4'	9:A:2577:A:OP1	1.80	0.78
9:A:2585:U:H5'	9:A:2586:U:OP2	1.83	0.78
8:7:76:A:C6	9:A:2451:A:H4'	2.18	0.78
6:5:91:ALA:C	6:5:93:ALA:H	1.87	0.78
9:A:2581:G:O2'	9:A:2610:C:N4	2.15	0.78
33:Y:18:LEU:O	33:Y:22:LEU:N	2.17	0.78
19:K:105:ARG:NH1	19:K:106:GLU:OE2	2.16	0.78
6:5:71:CYS:CA	6:5:117:LEU:CD1	2.62	0.77
9:A:1799:G:OP2	11:C:269:ARG:NH2	2.16	0.77
9:A:1509:A:O2'	9:A:1510:G:OP2	2.01	0.77
9:A:2063:C:H2'	9:A:2064:C:C5'	2.15	0.77
6:5:117:LEU:HD23	6:5:120:ALA:HA	1.65	0.77
6:5:35:VAL:HA	6:5:38:MET:SD	2.24	0.77
9:A:2611:C:H2'	9:A:2612:C:H6	1.47	0.77
12:D:184:ARG:NH1	24:P:6:GLN:OE1	2.17	0.77
9:A:2581:G:H2'	9:A:2581:G:N3	2.00	0.77
11:C:69:ASN:O	11:C:71:ASP:N	2.18	0.76
11:C:68:ARG:NH2	11:C:126:GLY:O	2.18	0.76
9:A:2580:U:C2'	9:A:2581:G:H5'	2.15	0.76
9:A:1187:G:OP1	26:R:85:LYS:NZ	2.19	0.75
9:A:1342:A:O2'	9:A:1344:U:OP2	2.04	0.75
6:5:131:THR:O	6:5:134:GLU:N	2.20	0.75
9:A:572:A:OP2	26:R:80:ARG:NH2	2.21	0.74
9:A:2592:G:N1	9:A:2603:G:C6	2.55	0.74
12:D:91:THR:O	12:D:93:GLY:N	2.21	0.74
6:5:57:ASN:O	6:5:59:LEU:N	2.21	0.74
5:4:11:CYS:SG	5:4:14:CYS:N	2.60	0.74
9:A:2707:U:O2	22:N:71:ARG:NH1	2.20	0.73
9:A:2611:C:H2'	9:A:2612:C:C6	2.24	0.73
9:A:1998:A:OP2	12:D:141:ARG:NH2	2.21	0.73
9:A:2331:G:O2'	31:W:39:GLN:O	2.04	0.73
18:J:43:GLU:O	18:J:45:THR:N	2.22	0.73
9:A:1799:G:O2'	11:C:179:GLU:OE2	2.07	0.72
15:G:22:VAL:HG12	15:G:36:LEU:CD1	2.19	0.72
9:A:2061:G:OP1	9:A:2061:G:H4'	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2579:C:H2'	9:A:2580:U:C5'	2.17	0.72
6:5:106:PHE:O	6:5:108:VAL:N	2.23	0.71
9:A:2060:A:O2'	9:A:2061:G:OP2	2.08	0.71
24:P:5:LYS:NZ	24:P:9:GLN:OE1	2.23	0.71
6:5:1:MET:SD	6:5:2:ALA:N	2.58	0.71
9:A:2063:C:C6	9:A:2064:C:C5	2.78	0.71
9:A:2599:G:C2'	9:A:2600:A:H5'	2.20	0.71
9:A:1993:U:H4'	12:D:133:THR:HG21	1.73	0.70
9:A:1805:A:N3	11:C:49:THR:OG1	2.24	0.70
8:7:76:A:C6	9:A:2451:A:C4'	2.74	0.70
9:A:161:A:H3'	9:A:162:U:H5''	1.72	0.70
9:A:2580:U:H2'	9:A:2581:G:C5'	2.20	0.70
9:A:2353:G:H1'	31:W:30:VAL:HG12	1.72	0.70
5:4:2:LYS:NZ	9:A:2478:A:OP2	2.23	0.70
9:A:971:G:OP2	9:A:974:G:N2	2.25	0.70
14:F:116:LEU:N	14:F:176:PHE:O	2.24	0.69
9:A:1783:A:N1	9:A:2587:A:H2'	2.07	0.69
9:A:587:C:OP2	20:L:21:ARG:NH1	2.25	0.69
9:A:2503:A:H3'	9:A:2503:A:OP2	1.92	0.69
9:A:2502:G:C5'	9:A:2503:A:H5''	2.22	0.69
34:Z:8:GLN:O	34:Z:10:ARG:N	2.25	0.69
21:M:66:ARG:NH1	21:M:104:GLU:OE1	2.26	0.69
9:A:2324:U:H3'	9:A:2325:G:H5''	1.74	0.68
6:5:26:VAL:O	6:5:27:VAL:HB	1.93	0.68
9:A:2061:G:N7	9:A:2501:C:H1'	2.09	0.68
9:A:2582:G:H2'	9:A:2583:G:H5'	1.75	0.68
6:5:25:ALA:O	6:5:26:VAL:HG13	1.94	0.68
9:A:2592:G:C2	9:A:2603:G:C6	2.82	0.68
6:5:129:LEU:O	6:5:131:THR:N	2.26	0.68
17:I:100:ILE:HB	17:I:139:VAL:HA	1.75	0.68
9:A:1820:U:OP1	11:C:176:ARG:NH2	2.27	0.68
9:A:1936:A:N6	9:A:1963:U:O2	2.26	0.68
9:A:2091:C:O2	32:X:33:HIS:NE2	2.26	0.68
6:5:24:SER:CB	6:5:116:GLU:HG2	2.24	0.68
9:A:301:G:OP2	29:U:81:ARG:NH1	2.26	0.68
12:D:149:ASN:OD1	12:D:150:GLN:N	2.26	0.68
20:L:93:ASN:O	20:L:95:LEU:N	2.27	0.67
10:B:73:A:C4	10:B:104:A:C2	2.82	0.67
9:A:2062:A:H62	36:A:9000:ERY:C27	2.05	0.67
18:J:4:PHE:N	18:J:44:TYR:OH	2.28	0.67
6:5:117:LEU:HD22	6:5:120:ALA:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:948:C:O2	9:A:984:A:O2'	2.12	0.67
19:K:76:VAL:HB	24:P:72:VAL:HG22	1.76	0.66
9:A:324:A:N6	9:A:338:G:O2'	2.27	0.66
19:K:18:ARG:HB2	19:K:45:GLU:HB2	1.77	0.66
20:L:93:ASN:OD1	20:L:94:THR:N	2.28	0.66
31:W:30:VAL:O	31:W:30:VAL:HG13	1.92	0.66
8:7:76:A:N6	9:A:2451:A:H4'	2.10	0.66
9:A:42:A:C2'	9:A:43:G:H5'	2.25	0.66
9:A:2142:A:H4'	9:A:2143:C:OP2	1.96	0.66
9:A:2063:C:C5	9:A:2064:C:C4	2.84	0.66
19:K:71:ARG:HB3	19:K:72:PRO:HD3	1.78	0.65
31:W:37:VAL:HG12	31:W:38:ARG:H	1.61	0.65
9:A:2582:G:C2'	9:A:2583:G:H5'	2.26	0.65
22:N:118:ARG:O	22:N:120:GLU:N	2.30	0.65
6:5:39:THR:HA	6:5:42:ARG:HD2	1.78	0.65
9:A:363:G:H2'	9:A:364:C:C6	2.32	0.65
8:7:76:A:N3	9:A:2451:A:H1'	2.12	0.65
9:A:2061:G:C2	9:A:2063:C:C4	2.84	0.65
9:A:2576:G:H3'	9:A:2576:G:N3	2.11	0.65
9:A:2503:A:H4'	9:A:2504:U:OP1	1.96	0.65
23:O:76:LYS:NZ	23:O:80:GLU:OE1	2.29	0.64
9:A:2604:U:O5'	9:A:2604:U:H6	1.80	0.64
11:C:43:ASN:OD1	11:C:44:ASN:N	2.30	0.64
9:A:1199:U:H5'	25:Q:4:LYS:HE3	1.79	0.64
24:P:50:ARG:HG3	24:P:57:ALA:O	1.97	0.64
13:E:58:LYS:NZ	13:E:70:SER:O	2.31	0.64
9:A:819:A:OP2	9:A:1187:G:N2	2.23	0.64
15:G:38:ASP:N	15:G:38:ASP:OD1	2.29	0.64
9:A:2063:C:C5	9:A:2064:C:H5	2.08	0.64
24:P:4:ILE:O	24:P:6:GLN:N	2.31	0.64
27:S:18:ARG:O	27:S:19:LEU:HB2	1.98	0.64
8:7:76:A:N1	9:A:2451:A:O4'	2.31	0.64
9:A:1482:G:H1'	9:A:1509:A:H61	1.62	0.63
29:U:73:ASN:ND2	29:U:80:ASP:OD2	2.31	0.63
10:B:87:U:H3'	10:B:88:C:H5'	1.80	0.63
18:J:44:TYR:HB2	25:Q:63:ARG:HB3	1.79	0.63
15:G:1:SER:O	15:G:3:VAL:N	2.31	0.63
9:A:1417:C:HO2'	9:A:1587:G:HO2'	1.45	0.63
8:7:75:C:O5'	8:7:75:C:H6	1.81	0.63
18:J:6:ALA:HB3	18:J:45:THR:HG21	1.78	0.63
9:A:2502:G:C5'	9:A:2503:A:C5'	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2608:G:O5'	9:A:2608:G:H8	1.82	0.63
9:A:1813:G:H1'	11:C:49:THR:HG21	1.81	0.63
9:A:861:A:N3	10:B:79:G:O2'	2.27	0.63
1:0:42:ILE:HD11	22:N:98:LEU:HB3	1.79	0.63
31:W:35:ILE:O	31:W:37:VAL:N	2.31	0.63
9:A:2346:A:H3'	9:A:2347:C:C5'	2.29	0.63
17:I:108:ILE:O	17:I:111:THR:OG1	2.17	0.63
9:A:1385:A:H1'	9:A:1386:C:C6	2.34	0.63
31:W:9:THR:OG1	31:W:10:ARG:N	2.31	0.62
9:A:2062:A:O2'	9:A:2063:C:O5'	2.17	0.62
17:I:131:THR:O	17:I:134:SER:OG	2.16	0.62
17:I:73:PRO:O	17:I:112:LYS:NZ	2.31	0.62
9:A:923:G:H1'	31:W:23:LYS:HD3	1.81	0.62
29:U:15:GLY:O	29:U:17:ASP:N	2.32	0.62
9:A:42:A:H2'	9:A:43:G:H5'	1.80	0.62
9:A:163:C:O2'	9:A:164:C:O5'	2.17	0.62
24:P:50:ARG:CB	24:P:57:ALA:H	2.11	0.62
9:A:2063:C:C6	9:A:2064:C:H5	2.17	0.62
9:A:546:U:O2'	9:A:547:A:H4'	1.99	0.62
22:N:73:ASN:HA	22:N:76:VAL:HG12	1.81	0.61
9:A:2603:G:C2	9:A:2604:U:C2	2.88	0.61
9:A:1248:G:N7	13:E:46:GLN:NE2	2.48	0.61
9:A:856:G:H21	31:W:19:ARG:NH1	1.97	0.61
28:T:32:LEU:H	28:T:83:ALA:HB3	1.63	0.61
9:A:2060:A:O2'	13:E:63:LYS:NZ	2.32	0.61
6:5:29:ASP:HA	6:5:108:VAL:HG11	1.82	0.61
22:N:98:LEU:O	22:N:112:TYR:N	2.34	0.61
9:A:1567:G:H5'	11:C:57:HIS:CD2	2.35	0.61
6:5:26:VAL:HG21	6:5:115:GLY:N	2.06	0.61
9:A:1930:G:O2'	9:A:1968:G:O6	2.17	0.61
5:4:36:ARG:HG2	5:4:37:GLN:H	1.66	0.61
6:5:27:VAL:HG13	6:5:83:ALA:HB3	1.83	0.61
9:A:616:A:H4'	13:E:101:TYR:CE2	2.36	0.61
12:D:118:PHE:HD1	12:D:119:ALA:H	1.49	0.60
9:A:2502:G:H5''	9:A:2503:A:H5''	1.81	0.60
17:I:100:ILE:HG22	17:I:101:SER:N	2.15	0.60
9:A:2502:G:H5'	9:A:2503:A:C5'	2.31	0.60
9:A:276:U:O2'	9:A:278:A:N7	2.34	0.60
9:A:2011:U:OP2	27:S:16:LYS:NZ	2.31	0.60
9:A:1338:G:O2'	28:T:18:GLU:OE1	2.20	0.60
23:O:105:ALA:O	23:O:107:ALA:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2581:G:HO2'	9:A:2610:C:H41	1.49	0.60
9:A:480:A:OP2	29:U:43:LYS:NZ	2.34	0.60
9:A:2579:C:C2'	9:A:2580:U:C5'	2.72	0.60
9:A:2595:G:N1	9:A:2599:G:C6	2.70	0.60
18:J:6:ALA:CB	18:J:45:THR:HG21	2.31	0.60
9:A:983:A:C6	9:A:984:A:C2	2.90	0.60
7:6:18:ASP:N	7:6:18:ASP:OD1	2.32	0.60
9:A:27:G:O2'	9:A:28:A:OP2	2.19	0.60
9:A:2353:G:N3	31:W:30:VAL:CG1	2.65	0.60
31:W:55:ASP:O	31:W:57:THR:N	2.34	0.60
9:A:1262:A:OP2	27:S:99:ARG:NH2	2.35	0.60
9:A:2681:C:OP2	12:D:114:LYS:NZ	2.33	0.60
6:5:15:VAL:HG22	6:5:66:GLY:HA3	1.84	0.60
9:A:2502:G:H5'	9:A:2503:A:H5''	1.82	0.59
9:A:635:C:OP2	20:L:126:ARG:NH1	2.35	0.59
23:O:89:ASP:HA	23:O:116:GLN:HB3	1.84	0.59
11:C:16:VAL:N	11:C:203:VAL:HG12	2.18	0.59
9:A:947:A:HO2'	9:A:984:A:H2	1.50	0.59
9:A:1803:A:O3'	11:C:256:THR:OG1	2.19	0.59
9:A:2592:G:N2	9:A:2603:G:C5	2.70	0.59
9:A:2800:A:H3'	9:A:2801:G:C5'	2.32	0.59
29:U:38:ILE:CG2	29:U:39:ASN:N	2.64	0.59
31:W:51:GLY:HA3	31:W:59:PHE:CE1	2.38	0.59
8:7:76:A:C4	9:A:2451:A:H1'	2.38	0.59
17:I:93:ASN:ND2	17:I:135:MET:O	2.36	0.59
24:P:63:ILE:HA	24:P:68:GLY:HA2	1.85	0.59
17:I:92:PRO:O	17:I:94:LYS:N	2.36	0.59
9:A:2063:C:C2'	9:A:2064:C:H5'	2.26	0.58
9:A:1076:C:H2'	9:A:1077:A:O4'	2.03	0.58
9:A:370:G:O2'	9:A:424:G:OP1	2.15	0.58
9:A:2780:G:OP2	18:J:120:ARG:NE	2.33	0.58
28:T:35:ALA:HB3	28:T:38:ALA:HB2	1.85	0.58
9:A:2581:G:HO2'	9:A:2610:C:H5	1.50	0.58
28:T:19:LYS:O	28:T:23:ALA:N	2.35	0.58
25:Q:63:ARG:NH1	25:Q:95:ALA:O	2.35	0.58
9:A:1131:G:OP1	18:J:82:GLY:HA2	2.02	0.58
6:5:62:ARG:NH2	9:A:1106:G:OP1	2.35	0.58
31:W:76:ARG:HH21	31:W:76:ARG:CG	2.16	0.58
5:4:2:LYS:HZ1	9:A:2478:A:P	2.27	0.58
9:A:784:G:O2'	9:A:785:G:OP2	2.15	0.58
25:Q:84:LYS:O	25:Q:86:SER:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:168:ASP:OD2	13:E:170:ARG:NH2	2.36	0.58
9:A:1076:C:H1'	17:I:93:ASN:HB3	1.86	0.58
31:W:51:GLY:HA3	31:W:59:PHE:CZ	2.38	0.58
28:T:54:GLU:HG3	28:T:88:LYS:HB2	1.86	0.58
9:A:2582:G:C2	9:A:2583:G:N7	2.71	0.58
9:A:2574:G:O2'	9:A:2575:C:H5'	2.04	0.57
6:5:45:GLY:HA2	6:5:49:GLY:HA2	1.85	0.57
9:A:1386:C:H2'	9:A:1387:A:C8	2.39	0.57
9:A:2517:C:C6	9:A:2542:A:N7	2.72	0.57
21:M:41:LEU:HD11	21:M:126:ILE:HD13	1.85	0.57
9:A:2061:G:C2	9:A:2063:C:N3	2.72	0.57
25:Q:63:ARG:HH22	25:Q:95:ALA:C	2.08	0.57
9:A:1936:A:H2	9:A:1943:U:C5	2.23	0.57
11:C:77:VAL:HG23	11:C:111:ALA:HA	1.86	0.57
9:A:422:A:C2	9:A:423:A:C4	2.92	0.57
25:Q:81:GLY:O	25:Q:85:ALA:N	2.37	0.57
9:A:2331:G:O2'	9:A:2336:A:N1	2.38	0.57
17:I:37:PHE:O	17:I:41:PHE:HB3	2.04	0.57
31:W:28:GLU:HB3	31:W:31:LEU:HD21	1.86	0.57
18:J:49:ASP:OD1	18:J:121:LYS:NZ	2.32	0.57
8:7:76:A:C2	9:A:2451:A:O4'	2.57	0.57
9:A:673:C:OP1	13:E:49:ARG:NH2	2.36	0.57
9:A:1654:A:O2'	12:D:118:PHE:CG	2.55	0.57
9:A:2063:C:C5	9:A:2064:C:N4	2.73	0.57
13:E:150:THR:HG21	13:E:153:LEU:HA	1.87	0.57
9:A:2583:G:N2	9:A:2584:U:C2	2.73	0.56
6:5:3:LEU:CD1	6:5:5:LEU:HG	2.35	0.56
9:A:1509:A:HO2'	9:A:1510:G:P	2.26	0.56
11:C:14:HIS:O	11:C:203:VAL:HG11	2.05	0.56
9:A:1324:G:C4	9:A:1328:A:N6	2.73	0.56
31:W:39:GLN:HG2	31:W:41:GLY:H	1.69	0.56
24:P:58:PHE:CD1	24:P:75:THR:HG22	2.40	0.56
17:I:100:ILE:HD11	17:I:137:LEU:HG	1.87	0.56
9:A:2548:U:O2	19:K:23:LYS:NZ	2.37	0.56
19:K:121:GLU:OE1	24:P:62:LYS:NZ	2.37	0.56
25:Q:105:PHE:O	25:Q:108:LEU:N	2.38	0.56
9:A:2574:G:H2'	9:A:2575:C:C5'	2.30	0.56
2:1:8:ILE:HD11	2:1:24:LYS:N	2.21	0.56
32:X:32:LEU:O	32:X:33:HIS:ND1	2.39	0.56
9:A:1773:A:N7	9:A:1829:A:H1'	2.20	0.56
9:A:2680:U:H5'	12:D:194:PRO:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y:56:LEU:O	33:Y:58:ASN:N	2.39	0.56
9:A:2061:G:OP2	13:E:63:LYS:HE2	2.06	0.56
6:5:132:TYR:CZ	7:6:23:ILE:HD11	2.40	0.56
6:5:58:THR:CG2	9:A:1107:G:H5''	2.36	0.56
24:P:50:ARG:HB3	24:P:57:ALA:N	2.17	0.56
18:J:81:ILE:HG13	18:J:82:GLY:N	2.21	0.56
9:A:443:A:N7	13:E:40:ARG:HD3	2.21	0.56
9:A:1353:A:C8	9:A:1378:A:N6	2.73	0.56
9:A:85:G:OP2	29:U:6:ARG:HG3	2.06	0.56
9:A:2585:U:C4	9:A:2608:G:O6	2.59	0.55
9:A:2603:G:H2'	9:A:2604:U:C6	2.41	0.55
9:A:2502:G:H5''	9:A:2503:A:C5'	2.36	0.55
17:I:135:MET:HB3	17:I:137:LEU:HD22	1.88	0.55
28:T:59:ASN:O	28:T:83:ALA:O	2.24	0.55
9:A:100:U:H4'	9:A:101:A:O5'	2.06	0.55
20:L:85:VAL:CG2	20:L:94:THR:HG22	2.36	0.55
31:W:18:LYS:HG3	31:W:19:ARG:N	2.21	0.55
14:F:151:LEU:HD12	14:F:152:ASP:N	2.21	0.55
9:A:1750:G:O2'	9:A:2860:A:N1	2.37	0.55
6:5:64:VAL:O	6:5:68:PRO:HD2	2.06	0.55
6:5:129:LEU:C	6:5:131:THR:H	2.10	0.55
9:A:811:U:C4	20:L:21:ARG:NH2	2.74	0.55
6:5:43:LYS:HZ3	6:5:98:GLU:HB2	1.71	0.55
23:O:2:ASP:OD1	23:O:3:LYS:N	2.39	0.55
6:5:56:ARG:O	6:5:57:ASN:ND2	2.39	0.55
28:T:32:LEU:N	28:T:83:ALA:HB3	2.21	0.55
26:R:39:LEU:O	26:R:49:ILE:HG23	2.07	0.55
17:I:116:MET:SD	17:I:124:MET:HE2	2.47	0.55
18:J:17:VAL:HG23	18:J:139:VAL:HA	1.88	0.55
12:D:118:PHE:O	12:D:120:GLY:N	2.36	0.55
9:A:1019:U:H3	9:A:1142:A:H62	1.53	0.55
9:A:1397:U:OP2	9:A:1398:C:N4	2.34	0.55
9:A:2061:G:C4	9:A:2063:C:N4	2.75	0.55
9:A:2582:G:N2	9:A:2583:G:N9	2.55	0.55
9:A:1482:G:C6	9:A:1508:A:C2	2.94	0.55
9:A:283:G:C2	9:A:284:U:H1'	2.41	0.55
1:0:2:VAL:HG22	9:A:2015:A:C2	2.41	0.55
5:4:36:ARG:NH1	9:A:2742:G:OP1	2.38	0.55
22:N:30:ARG:NH1	22:N:74:GLU:OE1	2.40	0.55
9:A:2355:G:H4'	31:W:20:LEU:HD13	1.88	0.55
9:A:2506:U:H6	9:A:2506:U:H3'	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:107:VAL:CG2	12:D:203:VAL:HG23	2.38	0.54
9:A:2757:A:N1	15:G:66:THR:HG21	2.21	0.54
9:A:834:G:C6	9:A:835:C:C4	2.95	0.54
25:Q:91:ARG:NH1	26:R:10:LYS:HB3	2.23	0.54
11:C:68:ARG:CD	11:C:103:ILE:HD11	2.37	0.54
6:5:81:LEU:HA	9:A:1107:G:H4'	1.88	0.54
9:A:1458:U:H4'	9:A:1459:G:O5'	2.07	0.54
9:A:2698:U:H2'	9:A:2699:C:H6	1.72	0.54
9:A:2576:G:HO2'	9:A:2577:A:P	2.30	0.54
9:A:1715:G:N2	9:A:1744:A:OP2	2.36	0.54
6:5:44:ALA:O	6:5:49:GLY:N	2.40	0.54
19:K:107:LEU:O	19:K:109:SER:N	2.38	0.54
9:A:1754:A:H4'	24:P:102:ARG:NH2	2.22	0.54
6:5:129:LEU:HB3	6:5:130:PRO:HD2	1.89	0.54
1:0:2:VAL:HG11	9:A:2016:U:H1'	1.89	0.54
9:A:1786:A:H1'	9:A:1938:A:N6	2.22	0.54
9:A:674:G:H1'	13:E:69:ARG:HE	1.72	0.54
9:A:396:G:OP2	32:X:9:LYS:NZ	2.40	0.54
9:A:2415:G:H4'	20:L:66:PHE:HB2	1.90	0.54
9:A:277:G:O2'	9:A:278:A:OP2	2.25	0.54
9:A:1936:A:N6	9:A:1963:U:H3	2.05	0.54
29:U:38:ILE:HG22	29:U:39:ASN:H	1.73	0.54
21:M:33:LEU:HD22	21:M:128:THR:HB	1.90	0.54
9:A:686:U:H2'	9:A:788:A:N1	2.21	0.54
9:A:877:A:C2	9:A:899:A:C2	2.95	0.54
9:A:2335:A:C6	9:A:2337:G:H1'	2.42	0.54
30:V:80:HIS:HD2	30:V:83:LYS:N	2.05	0.54
9:A:2533:U:OP1	9:A:2665:A:O2'	2.20	0.54
24:P:33:GLU:HB2	24:P:38:ARG:HH11	1.71	0.54
24:P:50:ARG:CG	24:P:57:ALA:O	2.55	0.54
9:A:1824:G:N3	11:C:251:THR:HG21	2.21	0.54
15:G:84:LYS:HG3	15:G:132:LEU:H	1.73	0.54
9:A:163:C:O2'	9:A:164:C:P	2.65	0.54
6:5:60:LEU:O	6:5:64:VAL:HB	2.08	0.54
12:D:12:THR:OG1	24:P:8:GLU:OE2	2.21	0.54
19:K:80:ASP:HB2	24:P:67:GLU:HG3	1.90	0.54
34:Z:5:LYS:H	34:Z:5:LYS:HD2	1.72	0.54
9:A:2580:U:O2'	9:A:2581:G:H5'	2.08	0.54
6:5:23:LEU:HG	6:5:24:SER:N	2.22	0.54
6:5:54:VAL:HA	6:5:84:TYR:O	2.07	0.54
24:P:4:ILE:HG22	24:P:5:LYS:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:81:GLY:HA2	25:Q:116:LEU:CD1	2.38	0.54
6:5:58:THR:HB	6:5:82:ILE:HB	1.89	0.54
9:A:1779:U:H5	9:A:1784:A:N7	2.06	0.54
9:A:910:A:N6	9:A:2277:G:O2'	2.36	0.54
20:L:77:ILE:CD1	20:L:108:ALA:HB1	2.38	0.54
28:T:50:LEU:C	28:T:52:GLU:H	2.11	0.54
9:A:84:A:P	29:U:5:ARG:NH2	2.81	0.54
25:Q:93:ILE:O	25:Q:96:ASP:N	2.39	0.54
26:R:49:ILE:HB	26:R:51:VAL:O	2.08	0.54
9:A:411:G:OP2	9:A:2406:A:O2'	2.25	0.54
18:J:32:LEU:HD22	18:J:54:ILE:HD12	1.90	0.54
12:D:106:LYS:HB3	12:D:206:ALA:HB3	1.89	0.54
19:K:43:ILE:CD1	19:K:52:VAL:HB	2.37	0.54
9:A:1772:A:N1	9:A:1980:G:C6	2.75	0.54
14:F:103:ILE:HG23	14:F:175:PRO:HD3	1.90	0.54
9:A:855:G:H1'	31:W:23:LYS:HE3	1.89	0.54
29:U:21:ARG:CZ	29:U:72:PHE:CE2	2.90	0.53
9:A:1187:G:H5''	26:R:83:TYR:CE2	2.44	0.53
31:W:46:ALA:HB3	31:W:80:SER:HB3	1.91	0.53
9:A:384:A:H2'	9:A:385:C:H5'	1.91	0.53
9:A:2505:G:C2'	9:A:2506:U:H5''	2.38	0.53
5:4:1:MET:N	9:A:2526:G:N3	2.57	0.53
9:A:2586:U:O2	9:A:2586:U:H2'	2.07	0.53
9:A:265:A:H4'	9:A:266:G:OP1	2.07	0.53
9:A:189:G:O6	9:A:205:G:O2'	2.19	0.53
12:D:120:GLY:HA2	12:D:162:ALA:CB	2.38	0.53
19:K:10:VAL:HG11	19:K:16:ALA:HB3	1.90	0.53
27:S:73:LYS:HB3	27:S:106:VAL:HB	1.90	0.53
25:Q:65:ASN:OD1	25:Q:69:ARG:NH2	2.42	0.53
17:I:98:GLY:HA3	17:I:137:LEU:HB3	1.90	0.53
26:R:49:ILE:HG22	26:R:54:VAL:HG13	1.89	0.53
18:J:39:LYS:HA	18:J:43:GLU:HG3	1.91	0.53
15:G:84:LYS:HB3	15:G:132:LEU:O	2.09	0.53
9:A:954:G:OP2	21:M:16:ARG:NH2	2.42	0.53
6:5:25:ALA:HB3	6:5:85:SER:OG	2.09	0.53
6:5:4:ASN:O	6:5:6:GLN:N	2.41	0.53
9:A:2505:G:HO2'	9:A:2506:U:H5''	1.70	0.53
28:T:50:LEU:H	28:T:50:LEU:HD12	1.74	0.53
9:A:2425:A:H5''	9:A:2427:C:O4'	2.09	0.53
1:0:12:ARG:NH1	9:A:1263:U:OP1	2.41	0.53
9:A:630:G:N2	9:A:633:A:OP2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:63:ARG:HH12	25:Q:96:ASP:CA	2.22	0.53
9:A:2053:G:H1	9:A:2616:C:H42	1.57	0.53
9:A:1069:A:C4	9:A:1073:A:N7	2.77	0.53
24:P:50:ARG:CD	24:P:51:ASN:N	2.72	0.53
9:A:273:G:N2	9:A:365:U:C2	2.77	0.53
9:A:2547:A:H2'	9:A:2548:U:C6	2.43	0.53
9:A:1080:A:H1'	17:I:127:SER:HA	1.91	0.53
23:O:31:THR:HG22	23:O:34:HIS:H	1.74	0.53
28:T:50:LEU:O	28:T:52:GLU:N	2.42	0.53
9:A:1535:A:H4'	9:A:1536:C:OP2	2.08	0.53
34:Z:48:ASN:O	34:Z:51:SER:OG	2.27	0.53
9:A:2297:A:N1	9:A:2321:U:H5	2.07	0.53
31:W:37:VAL:HG13	31:W:55:ASP:C	2.29	0.52
6:5:81:LEU:HD23	6:5:82:ILE:N	2.24	0.52
31:W:13:ARG:HG2	31:W:14:ASP:H	1.73	0.52
9:A:2092:U:H4'	9:A:2093:G:O5'	2.09	0.52
23:O:36:TYR:CD1	23:O:36:TYR:N	2.78	0.52
9:A:2582:G:H2'	9:A:2583:G:H8	1.74	0.52
9:A:1738:G:O2'	9:A:1739:A:O5'	2.25	0.52
9:A:1069:A:C5	9:A:1073:A:N7	2.77	0.52
31:W:37:VAL:HB	31:W:38:ARG:HH11	1.74	0.52
25:Q:31:TYR:O	25:Q:34:ALA:N	2.42	0.52
28:T:89:GLU:O	28:T:91:GLN:N	2.41	0.52
8:7:76:A:C2	9:A:2451:A:C1'	2.92	0.52
8:7:76:A:C2	9:A:2451:A:H1'	2.45	0.52
22:N:73:ASN:HA	22:N:76:VAL:CG1	2.39	0.52
1:0:2:VAL:CG1	9:A:2016:U:H1'	2.40	0.52
9:A:2232:C:P	32:X:26:ARG:HH22	2.32	0.52
19:K:70:ARG:HD3	19:K:76:VAL:HG22	1.90	0.52
9:A:1288:G:C4	9:A:1327:A:C2	2.98	0.52
6:5:43:LYS:NZ	6:5:98:GLU:HB2	2.24	0.52
9:A:1328:A:H2'	9:A:1330:C:C5	2.45	0.52
6:5:118:ILE:HB	6:5:119:PRO:CD	2.40	0.52
29:U:35:VAL:HB	29:U:38:ILE:HG21	1.90	0.52
2:1:33:LEU:N	2:1:51:ALA:HB3	2.25	0.52
29:U:82:VAL:HG12	29:U:83:GLY:N	2.25	0.52
9:A:2211:A:O2'	9:A:2212:A:OP1	2.25	0.52
34:Z:6:ILE:O	34:Z:34:THR:HA	2.10	0.52
28:T:44:LYS:HG3	28:T:55:VAL:HG11	1.90	0.52
26:R:61:ALA:HB2	26:R:98:ILE:HA	1.92	0.52
18:J:39:LYS:HA	18:J:43:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:36:ASP:O	6:5:39:THR:OG1	2.26	0.52
9:A:2504:U:O5'	9:A:2504:U:H6	1.93	0.52
18:J:55:ILE:HD11	18:J:130:HIS:CG	2.44	0.52
5:4:7:VAL:O	5:4:35:GLN:NE2	2.42	0.52
9:A:2507:C:H2'	9:A:2507:C:O2	2.08	0.52
9:A:2354:C:H4'	31:W:31:LEU:HD22	1.92	0.52
9:A:974:G:H8	9:A:990:A:H62	1.58	0.52
11:C:256:THR:O	11:C:256:THR:OG1	2.28	0.52
9:A:38:A:O2'	13:E:43:THR:HA	2.09	0.52
31:W:8:SER:O	31:W:9:THR:HG22	2.10	0.51
24:P:33:GLU:CD	24:P:34:GLY:N	2.63	0.51
15:G:83:THR:HA	15:G:84:LYS:CE	2.39	0.51
9:A:1759:A:HO2'	9:A:2714:G:HO2'	1.47	0.51
9:A:729:G:H2'	9:A:1775:U:H1'	1.91	0.51
19:K:13:ASN:O	19:K:15:GLY:N	2.43	0.51
11:C:255:LYS:O	11:C:257:ARG:N	2.43	0.51
12:D:151:THR:HG22	12:D:152:PRO:HD3	1.92	0.51
9:A:2313:C:H5''	14:F:87:LYS:HD3	1.92	0.51
9:A:2134:A:HO2'	9:A:2135:A:H8	1.56	0.51
9:A:2039:U:H2'	9:A:2040:G:C8	2.45	0.51
21:M:53:MET:HE3	21:M:63:ILE:HD13	1.92	0.51
9:A:2061:G:C2	9:A:2063:C:N4	2.78	0.51
6:5:3:LEU:HD12	6:5:5:LEU:H	1.76	0.51
9:A:2604:U:H2'	9:A:2605:U:C6	2.45	0.51
9:A:2387:U:O2'	31:W:38:ARG:NH2	2.43	0.51
21:M:73:ILE:HG21	21:M:91:TYR:CZ	2.45	0.51
9:A:2803:G:H2'	9:A:2804:U:C6	2.45	0.51
20:L:91:ASP:OD1	20:L:92:LEU:N	2.43	0.51
30:V:44:HIS:HE1	30:V:86:LEU:H	1.59	0.51
15:G:96:ALA:HB3	15:G:103:ASN:HB2	1.92	0.51
30:V:51:GLN:OE1	30:V:57:TYR:OH	2.28	0.51
9:A:2062:A:N6	36:A:9000:ERY:C27	2.54	0.51
25:Q:94:LEU:C	25:Q:96:ASP:H	2.14	0.51
9:A:1797:G:O2'	11:C:256:THR:CG2	2.59	0.51
17:I:36:GLU:HB3	17:I:66:PHE:CE1	2.46	0.51
6:5:94:ARG:O	6:5:97:LYS:N	2.43	0.51
13:E:148:ILE:HA	13:E:187:VAL:HB	1.93	0.51
9:A:1300:G:H4'	9:A:1301:A:H5'	1.92	0.51
16:H:41:LYS:HA	16:H:44:ILE:HG12	1.93	0.51
14:F:132:ARG:O	14:F:133:GLU:HB3	2.10	0.51
31:W:16:GLU:O	31:W:17:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1816:C:C5	11:C:61:TYR:CE2	2.98	0.51
6:5:25:ALA:O	6:5:116:GLU:OE1	2.28	0.51
25:Q:94:LEU:C	25:Q:96:ASP:N	2.64	0.51
12:D:91:THR:O	12:D:91:THR:OG1	2.28	0.51
30:V:9:ARG:NH2	30:V:12:GLN:HA	2.26	0.51
28:T:69:ARG:CG	28:T:70:HIS:H	2.23	0.51
3:2:27:GLY:O	3:2:30:VAL:HB	2.11	0.51
9:A:2063:C:C2'	9:A:2064:C:C5'	2.88	0.51
9:A:26:G:C6	9:A:27:G:N1	2.79	0.51
21:M:8:LYS:HE3	21:M:9:PHE:CE2	2.45	0.51
9:A:460:A:C2	9:A:470:A:C4	2.99	0.51
34:Z:41:PRO:HA	34:Z:44:ARG:HB3	1.93	0.51
9:A:565:C:H2'	9:A:566:U:O4'	2.11	0.51
9:A:84:A:N1	9:A:98:G:O2'	2.30	0.51
9:A:27:G:N2	9:A:512:G:H1'	2.26	0.51
18:J:81:ILE:CG1	18:J:82:GLY:N	2.74	0.51
9:A:1322:A:OP1	27:S:11:ARG:NE	2.38	0.51
9:A:489:G:N7	27:S:49:LYS:NZ	2.58	0.51
9:A:748:G:P	27:S:88:ARG:NH2	2.83	0.51
25:Q:91:ARG:HE	25:Q:93:ILE:CG2	2.25	0.50
9:A:2314:A:OP1	14:F:87:LYS:NZ	2.44	0.50
9:A:1394:U:H4'	9:A:1603:A:H4'	1.92	0.50
15:G:16:VAL:HG21	15:G:44:HIS:CD2	2.46	0.50
19:K:9:ASN:O	19:K:83:ALA:HA	2.11	0.50
9:A:1533:C:C2	9:A:1534:U:C4	2.99	0.50
5:4:3:VAL:HG23	5:4:4:ARG:H	1.74	0.50
20:L:81:ASP:O	20:L:83:ALA:N	2.41	0.50
31:W:76:ARG:HH21	31:W:76:ARG:HG2	1.76	0.50
9:A:391:A:C6	9:A:411:G:C2	3.00	0.50
9:A:1533:C:H2'	9:A:1534:U:C6	2.46	0.50
27:S:86:MET:HB2	27:S:96:ILE:HG21	1.92	0.50
15:G:30:GLY:O	15:G:32:LEU:N	2.38	0.50
28:T:29:THR:OG1	28:T:86:THR:N	2.43	0.50
9:A:1778:U:H2'	9:A:1784:A:N6	2.27	0.50
14:F:71:LYS:HD3	14:F:72:SER:N	2.26	0.50
9:A:945:A:C5	9:A:2448:A:C2	2.98	0.50
12:D:148:GLN:N	12:D:148:GLN:OE1	2.45	0.50
9:A:2074:U:H2'	9:A:2075:U:C6	2.46	0.50
3:2:34:ARG:NH1	3:2:41:ARG:O	2.45	0.50
9:A:1179:G:H2'	9:A:1180:U:O4'	2.12	0.50
18:J:44:TYR:O	18:J:45:THR:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:39:LEU:HA	26:R:49:ILE:HG21	1.92	0.50
9:A:322:A:H5'	9:A:340:A:H1'	1.94	0.50
21:M:35:ALA:O	21:M:36:VAL:HB	2.11	0.50
9:A:139:U:O2'	28:T:1:MET:HA	2.12	0.50
9:A:2352:A:C6	31:W:30:VAL:HG11	2.47	0.50
9:A:1654:A:H2'	9:A:1655:A:H8	1.76	0.50
9:A:2094:A:C2	9:A:2196:C:C2	2.99	0.50
9:A:2329:U:H2'	9:A:2330:G:C8	2.47	0.50
9:A:1203:U:O2'	20:L:4:ASN:OD1	2.28	0.50
9:A:1753:G:OP1	24:P:92:ARG:NE	2.38	0.50
22:N:52:ILE:HB	22:N:94:TYR:CD2	2.46	0.50
9:A:2576:G:N3	9:A:2576:G:C3'	2.75	0.50
34:Z:26:LEU:O	34:Z:37:ARG:NH1	2.44	0.50
33:Y:8:GLU:O	33:Y:12:GLU:HB2	2.12	0.50
19:K:19:VAL:CG1	19:K:41:ILE:HG12	2.40	0.50
9:A:2601:C:O2'	9:A:2602:A:O5'	2.26	0.50
9:A:504:A:HO2'	9:A:505:A:P	2.28	0.50
12:D:193:VAL:HG21	12:D:201:LEU:HD21	1.93	0.50
12:D:62:LYS:HB2	12:D:63:PRO:HD3	1.93	0.50
9:A:1437:C:H2'	9:A:1438:U:C6	2.46	0.50
9:A:654:A:H3'	9:A:654:A:N3	2.26	0.50
9:A:1475:G:O2'	9:A:1514:G:O6	2.30	0.50
9:A:118:A:N3	9:A:178:G:H1'	2.27	0.50
34:Z:30:ARG:HH11	34:Z:30:ARG:HB3	1.76	0.50
9:A:221:A:N1	9:A:265:A:O2'	2.45	0.50
9:A:1808:A:O2'	32:X:2:ARG:NH1	2.45	0.50
9:A:2061:G:O6	9:A:2501:C:O2	2.30	0.49
9:A:747:U:O2'	27:S:88:ARG:NH2	2.45	0.49
21:M:20:LEU:HD22	21:M:20:LEU:N	2.26	0.49
6:5:4:ASN:C	6:5:6:GLN:N	2.66	0.49
2:1:4:ILE:HG23	2:1:5:ARG:H	1.76	0.49
9:A:1869:G:H3'	9:A:1870:C:H5''	1.94	0.49
4:3:30:HIS:HD2	9:A:2421:G:N7	2.10	0.49
17:I:109:ALA:HB2	17:I:128:ILE:HG13	1.93	0.49
9:A:2604:U:H2'	9:A:2605:U:H6	1.75	0.49
31:W:9:THR:HG23	31:W:10:ARG:HD3	1.94	0.49
9:A:2571:U:O2'	12:D:151:THR:CG2	2.60	0.49
12:D:151:THR:CG2	12:D:152:PRO:HD3	2.43	0.49
9:A:748:G:OP1	27:S:88:ARG:NH2	2.45	0.49
6:5:138:ARG:NH2	7:6:26:MET:HA	2.27	0.49
23:O:51:ALA:HB3	23:O:78:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:96:ARG:NH2	22:N:114:GLU:OE1	2.44	0.49
6:5:95:LEU:H	6:5:95:LEU:HD22	1.77	0.49
28:T:54:GLU:CG	28:T:88:LYS:HB2	2.42	0.49
