



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 20, 2016 – 02:59 PM EST

PDB ID : 5LI0
EMDB ID: : EMD-4050
Title : 70S ribosome from Staphylococcus aureus
Authors : Khusainov, I.; Vicens, Q.; Bochler, A.; Grosse, F.; Myasnikov, A.; Menetret, J.F.; Chicher, J.; Marzi, S.; Romby, P.; Yusupova, G.; Yusupov, M.; Hashem, Y.
Deposited on : 2016-07-13
Resolution : 3.80 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

A user guide is available at

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

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

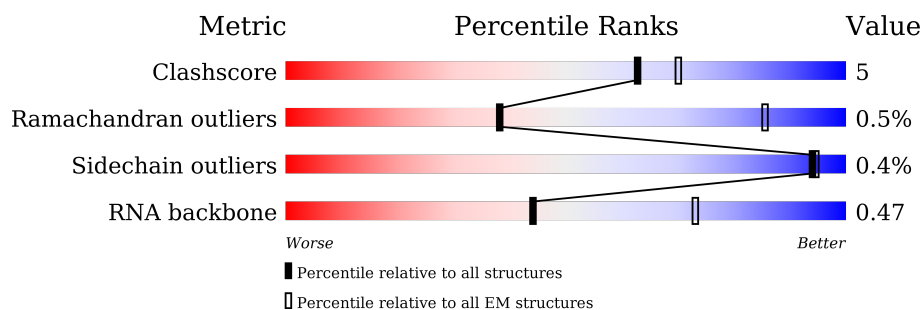
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	a	1547	79% 20% .
2	b	255	87% 12%
3	c	217	95% . .
4	d	199	98% ..
5	e	165	99% .
6	f	96	100%
7	g	150	96% ...
8	h	131	98% .











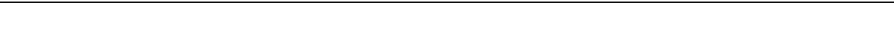

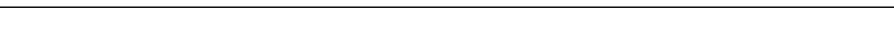
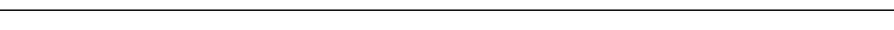
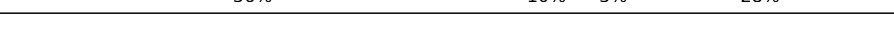


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Mol	Chain	Length	Quality of chain
9	i	128	99% .
10	j	102	100%
11	k	118	100%
12	l	135	100%
13	m	119	96% . .
14	n	60	97% .
15	o	88	100%
16	p	90	100%
17	q	86	95% . .
18	r	71	100%
19	s	84	96% .
20	t	80	100%
21	A	2918	60% 31% 8% .
22	B	114	58% 36% 6%
23	D	275	82% 17% .
24	E	218	87% 11% .
25	F	199	89% 10% .
26	G	166	95% 5%
27	H	164	87% 13%
28	M	145	94% 6%
29	N	122	84% 16% .
30	O	131	90% 8% .
31	P	141	91% 9%
32	Q	119	87% 13%
33	R	119	79% 21%

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Mol	Chain	Length	Quality of chain
34	S	110	 89% 11%
35	T	116	 89% 11%
36	U	102	 93% 7%
37	V	112	 90% 10%
38	W	89	 93% 6% .
39	X	100	 84% . 13%
40	Y	94	 80% 19% .
41	Z	82	 82% 18%
42	0	46	 83% 17%
43	1	65	 83% 17%
44	2	57	 95% 5%
45	3	84	 54% 36% 10% .
46	4	56	 89% 11%
47	5	39	 56% 10% 5% 28%
48	6	44	 75% 23% .
49	7	60	 77% 23%
50	8	37	 84% 16%

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 140825 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	1547	Total	C	N	O	P	0	0
			33126	14790	6036	10753	1547		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	224	Total	C	N	O	S	0	0
			1802	1147	315	333	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	208	Total	C	N	O	S	0	0
			1638	1032	306	298	2		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	197	Total	C	N	O	S	0	0
			1600	1009	300	289	2		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	165	Total	C	N	O	S	0	0
			1239	775	229	233	2		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	96	Total	C	N	O	S	0	0
			799	503	139	154	3		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	147	Total	C	N	O	S	0	0
			1189	744	227	214	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	128	Total	C	N	O	S	0	0
			1017	629	203	184	1		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	102	Total	C	N	O	S	0	0
			813	512	148	150	3		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	118	Total	C	N	O	S	0	0
			881	543	169	166	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	135	Total	C	N	O	S	0	0
			1063	658	218	185	2		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	119	Total	C	N	O	S	0	0
			946	581	188	176	1		

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			502	317	100	80	5		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			738	454	153	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	86	Total	C	N	O	S	0	0
			707	447	126	133	1		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	71	Total	C	N	O	S	0	0
			590	372	115	100	3		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	84	Total	C	N	O	S	0	0
			678	434	120	122	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total	C	N	O	S	0	0
			607	367	119	119	2		

- Molecule 21 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A	2914	Total	C	N	O	P	0	0
			62475	27892	11424	20245	2914		

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B	114	Total	C	N	O	P	0	0
			2427	1086	436	792	113		

- Molecule 23 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	275	Total	C	N	O	S	0	0
			2104	1309	417	373	5		

- Molecule 24 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E	218	Total	C	N	O	S	0	0
			1649	1030	304	310	5		

- Molecule 25 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	199	Total	C	N	O	S	0	0
			1525	955	281	287	2		

- Molecule 26 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	G	166	Total	C	N	O	S	0	0
			1312	832	223	251	6		

- Molecule 27 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	164	Total	C	N	O	S	0	0
			1285	799	232	251	3		

- Molecule 28 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	M	145	Total	C	N	O	S	0	0
			1151	717	211	220	3		

- Molecule 29 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 30 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	O	131	Total	C	N	O	S	0	0
			998	618	197	182	1		

- Molecule 31 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	P	141	Total	C	N	O	S	0	0
			1122	717	211	190	4		

- Molecule 32 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Q	119	Total	C	N	O	S	0	0
			940	575	181	183	1		

- Molecule 33 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	R	119	Total	C	N	O	S	0	0
			922	574	174	173	1		

- Molecule 34 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S	110	Total	C	N	O	S	0	0
			886	557	177	151	1		

- Molecule 35 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	T	116	Total	C	N	O	S	0	0
			944	593	189	158	4		

- Molecule 36 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	U	102	Total	C	N	O	S	0	0
			799	506	142	150	1		

- Molecule 37 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	V	112	Total	C	N	O	S	0	0
			863	537	164	159	3		

- Molecule 38 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	W	89	Total	C	N	O	S	0	0
			726	457	130	135	4		

- Molecule 39 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	X	87	Total	C	N	O	S	0	0
			669	423	122	123	1		

- Molecule 40 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 41 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Z	82	Total	C	N	O	0	0
			627	386	122	119		

- Molecule 42 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	0	46	Total	C	N	O	0	0
			374	231	83	60		

- Molecule 43 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	1	65	Total	C	N	O	0	0
			537	330	101	106		

- Molecule 44 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	2	57	Total	C	N	O	0	0
			442	274	83	85		

- Molecule 45 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3	83	Total	C	N	O	S	0	0
			677	430	116	128	3		

- Molecule 46 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4	56	Total	C	N	O	S	0	0
			444	268	92	79	5		

- Molecule 47 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5	28	Total	C	N	O	S	0	0
			229	137	45	43	4		

- Molecule 48 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	6	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

- Molecule 49 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	60	Total	C	N	O	S	0	0
			488	300	108	78	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 51 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	A	29	Total	Mg	0
			29	29	
51	a	2	Total	Mg	0
			2	2	

- Molecule 52 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		AltConf
52	A	9	Total	O	0
			9	9	

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	8	1	Total	Zn	0
			1	1	

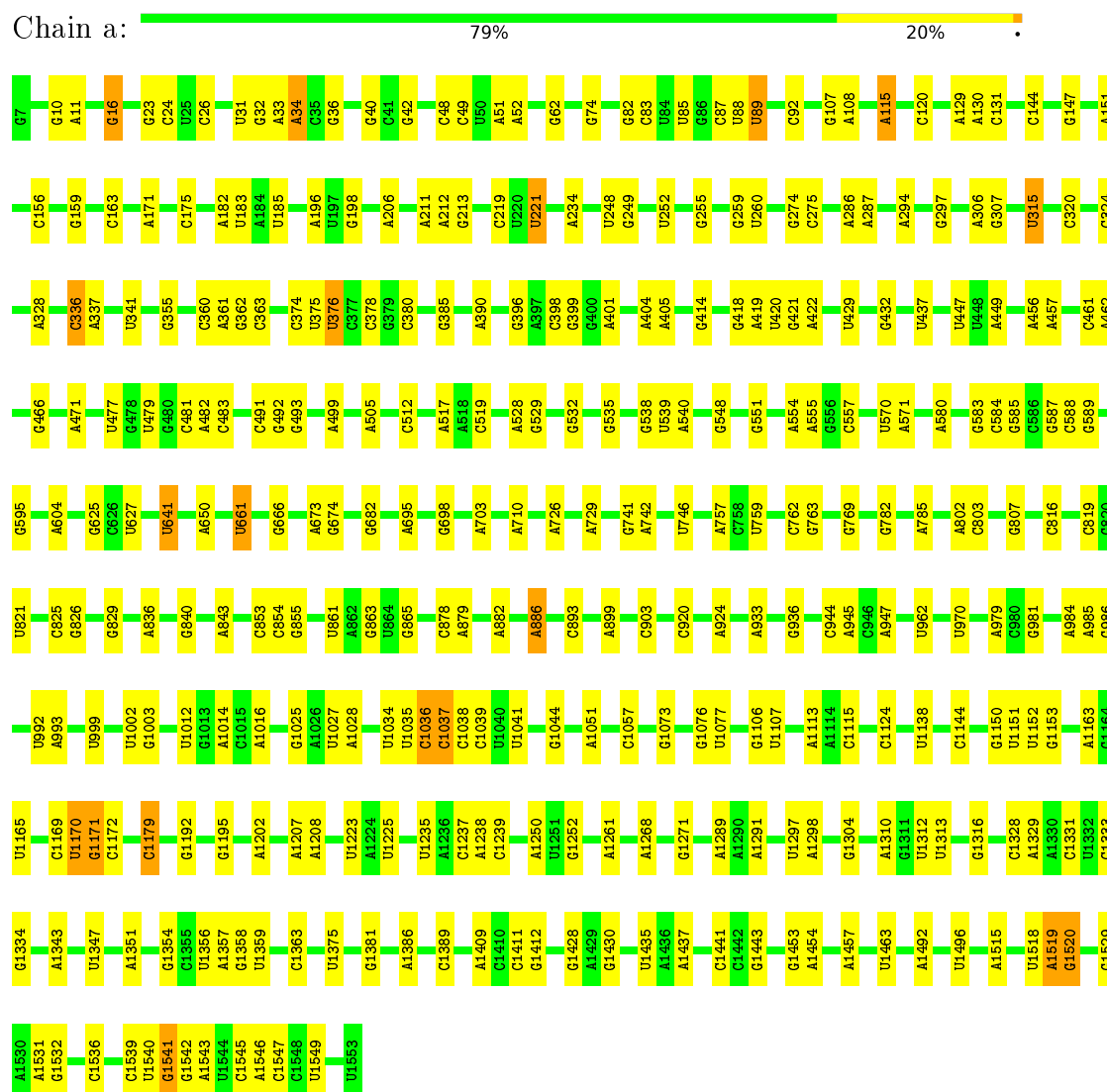
- Molecule 54 is water.

Mol	Chain	Residues	Atoms		AltConf
54	a	12	Total	O	0
			12	12	
54	A	143	Total	O	0
			143	143	
54	D	4	Total	O	0
			4	4	
54	T	2	Total	O	0
			2	2	
54	U	1	Total	O	0
			1	1	

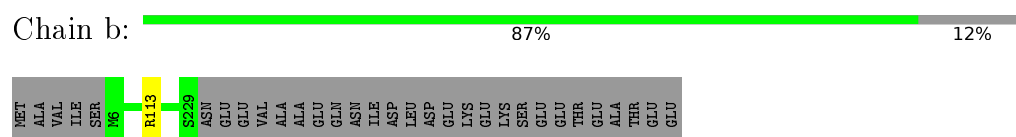
3 Residue-property plots

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

• Molecule 1: 16S ribosomal RNA

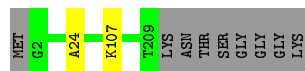


• Molecule 2: 30S ribosomal protein S2



- Molecule 3: 30S ribosomal protein S3

Chain c:  95% ..



- Molecule 4: 30S ribosomal protein S4

Chain d:  98% ..



- Molecule 5: 30S ribosomal protein S5

Chain e:  99% .



- Molecule 6: 30S ribosomal protein S6

Chain f:  100%

There are no outlier residues recorded for this chain.

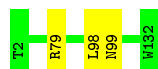
- Molecule 7: 30S ribosomal protein S7

Chain g:  96% ...



- Molecule 8: 30S ribosomal protein S8

Chain h:  98% .



- Molecule 9: 30S ribosomal protein S9

Chain i:  99% .



- Molecule 10: 30S ribosomal protein S10

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: 30S ribosomal protein S11

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: 30S ribosomal protein S12

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: 30S ribosomal protein S13

Chain m:  96% ..



- Molecule 14: 30S ribosomal protein S14 type Z

Chain n:  97% .



- Molecule 15: 30S ribosomal protein S15

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: 30S ribosomal protein S16

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 30S ribosomal protein S17

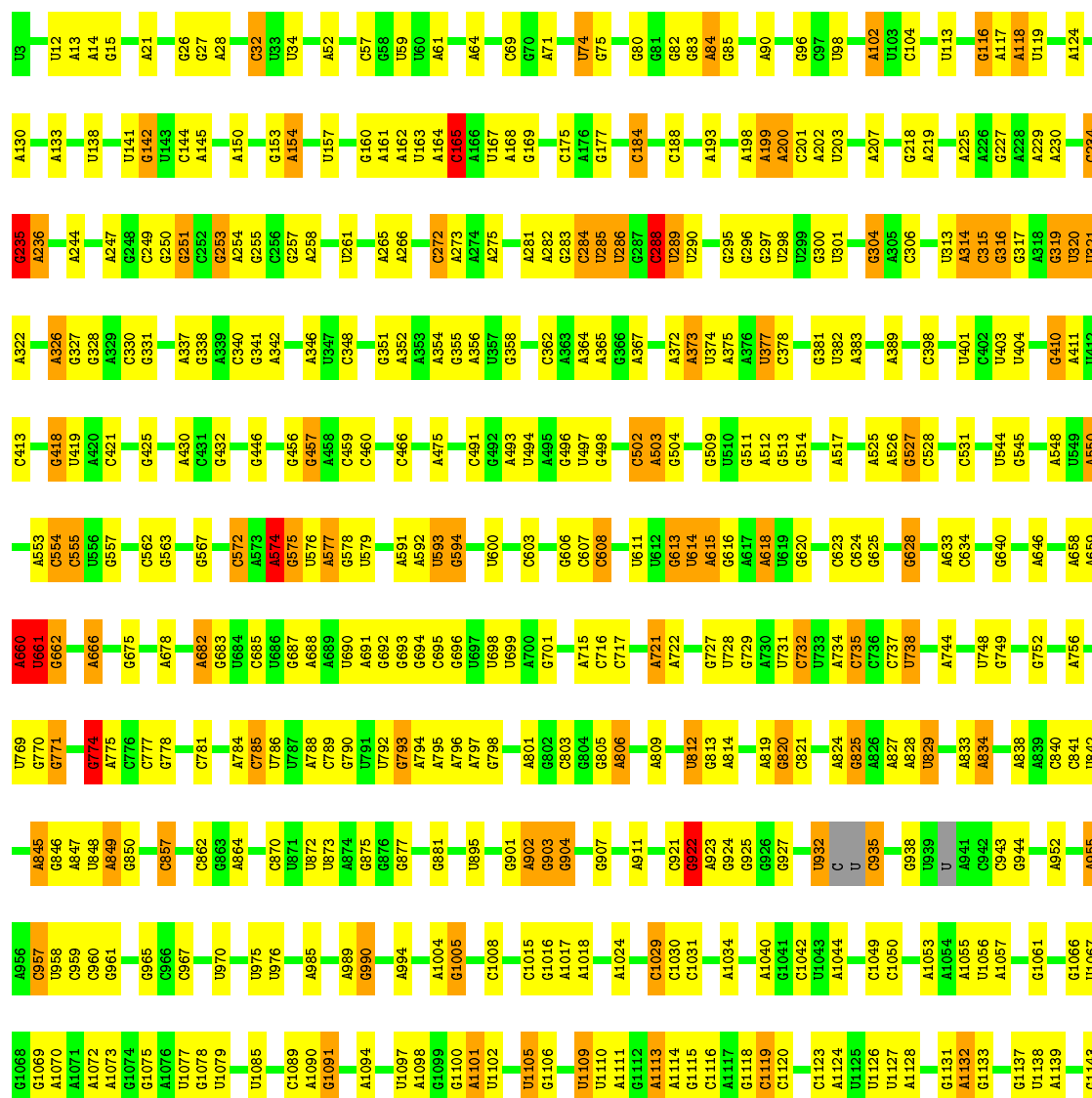
Chain q:  95% ..



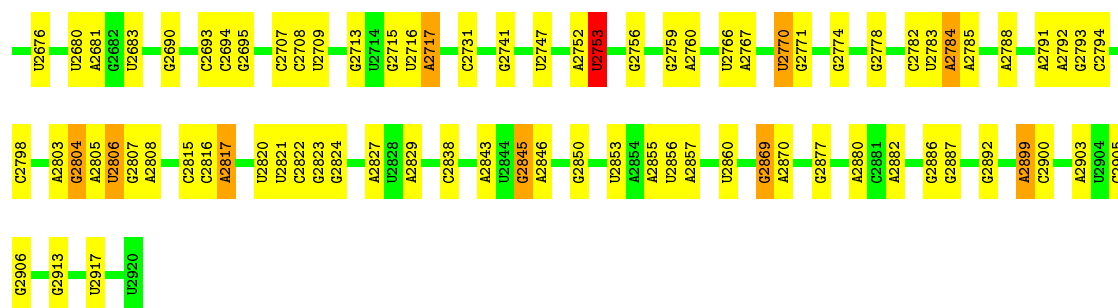
- Molecule 18: 30S ribosomal protein S18

Chain r:  100%

There are no outlier residues recorded for this chain.

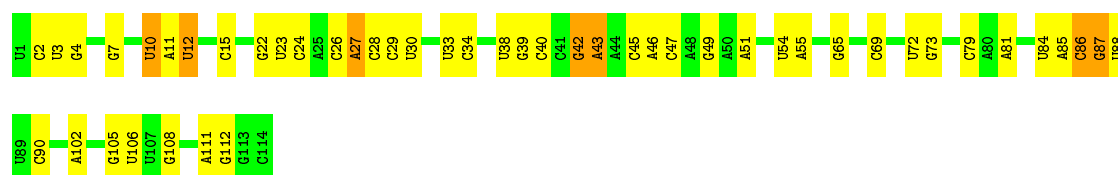


U2589	U2484	C2399	U2207	C2105	U2022	A	A1818	C1716	A1617	U1525	C1435	G1265	C1144
U2593	U2485	U2400	A2208	G2110	C2023	C1941	G1819	G1717	A1618	G1526	C1436	G1266	U1145
G2594	C2401	G2402	G2212	C2111	A2024	G1949	C1824	G1718	C1621	A1527	U1437	C1268	C1146
C2493	C2403	A2404	U2216	A2117	G2027	U1950	G1826	A1720	U1625	G1534	A1449	G1271	A1150
C2493	C2403	A2405	G2217	U2118	C2033	C1951	G1827	A1721	U1629	G1535	A1450	U1272	G1154
G2497	A2226	G2410	A2227	U2119	U2034	G1956	A1829	A1733	A1630	C1536	U1451	G1274	G1156
C2493	C2228	A2411	C2227	G2120	G2035	U1958	A1830	U1737	A1631	A1537	G1452	G1275	G1157
U2500	G2228	C2412	C2228	G2120	G2039	U1959	A1831	G1738	A1632	U1540	G1453	G1276	U1158
G2505	C2229	A2415	C2229	C2126	A2040	G1960	G1832	G1739	A1633	C1541	U1454	C1277	G1159
C2606	G2230	G2416	G2230	G2127	A2041	C1961	A1833	G1740	A1634	C1542	U1455	G1278	U1163
C2609	C2231	U2417	C2231	G2128	C2044	G1962	G1834	G1741	A1635	U1458	A1458	G1279	U1163
C2613	A2232	G2418	C2232	C2129	U2049	A1963	A1835	A1742	U1636	U1551	A1459	U1280	A1170
G2613	C2233	U2419	C2233	G2133	U2049	A1964	A1836	G1746	U1640	U1552	G1462	A1285	A1171
G2617	C2236	C2429	U2237	G2137	A2050	G1968	U1843	C1762	C1648	G1553	A1463	G1286	A1172
U2618	U2237	C2430	U2238	U2138	C2051	C1969	G1844	A1771	C1656	A1554	U1464	U1287	U1174
G2615	A2239	C2433	A2239	A2139	U2061	U1970	U1845	G1759	C1657	G1555	G1465	G1289	G1176
A2616	U2240	C2435	C2241	C2140	A2057	U1971	A1846	C1768	C1658	U1561	G1470	A1291	A1177
C2619	C2241	C2437	C2241	G2143	A2058	U1972	U1847	C1769	C1659	C1562	C1471	U1292	U1178
U2620	A2250	A2337	A2250	A2144	U2059	U1978	U1854	C1770	C1665	U1567	C1472	U1293	C1179
C2621	G2251	A2338	G2251	U2145	A2060	A1979	G1855	A1771	C1656	U1568	G1487	G1294	G1183
C2622	A2252	U2339	A2252	A2146	U2061	U1980	A1856	G1772	C1657	G1569	A1488	C1296	U1184
G2623	C2451	C2450	C2451	G2147	G2062	U1981	A1857	C1772	C1658	G1570	A1489	G1297	U1185
G2624	A2452	A2452	G2255	A2153	C2063	U1982	G1858	G1775	C1659	G1571	G1490	G1298	A1186
A2625	C2453	C2453	G2255	A2153	C2063	U1983	G1859	G1775	C1660	U1575	C1491	G1302	A1187
C2628	C2454	C2454	C2259	C2154	A2069	U1984	U1860	G1777	C1661	A1576	G1492	A1303	A1195
A2629	G2455	C2455	A2260	C2155	C2070	A1979	G1861	C1778	C1662	A1577	U1493	G1304	C1196
C2630	U2456	C2456	G2261	C2156	U2071	C1987	A1862	C1778	C1663	A1578	G1494	C1305	C1197
C2633	U2457	U2458	C2262	U2157	C2074	C1988	C1865	G1783	C1664	G1579	G1495	C1306	G1198
U2636	U2459	C2459	C2263	G2160	C2074	U1990	U1869	G1784	C1665	A1580	A1497	G1309	G1201
C2637	A2460	C2460	G2264	A2161	C2077	G1991	C1870	G1785	C1666	U1581	U1498	A1310	G1214
C2638	A2462	C2462	C2265	A2162	A2078	C1994	U1877	U1788	C1667	U1582	U1499	A1311	C1215
C2639	G2463	C2463	C2266	G2165	G2079	U1997	U1891	G1789	C1668	G1583	G1500	A1312	U1216
U2640	U2464	C2464	C2267	A2166	C2079	G1999	U1892	G1790	C1669	A1584	A1502	G1313	U1217
A2641	U2465	C2465	C2268	G2167	G2082	U2003	G1893	G1791	C1670	U1585	U1503	A1314	G1218
C2644	A2466	C2466	C2269	G2168	A2087	C2001	G1894	C1792	C1671	U1586	U1504	G1315	G1219
G2648	U2467	C2467	U2271	C2172	C2082	C2002	C1895	C1794	C1672	G1587	U1505	G1316	G1228
U2649	C2468	C2468	U2272	U2173	G2083	G2003	U1896	U1788	C1673	U1588	C1506	A1320	A1228
U2650	G2469	C2469	A2274	A2174	C2083	C2004	U1897	A1800	C1674	A1589	U1507	G1323	A1233
G2651	C2470	C2470	C2275	G2175	A2088	A2004	G1898	C1801	C1675	U1590	G1508	A1324	G1234
C2652	G2471	C2471	U2276	A2185	C2090	A2008	U1899	U1802	C1676	U1591	C1509	U1325	C1235
G2657	G2472	C2472	G2277	G2186	C2092	A2008	U1900	U1806	C1677	U1592	U1510	G1326	G1236
C2658	G2473	C2473	G2278	G2187	C2093	A2008	U1901	U1807	C1678	U1593	U1511	C1327	U1248
U2659	U2474	C2474	U2279	C2188	G2094	A2008	U1902	U1808	C1679	U1594	U1512	G1328	U1249
C2661	A2475	C2475	U2280	G2189	U2095	G2013	A1926	A1809	C1680	U1595	G1515	A1421	G1250
U2664	U2476	C2476	C2281	U2194	G2096	G2014	U1927	U1810	C1681	U1596	G1516	G1422	A1251
C2665	U2477	C2477	U2282	G2195	G2097	C2015	A1928	U1811	C1682	U1597	G1517	C1423	G1252
A2666	G2478	C2478	C2283	G2196	U2098	A2016	U1929	A1812	C1683	U1598	G1518	G1336	A1253
G2667	U2479	C2479	C2284	G2197	G2099	C2017	G1933	A1813	C1684	U1599	U1519	A1337	U1338
C2673	A2480	C2480	C2285	G2198	C2100	U2018	G1934	A1814	C1685	U1600	G1520	G1426	A1258
C2673	G2481	C2481	C2286	G2199	U2101	G2019	U1935	C1815	C1686	U1601	A1521	U1434	
	C2482	C2482	C2287	A2198	U2102	U2020	A1939	A1816	C1687	U1602	U1522		
	C2483	C2483	C2288	C2206		C2021		C1817	C1688	U1603			



