



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Aug 21, 2017 – 03:47 AM EDT

PDB ID : 5ND9
EMDB ID: : EMD-3625
Title : Hibernating ribosome from Staphylococcus aureus (Rotated state)
Authors : Khusainov, I.; Vicens, Q.; Ayupov, R.; Usachev, K.; Myasnikov, A.; Simonetti, A.; Validov, S.; Kieffer, B.; Yusupova, G.; Yusupov, M.; Hashem, Y.
Deposited on : unknown
Resolution : 3.70 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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

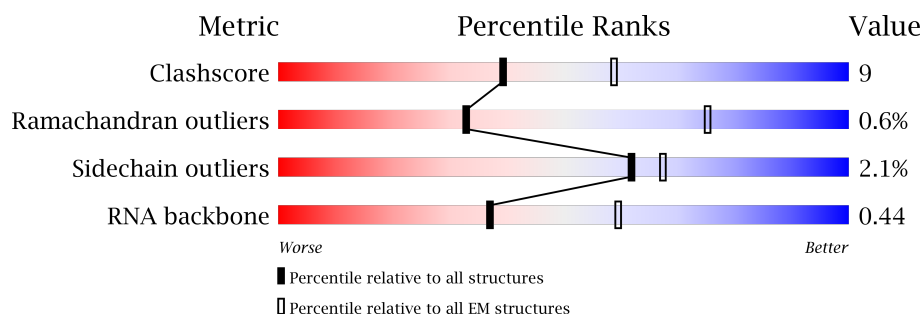
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



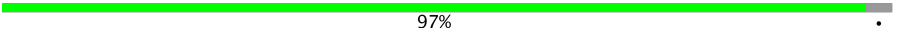
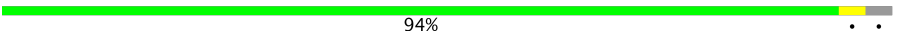




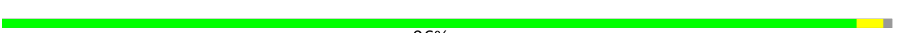


















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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	1556	70% 27% ..
2	b	255	84% . 13%
3	c	217	91% . 6%
4	d	200	97% ..
5	e	166	92% . .
6	f	98	93% . .
7	g	156	84% 6% . 8%
8	h	132	97% ..









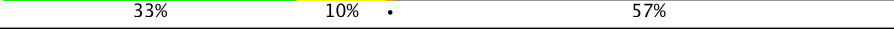


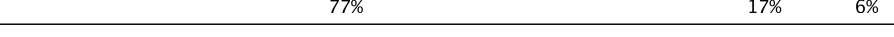

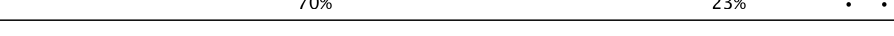

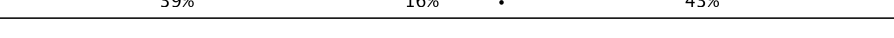
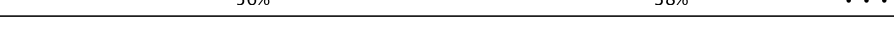

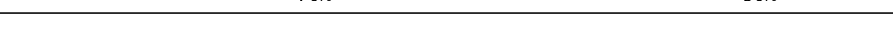
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Mol	Chain	Length	Quality of chain
9	i	132	 97% .
10	j	102	 94% . .
11	k	129	 87% . 11%
12	l	137	 93% 6% .
13	m	121	 89% . 9%
14	n	61	 93% 5% .
15	o	89	 96% . .
16	p	91	 97% . .
17	q	87	 95% . .
18	r	80	 69% . 30%
19	s	92	 90% . 9%
20	t	83	 95% . .
21	u	58	 59% 19% 22%
22	v	190	 35% 15% . 47%
23	A	2923	 51% 35% 12% .
24	B	114	 52% 42% 6%
25	D	277	 77% 21% . .
26	E	220	 81% 17% . .
27	F	207	 78% 18% .
28	G	179	 87% 6% 7%
29	H	178	 69% 23% 8%
30	M	145	 83% 16% .
31	N	122	 86% 13% .
32	O	146	 77% 12% . 10%
33	P	144	 71% 20% . 8%

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Mol	Chain	Length	Quality of chain
34	Q	122	
35	R	119	
36	S	116	
37	T	118	
38	U	102	
39	V	117	
40	W	91	
41	X	105	
42	Y	217	
43	Z	94	
44	0	62	
45	1	69	
46	2	59	
47	3	84	
48	4	58	
49	5	49	
50	6	45	
51	7	66	
52	8	37	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 141051 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	1541	Total	C	N	O	P	0	0
			33006	14736	6021	10708	1541		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	222	Total	C	N	O	S	0	0
			1788	1139	313	330	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	203	Total	C	N	O	S	0	0
			1600	1007	301	290	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	160	Total	C	N	O	S	0	0
			1194	750	218	224	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	94	Total	C	N	O	S	0	0
			781	494	137	147	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	143	Total	C	N	O	S	0	0
			1142	712	216	210	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	99	Total	C	N	O	S	0	0
			791	498	144	147	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	115	Total	C	N	O	S	0	0
			851	526	160	162	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
			1058	658	214	184	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	110	Total	C	N	O	S	0	0
			877	537	175	164	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	85	Total	C	N	O	S	0	0
			698	441	125	131	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	56	Total	C	N	O	S	0	0
			466	295	88	81	2		

- 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
			677	434	120	121	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
			606	367	119	118	2		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	u	45	Total	C	N	O	0	0
			377	233	76	68		

- Molecule 22 is a protein called Ribosome hibernation promotion factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	v	101	Total	C	N	O	0	0
			831	518	156	157		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A	2914	Total	C	N	O	P	0	0
			62480	27894	11427	20245	2914		