9:A:1614:A:N1	27:S:93:ALA:HB2	2.27	0.49
18:J:21:THR:HG22	18:J:22:GLY:N	2.27	0.49
32:X:70:LEU:O	32:X:75:GLU:N	2.45	0.49
9:A:2228:G:H22	32:X:33:HIS:HE2	1.61	0.49
9:A:2330:G:C2	9:A:2386:A:C2	3.01	0.49
17:I:123:ALA:HA	17:I:126:ARG:CZ	2.43	0.49
9:A:1199:U:H5'	25:Q:4:LYS:CE	2.42	0.49
9:A:443:A:C5	13:E:40:ARG:HD3	2.47	0.49
9:A:250:G:C6	9:A:251:A:C6	3.01	0.49
27:S:20:VAL:HG11	27:S:44:ALA:HA	1.93	0.49
9:A:2109:U:H2'	9:A:2110:G:H5'	1.94	0.49
17:I:48:ILE:HG13	17:I:49:GLU:H	1.77	0.49
25:Q:63:ARG:NH1	25:Q:96:ASP:HA	2.27	0.49
9:A:2755:C:HO2'	9:A:2756:U:H6	1.61	0.49
17:I:87:SER:OG	17:I:88:GLY:N	2.43	0.49
9:A:2609:U:H3'	9:A:2610:C:H5'	1.95	0.49
9:A:1567:G:H2'	11:C:84:PRO:HG3	1.95	0.49
6:5:68:PRO:HA	6:5:72:LEU:HD11	1.94	0.49
9:A:1844:C:O3'	11:C:255:LYS:NZ	2.43	0.49
13:E:112:LEU:HD13	13:E:186:VAL:HG11	1.94	0.49
14:F:5:ASP:OD1	14:F:8:LYS:NZ	2.46	0.49
9:A:2867:G:O2'	9:A:2868:A:OP2	2.28	0.49
9:A:107:G:H2'	9:A:108:G:H8	1.78	0.49
6:5:51:TYR:CD1	6:5:51:TYR:C	2.86	0.49
9:A:564:C:O2	9:A:578:G:N2	2.46	0.49
9:A:2580:U:C2'	9:A:2581:G:C5'	2.86	0.49
6:5:55:VAL:HG13	9:A:1084:A:H5'	1.93	0.49
9:A:223:A:C5	9:A:422:A:C8	3.00	0.49
15:G:84:LYS:HG3	15:G:132:LEU:N	2.28	0.49
28:T:34:VAL:O	28:T:34:VAL:CG2	2.61	0.49
9:A:1778:U:H2'	9:A:1784:A:H62	1.78	0.49
9:A:2211:A:O2'	9:A:2212:A:P	2.70	0.49
21:M:106:ASP:O	21:M:108:VAL:N	2.44	0.49
9:A:1474:U:H2'	9:A:1475:G:H5'	1.95	0.49
9:A:1022:G:C5	9:A:1140:C:C4	3.00	0.49
9:A:308:G:O2'	9:A:329:G:N2	2.46	0.49
27:S:13:SER:O	27:S:14:ALA:CB	2.60	0.49
9:A:2483:C:N3	21:M:123:LYS:NZ	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:12:ARG:CZ	22:N:20:MET:HE1	2.43	0.49
4:3:51:LYS:NZ	9:A:938:G:OP2	2.33	0.49
9:A:1730:C:OP1	9:A:1730:C:H4'	2.12	0.49
9:A:2701:U:H3'	9:A:2702:G:C5'	2.42	0.49
9:A:2063:C:C4	9:A:2064:C:C4	3.01	0.48
6:5:4:ASN:C	6:5:6:GLN:H	2.16	0.48
9:A:1327:A:N6	9:A:1328:A:C2	2.81	0.48
12:D:174:SER:OG	12:D:175:LEU:N	2.46	0.48
9:A:1607:C:H4'	9:A:1608:A:O5'	2.13	0.48
9:A:2393:U:H5'	20:L:60:ARG:O	2.13	0.48
9:A:1485:U:H2'	9:A:1486:U:C6	2.48	0.48
27:S:24:ILE:HG22	27:S:71:VAL:HG11	1.95	0.48
16:H:9:VAL:O	16:H:13:GLY:N	2.46	0.48
1:0:2:VAL:CG2	9:A:2015:A:C2	2.96	0.48
9:A:2016:U:H2'	9:A:2017:U:C6	2.48	0.48
15:G:73:SER:O	15:G:77:GLY:N	2.45	0.48
6:5:71:CYS:CA	6:5:117:LEU:HD13	2.31	0.48
9:A:2600:A:C2'	9:A:2601:C:C5'	2.86	0.48
18:J:43:GLU:O	18:J:45:THR:HG22	2.13	0.48
24:P:91:VAL:O	24:P:92:ARG:HG2	2.12	0.48
17:I:14:ALA:HB3	17:I:51:GLY:H	1.79	0.48
20:L:19:LEU:HB2	20:L:27:LEU:HB3	1.94	0.48
29:U:85:ARG:HD3	29:U:86:PHE:N	2.28	0.48
14:F:79:ARG:HB3	14:F:82:TYR:CE1	2.48	0.48
14:F:79:ARG:HB3	14:F:82:TYR:CZ	2.48	0.48
21:M:34:LYS:HD2	21:M:131:VAL:HG11	1.95	0.48
11:C:265:PHE:CD1	11:C:265:PHE:N	2.82	0.48
9:A:2580:U:O5'	9:A:2580:U:H6	1.96	0.48
9:A:856:G:O2'	31:W:22:VAL:HG23	2.14	0.48
9:A:856:G:H21	31:W:19:ARG:HH12	1.58	0.48
9:A:2747:G:O2'	15:G:66:THR:HG22	2.14	0.48
9:A:580:U:H2'	9:A:581:C:H6	1.79	0.48
9:A:1348:C:H2'	9:A:1349:C:H5'	1.96	0.48
32:X:39:VAL:HG22	32:X:44:ARG:O	2.14	0.48
6:5:77:VAL:O	6:5:79:PRO:HD2	2.13	0.48
31:W:18:LYS:HA	31:W:36:ILE:HG13	1.95	0.48
9:A:923:G:H1'	31:W:23:LYS:CD	2.43	0.48
9:A:2800:A:H3'	9:A:2801:G:H5''	1.96	0.48
9:A:391:A:C5	9:A:411:G:C2	3.02	0.48
32:X:70:LEU:O	32:X:74:GLY:N	2.46	0.48
9:A:1022:G:C6	9:A:1140:C:C4	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1135:C:N4	9:A:1139:G:C6	2.82	0.48
12:D:68:PHE:C	12:D:73:VAL:HG12	2.33	0.48
11:C:225:ASN:HB3	11:C:226:PRO:HD2	1.96	0.48
34:Z:38:GLU:O	34:Z:43:ILE:HG12	2.13	0.48
21:M:1:MET:O	21:M:2:LEU:CB	2.62	0.48
9:A:1760:C:H2'	9:A:1761:C:O4'	2.14	0.48
13:E:164:LEU:HB3	13:E:167:VAL:CG1	2.44	0.48
9:A:973:A:P	26:R:81:LYS:HZ3	2.35	0.48
14:F:110:ILE:O	14:F:112:ASP:N	2.46	0.48
9:A:301:G:H1'	9:A:302:C:C6	2.48	0.48
6:5:58:THR:HG23	9:A:1107:G:H5''	1.94	0.48
32:X:67:LEU:HD23	32:X:70:LEU:HD12	1.96	0.48
9:A:1277:G:C5'	22:N:20:MET:HE2	2.44	0.48
9:A:995:C:O2	18:J:3:THR:HG23	2.13	0.48
9:A:528:A:C2	9:A:2043:C:H4'	2.49	0.48
9:A:1996:C:OP1	19:K:31:ARG:NE	2.46	0.48
9:A:2678:C:H2'	9:A:2679:A:O4'	2.14	0.48
9:A:2230:G:O3'	32:X:29:LEU:HD23	2.14	0.48
9:A:1738:G:HO2'	9:A:1739:A:P	2.37	0.48
2:1:20:TYR:HH	9:A:2347:C:HO2'	1.59	0.48
9:A:2355:G:H4'	31:W:20:LEU:CD1	2.44	0.48
18:J:32:LEU:CD2	18:J:54:ILE:HD12	2.44	0.48
13:E:32:VAL:HG23	13:E:178:VAL:HG12	1.95	0.48
31:W:49:ASN:C	31:W:49:ASN:ND2	2.66	0.48
9:A:11:C:C3'	9:A:12:U:H5'	2.44	0.48
3:2:10:LEU:HD23	9:A:770:G:H5''	1.96	0.48
24:P:19:PHE:CD1	24:P:19:PHE:N	2.82	0.48
9:A:996:A:H4'	25:Q:91:ARG:NE	2.29	0.48
9:A:1069:A:C1'	9:A:1073:A:H62	2.26	0.48
15:G:22:VAL:O	15:G:22:VAL:HG23	2.14	0.48
31:W:18:LYS:CG	31:W:19:ARG:N	2.77	0.48
26:R:49:ILE:HD12	26:R:52:PRO:HA	1.95	0.48
9:A:1327:A:H2'	9:A:1328:A:O4'	2.14	0.48
14:F:10:GLU:O	14:F:12:VAL:N	2.44	0.48
15:G:23:ILE:HG21	15:G:71:LEU:HD11	1.95	0.48
18:J:44:TYR:CD1	25:Q:63:ARG:HG2	2.49	0.48
9:A:1799:G:C5	11:C:175:LEU:HD23	2.49	0.48
12:D:148:GLN:HB2	12:D:152:PRO:HG2	1.96	0.48
15:G:15:ASP:O	15:G:16:VAL:HG13	2.12	0.48
9:A:995:C:N4	18:J:2:LYS:HB3	2.29	0.48
31:W:44:PHE:HD1	31:W:45:HIS:CE1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:749:A:C6	9:A:1618:A:C2	3.01	0.48
15:G:104:LEU:HB2	15:G:112:VAL:HG21	1.96	0.48
9:A:2062:A:H61	36:A:9000:ERY:H273	1.70	0.47
9:A:2592:G:C6	9:A:2603:G:O6	2.67	0.47
9:A:983:A:N6	9:A:984:A:C2	2.82	0.47
9:A:1417:C:N3	9:A:1581:G:N2	2.60	0.47
9:A:479:A:C2	9:A:480:A:C4	3.01	0.47
17:I:60:VAL:HG22	17:I:66:PHE:HB3	1.95	0.47
24:P:105:LYS:HA	24:P:108:ARG:HD2	1.95	0.47
15:G:118:ALA:O	15:G:120:ILE:N	2.41	0.47
6:5:110:ALA:HB1	6:5:113:PHE:CZ	2.49	0.47
31:W:23:LYS:HE2	31:W:24:ARG:H	1.78	0.47
27:S:24:ILE:HD11	27:S:36:LEU:HD13	1.96	0.47
11:C:232:GLY:H	11:C:241:LYS:HE3	1.79	0.47
9:A:1814:G:C6	9:A:1815:A:N6	2.82	0.47
14:F:134:GLN:O	14:F:136:ILE:N	2.47	0.47
27:S:63:GLY:O	27:S:64:ALA:CB	2.62	0.47
17:I:100:ILE:HD13	17:I:137:LEU:HD12	1.96	0.47
19:K:72:PRO:O	19:K:74:GLY:N	2.43	0.47
31:W:47:GLY:H	31:W:80:SER:HB3	1.80	0.47
26:R:68:ARG:HD3	26:R:92:TRP:CZ2	2.49	0.47
14:F:64:PRO:HA	14:F:88:VAL:HG22	1.95	0.47
18:J:84:ILE:HG23	18:J:84:ILE:O	2.15	0.47
6:5:23:LEU:H	6:5:87:GLU:HB2	1.79	0.47
31:W:42:THR:HG22	31:W:43:LYS:HZ2	1.80	0.47
9:A:983:A:N6	9:A:984:A:N1	2.62	0.47
9:A:2406:A:C2	20:L:69:ARG:NH2	2.82	0.47
14:F:69:ALA:N	14:F:82:TYR:O	2.47	0.47
32:X:39:VAL:HG21	32:X:42:GLU:HB2	1.96	0.47
6:5:110:ALA:HB1	6:5:113:PHE:CE1	2.49	0.47
9:A:2862:G:C5	9:A:2863:C:C5	3.02	0.47
31:W:63:ASP:N	31:W:63:ASP:OD1	2.35	0.47
25:Q:91:ARG:HH21	25:Q:93:ILE:HD13	1.80	0.47
9:A:587:C:P	20:L:21:ARG:NH1	2.88	0.47
31:W:49:ASN:HA	31:W:61:LYS:HB2	1.94	0.47
2:1:16:THR:HG21	2:1:41:VAL:HG13	1.97	0.47
6:5:127:ALA:O	6:5:129:LEU:N	2.48	0.47
9:A:2346:A:H3'	9:A:2347:C:H5''	1.95	0.47
9:A:478:A:C6	9:A:480:A:C6	3.03	0.47
6:5:15:VAL:HG21	6:5:66:GLY:HA2	1.96	0.47
33:Y:56:LEU:O	33:Y:57:LEU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:24:VAL:HG13	19:K:33:ALA:HB2	1.95	0.47
9:A:451:U:C2	9:A:453:A:N7	2.83	0.47
5:4:6:SER:HB2	9:A:1031:G:H4'	1.95	0.47
20:L:82:LEU:CD1	20:L:116:VAL:HG23	2.44	0.47
6:5:123:ILE:HG12	6:5:124:ASP:N	2.30	0.47
9:A:2061:G:N2	9:A:2063:C:N3	2.63	0.47
6:5:39:THR:HA	6:5:42:ARG:CD	2.43	0.47
31:W:39:GLN:HG2	31:W:40:ARG:N	2.28	0.47
17:I:89:SER:OG	17:I:135:MET:SD	2.68	0.47
17:I:135:MET:HB3	17:I:137:LEU:CD2	2.43	0.47
9:A:1417:C:O2'	9:A:1587:G:O2'	2.19	0.47
6:5:60:LEU:HD23	6:5:78:GLY:HA3	1.97	0.47
9:A:2425:A:C5'	9:A:2427:C:O4'	2.62	0.47
9:A:1474:U:C2'	9:A:1475:G:H5'	2.44	0.47
9:A:419:U:H2'	9:A:420:C:C6	2.50	0.47
9:A:725:G:C6	9:A:726:G:N1	2.82	0.47
33:Y:1:MET:H3	33:Y:2:LYS:HD2	1.79	0.47
6:5:88:HIS:CB	6:5:89:PRO:HD3	2.44	0.47
28:T:61:LEU:C	28:T:61:LEU:HD12	2.35	0.47
9:A:1090:A:C2	9:A:1102:C:H1'	2.50	0.47
11:C:246:PRO:HG2	11:C:247:TRP:CZ3	2.50	0.47
26:R:64:VAL:HG21	26:R:97:LYS:HB2	1.97	0.47
6:5:100:ALA:HB2	6:5:125:ARG:HE	1.79	0.47
36:A:9000:ERY:H8	36:A:9000:ERY:H321	1.58	0.47
31:W:9:THR:HG23	31:W:10:ARG:N	2.30	0.47
24:P:50:ARG:HG2	24:P:57:ALA:N	2.30	0.47
31:W:60:ALA:HA	31:W:81:ILE:HD12	1.97	0.47
9:A:947:A:O2'	9:A:984:A:H2	1.98	0.47
6:5:15:VAL:HG22	6:5:66:GLY:CA	2.44	0.47
18:J:36:LEU:O	18:J:121:LYS:NZ	2.39	0.47
9:A:2210:U:H4'	9:A:2211:A:H5'	1.97	0.47
9:A:1614:A:N6	27:S:92:ARG:O	2.43	0.47
9:A:2902:C:C2'	9:A:2903:U:O5'	2.63	0.47
17:I:40:ALA:O	17:I:43:ALA:HB3	2.14	0.47
9:A:523:C:H5''	9:A:540:C:O2'	2.15	0.47
9:A:1478:G:C2	9:A:1479:G:N7	2.83	0.47
10:B:55:U:O3'	14:F:23:SER:OG	2.21	0.47
9:A:2063:C:H5	9:A:2064:C:H41	1.63	0.47
9:A:2609:U:C3'	9:A:2610:C:H5'	2.44	0.47
31:W:28:GLU:O	31:W:30:VAL:N	2.48	0.47
31:W:30:VAL:HG23	31:W:60:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1198:U:O3'	25:Q:4:LYS:HE3	2.15	0.47
14:F:131:VAL:HG22	14:F:151:LEU:H	1.80	0.47
6:5:51:TYR:HD1	6:5:52:MET:N	2.12	0.47
9:A:1161:C:H1'	26:R:8:GLY:O	2.15	0.47
1:0:9:ARG:NH2	9:A:517:C:OP2	2.48	0.47
9:A:2839:G:N2	9:A:2880:C:C4	2.82	0.47
6:5:54:VAL:HG22	6:5:83:ALA:HB1	1.97	0.47
9:A:479:A:H4'	9:A:480:A:OP1	2.15	0.47
9:A:1088:A:HO2'	9:A:1089:A:P	2.37	0.47
9:A:1079:C:O2	17:I:130:GLY:HA3	2.15	0.47
21:M:46:ILE:HD13	21:M:47:GLU:N	2.30	0.47
11:C:38:LYS:NZ	11:C:57:HIS:O	2.39	0.46
28:T:69:ARG:CD	28:T:70:HIS:H	2.28	0.46
17:I:14:ALA:HB1	17:I:45:THR:HG23	1.97	0.46
15:G:112:VAL:HG23	15:G:113:ASP:N	2.28	0.46
26:R:68:ARG:HD3	26:R:92:TRP:CE2	2.50	0.46
9:A:1817:G:H2'	9:A:1818:U:H5'	1.97	0.46
22:N:103:ARG:HD3	22:N:110:MET:HE3	1.97	0.46
9:A:657:U:H2'	9:A:658:U:C6	2.50	0.46
20:L:23:ILE:HD12	26:R:84:ARG:CZ	2.45	0.46
12:D:169:ARG:O	12:D:170:VAL:HG13	2.15	0.46
13:E:44:ARG:HH21	13:E:44:ARG:HG3	1.80	0.46
25:Q:63:ARG:HH22	25:Q:96:ASP:N	2.12	0.46
9:A:1509:A:C4	9:A:1510:G:C8	3.04	0.46
9:A:1392:A:N6	9:A:1393:A:N6	2.63	0.46
20:L:68:SER:O	20:L:69:ARG:HB3	2.15	0.46
9:A:747:U:C2'	27:S:88:ARG:NH2	2.78	0.46
16:H:8:LYS:O	16:H:9:VAL:HB	2.15	0.46
19:K:24:VAL:CG1	19:K:30:ARG:HD3	2.45	0.46
9:A:1219:U:OP2	25:Q:18:LYS:NZ	2.46	0.46
9:A:2365:G:H4'	31:W:59:PHE:CZ	2.51	0.46
28:T:54:GLU:N	28:T:54:GLU:OE1	2.48	0.46
9:A:1378:A:O2'	9:A:1380:G:N7	2.27	0.46
15:G:123:GLU:HG2	15:G:124:CYS:N	2.30	0.46
18:J:37:ARG:HA	18:J:118:MET:CE	2.45	0.46
9:A:2889:C:N4	9:A:2890:G:C6	2.83	0.46
14:F:39:VAL:HG13	14:F:40:GLY:N	2.31	0.46
31:W:72:GLY:N	31:W:73:PRO:CD	2.78	0.46
19:K:98:ARG:HA	19:K:118:LEU:HD23	1.97	0.46
21:M:22:GLN:O	21:M:24:THR:N	2.48	0.46
16:H:21:VAL:CG2	16:H:25:TYR:CD2	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2318:G:C6	9:A:2319:G:C6	3.03	0.46
9:A:2583:G:N2	9:A:2584:U:O2	2.48	0.46
20:L:85:VAL:HG22	20:L:94:THR:HG22	1.97	0.46
25:Q:4:LYS:NZ	25:Q:7:VAL:CG1	2.79	0.46
26:R:49:ILE:HG22	26:R:53:PHE:C	2.36	0.46
6:5:68:PRO:HA	6:5:72:LEU:CG	2.46	0.46
9:A:2335:A:C5	9:A:2337:G:C4	3.02	0.46
15:G:23:ILE:H	15:G:23:ILE:HD12	1.81	0.46
19:K:30:ARG:NH1	19:K:32:TYR:O	2.45	0.46
17:I:19:PRO:CG	17:I:23:VAL:HG23	2.45	0.46
25:Q:91:ARG:HH21	25:Q:93:ILE:HG21	1.81	0.46
1:0:42:ILE:H	1:0:42:ILE:HD12	1.80	0.46
9:A:2698:U:H2'	9:A:2699:C:C6	2.51	0.46
17:I:120:ASP:O	17:I:123:ALA:N	2.46	0.46
20:L:19:LEU:HD23	20:L:19:LEU:C	2.35	0.46
11:C:67:LYS:HG2	11:C:150:GLY:HA2	1.97	0.46
16:H:31:VAL:HB	16:H:32:PRO:CD	2.46	0.46
13:E:119:ILE:O	13:E:119:ILE:HG13	2.16	0.46
9:A:2436:G:C2	9:A:2437:G:C8	3.04	0.46
9:A:2581:G:H4'	9:A:2582:G:C8	2.51	0.46
9:A:1567:G:C2'	11:C:84:PRO:HG3	2.46	0.46
9:A:747:U:H2'	27:S:88:ARG:NH2	2.30	0.46
9:A:1313:U:H2'	9:A:1610:A:C2	2.51	0.46
6:5:136:ILE:HG13	6:5:139:LEU:HD12	1.98	0.46
14:F:30:VAL:CG1	14:F:96:TRP:CH2	2.99	0.46
9:A:1569:A:N6	9:A:1570:A:C6	2.84	0.46
11:C:75:ALA:HB2	11:C:95:TYR:HA	1.97	0.46
12:D:1:MET:HG2	12:D:205:PRO:HG3	1.98	0.46
10:B:29:A:H2'	10:B:30:C:C6	2.50	0.46
9:A:1838:C:H4'	9:A:1839:G:C8	2.51	0.46
10:B:37:C:C5	10:B:38:C:C4	3.04	0.46
31:W:9:THR:CG2	31:W:10:ARG:HD3	2.44	0.46
29:U:73:ASN:HA	29:U:95:PHE:CE2	2.51	0.46
9:A:1939:U:O2	9:A:1967:C:H4'	2.15	0.46
9:A:2701:U:H3'	9:A:2702:G:H5''	1.96	0.46
17:I:57:VAL:HG23	17:I:71:LYS:CE	2.46	0.46
23:O:79:ALA:O	23:O:82:ALA:N	2.49	0.46
9:A:2897:U:H2'	9:A:2898:U:C6	2.51	0.46
26:R:66:HIS:CG	26:R:94:THR:HG22	2.49	0.46
24:P:50:ARG:CB	24:P:57:ALA:N	2.78	0.46
9:A:2024:G:C4	9:A:2040:G:N2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:29:THR:HB	28:T:86:THR:HG22	1.98	0.46
28:T:29:THR:CB	28:T:86:THR:H	2.29	0.46
14:F:147:ARG:HG3	14:F:148:VAL:N	2.30	0.46
17:I:24:GLY:O	17:I:27:LEU:HG	2.16	0.46
11:C:93:VAL:HG12	11:C:94:LEU:N	2.31	0.46
9:A:2793:C:H2'	9:A:2794:C:C6	2.50	0.46
17:I:61:TYR:CD1	17:I:61:TYR:N	2.82	0.46
17:I:100:ILE:CG2	17:I:101:SER:N	2.79	0.46
24:P:72:VAL:HG23	24:P:72:VAL:O	2.15	0.46
31:W:19:ARG:CZ	31:W:22:VAL:HB	2.46	0.46
24:P:58:PHE:CE1	24:P:75:THR:HG22	2.51	0.46
2:1:4:ILE:HD11	2:1:27:ARG:HB2	1.97	0.46
9:A:751:A:C6	9:A:789:A:C5	3.04	0.46
9:A:247:G:H4'	9:A:386:G:C5	2.51	0.46
15:G:163:TYR:O	15:G:164:ALA:HB2	2.16	0.46
19:K:61:VAL:HG22	19:K:87:LEU:HD11	1.98	0.46
9:A:959:A:H62	21:M:82:MET:CE	2.28	0.46
20:L:132:ARG:HG3	20:L:142:ILE:HD12	1.98	0.46
9:A:593:U:H2'	9:A:594:U:C6	2.51	0.46
14:F:62:GLN:NE2	14:F:89:THR:O	2.47	0.46
14:F:113:PHE:HE1	14:F:116:LEU:HD13	1.81	0.46
12:D:193:VAL:HB	12:D:194:PRO:HD2	1.98	0.46
6:5:71:CYS:CA	6:5:117:LEU:HD11	2.43	0.45
6:5:63:ALA:HB3	6:5:84:TYR:CE2	2.52	0.45
18:J:44:TYR:O	18:J:45:THR:CB	2.64	0.45
8:7:76:A:C6	9:A:2451:A:O4'	2.69	0.45
9:A:1936:A:N6	9:A:1963:U:C2	2.84	0.45
19:K:13:ASN:O	19:K:14:SER:OG	2.29	0.45
9:A:1060:U:H3	9:A:1088:A:H2	1.64	0.45
9:A:1057:A:C6	9:A:1086:A:C2	3.04	0.45
9:A:281:C:H2'	9:A:282:A:C8	2.51	0.45
18:J:12:LYS:O	18:J:13:ARG:HB2	2.15	0.45
9:A:1248:G:C5	13:E:46:GLN:NE2	2.84	0.45
17:I:137:LEU:HD23	17:I:137:LEU:H	1.81	0.45
9:A:923:G:N3	31:W:23:LYS:HD2	2.31	0.45
1:0:3:GLN:HA	9:A:2615:U:C2	2.51	0.45
9:A:1171:G:C6	9:A:1172:C:C4	3.04	0.45
9:A:118:A:C8	9:A:119:A:C8	3.04	0.45
9:A:11:C:H2'	9:A:12:U:H5'	1.98	0.45
9:A:33:C:O2	9:A:447:A:N6	2.50	0.45
9:A:833:A:OP2	20:L:39:LYS:NZ	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1662:U:O2	9:A:2687:U:H4'	2.17	0.45
9:A:1593:A:H2'	9:A:1594:U:O4'	2.17	0.45
11:C:24:HIS:NE2	11:C:79:ARG:NH2	2.65	0.45
9:A:597:G:C2	9:A:661:A:C2	3.04	0.45
31:W:39:GLN:HG3	31:W:42:THR:H	1.81	0.45
9:A:1783:A:N1	9:A:2587:A:C4	2.85	0.45
9:A:271:G:H4'	9:A:272:A:OP1	2.17	0.45
30:V:80:HIS:HD2	30:V:83:LYS:H	1.62	0.45
19:K:80:ASP:CB	24:P:67:GLU:HG3	2.47	0.45
9:A:141:G:N1	28:T:1:MET:O	2.44	0.45
19:K:98:ARG:HA	19:K:118:LEU:CD2	2.47	0.45
10:B:51:G:OP2	23:O:64:TYR:HD2	1.98	0.45
4:3:21:PHE:O	4:3:22:LYS:O	2.33	0.45
23:O:15:ARG:NE	23:O:93:ASP:OD2	2.44	0.45
27:S:1:MET:O	27:S:108:SER:HB2	2.16	0.45
22:N:70:THR:HB	22:N:75:ILE:CD1	2.46	0.45
5:4:36:ARG:O	5:4:37:GLN:C	2.55	0.45
30:V:80:HIS:CD2	30:V:83:LYS:HB2	2.52	0.45
9:A:2862:G:C6	9:A:2863:C:C4	3.04	0.45
19:K:99:ILE:HG21	19:K:119:ALA:HB2	1.98	0.45
18:J:12:LYS:O	18:J:13:ARG:CB	2.64	0.45
4:3:12:ARG:HD3	20:L:61:LEU:O	2.16	0.45
9:A:2262:U:H4'	9:A:2328:A:C2	2.52	0.45
9:A:1150:C:H2'	9:A:1151:A:O5'	2.17	0.45
12:D:70:LYS:O	12:D:71:ALA:HB3	2.17	0.45
4:3:3:ILE:HG21	4:3:62:PRO:HG3	1.98	0.45
1:0:8:THR:HG21	9:A:2021:C:P	2.56	0.45
9:A:2852:G:C6	9:A:2853:C:N3	2.84	0.45
9:A:2144:G:H3'	9:A:2144:G:N3	2.31	0.45
9:A:2581:G:N3	9:A:2581:G:C2'	2.75	0.45
25:Q:91:ARG:HH12	26:R:10:LYS:HB3	1.82	0.45
27:S:18:ARG:HG3	27:S:76:VAL:HG13	1.98	0.45
2:1:33:LEU:N	2:1:51:ALA:CB	2.80	0.45
9:A:85:G:OP1	29:U:6:ARG:N	2.49	0.45
18:J:55:ILE:HD11	18:J:130:HIS:CD2	2.51	0.45
9:A:2108:A:C2'	9:A:2109:U:O5'	2.65	0.45
5:4:8:LYS:NZ	9:A:2467:C:OP1	2.48	0.45
9:A:2649:C:H2'	9:A:2650:U:C6	2.50	0.45
9:A:799:G:C6	9:A:800:A:C6	3.05	0.45
9:A:2758:A:H2'	9:A:2759:G:H5'	1.99	0.45
16:H:14:SER:OG	16:H:17:ASP:CG	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:11:C:O2'	10:B:15:A:N6	2.50	0.45
9:A:2326:C:C6	9:A:2326:C:H3'	2.52	0.45
9:A:2326:C:H4'	9:A:2327:A:OP1	2.16	0.45
13:E:154:ASP:OD1	13:E:154:ASP:N	2.50	0.45
6:5:71:CYS:HA	6:5:117:LEU:HD11	1.96	0.45
9:A:2592:G:C2	9:A:2603:G:C5	3.05	0.45
9:A:2478:A:H2'	9:A:2479:U:H5'	1.98	0.45
25:Q:4:LYS:NZ	25:Q:7:VAL:HG11	2.31	0.45
1:0:42:ILE:HD11	22:N:98:LEU:CB	2.46	0.45
4:3:38:LYS:NZ	9:A:2365:G:N7	2.52	0.45
2:1:4:ILE:HG23	2:1:5:ARG:N	2.32	0.45
6:5:48:ALA:HB3	6:5:51:TYR:HB3	1.98	0.45
24:P:21:PRO:HD3	24:P:49:ILE:HD12	1.98	0.45
9:A:2740:A:C6	9:A:2764:A:C8	3.04	0.45
22:N:33:ILE:CD1	22:N:118:ARG:NE	2.80	0.45
9:A:855:G:H21	31:W:23:LYS:HG2	1.82	0.45
9:A:1141:U:H4'	9:A:1142:A:O4'	2.17	0.45
30:V:80:HIS:CD2	30:V:82:TYR:H	2.35	0.45
13:E:187:VAL:O	13:E:188:MET:HB3	2.16	0.45
24:P:91:VAL:HG11	24:P:96:LEU:HD21	1.98	0.45
34:Z:3:THR:HA	34:Z:37:ARG:O	2.16	0.45
17:I:125:THR:O	17:I:128:ILE:N	2.48	0.45
6:5:110:ALA:O	6:5:113:PHE:N	2.46	0.45
9:A:1428:C:C5	9:A:1569:A:H5''	2.52	0.45
2:1:6:GLU:OE1	2:1:52:LYS:CE	2.64	0.45
16:H:40:THR:C	16:H:42:LYS:H	2.19	0.45
9:A:2058:A:C5	9:A:2059:A:N6	2.85	0.45
9:A:996:A:H4'	25:Q:91:ARG:CD	2.47	0.45
9:A:728:G:H4'	11:C:12:ARG:HD3	1.98	0.45
12:D:86:GLU:N	12:D:86:GLU:CD	2.69	0.45
14:F:127:TYR:O	14:F:128:SER:CB	2.65	0.45
25:Q:91:ARG:HH11	26:R:11:GLN:H	1.64	0.45
2:1:8:ILE:HG21	2:1:51:ALA:HA	1.98	0.45
24:P:102:ARG:O	24:P:103:THR:HG22	2.17	0.45
9:A:2405:G:O2'	9:A:2406:A:OP1	2.26	0.45
6:5:125:ARG:CZ	6:5:125:ARG:HA	2.46	0.45
22:N:103:ARG:CZ	22:N:110:MET:CE	2.95	0.45
23:O:43:ASN:O	23:O:45:SER:N	2.50	0.45
11:C:163:ILE:HG23	11:C:171:VAL:CG1	2.47	0.45
9:A:2407:A:C2	9:A:2408:U:C2	3.05	0.45
6:5:129:LEU:CB	6:5:130:PRO:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:107:VAL:HG11	14:F:116:LEU:HD21	1.99	0.45
25:Q:7:VAL:HG13	25:Q:8:ILE:N	2.32	0.45
31:W:17:ALA:O	31:W:18:LYS:CB	2.64	0.45
12:D:73:VAL:HG23	12:D:74:GLU:H	1.82	0.45
5:4:6:SER:HB2	9:A:1031:G:C4'	2.47	0.45
14:F:128:SER:HA	14:F:154:THR:HA	1.99	0.45
9:A:2564:A:C2	9:A:2647:U:H4'	2.52	0.45
18:J:30:THR:HG22	18:J:31:GLU:N	2.32	0.45
9:A:973:A:O4'	9:A:1188:U:C6	2.70	0.44
15:G:83:THR:C	15:G:84:LYS:HD3	2.37	0.44
16:H:8:LYS:O	16:H:13:GLY:HA2	2.16	0.44
9:A:2043:C:OP1	9:A:2777:G:O2'	2.24	0.44
19:K:118:LEU:O	19:K:119:ALA:HB3	2.17	0.44
10:B:51:G:H5''	23:O:64:TYR:CD2	2.52	0.44
9:A:980:A:C4	9:A:1136:G:O4'	2.70	0.44
9:A:2283:C:H5''	9:A:2389:G:O2'	2.18	0.44
9:A:627:A:C6	9:A:637:A:C8	3.04	0.44
12:D:121:THR:O	12:D:122:VAL:HB	2.17	0.44
21:M:102:LEU:HD12	21:M:102:LEU:N	2.32	0.44
31:W:37:VAL:HG11	31:W:55:ASP:HB2	1.99	0.44
9:A:1387:A:H5'	9:A:1469:A:H1'	2.00	0.44
17:I:109:ALA:CB	17:I:128:ILE:HG13	2.48	0.44
12:D:44:GLY:HA3	12:D:45:TYR:HD1	1.82	0.44
9:A:1181:U:H2'	9:A:1182:G:C8	2.53	0.44
9:A:646:U:H3'	9:A:647:G:H5''	1.99	0.44
9:A:2307:G:N2	9:A:2311:A:C8	2.85	0.44
28:T:40:LYS:HG2	28:T:58:VAL:HG22	1.99	0.44
29:U:53:GLN:N	29:U:54:PRO:CD	2.80	0.44
34:Z:15:ARG:HG2	34:Z:15:ARG:HH11	1.82	0.44
9:A:81:G:O2'	9:A:295:G:O2'	2.26	0.44
9:A:819:A:C4	9:A:1189:A:C2	3.05	0.44
9:A:1936:A:C2	9:A:1943:U:C5	3.03	0.44
6:5:15:VAL:CG2	6:5:66:GLY:HA2	2.47	0.44
18:J:80:HIS:O	18:J:82:GLY:N	2.50	0.44
29:U:6:ARG:O	29:U:24:VAL:HB	2.17	0.44
14:F:72:SER:HB2	14:F:80:GLN:HB2	2.00	0.44
6:5:139:LEU:O	6:5:142:THR:OG1	2.26	0.44
9:A:315:G:H2'	9:A:316:C:C6	2.52	0.44
9:A:792:A:C6	9:A:2440:C:C6	3.05	0.44
9:A:1686:C:C2	9:A:1703:G:C2	3.05	0.44
12:D:3:GLY:HA3	12:D:204:LYS:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1443:U:H2'	9:A:1444:G:C8	2.53	0.44
9:A:750:A:OP1	9:A:1615:C:N4	2.40	0.44
9:A:277:G:H2'	9:A:361:G:O6	2.17	0.44
17:I:100:ILE:HD11	17:I:137:LEU:CG	2.48	0.44
9:A:2683:C:O2	19:K:70:ARG:NH2	2.38	0.44
31:W:19:ARG:NH1	31:W:22:VAL:HG21	2.33	0.44
9:A:635:C:O2'	9:A:639:U:OP1	2.34	0.44
6:5:100:ALA:HB3	6:5:125:ARG:HD2	1.98	0.44
9:A:2344:U:H4'	9:A:2345:G:OP1	2.17	0.44
25:Q:103:VAL:HG23	25:Q:104:ALA:N	2.32	0.44
15:G:24:THR:HG23	15:G:34:ARG:HG2	1.99	0.44
9:A:818:G:H5'	9:A:839:U:OP1	2.18	0.44
9:A:1867:G:C5	9:A:1868:C:C5	3.06	0.44
15:G:60:GLY:O	15:G:61:TRP:HB2	2.17	0.44
9:A:2582:G:C2	9:A:2583:G:N9	2.86	0.44
9:A:2584:U:H5''	9:A:2584:U:H6	1.82	0.44
9:A:994:C:H1'	26:R:10:LYS:CE	2.47	0.44
9:A:1482:G:H1'	9:A:1509:A:N6	2.30	0.44
31:W:19:ARG:C	31:W:19:ARG:CD	2.85	0.44
1:0:3:GLN:NE2	9:A:2016:U:O2	2.46	0.44
9:A:2747:G:O6	9:A:2755:C:H5''	2.18	0.44
34:Z:5:LYS:N	34:Z:5:LYS:HD2	2.32	0.44
9:A:2108:A:H2'	9:A:2109:U:O5'	2.17	0.44
13:E:147:LEU:HB3	13:E:186:VAL:HG23	1.99	0.44
15:G:104:LEU:HB2	15:G:112:VAL:CG2	2.47	0.44
9:A:2283:C:C2	9:A:2389:G:C2	3.06	0.44
9:A:1045:C:C3'	9:A:1046:A:H5'	2.48	0.44
9:A:2276:G:P	21:M:83:GLY:O	2.76	0.44
9:A:1523:U:O2'	9:A:1524:G:H5'	2.18	0.44
9:A:2745:C:C4	9:A:2746:U:C4	3.05	0.44
9:A:2846:G:H2'	9:A:2847:U:O4'	2.17	0.44
9:A:666:A:H4'	20:L:48:ARG:HD2	1.99	0.44
9:A:2582:G:C2	9:A:2583:G:C5	3.06	0.44
9:A:2577:A:OP2	9:A:2577:A:H8	1.99	0.44
9:A:1197:G:H2'	9:A:1198:U:H6	1.83	0.44
19:K:10:VAL:HG21	19:K:17:ARG:H	1.81	0.44
6:5:51:TYR:CE1	6:5:52:MET:HG2	2.53	0.44
9:A:2902:C:H2'	9:A:2903:U:O5'	2.18	0.44
9:A:336:C:N3	9:A:337:C:C5	2.86	0.44
9:A:820:A:H2'	9:A:821:A:O4'	2.16	0.44
27:S:66:ILE:HD13	27:S:67:ASP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2788:C:H2'	9:A:2789:C:C6	2.53	0.44
14:F:94:ARG:CG	14:F:94:ARG:HH11	2.31	0.44
17:I:46:ASP:HA	17:I:50:LYS:HD2	2.00	0.44
18:J:44:TYR:HA	25:Q:59:LEU:CD2	2.48	0.44
9:A:1737:G:H5''	9:A:1738:G:OP2	2.17	0.44
9:A:2577:A:OP2	9:A:2577:A:C8	2.70	0.44
9:A:278:A:N1	9:A:362:A:C8	2.85	0.44
10:B:78:A:H2'	10:B:79:G:O4'	2.18	0.44
31:W:17:ALA:O	31:W:18:LYS:HB2	2.18	0.44
9:A:855:G:H21	31:W:23:LYS:CG	2.31	0.44
9:A:1779:U:C5	9:A:1784:A:N7	2.86	0.44
28:T:48:GLN:O	28:T:52:GLU:HA	2.17	0.44
4:3:31:ILE:HG13	4:3:31:ILE:O	2.17	0.44
17:I:40:ALA:O	17:I:68:PHE:CZ	2.71	0.44
11:C:24:HIS:CE1	11:C:79:ARG:HH21	2.36	0.44
9:A:979:A:H2'	9:A:982:C:H42	1.82	0.44
3:2:12:ARG:HH11	3:2:44:VAL:HG11	1.82	0.44
9:A:1340:U:H4'	9:A:1341:G:OP2	2.17	0.44
9:A:1542:U:H2'	9:A:1543:G:O4'	2.16	0.44
9:A:61:C:H2'	9:A:62:U:H5'	2.00	0.44
9:A:948:C:H1'	9:A:984:A:O2'	2.18	0.44
22:N:20:MET:HE1	22:N:40:LYS:HE2	2.00	0.44
12:D:69:ALA:HA	12:D:73:VAL:CG1	2.47	0.44
9:A:132:G:C2'	9:A:133:U:H5'	2.48	0.44
9:A:1232:G:C5	9:A:1233:C:C5	3.06	0.44
9:A:222:A:N6	9:A:231:A:C2	2.86	0.44
21:M:13:HIS:O	21:M:14:LYS:CB	2.66	0.44
9:A:2103:C:H2'	9:A:2104:C:C5'	2.47	0.44
22:N:38:LEU:HB3	22:N:39:PRO:CD	2.48	0.44
9:A:201:C:OP1	32:X:17:ARG:NH1	2.51	0.44
13:E:44:ARG:CG	13:E:44:ARG:HH21	2.31	0.44
18:J:44:TYR:O	18:J:44:TYR:CD2	2.71	0.44
15:G:35:THR:HG22	15:G:36:LEU:N	2.33	0.44
10:B:78:A:C2	10:B:99:A:C4	3.06	0.44
31:W:18:LYS:N	31:W:36:ILE:HG13	2.33	0.44
2:1:8:ILE:CD1	2:1:24:LYS:HG2	2.48	0.44
28:T:69:ARG:CG	28:T:70:HIS:N	2.81	0.44
9:A:2661:G:C6	9:A:2662:A:C2	3.06	0.44
