



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Feb 14, 2018 – 09:13 PM EST

PDB ID : 5T7V  
EMDB ID: : EMD-8369  
Title : Methicillin Resistant, Linezolid resistant Staphylococcus aureus 70S ribosome  
(delta S145 uL3)  
Authors : Belousoff, M.J.; Lithgow, T.; Eyal, Z.; Yonath, A.; Radjainia, M.  
Deposited on : 2016-09-06  
Resolution : 3.60 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

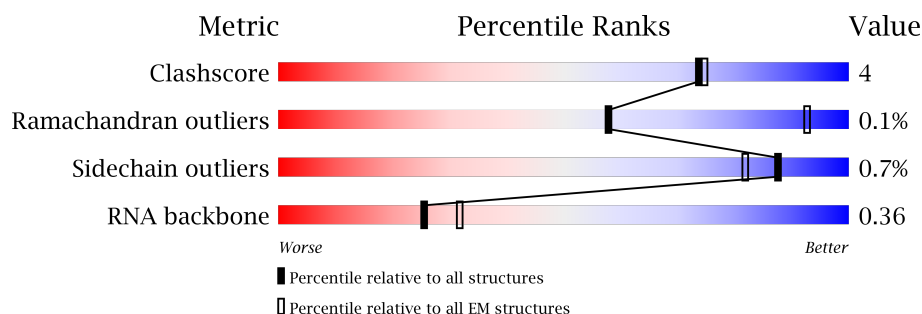
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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.























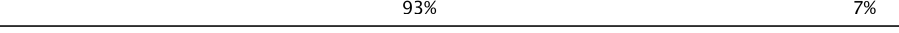

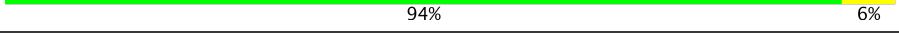


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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  $\geq 3$ , 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	A	1547	46% 37% 9% 8%
2	S1	82	90% 10%
3	S2	115	87% 13%
4	S3	136	78% 18% .
5	S6	87	86% 14%
6	S7	76	79% 21%
7	S8	82	87% 13%
8	S9	55	85% 15%










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Mol	Chain	Length	Quality of chain
9	SA	76	 83% 16%
10	SC	198	 81% 19%
11	SD	154	 84% 15%
12	SE	92	 84% 16%
13	SF	130	 87% 13%
14	B	2919	 59% 30% 6% 5%
15	C	114	 57% 37% 6%
16	L1	113	 81% 19%
17	L2	275	 87% 13%
18	L3	116	 89% 11%
19	L4	100	 85% 15%
20	L5	111	 92% 7%
21	L6	87	 93% 7%
22	L7	101	 89% 11%
23	L8	93	 92% 8%
24	L9	78	 79% 19%
25	LA	59	 88% 12%
26	LB	61	 85% 15%
27	LC	214	 89% 11%
28	LD	57	 93% 7%
29	LE	53	 79% 21%
30	LF	47	 94% 6%
31	LG	44	 91% 9%
32	LH	64	 84% 16%
33	LI	37	 95% 5%

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Mol	Chain	Length	Quality of chain
34	LJ	204	 91% 9%
35	LL	174	 86% 14% .
36	LM	143	 89% 10% .
37	LN	121	 90% 10%
38	LO	144	 92% 8%
39	LP	136	 93% 7%
40	LQ	121	 83% 17%
41	LR	116	 84% 15% .
42	D	74	 41% 47% 12%

## 2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 126001 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1419	Total	C	N	O	P	0	0
			30390	13573	5558	9844	1415		

- Molecule 2 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S1	82	Total	C	N	O	S	0	0
			647	405	117	124	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S1	57	GLY	LYS	conflict	UNP A0A0H2K0A0

- Molecule 3 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S2	115	Total	C	N	O	S	0	0
			850	525	161	161	3		

- Molecule 4 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S3	136	Total	C	N	O	S	0	0
			1011	622	205	183	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S3	43	ALA	LYS	conflict	UNP W8U1C6

- Molecule 5 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S6	87	Total	C	N	O	S	0	0
			725	448	149	127	1		

- Molecule 6 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S7	76	Total	C	N	O		0	0
			594	374	112	108			

- Molecule 7 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S8	82	Total	C	N	O	S	0	0
			674	427	122	124	1		

- Molecule 8 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S9	55	Total	C	N	O	S	0	0
			456	290	87	77	2		

- Molecule 9 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	SA	76	Total	C	N	O	0	0
			475	290	96	89		

- Molecule 10 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SC	198	Total	C	N	O	S	0	0
			1604	1014	298	290	2		

- Molecule 11 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SD	154	Total	C	N	O	S	0	0
			1132	711	209	210	2		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SE	92	Total	C	N	O	S	0	0
			763	484	135	142	2		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SF	130	Total	C	N	O	S	0	0
			1012	638	180	190	4		

- Molecule 14 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	2768	Total	C	N	O	P	0	0
			59339	26499	10863	19214	2763		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1866	A	G	conflict	GB 1015534143

- Molecule 15 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	114	Total	C	N	O	P	0	0
			2424	1085	434	792	113		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	68	A	U	conflict	GB 1043615627
C	?	-	G	deletion	GB 1043615627

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L1	113	Total	C	N	O		0	0
			914	576	184	154			

- Molecule 17 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L2	275	Total	C	N	O	S	0	0
			2086	1301	416	364	5		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L3	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L4	100	Total	C	N	O	S	0	0
			784	499	139	145	1		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L5	111	Total	C	N	O	S	0	0
			852	532	163	154	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L6	87	Total	C	N	O	S	0	0
			684	430	121	130	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L6	87	ASP	ILE	conflict	UNP W8TUB4

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L7	101	Total	C	N	O	S	0	0
			758	479	141	137	1		

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L8	93	Total	C	N	O	S	0	0
			726	465	129	131	1		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L9	78	Total	C	N	O	S	0	0
			590	365	116	109			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LA	59	Total	C	N	O	S	0	0
			462	287	99	75	1		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LB	61	Total	C	N	O	S	0	0
			502	310	95	96	1		

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LC	214	Total	C	N	O	S	0	0
			1617	1012	297	303	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LC	?	-	SER	deletion	UNP W8U3W0

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LD	57	Total	C	N	O	S	0	0
			440	274	83	83			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LE	53	Total	C	N	O	S	0	0
			421	256	86	74	5		

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LF	47	Total	C	N	O	S	0	0
			386	232	79	70	5		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LG	44	Total	C	N	O	S	0	0
			371	228	90	52	1		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LH	64	Total	C	N	O	S	0	0
			520	324	113	81	2		

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LI	37	Total	C	N	O	S	0	0
			295	186	60	44	5		

- Molecule 34 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LJ	204	Total	C	N	O	S	0	0
			1538	965	283	288	2		

- Molecule 35 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LL	174	Total	C	N	O	S	0	0
			1357	845	248	261	3		

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LM	143	Total	C	N	O	S	0	0
			1137	710	209	216	2		

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LN	121	Total	C	N	O	S	0	0
			910	566	173	167	4		

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LO	144	Total	C	N	O		0	0
			1081	669	213	199			

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LP	136	Total	C	N	O	S	0	0
			1088	698	206	180	4		

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LQ	121	Total	C	N	O	S	0	0
			954	586	183	184	1		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LR	116	Total	C	N	O		0	0
			896	559	171	166			

- Molecule 42 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	D	74	Total	C	N	O	P	0	0
			1577	704	282	518	73		

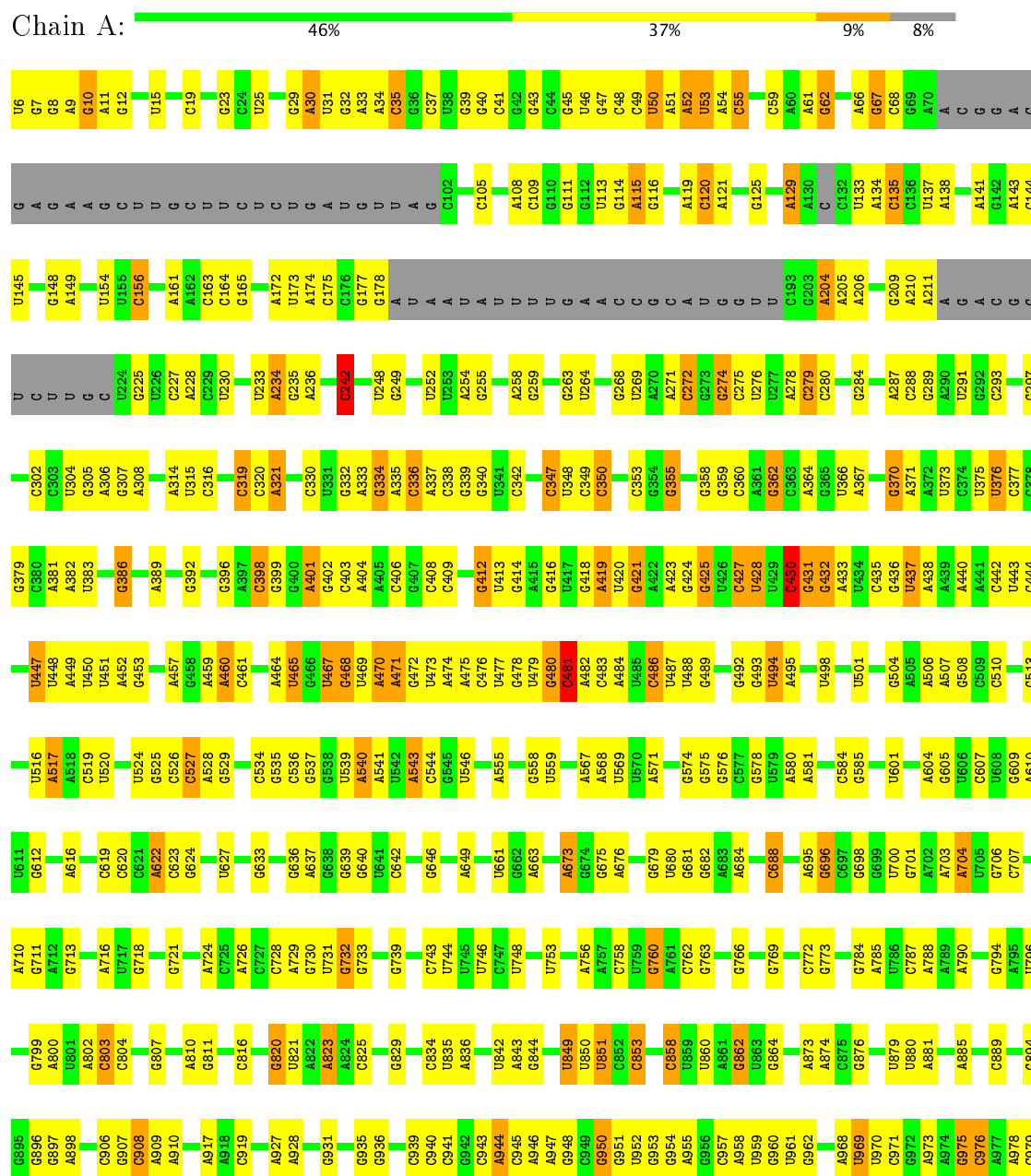
- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	B	13	Total 13	Mg 13	0
43	A	4	Total 4	Mg 4	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: 16S ribosomal RNA







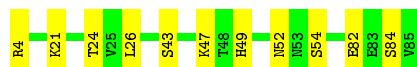
- Molecule 6: 30S ribosomal protein S16

Chain S7: 79% 21%



- Molecule 7: 30S ribosomal protein S17

Chain S8: 87% 13%



- Molecule 8: 30S ribosomal protein S18

Chain S9: 85% 15%



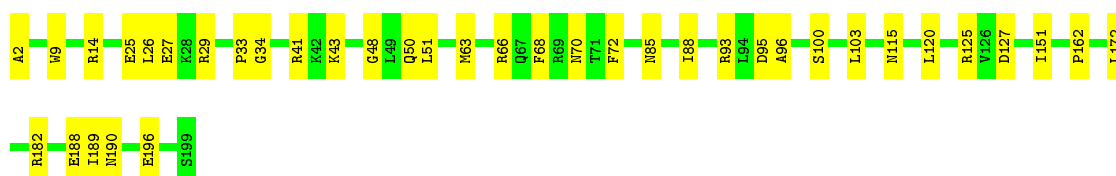
- Molecule 9: 30S ribosomal protein S20

Chain SA: 83% 16%



- Molecule 10: 30S ribosomal protein S4

Chain SC: 81% 19%



- Molecule 11: 30S ribosomal protein S5

Chain SD: 84% 15%



- Molecule 12: 30S ribosomal protein S6

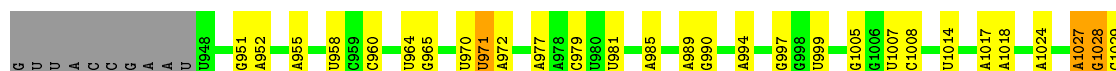
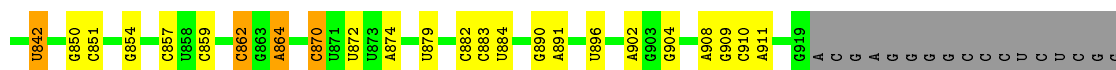
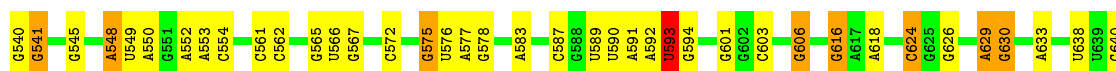
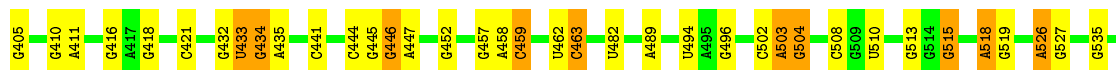
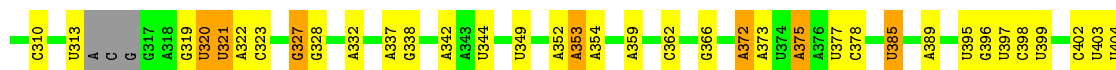
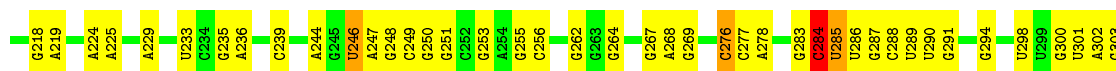
Chain SE: 84% 16%