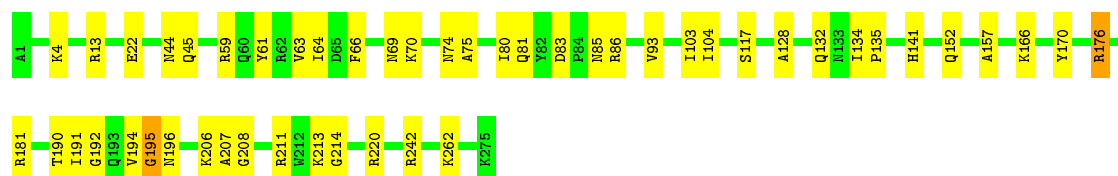
- Molecule 22: 5S ribosomal RNA

Chain B: 58% 36% 6%



- Molecule 23: 50S ribosomal protein L2

Chain D: 82% 17%



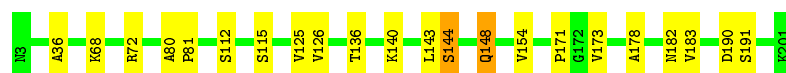
- Molecule 24: 50S ribosomal protein L3

Chain E: 87% 11%



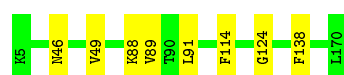
- Molecule 25: 50S ribosomal protein L4

Chain F: 89% 10%




- Molecule 26: 50S ribosomal protein L5

Chain G: 95% 5%



- Molecule 27: 50S ribosomal protein L6

Chain H:  87% 13%




- Molecule 28: 50S ribosomal protein L13

Chain M:  94% 6%



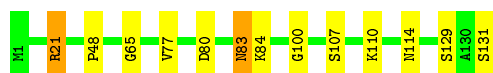
- Molecule 29: 50S ribosomal protein L14

Chain N:  84% 16%



- Molecule 30: 50S ribosomal protein L15

Chain O:  90% 8%




- Molecule 31: 50S ribosomal protein L16

Chain P:  91% 9%




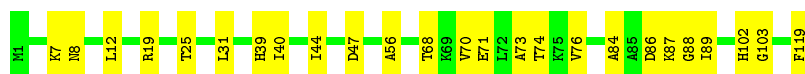
- Molecule 32: 50S ribosomal protein L17

Chain Q:  87% 13%




- Molecule 33: 50S ribosomal protein L18

Chain R:  79% 21%



- Molecule 34: 50S ribosomal protein L19

Chain S:  89% 11%



- Molecule 35: 50S ribosomal protein L20

Chain T: 89% 11%



- Molecule 36: 50S ribosomal protein L21

Chain U: 93% 7%



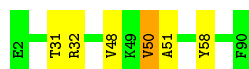
- Molecule 37: 50S ribosomal protein L22

Chain V: 90% 10%



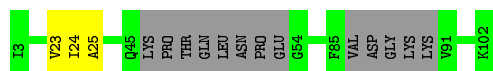
- Molecule 38: 50S ribosomal protein L23

Chain W: 93% 6%



- Molecule 39: 50S ribosomal protein L24

Chain X: 84% 13%



- Molecule 40: 50S ribosomal protein L25

Chain Y: 80% 19%




- Molecule 41: 50S ribosomal protein L27

Chain Z: 82% 18%




- Molecule 42: 50S ribosomal protein L28

Chain 0:  83% 17%



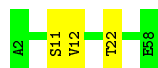
- Molecule 43: 50S ribosomal protein L29

Chain 1:  83% 17%



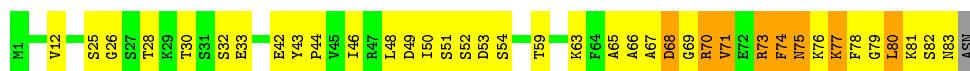
- Molecule 44: 50S ribosomal protein L30

Chain 2:  95% 5%



- Molecule 45: 50S ribosomal protein L31 type B

Chain 3:  54% 36% 10%



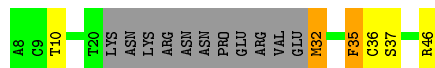
- Molecule 46: 50S ribosomal protein L32

Chain 4:  89% 11%



- Molecule 47: 50S ribosomal protein L33 2

Chain 5:  56% 10% 5% 28%




- Molecule 48: 50S ribosomal protein L34

Chain 6:  75% 23%

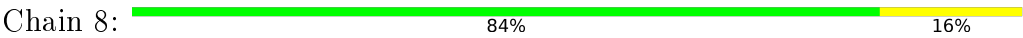


- Molecule 49: 50S ribosomal protein L35

Chain 7:  77% 23%



- Molecule 50: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	110000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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, ZN, O

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	0.89	0/37086	1.18	125/57833 (0.2%)
10	j	0.43	0/825	0.67	0/1110
11	k	0.46	0/896	0.69	0/1207
12	l	0.53	0/1080	0.78	0/1445
13	m	0.41	0/953	0.77	0/1275
14	n	0.54	0/512	0.70	0/678
15	o	0.51	0/747	0.68	0/996
16	p	0.55	0/723	0.67	0/971
17	q	0.57	0/715	0.79	0/955
18	r	0.45	0/599	0.72	0/797
19	s	0.41	0/696	0.73	0/934
2	b	0.39	0/1829	0.63	1/2454 (0.0%)
20	t	0.44	0/607	0.61	0/810
21	A	2.04	70/69965 (0.1%)	1.80	586/109115 (0.5%)
22	B	0.85	0/2714	1.14	4/4228 (0.1%)
23	D	0.73	0/2139	0.75	0/2869
24	E	0.67	0/1673	0.69	0/2243
25	F	0.62	0/1548	0.66	0/2088
26	G	0.42	0/1327	0.70	1/1780 (0.1%)
27	H	0.47	0/1303	0.65	0/1757
28	M	0.65	0/1173	0.65	0/1578
29	N	0.71	0/927	0.76	0/1243
3	c	0.44	0/1661	0.64	0/2233
30	O	0.60	0/1011	0.80	1/1344 (0.1%)
31	P	0.66	0/1146	0.75	0/1536
32	Q	0.56	0/943	0.69	0/1259
33	R	0.53	0/931	0.69	0/1244
34	S	0.66	0/898	0.72	0/1199
35	T	0.73	0/956	0.77	1/1265 (0.1%)
36	U	0.63	0/809	0.69	1/1080 (0.1%)
37	V	0.63	0/871	0.76	0/1171
38	W	0.60	0/734	0.71	0/978

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	X	0.49	0/673	0.64	0/893
4	d	0.51	0/1629	0.68	0/2185
40	Y	0.50	0/746	0.69	0/1000
41	Z	0.72	0/633	0.77	0/838
42	0	0.54	0/379	0.78	0/504
43	1	0.49	0/538	0.63	0/714
44	2	0.58	0/444	0.66	0/597
45	3	0.46	0/694	0.74	1/930 (0.1%)
46	4	0.65	0/451	0.73	0/599
47	5	0.51	0/230	0.79	0/303
48	6	0.72	0/377	0.79	0/491
49	7	0.61	0/492	0.87	0/643
5	e	0.55	0/1253	0.69	0/1687
50	8	0.73	0/300	0.72	1/393 (0.3%)
6	f	0.60	0/810	0.63	0/1085
7	g	0.41	0/1207	0.65	0/1625
8	h	0.57	0/1044	0.72	0/1401
9	i	0.41	0/1033	0.70	0/1386
All	All	1.48	70/152930 (0.0%)	1.43	722/228949 (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
13	m	0	5
14	n	0	2
17	q	0	3
19	s	0	3
23	D	0	1
24	E	0	6
25	F	0	5
26	G	0	4
28	M	0	2
29	N	0	1
3	c	0	2
30	O	0	4
31	P	0	1
33	R	0	2
34	S	0	1
35	T	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	U	0	1
38	W	0	2
40	Y	0	1
41	Z	0	4
45	3	0	3
46	4	0	2
47	5	0	1
48	6	0	2
49	7	0	2
5	e	0	1
7	g	0	3
8	h	0	2
All	All	0	67

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1288	G	C6-N1	171.20	2.59	1.39
21	A	1288	G	N3-C4	147.91	2.38	1.35
21	A	857	C	C5-C6	139.70	2.46	1.34
21	A	1288	G	N1-C2	138.56	2.48	1.37
21	A	1288	G	C2-N3	124.17	2.32	1.32
21	A	1288	G	C5-C4	122.56	2.24	1.38
21	A	1828	U	C2-N3	119.86	2.21	1.37
21	A	857	C	C2-N3	104.60	2.19	1.35
21	A	1828	U	N1-C2	98.17	2.27	1.38
21	A	1288	G	C5-C6	96.06	2.38	1.42
21	A	1828	U	N3-C4	92.48	2.21	1.38
21	A	1828	U	N1-C6	90.20	2.19	1.38
21	A	1828	U	C4-C5	83.56	2.18	1.43
21	A	1828	U	C5-C6	81.51	2.07	1.34
21	A	2230	G	C1'-N9	63.59	2.44	1.48
21	A	2230	G	N9-C4	38.43	1.68	1.38
21	A	857	C	N3-C4	37.14	1.59	1.33
21	A	2230	G	N9-C8	33.27	1.61	1.37
21	A	2230	G	N7-C5	-21.24	1.26	1.39
21	A	857	C	C4-C5	-18.54	1.28	1.43
21	A	1510	U	O3'-P	-17.20	1.40	1.61
21	A	1288	G	C8-N7	12.87	1.38	1.30
21	A	857	C	C2-O2	12.24	1.35	1.24
21	A	1288	G	N9-C4	-10.87	1.29	1.38
21	A	857	C	N1-C6	-10.07	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	2002	G	N3-C4	-9.93	1.28	1.35
21	A	1511	C	O3'-P	7.92	1.70	1.61
21	A	1858	G	N3-C4	-7.06	1.30	1.35
21	A	1815	C	C4-C5	-6.72	1.37	1.43
21	A	2002	G	C2-N3	-6.56	1.27	1.32
21	A	2230	G	N3-C4	6.12	1.39	1.35
21	A	1857	C	C2-N3	5.87	1.40	1.35
21	A	806	A	C5-C6	-5.85	1.35	1.41
21	A	2606	C	N1-C6	-5.80	1.33	1.37
21	A	824	A	N9-C4	-5.78	1.34	1.37
21	A	1024	A	N9-C4	-5.68	1.34	1.37
21	A	1031	C	C4-C5	-5.66	1.38	1.43
21	A	864	A	N9-C4	-5.62	1.34	1.37
21	A	2230	G	C8-N7	-5.54	1.27	1.30
21	A	1857	C	C4-C5	-5.52	1.38	1.43
21	A	1984	C	C4-C5	-5.51	1.38	1.43
21	A	903	G	N9-C4	-5.50	1.33	1.38
21	A	2644	C	N1-C6	-5.49	1.33	1.37
21	A	2230	G	C2'-C1'	5.48	1.59	1.53
21	A	2616	A	N9-C4	-5.46	1.34	1.37
21	A	2002	G	C2-N2	-5.46	1.29	1.34
21	A	2082	C	N1-C6	-5.43	1.33	1.37
21	A	2091	C	C4-C5	-5.43	1.38	1.43
21	A	1029	C	C4-C5	-5.41	1.38	1.43
21	A	2002	G	C5-C4	-5.41	1.34	1.38
21	A	2483	C	C4-C5	-5.38	1.38	1.43
21	A	1858	G	N9-C4	-5.33	1.33	1.38
21	A	2470	C	N1-C6	-5.30	1.33	1.37
21	A	903	G	N3-C4	-5.29	1.31	1.35
21	A	2002	G	N9-C4	-5.28	1.33	1.38
21	A	1708	A	N7-C5	-5.28	1.36	1.39
21	A	57	C	C4-C5	-5.27	1.38	1.43
21	A	555	C	C4-C5	-5.26	1.38	1.43
21	A	2443	C	C4-C5	-5.18	1.38	1.43
21	A	1858	G	C2-N3	-5.18	1.28	1.32
21	A	2001	C	N1-C6	-5.17	1.34	1.37
21	A	2474	G	N9-C8	-5.15	1.34	1.37
21	A	1435	C	C4-C5	-5.12	1.38	1.43
21	A	735	C	C4-C5	-5.11	1.38	1.43
21	A	2633	C	C4-C5	-5.09	1.38	1.43
21	A	1618	A	N9-C4	-5.06	1.34	1.37
21	A	1768	C	N1-C6	-5.02	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1029	C	N3-C4	-5.02	1.30	1.33
21	A	201	C	C4-C5	-5.01	1.39	1.43
21	A	567	G	N7-C5	-5.00	1.36	1.39