9:A:288:U:H2'	9:A:289:G:C8	2.52	0.44
30:V:29:ILE:HD13	30:V:30:ILE:N	2.33	0.44
9:A:2603:G:C2'	9:A:2604:U:H5'	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:J:44:TYR:HD1	25:Q:63:ARG:HG2	1.81	0.43
31:W:19:ARG:HA	31:W:34:SER:HA	2.00	0.43
9:A:2335:A:N6	9:A:2337:G:H1'	2.33	0.43
9:A:2657:A:C2	9:A:2665:A:C4	3.06	0.43
9:A:1071:G:H1'	9:A:1089:A:C5	2.53	0.43
9:A:980:A:C6	9:A:981:A:N1	2.86	0.43
9:A:720:U:H2'	9:A:721:A:C8	2.53	0.43
33:Y:45:GLN:O	33:Y:46:VAL:HB	2.17	0.43
20:L:112:LEU:HD23	20:L:114:GLY:H	1.83	0.43
9:A:2423:U:H5'	9:A:2423:U:H6	1.83	0.43
11:C:76:VAL:HG22	11:C:76:VAL:O	2.17	0.43
6:5:3:LEU:HB2	6:5:4:ASN:H	1.68	0.43
18:J:4:PHE:O	18:J:44:TYR:OH	2.34	0.43
25:Q:91:ARG:HH11	26:R:11:GLN:N	2.16	0.43
9:A:1786:A:N6	9:A:2606:C:O4'	2.46	0.43
11:C:265:PHE:HD1	11:C:265:PHE:N	2.15	0.43
9:A:1857:G:C2	9:A:1884:G:N3	2.86	0.43
18:J:110:PRO:HB2	18:J:111:LYS:HG3	2.00	0.43
20:L:2:ARG:HA	20:L:5:THR:CG2	2.48	0.43
9:A:1439:A:C2	9:A:1553:A:C4	3.06	0.43
9:A:1584:U:H2'	9:A:1585:C:H5'	2.00	0.43
6:5:71:CYS:HB3	6:5:74:ASP:OD2	2.18	0.43
9:A:2595:G:C6	9:A:2599:G:O6	2.72	0.43
15:G:36:LEU:HD22	15:G:36:LEU:N	2.33	0.43
31:W:24:ARG:HD3	31:W:65:LYS:CD	2.48	0.43
9:A:545:U:H6	9:A:545:U:O5'	2.02	0.43
9:A:2517:C:C5	9:A:2542:A:C5	3.06	0.43
4:3:31:ILE:CG1	4:3:31:ILE:O	2.66	0.43
9:A:581:C:H2'	9:A:582:A:C8	2.53	0.43
6:5:17:GLU:OE1	6:5:53:ARG:NH1	2.51	0.43
12:D:45:TYR:CD1	12:D:45:TYR:N	2.86	0.43
9:A:1252:G:C2	25:Q:32:ARG:HG2	2.52	0.43
11:C:109:LEU:HD23	11:C:110:LYS:H	1.83	0.43
9:A:2180:U:C2	9:A:2181:U:C5	3.06	0.43
19:K:47:ILE:HG13	19:K:48:PRO:HD2	2.00	0.43
7:6:13:ALA:HB1	7:6:17:MET:CE	2.49	0.43
9:A:2031:A:C6	9:A:2498:C:H1'	2.53	0.43
9:A:936:A:H2'	9:A:937:C:C6	2.54	0.43
20:L:111:ILE:HD12	20:L:111:ILE:N	2.33	0.43
12:D:133:THR:HG23	12:D:134:HIS:N	2.33	0.43
25:Q:4:LYS:HZ3	25:Q:7:VAL:CG1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:82:ALA:HB1	17:I:108:ILE:HG21	2.00	0.43
9:A:2134:A:O2'	9:A:2135:A:O4'	2.36	0.43
14:F:134:GLN:OE1	14:F:149:ARG:HB3	2.18	0.43
6:5:17:GLU:HA	6:5:88:HIS:CE1	2.54	0.43
26:R:64:VAL:O	26:R:65:ALA:HB3	2.18	0.43
15:G:123:GLU:HG2	15:G:125:PRO:HD3	2.00	0.43
13:E:158:PHE:HD2	13:E:159:LEU:HD12	1.83	0.43
9:A:172:A:H2'	9:A:173:A:C8	2.53	0.43
9:A:1914:C:H2'	9:A:1915:U:O4'	2.18	0.43
9:A:822:G:H2'	9:A:823:C:H6	1.83	0.43
10:B:27:C:C5	10:B:28:C:C5	3.06	0.43
26:R:74:ILE:HB	26:R:87:GLN:O	2.18	0.43
9:A:684:G:C2	9:A:794:A:C2	3.06	0.43
13:E:160:ALA:O	13:E:161:ALA:HB3	2.18	0.43
6:5:71:CYS:SG	6:5:117:LEU:HD12	2.58	0.43
9:A:1171:G:N2	9:A:1179:G:C4	2.86	0.43
31:W:49:ASN:ND2	31:W:50:VAL:N	2.67	0.43
22:N:70:THR:HB	22:N:75:ILE:HD11	2.01	0.43
12:D:124:ARG:HA	12:D:165:MET:SD	2.58	0.43
9:A:2582:G:N3	9:A:2582:G:H2'	2.34	0.43
6:5:54:VAL:O	6:5:55:VAL:C	2.57	0.43
25:Q:94:LEU:CD1	26:R:13:ARG:HB2	2.49	0.43
29:U:73:ASN:O	29:U:74:ALA:HB3	2.17	0.43
31:W:24:ARG:HD3	31:W:65:LYS:HG2	2.00	0.43
2:1:5:ARG:CZ	2:1:24:LYS:HA	2.49	0.43
9:A:247:G:N7	9:A:249:C:C2	2.86	0.43
9:A:959:A:H62	21:M:82:MET:HE1	1.84	0.43
20:L:2:ARG:HA	20:L:5:THR:HG21	2.01	0.43
19:K:35:VAL:HG12	19:K:36:GLY:N	2.34	0.43
33:Y:21:LEU:HA	33:Y:25:GLN:HB3	2.01	0.43
18:J:11:VAL:HG11	18:J:50:THR:HA	2.01	0.43
6:5:87:GLU:OE2	6:5:95:LEU:HD23	2.18	0.43
25:Q:60:TRP:CE2	25:Q:93:ILE:HB	2.54	0.43
9:A:323:C:OP1	9:A:338:G:N2	2.51	0.43
9:A:545:U:H2'	9:A:546:U:O3'	2.18	0.43
14:F:103:ILE:HG21	14:F:173:ASP:HB2	2.01	0.43
9:A:1536:C:H1'	9:A:1537:G:N2	2.34	0.43
28:T:29:THR:HB	28:T:86:THR:HA	2.01	0.43
2:1:7:LYS:NZ	9:A:2421:G:P	2.92	0.43
9:A:1485:U:H2'	9:A:1486:U:H6	1.82	0.43
9:A:580:U:O3'	25:Q:30:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:122:VAL:CG1	20:L:142:ILE:HG12	2.47	0.43
34:Z:15:ARG:HD3	34:Z:53:MET:SD	2.59	0.43
10:B:90:C:H5''	10:B:90:C:H6	1.83	0.43
19:K:3:GLN:HG3	19:K:4:GLU:N	2.34	0.43
9:A:1956:U:H2'	9:A:1957:C:H5'	2.01	0.43
9:A:2204:G:OP2	11:C:146:LYS:NZ	2.34	0.43
9:A:744:U:H2'	9:A:745:G:O4'	2.19	0.43
21:M:26:VAL:HB	21:M:133:LYS:HA	2.00	0.43
9:A:2601:C:HO2'	9:A:2602:A:P	2.41	0.43
9:A:994:C:O2'	9:A:996:A:OP1	2.25	0.43
9:A:2576:G:C5'	9:A:2576:G:N3	2.76	0.43
9:A:1188:U:H4'	26:R:81:LYS:O	2.19	0.43
9:A:2353:G:N3	31:W:30:VAL:HG12	2.32	0.43
9:A:975:A:C5	9:A:990:A:N7	2.86	0.43
9:A:274:C:H2'	9:A:275:C:O4'	2.19	0.43
22:N:117:ASP:O	22:N:118:ARG:C	2.57	0.43
9:A:479:A:N3	9:A:481:G:H5''	2.34	0.43
9:A:1378:A:C4	9:A:1380:G:N7	2.87	0.43
13:E:187:VAL:O	13:E:188:MET:CB	2.67	0.43
9:A:2094:A:P	16:H:22:LYS:HD2	2.59	0.43
32:X:67:LEU:HD22	32:X:77:TYR:CE1	2.53	0.43
17:I:45:THR:O	17:I:48:ILE:HG13	2.18	0.43
16:H:8:LYS:O	16:H:9:VAL:CB	2.66	0.43
4:3:22:LYS:HA	4:3:47:ALA:O	2.19	0.43
9:A:1441:G:H2'	9:A:1442:U:C6	2.53	0.43
33:Y:31:GLN:HG2	33:Y:36:GLN:HB2	2.01	0.43
9:A:1003:G:N2	9:A:1004:U:C2	2.86	0.43
9:A:1494:A:C2	9:A:1495:A:C4	3.06	0.43
9:A:645:C:O2'	9:A:645:C:O2	2.35	0.43
9:A:1509:A:O2'	9:A:1510:G:P	2.76	0.43
31:W:36:ILE:O	31:W:36:ILE:HG22	2.18	0.43
29:U:35:VAL:O	29:U:38:ILE:HB	2.19	0.43
33:Y:56:LEU:H	33:Y:56:LEU:HD22	1.84	0.43
31:W:44:PHE:O	31:W:78:PHE:HA	2.19	0.43
25:Q:20:ALA:HA	25:Q:23:TYR:CE2	2.54	0.43
9:A:764:A:C6	9:A:781:A:C2	3.06	0.43
9:A:570:G:C4	9:A:2030:A:N7	2.87	0.43
9:A:2682:A:C8	12:D:11:MET:HG3	2.53	0.43
18:J:60:ASP:N	18:J:60:ASP:OD1	2.52	0.43
9:A:2507:C:C2	9:A:2508:G:C8	3.07	0.43
9:A:1476:U:C5	9:A:1514:G:C2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:528:A:P	18:J:116:ARG:HH21	2.42	0.43
9:A:1223:G:P	26:R:68:ARG:HH11	2.41	0.43
9:A:2070:A:H2'	9:A:2071:A:O4'	2.19	0.43
9:A:1096:A:H2'	9:A:1097:U:H5''	2.01	0.43
9:A:742:A:H2'	9:A:743:A:C8	2.53	0.43
9:A:476:G:H4'	9:A:502:A:N1	2.33	0.43
9:A:2611:C:C6	9:A:2611:C:C3'	3.02	0.42
1:O:42:ILE:HG22	1:O:43:THR:O	2.19	0.42
9:A:1338:G:O2'	9:A:1393:A:N1	2.44	0.42
9:A:2516:A:N6	9:A:2517:C:N4	2.67	0.42
19:K:13:ASN:O	19:K:14:SER:CB	2.67	0.42
28:T:69:ARG:HG3	28:T:70:HIS:H	1.83	0.42
10:B:72:G:N2	10:B:103:U:C5	2.87	0.42
23:O:41:ALA:O	23:O:44:GLY:N	2.41	0.42
30:V:72:VAL:HG12	30:V:93:ARG:HA	2.01	0.42
12:D:110:THR:HG23	12:D:171:THR:HG22	2.00	0.42
22:N:8:ARG:HB3	22:N:10:LEU:CD2	2.48	0.42
18:J:88:THR:HG22	18:J:91:GLU:CG	2.49	0.42
9:A:1281:G:C2	9:A:1290:C:C2	3.07	0.42
11:C:180:MET:O	11:C:267:VAL:N	2.42	0.42
28:T:76:ARG:HG3	28:T:77:ARG:N	2.34	0.42
17:I:93:ASN:HB2	17:I:135:MET:SD	2.59	0.42
12:D:118:PHE:HZ	22:N:1:MET:HB2	1.85	0.42
25:Q:86:SER:O	26:R:51:VAL:HA	2.18	0.42
6:5:67:THR:C	6:5:69:PHE:N	2.73	0.42
9:A:580:U:H2'	9:A:581:C:C6	2.54	0.42
27:S:59:GLU:HA	27:S:64:ALA:CB	2.50	0.42
9:A:833:A:OP1	20:L:39:LYS:HE3	2.19	0.42
9:A:226:A:C6	9:A:227:A:C6	3.07	0.42
9:A:1747:U:H2'	9:A:1748:C:C6	2.55	0.42
33:Y:14:LEU:HA	33:Y:17:GLU:HB3	2.01	0.42
9:A:2823:A:C5	9:A:2824:C:C5	3.07	0.42
9:A:348:A:C5	9:A:349:U:C5	3.07	0.42
26:R:5:PHE:HB3	26:R:59:ILE:HD12	2.01	0.42
6:5:67:THR:CG2	6:5:72:LEU:HA	2.49	0.42
9:A:2748:A:H1'	15:G:66:THR:CG2	2.49	0.42
9:A:864:G:OP2	21:M:22:GLN:NE2	2.52	0.42
6:5:142:THR:OG1	6:5:143:MET:N	2.52	0.42
10:B:89:U:H3'	10:B:90:C:C5'	2.49	0.42
9:A:1094:U:N3	9:A:1097:U:OP2	2.51	0.42
25:Q:27:ARG:HA	25:Q:33:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:V:75:GLN:HB2	30:V:92:VAL:CG2	2.48	0.42
15:G:39:ALA:HB2	15:G:57:TYR:CD2	2.54	0.42
13:E:52:VAL:HG11	13:E:81:GLY:HA3	2.01	0.42
9:A:2047:C:O2'	9:A:2048:G:H5'	2.19	0.42
9:A:1224:U:H4'	26:R:88:GLY:O	2.18	0.42
12:D:149:ASN:CG	12:D:150:GLN:H	2.21	0.42
13:E:188:MET:HE3	13:E:196:VAL:HG21	2.01	0.42
9:A:726:G:O2'	9:A:727:A:OP2	2.37	0.42
9:A:1312:U:H4'	9:A:1313:U:O5'	2.20	0.42
9:A:959:A:N6	21:M:82:MET:CE	2.82	0.42
22:N:79:LEU:O	22:N:80:PHE:HB2	2.19	0.42
9:A:2287:A:C8	9:A:2289:G:C8	3.08	0.42
32:X:52:ALA:O	32:X:53:LYS:CB	2.67	0.42
9:A:1112:G:C5	9:A:1113:U:C5	3.07	0.42
9:A:1681:G:N2	9:A:1763:G:OP2	2.45	0.42
14:F:111:ARG:HA	14:F:111:ARG:NE	2.34	0.42
6:5:108:VAL:CG1	6:5:109:LYS:N	2.82	0.42
31:W:37:VAL:HB	31:W:38:ARG:NH1	2.34	0.42
9:A:1937:A:N7	9:A:1939:U:H2'	2.35	0.42
9:A:479:A:C2	9:A:480:A:C5	3.08	0.42
9:A:2526:G:C5	9:A:2527:C:C5	3.08	0.42
9:A:1814:G:C6	9:A:1815:A:C6	3.08	0.42
14:F:134:GLN:HG2	14:F:135:ILE:N	2.34	0.42
9:A:966:G:C6	9:A:967:U:C4	3.07	0.42
9:A:146:A:H2'	9:A:147:C:C6	2.54	0.42
29:U:10:VAL:HG12	29:U:71:ILE:HA	2.01	0.42
9:A:1204:A:C2	9:A:1240:U:N3	2.87	0.42
9:A:1239:G:H2'	9:A:1240:U:O4'	2.19	0.42
17:I:91:LYS:HB2	17:I:95:ASP:HB2	2.00	0.42
7:6:15:SER:OG	7:6:16:VAL:N	2.53	0.42
22:N:24:MET:HE2	22:N:44:LEU:HD22	2.02	0.42
9:A:846:U:HO2'	9:A:847:U:P	2.41	0.42
9:A:573:U:O2'	9:A:574:A:H3'	2.19	0.42
21:M:8:LYS:CE	21:M:9:PHE:CE2	3.02	0.42
9:A:2582:G:C4	9:A:2583:G:N7	2.88	0.42
6:5:47:GLU:HG2	6:5:95:LEU:HD21	2.00	0.42
18:J:43:GLU:O	18:J:44:TYR:C	2.58	0.42
12:D:120:GLY:HA2	12:D:162:ALA:HA	2.00	0.42
29:U:38:ILE:HG23	29:U:39:ASN:N	2.33	0.42
26:R:16:GLU:HA	26:R:98:ILE:HG22	2.01	0.42
9:A:2039:U:H2'	9:A:2040:G:H8	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:945:A:C4	9:A:2448:A:C2	3.07	0.42
24:P:92:ARG:CG	24:P:92:ARG:O	2.68	0.42
9:A:2274:A:C5	9:A:2276:G:C8	3.07	0.42
14:F:94:ARG:HH11	14:F:94:ARG:HB2	1.84	0.42
26:R:74:ILE:HD12	26:R:74:ILE:N	2.34	0.42
9:A:1638:C:H4'	9:A:2710:C:O2	2.18	0.42
9:A:2727:A:C6	9:A:2728:U:O4	2.73	0.42
9:A:2637:U:C2'	9:A:2638:G:H5'	2.50	0.42
18:J:64:VAL:HG13	18:J:65:THR:N	2.35	0.42
9:A:2557:G:H2'	9:A:2558:C:C6	2.54	0.42
25:Q:6:GLY:HA2	25:Q:9:ALA:HB3	2.02	0.42
2:1:18:HIS:CE1	2:1:40:PRO:HD3	2.54	0.42
9:A:2062:A:O2'	9:A:2063:C:C6	2.70	0.42
9:A:996:A:C5	9:A:1160:G:C2	3.08	0.42
25:Q:91:ARG:HE	25:Q:93:ILE:HG23	1.85	0.42
11:C:16:VAL:N	11:C:203:VAL:CG1	2.82	0.42
27:S:96:ILE:HG13	27:S:96:ILE:O	2.20	0.42
9:A:1179:G:C6	9:A:1180:U:C4	3.08	0.42
9:A:2661:G:H2'	9:A:2662:A:O4'	2.20	0.42
10:B:106:G:H2'	10:B:107:G:O4'	2.19	0.42
9:A:2821:A:C2	9:A:2822:G:C4	3.08	0.42
9:A:356:G:C6	9:A:357:C:C4	3.07	0.42
9:A:19:A:H2'	9:A:20:C:O4'	2.20	0.42
9:A:126:A:C6	9:A:127:A:N1	2.88	0.42
9:A:372:G:C4	32:X:60:LYS:HE2	2.54	0.42
17:I:20:SER:HB3	17:I:21:PRO:HD3	2.02	0.42
9:A:2585:U:C5	9:A:2608:G:O6	2.73	0.42
9:A:2611:C:H5'	36:A:9000:ERY:H301	2.01	0.42
9:A:1084:A:C6	9:A:1085:A:C6	3.08	0.42
6:5:3:LEU:HD12	6:5:5:LEU:N	2.35	0.42
11:C:203:VAL:O	11:C:205:GLY:N	2.53	0.42
10:B:16:G:C5	10:B:69:G:C2	3.07	0.42
20:L:77:ILE:HD13	20:L:108:ALA:HB1	2.02	0.42
13:E:42:GLY:O	13:E:43:THR:OG1	2.35	0.42
9:A:1171:G:H1	9:A:1178:C:H42	1.66	0.42
9:A:2071:A:H2'	9:A:2072:C:C6	2.54	0.42
9:A:1238:G:O2'	9:A:1239:G:H5'	2.19	0.42
9:A:2543:G:C6	9:A:2544:G:C6	3.08	0.42
12:D:24:VAL:HA	12:D:191:GLY:H	1.85	0.42
9:A:636:G:OP2	20:L:109:LYS:NZ	2.45	0.42
9:A:1183:U:H2'	9:A:1184:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1465:G:H2'	9:A:1466:U:O4'	2.19	0.42
23:O:14:ALA:O	23:O:17:LYS:N	2.52	0.42
6:5:22:ALA:N	6:5:87:GLU:O	2.53	0.42
18:J:38:GLY:O	18:J:43:GLU:HB2	2.19	0.42
18:J:4:PHE:CD2	18:J:44:TYR:CE2	3.08	0.42
9:A:2506:U:C3'	9:A:2506:U:C6	3.02	0.42
23:O:31:THR:HG22	23:O:34:HIS:N	2.33	0.42
24:P:58:PHE:HD1	24:P:75:THR:HG22	1.83	0.42
21:M:53:MET:CE	21:M:63:ILE:HG21	2.50	0.42
9:A:2803:G:H2'	9:A:2804:U:H6	1.84	0.42
6:5:88:HIS:CB	6:5:89:PRO:CD	2.97	0.42
17:I:9:LYS:HB3	17:I:71:LYS:NZ	2.34	0.42
9:A:1789:A:H2'	9:A:1790:C:O4'	2.20	0.42
9:A:803:U:C4	9:A:804:A:N7	2.88	0.42
9:A:1268:A:H2'	9:A:1269:A:O4'	2.20	0.42
9:A:1026:G:H2'	9:A:1027:A:C8	2.55	0.42
31:W:39:GLN:HG2	31:W:41:GLY:N	2.34	0.42
9:A:2352:A:N1	31:W:30:VAL:HG21	2.35	0.42
14:F:107:VAL:HG13	14:F:110:ILE:HD12	2.02	0.42
19:K:71:ARG:HB3	19:K:72:PRO:CD	2.49	0.42
18:J:81:ILE:CG1	18:J:82:GLY:H	2.33	0.42
9:A:653:U:H5	9:A:654:A:C2	2.38	0.42
29:U:84:PHE:O	29:U:85:ARG:HB3	2.19	0.42
12:D:35:THR:N	12:D:49:GLN:O	2.41	0.42
23:O:75:GLY:HA3	23:O:109:ALA:HB3	2.00	0.42
20:L:40:SER:O	20:L:41:ARG:CB	2.67	0.42
9:A:2796:U:C4	9:A:2798:U:C5	3.08	0.42
29:U:98:ASN:ND2	29:U:100:GLU:OE1	2.53	0.41
6:5:33:VAL:HB	6:5:36:ASP:OD1	2.20	0.41
9:A:1414:C:O2	9:A:1588:G:N2	2.44	0.41
11:C:16:VAL:HB	11:C:203:VAL:HG12	2.02	0.41
9:A:2755:C:O2'	9:A:2756:U:H2'	2.19	0.41
34:Z:4:ILE:HD13	34:Z:44:ARG:NH1	2.34	0.41
9:A:2869:G:C6	9:A:2870:C:C4	3.09	0.41
9:A:1607:C:H42	9:A:1622:G:P	2.43	0.41
9:A:1486:U:H2'	9:A:1487:U:C6	2.55	0.41
9:A:528:A:H2	9:A:2043:C:H5'	1.85	0.41
9:A:2636:C:O2'	12:D:45:TYR:OH	2.25	0.41
14:F:28:PRO:HB2	14:F:168:LEU:HD22	2.02	0.41
9:A:1770:G:C6	9:A:1983:G:C6	3.07	0.41
9:A:75:G:H4'	33:Y:48:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1194:A:C2'	9:A:1195:G:O5'	2.68	0.41
9:A:1298:C:C2	9:A:1643:G:N2	2.88	0.41
9:A:2609:U:C3'	9:A:2610:C:C5'	2.98	0.41
31:W:60:ALA:CB	31:W:81:ILE:CD1	2.98	0.41
9:A:1936:A:C2	9:A:1943:U:H5	2.38	0.41
9:A:2676:C:P	19:K:31:ARG:HH12	2.44	0.41
13:E:134:LEU:CD2	13:E:161:ALA:HB2	2.50	0.41
9:A:518:G:H2'	9:A:519:U:C6	2.54	0.41
34:Z:13:ILE:HG22	34:Z:14:GLY:N	2.34	0.41
9:A:866:A:N7	9:A:914:G:C6	2.89	0.41
13:E:129:PRO:HG3	13:E:156:ASN:OD1	2.21	0.41
9:A:45:G:H5'	9:A:46:G:H5'	2.02	0.41
9:A:1591:A:H2'	9:A:1592:C:C6	2.55	0.41
9:A:1945:G:C6	9:A:1946:U:C4	3.09	0.41
13:E:12:LEU:HD12	13:E:193:VAL:HG11	2.01	0.41
9:A:485:C:C2	9:A:496:G:N2	2.88	0.41
6:5:131:THR:HA	6:5:134:GLU:CG	2.50	0.41
31:W:24:ARG:HH11	31:W:65:LYS:HG2	1.85	0.41
11:C:16:VAL:H	11:C:203:VAL:HG12	1.84	0.41
9:A:1019:U:H3	9:A:1142:A:N6	2.17	0.41
28:T:70:HIS:HB3	28:T:73:ARG:O	2.19	0.41
28:T:34:VAL:O	28:T:34:VAL:HG22	2.20	0.41
9:A:1817:G:C2'	9:A:1818:U:H5'	2.51	0.41
9:A:2058:A:C6	9:A:2059:A:N6	2.88	0.41
9:A:1669:A:O2'	9:A:2549:G:OP1	2.36	0.41
15:G:26:LYS:CG	15:G:27:GLY:N	2.83	0.41
9:A:685:A:C2	9:A:689:A:C6	3.08	0.41
9:A:2341:G:H2'	9:A:2342:C:C6	2.55	0.41
9:A:2478:A:C2'	9:A:2479:U:H5'	2.51	0.41
25:Q:4:LYS:HZ3	25:Q:7:VAL:HG11	1.86	0.41
9:A:2685:G:H1	9:A:2724:U:H3	1.68	0.41
11:C:77:VAL:O	11:C:77:VAL:HG23	2.20	0.41
9:A:2259:U:H1'	9:A:2427:C:C2	2.56	0.41
6:5:51:TYR:CD1	6:5:52:MET:HG2	2.55	0.41
9:A:527:C:H4'	9:A:528:A:O5'	2.21	0.41
22:N:8:ARG:HB3	22:N:10:LEU:HD22	2.01	0.41
9:A:1747:U:H2'	9:A:1748:C:H6	1.85	0.41
9:A:109:C:H4'	9:A:348:A:H4'	2.02	0.41
15:G:31:GLU:O	15:G:33:THR:N	2.52	0.41
9:A:2201:G:C6	9:A:2202:U:C4	3.08	0.41
25:Q:82:LEU:HD12	25:Q:112:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1843:C:O2'	11:C:253:GLY:O	2.29	0.41
9:A:2063:C:N4	9:A:2064:C:N4	2.69	0.41
9:A:2580:U:C5	9:A:2581:G:C6	3.08	0.41
18:J:4:PHE:HB3	18:J:44:TYR:CE2	2.55	0.41
6:5:108:VAL:HG12	6:5:109:LYS:N	2.35	0.41
1:0:42:ILE:HD12	22:N:99:LYS:O	2.20	0.41
14:F:151:LEU:CD1	14:F:153:ILE:HG23	2.51	0.41
26:R:61:ALA:HB1	26:R:98:ILE:H	1.84	0.41
27:S:63:GLY:O	27:S:64:ALA:HB3	2.21	0.41
18:J:65:THR:HG22	18:J:68:LYS:NZ	2.36	0.41
17:I:74:PRO:HG2	17:I:77:VAL:HB	2.01	0.41
9:A:179:C:C2	9:A:180:G:C8	3.08	0.41
13:E:79:ARG:HG2	13:E:80:SER:N	2.35	0.41
9:A:1674:G:N2	9:A:1677:A:N1	2.69	0.41
9:A:2618:G:C6	9:A:2619:C:C4	3.09	0.41
17:I:52:LEU:HB3	17:I:53:PRO:HD2	2.03	0.41
9:A:2063:C:H41	9:A:2064:C:N4	2.18	0.41
9:A:1722:A:C2	9:A:1739:A:N3	2.89	0.41
6:5:106:PHE:CG	6:5:107:GLU:N	2.87	0.41
9:A:1587:G:C4	9:A:1588:G:C8	3.09	0.41
31:W:19:ARG:HG2	31:W:19:ARG:HH21	1.86	0.41
9:A:1020:A:C2	9:A:1141:U:C2	3.09	0.41
19:K:15:GLY:O	19:K:46:ALA:HA	2.20	0.41
21:M:63:ILE:HG22	21:M:64:TRP:N	2.36	0.41
16:H:39:ALA:HB1	16:H:44:ILE:HG22	2.01	0.41
27:S:88:ARG:HD2	27:S:94:ASP:OD2	2.20	0.41
24:P:92:ARG:HB2	24:P:92:ARG:HH11	1.85	0.41
14:F:10:GLU:HG2	14:F:13:LYS:HD3	2.02	0.41
12:D:46:ARG:HB3	12:D:46:ARG:CZ	2.50	0.41
9:A:1494:A:C6	9:A:1495:A:C5	3.08	0.41
9:A:1843:C:H5'	11:C:250:GLN:NE2	2.36	0.41
9:A:1691:C:C4	9:A:1692:U:C4	3.08	0.41
30:V:6:ALA:HB1	30:V:40:ILE:CG2	2.50	0.41
14:F:169:LEU:O	14:F:174:PHE:HB2	2.21	0.41
9:A:608:A:C8	9:A:621:A:N6	2.89	0.41
20:L:29:LYS:HG2	20:L:30:THR:N	2.36	0.41
27:S:69:LEU:HG	27:S:107:VAL:HG22	2.03	0.41
9:A:1381:G:H1'	9:A:1571:A:N1	2.36	0.41
9:A:1647:U:H3'	9:A:1647:U:P	2.60	0.41
9:A:996:A:C6	9:A:1160:G:C2	3.08	0.41
9:A:1069:A:C2'	9:A:1070:A:OP2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:301:G:H2'	9:A:334:C:H2'	2.01	0.41
9:A:1392:A:C6	9:A:1393:A:C6	3.09	0.41
9:A:2298:A:C6	9:A:2321:U:C4	3.09	0.41
9:A:1301:A:H2'	9:A:1301:A:N3	2.35	0.41
13:E:109:LEU:O	13:E:112:LEU:N	2.54	0.41
9:A:1868:C:O2	9:A:1873:G:N2	2.44	0.41
9:A:1494:A:C6	9:A:1495:A:C6	3.08	0.41
18:J:88:THR:HG23	18:J:91:GLU:H	1.86	0.41
22:N:24:MET:CE	22:N:36:THR:HG21	2.51	0.41
9:A:58:G:N2	9:A:70:G:C4	2.89	0.41
23:O:49:VAL:HG12	23:O:50:ALA:N	2.35	0.41
18:J:35:ARG:HG2	18:J:40:HIS:HD2	1.85	0.41
22:N:87:PHE:O	22:N:89:SER:N	2.54	0.41
34:Z:2:LYS:CB	34:Z:39:ASP:HB3	2.51	0.41
9:A:2409:G:H2'	9:A:2410:G:O4'	2.20	0.41
9:A:2601:C:C2	9:A:2603:G:N7	2.89	0.41
9:A:1069:A:N3	9:A:1073:A:C6	2.88	0.41
24:P:50:ARG:CD	24:P:56:SER:HB3	2.51	0.41
9:A:1509:A:H1'	9:A:1510:G:O5'	2.20	0.41
6:5:131:THR:HA	6:5:134:GLU:HG3	2.03	0.41
27:S:18:ARG:HG3	27:S:76:VAL:CG1	2.50	0.41
9:A:1714:U:H5'	9:A:1715:G:H5'	2.02	0.41
26:R:38:VAL:O	26:R:53:PHE:HA	2.20	0.41
33:Y:12:GLU:O	33:Y:15:ASN:HB2	2.21	0.41
22:N:51:LEU:HD21	22:N:70:THR:CG2	2.51	0.41
9:A:2180:U:N3	9:A:2181:U:C5	2.89	0.41
9:A:2682:A:C8	12:D:11:MET:CG	3.04	0.41
9:A:2070:A:C2	9:A:2071:A:C4	3.09	0.41
9:A:1403:A:C2	9:A:1404:C:C2	3.09	0.41
17:I:104:GLN:O	17:I:105:LEU:CB	2.69	0.41
9:A:535:G:C6	9:A:559:G:C6	3.09	0.41
6:5:47:GLU:CG	6:5:95:LEU:HD21	2.51	0.41
29:U:98:ASN:O	29:U:99:SER:C	2.59	0.41
9:A:1068:G:H3'	9:A:1069:A:H5''	2.03	0.41
26:R:80:ARG:O	26:R:81:LYS:HD3	2.20	0.41
6:5:59:LEU:HD23	6:5:62:ARG:HE	1.85	0.41
5:4:32:LYS:HD3	9:A:2478:A:H5'	2.02	0.41
14:F:112:ASP:OD1	14:F:112:ASP:N	2.54	0.41
19:K:71:ARG:O	19:K:72:PRO:O	2.39	0.41
31:W:19:ARG:NH2	31:W:22:VAL:CG2	2.83	0.41
9:A:1378:A:H4'	9:A:1379:U:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2017:U:H5''	9:A:2018:G:P	2.61	0.41
1:0:12:ARG:HD2	1:0:16:ARG:NH2	2.36	0.41
9:A:2038:G:H2'	9:A:2039:U:O4'	2.21	0.41
13:E:187:VAL:HG12	13:E:188:MET:N	2.36	0.41
9:A:138:U:H5'	9:A:139:U:C5'	2.51	0.41
22:N:12:ARG:HB3	22:N:16:HIS:HB3	2.01	0.41
9:A:749:A:C5	9:A:1618:A:C2	3.09	0.41
9:A:2674:G:H4'	19:K:30:ARG:HG3	2.02	0.41
33:Y:2:LYS:N	33:Y:2:LYS:HD2	2.36	0.41
9:A:1078:U:H5''	9:A:1079:C:OP1	2.20	0.41
9:A:2103:C:N4	9:A:2186:G:H1	2.19	0.41
23:O:75:GLY:HA3	23:O:106:LEU:HA	2.03	0.41
17:I:52:LEU:HB3	17:I:53:PRO:CD	2.51	0.41
9:A:659:G:H4'	13:E:95:LYS:HD3	2.02	0.41
10:B:114:C:H1'	23:O:47:VAL:HG11	2.03	0.41
9:A:1063:G:H2'	9:A:1064:C:O4'	2.20	0.41
9:A:307:G:N2	9:A:310:A:C8	2.89	0.41
11:C:143:VAL:HB	11:C:153:LEU:HB2	2.02	0.41
15:G:68:ARG:HH21	15:G:72:ASN:ND2	2.19	0.41
9:A:2145:C:N3	9:A:2146:C:N3	2.69	0.41
14:F:46:LYS:H	14:F:46:LYS:HD3	1.86	0.41
9:A:2845:U:H5''	24:P:51:ASN:O	2.20	0.41
15:G:19:ASN:O	15:G:22:VAL:HG22	2.21	0.41
9:A:301:G:C6	9:A:317:G:C6	3.09	0.41
31:W:22:VAL:O	31:W:23:LYS:HG3	2.21	0.41
12:D:104:VAL:HG12	12:D:106:LYS:H	1.86	0.41
19:K:19:VAL:HG13	19:K:41:ILE:HG12	2.02	0.41
14:F:148:VAL:HG23	14:F:149:ARG:N	2.36	0.41
6:5:88:HIS:HB3	6:5:89:PRO:HD3	2.03	0.41
25:Q:46:TYR:CZ	25:Q:50:ARG:NH2	2.89	0.41
16:H:24:GLY:O	16:H:28:ASN:HB2	2.21	0.41
9:A:629:G:H4'	9:A:650:C:O2	2.21	0.41
21:M:12:MET:HE3	21:M:71:LYS:HG3	2.03	0.41
6:5:23:LEU:HD22	6:5:92:ALA:O	2.21	0.40
9:A:996:A:C5	9:A:1160:G:N2	2.89	0.40
31:W:39:GLN:OE1	31:W:43:LYS:HB2	2.21	0.40
9:A:635:C:P	20:L:126:ARG:HH11	2.44	0.40
9:A:783:A:C8	9:A:784:G:H4'	2.56	0.40
9:A:2868:A:C2	9:A:2869:G:C4	3.09	0.40
6:5:111:ALA:C	6:5:113:PHE:N	2.75	0.40
17:I:19:PRO:HG2	17:I:24:GLY:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:46:ARG:HH21	12:D:86:GLU:H	1.69	0.40
11:C:158:GLY:H	11:C:194:VAL:HG22	1.86	0.40
31:W:67:LYS:O	31:W:68:PHE:HB2	2.20	0.40
9:A:176:A:N7	9:A:177:G:C6	2.89	0.40
24:P:30:TRP:CE3	24:P:39:LEU:HD12	2.56	0.40
11:C:184:GLU:O	11:C:185:ALA:HB3	2.20	0.40
23:O:7:ARG:HA	23:O:10:ARG:NH2	2.36	0.40
9:A:84:A:P	29:U:5:ARG:HH22	2.42	0.40
9:A:1905:C:N4	9:A:1930:G:C2	2.89	0.40
21:M:64:TRP:HZ3	21:M:106:ASP:HB2	1.86	0.40
32:X:67:LEU:HD22	32:X:77:TYR:CZ	2.57	0.40
9:A:580:U:O3'	25:Q:30:VAL:CG1	2.70	0.40
12:D:68:PHE:CE2	12:D:75:ALA:HB1	2.56	0.40
9:A:1613:G:O6	9:A:1617:C:H2'	2.21	0.40
11:C:172:THR:HG22	11:C:182:LYS:HG2	2.02	0.40
9:A:1579:A:H2'	9:A:1580:A:C8	2.56	0.40
9:A:2766:A:H2'	9:A:2766:A:N3	2.36	0.40
9:A:811:U:H2'	20:L:21:ARG:HA	2.04	0.40
17:I:100:ILE:CD1	17:I:137:LEU:HD12	2.51	0.40
9:A:364:C:H2'	9:A:365:U:H6	1.87	0.40
9:A:2347:C:H2'	9:A:2348:U:C6	2.56	0.40
11:C:254:LYS:O	11:C:256:THR:N	2.51	0.40
9:A:1773:A:N7	9:A:1829:A:C1'	2.85	0.40
29:U:82:VAL:HG13	29:U:93:ARG:HB3	2.03	0.40
14:F:148:VAL:HG23	14:F:149:ARG:H	1.87	0.40
20:L:127:VAL:HG11	20:L:142:ILE:HG21	2.03	0.40
9:A:230:G:N2	9:A:231:A:C4	2.90	0.40
15:G:10:VAL:HG22	15:G:47:ASN:C	2.41	0.40
3:2:9:VAL:HG13	9:A:1309:G:OP1	2.21	0.40
5:4:38:GLY:OXT	9:A:1124:G:H1'	2.21	0.40
9:A:544:C:N4	9:A:548:G:OP1	2.45	0.40
10:B:77:U:OP1	30:V:21:ARG:NH1	2.54	0.40
36:A:9000:ERY:H343	36:A:9000:ERY:O13	2.21	0.40
6:5:91:ALA:C	6:5:93:ALA:N	2.66	0.40
9:A:1967:C:H2'	9:A:1968:G:H5'	2.03	0.40
12:D:106:LYS:HB3	12:D:206:ALA:CB	2.52	0.40
19:K:39:ILE:HD12	19:K:41:ILE:HD11	2.02	0.40
9:A:1365:A:OP1	32:X:2:ARG:NE	2.48	0.40
4:3:30:HIS:ND1	4:3:31:ILE:HG23	2.37	0.40
9:A:2318:G:C5	9:A:2319:G:C6	3.10	0.40
9:A:1149:G:H2'	9:A:1150:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1096:A:N6	9:A:1097:U:C4	2.89	0.40
9:A:347:A:C2	9:A:348:A:C4	3.09	0.40
14:F:111:ARG:HA	14:F:111:ARG:CZ	2.51	0.40
15:G:137:LYS:HA	15:G:140:ILE:HG22	2.02	0.40
9:A:136:G:H1	9:A:143:C:H42	1.69	0.40
9:A:2555:U:C5	9:A:2556:C:C2	3.09	0.40
9:A:2469:A:C6	9:A:2482:A:C8	3.10	0.40
1:O:33:SER:OG	1:O:35:GLU:HG3	2.21	0.40
2:1:35:LEU:HD22	2:1:35:LEU:N	2.37	0.40
17:I:11:GLN:OE1	17:I:11:GLN:N	2.43	0.40
9:A:669:G:C2'	9:A:669:G:N3	2.83	0.40
6:5:34:THR:O	6:5:38:MET:HG3	2.22	0.40
19:K:76:VAL:HG12	19:K:77:ILE:N	2.37	0.40
31:W:19:ARG:HG2	31:W:19:ARG:NH2	2.37	0.40
9:A:2684:U:C4	9:A:2685:G:N7	2.90	0.40
9:A:2681:C:C2	9:A:2724:U:O4	2.74	0.40
29:U:12:VAL:HG21	29:U:38:ILE:CD1	2.52	0.40
6:5:132:TYR:HE1	7:6:19:VAL:HG13	1.85	0.40
9:A:2134:A:H2'	9:A:2135:A:H8	1.85	0.40
17:I:14:ALA:HB1	17:I:45:THR:CG2	2.52	0.40
9:A:841:G:C2	9:A:938:G:C2	3.10	0.40
9:A:528:A:H2	9:A:2043:C:C5'	2.34	0.40
13:E:178:VAL:HG23	13:E:179:SER:N	2.36	0.40
9:A:45:G:C5'	9:A:46:G:H5'	2.51	0.40
9:A:1864:U:O3'	9:A:2409:G:N2	2.54	0.40
9:A:2514:U:H2'	9:A:2515:C:C6	2.57	0.40
9:A:2537:U:C4	9:A:2538:C:N4	2.89	0.40
11:C:115:ILE:HG22	11:C:116:GLN:N	2.36	0.40
12:D:88:GLU:O	12:D:89:GLU:HG3	2.21	0.40
18:J:26:GLY:HA2	18:J:29:ALA:HB3	2.02	0.40
9:A:1847:A:H4'	9:A:1848:A:OP2	2.21	0.40
14:F:114:ARG:N	14:F:114:ARG:HD2	2.37	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 PDB entries followed by that with respect to all EM