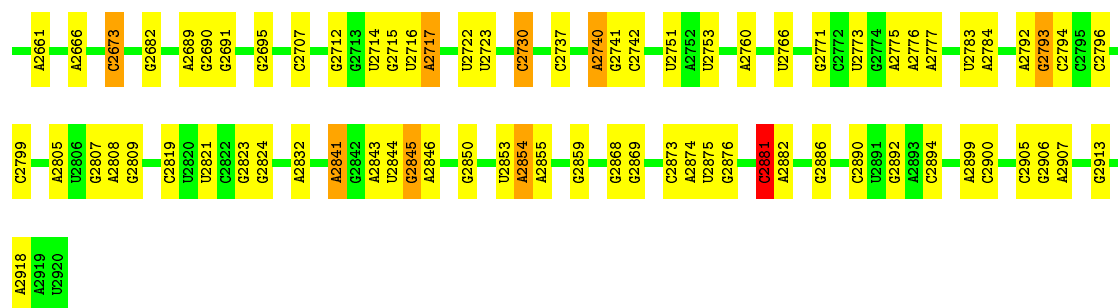
- Molecule 13: 30S ribosomal protein S8



- Molecule 14: 23S ribosomal RNA

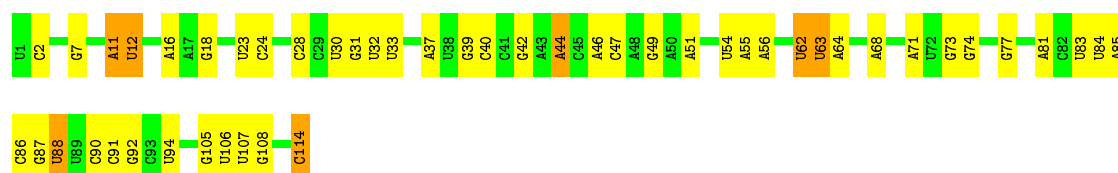


U2555	A2445	A2349	G2245	A	C2111	U2020	C1914	C1822	C1735	C1624	G1544	A1478	G1395	C1296	A1170
G2556	A2452	G2352	U2246	G	G2114	C2021	G1915	U1823	C1736	U1625	U1545	U1482	C1398	G1300	A1173
U2557	A2453	U2353	U2247	C	U2115	C2022	A1926	U1825	U1737	A1626	A1546	U1483	C1399	U1301	U1174
G2561	G2456	A2354	A2252	U	U2116	C2023	A1927	U1826	C1738	U1627	C1547	G1484	U1484	G1302	U1175
G2562	G2457	G2358	C2253	A	G2117	A2025	G1932	C1827	G1739	U1628	U1548	U1485	A1402	U1305	U1176
G2563	U2458	U2359	G2261	C	U2118	C2026	G1933	U1828	G1740	A1630	G1550	G1487	C1403	U1306	A1177
G2564	G2459	C2359	U2262	G	U2119	A2027	A1939	U1835	G1741	U1631	U	A1488	A1404	U1307	C1178
G2565	G2460	U2360	G2263	U	G2120	A2028	A1940	U1836	U1742	A1632	U	A1489	A1405	C1308	C1179
G2566	A2461	U2361	G2264	G	A2121	U2029	G1941	A1837	G1743	A1633	A	G1490	G1406	A	G1182
C2567	C2462	A2362	G2265	G	A2122	U2030	C1942	U1838	U1744	A1634	A	C1491	C1407	A1310	U1183
G2568	C2463	A2363	U2270	A	A2123	C2035	U1942	G1839	A1745	A1635	G1555	G1492	G1408	A1311	C1184
G2569	C2464	G2364	U2271	G	G2124	G2036	U1943	U1840	G1746	U1636	G1556	U1493	U1409	A1312	C1185
G2570	C2465	U2365	U2272	G	U2125	G2037	U1944	U1841	G1747	U1637	C1557	G1494	A1410	G1313	U1186
G2571	C2466	G2366	U2273	C	G2126	A2038	A1945	U1842	G1748	A1638	U1558	C1495	G1412	A1314	A1187
U2581	U2582	G2367	G2277	C	G2127	A2039	C1946	U1843	U1749	U1639	U1559	C1496	G1413	C1315	A1188
U2582	G2368	U2368	G2278	G	G2128	A2040	C1947	U1844	U1750	A1640	U1560	U1497	U1416	G1316	C1189
U2583	U2369	U2369	G2279	C	C2129	A2041	A1948	U1845	U1751	A1641	G1561	U1498	U1417	U1210	U1210
G2584	U2370	U2370	G2280	U	A2130	C2042	U1949	U1846	U1752	A1642	G1562	U1500	G1418	G1322	U1211
G2585	U2371	U2371	G2281	C	A2131	A2043	U1950	U1847	U1753	A1643	G1563	U1501	A1421	C1323	C1213
A2591	C2473	C2374	U2282	G	A2132	A2044	G1951	U1848	U1754	A1644	G1564	U1502	A1422	C1324	C1214
A2592	U2474	U2375	U2283	U	G2133	A2045	G1952	U1849	U1755	A1645	G1565	U1503	A1423	C1325	U1215
A2593	U2475	U2376	G2284	C	G2134	U2046	G1953	U1850	U1756	A1646	G1566	U1504	A1424	C1326	U1216
G2594	C2476	G2377	G2285	G	U2135	U2047	G1954	U1851	U1757	A1647	G1567	U1505	A1425	C1327	U1217
C2595	U2477	U2378	A2293	G	U2136	U2048	G1955	U1852	U1758	U1648	G1568	U1506	U1426	C1328	U1218
C2596	U2478	U2379	G2294	C	U2137	A2049	G1956	U1853	U1759	A1649	G1569	U1507	U1427	C1329	U1219
C2597	U2479	U2380	G2295	A	U2138	C2050	G1957	U1854	U1760	A1650	G1570	U1508	U1428	C1330	U1220
C2598	U2480	A2381	G2296	U	U2139	C2051	G1958	U1855	U1761	A1651	G1571	U1509	U1429	C1331	U1221
C2599	C2481	U2382	G2297	C	U2140	A2052	G1959	U1856	U1762	A1652	G1572	U1510	U1430	C1332	U1222
C2600	U2482	U2383	G2298	G	A2141	U2053	G1960	U1857	U1763	A1653	G1573	U1511	U1431	C1333	U1223
C2601	U2483	U2384	U2299	C	A2142	A2054	G1961	U1858	U1764	A1654	G1574	U1512	U1432	C1334	U1224
C2602	U2484	U2385	G2300	U	G2143	U2055	G1962	U1859	U1765	A1655	G1575	U1513	U1433	C1335	U1225
C2603	U2485	U2386	A2301	G	U2144	C2056	G1963	U1860	U1766	A1656	G1576	U1514	U1434	C1336	U1226
C2604	U2486	U2387	U2302	C	U2145	A2057	G1964	U1861	U1767	A1657	G1577	U1515	U1435	C1337	U1227
C2605	U2487	U2388	G2303	A	U2146	U2058	G1965	U1862	U1768	A1658	G1578	U1516	U1436	C1338	U1228
C2606	U2488	U2389	U2304	C	U2147	A2059	G1966	U1863	U1769	A1659	G1579	U1517	U1437	C1339	U1229
C2607	U2489	U2390	G2305	G	U2148	U2060	G1967	U1864	U1770	A1660	G1580	U1518	U1438	C1340	U1230
C2608	U2490	U2391	U2306	C	U2149	C2061	G1968	U1865	U1771	A1661	G1581	U1519	U1439	C1341	U1231
C2609	U2491	U2392	G2307	C	U2150	U2062	G1969	U1866	U1772	A1662	G1582	U1520	U1440	C1342	U1232
C2610	U2492	U2393	U2308	C	U2151	C2063	G1970	U1867	U1773	A1663	G1583	U1521	U1441	C1343	U1233
C2611	U2493	U2394	U2309	C	U2152	U2064	G1971	U1868	U1774	A1664	G1584	U1522	U1442	C1344	U1234
C2612	U2494	U2395	G2310	C	U2153	A2065	G1972	U1869	U1775	A1665	G1585	U1523	U1443	C1345	U1235
C2613	U2495	U2396	U2311	C	U2154	C2066	G1973	U1870	U1776	A1666	G1586	U1524	U1444	C1346	U1236
C2614	U2496	U2397	U2312	C	U2155	U2067	G1974	U1871	U1777	A1667	G1587	U1525	U1445	C1347	U1237
C2615	U2497	U2398	U2313	C	U2156	A2068	G1975	U1872	U1778	A1668	G1588	U1526	U1446	C1348	U1238
C2616	U2498	U2399	U2314	C	U2157	U2069	G1976	U1873	U1779	A1669	G1589	U1527	U1447	C1349	U1239
C2617	U2499	U2400	U2315	C	U2158	C2070	G1977	U1874	U1780	A1670	G1590	U1528	U1448	C1350	U1240
C2618	U2500	U2401	G2316	C	U2159	U2071	G1978	U1875	U1781	A1671	G1591	U1529	U1449	C1351	U1241
C2619	U2501	U2402	U2317	C	U2160	C2072	G1979	U1876	U1782	A1672	G1592	U1530	U1450	C1352	U1242
C2620	U2502	U2403	U2318	C	U2161	U2073	G1980	U1877	U1783	A1673	G1593	U1531	U1451	C1353	U1243
C2621	U2503	U2404	U2319	C	U2162	C2074	G1981	U1878	U1784	A1674	G1594	U1532	U1452	C1354	U1244
C2622	U2504	U2405	U2320	C	U2163	U2075	G1982	U1879	U1785	A1675	G1595	U1533	U1453	C1355	U1245
C2623	U2505	U2406	U2321	C	U2164	C2076	G1983	U1880	U1786	A1676	G1596	U1534	U1454	C1356	U1246
C2624	U2506	U2407	U2322	C	U2165	U2077	G1984	U1881	U1787	A1677	G1597	U1535	U1455	C1357	U1247
C2625	U2507	U2408	U2323	C	U2166	C2078	G1985	U1882	U1788	A1678	G1598	U1536	U1456	C1358	U1248
C2626	U2508	U2409	U2324	C	U2167	U2079	G1986	U1883	U1789	A1679	G1599	U1537	U1457	C1359	U1249
C2627	U2509	U2410	U2325	C	U2168	C2080	G1987	U1884	U1790	A1680	G1600	U1538	U1458	C1360	U1250
C2628	U2510	U2411	U2326	C	U2169	U2081	G1988	U1885	U1791	A1681	G1601	U1539	U1459	C1361	U1251
C2629	U2511	U2412	U2327	C	U2170	C2082	G1989	U1886	U1792	A1682	G1602	U1540	U1460	C1362	U1252
C2630	U2512	U2413	U2328	C	U2171	U2083	G1990	U1887	U1793	A1683	G1603	U1541	U1461	C1363	U1253
C2631	U2513	U2414	U2329	C	U2172	A2084	G1991	U1888	U1794	A1684	G1604	U1542	U1462	C1364	U1254
C2632	U2514	U2415	U2330	C	U2173	C2085	G1992	U1889	U1795	A1685	G1605	U1543	U1463	C1365	U1255
C2633	U2515	U2416	U2331	C	U2174	U2086	G1993	U1890	U1796	A1686	G1606	U1544	U1464	C1366	U1256
C2634	U2516	U2417	U2332	C	U2175	A2087	G1994	U1891	U1797	A1687	G1607	U1545	U1465	C1367	U1257
C2635	U2517	U2418	U2333	C	U2176	C2088	G1995	U1892	U1798	A1688	G1608	U1546	U1466	C1368	U1258
C2636	U2518	U2419	U2334	C	U2177	U2089	G1996	U1893	U1799	A1689	G1609	U1547	U1467	C1369	U1259
C2637	U2519	U2420	U2335	C	U2178	C2090	G1997	U1894	U1800	A1690	G1610	U1548	U1468	C1370	U1260
C2638	U2520	U2421	U2336	C	U2179	U2091	G1998	U1895	U1801	A1691	G1611	U1549	U1469	C1371	U1261
C2639	U2521	U2422	U2337	C	U2180	C2092	G1999	U1896	U1802	A1692	G1612	U1550	U1470	C1372	U1262
C2640	U2522	U2423	U2338	C	U2181	U2093	G2000	U1897	U1803	A1693	G1613	U1551	U1471	C1373	U1263
C2641	U2523	U2424	U2339	C	U2182	A2094	G2001	U1898	U1804	A1694	G1614	U1552	U1472	C1374	U1264
C2642	U2524	U2425	U2340	C	U2183	C2095	G2002	U1899	U1805	A1695	G1615	U1553	U1473	C1375	U1265
C2643	U2525	U2426	U2341	C	U2184	U2096	G2003	U1900	U1806	A1696	G1616	U1554	U1474	C1376	U1266
C2644	U2526	U2427	U2342	C	U2185	C2097	G2004	U1901	U1807	A1697	G1617	U1555	U1475	C1377	U1267
C2645	U2527	U2428	U2343	C	U2186	U2098	G2005	U1902	U1808	A1698	G1618	U1556	U1476	C1378	U1268
C2646	U2528	U2429	U2344	C	U2187	C2099	G2006	U1903	U1809	A1699	G1619	U1557	U1477	C1379	U1269
C2647	U2529	U2430	U2345	C	U2188	U2100	G2007	U1904	U1810	A1700	G1620	U1558	U1478	C1380	U1270
C2648	U2530	U2431	U2346	C	U2189	C2101	G2008	U1905	U1811	A1701	G1621	U1559	U1479	C1381	U1271
C2649	U2531	U2432	U2347	C	U2190	U2102	G2009	U1906	U1812	A1702	G1622	U1560	U1480	C1382	U1272
C2650	U2532	U2433	U2348	C	U2191	U2103	G2010	U1907	U1813	A1703	G1623	U1561	U1481	C1383	U1273
C2651	U2533	U2434	U2349	C	U2192	C2104	G2011	U1908	U1814	A1704	G1624	U1562	U1482	C1384	U1274
C2652	U2534	U2435	U2350	C	U2193	U2105	G2012	U1909	U1815	A17					



- Molecule 15: 5S ribosomal RNA

Chain C: 57% 37% 6%



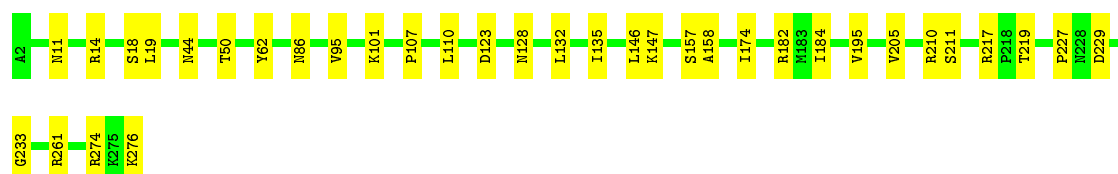
- Molecule 16: 50S ribosomal protein L19

Chain L1: 81% 19%



- Molecule 17: 50S ribosomal protein L2

Chain L2: 87% 13%



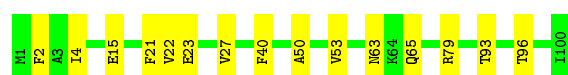
- Molecule 18: 50S ribosomal protein L20

Chain L3: 89% 11%



- Molecule 19: 50S ribosomal protein L21

Chain L4: 85% 15%



- Molecule 20: 50S ribosomal protein L22

Chain L5:  92% 7%



- Molecule 21: 50S ribosomal protein L23

Chain L6:  93% 7%



- Molecule 22: 50S ribosomal protein L24

Chain L7:  89% 11%




- Molecule 23: 50S ribosomal protein L25

Chain L8:  92% 8%



- Molecule 24: 50S ribosomal protein L27

Chain L9:  79% 19%




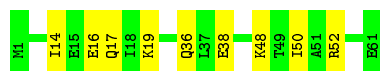
- Molecule 25: 50S ribosomal protein L28

Chain LA:  88% 12%



- Molecule 26: 50S ribosomal protein L29

Chain LB:  85% 15%



- Molecule 27: 50S ribosomal protein L3

Chain LC:  89% 11%



- Molecule 28: 50S ribosomal protein L30

Chain LD: 93% 7%



- Molecule 29: 50S ribosomal protein L32

Chain LE: 79% 21%



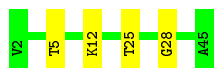
- Molecule 30: 50S ribosomal protein L33

Chain LF: 94% 6%



- Molecule 31: 50S ribosomal protein L34

Chain LG: 91% 9%



- Molecule 32: 50S ribosomal protein L35

Chain LH: 84% 16%



- Molecule 33: 50S ribosomal protein L36

Chain LI: 95% 5%

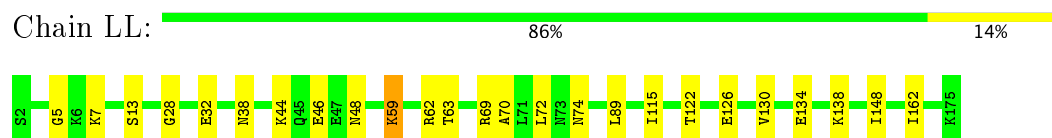


- Molecule 34: 50S ribosomal protein L4

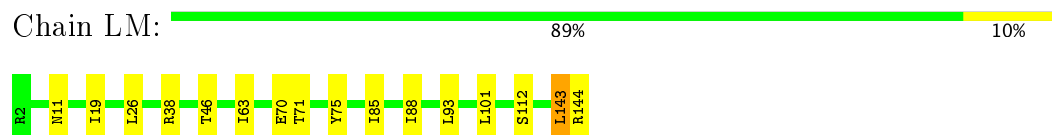
Chain LJ: 91% 9%



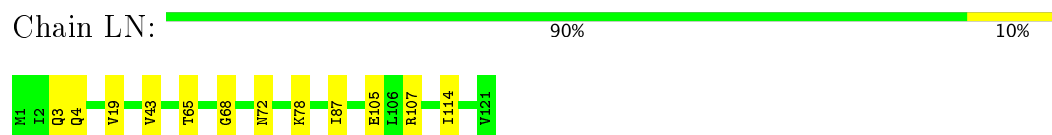
- Molecule 35: 50S ribosomal protein L6



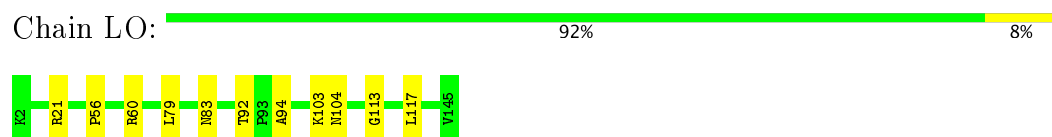
- Molecule 36: 50S ribosomal protein L13



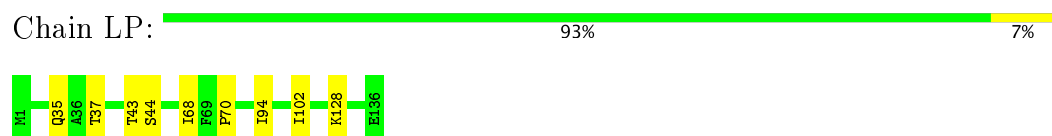
- Molecule 37: 50S ribosomal protein L14



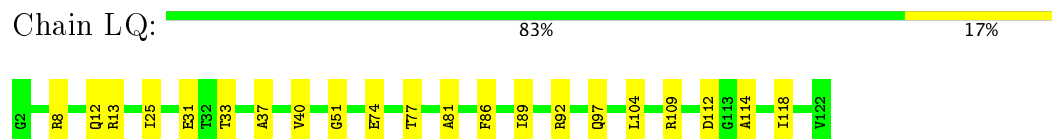
- Molecule 38: 50S ribosomal protein L15



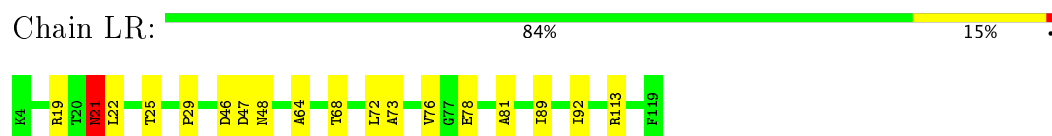
- Molecule 39: 50S ribosomal protein L16



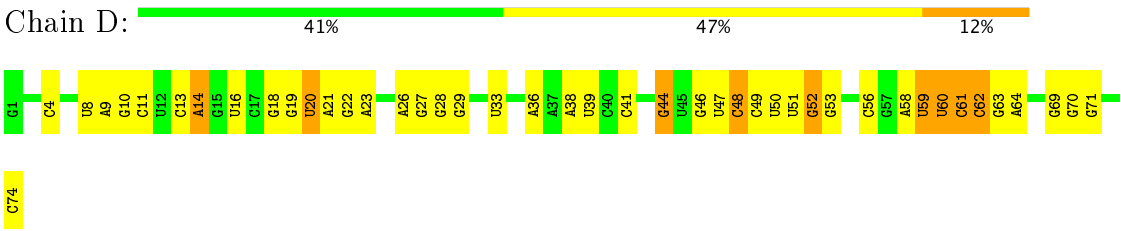
- Molecule 40: 50S ribosomal protein L17



- Molecule 41: 50S ribosomal protein L18



- Molecule 42: E-site tRNA



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	80500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 2$	RMSZ	# $ Z  > 2$
1	A	0.55	0/34022	1.12	160/53044 (0.3%)
10	SC	0.31	0/1634	0.56	0/2196
11	SD	0.35	0/1145	0.62	0/1546
12	SE	0.36	0/774	0.62	0/1039
13	SF	0.31	0/1022	0.56	0/1373
14	B	0.97	5/66453 (0.0%)	1.16	377/103631 (0.4%)
15	C	0.65	0/2710	1.15	20/4221 (0.5%)
16	L1	0.45	0/926	0.63	1/1238 (0.1%)
17	L2	0.53	0/2121	0.66	0/2849
18	L3	0.52	0/954	0.64	0/1264
19	L4	0.45	0/794	0.62	0/1061
2	S1	0.30	0/659	0.52	0/893
20	L5	0.46	0/860	0.66	0/1158
21	L6	0.48	0/691	0.61	0/926
22	L7	0.36	0/765	0.60	0/1021
23	L8	0.36	0/734	0.59	0/985
24	L9	0.52	0/596	0.74	0/792
25	LA	0.43	0/468	0.60	1/624 (0.2%)
26	LB	0.35	0/503	0.63	0/669
27	LC	0.50	0/1641	0.66	1/2203 (0.0%)
28	LD	0.40	0/442	0.64	0/596
29	LE	0.47	0/428	0.63	0/570
3	S2	0.29	0/865	0.55	0/1170
30	LF	0.39	0/389	0.55	0/518
31	LG	0.55	0/375	0.60	0/490
32	LH	0.44	0/525	0.61	0/689
33	LI	0.45	0/298	0.56	0/392
34	LJ	0.45	0/1561	0.62	0/2110
35	LL	0.36	0/1375	0.58	0/1850
36	LM	0.48	0/1159	0.60	1/1562 (0.1%)
37	LN	0.53	0/917	0.67	0/1231
38	LO	0.47	0/1095	0.63	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	LP	0.45	0/1112	0.59	0/1492
4	S3	0.34	0/1026	0.77	3/1385 (0.2%)
40	LQ	0.46	0/958	0.67	0/1281
41	LR	0.38	0/905	0.67	0/1211
42	D	0.41	0/1762	1.06	5/2746 (0.2%)
5	S6	0.32	0/734	0.53	0/981
6	S7	0.29	0/604	0.60	0/819
7	S8	0.34	0/682	0.63	0/912
8	S9	0.31	0/463	0.59	0/619
9	SA	0.28	0/475	0.57	1/645 (0.2%)
All	All	0.77	5/137622 (0.0%)	1.05	570/207462 (0.3%)

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	SD	0	1
18	L3	0	1
19	L4	0	1
24	L9	0	1
36	LM	0	1
37	LN	0	1
4	S3	0	1
41	LR	0	2
9	SA	0	1
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1289	A	N9-C4	-6.20	1.34	1.37
14	B	1599	G	N3-C4	-5.57	1.31	1.35
14	B	2740	A	N9-C4	-5.20	1.34	1.37
14	B	2625	A	N7-C5	-5.20	1.36	1.39
14	B	1566	G	N9-C4	-5.15	1.33	1.38