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B	114	Total	C	N	O	P	0	0
			2430	1086	436	794	114		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D	275	Total	C	N	O	S	0	0
			2103	1309	417	372	5		

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	199	Total	C	N	O	S	0	0
			1524	955	281	286	2		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	166	Total	C	N	O	S	0	0
			1311	832	223	250	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H	164	Total	C	N	O	S	0	0
			1284	799	232	250	3		

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	O	131	Total	C	N	O	S	0	0
			997	618	197	181	1		

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	P	133	Total	C	N	O	S	0	0
			1065	681	203	178	3		

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Q	117	Total	C	N	O	S	0	0
			924	564	179	180	1		

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	S	107	Total	C	N	O	S	0	0
			862	544	173	145			

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	T	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	V	112	Total	C	N	O	S	0	0
			862	537	164	158	3		

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	W	89	Total	C	N	O	S	0	0
			725	457	130	134	4		

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	X	87	Total	C	N	O	S	0	0
			668	423	122	122	1		

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	Z	77	Total	C	N	O	0	0
			591	364	115	112		

- Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	0	46	Total	C	N	O	0	0
			373	231	83	59		

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	1	65	Total	C	N	O	0	0
			536	330	101	105		

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	2	57	Total	C	N	O	0	0
			441	274	83	84		

- Molecule 47 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	81	Total	C	N	O	S	0	0
			663	423	113	124	3		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	44	Total	C	N	O	S	0	0
			360	220	78	58	4		

- Molecule 49 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5	28	Total	C	N	O	S	0	0
			229	137	45	43	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	6	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	7	60	Total	C	N	O	S	0	0
			487	300	108	77	2		

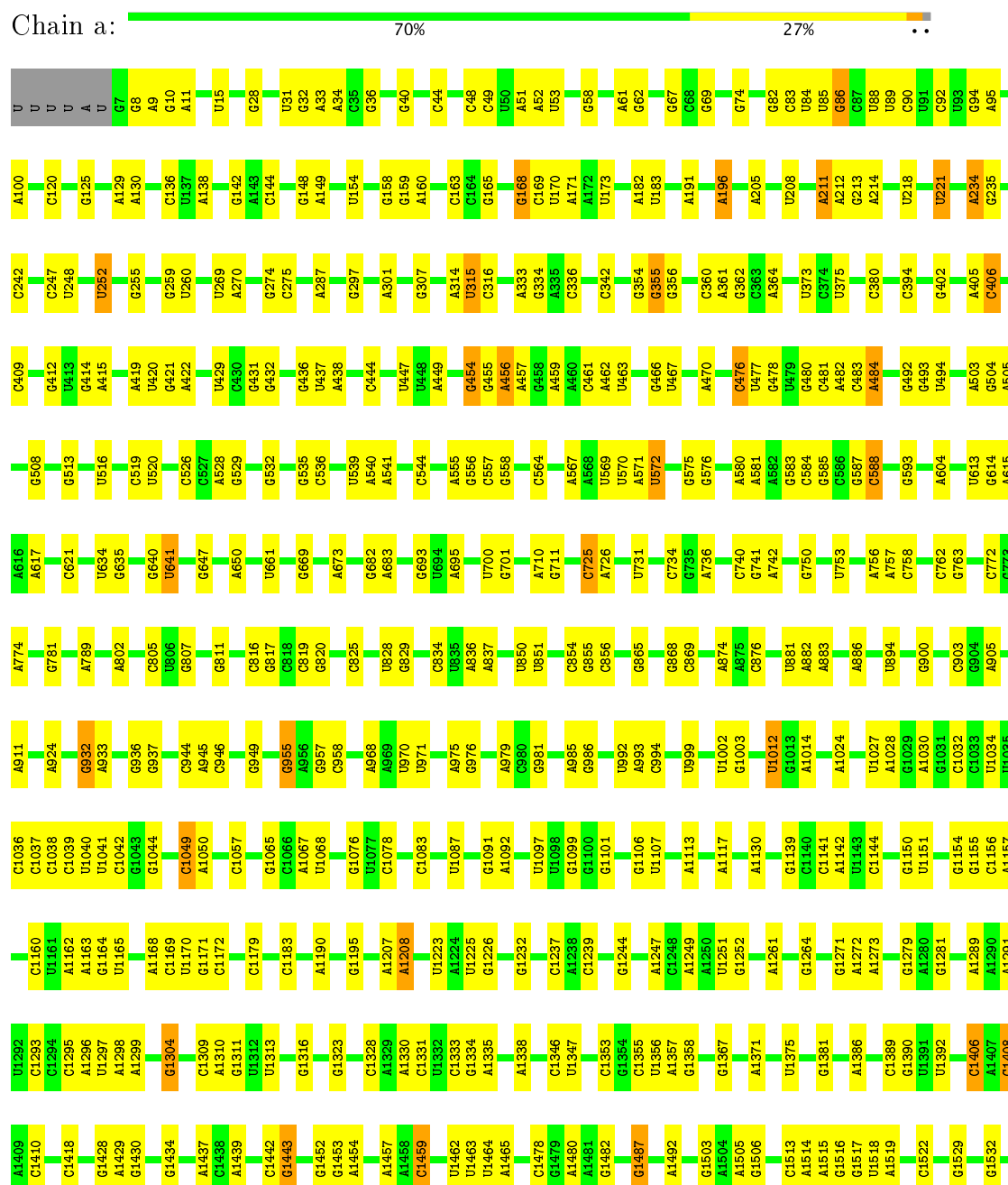
- Molecule 52 is a protein called 50S ribosomal protein L36.