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	21
2	1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	2	26
3	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
4	3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	5	43
5	4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	18
6	5	146/165 (88%)	77 (53%)	40 (27%)	29 (20%)	0	2
7	6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	4	40
11	C	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	2	29
12	D	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1	24
13	E	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	3	31
14	F	175/179 (98%)	141 (81%)	30 (17%)	4 (2%)	8	50
15	G	174/177 (98%)	127 (73%)	30 (17%)	17 (10%)	1	14
16	H	48/149 (32%)	29 (60%)	14 (29%)	5 (10%)	1	12
17	I	139/142 (98%)	97 (70%)	33 (24%)	9 (6%)	1	26
18	J	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	2	26
19	K	120/123 (98%)	95 (79%)	15 (12%)	10 (8%)	1	18
20	L	141/144 (98%)	104 (74%)	32 (23%)	5 (4%)	4	41
21	M	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1	18
22	N	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	24	68
23	O	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	21	65
24	P	112/115 (97%)	86 (77%)	17 (15%)	9 (8%)	1	19
25	Q	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	4	41
26	R	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	5	44
27	S	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	3	33
28	T	91/100 (91%)	57 (63%)	24 (26%)	10 (11%)	0	10
29	U	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	1	13
30	V	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
31	W	77/85 (91%)	39 (51%)	22 (29%)	16 (21%)	0	2
32	X	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	4	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Y	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	25
34	Z	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	4	40
35	a	1/19 (5%)	1 (100%)	0	0	100	100
All	All	3385/3714 (91%)	2613 (77%)	553 (16%)	219 (6%)	3	26