All (570) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1168	C	N1-C2-O2	12.01	126.10	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	12	U	C2-N1-C1'	11.85	131.92	117.70
14	B	1350	U	N3-C2-O2	-10.99	114.50	122.20
1	A	373	U	C2-N1-C1'	10.92	130.80	117.70
1	A	1168	C	C2-N1-C1'	10.73	130.61	118.80
14	B	1835	U	C5-C6-N1	10.44	127.92	122.70
14	B	12	U	N1-C2-O2	10.13	129.89	122.80
14	B	1350	U	N1-C2-O2	9.98	129.79	122.80
1	A	376	U	C2-N1-C1'	9.95	129.64	117.70
1	A	758	C	C6-N1-C2	-9.88	116.35	120.30
1	A	373	U	N1-C2-O2	9.84	129.69	122.80
14	B	402	C	C2-N1-C1'	9.47	129.22	118.80
1	A	1168	C	N3-C2-O2	-9.31	115.39	121.90
14	B	12	U	N3-C2-O2	-9.18	115.78	122.20
14	B	1215	U	C2-N1-C1'	9.11	128.64	117.70
4	S3	38	LEU	CA-CB-CG	9.02	136.05	115.30
14	B	402	C	N1-C2-O2	9.01	124.31	118.90
14	B	1835	U	C2-N1-C1'	9.01	128.51	117.70
1	A	135	C	N1-C2-O2	8.94	124.26	118.90
14	B	1514	A	C5-C6-N6	-8.81	116.65	123.70
1	A	376	U	N1-C2-O2	8.79	128.95	122.80
14	B	1215	U	N1-C2-O2	8.51	128.76	122.80
1	A	373	U	N3-C2-O2	-8.49	116.26	122.20
14	B	835	U	N3-C2-O2	-8.38	116.34	122.20
14	B	2017	C	C6-N1-C2	-8.37	116.95	120.30
1	A	135	C	C2-N1-C1'	8.36	128.00	118.80
1	A	288	C	N1-C2-O2	8.33	123.90	118.90
14	B	1370	C	C6-N1-C2	-8.30	116.98	120.30
1	A	376	U	N3-C2-O2	-8.25	116.42	122.20
14	B	2534	C	N1-C2-O2	8.18	123.81	118.90
14	B	1028	G	N3-C4-N9	8.16	130.90	126.00
14	B	999	U	C5-C6-N1	8.15	126.78	122.70
14	B	759	U	C2-N1-C1'	8.06	127.37	117.70
14	B	403	U	C2-N1-C1'	8.02	127.32	117.70
14	B	2035	C	C6-N1-C2	-7.93	117.13	120.30
14	B	1941	C	N1-C2-O2	7.91	123.65	118.90
1	A	758	C	C5-C6-N1	7.90	124.95	121.00
1	A	288	C	C2-N1-C1'	7.87	127.46	118.80
14	B	12	U	C5-C6-N1	7.85	126.62	122.70
15	C	86	C	C2-N1-C1'	7.84	127.43	118.80
1	A	1168	C	C6-N1-C2	-7.78	117.19	120.30
14	B	12	U	C6-N1-C1'	-7.78	110.31	121.20
1	A	319	C	C6-N1-C2	-7.77	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1524	C	C6-N1-C2	-7.76	117.19	120.30
1	A	135	C	N3-C2-O2	-7.76	116.47	121.90
14	B	1514	A	N9-C4-C5	-7.74	102.70	105.80
1	A	1002	G	N3-C4-C5	-7.71	124.75	128.60
14	B	803	C	C6-N1-C2	-7.69	117.22	120.30
1	A	758	C	N1-C2-O2	7.69	123.52	118.90
14	B	1932	C	C2-N1-C1'	7.68	127.25	118.80
14	B	2539	C	C6-N1-C2	-7.67	117.23	120.30
14	B	1961	C	C6-N1-C2	-7.65	117.24	120.30
14	B	2429	U	N1-C2-O2	7.63	128.14	122.80
14	B	1591	G	N3-C4-N9	7.58	130.55	126.00
1	A	6	U	C2-N1-C1'	7.56	126.78	117.70
14	B	1591	G	N3-C4-C5	-7.55	124.83	128.60
14	B	1085	U	N3-C2-O2	-7.55	116.92	122.20
14	B	1778	C	C6-N1-C2	-7.52	117.29	120.30
1	A	476	C	C6-N1-C2	-7.52	117.29	120.30
14	B	2429	U	N3-C2-O2	-7.52	116.94	122.20
14	B	1941	C	C2-N1-C1'	7.51	127.06	118.80
1	A	1002	G	C4-N9-C1'	7.50	136.25	126.50
14	B	2287	C	C6-N1-C2	-7.49	117.30	120.30
14	B	403	U	N3-C2-O2	-7.44	117.00	122.20
1	A	373	U	C6-N1-C1'	-7.43	110.79	121.20
14	B	1350	U	C2-N1-C1'	7.43	126.61	117.70
14	B	1085	U	N1-C2-O2	7.37	127.96	122.80
14	B	1514	A	C4-C5-N7	7.33	114.36	110.70
14	B	402	C	N3-C2-O2	-7.28	116.81	121.90
14	B	1524	C	C5-C6-N1	7.28	124.64	121.00
14	B	320	U	C2-N1-C1'	7.27	126.43	117.70
14	B	1591	G	C4-N9-C1'	7.27	135.95	126.50
14	B	1215	U	N3-C2-O2	-7.25	117.12	122.20
14	B	2621	C	C6-N1-C2	-7.19	117.42	120.30
14	B	835	U	N1-C2-O2	7.18	127.83	122.80
1	A	1168	C	C6-N1-C1'	-7.17	112.20	120.80
4	S3	24	LEU	CA-CB-CG	7.17	131.78	115.30
1	A	336	C	P-O3'-C3'	7.16	128.29	119.70
15	C	63	U	C2-N1-C1'	7.13	126.25	117.70
14	B	249	C	C6-N1-C2	-7.12	117.45	120.30
1	A	1193	U	N1-C2-O2	7.09	127.76	122.80
14	B	1216	U	C2-N1-C1'	7.09	126.21	117.70
14	B	2534	C	N3-C2-O2	-7.09	116.94	121.90
14	B	1503	U	P-O3'-C3'	7.08	128.20	119.70
14	B	781	C	C6-N1-C2	-7.07	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1042	C	C6-N1-C2	-7.07	117.47	120.30
14	B	403	U	N1-C2-O2	7.06	127.74	122.80
14	B	1028	G	N3-C4-C5	-7.06	125.07	128.60
1	A	1219	C	C2-N1-C1'	7.05	126.56	118.80
14	B	515	G	O4'-C1'-N9	7.04	113.83	108.20
1	A	1087	C	C6-N1-C2	-7.02	117.49	120.30
1	A	758	C	N3-C2-O2	-7.02	116.99	121.90
1	A	758	C	C2-N1-C1'	7.01	126.51	118.80
1	A	1219	C	N1-C2-O2	6.99	123.09	118.90
1	A	430	C	N1-C2-O2	6.99	123.09	118.90
14	B	1395	G	C4-C5-N7	6.98	113.59	110.80
14	B	1599	G	C2-N3-C4	-6.97	108.41	111.90
14	B	1835	U	N1-C2-O2	6.92	127.64	122.80
14	B	1289	A	C5-N7-C8	-6.89	100.45	103.90
14	B	2264	G	C8-N9-C4	-6.86	103.66	106.40
15	C	86	C	N1-C2-O2	6.86	123.01	118.90
1	A	851	U	C2-N1-C1'	6.84	125.91	117.70
1	A	1193	U	C2-N1-C1'	6.84	125.91	117.70
14	B	835	U	C2-N1-C1'	6.82	125.88	117.70
14	B	211	C	N1-C2-O2	6.80	122.98	118.90
14	B	2737	C	C6-N1-C2	-6.78	117.59	120.30
15	C	63	U	N1-C2-O2	6.77	127.54	122.80
1	A	510	C	C6-N1-C2	-6.76	117.60	120.30
14	B	811	C	C6-N1-C2	-6.74	117.60	120.30
14	B	1514	A	C5-C6-N1	6.74	121.07	117.70
15	C	86	C	N3-C2-O2	-6.73	117.19	121.90
14	B	1835	U	C6-N1-C2	-6.71	116.97	121.00
14	B	503	A	O4'-C1'-N9	6.71	113.57	108.20
14	B	2386	C	C5-C6-N1	6.70	124.35	121.00
14	B	402	C	C6-N1-C1'	-6.68	112.78	120.80
1	A	820	G	N3-C4-N9	6.67	130.00	126.00
14	B	561	C	C5-C6-N1	6.67	124.33	121.00
1	A	476	C	C5-C6-N1	6.66	124.33	121.00
14	B	1370	C	C5-C6-N1	6.66	124.33	121.00
14	B	1029	C	C5-C6-N1	6.64	124.32	121.00
14	B	2321	C	C6-N1-C2	-6.63	117.65	120.30
14	B	759	U	N1-C2-O2	6.59	127.42	122.80
14	B	1028	G	C4-N9-C1'	6.59	135.07	126.50
14	B	103	U	N3-C2-O2	-6.58	117.59	122.20
14	B	1466	G	C4-N9-C1'	6.58	135.05	126.50
14	B	714	G	N3-C4-N9	6.57	129.94	126.00
15	C	33	U	N1-C2-O2	6.57	127.40	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2035	C	C5-C6-N1	6.55	124.28	121.00
1	A	1211	A	P-O3'-C3'	6.54	127.55	119.70
14	B	680	C	N3-C2-O2	-6.54	117.32	121.90
1	A	1269	C	C6-N1-C2	-6.54	117.69	120.30
1	A	1002	G	N3-C4-N9	6.54	129.92	126.00
14	B	2469	C	C6-N1-C2	-6.54	117.69	120.30
14	B	1566	G	N3-C4-N9	-6.53	122.08	126.00
1	A	851	U	N1-C2-O2	6.52	127.36	122.80
14	B	1599	G	N3-C4-N9	-6.52	122.09	126.00
1	A	851	U	N3-C2-O2	-6.49	117.66	122.20
14	B	695	C	C5-C6-N1	6.49	124.24	121.00
14	B	162	A	OP1-P-OP2	-6.48	109.88	119.60
14	B	1351	C	C2-N1-C1'	6.47	125.92	118.80
14	B	1729	C	C6-N1-C2	-6.47	117.71	120.30
1	A	442	C	N1-C2-O2	6.46	122.78	118.90
14	B	1008	C	C6-N1-C2	-6.46	117.72	120.30
14	B	2609	G	C4-N9-C1'	6.46	134.89	126.50
1	A	288	C	N3-C2-O2	-6.45	117.39	121.90
15	C	33	U	C2-N1-C1'	6.45	125.44	117.70
14	B	518	A	C4-C5-N7	6.44	113.92	110.70
14	B	18	C	C6-N1-C2	-6.43	117.73	120.30
14	B	2881	C	C5-C6-N1	6.43	124.22	121.00
14	B	811	C	C5-C6-N1	6.42	124.21	121.00
14	B	1700	C	C6-N1-C2	-6.41	117.74	120.30
14	B	103	U	N1-C2-O2	6.40	127.28	122.80
1	A	820	G	N3-C4-C5	-6.39	125.40	128.60
14	B	1466	G	N3-C4-N9	6.37	129.82	126.00
14	B	31	C	C5-C6-N1	6.37	124.19	121.00
1	A	376	U	C6-N1-C1'	-6.36	112.29	121.20
14	B	515	G	N1-C6-O6	6.35	123.71	119.90
9	SA	49	LEU	CA-CB-CG	6.34	129.89	115.30
14	B	1865	C	N1-C2-O2	6.34	122.71	118.90
14	B	624	C	C6-N1-C2	-6.33	117.77	120.30
14	B	1409	U	N3-C2-O2	-6.32	117.78	122.20
14	B	2021	C	C6-N1-C2	-6.32	117.77	120.30
14	B	2539	C	C5-C6-N1	6.31	124.16	121.00
14	B	2017	C	C5-C6-N1	6.31	124.15	121.00
1	A	1517	U	N3-C2-O2	-6.31	117.78	122.20
14	B	2469	C	C5-C6-N1	6.28	124.14	121.00
14	B	680	C	N1-C2-O2	6.27	122.66	118.90
14	B	284	C	C2-N1-C1'	6.27	125.69	118.80
1	A	177	G	O4'-C1'-N9	6.26	113.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	C	C6-N1-C2	-6.26	117.80	120.30
1	A	607	C	C6-N1-C2	-6.26	117.80	120.30
15	C	33	U	C5-C6-N1	6.26	125.83	122.70
14	B	1215	U	C6-N1-C1'	-6.25	112.46	121.20
1	A	373	U	C5-C6-N1	6.24	125.82	122.70
1	A	1007	C	C2-N1-C1'	6.23	125.65	118.80
1	A	1193	U	N3-C2-O2	-6.22	117.85	122.20
14	B	515	G	C4-C5-N7	6.21	113.29	110.80
1	A	1168	C	C5-C6-N1	6.21	124.10	121.00
1	A	15	U	C2-N1-C1'	6.20	125.14	117.70
1	A	1158	U	C2-N1-C1'	6.20	125.14	117.70
14	B	2111	C	C5-C6-N1	6.20	124.10	121.00
14	B	1865	C	C2-N1-C1'	6.19	125.61	118.80
1	A	858	C	N1-C2-O2	6.19	122.61	118.90
14	B	2020	U	C5-C6-N1	6.18	125.79	122.70
14	B	680	C	C6-N1-C2	-6.18	117.83	120.30
15	C	63	U	N3-C2-O2	-6.18	117.88	122.20
1	A	105	C	C6-N1-C2	-6.17	117.83	120.30
14	B	508	C	C6-N1-C2	-6.16	117.83	120.30
14	B	1584	U	N1-C2-O2	6.16	127.11	122.80
42	D	39	U	C2-N1-C1'	6.16	125.09	117.70
14	B	2905	C	C5-C6-N1	6.15	124.08	121.00
14	B	1585	G	N3-C4-C5	-6.15	125.52	128.60
1	A	1374	U	C2-N1-C1'	6.15	125.08	117.70
1	A	272	C	C6-N1-C2	-6.14	117.84	120.30
1	A	442	C	C6-N1-C2	-6.14	117.84	120.30
1	A	969	U	P-O3'-C3'	6.14	127.07	119.70
14	B	2429	U	C2-N1-C1'	6.14	125.07	117.70
14	B	1514	A	N1-C6-N6	6.13	122.28	118.60
1	A	53	U	N1-C2-O2	6.13	127.09	122.80
14	B	698	U	C2-N1-C1'	6.12	125.04	117.70
14	B	1035	C	C5-C6-N1	6.12	124.06	121.00
14	B	256	C	C6-N1-C2	-6.11	117.85	120.30
14	B	1591	G	C8-N9-C1'	-6.11	119.05	127.00
1	A	483	C	C6-N1-C2	-6.10	117.86	120.30
14	B	714	G	N3-C4-C5	-6.10	125.55	128.60
14	B	515	G	C5-N7-C8	-6.09	101.25	104.30
14	B	2483	C	C5-C6-N1	6.09	124.05	121.00
14	B	1395	G	C6-C5-N7	-6.09	126.75	130.40
14	B	603	C	C5-C6-N1	6.09	124.04	121.00
1	A	336	C	N1-C2-O2	6.08	122.55	118.90
1	A	1533	U	C5-C6-N1	6.08	125.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	999	U	C6-N1-C2	-6.08	117.35	121.00
14	B	250	G	N3-C4-N9	6.07	129.64	126.00
14	B	1029	C	C6-N1-C2	-6.07	117.87	120.30
14	B	1035	C	C6-N1-C2	-6.06	117.88	120.30
14	B	1566	G	N3-C4-C5	6.06	131.63	128.60
15	C	114	C	C6-N1-C2	-6.05	117.88	120.30
1	A	227	C	C6-N1-C2	-6.05	117.88	120.30
14	B	1042	C	C5-C6-N1	6.04	124.02	121.00
14	B	733	U	C5-C6-N1	6.03	125.72	122.70
14	B	1153	C	C6-N1-C2	-6.03	117.89	120.30
14	B	1370	C	N1-C2-O2	6.03	122.52	118.90
14	B	1028	G	C8-N9-C1'	-6.02	119.17	127.00
1	A	68	C	C6-N1-C2	-6.01	117.89	120.30
14	B	1466	G	N3-C4-C5	-6.01	125.59	128.60
1	A	442	C	C5-C6-N1	6.01	124.00	121.00
14	B	1487	G	C8-N9-C4	-6.00	104.00	106.40
14	B	698	U	N1-C2-O2	6.00	127.00	122.80
14	B	2621	C	C5-C6-N1	6.00	124.00	121.00
14	B	1591	G	C2-N3-C4	6.00	114.90	111.90
14	B	1585	G	C4-N9-C1'	5.99	134.29	126.50
14	B	842	U	C5-C6-N1	5.99	125.69	122.70
1	A	480	G	P-O3'-C3'	5.98	126.88	119.70
14	B	1985	C	C6-N1-C2	-5.97	117.91	120.30
14	B	1599	G	N1-C2-N3	5.96	127.48	123.90
1	A	376	U	C5-C6-N1	5.96	125.68	122.70
14	B	1773	A	N7-C8-N9	5.96	116.78	113.80
1	A	976	C	C6-N1-C2	-5.95	117.92	120.30
1	A	1200	G	P-O3'-C3'	5.95	126.84	119.70
14	B	1801	C	N3-C2-O2	-5.95	117.73	121.90
14	B	2233	C	C5-C6-N1	5.95	123.97	121.00
14	B	1985	C	C5-C6-N1	5.95	123.97	121.00
14	B	1179	C	N1-C2-O2	5.94	122.46	118.90
1	A	6	U	N1-C2-O2	5.93	126.95	122.80
14	B	803	C	N3-C2-O2	-5.93	117.75	121.90
1	A	481	C	C2-N1-C1'	5.93	125.33	118.80
14	B	593	U	N1-C2-O2	5.93	126.95	122.80
14	B	515	G	C6-C5-N7	-5.92	126.85	130.40
14	B	1599	G	N3-C2-N2	-5.92	115.76	119.90
14	B	2534	C	C2-N1-C1'	5.91	125.30	118.80
14	B	759	U	C6-N1-C1'	-5.90	112.94	121.20
14	B	2020	U	N3-C2-O2	-5.90	118.07	122.20
14	B	1585	G	N3-C4-N9	5.90	129.54	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2386	C	C6-N1-C2	-5.89	117.94	120.30
14	B	1460	U	N1-C2-O2	5.89	126.92	122.80
1	A	1007	C	N1-C2-O2	5.89	122.43	118.90
14	B	1941	C	N3-C2-O2	-5.88	117.78	121.90
14	B	1409	U	N1-C2-O2	5.86	126.90	122.80
1	A	1137	U	N1-C2-O2	5.85	126.89	122.80
14	B	714	G	C4-N9-C1'	5.84	134.10	126.50
14	B	1351	C	C5-C6-N1	5.84	123.92	121.00
14	B	1351	C	C6-N1-C2	-5.84	117.96	120.30
1	A	1292	C	N1-C2-O2	5.83	122.40	118.90
14	B	1030	C	C6-N1-C2	-5.83	117.97	120.30
14	B	831	C	C5-C6-N1	5.82	123.91	121.00
14	B	2070	C	C5-C6-N1	5.82	123.91	121.00
1	A	1218	C	C2-N1-C1'	5.82	125.20	118.80
1	A	1352	C	C6-N1-C2	-5.82	117.97	120.30
1	A	1324	C	C5-C6-N1	5.82	123.91	121.00
14	B	182	C	N3-C2-O2	-5.82	117.83	121.90
14	B	1466	G	OP1-P-O3'	5.82	118.00	105.20
14	B	828	A	C2-N3-C4	5.81	113.51	110.60
14	B	1380	G	C4-N9-C1'	5.81	134.05	126.50
14	B	2233	C	N1-C2-O2	5.81	122.39	118.90
1	A	1374	U	N3-C2-O2	-5.81	118.14	122.20
14	B	182	C	N1-C2-O2	5.81	122.38	118.90
14	B	2905	C	C6-N1-C2	-5.81	117.98	120.30
14	B	739	U	C5-C6-N1	5.80	125.60	122.70
14	B	2239	A	N7-C8-N9	5.80	116.70	113.80
15	C	88	U	N3-C2-O2	-5.80	118.14	122.20
14	B	1778	C	C5-C6-N1	5.79	123.90	121.00
1	A	52	A	P-O3'-C3'	5.79	126.65	119.70
14	B	2324	C	C6-N1-C2	-5.79	117.98	120.30
14	B	1289	A	C4-C5-N7	5.79	113.59	110.70
14	B	1515	G	C8-N9-C1'	-5.79	119.48	127.00
14	B	2070	C	N1-C2-O2	5.78	122.37	118.90
14	B	717	C	C6-N1-C2	-5.78	117.99	120.30
14	B	731	U	N3-C2-O2	-5.78	118.16	122.20
14	B	1370	C	N3-C2-O2	-5.78	117.86	121.90
1	A	1277	C	C2-N1-C1'	5.77	125.15	118.80
15	C	28	C	C5-C6-N1	5.77	123.88	121.00
1	A	272	C	N1-C2-O2	5.77	122.36	118.90
15	C	86	C	C6-N1-C1'	-5.77	113.88	120.80
1	A	1374	U	N1-C2-O2	5.76	126.83	122.80
1	A	941	C	C6-N1-C2	-5.76	118.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2723	U	C5-C6-N1	5.75	125.58	122.70
14	B	402	C	C6-N1-C2	-5.75	118.00	120.30
14	B	759	U	O4'-C1'-N1	5.75	112.80	108.20
1	A	1372	C	C2-N1-C1'	5.75	125.12	118.80
14	B	31	C	C6-N1-C2	-5.75	118.00	120.30
14	B	1584	U	C2-N1-C1'	5.75	124.60	117.70
1	A	430	C	C2-N1-C1'	5.75	125.12	118.80
14	B	2525	C	N1-C2-O2	5.74	122.34	118.90
1	A	1002	G	C8-N9-C1'	-5.74	119.55	127.00
14	B	2287	C	C5-C6-N1	5.74	123.87	121.00
14	B	561	C	C6-N1-C2	-5.73	118.01	120.30
1	A	849	U	C2-N1-C1'	5.73	124.58	117.70
1	A	1463	U	C2-N1-C1'	5.73	124.57	117.70
14	B	90	A	P-O3'-C3'	5.72	126.57	119.70
14	B	2348	G	N3-C4-N9	5.72	129.44	126.00
1	A	1292	C	N3-C2-O2	-5.72	117.89	121.90
14	B	1036	C	C6-N1-C2	-5.71	118.01	120.30
14	B	1466	G	C8-N9-C1'	-5.71	119.57	127.00
1	A	334	G	C4-N9-C1'	5.71	133.92	126.50
14	B	12	U	C6-N1-C2	-5.70	117.58	121.00
14	B	1351	C	N1-C2-O2	5.70	122.32	118.90
14	B	710	C	N1-C2-O2	5.70	122.32	118.90
14	B	782	C	C5-C6-N1	5.70	123.85	121.00
1	A	1211	A	OP2-P-O3'	5.70	117.73	105.20
14	B	323	C	C6-N1-C2	-5.70	118.02	120.30
14	B	1599	G	C8-N9-C4	-5.69	104.12	106.40
1	A	1213	C	C6-N1-C2	-5.69	118.02	120.30
14	B	2321	C	C5-C6-N1	5.68	123.84	121.00
1	A	59	C	C6-N1-C2	-5.68	118.03	120.30
14	B	1474	C	C6-N1-C2	-5.67	118.03	120.30
14	B	463	C	C5-C6-N1	5.67	123.83	121.00
14	B	1515	G	C4-N9-C1'	5.66	133.86	126.50
14	B	2369	C	C6-N1-C2	-5.65	118.04	120.30
42	D	62	C	C6-N1-C2	-5.65	118.04	120.30
14	B	1983	U	N3-C2-O2	-5.65	118.25	122.20
14	B	1815	C	C5-C6-N1	5.64	123.82	121.00
14	B	2490	C	C6-N1-C2	-5.64	118.04	120.30
1	A	1324	C	C6-N1-C2	-5.63	118.05	120.30
14	B	575	G	N3-C4-C5	-5.62	125.79	128.60
42	D	39	U	N1-C2-O2	5.61	126.73	122.80
14	B	1715	U	C6-N1-C2	-5.60	117.64	121.00
1	A	1219	C	C6-N1-C2	-5.60	118.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2369	C	C5-C6-N1	5.60	123.80	121.00
14	B	1216	U	N1-C2-O2	5.59	126.72	122.80
14	B	2277	G	C8-N9-C4	-5.59	104.16	106.40
14	B	1932	C	C6-N1-C1'	-5.59	114.09	120.80
1	A	607	C	C5-C6-N1	5.59	123.80	121.00
14	B	765	U	N1-C2-O2	5.59	126.71	122.80
1	A	135	C	C6-N1-C1'	-5.59	114.09	120.80
1	A	1002	G	C8-N9-C4	-5.59	104.16	106.40
1	A	1303	G	C4-N9-C1'	5.59	133.76	126.50
14	B	1932	C	N1-C2-O2	5.59	122.25	118.90
14	B	1399	C	C5-C6-N1	5.58	123.79	121.00
14	B	764	C	C5-C6-N1	5.58	123.79	121.00
1	A	1014	C	C6-N1-C2	-5.57	118.07	120.30
14	B	276	C	C2-N1-C1'	5.57	124.93	118.80
1	A	467	U	P-O3'-C3'	5.57	126.38	119.70
1	A	1168	C	C2-N3-C4	5.56	122.68	119.90
1	A	242	C	C6-N1-C2	-5.55	118.08	120.30
1	A	288	C	C6-N1-C2	-5.55	118.08	120.30
15	C	33	U	N3-C2-O2	-5.55	118.31	122.20
14	B	1627	G	P-O3'-C3'	5.55	126.36	119.70
1	A	853	C	N1-C2-O2	5.55	122.23	118.90
14	B	593	U	C2-N1-C1'	5.55	124.36	117.70
14	B	721	A	C5-N7-C8	-5.55	101.13	103.90
14	B	1835	U	N3-C2-O2	-5.55	118.32	122.20
14	B	1441	C	C6-N1-C2	-5.54	118.08	120.30
14	B	1516	C	C6-N1-C2	-5.54	118.08	120.30
15	C	114	C	C2-N1-C1'	5.54	124.90	118.80
1	A	483	C	N1-C2-O2	5.54	122.22	118.90
25	LA	54	LEU	CA-CB-CG	5.54	128.04	115.30
14	B	2487	U	C5-C6-N1	5.53	125.47	122.70
14	B	1296	C	C5-C6-N1	5.53	123.76	121.00
14	B	1363	U	N1-C2-O2	5.52	126.67	122.80
14	B	1865	C	C6-N1-C2	-5.52	118.09	120.30
14	B	249	C	C5-C6-N1	5.52	123.76	121.00
14	B	1007	U	C5-C6-N1	5.52	125.46	122.70
14	B	1305	U	N3-C2-O2	-5.52	118.34	122.20
14	B	2020	U	N1-C2-O2	5.52	126.66	122.80
14	B	385	U	N3-C2-O2	-5.51	118.34	122.20
14	B	1961	C	C5-C6-N1	5.51	123.76	121.00
14	B	2730	C	C6-N1-C2	-5.51	118.09	120.30
14	B	735	C	C5-C6-N1	5.51	123.76	121.00
14	B	764	C	C6-N1-C2	-5.51	118.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1503	A	P-O3'-C3'	5.51	126.31	119.70
14	B	320	U	N1-C2-O2	5.51	126.65	122.80
14	B	1460	U	C2-N1-C1'	5.51	124.31	117.70
14	B	526	A	C2-N3-C4	5.50	113.35	110.60
14	B	593	U	N3-C2-O2	-5.50	118.35	122.20
14	B	882	C	C6-N1-C2	-5.50	118.10	120.30
14	B	2051	C	C6-N1-C2	-5.50	118.10	120.30
1	A	1002	G	C2-N3-C4	5.49	114.64	111.90
14	B	518	A	C5-N7-C8	-5.48	101.16	103.90
14	B	2794	C	C6-N1-C2	-5.48	118.11	120.30
14	B	1168	C	C6-N1-C2	-5.48	118.11	120.30
1	A	534	C	N1-C2-O2	5.47	122.18	118.90
1	A	1219	C	C5-C6-N1	5.47	123.73	121.00
14	B	1492	G	N3-C4-N9	-5.47	122.72	126.00
1	A	319	C	C5-C6-N1	5.46	123.73	121.00
14	B	1953	U	C2-N1-C1'	5.46	124.25	117.70
1	A	6	U	C6-N1-C1'	-5.45	113.57	121.20
14	B	777	C	N1-C2-O2	5.45	122.17	118.90
14	B	1584	U	N3-C2-O2	-5.45	118.39	122.20
14	B	1941	C	C6-N1-C1'	-5.44	114.27	120.80
14	B	2722	U	C5-C6-N1	5.44	125.42	122.70
14	B	2092	C	C5-C6-N1	5.44	123.72	121.00
1	A	1137	U	C2-N1-C1'	5.43	124.22	117.70
1	A	330	C	C5-C6-N1	5.43	123.72	121.00
14	B	1235	C	C6-N1-C2	-5.43	118.13	120.30
14	B	2070	C	C6-N1-C2	-5.43	118.13	120.30
15	C	12	U	N1-C2-O2	5.43	126.60	122.80
14	B	1898	C	N1-C2-O2	5.42	122.15	118.90
14	B	239	C	C6-N1-C2	-5.42	118.13	120.30
14	B	1676	A	N7-C8-N9	5.42	116.51	113.80
27	LC	81	ASP	CB-CG-OD1	5.42	123.18	118.30
14	B	862	C	C6-N1-C2	-5.41	118.14	120.30
14	B	698	U	N3-C2-O2	-5.40	118.42	122.20
14	B	2595	C	C6-N1-C2	-5.40	118.14	120.30
14	B	2091	C	C6-N1-C2	-5.40	118.14	120.30
1	A	15	U	N3-C2-O2	-5.40	118.42	122.20
14	B	1779	C	C6-N1-C2	-5.40	118.14	120.30
14	B	2488	C	C6-N1-C2	-5.40	118.14	120.30
14	B	2609	G	C8-N9-C1'	-5.39	119.99	127.00
1	A	1219	C	N3-C2-O2	-5.39	118.13	121.90
1	A	35	C	C6-N1-C2	-5.39	118.14	120.30
14	B	1029	C	N1-C2-O2	5.38	122.13	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1399	C	C6-N1-C2	-5.37	118.15	120.30
1	A	430	C	N3-C2-O2	-5.37	118.14	121.90
1	A	1372	C	N3-C2-O2	-5.37	118.14	121.90
14	B	1380	G	C8-N9-C1'	-5.37	120.02	127.00
14	B	2348	G	C4-N9-C1'	5.36	133.47	126.50
15	C	28	C	C6-N1-C2	-5.36	118.16	120.30
1	A	1503	A	OP1-P-O3'	5.36	116.99	105.20
14	B	575	G	C4-N9-C1'	5.36	133.46	126.50
14	B	2537	C	C5-C6-N1	5.36	123.68	121.00
1	A	908	C	P-O3'-C3'	5.34	126.11	119.70
14	B	759	U	N3-C2-O2	-5.34	118.46	122.20
14	B	1766	C	N1-C2-O2	5.34	122.10	118.90
14	B	2074	C	C6-N1-C2	-5.34	118.16	120.30
42	D	20	U	C2-N1-C1'	5.34	124.11	117.70
1	A	1474	C	N1-C2-O2	5.34	122.10	118.90
14	B	1492	G	C8-N9-C1'	5.34	133.94	127.00
14	B	1729	C	N1-C2-O2	5.33	122.10	118.90
14	B	1914	C	C6-N1-C2	-5.33	118.17	120.30
14	B	320	U	N3-C2-O2	-5.33	118.47	122.20
14	B	1441	C	C5-C6-N1	5.33	123.66	121.00
1	A	52	A	OP2-P-O3'	5.32	116.90	105.20
14	B	2021	C	C2-N1-C1'	5.32	124.65	118.80
1	A	156	C	C6-N1-C2	-5.32	118.17	120.30
14	B	2264	G	N7-C8-N9	5.31	115.76	113.10
14	B	1865	C	N3-C2-O2	-5.31	118.18	121.90
1	A	773	G	C8-N9-C4	-5.31	104.28	106.40
14	B	1499	U	N3-C2-O2	-5.31	118.49	122.20
1	A	1292	C	C6-N1-C2	-5.30	118.18	120.30
1	A	336	C	N3-C2-O2	-5.30	118.19	121.90
14	B	2894	C	C6-N1-C2	-5.30	118.18	120.30
1	A	820	G	C2-N3-C4	5.30	114.55	111.90
14	B	1801	C	N1-C2-O2	5.30	122.08	118.90
14	B	1460	U	N3-C2-O2	-5.29	118.49	122.20
14	B	1050	C	C6-N1-C2	-5.29	118.18	120.30
1	A	288	C	C6-N1-C1'	-5.28	114.46	120.80
14	B	1492	G	N3-C4-C5	5.28	131.24	128.60
14	B	870	C	C6-N1-C2	-5.28	118.19	120.30
14	B	2547	C	C5-C6-N1	5.27	123.64	121.00
14	B	1729	C	C5-C6-N1	5.27	123.63	121.00
15	C	88	U	C2-N1-C1'	5.26	124.02	117.70
1	A	279	C	P-O3'-C3'	5.26	126.02	119.70
4	S3	94	LEU	CA-CB-CG	5.26	127.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2287	C	C6-N1-C1'	5.26	127.11	120.80
14	B	1542	C	C6-N1-C2	-5.26	118.20	120.30
14	B	710	C	C6-N1-C2	-5.25	118.20	120.30
14	B	575	G	N3-C4-N9	5.25	129.15	126.00
14	B	1953	U	N3-C2-O2	-5.25	118.53	122.20
36	LM	143	LEU	CA-CB-CG	5.25	127.37	115.30
14	B	2799	C	C6-N1-C2	-5.24	118.20	120.30
14	B	1515	G	C6-C5-N7	-5.24	127.26	130.40
15	C	114	C	N1-C2-O2	5.24	122.04	118.90
14	B	1773	A	C8-N9-C4	-5.23	103.71	105.80
14	B	2890	C	C6-N1-C2	-5.23	118.21	120.30
14	B	721	A	O4'-C1'-N9	5.23	112.38	108.20
14	B	103	U	C2-N1-C1'	5.22	123.97	117.70
14	B	710	C	N3-C2-O2	-5.22	118.24	121.90
14	B	1942	U	C2-N1-C1'	5.22	123.97	117.70
14	B	2737	C	C5-C6-N1	5.22	123.61	121.00
1	A	1394	C	C6-N1-C2	-5.21	118.21	120.30
14	B	1328	C	C6-N1-C2	-5.21	118.22	120.30
14	B	313	U	C2-N1-C1'	5.20	123.94	117.70
14	B	2623	U	N1-C2-O2	5.20	126.44	122.80
14	B	2071	C	C6-N1-C2	-5.20	118.22	120.30
1	A	762	C	C2-N1-C1'	5.19	124.51	118.80
14	B	152	C	C6-N1-C2	-5.19	118.22	120.30
14	B	2900	C	N1-C2-O2	5.19	122.01	118.90
14	B	2583	C	C5-C6-N1	5.18	123.59	121.00
14	B	660	A	O4'-C1'-N9	-5.18	104.06	108.20
14	B	1515	G	N3-C4-N9	5.18	129.11	126.00
1	A	481	C	N1-C2-O2	5.18	122.01	118.90
1	A	1327	C	N1-C2-O2	5.17	122.00	118.90
14	B	1545	U	N3-C2-O2	-5.17	118.58	122.20
14	B	1510	U	P-O3'-C3'	5.17	125.90	119.70
1	A	1461	U	N1-C2-O2	5.16	126.41	122.80
14	B	515	G	N7-C8-N9	5.16	115.68	113.10
14	B	1845	U	N1-C2-O2	5.16	126.41	122.80
14	B	2006	C	C6-N1-C2	-5.16	118.24	120.30
14	B	2020	U	C2-N1-C1'	5.16	123.89	117.70
14	B	731	U	C2-N1-C1'	5.15	123.88	117.70
1	A	1324	C	N1-C2-O2	5.14	121.99	118.90
1	A	330	C	C6-N1-C2	-5.14	118.24	120.30
14	B	2288	C	C6-N1-C2	-5.14	118.24	120.30
14	B	1715	U	C5-C6-N1	5.14	125.27	122.70
14	B	1998	A	C2-N3-C4	5.14	113.17	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1004	C	C6-N1-C2	-5.13	118.25	120.30
1	A	272	C	N3-C2-O2	-5.13	118.31	121.90
14	B	518	A	N7-C8-N9	5.13	116.36	113.80
14	B	2051	C	C5-C6-N1	5.12	123.56	121.00
1	A	1218	C	N1-C2-O2	5.12	121.97	118.90
14	B	1676	A	C5-N7-C8	-5.12	101.34	103.90
14	B	144	C	C6-N1-C2	-5.11	118.25	120.30
14	B	163	U	N3-C2-O2	-5.11	118.62	122.20
14	B	1277	C	C5-C6-N1	5.11	123.56	121.00
14	B	421	C	C6-N1-C2	-5.11	118.26	120.30
14	B	90	A	C4-N9-C1'	5.11	135.49	126.30
14	B	1216	U	N3-C2-O2	-5.10	118.63	122.20
14	B	1296	C	C6-N1-C2	-5.10	118.26	120.30
15	C	88	U	N1-C2-O2	5.10	126.37	122.80
14	B	1503	U	OP2-P-O3'	5.10	116.42	105.20
1	A	403	C	C6-N1-C2	-5.10	118.26	120.30
14	B	2723	U	C6-N1-C2	-5.09	117.94	121.00
1	A	46	U	C5-C6-N1	5.09	125.25	122.70
14	B	508	C	C5-C6-N1	5.09	123.55	121.00
14	B	2074	C	C5-C6-N1	5.09	123.55	121.00
1	A	1507	C	C6-N1-C2	-5.09	118.27	120.30
14	B	1704	C	C6-N1-C2	-5.08	118.27	120.30
14	B	385	U	N1-C2-O2	5.08	126.36	122.80
14	B	1785	G	C4-N9-C1'	5.08	133.11	126.50
1	A	1087	C	C5-C6-N1	5.08	123.54	121.00
14	B	2642	U	N1-C2-O2	5.08	126.36	122.80
16	L1	18	ASP	C-N-CA	5.08	134.40	121.70
14	B	2561	C	N1-C2-O2	5.08	121.94	118.90
1	A	1158	U	N3-C2-O2	-5.07	118.65	122.20
14	B	695	C	C6-N1-C2	-5.07	118.27	120.30
14	B	2583	C	N1-C2-O2	5.07	121.94	118.90
1	A	773	G	C4-N9-C1'	5.06	133.08	126.50
1	A	1254	C	C6-N1-C2	-5.06	118.28	120.30
14	B	1215	U	C5-C6-N1	5.06	125.23	122.70
1	A	849	U	N3-C2-O2	-5.06	118.66	122.20
14	B	1628	A	O5'-P-OP2	-5.05	101.15	105.70
14	B	2673	C	N1-C2-O2	5.05	121.93	118.90
1	A	816	C	C6-N1-C2	-5.05	118.28	120.30
14	B	2063	C	C5-C6-N1	5.04	123.52	121.00
14	B	1574	G	C6-C5-N7	-5.04	127.38	130.40
14	B	2347	A	C4-N9-C1'	5.04	135.37	126.30
42	D	36	A	C2-N3-C4	5.04	113.12	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1372	C	N1-C2-O2	5.04	121.92	118.90
14	B	421	C	C5-C6-N1	5.04	123.52	121.00
14	B	795	A	C4-N9-C1'	5.04	135.37	126.30
14	B	90	A	C2-N3-C4	5.03	113.12	110.60
14	B	1093	C	C6-N1-C2	-5.03	118.29	120.30
14	B	630	G	N3-C4-N9	5.03	129.02	126.00
14	B	518	A	N1-C6-N6	5.03	121.62	118.60
14	B	601	G	O5'-P-OP1	-5.03	101.17	105.70
1	A	1137	U	N3-C2-O2	-5.03	118.68	122.20
1	A	1394	C	C5-C6-N1	5.03	123.51	121.00
1	A	1010	U	C2-N1-C1'	5.03	123.73	117.70
14	B	2529	G	P-O3'-C3'	5.03	125.73	119.70
1	A	116	G	C4-N9-C1'	5.03	133.03	126.50
14	B	402	C	O4'-C1'-N1	5.03	112.22	108.20
14	B	2233	C	C6-N1-C2	-5.02	118.29	120.30
14	B	2566	C	C6-N1-C2	-5.02	118.29	120.30
14	B	403	U	C6-N1-C1'	-5.02	114.17	121.20
14	B	1289	A	C2-N3-C4	-5.02	108.09	110.60
14	B	723	C	C6-N1-C2	-5.01	118.30	120.30
14	B	2020	U	C6-N1-C2	-5.01	118.00	121.00
1	A	1542	A	N7-C8-N9	5.01	116.30	113.80
14	B	2673	C	C6-N1-C2	-5.01	118.30	120.30
14	B	603	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	L3	95	LEU	Peptide
19	L4	23	GLU	Peptide
24	L9	21	GLY	Peptide
36	LM	112	SER	Peptide
37	LN	105	GLU	Peptide
41	LR	21	ASN	Peptide
41	LR	68	THR	Peptide
4	S3	28	PHE	Peptide
9	SA	60	ALA	Peptide
11	SD	108	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30390	0	15318	185	0
2	S1	647	0	657	4	0
3	S2	850	0	860	8	0
4	S3	1011	0	1001	17	0
5	S6	725	0	756	9	0
6	S7	594	0	618	12	0
7	S8	674	0	716	6	0
8	S9	456	0	490	5	0
9	SA	475	0	406	8	0
10	SC	1604	0	1633	24	0
11	SD	1132	0	1188	13	0
12	SE	763	0	766	10	0
13	SF	1012	0	1061	10	0
14	B	59339	0	29847	185	0
15	C	2424	0	1230	11	0
16	L1	914	0	987	13	0
17	L2	2086	0	2194	20	0
18	L3	942	0	1014	9	0
19	L4	784	0	825	7	0
20	L5	852	0	914	7	0
21	L6	684	0	696	3	0
22	L7	758	0	801	7	0
23	L8	726	0	777	5	0
24	L9	590	0	603	11	0
25	LA	462	0	501	4	0
26	LB	502	0	536	5	0
27	LC	1617	0	1651	13	0
28	LD	440	0	478	2	0
29	LE	421	0	430	9	0
30	LF	386	0	394	2	0
31	LG	371	0	420	3	0
32	LH	520	0	586	8	0
33	LI	295	0	340	1	0
34	LJ	1538	0	1561	10	0
35	LL	1357	0	1388	16	0
36	LM	1137	0	1130	8	0
37	LN	910	0	970	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	LO	1081	0	1119	6	0
39	LP	1088	0	1155	4	0
40	LQ	954	0	1002	12	0
41	LR	896	0	935	9	0
42	D	1577	0	800	15	0
43	A	4	0	0	0	0
43	B	13	0	0	0	0
All	All	126001	0	80754	625	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 4.