All (722) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	857	C	N3-C4-C5	-238.20	26.62	121.90
21	A	857	C	C6-N1-C2	-227.33	29.37	120.30
21	A	2230	G	C8-N9-C4	-102.39	65.45	106.40
21	A	857	C	C2-N3-C4	83.55	161.67	119.90
21	A	857	C	C5-C6-N1	82.07	162.03	121.00
21	A	2230	G	N7-C8-N9	64.31	145.25	113.10
21	A	2230	G	N9-C4-C5	54.49	127.19	105.40
21	A	1288	G	C4-C5-N7	-52.34	89.86	110.80
21	A	857	C	C4-C5-C6	44.75	139.78	117.40
21	A	2230	G	N3-C4-C5	-42.21	107.50	128.60
21	A	2002	G	N3-C2-N2	-29.40	99.32	119.90
21	A	1288	G	C2-N3-C4	29.39	126.59	111.90
21	A	1288	G	N7-C8-N9	28.34	127.27	113.10
21	A	2230	G	C2-N3-C4	28.10	125.95	111.90
21	A	857	C	N3-C4-N4	27.49	137.24	118.00
21	A	1288	G	N1-C6-O6	-26.80	103.82	119.90
21	A	1288	G	C5-C6-O6	26.18	144.31	128.60
21	A	1288	G	C6-C5-N7	24.35	145.01	130.40
21	A	1288	G	N1-C2-N3	-20.86	111.39	123.90
21	A	1288	G	N3-C4-N9	20.13	138.08	126.00
21	A	2230	G	C4-C5-C6	19.20	130.32	118.80
21	A	1288	G	C5-N7-C8	18.78	113.69	104.30
21	A	1288	G	N3-C2-N2	18.02	132.51	119.90
21	A	2230	G	N9-C1'-C2'	17.32	136.51	114.00
21	A	857	C	C6-N1-C1'	17.22	141.46	120.80
21	A	1288	G	N3-C4-C5	-16.72	120.24	128.60
21	A	1858	G	N3-C2-N2	-16.17	108.58	119.90
21	A	2002	G	N1-C2-N2	16.09	130.68	116.20
21	A	2230	G	C8-N9-C1'	16.06	147.87	127.00
21	A	2002	G	C5-C6-O6	-15.95	119.03	128.60
21	A	2230	G	C5-N7-C8	-15.75	96.43	104.30
21	A	2230	G	C4-N9-C1'	15.52	146.68	126.50
21	A	857	C	N1-C2-N3	15.31	129.92	119.20
21	A	2002	G	C6-N1-C2	-14.81	116.21	125.10
21	A	1857	C	C2-N1-C1'	14.17	134.39	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	857	C	C5-C4-N4	-13.65	110.65	120.20
21	A	1511	C	OP2-P-O3'	13.65	135.22	105.20
21	A	1857	C	C6-N1-C2	-13.06	115.07	120.30
21	A	2230	G	C4-C5-N7	-12.92	105.63	110.80
21	A	806	A	C5-C6-N6	-12.01	114.09	123.70
21	A	1858	G	N1-C2-N2	11.65	126.68	116.20
21	A	1510	U	OP2-P-O3'	11.51	130.53	105.20
21	A	1510	U	P-O3'-C3'	-11.27	106.18	119.70
21	A	806	A	N1-C6-N6	11.22	125.33	118.60
21	A	2416	G	C5-C6-O6	-11.19	121.89	128.60
21	A	2002	G	N1-C6-O6	11.01	126.50	119.90
21	A	1235	C	C2-N3-C4	10.63	125.21	119.90
21	A	2230	G	C6-C5-N7	-10.60	124.04	130.40
21	A	1288	G	C4-C5-C6	10.51	125.11	118.80
21	A	2230	G	C6-N1-C2	-10.48	118.81	125.10
21	A	2416	G	N1-C6-O6	10.45	126.17	119.90
21	A	1235	C	N3-C4-C5	-10.03	117.89	121.90
21	A	857	C	N3-C2-O2	-9.94	114.94	121.90
21	A	1843	U	C2-N1-C1'	9.88	129.56	117.70
21	A	1828	U	N1-C2-N3	-9.81	109.02	114.90
21	A	1857	C	N3-C4-N4	9.74	124.82	118.00
21	A	2002	G	N1-C2-N3	9.74	129.75	123.90
21	A	1857	C	C5-C6-N1	9.48	125.74	121.00
21	A	2002	G	N9-C4-C5	9.42	109.17	105.40
21	A	903	G	N3-C4-N9	-9.41	120.35	126.00
21	A	2816	C	O4'-C1'-N1	9.41	115.73	108.20
21	A	1288	G	N9-C4-C5	-9.31	101.68	105.40
21	A	2105	C	N1-C2-O2	9.21	124.43	118.90
21	A	1857	C	C6-N1-C1'	-9.11	109.86	120.80
21	A	1858	G	N3-C4-N9	-9.06	120.56	126.00
21	A	806	A	C4-C5-N7	9.03	115.21	110.70
21	A	1656	C	N1-C2-O2	8.88	124.23	118.90
21	A	1364	C	C5-C4-N4	-8.84	114.01	120.20
21	A	1857	C	C5-C4-N4	-8.83	114.02	120.20
21	A	1004	A	N1-C6-N6	8.77	123.86	118.60
1	a	1536	C	C6-N1-C2	-8.76	116.80	120.30
21	A	857	C	N1-C2-O2	-8.69	113.68	118.90
21	A	806	A	C5-N7-C8	-8.56	99.62	103.90
21	A	2290	C	C6-N1-C2	-8.56	116.88	120.30
21	A	1235	C	C6-N1-C2	-8.51	116.90	120.30
21	A	2302	C	N1-C2-O2	8.51	124.01	118.90
21	A	737	C	C6-N1-C2	-8.47	116.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	735	C	C6-N1-C2	-8.46	116.92	120.30
21	A	165	C	C6-N1-C2	-8.40	116.94	120.30
21	A	1870	C	C6-N1-C2	-8.30	116.98	120.30
21	A	1368	C	N1-C2-O2	8.30	123.88	118.90
21	A	2063	C	C2-N1-C1'	8.28	127.90	118.80
21	A	201	C	N1-C2-O2	8.25	123.85	118.90
1	a	1179	C	C2-N1-C1'	8.21	127.83	118.80
22	B	79	C	C5-C4-N4	-8.19	114.47	120.20
1	a	1179	C	N1-C2-O2	8.18	123.81	118.90
21	A	1511	C	OP1-P-O3'	-8.06	87.47	105.20
21	A	1350	U	C2-N1-C1'	8.03	127.34	117.70
21	A	1815	C	C5-C4-N4	-8.00	114.60	120.20
21	A	1895	C	N3-C2-O2	-7.99	116.31	121.90
21	A	623	C	C5-C4-N4	-7.99	114.61	120.20
21	A	2057	A	N9-C4-C5	-7.96	102.62	105.80
21	A	1288	G	C4-N9-C1'	-7.89	116.25	126.50
21	A	1004	A	C5-C6-N6	-7.84	117.42	123.70
21	A	555	C	N1-C2-O2	7.70	123.52	118.90
21	A	1030	C	C6-N1-C2	-7.70	117.22	120.30
21	A	288	C	N1-C2-O2	7.64	123.48	118.90
21	A	1831	A	C5-C6-N6	-7.64	117.59	123.70
1	a	1179	C	N3-C2-O2	-7.60	116.58	121.90
21	A	788	A	C5-C6-N6	-7.58	117.64	123.70
21	A	935	C	C2-N1-C1'	7.52	127.08	118.80
21	A	1015	C	N1-C2-O2	7.52	123.41	118.90
21	A	2057	A	C8-N9-C4	7.50	108.80	105.80
21	A	2105	C	N3-C2-O2	-7.49	116.66	121.90
21	A	1895	C	N1-C2-O2	7.45	123.37	118.90
21	A	1984	C	N1-C2-O2	7.40	123.34	118.90
1	a	512	C	N1-C2-O2	7.37	123.32	118.90
1	a	115	A	N1-C6-N6	7.37	123.02	118.60
21	A	2063	C	C6-N1-C2	-7.37	117.35	120.30
1	a	399	G	C6-C5-N7	-7.37	125.98	130.40
21	A	845	A	N1-C6-N6	7.36	123.02	118.60
21	A	2619	G	C4-N9-C1'	7.35	136.05	126.50
1	a	641	U	C2-N1-C1'	7.24	126.39	117.70
21	A	1708	A	N1-C6-N6	7.23	122.94	118.60
21	A	234	C	N1-C2-O2	7.19	123.22	118.90
21	A	1843	U	N1-C2-O2	7.19	127.83	122.80
21	A	1828	U	C6-N1-C2	7.19	125.31	121.00
21	A	2105	C	C2-N1-C1'	7.17	126.68	118.80
21	A	732	C	C5-C4-N4	-7.15	115.20	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1288	G	C8-N9-C1'	7.13	136.27	127.00
1	a	1519	A	C5-C6-N6	-7.12	118.00	123.70
21	A	574	A	N1-C2-N3	7.12	132.86	129.30
21	A	2543	G	N7-C8-N9	7.11	116.66	113.10
1	a	853	C	N3-C2-O2	-7.11	116.92	121.90
21	A	2021	C	C6-N1-C2	-7.10	117.46	120.30
21	A	2416	G	C4-C5-N7	7.08	113.63	110.80
21	A	1605	A	C5-C6-N6	-7.07	118.04	123.70
21	A	935	C	C6-N1-C2	-7.05	117.48	120.30
21	A	806	A	N9-C4-C5	-7.04	102.98	105.80
1	a	893	C	N1-C2-O2	7.04	123.12	118.90
21	A	692	G	N3-C2-N2	7.03	124.82	119.90
21	A	1435	C	C5-C4-N4	-7.03	115.28	120.20
21	A	721	A	N1-C6-N6	7.03	122.82	118.60
21	A	845	A	C5-C6-N6	-7.03	118.08	123.70
21	A	1315	C	N1-C2-O2	7.01	123.11	118.90
21	A	935	C	N3-C2-O2	-7.01	116.99	121.90
21	A	1843	U	N3-C2-O2	-7.01	117.29	122.20
1	a	115	A	C5-C6-N6	-6.99	118.11	123.70
1	a	819	C	C6-N1-C2	-6.97	117.51	120.30
21	A	1982	U	C5-C4-O4	-6.96	121.72	125.90
1	a	1541	G	C8-N9-C4	-6.96	103.62	106.40
21	A	2001	C	C2-N3-C4	-6.95	116.43	119.90
21	A	574	A	N1-C6-N6	-6.94	114.44	118.60
21	A	692	G	N1-C2-N2	-6.94	109.96	116.20
21	A	1778	C	N1-C2-O2	6.93	123.06	118.90
21	A	1042	C	N1-C2-O2	6.92	123.06	118.90
21	A	1298	G	C5-C6-O6	-6.92	124.45	128.60
21	A	661	U	C5-C6-N1	6.91	126.16	122.70
21	A	165	C	N3-C2-O2	-6.91	117.06	121.90
1	a	398	C	C6-N1-C2	-6.90	117.54	120.30
21	A	1414	G	C2-N3-C4	-6.89	108.45	111.90
1	a	1536	C	C2-N1-C1'	6.89	126.38	118.80
21	A	1843	U	C6-N1-C1'	-6.87	111.58	121.20
21	A	1648	C	N1-C2-O2	6.85	123.01	118.90
21	A	562	C	N3-C2-O2	-6.84	117.11	121.90
1	a	1171	G	O4'-C1'-N9	6.84	113.67	108.20
21	A	1201	G	C6-C5-N7	-6.83	126.30	130.40
1	a	399	G	N3-C4-N9	6.82	130.09	126.00
21	A	1235	C	C5-C6-N1	6.81	124.41	121.00
21	A	1029	C	N1-C2-O2	6.81	122.98	118.90
21	A	903	G	N3-C4-C5	6.80	132.00	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	819	C	C2-N1-C1'	6.76	126.24	118.80
21	A	12	U	C2-N1-C1'	6.76	125.81	117.70
21	A	735	C	C5-C6-N1	6.76	124.38	121.00
21	A	1029	C	C6-N1-C2	-6.75	117.60	120.30
21	A	2105	C	C6-N1-C2	-6.75	117.60	120.30
21	A	1815	C	N3-C4-N4	6.74	122.72	118.00
21	A	1998	A	N1-C6-N6	6.74	122.64	118.60
21	A	1605	A	N1-C6-N6	6.71	122.62	118.60
21	A	2023	C	N1-C2-O2	6.71	122.92	118.90
21	A	2288	C	N1-C2-O2	6.69	122.91	118.90
1	a	26	C	N1-C2-O2	6.67	122.90	118.90
21	A	2707	C	C6-N1-C2	-6.67	117.63	120.30
21	A	735	C	N3-C4-N4	6.64	122.65	118.00
21	A	2753	U	N3-C4-O4	-6.64	114.75	119.40
21	A	2077	C	N1-C2-O2	6.63	122.88	118.90
21	A	1858	G	N3-C4-C5	6.61	131.91	128.60
21	A	2227	C	C6-N1-C2	-6.61	117.66	120.30
21	A	2002	G	C8-N9-C4	-6.61	103.76	106.40
21	A	2322	C	N1-C2-O2	6.60	122.86	118.90
21	A	2302	C	N3-C2-O2	-6.60	117.28	121.90
21	A	2271	U	N3-C4-O4	6.59	124.01	119.40
21	A	555	C	C2-N1-C1'	6.58	126.04	118.80
21	A	2543	G	C4-N9-C1'	6.58	135.05	126.50
21	A	623	C	N3-C4-N4	6.56	122.59	118.00
35	T	3	ARG	NE-CZ-NH2	-6.54	117.03	120.30
21	A	2429	U	C2-N1-C1'	6.54	125.55	117.70
21	A	562	C	N1-C2-O2	6.54	122.82	118.90
1	a	920	C	N1-C2-O2	6.53	122.82	118.90
21	A	1815	C	C2-N1-C1'	6.53	125.98	118.80
21	A	2500	U	C2-N1-C1'	6.52	125.53	117.70
21	A	820	G	O4'-C1'-N9	6.51	113.41	108.20
21	A	2633	C	N1-C2-O2	6.51	122.81	118.90
21	A	935	C	N1-C2-O2	6.51	122.81	118.90
21	A	1984	C	C5-C4-N4	-6.50	115.65	120.20
21	A	633	A	N7-C8-N9	6.50	117.05	113.80
21	A	2133	G	C6-C5-N7	-6.49	126.50	130.40
21	A	1435	C	N3-C4-N4	6.49	122.54	118.00
21	A	2619	G	C8-N9-C1'	-6.49	118.57	127.00
21	A	2356	A	N7-C8-N9	6.48	117.04	113.80
21	A	1197	C	N1-C2-O2	6.48	122.78	118.90
21	A	1858	G	N1-C6-O6	6.47	123.78	119.90
21	A	1435	C	C2-N1-C1'	6.46	125.91	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	355	G	C6-C5-N7	-6.45	126.53	130.40
21	A	2606	C	N1-C2-O2	6.42	122.75	118.90
21	A	2416	G	C6-C5-N7	-6.41	126.55	130.40
21	A	2002	G	N3-C4-N9	-6.40	122.16	126.00
21	A	272	C	C6-N1-C2	-6.40	117.74	120.30
21	A	1960	G	N3-C2-N2	6.39	124.38	119.90
21	A	1364	C	N3-C4-N4	6.39	122.47	118.00
1	a	746	U	C5-C6-N1	6.39	125.89	122.70
21	A	2483	C	C5-C4-N4	-6.38	115.73	120.20
21	A	721	A	C5-C6-N6	-6.38	118.60	123.70
21	A	777	C	C6-N1-C2	-6.37	117.75	120.30
21	A	806	A	C6-C5-N7	-6.37	127.84	132.30
21	A	2034	U	C5-C4-O4	-6.36	122.08	125.90
21	A	1201	G	C4-C5-N7	6.35	113.34	110.80
1	a	933	A	N7-C8-N9	6.34	116.97	113.80
21	A	721	A	C5-N7-C8	-6.34	100.73	103.90
21	A	527	G	O4'-C1'-N9	6.33	113.27	108.20
1	a	625	G	C6-C5-N7	-6.33	126.60	130.40
21	A	2001	C	C5-C4-N4	-6.32	115.77	120.20
21	A	2483	C	N3-C4-N4	6.32	122.43	118.00
21	A	69	C	N3-C2-O2	-6.32	117.48	121.90
21	A	2464	C	N1-C2-O2	6.31	122.69	118.90
21	A	1015	C	N3-C2-O2	-6.30	117.49	121.90
1	a	361	A	N1-C6-N6	6.29	122.38	118.60
21	A	1368	C	N3-C2-O2	-6.29	117.50	121.90
21	A	1410	A	N9-C4-C5	-6.28	103.29	105.80
21	A	2023	C	N3-C2-O2	-6.27	117.51	121.90
1	a	1539	C	N3-C2-O2	-6.27	117.51	121.90
21	A	2133	G	N3-C4-N9	6.26	129.76	126.00
21	A	1708	A	C5-C6-N6	-6.26	118.69	123.70
21	A	496	G	N1-C2-N2	-6.26	110.56	116.20
21	A	608	C	C5-C4-N4	-6.26	115.82	120.20
21	A	1611	C	N1-C2-O2	6.26	122.66	118.90
1	a	1169	C	C6-N1-C2	-6.26	117.80	120.30
21	A	1029	C	C2-N1-C1'	6.26	125.68	118.80
1	a	762	C	C2-N1-C1'	6.24	125.66	118.80
21	A	2098	A	C5-C6-N6	-6.23	118.72	123.70
21	A	1801	C	C2-N3-C4	-6.22	116.79	119.90
1	a	843	A	C5-C6-N6	-6.22	118.73	123.70
21	A	2034	U	N3-C4-O4	6.21	123.75	119.40
1	a	1443	G	O4'-C1'-N9	6.21	113.17	108.20
21	A	2619	G	C6-C5-N7	-6.20	126.68	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	555	C	N3-C2-O2	-6.19	117.57	121.90
21	A	841	C	N1-C2-O2	6.19	122.61	118.90
21	A	1388	C	N1-C2-O2	6.18	122.61	118.90
21	A	2528	C	C6-N1-C2	-6.18	117.83	120.30
21	A	788	A	C6-C5-N7	-6.17	127.98	132.30
21	A	69	C	N1-C2-O2	6.17	122.60	118.90
21	A	2074	C	N1-C2-O2	6.17	122.60	118.90
21	A	903	G	C2-N3-C4	-6.16	108.82	111.90
1	a	1170	U	N1-C2-O2	6.16	127.11	122.80
1	a	726	A	N1-C6-N6	6.16	122.30	118.60
21	A	2305	A	C5-C6-N6	-6.16	118.78	123.70
21	A	870	C	N1-C2-O2	6.15	122.59	118.90
21	A	1651	C	N3-C4-C5	6.14	124.36	121.90
21	A	2044	C	C5-C4-N4	-6.14	115.90	120.20
21	A	2041	A	N1-C6-N6	-6.13	114.92	118.60
1	a	1536	C	C5-C6-N1	6.12	124.06	121.00
21	A	1219	G	N3-C4-N9	6.12	129.67	126.00
21	A	1608	C	N1-C2-O2	6.12	122.57	118.90
26	G	91	LEU	CA-CB-CG	6.12	129.37	115.30
21	A	1197	C	C2-N1-C1'	6.11	125.52	118.80
21	A	666	A	N1-C6-N6	6.10	122.26	118.60
21	A	1201	G	C4-N9-C1'	6.10	134.43	126.50
21	A	2271	U	C5-C4-O4	-6.10	122.24	125.90
21	A	528	C	C2-N1-C1'	6.09	125.50	118.80
21	A	57	C	C5-C4-N4	-6.09	115.94	120.20
21	A	1649	C	C2-N1-C1'	6.09	125.50	118.80
1	a	376	U	C2-N1-C1'	6.08	125.00	117.70
1	a	1441	C	N1-C2-O2	6.08	122.55	118.90
21	A	1350	U	C6-N1-C1'	-6.08	112.69	121.20
21	A	1414	G	C6-C5-N7	-6.08	126.75	130.40
21	A	2237	U	C5-C4-O4	-6.08	122.25	125.90
21	A	2443	C	C5-C4-N4	-6.08	115.95	120.20
1	a	903	C	C5-C4-N4	-6.07	115.95	120.20
21	A	732	C	N3-C4-N4	6.07	122.25	118.00
21	A	2117	A	N9-C4-C5	-6.06	103.38	105.80
21	A	735	C	C2-N1-C1'	6.06	125.46	118.80
21	A	528	C	C6-N1-C2	-6.05	117.88	120.30
21	A	1233	A	C5-C6-N1	6.05	120.73	117.70
21	A	1714	C	N3-C4-C5	6.05	124.32	121.90
1	a	89	U	C5-C4-O4	-6.04	122.28	125.90
50	8	4	ARG	NE-CZ-NH1	6.03	123.31	120.30
21	A	1984	C	N3-C2-O2	-6.02	117.68	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1413	C	C5-C4-N4	-6.02	115.99	120.20
1	a	853	C	C6-N1-C2	-6.01	117.90	120.30
21	A	1938	U	P-O3'-C3'	6.01	126.91	119.70
21	A	1335	C	C2-N1-C1'	6.01	125.41	118.80
21	A	1984	C	C2-N1-C1'	6.00	125.40	118.80
21	A	2500	U	N3-C2-O2	-5.99	118.01	122.20
1	a	1343	A	N1-C6-N6	5.98	122.19	118.60
21	A	1778	C	N3-C2-O2	-5.97	117.72	121.90
1	a	1179	C	C6-N1-C2	-5.97	117.91	120.30
21	A	1831	A	N1-C6-N6	5.95	122.17	118.60
21	A	496	G	C2-N3-C4	-5.95	108.93	111.90
21	A	1351	C	C6-N1-C2	-5.95	117.92	120.30
21	A	1355	A	C5-C6-N6	-5.94	118.95	123.70
21	A	1031	C	C5-C4-N4	-5.93	116.05	120.20
21	A	1815	C	N1-C2-O2	5.93	122.46	118.90
1	a	341	U	C5-C4-O4	-5.93	122.34	125.90
21	A	555	C	C6-N1-C2	-5.90	117.94	120.30
21	A	1436	C	N1-C2-O2	5.90	122.44	118.90
45	3	80	LEU	C-N-CA	-5.90	106.95	121.70
21	A	1388	C	N3-C2-O2	-5.89	117.78	121.90
1	a	328	A	C5-C6-N1	5.89	120.64	117.70
21	A	1316	G	C6-C5-N7	-5.89	126.87	130.40
22	B	79	C	N3-C4-N4	5.88	122.12	118.00
21	A	661	U	C6-N1-C2	-5.88	117.47	121.00
21	A	201	C	N3-C2-O2	-5.88	117.78	121.90
1	a	1316	G	O4'-C1'-N9	5.88	112.90	108.20
21	A	2236	C	N1-C2-O2	5.88	122.42	118.90
21	A	355	G	C4-C5-N7	5.87	113.15	110.80
21	A	2002	G	C5-C6-N1	5.87	114.44	111.50
1	a	36	G	C4-N9-C1'	5.87	134.13	126.50
21	A	2236	C	N3-C2-O2	-5.87	117.79	121.90
21	A	2098	A	N1-C6-N6	5.86	122.11	118.60
21	A	2063	C	N3-C2-O2	-5.85	117.80	121.90
21	A	1502	A	N1-C6-N6	5.84	122.10	118.60
1	a	175	C	N1-C2-O2	5.83	122.40	118.90
21	A	1197	C	C5-C4-N4	-5.83	116.11	120.20
21	A	1612	C	C6-N1-C2	-5.83	117.97	120.30
21	A	2074	C	N3-C2-O2	-5.83	117.82	121.90
21	A	721	A	C4-C5-N7	5.83	113.61	110.70
1	a	399	G	C4-N9-C1'	5.83	134.07	126.50
21	A	144	C	C6-N1-C2	-5.83	117.97	120.30
21	A	1981	G	N3-C2-N2	5.83	123.98	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	399	G	C4-C5-N7	5.82	113.13	110.80
21	A	1360	G	C6-C5-N7	-5.81	126.92	130.40
21	A	1831	A	C4-C5-N7	5.80	113.60	110.70
21	A	531	C	N1-C2-O2	5.80	122.38	118.90
21	A	1814	A	C4-C5-N7	5.80	113.60	110.70
21	A	1494	G	C2-N3-C4	-5.79	109.00	111.90
21	A	2479	C	C5-C4-N4	-5.79	116.14	120.20
21	A	1360	G	N3-C4-N9	5.79	129.47	126.00
21	A	1869	G	C4-N9-C1'	5.79	134.03	126.50
21	A	1998	A	C5-C6-N6	-5.79	119.07	123.70
21	A	2100	C	C6-N1-C2	-5.79	117.98	120.30
21	A	1351	C	C5-C4-N4	-5.79	116.15	120.20
21	A	2569	A	C5-C6-N6	-5.79	119.07	123.70
21	A	2063	C	N1-C2-O2	5.77	122.36	118.90
1	a	320	C	N3-C2-O2	-5.77	117.86	121.90
1	a	1520	G	C4-N9-C1'	5.76	133.99	126.50
21	A	2077	C	C2-N1-C1'	5.76	125.13	118.80
21	A	1410	A	C8-N9-C4	5.76	108.10	105.80
21	A	1960	G	N1-C2-N2	-5.75	111.02	116.20
21	A	2063	C	C5-C4-N4	-5.75	116.17	120.20
21	A	2416	G	N9-C4-C5	-5.75	103.10	105.40
21	A	1831	A	N9-C4-C5	-5.75	103.50	105.80
21	A	2004	A	N9-C4-C5	-5.74	103.50	105.80
1	a	625	G	C4-N9-C1'	5.74	133.96	126.50
21	A	1828	U	N3-C2-O2	5.74	126.22	122.20
21	A	1004	A	C4-C5-N7	5.74	113.57	110.70
21	A	2112	C	C5-C4-N4	-5.74	116.18	120.20
21	A	2543	G	C8-N9-C4	-5.74	104.11	106.40
1	a	1536	C	N1-C2-O2	5.73	122.34	118.90
21	A	806	A	C5-C6-N1	5.73	120.56	117.70
21	A	1859	C	N1-C2-O2	5.73	122.34	118.90
21	A	2817	A	N1-C6-N6	-5.72	115.17	118.60
21	A	288	C	N3-C2-O2	-5.72	117.89	121.90
21	A	1661	C	C2-N1-C1'	5.72	125.09	118.80
21	A	2098	A	C6-C5-N7	-5.72	128.30	132.30
21	A	2290	C	C5-C6-N1	5.72	123.86	121.00
21	A	355	G	N3-C4-N9	5.71	129.43	126.00
21	A	1519	U	O4'-C1'-N1	5.71	112.77	108.20
21	A	1353	A	N7-C8-N9	5.71	116.66	113.80
21	A	2639	C	N1-C2-O2	5.70	122.32	118.90
1	a	878	C	N3-C2-O2	-5.70	117.91	121.90
21	A	788	A	C4-C5-N7	5.70	113.55	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	803	C	N3-C2-O2	-5.69	117.92	121.90
21	A	1828	U	C6-N1-C1'	-5.69	113.23	121.20
1	a	336	C	C6-N1-C2	-5.69	118.03	120.30
21	A	862	C	N1-C2-O2	5.69	122.31	118.90
1	a	878	C	N1-C2-O2	5.68	122.31	118.90
1	a	1536	C	N3-C2-O2	-5.68	117.92	121.90
21	A	608	C	C2-N3-C4	-5.68	117.06	119.90
1	a	491	C	C2-N1-C1'	5.68	125.05	118.80
21	A	57	C	C2-N1-C1'	5.67	125.04	118.80
21	A	1824	C	N3-C4-N4	5.67	121.97	118.00
21	A	1869	G	N7-C8-N9	5.67	115.94	113.10
21	A	2615	G	C4-C5-N7	5.67	113.07	110.80
21	A	2628	C	N1-C2-O2	5.67	122.30	118.90
1	a	479	U	N3-C2-O2	-5.66	118.24	122.20
21	A	2500	U	C6-N1-C2	-5.66	117.60	121.00
21	A	1414	G	C4-C5-N7	5.66	113.06	110.80
21	A	1351	C	C2-N1-C1'	5.66	125.02	118.80
1	a	1356	U	O4'-C1'-N1	5.65	112.72	108.20
21	A	737	C	C5-C6-N1	5.65	123.83	121.00
21	A	1649	C	N1-C2-O2	5.65	122.29	118.90
21	A	21	A	C5-C6-N6	-5.65	119.18	123.70
21	A	1984	C	N3-C4-N4	5.65	121.95	118.00
21	A	2449	C	C6-N1-C2	-5.65	118.04	120.30
21	A	1004	A	C6-C5-N7	-5.64	128.35	132.30
21	A	1542	C	C6-N1-C2	-5.64	118.04	120.30
21	A	2638	C	C5-C4-N4	-5.64	116.25	120.20
1	a	962	U	C5-C4-O4	-5.63	122.52	125.90
21	A	661	U	P-O3'-C3'	5.63	126.45	119.70
21	A	1858	G	C5-C6-O6	-5.63	125.22	128.60
21	A	2295	A	N7-C8-N9	5.63	116.61	113.80
21	A	2543	G	C6-C5-N7	-5.62	127.03	130.40
21	A	2092	C	C5-C4-N4	-5.62	116.27	120.20
21	A	903	G	N9-C4-C5	5.61	107.64	105.40
1	a	1354	G	C6-C5-N7	-5.61	127.04	130.40
21	A	1031	C	N1-C2-O2	5.61	122.26	118.90
1	a	36	G	C8-N9-C1'	-5.60	119.72	127.00
21	A	777	C	C2-N1-C1'	5.60	124.96	118.80
1	a	341	U	N3-C4-O4	5.59	123.31	119.40
21	A	774	G	C2-N3-C4	-5.58	109.11	111.90
21	A	2274	A	C5-C6-N6	-5.58	119.23	123.70
1	a	893	C	N3-C2-O2	-5.58	118.00	121.90
21	A	2239	A	O4'-C1'-N9	5.58	112.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	2559	G	C4-N9-C1'	5.58	133.75	126.50
21	A	1015	C	C2-N1-C1'	5.57	124.93	118.80
21	A	1869	G	C6-C5-N7	-5.57	127.06	130.40
21	A	1814	A	N9-C4-C5	-5.57	103.57	105.80
21	A	2233	C	C6-N1-C2	-5.56	118.08	120.30
21	A	1894	G	C6-C5-N7	-5.56	127.06	130.40
21	A	2048	G	C4-N9-C1'	5.56	133.73	126.50
21	A	2077	C	C5-C4-N4	-5.56	116.31	120.20
1	a	933	A	C5-N7-C8	-5.55	101.12	103.90
21	A	633	A	C6-C5-N7	-5.55	128.42	132.30
21	A	2707	C	N1-C2-O2	5.55	122.23	118.90
21	A	788	A	C6-N1-C2	-5.55	115.27	118.60
21	A	778	G	C2-N3-C4	-5.54	109.13	111.90
21	A	1435	C	N1-C2-O2	5.54	122.23	118.90
1	a	404	A	C5-C6-N6	-5.54	119.27	123.70
21	A	1870	C	C5-C6-N1	5.54	123.77	121.00
21	A	421	C	N1-C2-O2	5.54	122.22	118.90
21	A	1708	A	C4-C5-N7	5.54	113.47	110.70
1	a	588	C	N1-C2-O2	5.53	122.22	118.90
21	A	785	C	N1-C1'-C2'	5.53	121.19	114.00
21	A	2356	A	C5-N7-C8	-5.53	101.13	103.90
21	A	1801	C	C6-N1-C2	-5.53	118.09	120.30
21	A	624	C	N3-C2-O2	-5.53	118.03	121.90
21	A	1700	C	C6-N1-C2	-5.53	118.09	120.30
21	A	2090	C	C2-N1-C1'	5.53	124.88	118.80
21	A	2004	A	C8-N9-C4	5.52	108.01	105.80
21	A	1335	C	N3-C4-N4	5.52	121.86	118.00
1	a	933	A	C6-C5-N7	-5.52	128.44	132.30
21	A	788	A	C5-C6-N1	5.52	120.46	117.70
36	U	79	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	A	737	C	N3-C4-N4	5.51	121.86	118.00
1	a	819	C	C5-C4-N4	-5.51	116.34	120.20
21	A	1661	C	C6-N1-C1'	-5.51	114.19	120.80
21	A	2117	A	C4-C5-N7	5.51	113.45	110.70
1	a	762	C	C6-N1-C1'	-5.51	114.19	120.80
21	A	829	U	O4'-C1'-N1	5.51	112.61	108.20
21	A	1360	G	C4-C5-N7	5.50	113.00	110.80
21	A	355	G	N9-C4-C5	-5.50	103.20	105.40
21	A	555	C	C5-C4-N4	-5.50	116.35	120.20
21	A	1844	G	C4-N9-C1'	5.49	133.63	126.50
21	A	1870	C	N1-C2-O2	5.49	122.19	118.90
21	A	57	C	N1-C2-O2	5.48	122.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	2569	A	N1-C6-N6	5.48	121.89	118.60
21	A	1268	C	C6-N1-C2	-5.48	118.11	120.30
1	a	625	G	N7-C8-N9	5.47	115.84	113.10
1	a	1428	G	C2-N3-C4	-5.47	109.16	111.90
21	A	57	C	N3-C4-N4	5.47	121.83	118.00
21	A	1336	G	C2-N3-C4	-5.47	109.16	111.90
21	A	666	A	C5-N7-C8	-5.47	101.17	103.90
21	A	1510	U	OP1-P-O3'	-5.47	93.17	105.20
21	A	2798	C	C6-N1-C2	-5.47	118.11	120.30
21	A	608	C	N3-C4-C5	5.47	124.09	121.90
21	A	2305	A	C4-C5-N7	5.47	113.43	110.70
21	A	628	G	N7-C8-N9	5.46	115.83	113.10
1	a	1237	C	C6-N1-C2	-5.46	118.12	120.30
1	a	1179	C	C6-N1-C1'	-5.45	114.25	120.80
21	A	514	G	C8-N9-C1'	-5.45	119.91	127.00
1	a	315	U	N3-C2-O2	-5.45	118.38	122.20
21	A	1179	C	C6-N1-C2	-5.45	118.12	120.30
1	a	1541	G	N7-C8-N9	5.45	115.82	113.10
21	A	737	C	C2-N1-C1'	5.45	124.79	118.80
21	A	1360	G	N9-C4-C5	-5.45	103.22	105.40
21	A	1828	U	C5-C6-N1	-5.45	119.98	122.70
21	A	2641	A	C5-C6-N1	5.45	120.42	117.70
21	A	1436	C	C2-N1-C1'	5.44	124.78	118.80
21	A	235	G	O4'-C1'-N9	5.44	112.55	108.20
21	A	1004	A	N9-C4-C5	-5.43	103.63	105.80
21	A	1315	C	N3-C2-O2	-5.43	118.10	121.90
21	A	2857	A	C5-C6-N6	-5.43	119.36	123.70
22	B	86	C	C6-N1-C2	-5.43	118.13	120.30
21	A	2480	A	C5-C6-N6	-5.42	119.36	123.70
21	A	957	C	N1-C2-O2	5.42	122.15	118.90
1	a	1036	C	C6-N1-C2	-5.42	118.13	120.30
21	A	2088	G	O4'-C1'-N9	5.41	112.53	108.20
21	A	2621	C	C5-C4-N4	-5.41	116.41	120.20
21	A	1511	C	P-O3'-C3'	-5.41	113.21	119.70
21	A	2539	C	C5-C4-N4	-5.41	116.42	120.20
21	A	2676	U	C5-C4-O4	-5.41	122.66	125.90
21	A	32	C	N1-C2-O2	5.40	122.14	118.90
21	A	12	U	N3-C2-O2	-5.40	118.42	122.20
21	A	1201	G	C8-N9-C1'	-5.40	119.98	127.00
1	a	819	C	C5-C6-N1	5.39	123.70	121.00
21	A	2083	G	C4-N9-C1'	5.39	133.50	126.50
21	A	1559	G	N3-C4-N9	-5.39	122.77	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	841	C	N3-C2-O2	-5.38	118.13	121.90
21	A	1368	C	C2-N1-C1'	5.38	124.72	118.80
21	A	1179	C	C2-N1-C1'	5.38	124.72	118.80
21	A	2117	A	C6-C5-N7	-5.38	128.53	132.30
1	a	816	C	C5-C4-N4	-5.38	116.44	120.20
21	A	1328	C	N1-C2-O2	5.38	122.13	118.90
21	A	2464	C	N3-C2-O2	-5.38	118.13	121.90
21	A	2664	U	C5-C6-N1	5.38	125.39	122.70
21	A	2090	C	N3-C2-O2	-5.38	118.14	121.90
21	A	1656	C	N3-C2-O2	-5.37	118.14	121.90
1	a	512	C	N3-C2-O2	-5.36	118.15	121.90
21	A	1303	A	C5-C6-N6	-5.36	119.42	123.70
21	A	2074	C	C6-N1-C2	-5.35	118.16	120.30
21	A	788	A	N1-C6-N6	5.35	121.81	118.60
21	A	2619	G	N7-C8-N9	5.35	115.78	113.10
21	A	1793	C	C5-C4-N4	-5.35	116.46	120.20
1	a	1354	G	N7-C8-N9	5.34	115.77	113.10
1	a	641	U	N1-C2-O2	5.34	126.53	122.80
21	A	801	A	C5-C6-N6	-5.34	119.43	123.70
21	A	728	U	C5-C4-O4	-5.33	122.70	125.90
21	A	1877	G	C4-C5-N7	5.33	112.93	110.80
21	A	2500	U	N1-C2-O2	5.33	126.53	122.80
21	A	633	A	C4-N9-C1'	5.33	135.89	126.30
21	A	2051	C	C6-N1-C2	-5.33	118.17	120.30
21	A	1858	G	N9-C4-C5	5.33	107.53	105.40
1	a	583	G	N3-C4-N9	-5.33	122.80	126.00
21	A	1029	C	C5-C4-N4	-5.33	116.47	120.20
1	a	627	U	C2-N1-C1'	5.32	124.08	117.70
21	A	1656	C	C2-N1-C1'	5.32	124.65	118.80
21	A	2098	A	C4-C5-N7	5.32	113.36	110.70
21	A	840	C	N3-C2-O2	-5.31	118.18	121.90
21	A	781	C	C5-C4-N4	-5.31	116.48	120.20
21	A	1648	C	N3-C2-O2	-5.31	118.18	121.90
21	A	1708	A	C6-C5-N7	-5.31	128.58	132.30
21	A	2117	A	C5-C6-N6	-5.31	119.45	123.70
21	A	250	G	C2-N3-C4	-5.31	109.25	111.90
21	A	2559	G	C8-N9-C1'	-5.30	120.12	127.00
1	a	320	C	N1-C2-O2	5.29	122.08	118.90
21	A	1410	A	C5-C6-N6	-5.29	119.47	123.70
1	a	399	G	C8-N9-C1'	-5.29	120.12	127.00
21	A	1380	G	C4-N9-C1'	5.29	133.38	126.50
21	A	2071	C	C6-N1-C2	-5.28	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1073	G	C4-N9-C1'	5.28	133.36	126.50
21	A	2651	G	C4-C5-N7	5.28	112.91	110.80
1	a	363	C	N1-C2-O2	5.28	122.06	118.90
21	A	788	A	N3-C4-N9	5.28	131.62	127.40
21	A	1719	C	N3-C4-C5	5.28	124.01	121.90
1	a	641	U	N3-C2-O2	-5.27	118.51	122.20
21	A	1579	C	C6-N1-C2	-5.27	118.19	120.30
21	A	2540	A	C6-N1-C2	-5.27	115.44	118.60
21	A	842	U	C5-C4-O4	-5.26	122.74	125.90
21	A	2083	G	C8-N9-C1'	-5.26	120.16	127.00
1	a	221	U	C2-N1-C1'	5.26	124.01	117.70
21	A	1280	U	N3-C4-O4	5.26	123.08	119.40
21	A	812	U	C5-C6-N1	5.26	125.33	122.70
21	A	1981	G	N1-C2-N2	-5.26	111.47	116.20
21	A	2063	C	C6-N1-C1'	-5.26	114.49	120.80
21	A	514	G	C4-N9-C1'	5.26	133.33	126.50
1	a	682	G	C6-C5-N7	-5.25	127.25	130.40
21	A	633	A	N3-C4-N9	5.25	131.60	127.40
21	A	1694	A	C5-C6-N6	-5.25	119.50	123.70
21	A	1050	C	C5-C4-N4	-5.25	116.53	120.20
1	a	1519	A	N1-C6-N6	5.25	121.75	118.60
21	A	1355	A	N1-C6-N6	5.25	121.75	118.60
21	A	788	A	C5-N7-C8	-5.24	101.28	103.90
21	A	2628	C	N3-C4-C5	5.24	124.00	121.90
1	a	399	G	N9-C4-C5	-5.24	103.30	105.40
21	A	1518	G	N3-C2-N2	5.24	123.57	119.90
21	A	1682	C	N1-C2-O2	5.24	122.04	118.90
21	A	2639	C	N3-C2-O2	-5.24	118.23	121.90
1	a	26	C	N3-C4-C5	5.23	123.99	121.90
21	A	346	A	C5-C6-N6	-5.23	119.51	123.70
21	A	1495	C	N3-C2-O2	-5.23	118.24	121.90
1	a	83	C	C6-N1-C2	-5.23	118.21	120.30
21	A	356	A	C5-C6-N6	-5.23	119.52	123.70
21	A	2295	A	C4-N9-C1'	5.23	135.71	126.30
1	a	447	U	N3-C2-O2	-5.22	118.54	122.20
21	A	249	C	C5-C4-N4	-5.22	116.54	120.20
1	a	1115	C	N1-C2-O2	5.22	122.03	118.90
21	A	2290	C	N3-C4-N4	5.22	121.65	118.00
21	A	735	C	C5-C4-N4	-5.22	116.55	120.20
21	A	781	C	N1-C2-O2	5.22	122.03	118.90
21	A	1228	A	C5-N7-C8	-5.22	101.29	103.90
21	A	1559	G	C2-N3-C4	-5.22	109.29	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	2601	G	C4-C5-N7	5.22	112.89	110.80
21	A	701	G	C6-C5-N7	-5.21	127.27	130.40
21	A	1894	G	N3-C4-N9	5.21	129.13	126.00
21	A	634	C	N1-C2-O2	5.21	122.03	118.90
21	A	666	A	C5-C6-N6	-5.21	119.53	123.70
21	A	721	A	C6-C5-N7	-5.21	128.66	132.30
21	A	2117	A	N1-C6-N6	5.21	121.72	118.60
1	a	315	U	C5-C6-N1	5.20	125.30	122.70
21	A	1399	C	C2-N1-C1'	5.20	124.52	118.80
2	b	113	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	a	1520	G	C8-N9-C1'	-5.19	120.25	127.00
21	A	2540	A	C5-C6-N6	-5.19	119.55	123.70
1	a	661	U	N1-C2-O2	5.19	126.43	122.80
21	A	777	C	C5-C6-N1	5.19	123.60	121.00
21	A	1315	C	C2-N1-C1'	5.19	124.51	118.80
1	a	171	A	N1-C6-N6	-5.18	115.49	118.60
21	A	771	G	C2-N3-C4	-5.18	109.31	111.90
21	A	666	A	C4-C5-N7	5.18	113.29	110.70
1	a	341	U	C5-C6-N1	5.18	125.29	122.70
21	A	738	U	N3-C4-O4	5.18	123.03	119.40
21	A	1201	G	N3-C4-N9	5.18	129.10	126.00
21	A	1351	C	N3-C4-N4	5.17	121.62	118.00
21	A	348	C	N1-C2-O2	5.17	122.00	118.90
21	A	1219	G	C6-C5-N7	-5.17	127.30	130.40
21	A	2111	C	C5-C4-N4	-5.17	116.58	120.20
21	A	193	A	C5-C6-N6	-5.16	119.57	123.70
21	A	2794	C	C6-N1-C2	-5.16	118.23	120.30
1	a	89	U	N3-C4-O4	5.16	123.01	119.40
1	a	491	C	C6-N1-C1'	-5.16	114.61	120.80
21	A	1235	C	N3-C2-O2	5.15	125.51	121.90
21	A	607	C	N1-C2-O2	5.15	121.99	118.90
21	A	1502	A	N7-C8-N9	5.15	116.38	113.80
21	A	2056	G	C4-C5-N7	5.15	112.86	110.80
21	A	1029	C	N3-C2-O2	-5.15	118.30	121.90
21	A	2090	C	N1-C2-O2	5.15	121.99	118.90
1	a	1363	C	N1-C2-O2	5.14	121.99	118.90
21	A	1217	U	C2-N1-C1'	5.14	123.87	117.70
21	A	1274	G	C2-N3-C4	-5.14	109.33	111.90
21	A	1326	C	C6-N1-C2	-5.14	118.24	120.30
21	A	265	A	C5-C6-N6	-5.14	119.59	123.70
21	A	2816	C	N3-C2-O2	-5.14	118.30	121.90
22	B	81	A	C5-C6-N6	-5.14	119.59	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	738	U	C5-C4-O4	-5.13	122.82	125.90
21	A	348	C	C5-C4-N4	-5.13	116.61	120.20
21	A	1657	G	N3-C4-C5	5.13	131.17	128.60
21	A	2899	A	C5-C6-N6	-5.13	119.60	123.70
1	a	34	A	C6-C5-N7	-5.12	128.71	132.30
1	a	548	G	C4-C5-N7	5.12	112.85	110.80
21	A	2488	C	C5-C4-N4	-5.12	116.61	120.20
21	A	2526	C	O4'-C1'-N1	-5.12	104.10	108.20
1	a	16	G	C4-N9-C1'	5.12	133.16	126.50
21	A	1197	C	N3-C4-N4	5.12	121.58	118.00
21	A	2770	U	C5-C4-O4	-5.12	122.83	125.90
21	A	1615	G	N3-C4-N9	-5.12	122.93	126.00
21	A	788	A	N9-C4-C5	-5.12	103.75	105.80
30	O	21	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	a	1536	C	N3-C4-N4	5.12	121.58	118.00
1	a	461	C	C6-N1-C2	-5.11	118.25	120.30
21	A	734	A	N7-C8-N9	5.11	116.36	113.80
21	A	2259	C	C5-C4-N4	-5.11	116.62	120.20
1	a	306	A	N9-C4-C5	-5.11	103.76	105.80
21	A	272	C	C2-N1-C1'	5.11	124.42	118.80
21	A	491	C	N1-C2-O2	5.10	121.96	118.90
21	A	857	C	C2-N1-C1'	-5.10	113.19	118.80
21	A	840	C	N1-C2-O2	5.10	121.96	118.90
21	A	355	G	C4-N9-C1'	5.10	133.13	126.50
21	A	967	C	N1-C2-O2	5.10	121.96	118.90
21	A	1435	C	C6-N1-C2	-5.10	118.26	120.30
21	A	567	G	C6-C5-N7	-5.09	127.34	130.40
21	A	1366	U	C5-C6-N1	5.09	125.25	122.70
21	A	555	C	N3-C4-N4	5.09	121.56	118.00
21	A	1426	G	C6-C5-N7	-5.09	127.34	130.40
21	A	2335	G	O4'-C1'-N9	5.09	112.27	108.20
21	A	2275	C	N1-C2-O2	5.09	121.95	118.90
1	a	24	C	N1-C2-O2	5.09	121.95	118.90
1	a	698	G	N1-C2-N2	-5.08	111.62	116.20
21	A	777	C	N3-C4-N4	5.08	121.56	118.00
1	a	315	U	N1-C2-O2	5.08	126.36	122.80
21	A	1870	C	N3-C2-O2	-5.08	118.34	121.90
21	A	2129	C	C6-N1-C2	-5.08	118.27	120.30
21	A	2493	C	N1-C2-O2	5.08	121.95	118.90
21	A	1831	A	C5-C6-N1	5.08	120.24	117.70
21	A	1612	C	N3-C2-O2	-5.08	118.35	121.90
21	A	620	G	N7-C8-N9	5.07	115.64	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	2290	C	C2-N1-C1'	5.07	124.38	118.80
21	A	184	C	C6-N1-C2	-5.07	118.27	120.30
21	A	778	G	N1-C2-N2	-5.07	111.64	116.20
21	A	1663	G	C6-C5-N7	-5.07	127.36	130.40
1	a	682	G	N7-C8-N9	5.07	115.63	113.10
21	A	1335	C	C6-N1-C2	-5.06	118.28	120.30
21	A	922	G	C8-N9-C1'	5.06	133.57	127.00
21	A	1285	A	C5-C6-N1	5.06	120.23	117.70
1	a	1037	C	C6-N1-C2	-5.06	118.28	120.30
21	A	188	C	C5-C4-N4	-5.05	116.66	120.20
21	A	1172	A	C5-C6-N6	-5.05	119.66	123.70
21	A	903	G	N3-C2-N2	-5.05	116.36	119.90
1	a	551	G	C4-N9-C1'	5.05	133.06	126.50
1	a	1519	A	C5-C6-N1	5.05	120.22	117.70
21	A	620	G	C6-C5-N7	-5.05	127.37	130.40
1	a	886	A	C5-C6-N6	-5.04	119.67	123.70
21	A	2715	G	C2-N3-C4	-5.04	109.38	111.90
21	A	116	G	C2-N3-C4	-5.04	109.38	111.90
21	A	491	C	C2-N1-C1'	5.04	124.34	118.80
21	A	685	C	N1-C2-O2	5.04	121.92	118.90
21	A	805	G	N3-C4-N9	5.04	129.02	126.00
21	A	2074	C	C2-N1-C1'	5.04	124.34	118.80
21	A	304	G	C4-C5-N7	5.03	112.81	110.80
21	A	1298	G	N3-C2-N2	-5.03	116.38	119.90
21	A	2077	C	N3-C4-N4	5.03	121.52	118.00
21	A	2356	A	C4-N9-C1'	5.03	135.36	126.30
21	A	660	A	N1-C6-N6	5.03	121.62	118.60
21	A	1353	A	C5-N7-C8	-5.03	101.39	103.90
21	A	2667	G	C6-C5-N7	-5.03	127.38	130.40
1	a	315	U	C6-N1-C2	-5.02	117.99	121.00
1	a	1435	U	C5-C4-O4	-5.02	122.89	125.90
21	A	26	G	C8-N9-C1'	-5.02	120.47	127.00
21	A	717	C	N1-C2-O2	5.02	121.91	118.90
21	A	2077	C	N3-C2-O2	-5.02	118.39	121.90
21	A	2899	A	N1-C6-N6	5.02	121.61	118.60
1	a	378	C	C5-C4-N4	-5.02	116.69	120.20
21	A	640	G	N1-C2-N2	-5.02	111.68	116.20
21	A	1859	C	C5-C4-N4	-5.02	116.69	120.20
1	a	1539	C	N1-C2-O2	5.01	121.91	118.90
21	A	250	G	N1-C2-N2	-5.01	111.69	116.20
21	A	814	A	C6-N1-C2	-5.01	115.59	118.60
21	A	1870	C	C2-N1-C1'	5.01	124.31	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	2048	G	C8-N9-C1'	-5.01	120.48	127.00
21	A	2583	C	C5-C4-N4	-5.01	116.69	120.20
1	a	147	G	C4-N9-C1'	5.01	133.01	126.50
21	A	2713	G	C6-C5-N7	-5.01	127.39	130.40
21	A	306	C	C6-N1-C2	-5.01	118.30	120.30
1	a	1520	G	C6-C5-N7	-5.01	127.39	130.40
1	a	1541	G	C6-C5-N7	-5.01	127.40	130.40
21	A	498	G	C4-N9-C1'	5.01	133.01	126.50
21	A	1294	G	C4-N9-C1'	5.01	133.01	126.50
21	A	1648	C	C2-N1-C1'	5.01	124.31	118.80
21	A	528	C	N3-C2-O2	-5.00	118.40	121.90
21	A	721	A	N7-C8-N9	5.00	116.30	113.80
21	A	789	C	N1-C2-O2	5.00	121.90	118.90
21	A	1501	G	C4-N9-C1'	5.00	133.00	126.50
21	A	340	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
45	3	43	TYR	Peptide
45	3	44	PRO	Peptide
45	3	63	LYS	Peptide
46	4	32	ASN	Peptide
46	4	45	LYS	Peptide
47	5	10	THR	Peptide
48	6	14	SER	Peptide
48	6	15	LYS	Peptide
49	7	28	PHE	Peptide
49	7	33	PHE	Peptide
23	D	176	ARG	Peptide
24	E	140	PRO	Peptide
24	E	142	SER	Peptide
24	E	62	ASP	Peptide
24	E	64	LYS	Peptide
24	E	65	SER	Peptide
24	E	9	LYS	Peptide
25	F	143	LEU	Peptide
25	F	148	GLN	Peptide
25	F	154	VAL	Peptide
25	F	171	PRO	Peptide
25	F	183	VAL	Peptide