All (219) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	23	ALA
4	3	22	LYS
5	4	8	LYS
6	5	27	VAL
6	5	48	ALA
6	5	54	VAL
6	5	55	VAL
6	5	58	THR
6	5	69	PHE
6	5	93	ALA
6	5	107	GLU
6	5	108	VAL
6	5	120	ALA
6	5	124	ASP
6	5	130	PRO
11	C	70	LYS
11	C	104	LEU
11	C	121	ALA
11	C	140	VAL
12	D	43	ASP
12	D	73	VAL
12	D	170	VAL
13	E	79	ARG
14	F	111	ARG
15	G	2	ARG
15	G	16	VAL
15	G	28	LYS
15	G	31	GLU
15	G	84	LYS
15	G	164	ALA
15	G	168	VAL
16	H	3	VAL
18	J	13	ARG

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Mol	Chain	Res	Type
18	J	21	THR
18	J	44	TYR
18	J	45	THR
18	J	81	ILE
18	J	125	TYR
20	L	66	PHE
21	M	14	LYS
21	M	77	PRO
22	N	119	SER
24	P	50	ARG
24	P	51	ASN
24	P	93	LYS
27	S	3	THR
27	S	14	ALA
27	S	64	ALA
28	T	27	SER
28	T	29	THR
28	T	40	LYS
29	U	6	ARG
29	U	87	GLU
29	U	92	VAL
29	U	98	ASN
29	U	99	SER
31	W	9	THR
31	W	18	LYS
31	W	29	SER
31	W	36	ILE
31	W	56	HIS
34	Z	9	THR
1	0	35	GLU
2	1	4	ILE
2	1	50	GLU
6	5	3	LEU
6	5	33	VAL
6	5	88	HIS
6	5	92	ALA
6	5	116	GLU
6	5	119	PRO
11	C	37	SER
11	C	77	VAL
11	C	238	ASN
11	C	256	THR