All (625) 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)
14:B:2533:U:H5''	14:B:2533:U:C6	2.26	0.71
35:LL:5:GLY:HA2	35:LL:69:ARG:HD3	1.71	0.70
12:SE:10:VAL:HB	12:SE:59:PHE:HB2	1.73	0.70
14:B:262:G:H21	14:B:666:A:H8	1.40	0.69
14:B:2037:G:H5''	20:L5:42:ALA:HB2	1.72	0.68
26:LB:17:GLN:HE22	26:LB:50:ILE:HG23	1.58	0.68
1:A:1368:U:H3	1:A:1373:A:H61	1.40	0.68
14:B:1521:A:H61	14:B:1559:G:H1	1.42	0.68
14:B:540:G:H21	20:L5:61:ASN:HD22	1.40	0.67
1:A:1004:C:H42	1:A:1220:C:H42	1.41	0.67
1:A:1314:G:H21	1:A:1343:A:H62	1.42	0.67
2:S1:42:LEU:HD13	2:S1:73:LEU:H	1.60	0.67
1:A:696:G:H1	1:A:707:C:H42	1.43	0.67
1:A:612:G:H1	1:A:642:C:H42	1.41	0.66
14:B:606:G:H21	18:L3:37:GLN:HE22	1.41	0.66
1:A:519:C:H5'	10:SC:41:ARG:HD2	1.77	0.65
1:A:537:G:H22	4:S3:61:ALA:HB2	1.63	0.64
1:A:979:C:H2'	1:A:1241:G:H1'	1.79	0.64
1:A:263:G:O6	1:A:278:A:N6	2.31	0.64
14:B:2649:U:O2'	14:B:2845:G:N2	2.31	0.63
14:B:132:C:H42	14:B:147:G:H1	1.46	0.63
1:A:1075:G:N2	1:A:1201:A:OP2	2.31	0.63
1:A:10:G:H5'	11:SD:108:GLY:HA2	1.79	0.63
14:B:826:A:OP1	17:L2:217:ARG:NH2	2.32	0.63
10:SC:120:LEU:HD22	10:SC:125:ARG:HA	1.81	0.63
10:SC:9:TRP:NE1	10:SC:25:GLU:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L1:50:ILE:HD11	16:L1:64:ARG:HD2	1.79	0.63
39:LP:44:SER:HB2	39:LP:70:PRO:HG3	1.81	0.63
10:SC:188:GLU:HG2	10:SC:189:ILE:HG13	1.81	0.62
27:LC:186:GLN:HB2	27:LC:195:LEU:HD12	1.82	0.62
14:B:1448:U:H3	14:B:1635:A:H61	1.46	0.62
41:LR:25:THR:HA	41:LR:46:ASP:HB2	1.81	0.62
1:A:1362:C:H42	1:A:1380:G:H22	1.48	0.62
10:SC:100:SER:HB3	10:SC:162:PRO:HG3	1.82	0.62
14:B:1825:U:OP2	17:L2:274:ARG:NH2	2.33	0.62
22:L7:10:LYS:HB2	22:L7:71:LEU:HD23	1.81	0.62
41:LR:29:PRO:HG2	41:LR:89:ILE:HD11	1.81	0.62
6:S7:5:ILE:HD12	6:S7:67:PRO:HG3	1.81	0.61
27:LC:185:VAL:HG12	27:LC:186:GLN:HG3	1.81	0.61
6:S7:21:VAL:HG11	6:S7:33:ILE:HD12	1.83	0.61
1:A:1442:G:O2'	1:A:1478:G:N1	2.34	0.61
14:B:246:U:OP2	32:LH:8:ARG:NH1	2.34	0.61
14:B:349:U:H3	14:B:353:A:H62	1.47	0.61
29:LE:32:ASN:ND2	29:LE:50:ASN:OD1	2.33	0.61
1:A:1407:C:N4	1:A:1412:C:OP1	2.34	0.60
35:LL:28:GLY:H	35:LL:32:GLU:HG2	1.65	0.60
1:A:399:G:OP1	6:S7:9:ARG:NH1	2.34	0.60
41:LR:19:ARG:NH2	41:LR:47:ASP:OD2	2.35	0.60
14:B:1342:C:H42	14:B:1667:G:H1	1.49	0.60
41:LR:29:PRO:HD2	41:LR:92:ILE:HD12	1.82	0.60
7:S8:24:THR:HG22	7:S8:47:LYS:HG2	1.84	0.60
14:B:1651:C:N4	14:B:1666:A:OP2	2.35	0.60
35:LL:38:ASN:HD21	35:LL:72:LEU:HD11	1.66	0.60
14:B:2380:G:N2	24:L9:42:GLY:O	2.35	0.60
1:A:1460:U:H3	1:A:1464:A:H61	1.50	0.60
14:B:2533:U:C6	14:B:2533:U:C5'	2.85	0.60
14:B:2531:U:H2'	14:B:2532:G:H5''	1.84	0.60
1:A:62:G:O2'	1:A:386:G:N2	2.36	0.59
1:A:12:G:N2	1:A:25:U:O2	2.34	0.59
1:A:743:C:H5''	8:S9:62:THR:HG23	1.85	0.59
5:S6:18:HIS:ND1	5:S6:21:ASP:OD2	2.36	0.59
1:A:1247:C:O2'	1:A:1344:G:N2	2.36	0.59
1:A:54:A:N6	1:A:55:C:O2	2.36	0.59
1:A:412:G:N7	10:SC:2:ALA:N	2.51	0.59
14:B:1340:G:HO2'	14:B:1686:G:HO2'	1.44	0.58
25:LA:5:CYS:HB3	25:LA:9:GLY:H	1.68	0.58
1:A:120:C:H41	1:A:242:C:H3'	1.65	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:2233:C:H42	14:B:2245:G:H1	1.50	0.58
35:LL:126:GLU:HB2	35:LL:130:VAL:HB	1.85	0.58
11:SD:76:ARG:NH1	11:SD:119:GLY:O	2.36	0.58
1:A:305:G:N2	1:A:308:A:OP2	2.32	0.58
6:S7:34:ILE:HG22	6:S7:35:GLU:HG2	1.86	0.58
10:SC:50:GLN:HG2	10:SC:196:GLU:HB2	1.84	0.58
10:SC:85:ASN:HD22	10:SC:88:ILE:HD12	1.67	0.58
10:SC:14:ARG:NH2	10:SC:33:PRO:O	2.37	0.58
1:A:951:G:N2	1:A:1352:C:O2	2.34	0.58
42:D:27:G:N2	42:D:44:G:O2'	2.37	0.57
24:L9:75:VAL:HG12	24:L9:89:VAL:HG22	1.86	0.57
14:B:2533:U:H2'	14:B:2533:U:O2	2.03	0.57
14:B:1518:G:H1	14:B:1562:C:H42	1.52	0.57
39:LP:35:GLN:HB3	39:LP:102:ILE:HD13	1.86	0.57
14:B:1631:G:H21	14:B:1632:A:H1'	1.70	0.57
16:L1:73:GLU:HB2	37:LN:78:LYS:HB2	1.87	0.57
11:SD:82:PRO:HD2	11:SD:147:LEU:HD13	1.86	0.57
14:B:721:A:H8	14:B:2096:G:H21	1.52	0.57
14:B:2317:G:N1	14:B:2370:U:O2	2.33	0.57
1:A:419:A:N7	1:A:421:G:N2	2.53	0.57
1:A:469:U:O4	1:A:479:U:N3	2.37	0.56
18:L3:90:ILE:O	18:L3:92:ARG:NH1	2.37	0.56
12:SE:50:TYR:OH	12:SE:88:ARG:NH1	2.37	0.56
13:SF:18:ASN:ND2	13:SF:74:ILE:O	2.37	0.56
14:B:1501:G:N2	14:B:2730:C:O2	2.38	0.56
22:L7:10:LYS:HD3	22:L7:78:PRO:HG3	1.87	0.56
1:A:1222:U:O2	1:A:1223:A:N6	2.38	0.56
1:A:34:A:H61	1:A:559:U:H3	1.53	0.56
5:S6:88:ARG:NH2	14:B:759:U:O2	2.38	0.56
1:A:1315:G:H2'	1:A:1316:A:H8	1.70	0.56
14:B:1492:G:HO2'	14:B:1575:A:HO2'	1.47	0.56
1:A:950:G:N2	1:A:1360:A:OP1	2.39	0.56
14:B:1839:G:H21	17:L2:44:ASN:HD22	1.53	0.56
13:SF:117:GLU:O	13:SF:121:ARG:NH1	2.38	0.56
14:B:321:U:O2	14:B:327:G:N2	2.39	0.56
14:B:2298:G:OP1	24:L9:26:SER:OG	2.24	0.56
1:A:834:C:H4'	13:SF:13:ARG:HD3	1.87	0.56
12:SE:21:ALA:O	12:SE:25:ARG:NH1	2.39	0.56
1:A:1000:U:O2	1:A:1223:A:N6	2.38	0.56
14:B:2359:C:OP1	24:L9:84:LYS:NZ	2.38	0.56
15:C:31:G:N2	15:C:47:C:O2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L1:51:LYS:NZ	16:L1:100:TYR:OH	2.38	0.56
1:A:418:G:H21	1:A:440:A:H62	1.51	0.56
14:B:2532:G:H1'	14:B:2533:U:H5	1.71	0.56
36:LM:26:LEU:HD13	36:LM:63:ILE:HD12	1.88	0.56
1:A:435:C:H5'	10:SC:34:GLY:H	1.70	0.56
14:B:675:G:N2	14:B:678:A:OP2	2.38	0.56
1:A:1287:C:O2'	1:A:1289:A:N7	2.39	0.55
14:B:1335:C:H42	14:B:1686:G:H1	1.54	0.55
1:A:470:A:N6	1:A:477:U:O4	2.40	0.55
1:A:799:G:O6	1:A:800:A:N6	2.40	0.55
1:A:959:U:H2'	1:A:960:G:H8	1.70	0.55
17:L2:146:LEU:HD11	17:L2:182:ARG:HH21	1.70	0.55
35:LL:122:THR:HB	35:LL:134:GLU:HB3	1.88	0.55
39:LP:43:THR:HG22	39:LP:94:ILE:HG22	1.87	0.55
14:B:2445:A:OP1	32:LH:45:ARG:NH2	2.39	0.55
40:LQ:8:ARG:HB3	40:LQ:12:GLN:HB2	1.87	0.55
1:A:748:U:OP1	5:S6:2:ALA:N	2.39	0.55
1:A:578:G:O6	1:A:874:A:N6	2.39	0.55
14:B:2007:G:O2'	14:B:2009:U:OP2	2.23	0.55
11:SD:95:PHE:HB3	11:SD:125:SER:HB2	1.89	0.55
1:A:1454:G:O6	1:A:1469:C:N4	2.38	0.55
14:B:738:U:O2'	14:B:1390:A:N3	2.35	0.55
8:S9:38:ILE:HG22	8:S9:42:GLY:HA2	1.87	0.55
1:A:339:G:OP2	1:A:339:G:N2	2.40	0.55
1:A:381:A:H2'	1:A:382:A:H8	1.71	0.55
14:B:28:A:N3	18:L3:11:ARG:NH2	2.55	0.55
14:B:1288:G:OP2	38:LO:21:ARG:NH1	2.40	0.55
14:B:640:G:H1	14:B:705:U:H3	1.54	0.54
27:LC:48:ALA:HB2	27:LC:92:ARG:HG2	1.89	0.54
1:A:319:C:OP1	6:S7:32:ARG:NH1	2.39	0.54
11:SD:106:ILE:HD11	11:SD:124:LEU:H	1.72	0.54
14:B:1487:G:N2	14:B:1598:U:O2	2.39	0.54
37:LN:19:VAL:HG12	37:LN:43:VAL:HA	1.89	0.54
1:A:1366:G:N2	1:A:1376:C:O2	2.41	0.54
14:B:2602:C:H5'	27:LC:156:ALA:HB2	1.89	0.54
14:B:2869:G:N2	14:B:2886:G:O2'	2.40	0.54
42:D:53:G:O6	42:D:61:C:N4	2.40	0.54
35:LL:70:ALA:O	35:LL:74:ASN:ND2	2.41	0.54
1:A:605:G:N2	13:SF:88:TYR:OH	2.41	0.54
14:B:1967:U:OP2	14:B:2630:G:N2	2.40	0.54
14:B:2046:U:OP2	29:LE:6:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:LR:72:LEU:O	41:LR:76:VAL:N	2.39	0.54
11:SD:24:VAL:HG12	11:SD:25:VAL:HG23	1.88	0.54
12:SE:37:VAL:HG12	12:SE:65:VAL:HG23	1.90	0.54
17:L2:174:ILE:HG13	17:L2:184:ILE:HD12	1.89	0.54
14:B:545:G:N1	14:B:548:A:OP2	2.39	0.54
1:A:1352:C:H2'	1:A:1353:G:H8	1.72	0.54
1:A:141:A:H61	1:A:230:U:H3	1.56	0.54
14:B:1488:A:H61	14:B:1595:C:H42	1.55	0.54
13:SF:33:LYS:HG2	13:SF:36:ILE:HD12	1.90	0.54
18:L3:18:ILE:HD11	18:L3:32:TYR:HA	1.89	0.54
32:LH:58:VAL:HG13	32:LH:61:LEU:HD12	1.90	0.53
1:A:944:A:O2'	1:A:1394:C:N3	2.40	0.53
14:B:2773:U:H5''	35:LL:138:LYS:HE3	1.90	0.53
40:LQ:33:THR:HG23	40:LQ:114:ALA:HB1	1.89	0.53
40:LQ:37:ALA:HA	40:LQ:40:VAL:HG12	1.90	0.53
1:A:1392:C:N4	1:A:1395:G:O6	2.41	0.53
1:A:401:A:H2'	1:A:402:G:H8	1.73	0.53
1:A:559:U:O2'	4:S3:96:ARG:NH1	2.41	0.53
35:LL:59:LYS:HD3	35:LL:62:ARG:HH11	1.74	0.53
1:A:50:U:O2	1:A:370:G:O2'	2.26	0.53
38:LO:83:ASN:ND2	38:LO:117:LEU:O	2.42	0.53
17:L2:132:LEU:HD23	17:L2:135:ILE:HD12	1.90	0.53
34:LJ:182:ASN:ND2	34:LJ:185:ASP:OD2	2.41	0.53
14:B:433:U:H4'	14:B:434:G:H5'	1.89	0.53
15:C:11:A:OP1	24:L9:82:ARG:NH1	2.41	0.53
14:B:540:G:O2'	14:B:541:G:O5'	2.26	0.53
42:D:4:C:H42	42:D:69:G:H1	1.55	0.53
14:B:2650:G:O5'	14:B:2845:G:N2	2.42	0.53
35:LL:115:ILE:HD13	35:LL:148:ILE:HG12	1.91	0.53
1:A:1422:C:O2	1:A:1500:G:N2	2.42	0.52
14:B:1806:U:OP2	14:B:1811:A:N6	2.42	0.52
14:B:2386:C:O2'	32:LH:54:ASP:OD2	2.28	0.52
1:A:1316:A:N6	1:A:1341:G:O2'	2.42	0.52
1:A:947:A:HO2'	1:A:1386:U:HO2'	1.57	0.52
15:C:73:G:O2'	23:L8:88:HIS:NE2	2.36	0.52
26:LB:48:LYS:O	26:LB:52:ARG:NH2	2.42	0.52
12:SE:2:ARG:N	12:SE:67:SER:O	2.43	0.52
1:A:1109:C:O2'	1:A:1177:A:N6	2.39	0.52
18:L3:50:ARG:O	18:L3:54:LYS:NZ	2.39	0.52
1:A:1092:G:OP2	11:SD:52:LYS:NZ	2.42	0.52
1:A:1452:G:H21	1:A:1472:G:H22	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:81:A:H61	15:C:90:C:H42	1.58	0.52
41:LR:73:ALA:HA	41:LR:76:VAL:HG12	1.91	0.52
14:B:2082:C:H2'	14:B:2531:U:H5''	1.91	0.52
14:B:2033:C:O2'	14:B:2843:A:N3	2.43	0.52
14:B:2854:A:H2'	14:B:2899:A:H61	1.75	0.52
14:B:1302:G:OP1	29:LE:16:ARG:NH1	2.41	0.52
14:B:1823:U:OP2	17:L2:276:LYS:NZ	2.42	0.52
14:B:2127:G:H1	14:B:2216:U:H3	1.58	0.52
27:LC:145:HIS:O	27:LC:147:HIS:ND1	2.43	0.52
27:LC:111:VAL:HG12	27:LC:187:VAL:HG21	1.90	0.52
31:LG:25:THR:HG23	31:LG:28:GLY:H	1.74	0.52
13:SF:19:MET:O	13:SF:72:ARG:NH1	2.42	0.52
1:A:447:U:OP2	1:A:449:A:N6	2.43	0.52
15:C:18:G:N2	15:C:62:U:O2	2.41	0.52
27:LC:28:VAL:HG11	27:LC:210:ILE:HD11	1.92	0.52
1:A:1271:A:H62	1:A:1284:A:H2	1.57	0.52
1:A:421:G:N2	1:A:437:U:OP2	2.42	0.52
17:L2:227:PRO:HB3	17:L2:233:GLY:HA3	1.91	0.52
41:LR:21:ASN:HB3	41:LR:22:LEU:HD12	1.90	0.52
3:S2:23:ILE:HG12	3:S2:32:VAL:HG22	1.91	0.52
13:SF:21:ARG:HE	13:SF:72:ARG:HE	1.56	0.52
14:B:1599:G:OP1	14:B:1761:G:N2	2.38	0.52
17:L2:157:SER:OG	17:L2:158:ALA:N	2.43	0.52
22:L7:85:PHE:HB3	22:L7:90:LYS:HA	1.92	0.52
14:B:2389:G:OP1	32:LH:40:GLN:NE2	2.42	0.52
1:A:347:C:H42	1:A:358:G:H1	1.56	0.51
14:B:1179:C:N4	14:B:1182:G:OP2	2.43	0.51
14:B:1576:A:H61	14:B:1590:C:H42	1.58	0.51
14:B:862:C:O2'	14:B:884:U:OP1	2.25	0.51
1:A:571:A:HO2'	1:A:574:G:HO2'	1.55	0.51
1:A:1009:U:OP2	1:A:1016:A:N6	2.43	0.51
12:SE:38:LEU:HD12	12:SE:64:ARG:HG2	1.92	0.51
34:LJ:7:LEU:HG	34:LJ:14:SER:HB3	1.92	0.51
1:A:428:U:O2	1:A:432:G:N1	2.44	0.51
1:A:609:G:H2'	1:A:610:A:H8	1.75	0.51
16:L1:59:GLU:OE2	16:L1:79:HIS:NE2	2.44	0.51
14:B:2773:U:H4'	35:LL:138:LYS:HG3	1.92	0.51
4:S3:107:ARG:HD3	4:S3:108:TYR:HB3	1.91	0.51
1:A:1504:A:OP1	14:B:1940:A:N6	2.39	0.51
14:B:1318:G:N2	14:B:1327:C:O2	2.44	0.51
14:B:1398:G:HO2'	14:B:2242:G:HO2'	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LE:9:SER:OG	29:LE:10:LYS:N	2.44	0.51
14:B:629:A:H62	14:B:1289:A:H2	1.57	0.51
24:L9:55:PRO:HG3	24:L9:61:ARG:HB2	1.93	0.51
10:SC:182:ARG:NH2	10:SC:189:ILE:O	2.43	0.51
14:B:1083:G:H1	14:B:1160:C:H42	1.59	0.51
14:B:2026:C:O2	14:B:2714:U:O2'	2.29	0.51
33:LI:23:VAL:HB	33:LI:37:GLY:HA3	1.92	0.51
1:A:682:G:H5'	12:SE:88:ARG:HH22	1.76	0.51
1:A:430:C:O3'	1:A:431:G:N2	2.41	0.51
17:L2:123:ASP:O	17:L2:128:ASN:ND2	2.43	0.51
27:LC:55:ASP:HA	27:LC:85:LYS:HA	1.91	0.51
1:A:1505:G:H21	14:B:1939:A:H1'	1.74	0.51
1:A:494:U:H2'	1:A:495:A:H8	1.75	0.51
14:B:1450:A:N7	14:B:1634:A:N6	2.59	0.50
1:A:248:U:H2'	1:A:249:G:H8	1.77	0.50
14:B:2092:C:O2	14:B:2476:U:N3	2.43	0.50
16:L1:102:LEU:HD11	16:L1:112:ILE:HD11	1.93	0.50
1:A:1134:A:H2	1:A:1160:U:H3	1.59	0.50
17:L2:95:VAL:HG22	17:L2:101:LYS:HG2	1.92	0.50
23:L8:9:ARG:NH1	23:L8:41:VAL:O	2.44	0.50
13:SF:34:LYS:HD3	13:SF:52:VAL:HG22	1.94	0.50
40:LQ:109:ARG:HD2	40:LQ:112:ASP:HB3	1.93	0.50
1:A:481:C:H5'	6:S7:76:SER:HB3	1.93	0.50
1:A:897:G:N2	1:A:917:A:N7	2.60	0.50
14:B:1360:G:OP1	20:L5:84:ARG:NH2	2.36	0.50
42:D:26:A:N1	42:D:44:G:N2	2.58	0.50
14:B:459:C:HO2'	14:B:1907:U:HO2'	1.58	0.50
1:A:421:G:H22	10:SC:27:GLU:HB3	1.75	0.50
1:A:1171:C:H42	1:A:1185:G:H22	1.59	0.50
1:A:19:C:H4'	1:A:1089:U:H3	1.75	0.50
14:B:15:G:H4'	29:LE:18:THR:HG22	1.94	0.50
14:B:864:A:OP2	14:B:1226:G:N2	2.45	0.50
14:B:2381:A:O3'	24:L9:33:ARG:NH2	2.40	0.50
14:B:2106:U:O2'	25:LA:23:ASN:OD1	2.28	0.50
29:LE:54:VAL:HG11	40:LQ:104:LEU:HD13	1.94	0.50
32:LH:9:GLY:O	32:LH:13:ARG:NH2	2.42	0.50
14:B:2766:U:O2	14:B:2793:G:N2	2.44	0.50
21:L6:7:LEU:HD23	21:L6:29:VAL:HG12	1.94	0.50
29:LE:48:SER:HB3	29:LE:53:GLU:HA	1.94	0.50
1:A:67:G:N2	1:A:172:A:O2'	2.45	0.49
1:A:874:A:N3	1:A:927:A:O2'	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LQ:89:ILE:HD13	40:LQ:92:ARG:HH12	1.76	0.49
41:LR:78:GLU:HA	41:LR:81:ALA:HB3	1.94	0.49
14:B:1431:U:H4'	14:B:1647:A:H4'	1.93	0.49
1:A:113:U:H3	1:A:321:A:H61	1.60	0.49
27:LC:115:VAL:HB	27:LC:213:SER:HB2	1.94	0.49
35:LL:13:SER:OG	35:LL:48:ASN:ND2	2.45	0.49
4:S3:25:ASN:ND2	4:S3:40:SER:OG	2.46	0.49
26:LB:36:GLN:HG2	26:LB:38:GLU:H	1.77	0.49
8:S9:42:GLY:O	8:S9:68:ARG:NH2	2.45	0.49
1:A:1258:A:N7	1:A:1300:G:N2	2.60	0.49
14:B:2532:G:H1'	14:B:2533:U:C5	2.47	0.49
38:LO:79:LEU:HG	38:LO:113:GLY:HA2	1.94	0.49
6:S7:52:VAL:HG21	6:S7:75:LEU:HD21	1.95	0.49
14:B:1932:C:HO2'	14:B:1956:G:HO2'	1.52	0.49
14:B:2312:C:OP2	30:LF:2:ARG:NH2	2.37	0.49
14:B:2707:C:H1'	27:LC:199:ASN:HD22	1.77	0.49
15:C:37:A:O2'	15:C:44:A:N1	2.44	0.49
42:D:52:G:H2'	42:D:53:G:H8	1.78	0.49
17:L2:18:SER:OG	17:L2:19:LEU:N	2.41	0.49
29:LE:49:TYR:H	29:LE:54:VAL:H	1.61	0.49
40:LQ:74:GLU:HB3	40:LQ:77:THR:HB	1.94	0.49
1:A:175:C:OP1	9:SA:20:ARG:NH2	2.39	0.49
1:A:43:G:N2	1:A:409:C:O2	2.46	0.49
14:B:86:C:HO2'	14:B:103:U:HO2'	1.54	0.49
22:L7:5:LYS:HA	22:L7:23:VAL:HB	1.94	0.49
4:S3:120:VAL:O	4:S3:132:THR:OG1	2.29	0.49
9:SA:29:ARG:O	9:SA:33:LYS:N	2.39	0.49
1:A:427:C:N4	1:A:432:G:O6	2.46	0.49
1:A:823:A:N7	1:A:1520:C:O2'	2.44	0.49
14:B:1878:U:O2'	42:D:71:G:N3	2.45	0.49
14:B:902:A:H61	14:B:965:G:H1	1.61	0.49
42:D:18:G:O2'	42:D:59:U:OP1	2.30	0.49
1:A:1075:G:O2'	1:A:1200:G:N2	2.46	0.48
1:A:416:G:N2	1:A:443:U:O2'	2.45	0.48
1:A:1262:A:H61	1:A:1295:A:H61	1.59	0.48
10:SC:151:ILE:HG21	10:SC:172:LEU:HD11	1.94	0.48
1:A:35:C:H1'	4:S3:42:GLN:HE22	1.77	0.48
14:B:2751:U:OP2	27:LC:125:LYS:NZ	2.43	0.48
14:B:731:U:O5'	31:LG:12:LYS:NZ	2.44	0.48
17:L2:107:PRO:HA	17:L2:195:VAL:HA	1.95	0.48
21:L6:11:VAL:HG22	21:L6:13:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:A:C6	1:A:437:U:H5''	2.48	0.48
14:B:1711:G:O2'	14:B:2018:U:O4	2.32	0.48
14:B:2740:A:O2'	14:B:2742:C:OP2	2.29	0.48
5:S6:64:ARG:O	5:S6:68:ASN:ND2	2.46	0.48
14:B:1569:G:H3'	14:B:1570:G:H8	1.79	0.48
14:B:1478:A:H61	14:B:1605:A:H61	1.61	0.48
14:B:1894:G:H1	14:B:1901:C:H42	1.61	0.48
42:D:21:A:H5'	42:D:48:C:H41	1.79	0.48
1:A:753:U:H4'	1:A:844:G:H21	1.78	0.48
35:LL:7:LYS:O	35:LL:69:ARG:NH2	2.41	0.48
15:C:16:A:H61	15:C:105:G:H21	1.60	0.48
9:SA:57:VAL:HA	9:SA:60:ALA:HB3	1.96	0.48
5:S6:88:ARG:NH2	14:B:760:A:N7	2.62	0.48
18:L3:64:ARG:HH22	36:LM:46:THR:HG22	1.78	0.48
1:A:274:G:O6	1:A:278:A:N6	2.47	0.48
14:B:616:G:N1	14:B:2058:A:OP1	2.46	0.48
14:B:633:A:OP1	34:LJ:95:ARG:NH2	2.47	0.48
9:SA:55:LYS:O	9:SA:59:LYS:N	2.47	0.48
1:A:412:G:OP1	10:SC:115:ASN:ND2	2.46	0.48
22:L7:71:LEU:HA	22:L7:78:PRO:HA	1.96	0.47
4:S3:84:GLY:H	4:S3:120:VAL:HG13	1.79	0.47
7:S8:82:GLU:HG2	7:S8:84:SER:H	1.78	0.47