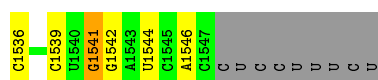
Mol	Chain	Residues	Atoms					AltConf	Trace
52	8	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

3 Residue-property plots

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

• Molecule 1: 16S ribosomal RNA





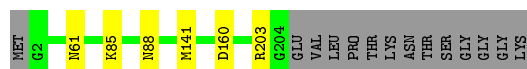
- Molecule 2: 30S ribosomal protein S2

Chain b: 84% 13%



- Molecule 3: 30S ribosomal protein S3

Chain c: 91% 6%



- Molecule 4: 30S ribosomal protein S4

Chain d: 97%



- Molecule 5: 30S ribosomal protein S5

Chain e: 92%



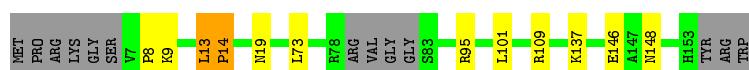
- Molecule 6: 30S ribosomal protein S6

Chain f: 93%



- Molecule 7: 30S ribosomal protein S7

Chain g: 84% 6% 8%



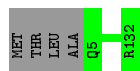
- Molecule 8: 30S ribosomal protein S8

Chain h: 97%



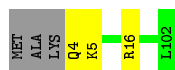
- Molecule 9: 30S ribosomal protein S9

Chain i:  97% .




- Molecule 10: 30S ribosomal protein S10

Chain j:  94% . .



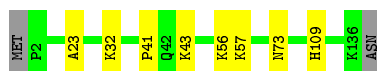
- Molecule 11: 30S ribosomal protein S11

Chain k:  87% . 11%



- Molecule 12: 30S ribosomal protein S12

Chain l:  93% 6% .



- Molecule 13: 30S ribosomal protein S13

Chain m:  89% . 9%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain n:  93% 5% .



- Molecule 15: 30S ribosomal protein S15

Chain o:  96% . .



- Molecule 16: 30S ribosomal protein S16

Chain p:  97%



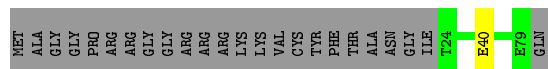
- Molecule 17: 30S ribosomal protein S17

Chain q:  95%




- Molecule 18: 30S ribosomal protein S18

Chain r:  69% 30%



- Molecule 19: 30S ribosomal protein S19

Chain s:  90% 9%



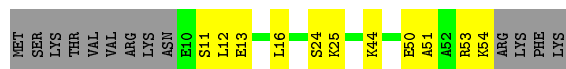
- Molecule 20: 30S ribosomal protein S20

Chain t:  95%




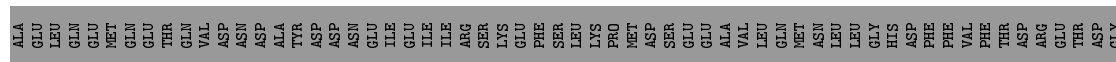
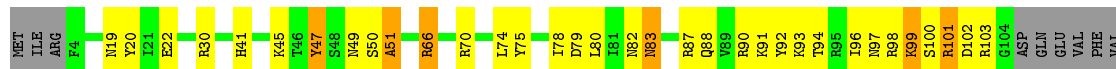
- Molecule 21: 30S ribosomal protein S21