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Mol	Chain	Res	Type	Group
26	G	114	PHE	Peptide
26	G	124	GLY	Peptide
26	G	138	PHE	Peptide
26	G	88	LYS	Peptide
28	M	68	ASN	Peptide
28	M	69	LYS	Peptide
29	N	89	ASP	Peptide
30	O	100	GLY	Peptide
30	O	65	GLY	Peptide
30	O	80	ASP	Peptide
30	O	83	ASN	Peptide
31	P	41	TRP	Peptide
33	R	103	GLY	Peptide
33	R	89	ILE	Peptide
34	S	104	SER	Peptide
35	T	91	ASN	Peptide
36	U	100	ILE	Peptide
38	W	48	VAL	Peptide
38	W	50	VAL	Peptide
40	Y	73	MET	Peptide
41	Z	16	SER	Peptide
41	Z	17	SER	Peptide
41	Z	19	LYS	Peptide
41	Z	22	ARG	Peptide
3	c	107	LYS	Peptide
3	c	24	ALA	Peptide
5	e	162	GLU	Peptide
7	g	13	LEU	Peptide
7	g	14	PRO	Peptide
7	g	17	ILE	Peptide
8	h	79	ARG	Peptide
8	h	98	LEU	Peptide
13	m	102	THR	Peptide
13	m	111	GLY	Peptide
13	m	64	LYS	Peptide
13	m	65	VAL	Peptide
13	m	84	SER	Peptide
14	n	18	VAL	Peptide
14	n	57	ARG	Peptide
17	q	5	ASN	Peptide
17	q	76	ARG	Peptide
17	q	85	VAL	Peptide