14:B:2103:U:OP2	14:B:2265:G:N2	2.47	0.47
14:B:1245:G:N2	14:B:1278:G:N7	2.62	0.47
14:B:2881:C:H2'	14:B:2882:A:H8	1.78	0.47
14:B:909:G:N2	14:B:958:U:O2	2.48	0.47
14:B:2231:C:OP1	17:L2:147:LYS:NZ	2.46	0.47
40:LQ:31:GLU:HG2	40:LQ:118:ILE:HG12	1.96	0.47
1:A:381:A:H62	1:A:399:G:H21	1.63	0.47
14:B:284:C:H3'	14:B:285:U:H4'	1.97	0.47
1:A:1237:A:O2'	1:A:1238:C:O4'	2.33	0.47
1:A:453:G:N2	1:A:498:U:O2	2.41	0.47
40:LQ:25:ILE:HD11	40:LQ:81:ALA:HB1	1.97	0.47
1:A:907:G:N2	1:A:910:A:OP2	2.36	0.47
14:B:687:G:H22	14:B:690:U:H5''	1.79	0.47
1:A:45:G:O6	1:A:404:A:N6	2.48	0.47
14:B:1308:C:H5''	14:B:1309:G:H5'	1.97	0.47
10:SC:68:PHE:O	10:SC:72:PHE:N	2.46	0.47
14:B:196:U:N3	14:B:206:U:O2	2.47	0.47
14:B:673:G:O2'	14:B:696:G:O2'	2.27	0.47
1:A:148:G:H22	1:A:174:A:H61	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:830:U:H4'	14:B:1806:U:H4'	1.97	0.47
7:S8:26:LEU:HD11	7:S8:43:SER:HB3	1.95	0.47
14:B:1520:A:O2'	14:B:1521:A:O5'	2.30	0.47
17:L2:62:TYR:HA	17:L2:86:ASN:HD21	1.81	0.46
14:B:2608:G:N3	14:B:2608:G:H2'	2.29	0.46
42:D:18:G:H4'	42:D:60:U:H3	1.80	0.46
1:A:1291:U:OP1	1:A:1293:C:N4	2.48	0.46
1:A:1384:A:H2'	1:A:1385:A:H8	1.80	0.46
14:B:2776:A:H1'	35:LL:63:THR:HG22	1.96	0.46
17:L2:107:PRO:HD2	17:L2:110:LEU:HD22	1.98	0.46
14:B:2717:A:OP2	40:LQ:13:ARG:NH2	2.48	0.46
14:B:1491:C:N3	14:B:1492:G:N1	2.64	0.46
14:B:1377:U:OP2	21:L6:58:TYR:OH	2.34	0.46
30:LF:35:PHE:HA	30:LF:42:GLN:HG2	1.98	0.46
1:A:733:G:OP1	1:A:862:G:N2	2.46	0.46
1:A:704:A:O2'	1:A:794:G:O2'	2.33	0.46
27:LC:4:GLY:HA2	27:LC:110:PHE:HZ	1.81	0.46
3:S2:23:ILE:HB	3:S2:86:VAL:HG12	1.98	0.46
10:SC:63:MET:HG3	10:SC:93:ARG:HH12	1.80	0.46
1:A:536:C:O2	1:A:543:A:O2'	2.30	0.46
1:A:619:C:N4	1:A:637:A:N1	2.63	0.46
1:A:746:U:OP1	12:SE:2:ARG:NH1	2.48	0.46
35:LL:122:THR:N	35:LL:134:GLU:O	2.44	0.46
1:A:129:A:OP1	7:S8:4:ARG:NH1	2.49	0.46
1:A:989:C:N4	1:A:992:A:N1	2.50	0.46
14:B:1517:A:H61	14:B:1563:U:H3	1.62	0.46
14:B:418:G:O2'	14:B:446:G:O6	2.30	0.46
14:B:624:C:OP2	18:L3:33:LYS:NZ	2.48	0.46
34:LJ:51:VAL:HG11	34:LJ:91:GLY:HA3	1.96	0.46
1:A:145:U:O2	1:A:178:G:N1	2.49	0.46
1:A:842:U:H2'	1:A:843:A:C8	2.50	0.46
14:B:2312:C:H42	14:B:2410:G:H1	1.62	0.46
14:B:2875:U:H2'	14:B:2876:G:H8	1.81	0.46
14:B:352:A:N3	14:B:372:A:O2'	2.49	0.46
1:A:1270:G:H21	1:A:1285:A:H62	1.64	0.46
1:A:952:U:H2'	1:A:953:G:H8	1.81	0.46
16:L1:51:LYS:HG2	16:L1:52:ARG:H	1.81	0.46
3:S2:100:LEU:HD22	3:S2:105:LEU:HD23	1.98	0.46
1:A:744:U:O2'	12:SE:91:VAL:O	2.33	0.46
14:B:342:A:N3	14:B:362:C:O2'	2.42	0.46
14:B:1658:A:N6	20:L5:92:ARG:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:LJ:157:GLU:O	34:LJ:177:THR:OG1	2.34	0.46
1:A:1504:A:O2'	14:B:1940:A:N7	2.49	0.45
14:B:1713:A:O2'	14:B:2576:G:OP1	2.31	0.45
14:B:2290:C:N4	24:L9:23:ASP:OD1	2.49	0.45
17:L2:229:ASP:OD1	17:L2:229:ASP:N	2.48	0.45
1:A:175:C:H5''	9:SA:20:ARG:HH21	1.82	0.45
14:B:2859:G:N2	40:LQ:97:GLN:O	2.43	0.45
7:S8:52:ASN:OD1	7:S8:54:SER:OG	2.32	0.45
1:A:145:U:H1'	1:A:178:G:H22	1.81	0.45
1:A:1265:G:H2'	1:A:1289:A:H61	1.81	0.45
1:A:633:G:OP1	6:S7:19:ARG:NH2	2.50	0.45
14:B:284:C:O2	14:B:285:U:O2'	2.28	0.45
1:A:1278:G:H8	1:A:1280:G:H22	1.63	0.45
14:B:188:C:O2	14:B:215:G:N2	2.49	0.45
14:B:2533:U:N1	14:B:2533:U:C5'	2.80	0.45
23:L8:3:SER:OG	23:L8:62:GLU:OE1	2.32	0.45
14:B:902:A:H5''	24:L9:85:LYS:HE2	1.99	0.45
28:LD:48:ASN:HA	28:LD:51:LYS:HB3	1.97	0.45
13:SF:5:ASP:OD2	13:SF:79:ARG:NH2	2.50	0.45
1:A:844:G:N2	1:A:860:U:O2	2.50	0.45
1:A:957:C:H2'	1:A:958:A:H8	1.81	0.45
1:A:961:U:H2'	1:A:962:G:H8	1.81	0.45
14:B:1407:C:O2'	14:B:1838:G:O2'	2.34	0.45
14:B:1591:G:N2	14:B:1592:A:H62	2.15	0.45
14:B:375:A:O2'	14:B:377:U:OP2	2.29	0.45
14:B:629:A:N1	14:B:854:G:O2'	2.38	0.45
14:B:441:C:HO2'	25:LA:13:SER:HG	1.64	0.45
1:A:546:U:H4'	4:S3:124:ARG:HH21	1.81	0.45
14:B:1520:A:N6	14:B:1560:A:O2'	2.46	0.45
37:LN:87:ILE:HD11	37:LN:114:ILE:HD11	1.98	0.45
3:S2:18:ASN:HD22	3:S2:81:THR:H	1.64	0.45
5:S6:9:ASN:HA	5:S6:12:ILE:HD12	1.99	0.45
28:LD:12:VAL:HB	28:LD:20:ARG:HG2	1.99	0.45
36:LM:93:LEU:HD23	36:LM:101:LEU:HD13	1.99	0.45
1:A:460:A:H62	1:A:488:U:H3	1.65	0.45
11:SD:99:ALA:HB2	11:SD:123:ILE:HG23	1.99	0.45
15:C:12:U:OP2	15:C:68:A:O2'	2.29	0.44
16:L1:34:ILE:HD12	16:L1:36:GLU:HB2	1.99	0.44
4:S3:77:ASN:HB2	4:S3:106:VAL:HA	1.99	0.44
4:S3:112:ARG:HA	4:S3:117:THR:HG22	1.98	0.44
9:SA:35:ALA:O	9:SA:39:VAL:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SC:26:LEU:HB2	10:SC:29:ARG:HE	1.82	0.44
14:B:2277:G:O2'	14:B:2523:C:OP1	2.26	0.44
11:SD:108:GLY:O	11:SD:111:VAL:N	2.43	0.44
11:SD:127:SER:HB2	11:SD:130:SER:HB2	1.98	0.44
1:A:810:A:H3'	1:A:811:G:H8	1.83	0.44
14:B:2869:G:O2'	14:B:2886:G:N2	2.49	0.44
2:S1:41:PRO:HG3	2:S1:72:ARG:HH12	1.82	0.44
4:S3:83:ILE:HD12	4:S3:122:GLY:HA3	2.00	0.44
6:S7:7:LEU:HD22	6:S7:18:TYR:HB3	1.98	0.44
8:S9:31:THR:HA	8:S9:34:LEU:HD13	1.99	0.44
1:A:111:G:H21	1:A:362:G:H4'	1.82	0.44
14:B:2022:U:O2	37:LN:3:GLN:NE2	2.51	0.44
7:S8:21:LYS:HB3	7:S8:49:HIS:CD2	2.52	0.44
10:SC:182:ARG:HH22	10:SC:190:ASN:HA	1.83	0.44
34:LJ:26:ILE:HD12	34:LJ:111:ARG:HD3	1.99	0.44
4:S3:80:ILE:HG13	4:S3:110:ILE:HD12	2.00	0.44
12:SE:53:ASN:HB2	12:SE:87:ILE:HD11	1.99	0.44
1:A:1514:A:OP1	1:A:1542:A:O2'	2.28	0.44
16:L1:77:PRO:HB2	16:L1:80:THR:HG23	2.00	0.44
19:L4:50:ALA:HB3	19:L4:53:VAL:HB	2.00	0.44
10:SC:66:ARG:O	10:SC:70:ASN:ND2	2.51	0.44
1:A:540:A:H2'	1:A:541:A:H2'	1.98	0.44
42:D:9:A:O2'	42:D:11:C:N4	2.37	0.44
35:LL:89:LEU:HG	35:LL:162:ILE:HG12	1.98	0.44
35:LL:44:LYS:HG2	35:LL:46:GLU:HG3	2.00	0.44
1:A:264:U:O4	1:A:274:G:N2	2.51	0.44
14:B:2532:G:N3	14:B:2532:G:H2'	2.33	0.44
5:S6:26:GLU:HB2	5:S6:77:ARG:HH21	1.83	0.44
9:SA:50:VAL:O	9:SA:54:VAL:N	2.43	0.44
11:SD:32:ARG:HE	11:SD:52:LYS:HE2	1.83	0.44
1:A:1009:U:H5''	1:A:1016:A:H62	1.82	0.43
19:L4:63:ASN:ND2	19:L4:96:THR:OG1	2.51	0.43
1:A:1306:C:H4'	1:A:1312:U:H3	1.82	0.43
1:A:1440:C:O2	1:A:1482:G:N2	2.51	0.43
1:A:425:G:O6	1:A:433:A:N6	2.51	0.43
1:A:796:U:H3	1:A:803:C:H41	1.66	0.43
1:A:961:U:H4'	1:A:973:A:H61	1.82	0.43
14:B:647:G:N7	38:LO:103:LYS:NZ	2.57	0.43
16:L1:34:ILE:HD11	16:L1:41:ARG:HE	1.82	0.43
4:S3:74:ILE:H	4:S3:74:ILE:HG12	1.74	0.43
1:A:398:C:H4'	6:S7:29:ARG:HH22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:G:N2	1:A:481:C:OP1	2.51	0.43
16:L1:60:THR:HG22	16:L1:77:PRO:HA	2.01	0.43
23:L8:80:ASP:OD1	23:L8:80:ASP:N	2.51	0.43
14:B:593:U:C2	19:L4:21:PHE:HE1	2.36	0.43
20:L5:12:ILE:HG12	20:L5:12:ILE:H	1.69	0.43
1:A:1099:G:H21	1:A:1179:A:H2	1.66	0.43
1:A:1262:A:N6	1:A:1295:A:H61	2.16	0.43
1:A:620:C:H42	1:A:636:G:H1	1.66	0.43
14:B:1893:A:N6	14:B:1902:G:O2'	2.51	0.43
14:B:2841:A:O2'	14:B:2846:A:N1	2.47	0.43
17:L2:205:VAL:HG11	17:L2:211:SER:HB2	2.00	0.43
2:S1:92:LEU:HD12	2:S1:93:PRO:HD2	1.99	0.43
14:B:1465:G:O2'	14:B:1539:A:N6	2.51	0.43
14:B:1962:G:N1	14:B:1989:C:O2'	2.51	0.43
14:B:2873:C:H2'	14:B:2874:A:H8	1.84	0.43
14:B:1293:U:H5''	14:B:1294:G:H5''	2.00	0.43
14:B:2358:G:O2'	14:B:2363:A:N1	2.44	0.43
1:A:1488:C:H2'	1:A:1489:A:C8	2.54	0.43
16:L1:22:PHE:O	16:L1:53:ARG:NH2	2.51	0.43
25:LA:39:LEU:HA	25:LA:44:PRO:HB3	2.00	0.43
34:LJ:4:TYR:OH	34:LJ:203:GLU:OE1	2.37	0.43
1:A:1323:U:H2'	1:A:1324:C:H6	1.84	0.43
1:A:842:U:H2'	1:A:843:A:H8	1.83	0.43
14:B:1091:G:O6	14:B:1154:G:O2'	2.31	0.43
14:B:2040:A:H61	14:B:2640:U:H3	1.67	0.43
1:A:673:A:H62	1:A:732:G:H1	1.66	0.42
36:LM:19:ILE:HD13	36:LM:143:LEU:HD23	2.00	0.42
8:S9:41:ARG:HG3	8:S9:76:VAL:HG13	1.99	0.42
1:A:517:A:OP2	10:SC:43:LYS:NZ	2.52	0.42
10:SC:95:ASP:OD1	10:SC:96:ALA:N	2.52	0.42
1:A:1364:U:H2'	1:A:1365:A:C8	2.54	0.42
14:B:1613:G:OP1	17:L2:210:ARG:NH2	2.52	0.42
14:B:2868:G:C8	16:L1:97:ALA:HB2	2.54	0.42
22:L7:80:ARG:HE	22:L7:96:LYS:HE3	1.84	0.42
1:A:1442:G:OP1	16:L1:108:LYS:N	2.52	0.42
1:A:688:C:H42	1:A:718:G:H1	1.68	0.42
14:B:1027:A:N6	14:B:1028:G:O6	2.51	0.42
14:B:1169:G:O6	14:B:1170:A:N6	2.52	0.42
19:L4:27:VAL:O	19:L4:65:GLN:NE2	2.51	0.42
1:A:680:U:H2'	1:A:681:G:H8	1.84	0.42
1:A:889:C:OP1	4:S3:5:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:U:H2'	1:A:960:G:C8	2.53	0.42
14:B:2318:U:O2'	14:B:2401:C:O2	2.37	0.42
14:B:247:A:OP2	32:LH:8:ARG:NH2	2.52	0.42
14:B:2047:A:H5'	29:LE:9:SER:HB2	2.01	0.42
14:B:1520:A:O2'	14:B:1521:A:O4'	2.36	0.42
10:SC:103:LEU:HD22	10:SC:172:LEU:HD23	2.00	0.42
11:SD:64:VAL:HG12	11:SD:68:LYS:HE2	2.01	0.42
14:B:2103:U:H5''	14:B:2265:G:H22	1.85	0.42
19:L4:22:VAL:O	19:L4:93:THR:N	2.53	0.42
4:S3:24:LEU:HD22	4:S3:107:ARG:HH12	1.84	0.42
4:S3:47:CYS:HA	4:S3:68:VAL:HG12	2.00	0.42
14:B:1051:C:OP1	36:LM:38:ARG:NH2	2.53	0.42
14:B:833:A:OP1	14:B:836:C:N4	2.49	0.42
34:LJ:49:HIS:HD2	34:LJ:92:PRO:HB3	1.84	0.42
42:D:51:U:H3	42:D:63:G:H22	1.66	0.42
15:C:74:G:OP2	23:L8:12:LYS:NZ	2.53	0.42
32:LH:31:HIS:CD2	32:LH:32:LEU:HG	2.55	0.42
13:SF:25:LEU:HD23	13:SF:62:LEU:HD12	2.02	0.42
24:L9:66:THR:O	24:L9:66:THR:OG1	2.32	0.42
1:A:156:C:O2	1:A:165:G:N1	2.47	0.42
14:B:86:C:O2'	14:B:103:U:O2'	2.28	0.42
36:LM:70:GLU:HG3	36:LM:71:THR:HG23	2.02	0.42
37:LN:65:THR:HG23	37:LN:68:GLY:H	1.85	0.42
38:LO:92:THR:HG22	38:LO:94:ALA:H	1.85	0.42
10:SC:48:GLY:HA2	10:SC:51:LEU:HB3	2.01	0.42
1:A:10:G:H2'	1:A:11:A:H8	1.84	0.41
1:A:968:A:O2'	1:A:993:C:O2	2.35	0.41
14:B:1545:U:O4	14:B:1546:A:N6	2.53	0.41
36:LM:144:ARG:H	36:LM:144:ARG:HG3	1.60	0.41
1:A:383:U:O2'	6:S7:7:LEU:O	2.37	0.41
9:SA:56:LEU:O	9:SA:60:ALA:N	2.52	0.41
1:A:1326:G:H2'	1:A:1327:C:H3'	2.02	0.41
20:L5:11:ARG:O	20:L5:98:LYS:NZ	2.44	0.41
20:L5:10:ILE:HG21	20:L5:46:VAL:HG11	2.02	0.41
1:A:115:A:H61	1:A:321:A:H2	1.67	0.41
1:A:1272:A:N7	1:A:1273:A:N6	2.69	0.41
1:A:471:A:N1	1:A:474:A:O2'	2.53	0.41
14:B:1773:A:H8	14:B:1774:A:C8	2.39	0.41
42:D:13:C:H2'	42:D:14:A:H8	1.85	0.41
19:L4:4:ILE:HD12	19:L4:40:PHE:HB3	2.02	0.41
40:LQ:51:GLY:HA2	40:LQ:86:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:1518:G:H22	14:B:1562:C:H42	1.69	0.41
14:B:2500:U:OP1	14:B:2556:G:N2	2.54	0.41
22:L7:40:ILE:HG22	22:L7:60:GLU:HG3	2.01	0.41
26:LB:16:GLU:HG3	26:LB:19:LYS:HE3	2.03	0.41
2:S1:39:PRO:HB3	2:S1:74:ILE:HG23	2.02	0.41
3:S2:122:ARG:HA	3:S2:123:PRO:HD3	1.87	0.41
1:A:676:A:O2'	5:S6:46:HIS:ND1	2.48	0.41
1:A:1128:A:H2'	1:A:1189:A:H2	1.85	0.41
1:A:1527:G:N2	1:A:1530:A:OP2	2.53	0.41
1:A:234:A:H2'	1:A:235:G:H8	1.86	0.41
1:A:568:A:H4'	1:A:569:U:H5''	2.02	0.41
1:A:975:G:OP1	1:A:976:C:N4	2.54	0.41
1:A:1416:U:H1'	1:A:1529:A:H4'	2.02	0.41
1:A:204:A:H2'	1:A:205:A:H8	1.86	0.41
1:A:760:G:OP1	5:S6:73:LYS:NZ	2.53	0.41
14:B:1540:U:O2	14:B:1624:C:O2'	2.29	0.41
14:B:735:C:O2'	14:B:825:G:OP1	2.37	0.41
14:B:758:G:H22	14:B:763:A:H8	1.67	0.41
1:A:1178:C:H5''	1:A:1179:A:H2'	2.02	0.41
1:A:1273:A:H61	1:A:1283:C:H42	1.69	0.41
1:A:787:C:H42	1:A:811:G:H1	1.68	0.41
14:B:1726:A:OP1	14:B:1743:G:N1	2.45	0.41
34:LJ:22:ALA:HB1	34:LJ:26:ILE:HD11	2.03	0.41
34:LJ:57:VAL:HG21	34:LJ:79:ARG:HB3	2.03	0.41
36:LM:75:TYR:HB2	36:LM:88:ILE:HG23	2.02	0.41
1:A:30:A:N6	1:A:31:U:O4	2.54	0.41
1:A:796:U:H3	1:A:803:C:N4	2.19	0.41
14:B:1063:U:OP1	14:B:1079:U:O2'	2.30	0.41
26:LB:14:ILE:HA	26:LB:17:GLN:HB3	2.02	0.41
3:S2:32:VAL:HG21	3:S2:67:SER:HA	2.02	0.41
11:SD:36:LEU:HD22	11:SD:134:ILE:HG12	2.02	0.41
41:LR:64:ALA:HA	41:LR:72:LEU:HD21	2.03	0.41
3:S2:30:THR:HB	3:S2:47:ALA:HB2	2.02	0.41
1:A:271:A:H2'	1:A:272:C:H6	1.86	0.41
1:A:527:C:H42	1:A:541:A:N6	2.19	0.41
1:A:622:A:N6	1:A:633:G:O6	2.54	0.41
14:B:1250:G:H2'	14:B:1274:G:H22	1.86	0.41
14:B:1290:G:OP2	18:L3:14:ARG:NH2	2.44	0.41
14:B:23:G:H1	14:B:562:C:H42	1.67	0.41
14:B:2850:G:H5'	27:LC:67:LYS:HE3	2.03	0.41
14:B:504:G:O2'	14:B:515:G:O6	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:971:U:H2'	14:B:972:A:C8	2.57	0.40
19:L4:2:PHE:HB3	19:L4:15:GLU:HG2	2.02	0.40
15:C:91:C:H2'	15:C:92:G:C8	2.56	0.40
42:D:13:C:H2'	42:D:14:A:C8	2.56	0.40
37:LN:3:GLN:HG2	37:LN:4:GLN:H	1.86	0.40
4:S3:83:ILE:H	4:S3:120:VAL:HG11	1.87	0.40
1:A:350:C:N4	1:A:355:G:O6	2.49	0.40
14:B:2050:A:H5'	14:B:2644:C:H4'	2.02	0.40
14:B:994:A:H5''	15:C:85:A:H61	1.85	0.40
24:L9:44:ILE:HG21	24:L9:47:ARG:HD3	2.02	0.40
14:B:732:C:H1'	31:LG:5:THR:HG22	2.02	0.40
38:LO:56:PRO:O	38:LO:60:ARG:NH1	2.54	0.40
1:A:1198:A:N6	1:A:1199:U:O2	2.54	0.40
1:A:1449:G:H1	1:A:1473:C:H42	1.70	0.40
1:A:29:G:H21	1:A:304:U:H5'	1.86	0.40
39:LP:37:THR:OG1	39:LP:128:LYS:O	2.29	0.40
1:A:109:C:O2'	6:S7:26:ARG:O	2.36	0.40
10:SC:125:ARG:NE	10:SC:127:ASP:OD2	2.55	0.40
1:A:465:U:H3	1:A:486:C:H41	1.67	0.40
14:B:2682:G:O2'	14:B:2691:G:O6	2.32	0.40
42:D:51:U:H3	42:D:63:G:H1	1.69	0.40
42:D:63:G:H2'	42:D:64:A:C8	2.56	0.40
17:L2:11:ASN:ND2	17:L2:14:ARG:HH21	2.19	0.40
18:L3:53:ARG:HH11	18:L3:53:ARG:HD3	1.76	0.40
3:S2:111:ARG:HG2	3:S2:113:VAL:HG23	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
2	S1	80/82 (98%)	70 (88%)	10 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S2	113/115 (98%)	104 (92%)	9 (8%)	0	100	100
4	S3	134/136 (98%)	109 (81%)	22 (16%)	3 (2%)	8	47
5	S6	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
6	S7	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
7	S8	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
8	S9	53/55 (96%)	46 (87%)	7 (13%)	0	100	100
9	SA	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
10	SC	196/198 (99%)	180 (92%)	16 (8%)	0	100	100
11	SD	152/154 (99%)	136 (90%)	16 (10%)	0	100	100
12	SE	90/92 (98%)	80 (89%)	10 (11%)	0	100	100
13	SF	128/130 (98%)	109 (85%)	19 (15%)	0	100	100
16	L1	111/113 (98%)	94 (85%)	17 (15%)	0	100	100
17	L2	273/275 (99%)	233 (85%)	39 (14%)	1 (0%)	38	77
18	L3	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
19	L4	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
20	L5	109/111 (98%)	101 (93%)	8 (7%)	0	100	100
21	L6	85/87 (98%)	71 (84%)	14 (16%)	0	100	100
22	L7	99/101 (98%)	87 (88%)	12 (12%)	0	100	100
23	L8	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
24	L9	76/78 (97%)	68 (90%)	8 (10%)	0	100	100
25	LA	57/59 (97%)	49 (86%)	8 (14%)	0	100	100
26	LB	59/61 (97%)	53 (90%)	6 (10%)	0	100	100
27	LC	212/214 (99%)	176 (83%)	36 (17%)	0	100	100
28	LD	55/57 (96%)	49 (89%)	6 (11%)	0	100	100
29	LE	51/53 (96%)	43 (84%)	8 (16%)	0	100	100
30	LF	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
31	LG	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
32	LH	62/64 (97%)	55 (89%)	7 (11%)	0	100	100
33	LI	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
34	LJ	202/204 (99%)	173 (86%)	29 (14%)	0	100	100
35	LL	172/174 (99%)	147 (86%)	24 (14%)	1 (1%)	28	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	LM	141/143 (99%)	122 (86%)	19 (14%)	0	100	100
37	LN	119/121 (98%)	108 (91%)	11 (9%)	0	100	100
38	LO	142/144 (99%)	121 (85%)	21 (15%)	0	100	100
39	LP	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
40	LQ	119/121 (98%)	107 (90%)	12 (10%)	0	100	100
41	LR	114/116 (98%)	99 (87%)	15 (13%)	0	100	100
All	All	4076/4152 (98%)	3590 (88%)	481 (12%)	5 (0%)	58	88