Chain u:  59% 19% 22%



- Molecule 22: Ribosome hibernation promotion factor

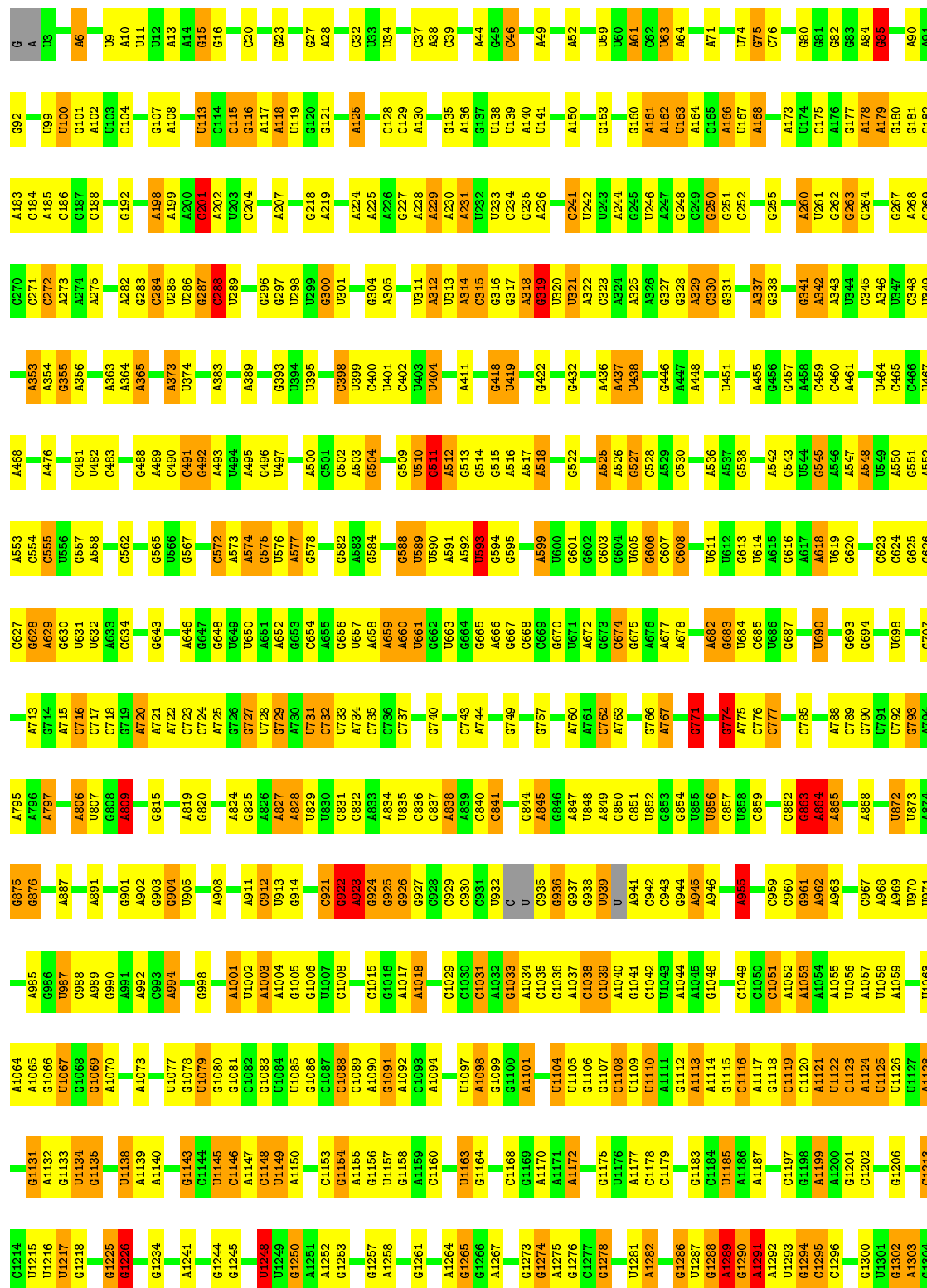
Chain v:  35% 15% 47%



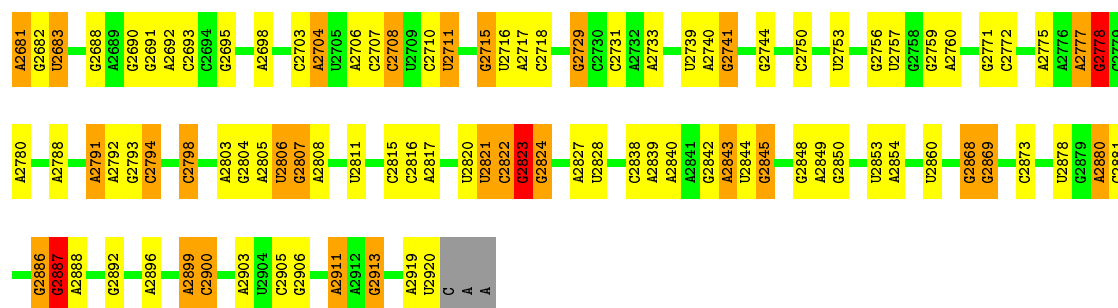
THR
SER
ILE
VAL
TYR
ARG
ARG
LYS
ASP
GLY
GLY
TYR
GLY
LEU
ILE
GLN
THR
SER
GLU
GLN

• Molecule 23: 23S ribosomal RNA

Chain A:  51% 35% 12%

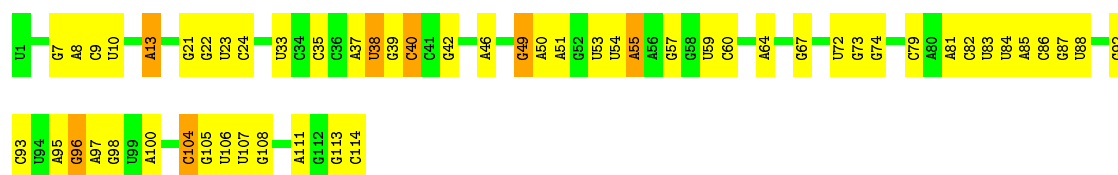


A2599	C2504	C2483	U2332	C2236	A2162	G2084	G2000	A1917	C1822	A1722	G1631	U1551	A1478	U1305
C2600	A2505	G2437	U2333	U2240	A2163	A2085	C2001	G1918	U1823	A1726	A1632	U1552	G1479	C1306
C2601	G2508	G2438	G2334	C2241	C2170	A2086	A2004	C1919	C1824	G1727	A1633	A1553	G1480	C1307
G2603	A2439	A2336	G2335	A2250	G2171	G2088	A2005	A2020	U1825	G1731	A1634	A1554	G1484	C1308
C2604	G2511	A2337	A2338	G2251	C2172	G2089	C2006	A1926	C1826	U1732	A1635	U1555	G1485	A1310
C2605	G2516	U2339	G2339	A2252	U2173	C2090	U2009	A1927	U1828	U1733	U1650	G1395	C1486	A1311
C2610	G2517	C2443	U2340	C2253	G2175	C2091	C2017	A1928	A1829	A1734	A1651	A1560	G1487	A1312
U2611	U2518	U2446	U2342	A2254	C2176	C2092	U2018	G1930	C1832	C1735	A1652	C1562	A1489	C1315
U2612	C2523	G2447	A2347	C2259	U2178	G2096	G2019	C1932	C1833	G1738	A1654	U1565	C1491	U1319
C2613	A2524	G2448	G2348	G2261	A1719	G2097	U2020	A1933	A1830	U1739	A1655	G1566	G1492	G1320
A2616	C2526	U2450	A2349	G2262	C2180	A2098	C2021	G1934	U1835	G1740	C1656	A1567	U1493	
U2617	U2527	C2451	U2354	C2263	G2183	G2099	U2022	U1938	A1837	G1741	G1657	U1568	G1494	A1323
C2618	G2528	A2452	A2355	G2264	U2101	U2102	A2024	A1943	U1842	G1743	A1658	G1495	C1495	A1324
C2619	G2529	A2453	A2356	G2265	A2185	U2103	C2026	A1944	U1845	U1744	A1660	G1496	G1497	U1325
U2620	A2530	C2454	G2357	G2266	G2186	U2104	G2027	U1942	U1843	G1751	C1661	U1574	U1498	C1328
C2621	U2531	G2455	G2358	U2270	G2187	A2105	A2028	U1944	U1844	G1759	A1662	U1575	U1499	A1333
G2622	G2532	G2456	A2360	U2271	G2188	U2106	U2034	A1945	U1846	G1767	G1667	U1576	G1500	A1334
U2623	U2533	A2457	U2361	U2272	G2189	G2107	C2033	U1946	U1847	G1768	A1668	U1577	U1501	C1335
C2624	C2534	U2458	C2190	G2273	C2190	G2107	A2040	A1946	U1851	U1781	A1678	U1585	U1510	G1336
	G2535		A2362	C2275	U2191	C2112	C2035	A1954	G1850		A1679	U1586	U1511	A1337
C2628	G2536		A2363	U2276	G2192		C2036	A1955	G1851		A1680	U1587	C1511	U1338
A2629	C2539	A2462	G2364	U2277	G2193	U2119	G2037	U1956	U1855	U1784	A1685	U1588	C1512	U1350
C2630	A2540	G2463	G2372	G2278	U2194	G2120	U2038	G1957	U1856	G1785	A1690	U1589	A1431	C1351