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Mol	Chain	Res	Type	Group
19	s	13	GLU	Peptide
19	s	7	LYS	Peptide
19	s	9	PRO	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	33126	0	16679	0	0
2	b	1802	0	1861	0	0
3	c	1638	0	1702	0	0
4	d	1600	0	1628	0	0
5	e	1239	0	1298	0	0
6	f	799	0	794	0	0
7	g	1189	0	1218	0	0
8	h	1032	0	1082	0	0
9	i	1017	0	1039	0	0
10	j	813	0	859	0	0
11	k	881	0	899	0	0
12	l	1063	0	1130	0	0
13	m	946	0	1001	0	0
14	n	502	0	527	0	0
15	o	738	0	769	0	0
16	p	712	0	744	0	0
17	q	707	0	749	0	0
18	r	590	0	628	0	0
19	s	678	0	672	0	0
20	t	607	0	650	0	0
21	A	62475	0	31402	495	0
22	B	2427	0	1230	24	0
23	D	2104	0	2221	35	0
24	E	1649	0	1689	15	0
25	F	1525	0	1570	12	0
26	G	1312	0	1366	1	0
27	H	1285	0	1301	13	0
28	M	1151	0	1145	5	0
29	N	920	0	981	10	0
30	O	998	0	1044	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	P	1122	0	1185	8	0
32	Q	940	0	990	12	0
33	R	922	0	968	14	0
34	S	886	0	957	6	0
35	T	944	0	1014	8	0
36	U	799	0	836	3	0
37	V	863	0	920	7	0
38	W	726	0	761	3	0
39	X	669	0	725	2	0
40	Y	738	0	787	11	0
41	Z	627	0	645	11	0
42	0	374	0	407	5	0
43	1	537	0	567	8	0
44	2	442	0	478	3	0
45	3	677	0	655	55	0
46	4	444	0	453	2	0
47	5	229	0	224	15	0
48	6	373	0	420	6	0
49	7	488	0	548	9	0
50	8	297	0	339	5	0
51	A	29	0	0	0	0
51	a	2	0	0	0	0
52	A	9	0	0	1	0
53	8	1	0	0	0	0
54	A	143	0	0	13	0
54	D	4	0	0	0	0
54	T	2	0	0	0	0
54	U	1	0	0	1	0
54	a	12	0	0	0	0
All	All	140825	0	93757	732	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 5.