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	LL	59	LYS
17	L2	50	THR
4	S3	57	LYS
4	S3	58	PRO
4	S3	41	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
2	S1	73/73 (100%)	73 (100%)	0	100	100
3	S2	91/91 (100%)	90 (99%)	1 (1%)	78	91
4	S3	103/117 (88%)	99 (96%)	4 (4%)	37	73
5	S6	79/79 (100%)	79 (100%)	0	100	100
6	S7	64/64 (100%)	64 (100%)	0	100	100
7	S8	77/77 (100%)	77 (100%)	0	100	100
8	S9	50/50 (100%)	50 (100%)	0	100	100
9	SA	29/64 (45%)	29 (100%)	0	100	100
10	SC	173/173 (100%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	SD	118/120 (98%)	116 (98%)	2 (2%)	66	88
12	SE	80/80 (100%)	80 (100%)	0	100	100
13	SF	110/111 (99%)	110 (100%)	0	100	100
16	L1	99/99 (100%)	99 (100%)	0	100	100
17	L2	217/222 (98%)	215 (99%)	2 (1%)	82	92
18	L3	96/96 (100%)	96 (100%)	0	100	100
19	L4	85/85 (100%)	84 (99%)	1 (1%)	75	90
20	L5	90/90 (100%)	89 (99%)	1 (1%)	78	91
21	L6	74/79 (94%)	73 (99%)	1 (1%)	71	89
22	L7	79/86 (92%)	79 (100%)	0	100	100
23	L8	81/81 (100%)	81 (100%)	0	100	100
24	L9	59/61 (97%)	57 (97%)	2 (3%)	42	77
25	LA	49/49 (100%)	49 (100%)	0	100	100
26	LB	55/55 (100%)	55 (100%)	0	100	100
27	LC	171/172 (99%)	169 (99%)	2 (1%)	75	90
28	LD	51/51 (100%)	51 (100%)	0	100	100
29	LE	48/48 (100%)	48 (100%)	0	100	100
30	LF	44/45 (98%)	44 (100%)	0	100	100
31	LG	39/39 (100%)	39 (100%)	0	100	100
32	LH	55/55 (100%)	55 (100%)	0	100	100
33	LI	35/35 (100%)	35 (100%)	0	100	100
34	LJ	160/167 (96%)	160 (100%)	0	100	100
35	LL	151/152 (99%)	151 (100%)	0	100	100
36	LM	122/122 (100%)	120 (98%)	2 (2%)	68	88
37	LN	99/99 (100%)	97 (98%)	2 (2%)	60	85
38	LO	110/110 (100%)	109 (99%)	1 (1%)	82	92
39	LP	113/113 (100%)	112 (99%)	1 (1%)	82	92
40	LQ	101/101 (100%)	101 (100%)	0	100	100
41	LR	91/92 (99%)	88 (97%)	3 (3%)	43	77
All	All	3421/3503 (98%)	3396 (99%)	25 (1%)	87	95