C2633	G2543	C2464	A2373	G2279	G2195	U2124	G2039	U1958	C1857	A1786	G1691	C1590	A1432	C1352
G2635	G2544	U2465	G2374	G2280	G2196	U2124	A2040	U1958	U1858	G1790	G1693	A1592	G1516	G1357
U2636	C2545	C2467	C2375	C2285	U2198	G2127	A2047	A1955	U1859	G1791	A1694	G1593	G1518	A1358
G2637	A2546	G2468	G2376	G2286	U2199		G2048	U1956	A1880	U1784	A1695	U1594	U1519	A1359
C2638	C2547	C2470	A2379	C2287	A2200	G2133	C2051	U1966	G1884	G1785	G1696	C1595	A1520	G1360
U2640	G2550	G2472	A2381	U2289	A2203	U2135	C2052	U1967	G1885	A1795	A1697	G1596	A1521	G1361
A2641	G2551	G2473	A2385	C2290	C2206	U2136	G2056	A1963	U1891	G1790	G1693	U1597	G1522	C1362
U2642	G2552	G2474	A2385	C2291	U2207	G2137	A2057	A1964	U1892	G1799	A1698	U1598	G1526	U1363
C2643	U2560	C2475	G2398	U2292	A2208	U2138	A2058	U1965	U1893	A1800	G1702	C1604	U1526	G1364
G2644	C2561	C2479	G2402	A2293	G2209	A2139	G2059	U1966	U1894	G1801	U1703	A1605	U1532	G1365
C2647	A2569	G2480	A2403	A2294	C2206	U2140	A2060	U1967	G1895	U1804	A1708	A1606	A1533	U1366
U2649	G2576	C2483	A2404	A2295	G2214	A2141	G2061	C1968	U1896	U1805	A1709	A1607	G1534	C1367
G2654	G2577	U2484	G2409	A2301	U2215	A2142	G2062	C1969	U1897	U1806	G1710	G1462	U1536	G1368
U2655	C2578	U2485	G2410	C2302	G2218	A2143	A2064	U1970	U1898	A1807	G1711	A1614	A1537	C1370
A2656	U2579	A2486	A2411	A2305	C2219	U2146	A2069	A1979	U1899	U1808	A1712	A1615	A1538	U1377
G2657	G2580	U2487	C2412	C2308	U2220	G2147	C2070	G1981	G1900	C1809	A1713	A1616	A1539	U1378
	U2581	C2488	U2417	G2309	U2221	U2149	C2071	U1982	G1902	U1809	A1714	A1618	C1542	A1379
A2661	U2582	C2492	G2418	C2310	A2225	A2150	C2072	C1989	U1907	U1810	G1717	U1625	A1546	U1381
U2662	C2583	A2419	A2419	A2314	A2226	G2151	G2073	G1990	A1908	C1809	A1718	A1626	C1547	C1382
G2667	C2587	C2493	C2493	G2317	C2229	A2152	C2074	G1991	A1909	C1810	A1719	A1627	A1475	G1383
A2668	U2588	C2494	C2422	G2317	G2230	G2154	A2077	A1993	C1909	A1811	G1717	U1628	A1546	U1384
	U2589	A2496	U2429	G2326	A2232	C2155	A2078	C1994	A1911	A1812	G1717	A1629	A1546	U1385
C2673	A2593	U2501	U2430	A2327	C2233	U2159	G2079	A1997	A1912	A1813	G1718	A1629	A1546	U1386
U2679	G2594	C2502	G2431	G2331	C2234	A2161	C2082	A1998	U1913	A1815	A1721	A1630	A1550	
U2680		A2503	G2432		A2235		G2083	G1999	A1916					



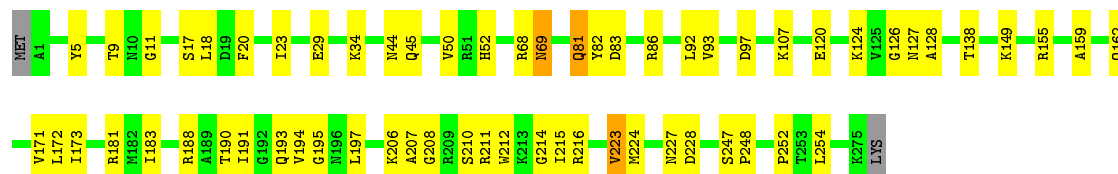
• Molecule 24: 5S ribosomal RNA

Chain B: 52% 42% 6%



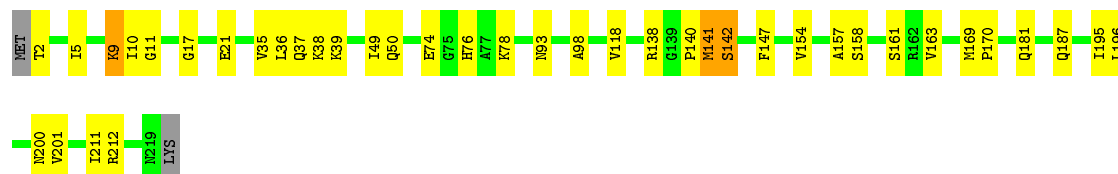
• Molecule 25: 50S ribosomal protein L2

Chain D: 77% 21% ..