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Mol	Chain	Res	Type
12	D	92	VAL
12	D	99	GLU
12	D	107	VAL
12	D	118	PHE
14	F	135	ILE
14	F	176	PHE
15	G	169	ARG
16	H	9	VAL
16	H	16	GLY
17	I	20	SER
17	I	79	LEU
18	J	111	LYS
19	K	35	VAL
19	K	71	ARG
20	L	111	ILE
21	M	2	LEU
21	M	36	VAL
21	M	56	ALA
26	R	65	ALA
27	S	19	LEU
27	S	96	ILE
28	T	36	LYS
28	T	49	LYS
29	U	51	LEU
31	W	14	ASP
31	W	47	GLY
31	W	50	VAL
31	W	74	LYS
33	Y	37	LEU
2	1	51	ALA
5	4	4	ARG
6	5	5	LEU
6	5	78	GLY
6	5	118	ILE
7	6	14	MET
11	C	110	LYS
12	D	95	SER
12	D	109	VAL
12	D	192	ALA
13	E	7	ASP
13	E	70	SER
13	E	123	LYS

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Mol	Chain	Res	Type
15	G	32	LEU
15	G	117	PRO
15	G	170	THR
16	H	10	ALA
17	I	11	GLN
18	J	74	TYR
19	K	13	ASN
19	K	46	ALA
19	K	93	GLN
21	M	69	PRO
23	O	3	LYS
24	P	113	LEU
26	R	98	ILE
29	U	85	ARG
29	U	101	THR
31	W	34	SER
32	X	17	ARG
32	X	34	SER
34	Z	34	THR
1	0	54	ILE
5	4	16	ILE
6	5	89	PRO
11	C	59	GLN
11	C	197	ALA
12	D	169	ARG
12	D	175	LEU
14	F	132	ARG
15	G	33	THR
15	G	173	ALA
17	I	64	ARG
19	K	119	ALA
20	L	29	LYS
21	M	23	GLY
21	M	134	THR
24	P	4	ILE
24	P	92	ARG
24	P	103	THR
25	Q	87	VAL
25	Q	88	GLU
25	Q	95	ALA
28	T	28	ASN
28	T	51	PHE