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S2	29	ASN
4	S3	25	ASN
4	S3	38	LEU
4	S3	74	ILE
4	S3	96	ARG
11	SD	23	LYS
11	SD	26	LYS
17	L2	219	THR
17	L2	261	ARG
19	L4	79	ARG
20	L5	84	ARG
21	L6	6	ILE
24	L9	61	ARG
24	L9	80	LYS
27	LC	66	ASN
27	LC	138	ARG
36	LM	11	ASN
36	LM	85	ILE
37	LN	72	ASN
37	LN	107	ARG
38	LO	104	ASN
39	LP	68	ILE
41	LR	21	ASN
41	LR	48	ASN
41	LR	113	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
3	S2	18	ASN
3	S2	29	ASN
4	S3	25	ASN
4	S3	72	ASN
4	S3	77	ASN
6	S7	62	ASN
10	SC	8	ASN
10	SC	67	GLN
10	SC	85	ASN
13	SF	31	ASN
17	L2	11	ASN
17	L2	86	ASN
17	L2	232	HIS
18	L3	44	GLN

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Mol	Chain	Res	Type
20	L5	60	HIS
20	L5	61	ASN
20	L5	77	ASN
22	L7	2	HIS
24	L9	37	GLN
26	LB	17	GLN
27	LC	66	ASN
29	LE	32	ASN
29	LE	50	ASN
32	LH	31	HIS
35	LL	38	ASN
35	LL	48	ASN
36	LM	11	ASN
37	LN	72	ASN
38	LO	83	ASN
38	LO	104	ASN
41	LR	21	ASN
41	LR	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1411/1547 (91%)	486 (34%)	14 (0%)
14	B	2759/2919 (94%)	765 (27%)	9 (0%)
15	C	113/114 (99%)	31 (27%)	1 (0%)
42	D	73/74 (98%)	28 (38%)	0
All	All	4356/4654 (93%)	1310 (30%)	24 (0%)

All (1310) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	G
1	A	9	A
1	A	10	G
1	A	23	G
1	A	30	A
1	A	32	G
1	A	33	A
1	A	37	C
1	A	39	G

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Mol	Chain	Res	Type
1	A	40	G
1	A	41	C
1	A	47	G
1	A	48	C
1	A	49	C
1	A	50	U
1	A	51	A
1	A	52	A
1	A	53	U
1	A	55	C
1	A	61	A
1	A	62	G
1	A	66	A
1	A	67	G
1	A	108	A
1	A	114	G
1	A	115	A
1	A	119	A
1	A	120	C
1	A	121	A
1	A	125	G
1	A	129	A
1	A	133	U
1	A	134	A
1	A	135	C
1	A	137	U
1	A	138	A
1	A	143	A
1	A	144	C
1	A	149	A
1	A	154	U
1	A	161	A
1	A	163	C
1	A	164	C
1	A	173	U
1	A	204	A
1	A	206	A
1	A	209	G
1	A	210	A
1	A	211	A
1	A	225	G
1	A	228	A

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Mol	Chain	Res	Type
1	A	233	U
1	A	234	A
1	A	236	A
1	A	242	C
1	A	252	U
1	A	254	A
1	A	255	G
1	A	258	A
1	A	259	G
1	A	268	G
1	A	269	U
1	A	274	G
1	A	275	C
1	A	276	U
1	A	280	C
1	A	284	G
1	A	287	A
1	A	289	G
1	A	291	U
1	A	293	C
1	A	297	G
1	A	302	C
1	A	306	A
1	A	307	G
1	A	314	A
1	A	315	U
1	A	316	C
1	A	320	C
1	A	321	A
1	A	332	G
1	A	333	A
1	A	334	G
1	A	335	A
1	A	336	C
1	A	337	A
1	A	338	C
1	A	340	G
1	A	342	C
1	A	347	C
1	A	348	U
1	A	349	C
1	A	350	C

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Mol	Chain	Res	Type
1	A	353	C
1	A	355	G
1	A	359	G
1	A	360	C
1	A	362	G
1	A	364	A
1	A	366	U
1	A	367	A
1	A	370	G
1	A	371	A
1	A	375	U
1	A	376	U
1	A	377	C
1	A	379	G
1	A	386	G
1	A	389	A
1	A	392	G
1	A	396	G
1	A	398	C
1	A	401	A
1	A	406	C
1	A	408	C
1	A	412	G
1	A	413	U
1	A	414	G
1	A	419	A
1	A	420	U
1	A	421	G
1	A	423	A
1	A	424	G
1	A	425	G
1	A	427	C
1	A	428	U
1	A	430	C
1	A	431	G
1	A	432	G
1	A	436	G
1	A	437	U
1	A	438	A
1	A	444	C
1	A	447	U
1	A	448	U

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Mol	Chain	Res	Type
1	A	450	U
1	A	451	U
1	A	452	A
1	A	457	A
1	A	459	A
1	A	460	A
1	A	461	C
1	A	464	A
1	A	465	U
1	A	467	U
1	A	468	G
1	A	470	A
1	A	471	A
1	A	472	G
1	A	473	U
1	A	475	A
1	A	478	G
1	A	481	C
1	A	482	A
1	A	484	A
1	A	486	C
1	A	487	U
1	A	489	G
1	A	492	G
1	A	493	G
1	A	494	U
1	A	501	U
1	A	504	G
1	A	506	A
1	A	507	A
1	A	508	G
1	A	513	G
1	A	516	U
1	A	517	A
1	A	520	U
1	A	524	U
1	A	525	G
1	A	526	C
1	A	527	C
1	A	528	A
1	A	529	G
1	A	535	G

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Mol	Chain	Res	Type
1	A	539	U
1	A	540	A
1	A	543	A
1	A	544	C
1	A	555	A
1	A	558	G
1	A	567	A
1	A	575	G
1	A	576	G
1	A	580	A
1	A	581	A
1	A	584	C
1	A	585	G
1	A	601	U
1	A	604	A
1	A	616	A
1	A	622	A
1	A	623	C
1	A	624	G
1	A	627	U
1	A	639	G
1	A	640	G
1	A	646	G
1	A	649	A
1	A	661	U
1	A	663	A
1	A	673	A
1	A	675	G
1	A	679	G
1	A	684	A
1	A	688	C
1	A	695	A
1	A	696	G
1	A	698	G
1	A	700	U
1	A	701	G
1	A	703	A
1	A	704	A
1	A	706	G
1	A	710	A
1	A	711	G
1	A	713	G

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Mol	Chain	Res	Type
1	A	716	A
1	A	721	G
1	A	724	A
1	A	726	A
1	A	728	C
1	A	729	A
1	A	730	G
1	A	731	U
1	A	732	G
1	A	739	G
1	A	756	A
1	A	760	G
1	A	763	G
1	A	766	G
1	A	769	G
1	A	772	C
1	A	784	G
1	A	785	A
1	A	788	A
1	A	790	A
1	A	802	A
1	A	803	C
1	A	804	C
1	A	807	G
1	A	820	G
1	A	821	U
1	A	823	A
1	A	825	C
1	A	829	G
1	A	835	U
1	A	836	A
1	A	849	U
1	A	850	U
1	A	851	U
1	A	853	C
1	A	858	C
1	A	862	G
1	A	864	G
1	A	873	A
1	A	876	G
1	A	879	U
1	A	880	U

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Mol	Chain	Res	Type
1	A	881	A
1	A	885	A
1	A	894	G
1	A	896	G
1	A	898	A
1	A	906	C
1	A	909	A
1	A	919	C
1	A	928	A
1	A	931	G
1	A	935	G
1	A	936	G
1	A	939	C
1	A	940	C
1	A	943	C
1	A	944	A
1	A	945	C
1	A	946	A
1	A	948	G
1	A	950	G
1	A	954	G
1	A	955	A
1	A	969	U
1	A	970	U
1	A	971	C
1	A	975	G
1	A	978	A
1	A	980	G
1	A	984	A
1	A	985	G
1	A	986	A
1	A	989	C
1	A	990	U
1	A	992	A
1	A	993	C
1	A	994	C
1	A	1002	G
1	A	1003	A
1	A	1006	U
1	A	1009	U
1	A	1010	U
1	A	1012	G

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Mol	Chain	Res	Type
1	A	1013	A
1	A	1014	C
1	A	1016	A
1	A	1065	C
1	A	1067	U
1	A	1068	G
1	A	1075	G
1	A	1076	U
1	A	1081	U
1	A	1090	G
1	A	1093	A
1	A	1096	U
1	A	1100	G
1	A	1103	A
1	A	1104	A
1	A	1105	G
1	A	1106	U
1	A	1109	C
1	A	1111	C
1	A	1112	A
1	A	1115	G
1	A	1121	A
1	A	1122	A
1	A	1124	C
1	A	1125	C
1	A	1126	U
1	A	1130	G
1	A	1134	A
1	A	1135	G
1	A	1136	U
1	A	1138	G
1	A	1140	C
1	A	1141	A
1	A	1143	C
1	A	1144	A
1	A	1145	U
1	A	1162	A
1	A	1164	U
1	A	1168	C
1	A	1169	U
1	A	1170	G
1	A	1173	G