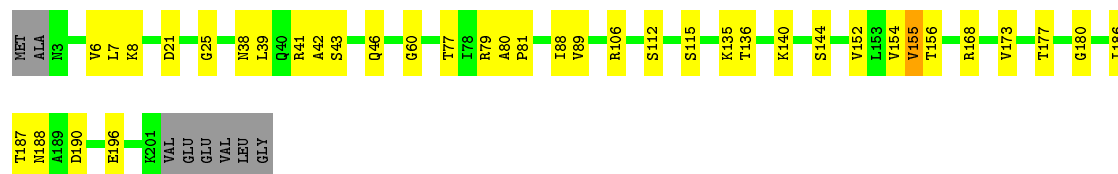
• Molecule 26: 50S ribosomal protein L3

Chain E: 81% 17% ..




• Molecule 27: 50S ribosomal protein L4

Chain F: 78% 18% .



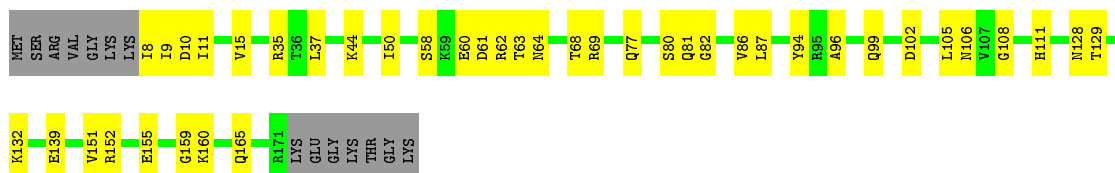
• Molecule 28: 50S ribosomal protein L5

Chain G:  87% 6% 7%




- Molecule 29: 50S ribosomal protein L6

Chain H:  69% 23% 8%




- Molecule 30: 50S ribosomal protein L13

Chain M:  83% 16% .




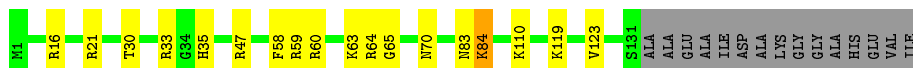
- Molecule 31: 50S ribosomal protein L14

Chain N:  86% 13% .



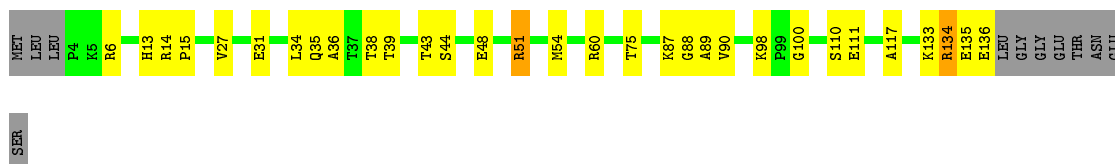
- Molecule 32: 50S ribosomal protein L15

Chain O:  77% 12% 10%



- Molecule 33: 50S ribosomal protein L16

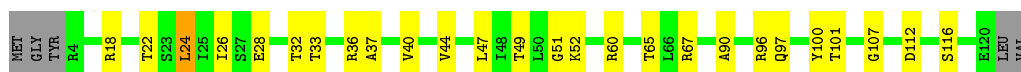
Chain P:  71% 20% 8%



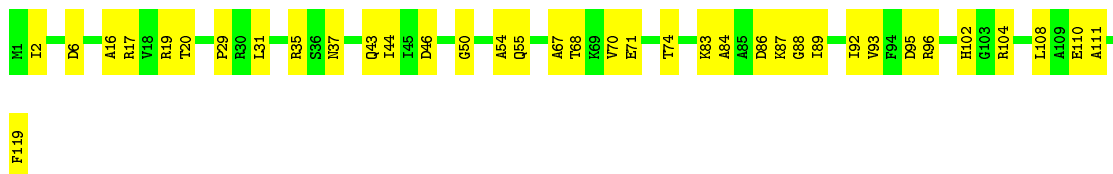
- Molecule 34: 50S ribosomal protein L17

Chain Q:  75% 20% . .





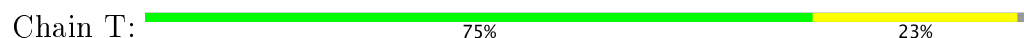
- Molecule 35: 50S ribosomal protein L18



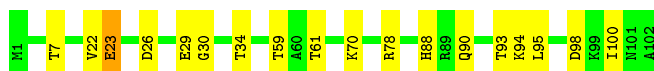
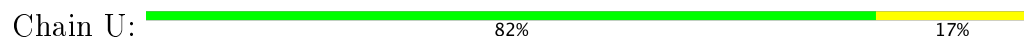
- Molecule 36: 50S ribosomal protein L19



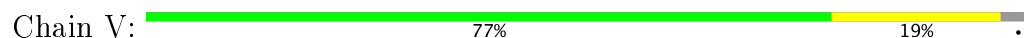
- Molecule 37: 50S ribosomal protein L20



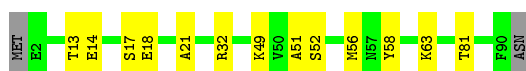
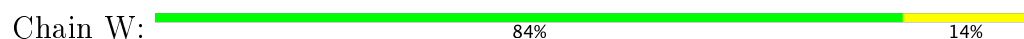
- Molecule 38: 50S ribosomal protein L21



- Molecule 39: 50S ribosomal protein L22



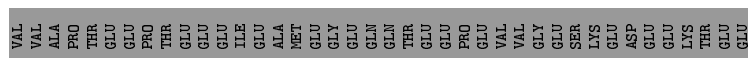
- Molecule 40: 50S ribosomal protein L23



- Molecule 41: 50S ribosomal protein L24



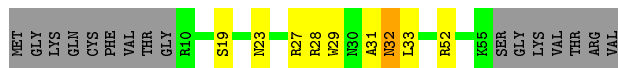
- Molecule 42: 50S ribosomal protein L25