All (732) 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)
21:A:1828:U:C6	21:A:1828:U:C5	2.07	1.42
21:A:2230:G:N9	21:A:2230:G:C4	1.68	1.39
21:A:857:C:C6	21:A:857:C:N3	1.94	1.34
21:A:1828:U:C5	21:A:1828:U:C4	2.18	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1288:G:C5	21:A:1288:G:C4	2.24	1.23
21:A:857:C:N3	21:A:1288:G:N1	1.96	1.14
21:A:1828:U:N1	21:A:2230:G:H1'	1.65	1.12
21:A:1794:C:C2	21:A:2013:G:N2	2.18	1.11
21:A:1288:G:C5	21:A:1288:G:C6	2.38	1.11
21:A:1828:U:C6	21:A:1828:U:N1	2.19	1.08
21:A:857:C:N3	21:A:857:C:C2	2.19	1.08
21:A:1828:U:N3	21:A:1828:U:C2	2.21	1.07
21:A:1828:U:C4	21:A:1828:U:N3	2.21	1.07
21:A:857:C:C6	21:A:857:C:C5	2.46	1.04
47:5:35:PHE:HD1	47:5:36:CYS:N	1.54	1.03
21:A:1828:U:N1	21:A:1828:U:C2	2.26	1.02
21:A:1793:C:C2	21:A:2014:G:N2	2.28	1.01
21:A:903:G:N1	21:A:2295:A:C2	2.28	1.01
45:3:71:VAL:HA	45:3:74:PHE:CE1	1.97	0.99
21:A:1288:G:N3	21:A:1288:G:C2	2.32	0.98
21:A:1828:U:N3	21:A:2230:G:O4'	2.01	0.94
45:3:75:ASN:HA	45:3:78:PHE:CE2	2.02	0.93
45:3:70:ARG:HD2	45:3:71:VAL:H	1.33	0.91
21:A:1288:G:C4	21:A:1288:G:N3	2.39	0.91
45:3:70:ARG:NE	45:3:71:VAL:HG23	1.89	0.88
21:A:857:C:C2	21:A:1288:G:N1	2.42	0.87
21:A:790:G:HO2'	21:A:793:G:HO2'	1.05	0.87
45:3:77:LYS:HE2	45:3:77:LYS:HA	1.56	0.87
21:A:628:G:C2	21:A:1289:A:N1	2.42	0.87
21:A:857:C:N3	21:A:1288:G:C6	2.42	0.87
21:A:857:C:C5	21:A:1288:G:C4	2.62	0.87
47:5:35:PHE:CD1	47:5:36:CYS:N	2.42	0.87
31:P:80:GLU:O	41:Z:12:LYS:NZ	2.08	0.86
45:3:70:ARG:CD	45:3:71:VAL:HG23	2.05	0.85
21:A:1828:U:C2	21:A:2230:G:C1'	2.58	0.85
21:A:857:C:N3	21:A:1288:G:C2	2.44	0.85
21:A:1828:U:C6	21:A:2230:G:N9	2.44	0.85
21:A:1971:U:O4'	21:A:1982:U:O2'	1.93	0.84
21:A:1306:C:C2	21:A:2040:A:C6	2.64	0.84
45:3:70:ARG:HD2	45:3:71:VAL:N	1.92	0.84
21:A:2397:G:N2	47:5:35:PHE:CE2	2.46	0.84
22:B:15:C:H42	22:B:105:G:H21	1.25	0.84
45:3:70:ARG:O	45:3:73:ARG:HG3	1.78	0.83
21:A:2397:G:H21	47:5:35:PHE:HE2	1.21	0.83
21:A:903:G:C6	21:A:2295:A:C2	2.66	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1828:U:C2	21:A:2230:G:N9	2.46	0.83
21:A:857:C:C6	21:A:1288:G:C4	2.67	0.83
21:A:1987:A:H5''	21:A:1987:A:H8	1.43	0.83
21:A:1288:G:N1	21:A:1288:G:C2	2.48	0.81
21:A:1828:U:N3	21:A:2230:G:N9	2.29	0.81
21:A:857:C:C5	21:A:1288:G:N3	2.49	0.81
21:A:1312:A:O4'	32:Q:12:GLN:NE2	2.14	0.81
21:A:1828:U:C4	21:A:2230:G:C1'	2.64	0.81
21:A:2230:G:N9	21:A:2230:G:C1'	2.44	0.81
21:A:2250:A:OP1	23:D:170:TYR:OH	1.99	0.81
21:A:1828:U:N3	21:A:2230:G:C1'	2.44	0.80
21:A:2471:G:OP2	25:F:68:LYS:NZ	2.15	0.80
21:A:321:U:OP1	21:A:326:A:N6	2.15	0.80
21:A:2649:U:O2'	21:A:2845:G:N2	2.15	0.80
21:A:1094:A:N3	21:A:2778:G:N2	2.29	0.79
21:A:2060:A:O2'	21:A:2062:G:OP2	1.99	0.79
45:3:75:ASN:HA	45:3:78:PHE:CD2	2.18	0.79
21:A:1987:A:O2'	21:A:1988:C:H5'	1.81	0.79
21:A:628:G:N2	21:A:1289:A:C2	2.51	0.79
21:A:1520:A:N6	21:A:1562:C:O2	2.16	0.79
21:A:1806:U:OP2	21:A:1811:A:N6	2.15	0.79
21:A:1569:G:H21	21:A:1570:G:H5'	1.46	0.78
21:A:1828:U:N1	21:A:2230:G:N9	2.30	0.78
21:A:83:G:N2	21:A:102:A:OP2	2.17	0.78
21:A:857:C:C5	21:A:1288:G:C2	2.70	0.78
21:A:275:A:H62	21:A:296:G:H21	1.29	0.78
21:A:1101:A:N6	21:A:1131:G:OP2	2.16	0.78
21:A:932:U:C2	21:A:935:C:N4	2.51	0.78
47:5:35:PHE:HE1	47:5:37:SER:N	1.81	0.78
21:A:575:G:O2'	21:A:577:A:N7	2.17	0.78
21:A:289:U:O2'	21:A:290:U:O4'	2.01	0.78
21:A:1415:A:O2'	21:A:1417:G:N7	2.17	0.78
21:A:857:C:C5	21:A:1288:G:C5	2.72	0.77
21:A:61:A:OP1	43:1:44:ARG:NE	2.17	0.77
22:B:29:C:O2	22:B:51:A:N6	2.17	0.77
21:A:2717:A:OP1	32:Q:4:ARG:NH2	2.17	0.77
25:F:112:SER:O	25:F:115:SER:OG	2.02	0.77
21:A:2285:C:O2'	21:A:2454:C:OP2	2.02	0.77
21:A:2102:U:OP1	23:D:242:ARG:NH2	2.17	0.77
47:5:35:PHE:CE1	47:5:37:SER:N	2.52	0.77
21:A:2017:C:OP2	54:A:3101:HOH:O	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1794:C:O2	21:A:2013:G:N2	2.18	0.76
29:N:64:ARG:NH1	29:N:100:GLY:O	2.18	0.76
21:A:661:U:O2'	21:A:662:G:OP2	2.02	0.76
21:A:1819:G:N7	54:A:3110:HOH:O	2.18	0.76
21:A:857:C:C6	21:A:1288:G:N3	2.54	0.76
45:3:70:ARG:HD2	45:3:71:VAL:HG23	1.67	0.76
21:A:1828:U:C4	21:A:2230:G:N9	2.53	0.76
21:A:304:G:O6	21:A:410:G:N2	2.17	0.76
21:A:797:A:C5	21:A:1808:U:O2	2.39	0.76
21:A:1828:U:C6	21:A:2230:G:C1'	2.69	0.76
21:A:2747:U:OP1	54:A:3103:HOH:O	2.04	0.76
25:F:144:SER:OG	25:F:148:GLN:NE2	2.19	0.76
21:A:834:A:N1	48:6:4:ARG:NH1	2.33	0.76
21:A:1828:U:C5	21:A:2230:G:N9	2.54	0.76
29:N:73:ASP:OD2	34:S:82:LYS:NZ	2.19	0.76
21:A:321:U:C2	21:A:326:A:N6	2.54	0.76
21:A:1323:A:O2'	21:A:1325:U:OP2	2.03	0.75
21:A:1828:U:N1	21:A:2230:G:C1'	2.47	0.75
21:A:628:G:N3	21:A:1289:A:C6	2.54	0.75
22:B:72:U:O2'	40:Y:38:ASN:ND2	2.18	0.75
21:A:628:G:C2	21:A:1289:A:C2	2.74	0.75
21:A:857:C:C6	21:A:1288:G:C2	2.75	0.75
21:A:907:G:OP2	54:A:3104:HOH:O	2.05	0.75
33:R:71:GLU:O	33:R:74:THR:OG1	2.03	0.75
21:A:955:A:OP1	54:A:3102:HOH:O	2.04	0.75
25:F:178:ALA:O	25:F:182:ASN:ND2	2.20	0.75
21:A:903:G:OP1	41:Z:52:LYS:NZ	2.18	0.75
21:A:2328:A:OP2	21:A:2336:A:N6	2.20	0.75
21:A:419:U:OP2	42:0:52:ARG:NH1	2.20	0.74
21:A:628:G:C2	21:A:1289:A:C6	2.75	0.74
32:Q:73:ASN:ND2	32:Q:77:THR:O	2.19	0.74
21:A:857:C:C2	21:A:1288:G:C6	2.75	0.74
21:A:1493:U:O4	21:A:1506:C:N3	2.20	0.74
21:A:2153:A:O2'	21:A:2189:G:N2	2.20	0.74
23:D:132:GLN:O	23:D:166:LYS:NZ	2.21	0.74
45:3:70:ARG:CD	45:3:71:VAL:H	2.01	0.74
21:A:1854:U:OP2	23:D:220:ARG:NH1	2.21	0.74
21:A:2126:C:O2'	21:A:2127:G:O4'	2.06	0.74
21:A:2667:G:OP1	28:M:100:ARG:NH1	2.20	0.73
45:3:71:VAL:HA	45:3:74:PHE:CD1	2.22	0.73
47:5:35:PHE:HE1	47:5:37:SER:CA	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:2272:U:O2'	21:A:2463:G:OP2	2.03	0.73
27:H:57:ASP:O	27:H:62:ARG:NH1	2.20	0.73
21:A:2157:U:O2'	21:A:2185:A:N1	2.19	0.73
21:A:59:U:O2'	21:A:74:U:OP2	2.07	0.73
27:H:60:GLU:O	27:H:63:THR:OG1	2.04	0.73
21:A:142:G:N2	21:A:1640:U:O3'	2.22	0.73
21:A:315:C:O2'	21:A:316:G:N7	2.17	0.73
21:A:375:A:O2'	21:A:377:U:OP2	2.04	0.73
21:A:2397:G:N2	47:5:35:PHE:CD2	2.57	0.72
21:A:2622:G:N2	21:A:2625:A:OP2	2.22	0.72
21:A:625:G:C6	21:A:1297:G:N1	2.57	0.72
32:Q:18:ARG:O	32:Q:22:THR:OG1	2.03	0.72
21:A:313:U:O2'	21:A:314:A:N3	2.19	0.72
21:A:774:G:C2	21:A:1802:U:C2	2.77	0.72
45:3:30:THR:OG1	45:3:33:GLU:O	2.06	0.72
21:A:2530:A:O2'	21:A:2532:G:OP2	2.08	0.72
22:B:65:G:O6	22:B:105:G:N2	2.19	0.72
21:A:1978:U:O2'	21:A:1980:A:N7	2.22	0.72
21:A:613:G:C6	21:A:2057:A:N6	2.57	0.72
43:1:46:VAL:O	43:1:49:THR:OG1	2.07	0.72
23:D:93:VAL:HG21	23:D:103:ILE:HD13	1.72	0.72
21:A:2804:G:OP2	21:A:2808:A:O2'	2.07	0.72
21:A:364:A:O2'	21:A:383:A:N3	2.23	0.72
22:B:29:C:O2'	22:B:51:A:N1	2.17	0.72
21:A:857:C:C6	21:A:1288:G:C5	2.78	0.71
21:A:425:G:O6	54:A:3105:HOH:O	2.05	0.71
21:A:1828:U:C5	21:A:2230:G:C1'	2.73	0.71
45:3:71:VAL:HA	45:3:74:PHE:HE1	1.52	0.71
21:A:1771:A:O2'	21:A:1772:G:O5'	2.06	0.71
21:A:1288:G:C6	21:A:1288:G:N1	2.59	0.71
21:A:614:U:O2'	21:A:616:G:OP2	2.09	0.70
21:A:283:G:N7	21:A:284:C:O2'	2.23	0.70
21:A:1488:A:N1	21:A:1490:G:C6	2.59	0.70
22:B:34:C:N4	22:B:47:C:O2	2.25	0.70
45:3:75:ASN:ND2	45:3:78:PHE:HE2	1.90	0.70
21:A:922:G:O6	21:A:943:C:N4	2.24	0.70
21:A:2815:C:O2'	21:A:2829:A:N3	2.23	0.69
42:0:29:TRP:CZ3	42:0:31:ALA:HB2	2.26	0.69
21:A:425:G:N7	54:A:3113:HOH:O	2.25	0.69
21:A:1987:A:C2'	21:A:1988:C:H5'	2.22	0.69
21:A:2015:C:OP2	54:A:3106:HOH:O	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1377:U:OP2	38:W:58:TYR:OH	2.11	0.69
21:A:688:A:N1	21:A:2396:A:O2'	2.21	0.69
21:A:1569:G:N3	21:A:1569:G:H3'	2.08	0.69
21:A:628:G:C4	21:A:1289:A:C6	2.81	0.69
21:A:2229:C:O2'	21:A:2231:C:OP1	2.10	0.69
21:A:2599:A:N7	24:E:158:SER:OG	2.23	0.68
21:A:321:U:N3	21:A:326:A:C6	2.61	0.68
21:A:1320:G:N2	21:A:1323:A:OP2	2.26	0.68
21:A:1658:A:N6	37:V:92:ARG:O	2.26	0.68
21:A:2019:G:N2	21:A:2023:C:O2	2.24	0.68
21:A:616:G:O2'	21:A:618:A:OP1	2.11	0.68
21:A:2089:A:OP1	54:A:3107:HOH:O	2.10	0.68
42:O:12:ALA:O	42:O:14:THR:OG1	2.11	0.68
21:A:2477:A:OP1	21:A:2524:A:O2'	2.08	0.68
21:A:903:G:N1	21:A:2295:A:H2	1.91	0.68
21:A:1816:A:OP1	23:D:220:ARG:NE	2.27	0.67
21:A:257:G:O2'	21:A:258:A:O4'	2.11	0.67
21:A:2695:G:O2'	27:H:111:HIS:NE2	2.25	0.67
21:A:1379:A:O2'	21:A:1381:U:OP2	2.11	0.67
22:B:38:U:O2'	22:B:43:A:N6	2.22	0.67
21:A:1455:U:O2	21:A:1631:G:N2	2.27	0.67
21:A:234:C:O2'	21:A:235:G:O4'	2.12	0.67
21:A:1897:U:O2'	21:A:1898:C:O4'	2.13	0.67
21:A:1465:G:O2'	21:A:1537:A:N6	2.27	0.67
23:D:4:LYS:NZ	23:D:13:ARG:O	2.17	0.67
45:3:70:ARG:CZ	45:3:71:VAL:HG23	2.24	0.66
21:A:613:G:N1	21:A:2057:A:N7	2.42	0.66
21:A:857:C:C4	21:A:1288:G:N1	2.63	0.66
21:A:2457:A:O2'	21:A:2458:U:O5'	2.12	0.66
21:A:2127:G:N2	21:A:2216:U:O2	2.29	0.66
21:A:32:C:N4	21:A:493:A:OP2	2.28	0.66
22:B:45:C:OP2	33:R:7:LYS:NZ	2.28	0.66
45:3:73:ARG:HG3	45:3:74:PHE:H	1.61	0.66
21:A:2717:A:N6	32:Q:39:GLU:OE1	2.27	0.66
23:D:208:GLY:O	23:D:211:ARG:N	2.29	0.66
49:7:26:ARG:O	49:7:40:GLN:NE2	2.28	0.66
21:A:1172:A:C6	21:A:2545:A:C6	2.84	0.65
21:A:592:A:O2'	21:A:593:U:O5'	2.13	0.65
21:A:1987:A:H2'	21:A:1988:C:C5'	2.25	0.65
21:A:675:G:N2	21:A:678:A:OP2	2.25	0.65
21:A:1053:A:N3	21:A:1197:C:O2'	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:199:A:O2'	21:A:200:A:OP1	2.12	0.65
50:8:2:LYS:NZ	50:8:31:LYS:O	2.22	0.65
21:A:857:C:O2	21:A:1288:G:N1	2.29	0.65
21:A:266:A:O2'	21:A:475:A:N3	2.23	0.65
21:A:1518:G:HO2'	21:A:1519:U:P	2.19	0.65
27:H:54:ARG:NH2	27:H:57:ASP:OD1	2.29	0.65
21:A:275:A:H62	21:A:296:G:N2	1.95	0.65
21:A:1313:G:OP2	21:A:1689:G:O2'	2.09	0.65
21:A:2505:A:OP1	50:8:31:LYS:NZ	2.29	0.65
22:B:84:U:O2'	22:B:86:C:O2	2.11	0.65
21:A:2747:U:OP2	54:A:3108:HOH:O	2.14	0.65
34:S:16:ARG:NH2	34:S:80:THR:O	2.30	0.65
23:D:83:ASP:OD2	23:D:86:ARG:NH2	2.30	0.64
21:A:138:U:N3	21:A:141:U:OP2	2.29	0.64
21:A:2752:A:O2'	21:A:2753:U:O5'	2.15	0.64
46:4:10:LYS:O	46:4:14:ASN:ND2	2.30	0.64
21:A:572:C:N4	21:A:2806:U:OP2	2.30	0.64
21:A:1359:A:O2'	37:V:84:ARG:NH2	2.31	0.64
21:A:2024:A:OP2	24:E:138:ARG:NH1	2.31	0.64
21:A:1570:G:O5'	21:A:1570:G:H8	1.80	0.64
21:A:2070:C:OP1	21:A:2804:G:O2'	2.15	0.64
21:A:1987:A:H2'	21:A:1988:C:H5'	1.80	0.64
21:A:1215:U:O2'	21:A:1217:U:OP2	2.14	0.63
21:A:1172:A:N6	21:A:2545:A:C6	2.66	0.63
47:5:35:PHE:HE1	47:5:37:SER:HA	1.63	0.63
21:A:230:A:H61	21:A:456:G:H21	1.46	0.63
21:A:1295:C:OP1	25:F:72:ARG:NH2	2.32	0.63
21:A:661:U:HO2'	21:A:662:G:P	2.22	0.63
25:F:144:SER:O	25:F:148:GLN:NE2	2.32	0.63
21:A:2717:A:OP2	32:Q:13:ARG:NH2	2.32	0.63
42:0:19:SER:N	42:0:27:ARG:O	2.30	0.63
21:A:1302:G:O6	21:A:1303:A:N6	2.31	0.63
21:A:1306:C:N3	21:A:2040:A:C6	2.67	0.63
21:A:2877:G:N2	21:A:2880:A:OP2	2.31	0.63
21:A:457:G:OP2	21:A:2433:C:O2'	2.14	0.63
21:A:1828:U:C6	21:A:2230:G:H1'	2.33	0.63
21:A:1845:U:O2'	23:D:152:GLN:O	2.11	0.63
21:A:2404:A:O2'	33:R:119:PHE:OXT	2.16	0.63
21:A:251:G:O2'	21:A:2459:A:OP1	2.09	0.63
21:A:2599:A:OP1	21:A:2601:G:O2'	2.12	0.62
22:B:7:G:OP1	33:R:19:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1578:A:N6	21:A:1591:G:N7	2.45	0.62
21:A:1395:G:O2'	21:A:1410:A:N6	2.31	0.62
37:V:23:LEU:O	37:V:27:LYS:NZ	2.22	0.62
21:A:1250:G:O2'	21:A:1274:G:N2	2.33	0.62
21:A:735:C:O2'	21:A:825:G:OP1	2.18	0.62
21:A:1612:C:O2'	21:A:1614:A:N7	2.30	0.62
21:A:1987:A:C8	21:A:1987:A:H5''	2.32	0.62
21:A:628:G:N2	21:A:1289:A:N1	2.46	0.62
21:A:1306:C:C2	21:A:2040:A:N6	2.67	0.62
21:A:774:G:OP2	23:D:206:LYS:NZ	2.31	0.62
21:A:460:C:O2	21:A:1891:U:O2'	2.18	0.62
21:A:1097:U:O4	21:A:1098:A:N6	2.33	0.61
21:A:74:U:OP1	43:1:47:ARG:NH2	2.34	0.61
21:A:2510:C:O2	31:P:49:SER:OG	2.15	0.61
21:A:790:G:H21	21:A:795:A:H61	1.46	0.61
21:A:1518:G:O2'	21:A:1519:U:O5'	2.12	0.61
25:F:136:THR:O	25:F:140:LYS:NZ	2.21	0.61
21:A:321:U:C2	21:A:326:A:C6	2.89	0.61
21:A:2418:G:OP1	49:7:26:ARG:NH2	2.34	0.61
21:A:857:C:N3	21:A:1288:G:C5	2.68	0.61
43:1:42:ARG:O	43:1:45:THR:OG1	2.16	0.61
39:X:24:ILE:HG22	39:X:25:ALA:H	1.65	0.61
21:A:284:C:N4	21:A:286:U:O4'	2.34	0.60
22:B:87:G:C2	31:P:39:THR:HA	2.34	0.60
29:N:42:THR:OG1	29:N:56:ASP:O	2.13	0.60
21:A:1793:C:C2	21:A:2014:G:C2	2.89	0.60
21:A:1828:U:C4	21:A:2230:G:C8	2.88	0.60
23:D:117:SER:HA	23:D:128:ALA:HB3	1.82	0.60
21:A:857:C:C5	21:A:1288:G:C6	2.86	0.60
21:A:1453:G:N2	21:A:1631:G:N7	2.49	0.60
21:A:321:U:N3	21:A:326:A:N6	2.50	0.60
21:A:965:G:N2	21:A:2296:A:OP2	2.35	0.60
21:A:1581:U:C5	21:A:1584:A:H8	2.19	0.60
21:A:2239:A:N7	21:A:2241:C:N4	2.50	0.60
21:A:1306:C:O2	21:A:2040:A:N1	2.34	0.59
21:A:2161:A:N6	21:A:2184:G:O2'	2.29	0.59
43:1:62:ILE:O	43:1:65:SER:OG	2.10	0.59
44:2:11:SER:OG	44:2:12:VAL:N	2.33	0.59
21:A:1172:A:C6	21:A:2545:A:N1	2.70	0.59
21:A:1938:U:O2'	21:A:1939:A:O5'	2.20	0.59
21:A:2650:G:O5'	21:A:2845:G:N2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:2575:G:O2'	29:N:4:GLN:OE1	2.20	0.59
21:A:236:A:H61	21:A:475:A:H61	1.50	0.59
27:H:22:ASN:OD1	27:H:23:HIS:N	2.36	0.59
21:A:628:G:C4	21:A:1289:A:N6	2.71	0.59
32:Q:46:LYS:O	32:Q:49:THR:OG1	2.17	0.59
21:A:1462:G:O2'	21:A:1463:A:O4'	2.18	0.59
21:A:2361:U:O2'	21:A:2362:A:OP1	2.17	0.59
45:3:67:ALA:O	45:3:68:ASP:HB2	2.01	0.58
21:A:153:G:O2'	21:A:154:A:O5'	2.21	0.58
21:A:1794:C:C2	21:A:2013:G:C2	2.90	0.58
21:A:774:G:N1	21:A:1802:U:N3	2.50	0.58
21:A:932:U:N3	21:A:935:C:N4	2.51	0.58
48:6:9:ASN:OD1	48:6:10:LYS:N	2.36	0.58
21:A:1290:G:OP2	35:T:13:ARG:NH2	2.34	0.58
47:5:35:PHE:HD1	47:5:36:CYS:H	1.40	0.58
21:A:1005:G:O6	21:A:2482:G:O2'	2.21	0.58
21:A:1079:U:OP1	27:H:59:LYS:NZ	2.33	0.58
21:A:2195:G:N1	21:A:2197:G:N7	2.52	0.58
21:A:1304:G:O2'	21:A:2039:G:O6	2.13	0.58
21:A:1828:U:C2	21:A:2230:G:H1'	2.37	0.58
21:A:1708:A:C6	21:A:2753:U:N3	2.72	0.57
31:P:39:THR:O	31:P:40:SER:OG	2.14	0.57
21:A:857:C:C2	21:A:1288:G:C2	2.89	0.57
21:A:990:G:O6	21:A:1016:G:N2	2.37	0.57
40:Y:47:GLU:O	40:Y:51:VAL:HG23	2.05	0.57
45:3:73:ARG:HD3	45:3:74:PHE:N	2.18	0.57
21:A:593:U:O2'	21:A:594:G:OP1	2.19	0.57
21:A:2402:G:N2	21:A:2405:A:OP2	2.26	0.57
21:A:895:U:HO2'	44:2:22:THR:HG1	1.53	0.57
21:A:1568:U:H5'	21:A:1570:G:H1'	1.87	0.57
21:A:833:A:N3	48:6:5:THR:OG1	2.37	0.57
21:A:1934:G:O6	21:A:1951:C:N4	2.38	0.57
41:Z:64:ASP:OD1	41:Z:66:THR:HG23	2.04	0.57
21:A:795:A:OP1	21:A:1659:C:N4	2.37	0.57
21:A:1091:G:N2	21:A:1154:G:HO2'	2.03	0.56
21:A:1458:A:N1	21:A:1459:A:N6	2.53	0.56
25:F:80:ALA:HB1	25:F:81:PRO:HD2	1.87	0.56
21:A:857:C:C4	21:A:1288:G:C6	2.94	0.56
21:A:1962:G:C4	21:A:1991:G:N2	2.74	0.56
21:A:2860:U:H5''	32:Q:49:THR:HG21	1.87	0.56
24:E:114:ASP:OD1	24:E:115:VAL:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3:69:GLY:O	45:3:73:ARG:HB3	2.05	0.56
21:A:2372:G:O6	21:A:2398:G:N2	2.37	0.56
21:A:579:U:O2'	35:T:49:ASP:OD2	2.12	0.56
21:A:1271:G:OP1	21:A:1295:C:O2'	44.55	0.55
46:4:30:CYS:N	46:4:35:ARG:O	2.40	0.55
21:A:1110:U:O2'	21:A:1113:A:N6	2.38	0.55
21:A:574:A:N6	21:A:2069:A:N3	2.54	0.55
21:A:1828:U:C5	21:A:2230:G:C8	2.94	0.55
21:A:613:G:N1	21:A:2057:A:C5	2.74	0.55
21:A:1659:C:OP2	21:A:1661:C:N4	2.37	0.55
21:A:796:A:N7	21:A:834:A:N6	2.54	0.55
21:A:83:G:O2'	21:A:84:A:OP2	2.24	0.55
40:Y:76:ASP:OD1	40:Y:77:TYR:N	2.39	0.55
45:3:77:LYS:HA	45:3:77:LYS:CE	2.34	0.55
21:A:1436:C:HO2'	21:A:1437:U:P	2.30	0.55
21:A:1491:C:H42	21:A:1508:C:H42	1.54	0.55
21:A:1788:U:O4	21:A:1789:A:N6	2.39	0.55
30:O:110:LYS:NZ	30:O:131:SER:OG	2.35	0.55
37:V:57:ASN:OD1	37:V:58:ALA:N	2.40	0.55
21:A:2680:U:OP2	21:A:2681:A:O2'	2.17	0.55
34:S:61:PHE:O	34:S:75:THR:OG1	2.19	0.55
21:A:904:G:O2'	21:A:961:G:O6	2.24	0.55
21:A:1569:G:H21	21:A:1570:G:C5'	2.19	0.55
21:A:1828:U:C2	21:A:2230:G:C4	2.94	0.55
21:A:903:G:O2'	21:A:904:G:O4'	2.25	0.55
21:A:1506:C:O2'	21:A:1507:A:O4'	2.21	0.54
30:O:77:VAL:O	30:O:107:SER:OG	2.11	0.54
21:A:254:A:OP1	49:7:7:HIS:NE2	2.41	0.54
23:D:44:ASN:OD1	23:D:45:GLN:N	2.40	0.54
21:A:806:A:N6	52:A:3004:O:O	2.41	0.54
34:S:102:LEU:O	34:S:103:ARG:NH1	2.36	0.54
21:A:857:C:H5	21:A:1288:G:C4	2.23	0.54
21:A:2089:A:N6	21:A:2530:A:N7	2.56	0.54
23:D:74:ASN:OD1	23:D:75:ALA:N	2.40	0.54
21:A:1569:G:N2	21:A:1570:G:H5'	2.20	0.54
21:A:545:G:N1	21:A:548:A:OP2	2.40	0.54
21:A:2276:U:N3	21:A:2280:G:OP2	2.41	0.54
45:3:75:ASN:CA	45:3:78:PHE:CE2	2.86	0.54
21:A:283:G:N2	21:A:289:U:O2	2.40	0.54
45:3:46:ILE:HD12	45:3:48:LEU:HD11	1.90	0.54
21:A:342:A:N3	21:A:362:C:O2'	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:2869:G:O3'	21:A:2886:G:N2	2.34	0.53
36:U:81:ASN:ND2	54:U:201:HOH:O	2.41	0.53
45:3:51:SER:O	45:3:52:SER:OG	2.20	0.53
21:A:903:G:C2	21:A:2295:A:C2	2.96	0.53
29:N:64:ARG:NE	29:N:81:GLU:OE2	2.40	0.53
21:A:1581:U:C6	21:A:1584:A:H8	2.27	0.53
21:A:2465:U:O2'	21:A:2467:C:OP1	2.26	0.53
48:6:19:PHE:O	48:6:22:ARG:N	2.42	0.53
21:A:994:A:O3'	22:B:85:A:N6	2.42	0.53
45:3:75:ASN:HA	45:3:78:PHE:HE2	1.64	0.53
40:Y:15:ARG:O	40:Y:17:ASP:N	2.41	0.53
21:A:2282:G:N2	41:Z:14:GLY:O	2.42	0.53
45:3:74:PHE:CD2	45:3:75:ASN:N	2.77	0.53
21:A:418:G:O2'	21:A:446:G:O6	2.10	0.53
21:A:625:G:C4	21:A:1297:G:N2	2.77	0.53
21:A:2693:C:H42	27:H:109:TYR:HA	1.74	0.53
21:A:1712:A:N3	21:A:1714:C:N4	2.57	0.53
21:A:615:A:H61	21:A:2056:G:H21	1.58	0.52
21:A:2281:C:H42	41:Z:14:GLY:HA3	1.73	0.52
21:A:857:C:C6	21:A:1288:G:C6	2.94	0.52
27:H:10:ASP:OD1	27:H:11:ILE:N	2.42	0.52
21:A:1794:C:N3	21:A:2013:G:C2	2.77	0.52
23:D:61:TYR:CE2	23:D:63:VAL:HG22	2.45	0.52