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Mol	Chain	Res	Type
1	A	1177	A
1	A	1179	A
1	A	1180	A
1	A	1184	G
1	A	1185	G
1	A	1186	A
1	A	1187	G
1	A	1188	G
1	A	1189	A
1	A	1191	G
1	A	1192	G
1	A	1197	G
1	A	1198	A
1	A	1199	U
1	A	1200	G
1	A	1201	A
1	A	1206	A
1	A	1207	A
1	A	1208	A
1	A	1210	C
1	A	1212	U
1	A	1213	C
1	A	1217	C
1	A	1218	C
1	A	1219	C
1	A	1220	C
1	A	1222	U
1	A	1223	A
1	A	1224	U
1	A	1225	G
1	A	1228	U
1	A	1235	A
1	A	1236	C
1	A	1238	C
1	A	1243	G
1	A	1246	A
1	A	1247	C
1	A	1248	A
1	A	1251	G
1	A	1254	C
1	A	1255	A
1	A	1257	U

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Mol	Chain	Res	Type
1	A	1264	G
1	A	1266	C
1	A	1267	A
1	A	1268	G
1	A	1271	A
1	A	1273	A
1	A	1275	C
1	A	1279	A
1	A	1280	G
1	A	1281	G
1	A	1288	A
1	A	1289	A
1	A	1290	A
1	A	1291	U
1	A	1292	C
1	A	1296	U
1	A	1297	A
1	A	1299	A
1	A	1304	U
1	A	1305	U
1	A	1308	C
1	A	1309	A
1	A	1310	G
1	A	1311	U
1	A	1315	G
1	A	1332	C
1	A	1333	G
1	A	1335	C
1	A	1336	U
1	A	1342	A
1	A	1343	A
1	A	1347	G
1	A	1350	A
1	A	1355	U
1	A	1357	G
1	A	1358	U
1	A	1361	U
1	A	1362	C
1	A	1364	U
1	A	1374	U
1	A	1380	G
1	A	1381	G

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Mol	Chain	Res	Type
1	A	1388	C
1	A	1389	G
1	A	1392	C
1	A	1394	C
1	A	1395	G
1	A	1397	G
1	A	1404	A
1	A	1407	C
1	A	1408	A
1	A	1410	C
1	A	1411	G
1	A	1416	U
1	A	1429	G
1	A	1442	G
1	A	1444	A
1	A	1446	C
1	A	1451	G
1	A	1452	G
1	A	1453	A
1	A	1456	A
1	A	1458	C
1	A	1461	U
1	A	1462	U
1	A	1463	U
1	A	1464	A
1	A	1465	G
1	A	1469	C
1	A	1479	A
1	A	1485	G
1	A	1486	G
1	A	1495	U
1	A	1498	G
1	A	1501	U
1	A	1502	G
1	A	1503	A
1	A	1504	A
1	A	1505	G
1	A	1508	G
1	A	1510	A
1	A	1514	A
1	A	1516	G
1	A	1517	U

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Mol	Chain	Res	Type
1	A	1518	A
1	A	1519	G
1	A	1522	G
1	A	1524	A
1	A	1528	G
1	A	1530	A
1	A	1531	G
1	A	1540	G
1	A	1541	G
1	A	1542	A
1	A	1544	C
1	A	1545	A
1	A	1546	C
1	A	1547	C
14	B	2	A
14	B	3	U
14	B	4	U
14	B	8	U
14	B	12	U
14	B	13	A
14	B	25	U
14	B	32	C
14	B	34	U
14	B	42	G
14	B	43	A
14	B	49	A
14	B	51	G
14	B	54	G
14	B	56	A
14	B	60	U
14	B	64	A
14	B	71	A
14	B	75	G
14	B	88	G
14	B	89	U
14	B	90	A
14	B	91	A
14	B	93	U
14	B	96	G
14	B	99	U
14	B	102	A
14	B	103	U

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Mol	Chain	Res	Type
14	B	109	G
14	B	114	C
14	B	117	A
14	B	118	A
14	B	119	U
14	B	124	A
14	B	130	A
14	B	148	U
14	B	152	C
14	B	153	G
14	B	154	A
14	B	156	A
14	B	157	U
14	B	160	G
14	B	161	A
14	B	162	A
14	B	163	U
14	B	169	G
14	B	174	U
14	B	176	A
14	B	182	C
14	B	183	A
14	B	184	C
14	B	185	A
14	B	189	G
14	B	191	A
14	B	194	A
14	B	199	A
14	B	202	A
14	B	218	G
14	B	219	A
14	B	224	A
14	B	225	A
14	B	229	A
14	B	233	U
14	B	235	G
14	B	236	A
14	B	244	A
14	B	246	U
14	B	248	G
14	B	251	G
14	B	253	G

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Mol	Chain	Res	Type
14	B	255	G
14	B	264	G
14	B	267	G
14	B	268	A
14	B	269	G
14	B	276	C
14	B	277	C
14	B	278	A
14	B	283	G
14	B	284	C
14	B	285	U
14	B	286	U
14	B	287	G
14	B	288	C
14	B	289	U
14	B	290	U
14	B	291	G
14	B	294	G
14	B	298	U
14	B	300	G
14	B	301	U
14	B	302	A
14	B	303	G
14	B	310	C
14	B	319	G
14	B	320	U
14	B	321	U
14	B	322	A
14	B	327	G
14	B	328	G
14	B	332	A
14	B	337	A
14	B	338	G
14	B	344	U
14	B	353	A
14	B	354	A
14	B	359	A
14	B	366	G
14	B	372	A
14	B	373	A
14	B	375	A
14	B	378	C

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Mol	Chain	Res	Type
14	B	385	U
14	B	389	A
14	B	395	U
14	B	396	G
14	B	397	U
14	B	398	C
14	B	399	U
14	B	404	U
14	B	405	G
14	B	410	G
14	B	411	A
14	B	416	G
14	B	432	G
14	B	433	U
14	B	434	G
14	B	435	A
14	B	444	C
14	B	445	G
14	B	446	G
14	B	447	A
14	B	452	G
14	B	457	G
14	B	458	A
14	B	459	C
14	B	462	U
14	B	463	C
14	B	482	U
14	B	489	A
14	B	494	U
14	B	496	G
14	B	502	C
14	B	503	A
14	B	504	G
14	B	510	U
14	B	513	G
14	B	518	A
14	B	519	G
14	B	526	A
14	B	527	G
14	B	535	G
14	B	541	G
14	B	548	A

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Mol	Chain	Res	Type
14	B	549	U
14	B	550	A
14	B	552	A
14	B	553	A
14	B	554	C
14	B	565	G
14	B	566	U
14	B	567	G
14	B	572	C
14	B	575	G
14	B	576	U
14	B	577	A
14	B	578	G
14	B	583	A
14	B	587	C
14	B	589	U
14	B	590	U
14	B	591	A
14	B	592	A
14	B	593	U
14	B	594	G
14	B	606	G
14	B	616	G
14	B	618	A
14	B	626	G
14	B	629	A
14	B	630	G
14	B	638	U
14	B	644	C
14	B	646	A
14	B	647	G
14	B	648	G
14	B	658	A
14	B	659	A
14	B	660	A
14	B	661	U
14	B	662	G
14	B	667	G
14	B	673	G
14	B	679	G
14	B	681	G
14	B	682	A

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Mol	Chain	Res	Type
14	B	683	G
14	B	691	A
14	B	696	G
14	B	698	U
14	B	702	U
14	B	705	U
14	B	715	A
14	B	716	C
14	B	722	A
14	B	731	U
14	B	735	C
14	B	745	G
14	B	748	U
14	B	751	A
14	B	752	G
14	B	759	U
14	B	761	A
14	B	762	C
14	B	763	A
14	B	764	C
14	B	768	A
14	B	773	G
14	B	775	A
14	B	793	G
14	B	794	A
14	B	795	A
14	B	799	U
14	B	802	G
14	B	809	A
14	B	820	G
14	B	822	G
14	B	823	G
14	B	827	A
14	B	828	A
14	B	829	U
14	B	837	G
14	B	838	A
14	B	842	U
14	B	850	G
14	B	851	C
14	B	857	C
14	B	859	C

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Mol	Chain	Res	Type
14	B	864	A
14	B	870	C
14	B	872	U
14	B	874	A
14	B	879	U
14	B	883	C
14	B	890	G
14	B	891	A
14	B	896	U
14	B	904	G
14	B	908	A
14	B	910	C
14	B	911	A
14	B	951	G
14	B	952	A
14	B	955	A
14	B	960	C
14	B	964	U
14	B	970	U
14	B	971	U
14	B	977	A
14	B	979	C
14	B	981	U
14	B	985	A
14	B	989	A
14	B	990	G
14	B	997	G
14	B	1005	G
14	B	1014	U
14	B	1017	A
14	B	1018	A
14	B	1024	A
14	B	1027	A
14	B	1033	G
14	B	1040	A
14	B	1045	A
14	B	1048	U
14	B	1049	C
14	B	1052	A
14	B	1053	A
14	B	1055	A
14	B	1056	U

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Mol	Chain	Res	Type
14	B	1057	A
14	B	1061	G
14	B	1066	G
14	B	1067	U
14	B	1069	G
14	B	1070	A
14	B	1074	G
14	B	1077	U
14	B	1081	G
14	B	1082	C
14	B	1083	G
14	B	1086	G
14	B	1090	A
14	B	1091	G
14	B	1092	A
14	B	1093	C
14	B	1095	A
14	B	1132	A
14	B	1134	U
14	B	1136	C
14	B	1138	U
14	B	1139	A
14	B	1140	A
14	B	1141	U
14	B	1142	A
14	B	1143	G
14	B	1147	A
14	B	1148	C
14	B	1151	G
14	B	1154	G
14	B	1155	A
14	B	1156	G
14	B	1158	G
14	B	1160	C
14	B	1162	C
14	B	1163	U
14	B	1170	A
14	B	1173	A
14	B	1174	U
14	B	1176	U
14	B	1178	C
14	B	1183	G

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Mol	Chain	Res	Type
14	B	1185	U
14	B	1186	A
14	B	1187	A
14	B	1189	C
14	B	1210	U
14	B	1213	C
14	B	1215	U
14	B	1217	U
14	B	1223	A
14	B	1229	G
14	B	1250	G
14	B	1258	A
14	B	1270	U
14	B	1273	G
14	B	1274	G
14	B	1276	G
14	B	1278	G
14	B	1285	A
14	B	1288	G
14	B	1291	A
14	B	1293	U
14	B	1294	G
14	B	1296	C
14	B	1300	G
14	B	1309	G
14	B	1310	A
14	B	1312	A
14	B	1313	G
14	B	1315	C
14	B	1318	G
14	B	1322	G
14	B	1333	A
14	B	1337	A
14	B	1338	U
14	B	1339	U
14	B	1350	U
14	B	1355	A
14	B	1364	C
14	B	1366	U
14	B	1378	U
14	B	1382	C
14	B	1383	G

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Mol	Chain	Res	Type
14	B	1389	U
14	B	1390	A
14	B	1402	A
14	B	1403	C
14	B	1405	G
14	B	1410	A
14	B	1412	G
14	B	1416	U
14	B	1417	G
14	B	1421	A
14	B	1424	A
14	B	1432	A
14	B	1437	U
14	B	1439	U
14	B	1447	A
14	B	1448	U
14	B	1449	A
14	B	1451	U
14	B	1452	C
14	B	1453	G
14	B	1454	U
14	B	1460	U
14	B	1462	G
14	B	1464	U
14	B	1466	G
14	B	1467	G
14	B	1471	A
14	B	1472	C
14	B	1473	G
14	B	1482	U
14	B	1484	G
14	B	1489	A
14	B	1490	G
14	B	1491	C
14	B	1494	G
14	B	1495	C
14	B	1496	G
14	B	1503	U
14	B	1504	U
14	B	1505	G
14	B	1507	A
14	B	1508	C

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Mol	Chain	Res	Type
14	B	1509	G
14	B	1510	U
14	B	1511	C
14	B	1515	G
14	B	1517	A
14	B	1518	G
14	B	1519	U
14	B	1520	A
14	B	1521	A
14	B	1524	C
14	B	1526	G
14	B	1527	A
14	B	1528	G
14	B	1530	A
14	B	1540	U
14	B	1541	C
14	B	1542	C
14	B	1544	G
14	B	1546	A
14	B	1548	U
14	B	1550	G
14	B	1556	G
14	B	1557	C
14	B	1559	G
14	B	1561	G
14	B	1568	U
14	B	1570	G
14	B	1572	G
14	B	1575	A
14	B	1578	A
14	B	1581	U
14	B	1582	U
14	B	1583	G
14	B	1584	U
14	B	1586	U
14	B	1590	C
14	B	1592	A
14	B	1598	U
14	B	1599	G
14	B	1605	A
14	B	1613	G
14	B	1614	A

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Mol	Chain	Res	Type
14	B	1616	A
14	B	1618	A
14	B	1625	U
14	B	1627	G
14	B	1628	A
14	B	1629	U
14	B	1630	A
14	B	1631	G
14	B	1633	A
14	B	1646	U
14	B	1647	A
14	B	1652	A
14	B	1653	A
14	B	1654	A
14	B	1656	C
14	B	1660	A
14	B	1676	A
14	B	1687	G
14	B	1690	A
14	B	1691	G
14	B	1692	C
14	B	1697	G
14	B	1698	A
14	B	1712	A
14	B	1718	G
14	B	1719	C
14	B	1721	A
14	B	1735	C
14	B	1736	U
14	B	1737	U
14	B	1738	C
14	B	1739	G
14	B	1740	G
14	B	1742	A
14	B	1743	G
14	B	1745	A
14	B	1747	G
14	B	1748	G
14	B	1751	G
14	B	1756	U
14	B	1759	G
14	B	1765	A

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Mol	Chain	Res	Type
14	B	1766	C
14	B	1772	G
14	B	1783	G
14	B	1785	G
14	B	1790	G
14	B	1791	G
14	B	1796	A
14	B	1800	A
14	B	1803	G
14	B	1808	U
14	B	1809	C
14	B	1811	A
14	B	1812	A
14	B	1813	A
14	B	1821	U
14	B	1826	G
14	B	1827	C
14	B	1828	U
14	B	1835	U
14	B	1836	A
14	B	1838	G
14	B	1839	G
14	B	1842	A
14	B	1843	U
14	B	1844	G
14	B	1845	U
14	B	1851	G
14	B	1853	C
14	B	1855	G
14	B	1856	A
14	B	1863	C
14	B	1866	A
14	B	1867	G
14	B	1873	G
14	B	1875	A
14	B	1878	U
14	B	1881	A
14	B	1884	G
14	B	1893	A
14	B	1896	U
14	B	1899	U
14	B	1900	G

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Mol	Chain	Res	Type
14	B	1902	G
14	B	1905	G
14	B	1911	A
14	B	1912	A
14	B	1915	G
14	B	1926	A
14	B	1933	G
14	B	1940	A
14	B	1941	C
14	B	1943	A
14	B	1944	U
14	B	1945	A
14	B	1946	A
14	B	1947	C
14	B	1957	G
14	B	1961	C
14	B	1965	A
14	B	1967	U
14	B	1982	U
14	B	1990	C
14	B	1991	G
14	B	1992	C
14	B	1994	C
14	B	1997	A
14	B	1998	A
14	B	1999	G
14	B	2002	G
14	B	2009	U
14	B	2012	G
14	B	2015	C
14	B	2018	U
14	B	2019	G
14	B	2020	U
14	B	2023	C
14	B	2024	A
14	B	2032	A
14	B	2034	U
14	B	2044	C
14	B	2048	G
14	B	2050	A
14	B	2058	A
14	B	2059	G

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Mol	Chain	Res	Type
14	B	2060	A
14	B	2063	C
14	B	2068	U
14	B	2070	C
14	B	2073	G
14	B	2079	G
14	B	2081	A
14	B	2082	C
14	B	2083	G
14	B	2086	A
14	B	2087	A
14	B	2088	G
14	B	2089	A
14	B	2090	C
14	B	2096	G
14	B	2102	U
14	B	2111	C
14	B	2114	G
14	B	2116	U
14	B	2119	U
14	B	2121	A
14	B	2123	A
14	B	2129	C
14	B	2131	C
14	B	2132	A
14	B	2133	G
14	B	2210	C
14	B	2214	G
14	B	2215	U
14	B	2218	G
14	B	2220	U
14	B	2225	A
14	B	2226	A
14	B	2230	G
14	B	2231	C
14	B	2232	A
14	B	2233	C
14	B	2237	U
14	B	2238	U
14	B	2240	U
14	B	2241	C
14	B	2242	G

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Mol	Chain	Res	Type
14	B	2246	U
14	B	2252	A
14	B	2253	C
14	B	2261	G
14	B	2265	G
14	B	2270	U
14	B	2278	G
14	B	2293	A
14	B	2296	A
14	B	2297	G
14	B	2307	G
14	B	2310	C
14	B	2312	C
14	B	2314	A
14	B	2315	A
14	B	2321	C
14	B	2330	G
14	B	2331	G
14	B	2333	U
14	B	2335	G
14	B	2337	A
14	B	2338	A
14	B	2339	U
14	B	2341	A
14	B	2346	U
14	B	2349	A
14	B	2352	G
14	B	2353	U
14	B	2354	A
14	B	2360	A
14	B	2362	A
14	B	2367	A
14	B	2370	U
14	B	2371	U
14	B	2374	C
14	B	2375	U
14	B	2377	C
14	B	2380	G
14	B	2381	A
14	B	2384	U
14	B	2385	A
14	B	2396	A

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Mol	Chain	Res	Type
14	B	2397	G
14	B	2398	G
14	B	2406	G
14	B	2409	G
14	B	2410	G
14	B	2411	A
14	B	2412	C
14	B	2414	U
14	B	2419	A
14	B	2429	U
14	B	2432	G
14	B	2433	C
14	B	2438	A
14	B	2440	G
14	B	2441	G
14	B	2452	A
14	B	2453	A
14	B	2456	G
14	B	2457	A
14	B	2458	U
14	B	2463	G
14	B	2467	C
14	B	2468	C
14	B	2470	C
14	B	2475	A
14	B	2490	C
14	B	2492	C
14	B	2497	G
14	B	2499	G
14	B	2502	C
14	B	2505	A
14	B	2521	G
14	B	2528	C
14	B	2529	G
14	B	2530	A
14	B	2531	U
14	B	2532	G
14	B	2533	U
14	B	2534	C
14	B	2545	A
14	B	2546	U
14	B	2547	C

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Mol	Chain	Res	Type
14	B	2554	C
14	B	2556	G
14	B	2557	U
14	B	2561	C
14	B	2562	G
14	B	2564	U
14	B	2567	C
14	B	2581	U
14	B	2583	C
14	B	2584	G
14	B	2591	A
14	B	2593	A
14	B	2594	G
14	B	2600	C
14	B	2610	G
14	B	2611	U
14	B	2613	C
14	B	2624	G
14	B	2631	U
14	B	2636	U
14	B	2640	U
14	B	2642	U
14	B	2656	A
14	B	2657	G
14	B	2661	A
14	B	2666	A
14	B	2673	C
14	B	2689	A
14	B	2690	G
14	B	2695	G
14	B	2712	G
14	B	2715	G
14	B	2716	U
14	B	2717	A
14	B	2741	G
14	B	2753	U
14	B	2760	A
14	B	2771	G
14	B	2775	A
14	B	2777	A
14	B	2784	A
14	B	2792	A

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Mol	Chain	Res	Type
14	B	2793	G
14	B	2796	C
14	B	2805	A
14	B	2807	G
14	B	2808	A
14	B	2809	G
14	B	2819	C
14	B	2821	U
14	B	2823	G
14	B	2824	G
14	B	2832	A
14	B	2841	A
14	B	2844	U
14	B	2845	G
14	B	2853	U
14	B	2854	A
14	B	2855	A
14	B	2881	C
14	B	2892	G
14	B	2906	G
14	B	2907	A
14	B	2913	G
14	B	2918	A
15	C	2	C
15	C	7	G
15	C	11	A
15	C	23	U
15	C	24	C
15	C	30	U
15	C	32	U
15	C	39	G
15	C	40	C
15	C	42	G
15	C	44	A
15	C	46	A
15	C	49	G
15	C	51	A
15	C	54	U
15	C	55	A
15	C	56	A
15	C	62	U
15	C	63	U

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Mol	Chain	Res	Type
15	C	64	A
15	C	71	A
15	C	77	G
15	C	83	U
15	C	84	U
15	C	87	G
15	C	88	U
15	C	94	U
15	C	106	U
15	C	107	U
15	C	108	G
15	C	114	C
42	D	8	U
42	D	10	G
42	D	14	A
42	D	16	U
42	D	19	G
42	D	20	U
42	D	22	G
42	D	23	A
42	D	28	G
42	D	29	G
42	D	33	U
42	D	38	A
42	D	41	C
42	D	44	G
42	D	46	G
42	D	47	U
42	D	48	C
42	D	49	C
42	D	50	U
42	D	52	G
42	D	56	C
42	D	58	A
42	D	59	U
42	D	60	U
42	D	61	C
42	D	62	C
42	D	70	G
42	D	74	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	52	A
1	A	279	C
1	A	336	C
1	A	467	U
1	A	480	G
1	A	908	C
1	A	935	G
1	A	969	U
1	A	970	U
1	A	1089	U
1	A	1200	G
1	A	1211	A
1	A	1354	C
1	A	1503	A
14	B	90	A
14	B	660	A
14	B	1503	U
14	B	1510	U
14	B	1940	A
14	B	2530	A
14	B	2533	U
14	B	2608	G
14	B	2783	U
15	C	55	A

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	193:C	O3'	203:G	P	30.87