- Molecule 43: 50S ribosomal protein L27



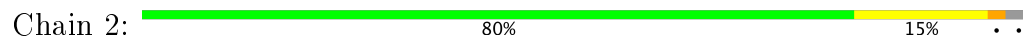
- Molecule 44: 50S ribosomal protein L28



- Molecule 45: 50S ribosomal protein L29




- Molecule 46: 50S ribosomal protein L30

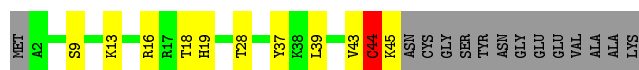


- Molecule 47: 50S ribosomal protein L31 type B



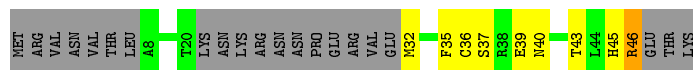
- Molecule 48: 50S ribosomal protein L32

Chain 4:  57% 17% • 24%



- Molecule 49: 50S ribosomal protein L33 2

Chain 5:  39% 16% • 43%



- Molecule 50: 50S ribosomal protein L34

Chain 6:  56% 38% • • •



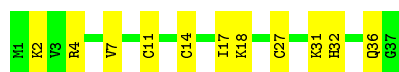
- Molecule 51: 50S ribosomal protein L35

Chain 7:  67% 23% • 9%



- Molecule 52: 50S ribosomal protein L36

Chain 8:  70% 30%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	83000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.97	3/36954 (0.0%)	1.25	166/57629 (0.3%)
10	j	0.42	0/803	0.69	0/1082
11	k	0.48	0/866	0.67	1/1169 (0.1%)
12	l	0.62	0/1075	0.80	0/1439
13	m	0.42	0/883	0.79	0/1182
14	n	0.46	0/512	0.81	0/678
15	o	0.53	0/747	0.80	0/996
16	p	0.56	0/723	0.69	0/971
17	q	0.57	0/706	0.73	0/944
18	r	0.51	0/473	0.76	0/632
19	s	0.40	0/695	0.68	0/934
2	b	0.47	0/1815	0.72	3/2436 (0.1%)
20	t	0.43	0/606	0.69	0/810
21	u	0.35	0/380	0.53	0/498
22	v	0.37	0/841	0.72	0/1131
23	A	1.33	155/69971 (0.2%)	1.40	719/109124 (0.7%)
24	B	0.94	1/2717 (0.0%)	1.26	19/4232 (0.4%)
25	D	0.86	2/2138 (0.1%)	0.82	2/2869 (0.1%)
26	E	0.78	2/1673 (0.1%)	0.73	0/2243
27	F	0.72	0/1547	0.76	1/2088 (0.0%)
28	G	0.42	0/1326	0.73	0/1780
29	H	0.51	1/1302 (0.1%)	0.70	0/1757
3	c	0.39	0/1622	0.68	0/2178
30	M	0.68	0/1173	0.71	0/1578
31	N	0.77	0/927	0.83	0/1243
32	O	0.70	0/1010	0.89	4/1344 (0.3%)
33	P	0.75	0/1089	0.84	0/1460
34	Q	0.63	0/927	0.77	1/1238 (0.1%)
35	R	0.48	0/931	0.74	0/1244
36	S	0.70	0/874	0.86	2/1168 (0.2%)
37	T	0.81	0/955	0.82	3/1265 (0.2%)
38	U	0.72	0/809	0.75	1/1080 (0.1%)
39	V	0.69	0/870	0.78	0/1171
4	d	0.46	0/1629	0.69	0/2185

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	W	0.69	0/733	0.76	0/978
41	X	0.50	0/672	0.66	0/893
42	Y	0.76	1/746 (0.1%)	1.56	4/1000 (0.4%)
43	Z	0.72	0/597	0.69	0/793
44	0	0.59	0/378	0.90	0/504
45	1	0.53	0/537	0.71	0/714
46	2	0.64	0/443	0.76	1/597 (0.2%)
47	3	0.47	0/680	0.83	1/911 (0.1%)
48	4	0.73	0/366	0.76	0/485
49	5	0.40	0/230	0.85	0/303
5	e	0.53	0/1208	0.73	0/1628
50	6	0.91	0/377	0.89	1/491 (0.2%)
51	7	0.73	0/491	0.96	2/643 (0.3%)
52	8	0.70	0/300	0.88	2/393 (0.5%)
6	f	0.54	0/792	0.68	0/1062
7	g	0.45	0/1157	0.73	2/1557 (0.1%)
8	h	0.58	0/1044	0.75	0/1401
9	i	0.41	0/1033	0.71	0/1386
All	All	1.08	165/153353 (0.1%)	1.23	935/229517 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	k	0	1
12	l	0	3
13	m	0	1
14	n	0	2
17	q	0	2
19	s	0	1
2	b	0	2
22	v	0	7
25	D	0	2
26	E	0	5
27	F	0	2
3	c	0	1
30	M	0	1
31	N	0	1
32	O	0	4
33	P	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
35	R	0	3
36	S	0	2
37	T	0	1
38	U	0	1
4	d	0	2
41	X	0	1
43	Z	0	1
46	2	0	1
47	3	0	3
5	e	0	1
50	6	0	2
51	7	0	2
6	f	0	1
7	g	0	6
All	All	0	65