37:V:30:ALA:HA	37:V:33:ILE:HD12	1.92	0.52
29:N:63:VAL:HG21	29:N:102:VAL:HG23	1.91	0.52
50:8:19:ARG:NE	50:8:24:MET:SD	2.82	0.52
21:A:628:G:N3	21:A:1289:A:N6	2.57	0.52
21:A:2059:G:N2	24:E:159:ASP:OD2	2.42	0.52
21:A:1828:U:N1	21:A:2230:G:C4	2.78	0.52
21:A:608:C:O3'	54:A:3111:HOH:O	2.19	0.52
21:A:2255:G:P	23:D:262:LYS:HZ1	2.32	0.52
45:3:73:ARG:CG	45:3:74:PHE:N	2.73	0.52
25:F:190:ASP:OD1	25:F:191:SER:N	2.42	0.52
21:A:550:A:HO2'	21:A:554:C:HO2'	1.53	0.52
21:A:2260:A:O2'	21:A:2261:G:H5'	2.10	0.52
21:A:903:G:C6	21:A:2295:A:N1	2.78	0.52
21:A:932:U:N3	21:A:935:C:C4	2.78	0.52
21:A:1288:G:OP2	30:O:21:ARG:NH2	2.43	0.52
21:A:1569:G:N3	21:A:1569:G:C2'	2.73	0.51
21:A:1987:A:C2'	21:A:1988:C:C5'	2.85	0.51
21:A:1710:G:N1	21:A:2022:U:O4	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:2110:G:O6	21:A:2264:G:N2	2.43	0.51
45:3:78:PHE:CD1	45:3:79:GLY:N	2.78	0.51
21:A:13:A:O2'	21:A:15:G:N7	2.43	0.51
21:A:352:A:N7	21:A:373:A:N6	2.58	0.51
21:A:1075:G:H21	50:8:36:GLN:HE22	1.58	0.51
21:A:1568:U:O4'	21:A:1570:G:C4	2.64	0.51
21:A:1569:G:C3'	21:A:1569:G:N3	2.73	0.51
21:A:1570:G:H2'	21:A:1571:G:C8	2.45	0.51
22:B:22:G:N7	22:B:54:U:O2'	2.31	0.51
34:S:29:ARG:NH1	34:S:46:GLU:OE2	2.44	0.51
41:Z:48:GLN:OE1	41:Z:53:ILE:N	2.44	0.51
21:A:1581:U:C5	21:A:1584:A:C8	2.98	0.51
21:A:752:G:O6	21:A:770:G:N2	2.44	0.51
22:B:38:U:N3	22:B:42:G:OP2	2.44	0.51
23:D:69:ASN:OD1	23:D:70:LYS:N	2.43	0.51
21:A:1519:U:O2'	21:A:1560:A:N1	2.43	0.51
21:A:1570:G:P	21:A:1570:G:H8	2.33	0.51
21:A:1172:A:C5	21:A:2545:A:N1	2.79	0.51
21:A:1708:A:N6	21:A:2753:U:C4	2.78	0.51
21:A:550:A:O2'	21:A:554:C:O2'	2.26	0.51
21:A:1175:G:N7	24:E:162:ARG:NH2	2.59	0.51
21:A:1568:U:C5'	21:A:1570:G:H1'	2.39	0.51
21:A:1962:G:O2'	21:A:1963:A:O5'	2.26	0.51
21:A:2002:G:O6	21:A:2003:U:N3	2.43	0.51
22:B:90:C:OP1	40:Y:19:LYS:NZ	2.40	0.51
31:P:110:SER:OG	31:P:111:GLU:N	2.44	0.51
45:3:33:GLU:O	45:3:51:SER:OG	2.26	0.51
21:A:1306:C:C2	21:A:2040:A:N1	2.78	0.51
31:P:22:LYS:NZ	31:P:23:GLY:O	2.42	0.51
21:A:563:G:O5'	37:V:18:ARG:NH1	2.44	0.51
21:A:1235:C:N3	21:A:1288:G:N1	2.49	0.50
21:A:749:G:O2'	21:A:771:G:N2	2.44	0.50
21:A:1250:G:HO2'	21:A:1274:G:N2	2.09	0.50
21:A:1711:G:O2'	21:A:2018:U:O4	2.24	0.50
40:Y:27:VAL:N	40:Y:43:VAL:O	2.44	0.50
42:0:18:ARG:O	42:0:29:TRP:NE1	2.44	0.50
21:A:1123:C:N4	21:A:1132:A:O4'	2.43	0.50
21:A:1836:A:O2'	21:A:1837:A:O4'	2.20	0.50
21:A:1897:U:HO2'	21:A:1898:C:C1'	2.24	0.50
24:E:83:ALA:O	24:E:85:LYS:NZ	2.42	0.50
21:A:2860:U:C5'	32:Q:49:THR:HG21	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R:84:ALA:O	33:R:88:GLY:N	2.39	0.50
21:A:1494:G:N2	21:A:1506:C:N3	2.53	0.50
23:D:190:THR:OG1	23:D:191:ILE:N	2.45	0.50
45:3:66:ALA:HA	45:3:67:ALA:HB3	1.94	0.50
21:A:1855:G:N2	54:A:3126:HOH:O	2.45	0.50
21:A:2140:C:N4	21:A:2195:G:O2'	2.44	0.50
21:A:319:G:N2	21:A:320:U:O3'	2.44	0.50
21:A:1236:G:H1'	21:A:1288:G:H21	1.77	0.50
21:A:902:A:N1	21:A:903:G:N2	2.59	0.50
21:A:687:G:H21	21:A:691:A:H62	1.59	0.50
24:E:41:VAL:N	24:E:47:ASN:OD1	2.43	0.50
45:3:74:PHE:CD2	45:3:74:PHE:C	2.85	0.49
21:A:164:A:O2'	21:A:165:C:O2	2.22	0.49
45:3:75:ASN:ND2	45:3:78:PHE:CE2	2.78	0.49
21:A:1463:A:HO2'	21:A:1464:U:P	2.36	0.49
21:A:198:A:OP2	21:A:199:A:O2'	2.29	0.49
21:A:2362:A:N6	21:A:2364:G:N3	2.59	0.49
45:3:78:PHE:C	45:3:78:PHE:CD1	2.85	0.49
21:A:1292:A:O2'	21:A:1293:U:OP1	2.30	0.49
48:6:15:LYS:O	48:6:18:GLY:N	2.44	0.49
21:A:2603:G:O2'	21:A:2606:C:OP2	2.31	0.49
21:A:285:U:OP1	21:A:288:C:N4	2.42	0.49
49:7:34:ALA:O	49:7:38:THR:OG1	2.18	0.49
21:A:613:G:C5	21:A:2057:A:N6	2.80	0.49
45:3:70:ARG:CZ	45:3:71:VAL:CG2	2.90	0.49
21:A:1510:U:C2'	21:A:1511:C:H5'	2.43	0.49
21:A:682:A:N1	21:A:696:G:O2'	2.34	0.49
21:A:738:U:O2'	21:A:1390:A:N3	2.42	0.49
21:A:790:G:N2	21:A:795:A:H61	2.10	0.49
36:U:23:GLU:OE1	36:U:90:GLN:NE2	2.45	0.49
21:A:1828:U:C5	21:A:2230:G:C2'	2.96	0.49
21:A:613:G:C6	21:A:2057:A:C6	3.00	0.49
21:A:230:A:H61	21:A:456:G:N2	2.11	0.49
21:A:281:A:N1	21:A:282:A:N6	2.60	0.49
27:H:96:ALA:N	27:H:128:ASN:O	2.38	0.49
21:A:1752:C:H42	21:A:1777:G:H1	1.61	0.48
41:Z:35:ASP:OD1	41:Z:36:GLY:N	2.46	0.48
21:A:2268:A:N7	54:A:3121:HOH:O	2.35	0.48
21:A:1708:A:N6	21:A:2753:U:N3	2.62	0.48
43:1:38:GLU:N	43:1:38:GLU:OE1	2.46	0.48
45:3:28:THR:HG23	45:3:48:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:2616:A:N1	21:A:2633:C:N4	2.61	0.48
23:D:64:ILE:HD11	23:D:86:ARG:HH22	1.77	0.48
45:3:71:VAL:CA	45:3:74:PHE:CE1	2.86	0.48
21:A:1828:U:C6	21:A:2230:G:C2'	2.96	0.48
32:Q:9:THR:OG1	32:Q:10:SER:N	2.45	0.48
40:Y:32:TYR:O	40:Y:93:ALA:N	2.41	0.48
47:5:35:PHE:HE1	47:5:37:SER:H	1.38	0.48
21:A:796:A:H62	21:A:834:A:H62	1.59	0.48
45:3:42:GLU:N	45:3:42:GLU:OE1	2.46	0.48
21:A:1187:A:N7	28:M:28:ARG:NH1	2.62	0.48
47:5:32:MET:SD	47:5:32:MET:N	2.87	0.48
21:A:1105:U:O2'	21:A:1109:U:O4	2.32	0.48
21:A:2126:C:HO2'	21:A:2127:G:H8	1.62	0.48
21:A:749:G:O2'	21:A:771:G:N1	2.46	0.48
29:N:98:ILE:HG22	29:N:99:PHE:O	2.13	0.48
21:A:1793:C:N1	21:A:2014:G:N2	2.60	0.48
22:B:15:C:N4	22:B:105:G:H21	2.03	0.48
45:3:75:ASN:CG	45:3:78:PHE:HE2	2.17	0.48
47:5:35:PHE:C	47:5:35:PHE:CD1	2.86	0.48
21:A:1828:U:C6	21:A:2230:G:H2'	2.49	0.48
21:A:1072:A:N3	21:A:2513:G:O2'	2.41	0.47
21:A:1306:C:N3	21:A:2040:A:C5	2.81	0.47
38:W:31:THR:HG22	38:W:32:ARG:H	1.78	0.47
45:3:77:LYS:HE2	45:3:77:LYS:CA	2.37	0.47
23:D:141:HIS:ND1	23:D:192:GLY:O	2.44	0.47
21:A:2355:A:H2'	21:A:2356:A:C8	2.49	0.47
21:A:895:U:O2'	44:2:22:THR:OG1	2.24	0.47
21:A:2510:C:H42	31:P:124:LYS:HE2	1.79	0.47
21:A:1709:A:N1	21:A:2023:C:N4	2.58	0.47
21:A:1252:A:N6	21:A:1273:G:O2'	2.39	0.47
21:A:1450:A:H3'	21:A:1634:A:H61	1.79	0.47
21:A:1982:U:H3	21:A:2579:U:C4'	2.28	0.47
21:A:330:C:N4	21:A:337:A:N7	25.40	0.47
35:T:70:ARG:NH1	35:T:75:SER:OG	2.48	0.47
21:A:2870:A:P	21:A:2886:G:H22	2.37	0.47
21:A:446:G:O2'	21:A:502:C:N4	85.00	0.47
36:U:60:ALA:HB1	36:U:96:THR:O	2.15	0.47
21:A:1469:G:N2	21:A:1621:C:N3	2.63	0.47
33:R:70:VAL:O	33:R:73:ALA:HB3	2.15	0.47
38:W:31:THR:HG22	38:W:32:ARG:N	2.30	0.47
40:Y:27:VAL:HB	40:Y:43:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:164:A:O2'	21:A:165:C:O5'	2.32	0.47
21:A:2822:C:O2'	21:A:2823:G:O4'	2.33	0.47
21:A:1817:C:O2'	23:D:207:ALA:HB2	2.15	0.47
45:3:65:ALA:O	45:3:67:ALA:HB3	2.15	0.47
45:3:80:LEU:HA	45:3:80:LEU:HD23	1.77	0.47
22:B:69:C:H42	22:B:102:A:H61	1.61	0.47
21:A:82:G:N1	21:A:102:A:OP2	2.44	0.46
21:A:1436:C:O2'	21:A:1437:U:O5'	2.31	0.46
33:R:31:LEU:HD13	33:R:44:ILE:HG13	1.98	0.46
45:3:73:ARG:HG3	45:3:74:PHE:N	2.25	0.46
21:A:1172:A:N6	21:A:2545:A:N6	2.63	0.46
22:B:4:G:H1	22:B:111:A:H62	1.62	0.46
21:A:319:G:H21	21:A:320:U:C4'	2.29	0.46
22:B:10:U:O2'	22:B:12:U:OP1	2.32	0.46
32:Q:90:ALA:O	32:Q:94:THR:HG23	2.15	0.46
21:A:1091:G:N2	21:A:1154:G:O2'	2.47	0.46
21:A:1858:G:H22	21:A:2002:G:N2	2.13	0.46
21:A:203:U:O4	21:A:253:G:N2	2.30	0.46
21:A:1390:A:OP2	21:A:1414:G:N1	2.42	0.46
21:A:695:C:N4	21:A:696:G:O6	2.48	0.46
22:B:11:A:OP1	41:Z:82:ARG:NE	2.44	0.46
21:A:1704:C:H42	21:A:2027:G:H1	1.64	0.46
21:A:2093:C:N4	21:A:2094:G:O6	2.49	0.46
21:A:2485:U:HO2'	21:A:2517:G:H1	1.63	0.46
21:A:1044:A:OP2	21:A:1198:G:N1	2.40	0.46
45:3:53:ASP:OD1	45:3:59:THR:OG1	2.34	0.46
21:A:446:G:N2	21:A:504:G:O6	61.35	0.46
23:D:64:ILE:HG21	23:D:66:PHE:CE1	2.51	0.46
21:A:2039:G:O2'	21:A:2040:A:O5'	2.29	0.46
21:A:1008:C:O2'	21:A:2300:A:N3	2.38	0.46
21:A:2375:U:OP2	49:7:35:ASN:ND2	2.43	0.46
24:E:63:ALA:HB1	24:E:68:TYR:HD2	1.81	0.46
40:Y:18:LEU:O	40:Y:21:LEU:N	2.47	0.46
21:A:1579:C:HO2'	21:A:1580:A:H2	1.62	0.45
21:A:1488:A:N7	21:A:1596:G:N1	2.63	0.45
21:A:786:U:O4	21:A:812:U:N3	28.01	0.45
21:A:600:U:OP1	28:M:114:ARG:NH1	2.47	0.45
33:R:8:ASN:O	33:R:12:LEU:N	2.49	0.45
21:A:625:G:C6	21:A:1297:G:C6	3.04	0.45
21:A:1927:A:O2'	21:A:1928:A:OP1	2.32	0.45
21:A:2127:G:C2	21:A:2216:U:O2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3:67:ALA:O	45:3:68:ASP:CB	2.65	0.45
49:7:18:ALA:O	49:7:19:SER:OG	2.29	0.45
21:A:175:C:N4	21:A:177:G:O6	2.50	0.45
21:A:1718:G:H21	21:A:1721:A:H61	1.64	0.45
24:E:142:SER:O	24:E:143:HIS:ND1	2.48	0.45
21:A:1989:C:O5'	21:A:1989:C:H6	2.00	0.45
21:A:903:G:O6	21:A:2295:A:N1	2.50	0.45
43:1:45:THR:O	43:1:49:THR:HG23	2.16	0.45
21:A:116:G:OP2	21:A:118:A:O2'	2.35	0.45
45:3:32:SER:OG	45:3:54:SER:OG	2.19	0.45
45:3:75:ASN:O	45:3:78:PHE:CD2	2.70	0.45
21:A:2354:A:N7	21:A:2415:A:N6	2.65	0.45
30:O:114:ASN:ND2	30:O:129:SER:O	2.50	0.45
21:A:261:U:C1'	21:A:283:G:H21	62.01	0.44
21:A:729:G:N2	21:A:819:A:N1	2.65	0.44
31:P:60:ARG:NH1	31:P:108:GLY:O	2.45	0.44
37:V:5:ALA:HB3	37:V:54:ALA:HB2	1.98	0.44
21:A:1865:C:H41	21:A:1926:A:H5'	1.82	0.44
21:A:2370:U:HO2'	21:A:2400:U:HO2'	1.58	0.44
21:A:721:A:H2	21:A:847:A:H61	1.64	0.44
32:Q:45:GLU:O	32:Q:49:THR:HG23	2.18	0.44
41:Z:64:ASP:CG	41:Z:66:THR:HG23	2.38	0.44
45:3:71:VAL:O	45:3:74:PHE:CD1	2.70	0.44
21:A:1793:C:N3	21:A:2014:G:C2	2.85	0.44
21:A:1847:U:O2'	23:D:157:ALA:HB3	2.18	0.44
23:D:59:ARG:NH2	23:D:213:LYS:O	2.50	0.44
47:5:35:PHE:CD1	47:5:37:SER:N	2.81	0.44
21:A:1357:G:N1	21:A:1367:C:OP2	2.48	0.44
21:A:1828:U:H3'	21:A:1829:A:C5'	2.48	0.44
21:A:2195:G:N2	21:A:2197:G:O6	2.50	0.44
21:A:2458:U:N3	21:A:2461:A:OP2	2.45	0.44
21:A:748:U:HO2'	21:A:749:G:C5'	3.18	0.44
24:E:9:LYS:O	24:E:11:GLY:N	2.51	0.44
27:H:83:TYR:N	27:H:135:GLY:O	2.47	0.44
21:A:877:G:N2	30:O:48:PRO:O	2.47	0.44
21:A:1515:G:HO2'	21:A:1516:C:H6	1.65	0.44
21:A:660:A:C2	25:F:36:ALA:HB1	2.53	0.44
45:3:46:ILE:HD12	45:3:48:LEU:CD1	2.48	0.43
49:7:49:LEU:HD12	49:7:49:LEU:N	2.32	0.43
21:A:628:G:H2'	21:A:1289:A:H62	1.82	0.43
21:A:2033:C:O2'	21:A:2843:A:N3	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:22:GLU:O	23:D:80:ILE:HG21	2.18	0.43
33:R:68:THR:O	33:R:68:THR:HG23	2.18	0.43
40:Y:38:ASN:OD1	40:Y:39:VAL:N	2.51	0.43
45:3:25:SER:OG	45:3:26:GLY:N	2.52	0.43
21:A:1198:G:OP2	35:T:58:ARG:NE	2.35	0.43
21:A:1828:U:C4	21:A:2230:G:O4'	2.71	0.43
49:7:24:ARG:NH2	49:7:43:GLN:O	2.49	0.43
21:A:1569:G:N3	21:A:1569:G:H2'	2.33	0.43
21:A:1570:G:H2'	21:A:1571:G:H8	1.82	0.43
23:D:80:ILE:HG22	23:D:81:GLN:N	2.33	0.43
30:O:83:ASN:OD1	30:O:84:LYS:N	2.51	0.43
33:R:39:HIS:HA	33:R:40:ILE:HD12	2.00	0.43
33:R:86:ASP:OD1	33:R:87:LYS:N	2.51	0.43
21:A:1118:G:O2'	21:A:1119:C:O5'	2.33	0.43
21:A:1575:A:O2'	21:A:1577:G:O6	2.23	0.43
21:A:2673:C:OP2	21:A:2759:G:O2'	2.35	0.43
21:A:932:U:C2	21:A:935:C:C4	3.07	0.43
28:M:76:TYR:HE1	28:M:87:SER:HG	1.66	0.43
45:3:49:ASP:OD1	45:3:50:ILE:N	2.51	0.43
21:A:1816:A:H2'	21:A:1817:C:O4'	2.19	0.43
21:A:1827:C:OP2	23:D:181:ARG:NH1	2.51	0.43
21:A:27:G:O2'	21:A:557:G:N2	2.51	0.43
22:B:26:C:H2'	22:B:27:A:O4'	2.18	0.43
24:E:65:SER:O	24:E:67:LYS:N	2.52	0.43
21:A:273:A:OP2	21:A:297:G:N1	2.45	0.43
21:A:503:A:N6	21:A:517:A:OP2	2.49	0.43
21:A:2137:G:O6	21:A:2206:C:N4	2.52	0.43
21:A:790:G:H21	21:A:795:A:N6	2.15	0.43
24:E:9:LYS:HG2	24:E:9:LYS:O	2.19	0.43
40:Y:72:VAL:HG21	40:Y:91:PHE:CD1	2.54	0.43
45:3:75:ASN:CG	45:3:78:PHE:CE2	2.92	0.43
21:A:903:G:H1	21:A:2295:A:H2	1.60	0.43
21:A:903:G:H22	21:A:965:G:H1	1.67	0.43
21:A:975:U:O2'	21:A:976:U:O4'	2.35	0.43
21:A:1707:U:HO2'	21:A:1708:A:H8	1.67	0.43
22:B:3:U:H3	22:B:112:G:H22	1.67	0.43
21:A:1510:U:O2'	21:A:1511:C:H5'	2.19	0.42
21:A:1987:A:H2'	21:A:1988:C:O5'	2.18	0.42
23:D:157:ALA:O	23:D:176:ARG:NH2	2.51	0.42
27:H:117:ALA:HB2	27:H:123:PHE:CE2	2.54	0.42
21:A:628:G:N3	21:A:1289:A:N1	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1989:C:O2'	21:A:1991:G:OP2	2.32	0.42
21:A:1828:U:C5	21:A:2230:G:H2'	2.54	0.42
25:F:125:VAL:HG22	25:F:126:VAL:N	2.34	0.42
28:M:5:PHE:O	35:T:64:ARG:NH2	2.46	0.42
21:A:848:U:O4	21:A:849:A:N6	2.52	0.42
29:N:13:ASN:OD1	29:N:96:THR:OG1	2.28	0.42
48:6:2:VAL:HG21	48:6:4:ARG:HE	1.84	0.42
21:A:247:A:OP2	49:7:8:ARG:NH1	2.50	0.42
23:D:194:VAL:HG12	23:D:195:GLY:N	2.35	0.42
24:E:141:MET:SD	24:E:148:HIS:ND1	2.92	0.42
34:S:28:LEU:HD11	34:S:86:ILE:CG2	2.49	0.42
45:3:28:THR:OG1	45:3:46:ILE:HD11	2.20	0.42
45:3:73:ARG:HE	45:3:73:ARG:HB2	1.64	0.42
23:D:213:LYS:N	23:D:214:GLY:HA2	2.35	0.42
21:A:1344:A:OP2	21:A:1650:G:N1	2.49	0.42
21:A:1396:A:OP2	21:A:1408:G:N2	2.51	0.42
21:A:319:G:H21	21:A:320:U:H4'	1.84	0.42
27:H:46:GLU:HB2	27:H:49:THR:HG23	2.01	0.42
33:R:25:THR:OG1	33:R:47:ASP:N	2.52	0.42
21:A:1378:U:OP1	21:A:1434:U:N3	2.53	0.42
21:A:2774:G:H21	21:A:2784:A:H62	1.67	0.42
23:D:103:ILE:HG22	23:D:104:ILE:O	2.20	0.42
41:Z:64:ASP:OD1	41:Z:64:ASP:N	2.52	0.41
21:A:153:G:HO2'	21:A:154:A:P	2.43	0.41
21:A:1949:G:H2'	21:A:1950:U:O4'	2.20	0.41
21:A:1693:G:H1	21:A:2035:C:H42	1.67	0.41
21:A:2694:C:O2	27:H:110:SER:OG	2.24	0.41
21:A:922:G:N2	21:A:944:G:O6	2.47	0.41
33:R:56:ALA:HB1	33:R:76:VAL:HG13	2.02	0.41
35:T:35:ALA:O	35:T:39:VAL:HG23	2.20	0.41
21:A:2023:C:O2'	21:A:2023:C:O2	2.36	0.41
23:D:80:ILE:HG22	23:D:81:GLN:H	1.84	0.41
29:N:21:THR:HG22	29:N:39:ILE:HD12	2.01	0.41
21:A:1858:G:H1	21:A:2002:G:N2	2.19	0.41
21:A:688:A:H61	21:A:2396:A:H1'	1.85	0.41
25:F:173:VAL:HG22	25:F:173:VAL:O	2.20	0.41
45:3:73:ARG:CD	45:3:74:PHE:N	2.84	0.41
21:A:2207:U:O4	21:A:2208:A:N6	2.52	0.41
21:A:2770:U:OP2	21:A:2782:C:N4	2.54	0.41
22:B:28:C:H1'	22:B:55:A:H61	1.86	0.41
23:D:194:VAL:HG12	23:D:195:GLY:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:E:51:VAL:HG12	24:E:52:GLY:N	2.35	0.41
21:A:1487:G:N2	21:A:1597:U:O2	2.54	0.41
21:A:1733:A:OP2	21:A:1742:A:N6	2.51	0.41
21:A:1865:C:N4	21:A:1926:A:O4'	2.54	0.41
21:A:341:G:N1	21:A:382:U:OP2	2.54	0.41
21:A:509:G:N2	21:A:512:A:OP2	2.53	0.41
21:A:2397:G:N2	47:5:35:PHE:HE2	2.00	0.41
21:A:901:G:H2'	21:A:902:A:C8	2.56	0.41
23:D:134:ILE:HG22	23:D:135:PRO:O	2.21	0.41
23:D:157:ALA:HB1	23:D:196:ASN:O	2.21	0.41
45:3:77:LYS:HD3	45:3:77:LYS:C	2.40	0.41
21:A:2146:A:H61	21:A:2195:G:H1	1.69	0.41
21:A:1828:U:C2	21:A:2230:G:N3	2.89	0.41
21:A:2261:G:C6	21:A:2262:G:C6	3.08	0.41
21:A:236:A:H61	21:A:475:A:N6	2.16	0.41
22:B:46:A:O3'	33:R:102:HIS:NE2	2.46	0.41
29:N:7:ARG:C	29:N:8:LEU:HD12	2.42	0.41
35:T:92:ARG:O	35:T:93:LYS:HG2	2.21	0.40
21:A:1500:G:N2	21:A:2731:C:C2	2.90	0.40
21:A:603:C:O2'	35:T:48:ARG:NH2	2.54	0.40
26:G:46:ASN:O	26:G:49:VAL:N	2.54	0.40
21:A:1712:A:O2'	21:A:1718:G:N7	2.52	0.40
21:A:1770:C:H42	21:A:1771:A:N6	2.19	0.40
21:A:1818:A:H2	21:A:1856:A:HO2'	1.66	0.40
21:A:2357:G:H21	41:Z:50:GLY:N	2.20	0.40
21:A:2593:A:HO2'	21:A:2594:G:P	2.44	0.40
21:A:327:G:N1	21:A:328:G:N7	2.70	0.40
43:1:25:LEU:O	43:1:28:LEU:N	2.55	0.40
21:A:1075:G:N2	50:8:36:GLN:HE22	2.18	0.40
24:E:178:VAL:HG12	24:E:179:THR:N	2.36	0.40
39:X:23:VAL:O	39:X:24:ILE:HD13	2.20	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	b	222/255 (87%)	199 (90%)	23 (10%)	0	100	100
3	c	206/217 (95%)	172 (84%)	34 (16%)	0	100	100
4	d	193/199 (97%)	171 (89%)	21 (11%)	1 (0%)	34	77
5	e	163/165 (99%)	140 (86%)	23 (14%)	0	100	100
6	f	94/96 (98%)	85 (90%)	9 (10%)	0	100	100
7	g	143/150 (95%)	124 (87%)	17 (12%)	2 (1%)	14	59
8	h	129/131 (98%)	109 (84%)	19 (15%)	1 (1%)	24	70
9	i	126/128 (98%)	114 (90%)	12 (10%)	0	100	100
10	j	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
11	k	116/118 (98%)	99 (85%)	17 (15%)	0	100	100
12	l	133/135 (98%)	103 (77%)	30 (23%)	0	100	100
13	m	117/119 (98%)	92 (79%)	23 (20%)	2 (2%)	11	56
14	n	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
15	o	86/88 (98%)	75 (87%)	11 (13%)	0	100	100
16	p	88/90 (98%)	74 (84%)	14 (16%)	0	100	100
17	q	84/86 (98%)	66 (79%)	17 (20%)	1 (1%)	16	63
18	r	69/71 (97%)	58 (84%)	11 (16%)	0	100	100
19	s	82/84 (98%)	66 (80%)	16 (20%)	0	100	100
20	t	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
23	D	273/275 (99%)	236 (86%)	36 (13%)	1 (0%)	39	80
24	E	216/218 (99%)	181 (84%)	33 (15%)	2 (1%)	21	68
25	F	197/199 (99%)	166 (84%)	30 (15%)	1 (0%)	34	77
26	G	164/166 (99%)	132 (80%)	31 (19%)	1 (1%)	30	74
27	H	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
28	M	143/145 (99%)	126 (88%)	17 (12%)	0	100	100
29	N	120/122 (98%)	98 (82%)	19 (16%)	3 (2%)	7	49
30	O	129/131 (98%)	90 (70%)	39 (30%)	0	100	100
31	P	139/141 (99%)	106 (76%)	33 (24%)	0	100	100
32	Q	117/119 (98%)	104 (89%)	13 (11%)	0	100	100
33	R	117/119 (98%)	104 (89%)	13 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	S	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
35	T	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
36	U	100/102 (98%)	82 (82%)	18 (18%)	0	100	100
37	V	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
38	W	87/89 (98%)	75 (86%)	10 (12%)	2 (2%)	8	51
39	X	81/100 (81%)	66 (82%)	15 (18%)	0	100	100
40	Y	92/94 (98%)	73 (79%)	17 (18%)	2 (2%)	8	52
41	Z	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
42	0	44/46 (96%)	30 (68%)	14 (32%)	0	100	100
43	1	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
44	2	55/57 (96%)	48 (87%)	7 (13%)	0	100	100
45	3	81/84 (96%)	54 (67%)	24 (30%)	3 (4%)	4	40
46	4	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
47	5	24/39 (62%)	15 (62%)	9 (38%)	0	100	100
48	6	42/44 (96%)	35 (83%)	5 (12%)	2 (5%)	3	32
49	7	58/60 (97%)	47 (81%)	11 (19%)	0	100	100
50	8	35/37 (95%)	29 (83%)	6 (17%)	0	100	100
All	All	5292/5466 (97%)	4481 (85%)	787 (15%)	24 (0%)	38	77