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Mol	Chain	Res	Type
28	T	55	VAL
31	W	37	VAL
32	X	76	LYS
33	Y	7	ARG
6	5	36	ASP
6	5	72	LEU
6	5	128	THR
11	C	64	VAL
11	C	120	ASP
11	C	196	ASN
12	D	183	GLU
13	E	46	GLN
13	E	96	VAL
15	G	97	VAL
15	G	163	TYR
15	G	166	GLU
17	I	12	VAL
17	I	71	LYS
18	J	65	THR
19	K	49	ARG
19	K	108	ARG
20	L	5	THR
20	L	41	ARG
21	M	35	ALA
21	M	73	ILE
24	P	34	GLY
25	Q	85	ALA
28	T	86	THR
28	T	89	GLU
29	U	88	ASP
31	W	46	ALA
31	W	76	ARG
33	Y	9	LYS
6	5	59	LEU
6	5	94	ARG
6	5	102	ALA
13	E	83	VAL
13	E	153	LEU
15	G	118	ALA
16	H	14	SER
17	I	93	ASN
19	K	6	THR

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Mol	Chain	Res	Type
19	K	50	GLY
21	M	13	HIS
26	R	40	MET
29	U	16	LYS
31	W	10	ARG
31	W	78	PHE
24	P	63	ILE
31	W	41	GLY
6	5	32	GLY
13	E	148	ILE
33	Y	62	GLY
4	3	6	VAL
11	C	232	GLY
12	D	122	VAL
17	I	22	PRO
17	I	88	GLY
1	0	24	VAL
13	E	71	GLY

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/48 (98%)	46 (98%)	1 (2%)	61	85
2	1	45/49 (92%)	42 (93%)	3 (7%)	20	60
3	2	38/38 (100%)	35 (92%)	3 (8%)	15	54
4	3	51/52 (98%)	46 (90%)	5 (10%)	10	43
5	4	34/34 (100%)	31 (91%)	3 (9%)	12	48
6	5	112/123 (91%)	93 (83%)	19 (17%)	2	20
7	6	26/85 (31%)	22 (85%)	4 (15%)	3	24
11	C	216/218 (99%)	202 (94%)	14 (6%)	21	61
12	D	164/164 (100%)	151 (92%)	13 (8%)	15	54
13	E	165/165 (100%)	146 (88%)	19 (12%)	7	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	F	148/150 (99%)	138 (93%)	10 (7%)	20	59
15	G	137/138 (99%)	122 (89%)	15 (11%)	8	39
16	H	40/114 (35%)	39 (98%)	1 (2%)	55	82
17	I	109/110 (99%)	105 (96%)	4 (4%)	41	75
18	J	116/116 (100%)	100 (86%)	16 (14%)	4	29
19	K	103/104 (99%)	92 (89%)	11 (11%)	8	39
20	L	102/103 (99%)	95 (93%)	7 (7%)	19	59
21	M	109/109 (100%)	93 (85%)	16 (15%)	4	26
22	N	100/103 (97%)	93 (93%)	7 (7%)	19	58
23	O	86/87 (99%)	78 (91%)	8 (9%)	11	46
24	P	99/100 (99%)	91 (92%)	8 (8%)	15	53
25	Q	89/90 (99%)	81 (91%)	8 (9%)	12	47
26	R	84/84 (100%)	78 (93%)	6 (7%)	18	58
27	S	93/93 (100%)	84 (90%)	9 (10%)	10	43
28	T	80/84 (95%)	77 (96%)	3 (4%)	40	74
29	U	83/85 (98%)	76 (92%)	7 (8%)	14	51
30	V	78/78 (100%)	75 (96%)	3 (4%)	40	74
31	W	59/63 (94%)	53 (90%)	6 (10%)	9	41
32	X	67/68 (98%)	61 (91%)	6 (9%)	12	47
33	Y	55/55 (100%)	52 (94%)	3 (6%)	27	66
34	Z	48/49 (98%)	40 (83%)	8 (17%)	3	21
35	a	4/18 (22%)	4 (100%)	0	100	100
All	All	2787/2977 (94%)	2541 (91%)	246 (9%)	17	48