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	g	13	LEU
8	h	99	ASN
38	W	50	VAL
45	3	12	VAL
45	3	68	ASP
24	E	10	ILE
29	N	100	GLY
48	6	15	LYS
48	6	16	VAL
13	m	111	GLY
24	E	142	SER
4	d	143	GLU
25	F	144	SER
29	N	25	LEU

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Mol	Chain	Res	Type
40	Y	15	ARG
7	g	14	PRO
38	W	51	ALA
40	Y	16	SER
23	D	195	GLY
45	3	71	VAL
29	N	101	PRO
13	m	65	VAL
26	G	89	VAL
17	q	86	ILE

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	b	194/221 (88%)	194 (100%)	0	100	100
3	c	169/175 (97%)	169 (100%)	0	100	100
4	d	172/174 (99%)	172 (100%)	0	100	100
5	e	130/130 (100%)	129 (99%)	1 (1%)	86	94
6	f	84/84 (100%)	84 (100%)	0	100	100
7	g	126/127 (99%)	126 (100%)	0	100	100
8	h	112/112 (100%)	112 (100%)	0	100	100
9	i	106/106 (100%)	105 (99%)	1 (1%)	84	93
10	j	91/91 (100%)	91 (100%)	0	100	100
11	k	94/94 (100%)	94 (100%)	0	100	100
12	l	117/117 (100%)	117 (100%)	0	100	100
13	m	102/102 (100%)	102 (100%)	0	100	100
14	n	52/52 (100%)	52 (100%)	0	100	100
15	o	80/80 (100%)	80 (100%)	0	100	100
16	p	76/76 (100%)	76 (100%)	0	100	100
17	q	81/81 (100%)	80 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	r	63/63 (100%)	63 (100%)	0	100	100
19	s	73/73 (100%)	73 (100%)	0	100	100
20	t	67/67 (100%)	67 (100%)	0	100	100
23	D	222/222 (100%)	221 (100%)	1 (0%)	92	97
24	E	175/175 (100%)	175 (100%)	0	100	100
25	F	163/163 (100%)	163 (100%)	0	100	100
26	G	147/147 (100%)	147 (100%)	0	100	100
27	H	144/144 (100%)	144 (100%)	0	100	100
28	M	123/123 (100%)	123 (100%)	0	100	100
29	N	100/100 (100%)	100 (100%)	0	100	100
30	O	104/104 (100%)	104 (100%)	0	100	100
31	P	116/116 (100%)	116 (100%)	0	100	100
32	Q	100/100 (100%)	100 (100%)	0	100	100
33	R	95/95 (100%)	95 (100%)	0	100	100
34	S	96/96 (100%)	96 (100%)	0	100	100
35	T	96/96 (100%)	96 (100%)	0	100	100
36	U	86/86 (100%)	86 (100%)	0	100	100
37	V	91/91 (100%)	91 (100%)	0	100	100
38	W	80/80 (100%)	80 (100%)	0	100	100
39	X	73/85 (86%)	73 (100%)	0	100	100
40	Y	83/83 (100%)	83 (100%)	0	100	100
41	Z	64/64 (100%)	64 (100%)	0	100	100
42	0	39/39 (100%)	39 (100%)	0	100	100
43	1	59/59 (100%)	59 (100%)	0	100	100
44	2	51/51 (100%)	51 (100%)	0	100	100
45	3	74/75 (99%)	65 (88%)	9 (12%)	6	34
46	4	49/49 (100%)	49 (100%)	0	100	100
47	5	26/37 (70%)	23 (88%)	3 (12%)	7	37
48	6	39/39 (100%)	39 (100%)	0	100	100
49	7	52/52 (100%)	52 (100%)	0	100	100
50	8	35/35 (100%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4571/4631 (99%)	4555 (100%)	16 (0%)	94 97

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	45	ARG
9	i	16	ASN
17	q	5	ASN
23	D	85	ASN
45	3	70	ARG
45	3	73	ARG
45	3	74	PHE
45	3	75	ASN
45	3	76	LYS
45	3	77	LYS
45	3	81	LYS
45	3	82	SER
45	3	83	ASN
47	5	32	MET
47	5	35	PHE
47	5	46	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	3	GLN
7	g	106	ASN
7	g	129	ASN
9	i	16	ASN
9	i	77	GLN
12	l	42	GLN
13	m	76	ASN
15	o	9	ASN
18	r	57	GLN
19	s	22	GLN
19	s	43	ASN
20	t	64	ASN
24	E	66	ASN
25	F	148	GLN
36	U	81	ASN
40	Y	38	ASN

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Mol	Chain	Res	Type
40	Y	78	GLN
46	4	14	ASN
46	4	51	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1546/1547 (99%)	268 (17%)	0
21	A	2910/2918 (99%)	631 (21%)	8 (0%)
22	B	113/114 (99%)	18 (15%)	0
All	All	4569/4579 (99%)	917 (20%)	8 (0%)

All (917) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	G
1	a	11	A
1	a	16	G
1	a	23	G
1	a	31	U
1	a	32	G
1	a	33	A
1	a	34	A
1	a	40	G
1	a	42	G
1	a	48	C
1	a	49	C
1	a	51	A
1	a	52	A
1	a	62	G
1	a	74	G
1	a	82	G
1	a	85	U
1	a	87	C
1	a	88	U
1	a	89	U
1	a	92	C
1	a	107	G
1	a	108	A
1	a	115	A
1	a	120	C

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Mol	Chain	Res	Type
1	a	129	A
1	a	130	A
1	a	131	C
1	a	144	C
1	a	151	A
1	a	156	C
1	a	159	G
1	a	163	C
1	a	182	A
1	a	183	U
1	a	185	U
1	a	196	A
1	a	198	G
1	a	206	A
1	a	211	A
1	a	212	A
1	a	213	G
1	a	219	C
1	a	221	U
1	a	234	A
1	a	248	U
1	a	249	G
1	a	252	U
1	a	255	G
1	a	259	G
1	a	260	U
1	a	274	G
1	a	275	C
1	a	286	A
1	a	287	A
1	a	294	A
1	a	297	G
1	a	307	G
1	a	315	U
1	a	324	C
1	a	336	C
1	a	337	A
1	a	355	G
1	a	360	C
1	a	362	G
1	a	374	C
1	a	375	U

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Mol	Chain	Res	Type
1	a	376	U
1	a	380	C
1	a	385	G
1	a	390	A
1	a	396	G
1	a	401	A
1	a	405	A
1	a	414	G
1	a	418	G
1	a	419	A
1	a	420	U
1	a	421	G
1	a	422	A
1	a	429	U
1	a	432	G
1	a	437	U
1	a	449	A
1	a	456	A
1	a	457	A
1	a	462	A
1	a	466	G
1	a	471	A
1	a	477	U
1	a	481	C
1	a	482	A
1	a	483	C
1	a	492	G
1	a	493	G
1	a	499	A
1	a	505	A
1	a	517	A
1	a	519	C
1	a	528	A
1	a	529	G
1	a	532	G
1	a	535	G
1	a	538	G
1	a	539	U
1	a	540	A
1	a	554	A
1	a	555	A
1	a	557	C

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Mol	Chain	Res	Type
1	a	570	U
1	a	571	A
1	a	580	A
1	a	584	C
1	a	585	G
1	a	587	G
1	a	589	G
1	a	595	G
1	a	604	A
1	a	641	U
1	a	650	A
1	a	661	U
1	a	666	G
1	a	673	A
1	a	674	G
1	a	695	A
1	a	703	A
1	a	710	A
1	a	729	A
1	a	741	G
1	a	742	A
1	a	757	A
1	a	759	U
1	a	763	G
1	a	769	G
1	a	782	G
1	a	785	A
1	a	802	A
1	a	803	C
1	a	807	G
1	a	821	U
1	a	825	C
1	a	826	G
1	a	829	G
1	a	836	A
1	a	840	G
1	a	854	C
1	a	855	G
1	a	861	U
1	a	863	G
1	a	865	G
1	a	879	A

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Mol	Chain	Res	Type
1	a	882	A
1	a	886	A
1	a	899	A
1	a	924	A
1	a	936	G
1	a	944	C
1	a	945	A
1	a	947	A
1	a	970	U
1	a	979	A
1	a	981	G
1	a	984	A
1	a	985	A
1	a	986	G
1	a	992	U
1	a	993	A
1	a	999	U
1	a	1002	U
1	a	1003	G
1	a	1012	U
1	a	1014	A
1	a	1016	A
1	a	1025	G
1	a	1027	U
1	a	1028	A
1	a	1034	U
1	a	1035	U
1	a	1036	C
1	a	1037	C
1	a	1038	C
1	a	1039	C
1	a	1041	U
1	a	1044	G
1	a	1051	A
1	a	1057	C
1	a	1076	G
1	a	1077	U
1	a	1106	G
1	a	1107	U
1	a	1113	A
1	a	1124	C
1	a	1138	U

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Mol	Chain	Res	Type
1	a	1144	C
1	a	1150	G
1	a	1151	U
1	a	1152	U
1	a	1153	G
1	a	1163	A
1	a	1165	U
1	a	1170	U
1	a	1171	G
1	a	1172	C
1	a	1179	C
1	a	1192	G
1	a	1195	G
1	a	1202	A
1	a	1207	A
1	a	1208	A
1	a	1223	U
1	a	1225	U
1	a	1235	U
1	a	1238	A
1	a	1239	C
1	a	1250	A
1	a	1252	G
1	a	1261	A
1	a	1268	A
1	a	1271	G
1	a	1289	A
1	a	1291	A
1	a	1297	U
1	a	1298	A
1	a	1304	G
1	a	1310	A
1	a	1312	U
1	a	1313	U
1	a	1328	C
1	a	1329	A
1	a	1331	C
1	a	1333	C
1	a	1334	G
1	a	1347	U
1	a	1351	A
1	a	1357	A

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Mol	Chain	Res	Type
1	a	1358	G
1	a	1359	U
1	a	1375	U
1	a	1381	G
1	a	1386	A
1	a	1389	C
1	a	1409	A
1	a	1411	C
1	a	1412	G
1	a	1430	G
1	a	1437	A
1	a	1453	G
1	a	1454	A
1	a	1457	A
1	a	1463	U
1	a	1492	A
1	a	1496	U
1	a	1515	A
1	a	1518	U
1	a	1519	A
1	a	1520	G
1	a	1529	G
1	a	1531	A
1	a	1532	G
1	a	1540	U
1	a	1541	G
1	a	1542	G
1	a	1543	A
1	a	1545	C
1	a	1546	A
1	a	1547	C
1	a	1549	U
21	A	14	A
21	A	28	A
21	A	34	U
21	A	52	A
21	A	64	A
21	A	71	A
21	A	74	U
21	A	75	G
21	A	80	G
21	A	84	A

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Mol	Chain	Res	Type
21	A	85	G
21	A	90	A
21	A	96	G
21	A	98	U
21	A	102	A
21	A	104	C
21	A	113	U
21	A	117	A
21	A	118	A
21	A	119	U
21	A	124	A
21	A	130	A
21	A	133	A
21	A	142	G
21	A	145	A
21	A	150	A
21	A	154	A
21	A	157	U
21	A	160	G
21	A	161	A
21	A	162	A
21	A	163	U
21	A	165	C
21	A	167	U
21	A	168	A
21	A	169	G
21	A	184	C
21	A	199	A
21	A	200	A
21	A	202	A
21	A	207	A
21	A	218	G
21	A	219	A
21	A	225	A
21	A	227	G
21	A	229	A
21	A	235	G
21	A	236	A
21	A	244	A
21	A	251	G
21	A	253	G
21	A	255	G

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Mol	Chain	Res	Type
21	A	272	C
21	A	284	C
21	A	285	U
21	A	286	U
21	A	288	C
21	A	289	U
21	A	295	G
21	A	298	U
21	A	300	G
21	A	301	U
21	A	314	A
21	A	315	C
21	A	316	G
21	A	317	G
21	A	319	G
21	A	320	U
21	A	321	U
21	A	322	A
21	A	326	A
21	A	331	G
21	A	338	G
21	A	351	G
21	A	354	A
21	A	358	G
21	A	365	A
21	A	367	A
21	A	372	A
21	A	373	A
21	A	374	U
21	A	378	C
21	A	381	G
21	A	389	A
21	A	398	C
21	A	401	U
21	A	403	U
21	A	404	U
21	A	410	G
21	A	411	A
21	A	413	C
21	A	418	G
21	A	430	A
21	A	432	G

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Mol	Chain	Res	Type
21	A	457	G
21	A	459	C
21	A	466	C
21	A	494	U
21	A	497	U
21	A	502	C
21	A	503	A
21	A	511	G
21	A	513	G
21	A	525	A
21	A	526	A
21	A	527	G
21	A	544	U
21	A	550	A
21	A	553	A
21	A	554	C
21	A	555	C
21	A	572	C
21	A	574	A
21	A	575	G
21	A	576	U
21	A	577	A
21	A	578	G
21	A	591	A
21	A	593	U
21	A	594	G
21	A	606	G
21	A	611	U
21	A	613	G
21	A	614	U
21	A	615	A
21	A	618	A
21	A	646	A
21	A	658	A
21	A	659	A
21	A	660	A
21	A	661	U
21	A	662	G
21	A	666	A
21	A	682	A
21	A	683	G
21	A	690	U

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Mol	Chain	Res	Type
21	A	693	G
21	A	694	G
21	A	698	U
21	A	699	U
21	A	715	A
21	A	716	C
21	A	722	A
21	A	727	G
21	A	731	U
21	A	732	C
21	A	744	A
21	A	756	A
21	A	769	U
21	A	774	G
21	A	775	A
21	A	784	A
21	A	785	C
21	A	792	U
21	A	793	G
21	A	794	A
21	A	798	G
21	A	809	A
21	A	813	G
21	A	820	G
21	A	821	C
21	A	825	G
21	A	827	A
21	A	828	A
21	A	829	U
21	A	834	A
21	A	838	A
21	A	845	A
21	A	846	G
21	A	849	A
21	A	850	G
21	A	872	U
21	A	873	U
21	A	875	G
21	A	881	G
21	A	902	A
21	A	904	G
21	A	911	A

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Mol	Chain	Res	Type
21	A	921	C
21	A	922	G
21	A	923	A
21	A	924	G
21	A	925	G
21	A	927	G
21	A	932	U
21	A	938	G
21	A	952	A
21	A	955	A
21	A	957	C
21	A	958	U
21	A	959	C
21	A	960	C
21	A	970	U
21	A	985	A
21	A	989	A
21	A	990	G
21	A	1005	G
21	A	1017	A
21	A	1018	A
21	A	1029	C
21	A	1034	A
21	A	1040	A
21	A	1049	C
21	A	1055	A
21	A	1056	U
21	A	1057	A
21	A	1061	G
21	A	1066	G
21	A	1067	U
21	A	1069	G
21	A	1070	A
21	A	1073	A
21	A	1077	U
21	A	1078	G
21	A	1085	U
21	A	1089	C
21	A	1090	A
21	A	1091	G
21	A	1100	G
21	A	1101	A

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Mol	Chain	Res	Type
21	A	1102	U
21	A	1105	U
21	A	1106	G
21	A	1109	U
21	A	1111	A
21	A	1113	A
21	A	1114	A
21	A	1115	G
21	A	1116	C
21	A	1119	C
21	A	1120	C
21	A	1124	A
21	A	1126	U
21	A	1127	U
21	A	1128	A
21	A	1132	A
21	A	1133	G
21	A	1137	G
21	A	1138	U
21	A	1139	A
21	A	1143	G
21	A	1145	U
21	A	1146	C
21	A	1150	A
21	A	1154	G
21	A	1155	A
21	A	1156	G
21	A	1158	G
21	A	1163	U
21	A	1170	A
21	A	1171	A
21	A	1172	A
21	A	1174	U
21	A	1175	G
21	A	1177	A
21	A	1178	C
21	A	1179	C
21	A	1183	G
21	A	1184	C
21	A	1186	A
21	A	1195	A
21	A	1214	C

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Mol	Chain	Res	Type
21	A	1218	G
21	A	1248	U
21	A	1250	G
21	A	1258	A
21	A	1265	G
21	A	1273	G
21	A	1276	G
21	A	1277	C
21	A	1278	G
21	A	1285	A
21	A	1286	G
21	A	1288	G
21	A	1289	A
21	A	1291	A
21	A	1292	A
21	A	1293	U
21	A	1294	G
21	A	1303	A
21	A	1306	C
21	A	1309	G
21	A	1310	A
21	A	1337	A
21	A	1338	U
21	A	1355	A
21	A	1362	C
21	A	1376	G
21	A	1378	U
21	A	1379	A
21	A	1383	G
21	A	1403	C
21	A	1405	G
21	A	1416	U
21	A	1421	A
21	A	1423	C
21	A	1437	U
21	A	1449	A
21	A	1450	A
21	A	1451	U
21	A	1454	U
21	A	1455	U
21	A	1459	A
21	A	1463	A

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Mol	Chain	Res	Type
21	A	1464	U
21	A	1471	A
21	A	1472	C
21	A	1489	A
21	A	1490	G
21	A	1491	C
21	A	1494	G
21	A	1495	C
21	A	1496	G
21	A	1497	A
21	A	1498	U
21	A	1499	U
21	A	1504	U
21	A	1505	G
21	A	1506	C
21	A	1510	U
21	A	1512	U
21	A	1516	C
21	A	1519	U
21	A	1520	A
21	A	1521	A
21	A	1525	U
21	A	1527	A
21	A	1534	G
21	A	1536	C
21	A	1537	A
21	A	1540	U
21	A	1551	U
21	A	1552	U
21	A	1553	A
21	A	1555	G
21	A	1561	G
21	A	1567	A
21	A	1568	U
21	A	1569	G
21	A	1570	G
21	A	1571	G
21	A	1576	A
21	A	1577	G
21	A	1579	C
21	A	1580	A
21	A	1582	U

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Mol	Chain	Res	Type
21	A	1583	G
21	A	1584	A
21	A	1585	G
21	A	1586	U
21	A	1587	C
21	A	1605	A
21	A	1606	C
21	A	1613	G
21	A	1614	A
21	A	1616	A
21	A	1621	C
21	A	1625	U
21	A	1629	U
21	A	1631	G
21	A	1632	A
21	A	1633	A
21	A	1636	U
21	A	1651	C
21	A	1652	A
21	A	1655	C
21	A	1659	C
21	A	1660	A
21	A	1662	A
21	A	1678	A
21	A	1684	A
21	A	1690	A
21	A	1691	G
21	A	1692	C
21	A	1704	C
21	A	1709	A
21	A	1716	C
21	A	1717	G
21	A	1718	G
21	A	1737	U
21	A	1738	C
21	A	1739	G
21	A	1740	G
21	A	1742	A
21	A	1746	G
21	A	1759	G
21	A	1768	C
21	A	1772	G

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Mol	Chain	Res	Type
21	A	1775	G
21	A	1777	G
21	A	1782	A
21	A	1783	G
21	A	1785	G
21	A	1790	G
21	A	1791	G
21	A	1800	A
21	A	1801	C
21	A	1808	U
21	A	1811	A
21	A	1818	A
21	A	1826	G
21	A	1827	C
21	A	1828	U
21	A	1829	A
21	A	1833	C
21	A	1835	U
21	A	1843	U
21	A	1844	G
21	A	1846	A
21	A	1855	G
21	A	1856	A
21	A	1861	U
21	A	1862	G
21	A	1865	C
21	A	1893	A
21	A	1895	C
21	A	1897	U
21	A	1899	U
21	A	1926	A
21	A	1928	A
21	A	1933	G
21	A	1939	A
21	A	1950	U
21	A	1956	G
21	A	1957	G
21	A	1958	U
21	A	1963	A
21	A	1964	A
21	A	1965	A
21	A	1968	C

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Mol	Chain	Res	Type
21	A	1969	C
21	A	1970	U
21	A	1972	G
21	A	1982	U
21	A	1983	U
21	A	1989	C
21	A	1994	C
21	A	1997	A
21	A	1998	A
21	A	1999	G
21	A	2002	G
21	A	2008	A
21	A	2018	U
21	A	2020	U
21	A	2048	G
21	A	2050	A
21	A	2057	A
21	A	2058	A
21	A	2059	G
21	A	2060	A
21	A	2061	U
21	A	2070	C
21	A	2079	G
21	A	2082	C
21	A	2083	G
21	A	2087	A
21	A	2088	G
21	A	2096	G
21	A	2119	U
21	A	2120	G
21	A	2127	G
21	A	2139	A
21	A	2140	C
21	A	2143	G
21	A	2145	U
21	A	2147	G
21	A	2155	C
21	A	2160	G
21	A	2161	A
21	A	2162	A
21	A	2165	G
21	A	2172	C

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Mol	Chain	Res	Type
21	A	2173	U
21	A	2174	A
21	A	2175	G
21	A	2185	A
21	A	2186	G
21	A	2188	C
21	A	2194	U
21	A	2195	G
21	A	2198	A
21	A	2208	A
21	A	2212	G
21	A	2217	G
21	A	2226	A
21	A	2230	G
21	A	2231	C
21	A	2238	U
21	A	2240	U
21	A	2241	C
21	A	2252	A
21	A	2265	G
21	A	2266	G
21	A	2275	C
21	A	2278	G
21	A	2290	C
21	A	2293	A
21	A	2294	A
21	A	2295	A
21	A	2305	A
21	A	2306	G
21	A	2310	C
21	A	2314	A
21	A	2333	U
21	A	2334	G
21	A	2335	G
21	A	2337	A
21	A	2339	U
21	A	2342	U
21	A	2346	U
21	A	2347	A
21	A	2348	G
21	A	2349	A
21	A	2352	G

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Mol	Chain	Res	Type
21	A	2353	U
21	A	2354	A
21	A	2358	G
21	A	2361	U
21	A	2362	A
21	A	2363	A
21	A	2372	G
21	A	2374	C
21	A	2377	C
21	A	2410	G
21	A	2412	C
21	A	2415	A
21	A	2419	A
21	A	2429	U
21	A	2430	C
21	A	2433	C
21	A	2449	C
21	A	2450	U
21	A	2452	A
21	A	2456	G
21	A	2457	A
21	A	2458	U
21	A	2462	A
21	A	2467	C
21	A	2468	C
21	A	2472	G
21	A	2475	A
21	A	2492	C
21	A	2497	G
21	A	2505	A
21	A	2518	U
21	A	2521	G
21	A	2525	C
21	A	2526	C
21	A	2529	G
21	A	2530	A
21	A	2532	G
21	A	2533	U
21	A	2540	A
21	A	2545	A
21	A	2549	U
21	A	2552	G

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Mol	Chain	Res	Type
21	A	2560	U
21	A	2561	C
21	A	2562	G
21	A	2576	G
21	A	2579	U
21	A	2582	U
21	A	2583	C
21	A	2589	U
21	A	2593	A
21	A	2594	G
21	A	2599	A
21	A	2600	C
21	A	2601	G
21	A	2605	G
21	A	2609	G
21	A	2612	U
21	A	2613	C
21	A	2624	G
21	A	2629	A
21	A	2630	G
21	A	2636	U
21	A	2638	C
21	A	2640	U
21	A	2648	G
21	A	2657	G
21	A	2661	A
21	A	2666	A
21	A	2683	U
21	A	2690	G
21	A	2708	C
21	A	2709	U
21	A	2716	U
21	A	2717	A
21	A	2741	G
21	A	2753	U
21	A	2756	G
21	A	2760	A
21	A	2766	U
21	A	2767	A
21	A	2771	G
21	A	2783	U
21	A	2784	A

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Mol	Chain	Res	Type
21	A	2785	A
21	A	2788	A
21	A	2791	A
21	A	2792	A
21	A	2793	G
21	A	2803	A
21	A	2804	G
21	A	2805	A
21	A	2806	U
21	A	2807	G
21	A	2817	A
21	A	2820	U
21	A	2821	U
21	A	2824	G
21	A	2827	A
21	A	2838	C
21	A	2845	G
21	A	2846	A
21	A	2850	G
21	A	2853	U
21	A	2855	A
21	A	2856	U
21	A	2869	G
21	A	2882	A
21	A	2887	G
21	A	2892	G
21	A	2899	A
21	A	2900	C
21	A	2903	A
21	A	2905	C
21	A	2906	G
21	A	2913	G
21	A	2917	U
22	B	2	C
22	B	10	U
22	B	12	U
22	B	23	U
22	B	24	C
22	B	27	A
22	B	30	U
22	B	33	U
22	B	39	G

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Mol	Chain	Res	Type
22	B	40	C
22	B	42	G
22	B	43	A
22	B	49	G
22	B	73	G
22	B	87	G
22	B	88	U
22	B	106	U
22	B	108	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	A	160	G
21	A	199	A
21	A	377	U
21	A	661	U
21	A	1127	U
21	A	1938	U
21	A	1962	G
21	A	2230	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 41 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 ⓘ

There are no chain breaks in this entry.