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	24	VAL
2	1	8	ILE
2	1	35	LEU
2	1	47	ILE
3	2	8	SER
3	2	9	VAL
3	2	24	THR

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Mol	Chain	Res	Type
4	3	7	ARG
4	3	30	HIS
4	3	31	ILE
4	3	49	VAL
4	3	56	LEU
5	4	4	ARG
5	4	15	LYS
5	4	27	CYS
6	5	1	MET
6	5	3	LEU
6	5	26	VAL
6	5	42	ARG
6	5	51	TYR
6	5	54	VAL
6	5	59	LEU
6	5	65	GLU
6	5	69	PHE
6	5	70	GLU
6	5	96	PHE
6	5	106	PHE
6	5	107	GLU
6	5	116	GLU
6	5	121	SER
6	5	125	ARG
6	5	130	PRO
6	5	132	TYR
6	5	143	MET
7	6	17	MET
7	6	18	ASP
7	6	24	SER
7	6	26	MET
11	C	51	ARG
11	C	57	HIS
11	C	109	LEU
11	C	117	SER
11	C	124	LYS
11	C	129	LEU
11	C	142	ASN
11	C	155	ARG
11	C	166	ARG
11	C	176	ARG
11	C	194	VAL

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Mol	Chain	Res	Type
11	C	212	TRP
11	C	251	THR
11	C	270	ARG
12	D	33	ARG
12	D	37	VAL
12	D	97	SER
12	D	103	ASP
12	D	107	VAL
12	D	118	PHE
12	D	124	ARG
12	D	170	VAL
12	D	171	THR
12	D	177	VAL
12	D	183	GLU
12	D	201	LEU
12	D	203	VAL
13	E	5	LEU
13	E	12	LEU
13	E	21	ARG
13	E	40	ARG
13	E	44	ARG
13	E	65	THR
13	E	69	ARG
13	E	70	SER
13	E	78	TRP
13	E	88	ARG
13	E	109	LEU
13	E	113	VAL
13	E	118	LEU
13	E	120	VAL
13	E	126	VAL
13	E	131	THR
13	E	149	ILE
13	E	167	VAL
13	E	171	ASP
14	F	9	ASP
14	F	16	MET
14	F	34	THR
14	F	41	GLU
14	F	46	LYS
14	F	90	LEU
14	F	94	ARG

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Mol	Chain	Res	Type
14	F	111	ARG
14	F	114	ARG
14	F	154	THR
15	G	3	VAL
15	G	16	VAL
15	G	44	HIS
15	G	68	ARG
15	G	84	LYS
15	G	94	ARG
15	G	103	ASN
15	G	110	HIS
15	G	121	THR
15	G	126	THR
15	G	131	VAL
15	G	132	LEU
15	G	151	ARG
15	G	170	THR
15	G	176	LYS
16	H	3	VAL
17	I	23	VAL
17	I	63	ASP
17	I	102	ARG
17	I	137	LEU
18	J	2	LYS
18	J	17	VAL
18	J	24	THR
18	J	30	THR
18	J	36	LEU
18	J	40	HIS
18	J	54	ILE
18	J	55	ILE
18	J	65	THR
18	J	72	LYS
18	J	73	VAL
18	J	95	ARG
18	J	103	ILE
18	J	129	GLU
18	J	131	ASN
18	J	140	LEU
19	K	3	GLN
19	K	8	LEU
19	K	13	ASN

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Mol	Chain	Res	Type
19	K	18	ARG
19	K	21	CYS
19	K	23	LYS
19	K	41	ILE
19	K	54	LYS
19	K	73	ASP
19	K	93	GLN
19	K	105	ARG
20	L	5	THR
20	L	19	LEU
20	L	82	LEU
20	L	91	ASP
20	L	100	ILE
20	L	121	THR
20	L	144	GLU
21	M	12	MET
21	M	13	HIS
21	M	31	PHE
21	M	33	LEU
21	M	46	ILE
21	M	53	MET
21	M	70	ASP
21	M	72	PRO
21	M	81	ARG
21	M	88	ASN
21	M	95	LEU
21	M	96	ILE
21	M	97	GLN
21	M	100	LYS
21	M	110	GLU
21	M	134	THR
22	N	6	SER
22	N	8	ARG
22	N	33	ILE
22	N	65	LEU
22	N	69	ARG
22	N	70	THR
22	N	71	ARG
23	O	18	LEU
23	O	31	THR
23	O	33	ARG
23	O	36	TYR

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Mol	Chain	Res	Type
23	O	38	GLN
23	O	47	VAL
23	O	106	LEU
23	O	115	LEU
24	P	16	VAL
24	P	19	PHE
24	P	62	LYS
24	P	83	ILE
24	P	85	VAL
24	P	92	ARG
24	P	95	LYS
24	P	103	THR
25	Q	16	ILE
25	Q	40	LYS
25	Q	50	ARG
25	Q	59	LEU
25	Q	63	ARG
25	Q	88	GLU
25	Q	93	ILE
25	Q	97	ILE
26	R	4	VAL
26	R	29	THR
26	R	38	VAL
26	R	46	GLU
26	R	48	LYS
26	R	63	VAL
27	S	3	THR
27	S	4	ILE
27	S	7	HIS
27	S	36	LEU
27	S	45	VAL
27	S	66	ILE
27	S	76	VAL
27	S	96	ILE
27	S	101	SER
28	T	32	LEU
28	T	43	ILE
28	T	58	VAL
29	U	6	ARG
29	U	26	ASN
29	U	30	SER
29	U	38	ILE

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Mol	Chain	Res	Type
29	U	61	GLU
29	U	86	PHE
29	U	92	VAL
30	V	29	ILE
30	V	61	LEU
30	V	87	GLN
31	W	19	ARG
31	W	23	LYS
31	W	25	PHE
31	W	30	VAL
31	W	49	ASN
31	W	63	ASP
32	X	19	HIS
32	X	24	THR
32	X	26	ARG
32	X	29	LEU
32	X	34	SER
32	X	77	TYR
33	Y	10	SER
33	Y	16	THR
33	Y	57	LEU
34	Z	2	LYS
34	Z	9	THR
34	Z	15	ARG
34	Z	23	LEU
34	Z	30	ARG
34	Z	31	ILE
34	Z	37	ARG
34	Z	40	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	30	HIS
14	F	26	GLN
27	S	15	GLN
30	V	44	HIS
30	V	80	HIS
33	Y	41	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	117/118 (99%)	17 (14%)	0
8	7	1/3 (33%)	0	0
9	A	2850/2903 (98%)	466 (16%)	43 (1%)
All	All	2968/3024 (98%)	483 (16%)	43 (1%)

All (483) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	10	A
9	A	12	U
9	A	15	G
9	A	34	U
9	A	35	G
9	A	42	A
9	A	43	G
9	A	45	G
9	A	46	G
9	A	51	G
9	A	61	C
9	A	71	A
9	A	74	A
9	A	75	G
9	A	80	G
9	A	82	U
9	A	84	A
9	A	96	C
9	A	101	A
9	A	118	A
9	A	119	A
9	A	120	U
9	A	131	A
9	A	135	U
9	A	136	G
9	A	137	U
9	A	138	U
9	A	139	U
9	A	140	C
9	A	141	G
9	A	142	A
9	A	144	A
9	A	149	A
9	A	162	U
9	A	163	C

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Mol	Chain	Res	Type
9	A	164	C
9	A	181	A
9	A	188	G
9	A	196	A
9	A	199	A
9	A	215	G
9	A	216	A
9	A	222	A
9	A	226	A
9	A	230	G
9	A	248	G
9	A	255	A
9	A	264	C
9	A	265	A
9	A	266	G
9	A	267	C
9	A	272	A
9	A	273	G
9	A	276	U
9	A	277	G
9	A	278	A
9	A	281	C
9	A	285	G
9	A	302	C
9	A	311	A
9	A	329	G
9	A	330	A
9	A	346	A
9	A	347	A
9	A	353	C
9	A	355	U
9	A	361	G
9	A	362	A
9	A	371	A
9	A	372	G
9	A	382	A
9	A	383	C
9	A	386	G
9	A	388	G
9	A	396	G
9	A	404	A
9	A	405	U

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Mol	Chain	Res	Type
9	A	411	G
9	A	412	A
9	A	424	G
9	A	451	U
9	A	455	C
9	A	481	G
9	A	491	G
9	A	503	A
9	A	504	A
9	A	505	A
9	A	509	C
9	A	528	A
9	A	531	C
9	A	532	A
9	A	533	G
9	A	538	A
9	A	543	G
9	A	544	C
9	A	546	U
9	A	547	A
9	A	548	G
9	A	549	G
9	A	563	A
9	A	573	U
9	A	575	A
9	A	586	A
9	A	603	A
9	A	604	G
9	A	613	A
9	A	614	A
9	A	615	U
9	A	627	A
9	A	631	A
9	A	637	A
9	A	645	C
9	A	646	U
9	A	647	G
9	A	648	G
9	A	654	A
9	A	655	A
9	A	656	G
9	A	686	U

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Mol	Chain	Res	Type
9	A	714	U
9	A	715	A
9	A	730	A
9	A	738	G
9	A	747	U
9	A	775	G
9	A	776	G
9	A	782	A
9	A	784	G
9	A	785	G
9	A	805	G
9	A	812	C
9	A	819	A
9	A	827	U
9	A	828	U
9	A	845	A
9	A	846	U
9	A	847	U
9	A	859	G
9	A	878	A
9	A	883	G
9	A	884	U
9	A	896	A
9	A	897	C
9	A	910	A
9	A	914	G
9	A	915	C
9	A	932	U
9	A	941	A
9	A	946	C
9	A	961	C
9	A	974	G
9	A	983	A
9	A	985	C
9	A	995	C
9	A	996	A
9	A	1003	G
9	A	1012	U
9	A	1013	C
9	A	1021	A
9	A	1022	G
9	A	1023	U

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Mol	Chain	Res	Type
9	A	1025	G
9	A	1026	G
9	A	1033	U
9	A	1045	C
9	A	1046	A
9	A	1047	G
9	A	1051	G
9	A	1053	C
9	A	1059	G
9	A	1060	U
9	A	1061	U
9	A	1062	G
9	A	1067	A
9	A	1069	A
9	A	1070	A
9	A	1072	C
9	A	1074	G
9	A	1078	U
9	A	1083	U
9	A	1084	A
9	A	1088	A
9	A	1089	A
9	A	1090	A
9	A	1091	G
9	A	1097	U
9	A	1098	A
9	A	1110	G
9	A	1111	A
9	A	1112	G
9	A	1129	A
9	A	1132	U
9	A	1133	A
9	A	1135	C
9	A	1136	G
9	A	1139	G
9	A	1142	A
9	A	1151	A
9	A	1155	A
9	A	1169	A
9	A	1170	C
9	A	1172	C
9	A	1174	U

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Mol	Chain	Res	Type
9	A	1175	A
9	A	1176	U
9	A	1180	U
9	A	1186	G
9	A	1238	G
9	A	1248	G
9	A	1250	G
9	A	1253	A
9	A	1256	G
9	A	1266	G
9	A	1268	A
9	A	1271	G
9	A	1272	A
9	A	1273	U
9	A	1281	G
9	A	1300	G
9	A	1301	A
9	A	1313	U
9	A	1317	G
9	A	1352	U
9	A	1365	A
9	A	1368	G
9	A	1378	A
9	A	1379	U
9	A	1383	A
9	A	1395	A
9	A	1415	U
9	A	1416	G
9	A	1419	A
9	A	1420	A
9	A	1428	C
9	A	1435	G
9	A	1452	G
9	A	1459	G
9	A	1482	G
9	A	1493	C
9	A	1504	A
9	A	1508	A
9	A	1510	G
9	A	1515	A
9	A	1524	G
9	A	1533	C

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Mol	Chain	Res	Type
9	A	1534	U
9	A	1535	A
9	A	1536	C
9	A	1566	A
9	A	1569	A
9	A	1578	U
9	A	1583	A
9	A	1584	U
9	A	1585	C
9	A	1607	C
9	A	1608	A
9	A	1610	A
9	A	1613	G
9	A	1627	G
9	A	1647	U
9	A	1648	U
9	A	1649	G
9	A	1652	A
9	A	1653	G
9	A	1674	G
9	A	1714	U
9	A	1715	G
9	A	1723	G
9	A	1729	U
9	A	1730	C
9	A	1737	G
9	A	1738	G
9	A	1739	A
9	A	1744	A
9	A	1758	U
9	A	1764	C
9	A	1773	A
9	A	1776	G
9	A	1791	A
9	A	1800	C
9	A	1801	A
9	A	1802	A
9	A	1808	A
9	A	1811	G
9	A	1816	C
9	A	1829	A
9	A	1833	C

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Mol	Chain	Res	Type
9	A	1847	A
9	A	1848	A
9	A	1858	A
9	A	1869	G
9	A	1870	C
9	A	1871	A
9	A	1872	A
9	A	1873	G
9	A	1884	G
9	A	1906	G
9	A	1913	A
9	A	1914	C
9	A	1927	A
9	A	1929	G
9	A	1930	G
9	A	1937	A
9	A	1938	A
9	A	1955	U
9	A	1960	A
9	A	1966	A
9	A	1967	C
9	A	1970	A
9	A	1971	U
9	A	1972	G
9	A	1991	U
9	A	1993	U
9	A	1997	C
9	A	2017	U
9	A	2020	A
9	A	2022	U
9	A	2023	C
9	A	2031	A
9	A	2033	A
9	A	2043	C
9	A	2055	C
9	A	2056	G
9	A	2060	A
9	A	2061	G
9	A	2063	C
9	A	2064	C
9	A	2069	G
9	A	2072	C

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Mol	Chain	Res	Type
9	A	2093	G
9	A	2104	C
9	A	2106	U
9	A	2107	G
9	A	2108	A
9	A	2109	U
9	A	2110	G
9	A	2134	A
9	A	2135	A
9	A	2137	U
9	A	2138	G
9	A	2139	U
9	A	2140	G
9	A	2142	A
9	A	2143	C
9	A	2144	G
9	A	2145	C
9	A	2146	C
9	A	2147	A
9	A	2148	G
9	A	2149	U
9	A	2150	C
9	A	2151	U
9	A	2153	C
9	A	2154	A
9	A	2155	U
9	A	2156	G
9	A	2157	G
9	A	2180	U
9	A	2183	A
9	A	2185	U
9	A	2194	U
9	A	2198	A
9	A	2199	A
9	A	2204	G
9	A	2211	A
9	A	2212	A
9	A	2214	C
9	A	2225	A
9	A	2226	C
9	A	2238	G
9	A	2239	G

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Mol	Chain	Res	Type
9	A	2250	G
9	A	2268	A
9	A	2278	A
9	A	2283	C
9	A	2284	A
9	A	2286	G
9	A	2287	A
9	A	2305	U
9	A	2308	G
9	A	2311	A
9	A	2322	A
9	A	2325	G
9	A	2327	A
9	A	2333	A
9	A	2336	A
9	A	2347	C
9	A	2354	C
9	A	2361	G
9	A	2383	G
9	A	2385	C
9	A	2402	U
9	A	2403	C
9	A	2406	A
9	A	2423	U
9	A	2424	C
9	A	2425	A
9	A	2429	G
9	A	2430	A
9	A	2435	A
9	A	2441	U
9	A	2448	A
9	A	2470	G
9	A	2476	A
9	A	2491	U
9	A	2502	G
9	A	2503	A
9	A	2504	U
9	A	2505	G
9	A	2506	U
9	A	2508	G
9	A	2518	A
9	A	2529	G

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Mol	Chain	Res	Type
9	A	2554	U
9	A	2556	C
9	A	2566	A
9	A	2567	G
9	A	2572	A
9	A	2573	C
9	A	2575	C
9	A	2576	G
9	A	2577	A
9	A	2583	G
9	A	2585	U
9	A	2586	U
9	A	2587	A
9	A	2601	C
9	A	2602	A
9	A	2608	G
9	A	2609	U
9	A	2610	C
9	A	2611	C
9	A	2613	U
9	A	2629	U
9	A	2663	G
9	A	2671	G
9	A	2681	C
9	A	2682	A
9	A	2689	U
9	A	2690	U
9	A	2714	G
9	A	2716	C
9	A	2726	A
9	A	2733	A
9	A	2744	G
9	A	2748	A
9	A	2757	A
9	A	2760	C
9	A	2765	A
9	A	2778	A
9	A	2791	G
9	A	2798	U
9	A	2800	A
9	A	2801	G
9	A	2818	U

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Mol	Chain	Res	Type
9	A	2820	A
9	A	2821	A
9	A	2861	U
9	A	2867	G
9	A	2873	A
9	A	2874	C
9	A	2883	A
9	A	2884	U
9	A	2885	G
9	A	2891	U
9	A	2903	U
10	B	3	C
10	B	15	A
10	B	16	G
10	B	21	G
10	B	30	C
10	B	35	C
10	B	42	C
10	B	44	G
10	B	45	A
10	B	56	G
10	B	84	G
10	B	87	U
10	B	88	C
10	B	89	U
10	B	90	C
10	B	99	A
10	B	109	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	119	A
9	A	271	G
9	A	277	G
9	A	301	G
9	A	403	U
9	A	404	A
9	A	503	A
9	A	527	C
9	A	613	A
9	A	655	A

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Mol	Chain	Res	Type
9	A	784	G
9	A	827	U
9	A	846	U
9	A	882	G
9	A	931	U
9	A	1020	A
9	A	1025	G
9	A	1069	A
9	A	1088	A
9	A	1110	G
9	A	1247	A
9	A	1378	A
9	A	1458	U
9	A	1509	A
9	A	1535	A
9	A	1626	A
9	A	1738	G
9	A	1757	A
9	A	1847	A
9	A	1870	C
9	A	1939	U
9	A	2108	A
9	A	2142	A
9	A	2211	A
9	A	2286	G
9	A	2326	C
9	A	2423	U
9	A	2503	A
9	A	2576	G
9	A	2601	C
9	A	2756	U
9	A	2873	A
9	A	2902	C

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	ERY	A	9000	-	53,53,53	0.78	1 (1%)	82,82,82	1.64	15 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ERY	A	9000	-	-	0/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	9000	ERY	C6-C5	2.18	1.59	1.55

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	9000	ERY	C25-C24-C23	-4.98	102.73	110.05
36	A	9000	ERY	O7-C5-C6	-4.64	100.47	106.45
36	A	9000	ERY	C3-C2-C1	-3.57	102.94	109.85
36	A	9000	ERY	O2-C1-O1	-3.43	117.24	123.88
36	A	9000	ERY	C15-C16-C17	-2.97	104.03	107.82
36	A	9000	ERY	C27-C26-C25	-2.96	108.46	113.44
36	A	9000	ERY	C32-C6-C7	-2.88	106.19	110.99
36	A	9000	ERY	O3-C14-C15	-2.77	104.31	108.94
36	A	9000	ERY	O6-C17-C18	-2.75	104.78	109.24
36	A	9000	ERY	O3-C3-C4	-2.46	105.19	108.22
36	A	9000	ERY	O3-C3-C2	-2.28	106.78	111.10
36	A	9000	ERY	C16-C17-C18	-2.12	107.80	111.03
36	A	9000	ERY	O2-C13-C12	-2.06	103.62	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	9000	ERY	C32-C6-C5	2.14	114.17	110.29
36	A	9000	ERY	C19-C16-C17	2.31	116.20	111.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	9000	ERY	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.