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	Y	25	GLY	C-N	17.38	1.74	1.34
26	E	147	PHE	CA-CB	-8.04	1.36	1.53
23	A	806	A	C5-C6	-7.55	1.34	1.41
23	A	2606	C	N1-C6	-7.36	1.32	1.37
23	A	2503	A	N9-C4	-7.23	1.33	1.37
25	D	5	TYR	C-N	-7.06	1.17	1.34
23	A	732	C	C4-C5	-6.91	1.37	1.43
23	A	2708	C	N1-C6	-6.83	1.33	1.37
23	A	2082	C	N1-C6	-6.72	1.33	1.37
23	A	2021	C	C4-C5	-6.69	1.37	1.43
23	A	2451	C	N3-C4	-6.60	1.29	1.33
23	A	840	C	N1-C6	-6.54	1.33	1.37
23	A	558	A	N9-C4	-6.53	1.33	1.37
23	A	2078	A	N9-C4	-6.51	1.33	1.37
23	A	2017	C	N1-C6	-6.34	1.33	1.37
23	A	201	C	C4-C5	-6.32	1.37	1.43
23	A	827	A	N9-C4	-6.30	1.34	1.37
23	A	2616	A	N9-C4	-6.25	1.34	1.37
23	A	1618	A	N9-C4	-6.25	1.34	1.37
23	A	623	C	C4-C5	-6.23	1.38	1.43
23	A	2051	C	C4-C5	-6.18	1.38	1.43
23	A	629	A	N9-C4	-6.13	1.34	1.37
23	A	841	C	N1-C6	-6.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	491	C	N1-C6	-6.10	1.33	1.37
23	A	1714	C	C4-C5	-6.05	1.38	1.43
23	A	849	A	N9-C4	-6.05	1.34	1.37
23	A	721	A	N9-C4	-6.03	1.34	1.37
23	A	2021	C	N1-C6	-6.03	1.33	1.37
23	A	1029	C	C4-C5	-6.02	1.38	1.43
26	E	163	VAL	CB-CG1	-6.01	1.40	1.52
23	A	718	C	N1-C6	-5.98	1.33	1.37
23	A	2098	A	N9-C4	-5.96	1.34	1.37
23	A	737	C	C4-C5	-5.89	1.38	1.43
23	A	859	C	N1-C6	-5.85	1.33	1.37
23	A	836	C	N1-C6	-5.84	1.33	1.37
23	A	2052	C	C4-C5	-5.83	1.38	1.43
23	A	716	C	N1-C6	-5.83	1.33	1.37
23	A	1296	C	N1-C6	-5.79	1.33	1.37
23	A	1008	C	N1-C6	-5.78	1.33	1.37
23	A	716	C	C4-C5	-5.78	1.38	1.43
23	A	1850	G	N9-C8	-5.78	1.33	1.37
23	A	845	A	N9-C4	-5.77	1.34	1.37
23	A	1815	C	C4-C5	-5.75	1.38	1.43
23	A	2454	C	C4-C5	-5.74	1.38	1.43
23	A	716	C	N3-C4	-5.71	1.29	1.33
23	A	809	A	C6-N6	-5.70	1.29	1.33
23	A	1798	C	C4-C5	-5.70	1.38	1.43
23	A	1824	C	C4-C5	-5.69	1.38	1.43
23	A	2467	C	N1-C6	-5.68	1.33	1.37
23	A	2250	A	N9-C4	-5.68	1.34	1.37
23	A	1802	U	C4-C5	-5.67	1.38	1.43
23	A	2483	C	C4-C5	-5.67	1.38	1.43
23	A	832	C	N1-C6	-5.65	1.33	1.37
23	A	2091	C	C4-C5	-5.64	1.38	1.43
23	A	2079	G	N9-C8	-5.63	1.33	1.37
23	A	1721	A	N9-C4	-5.62	1.34	1.37
23	A	774	G	C6-N1	-5.61	1.35	1.39
23	A	1202	C	C4-C5	-5.58	1.38	1.43
23	A	511	G	N9-C8	-5.58	1.33	1.37
23	A	1712	A	N9-C4	-5.57	1.34	1.37
23	A	1172	A	N9-C4	-5.56	1.34	1.37
23	A	1370	C	C4-C5	-5.55	1.38	1.43
23	A	1616	A	N9-C4	-5.54	1.34	1.37
23	A	512	A	N9-C4	-5.53	1.34	1.37
23	A	2301	A	N9-C4	-5.53	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	2750	C	C4-C5	-5.52	1.38	1.43
23	A	1734	A	N9-C4	-5.51	1.34	1.37
23	A	2525	C	C4-C5	-5.50	1.38	1.43
23	A	2481	G	N9-C8	-5.48	1.34	1.37
23	A	2707	C	C4-C5	-5.48	1.38	1.43
23	A	2523	C	N1-C6	-5.46	1.33	1.37
23	A	743	C	N1-C6	-5.45	1.33	1.37
23	A	500	A	N9-C4	-5.45	1.34	1.37
23	A	865	A	N9-C4	-5.45	1.34	1.37
23	A	515	G	C6-N1	-5.43	1.35	1.39
23	A	625	G	N9-C8	-5.43	1.34	1.37
23	A	1566	G	N9-C4	-5.43	1.33	1.38
23	A	2470	C	N1-C6	-5.43	1.33	1.37
23	A	1661	C	N1-C6	-5.41	1.33	1.37
23	A	1347	G	N1-C2	-5.41	1.33	1.37
23	A	717	C	C4-C5	-5.40	1.38	1.43
23	A	1038	C	N1-C6	-5.39	1.33	1.37
23	A	603	C	N1-C6	-5.39	1.33	1.37
23	A	724	C	C4-C5	-5.39	1.38	1.43
23	A	201	C	N3-C4	-5.37	1.30	1.33
23	A	1833	C	N1-C6	-5.37	1.33	1.37
23	A	2057	A	N9-C4	-5.36	1.34	1.37
23	A	1367	C	N1-C6	-5.35	1.33	1.37
23	A	789	C	C4-C5	-5.34	1.38	1.43
23	A	2618	C	C4-C5	-5.33	1.38	1.43
23	A	2569	A	N9-C4	-5.33	1.34	1.37
23	A	735	C	N1-C6	-5.32	1.33	1.37
23	A	2471	G	N9-C8	-5.32	1.34	1.37
23	A	732	C	N1-C6	-5.31	1.33	1.37
23	A	836	C	C4-C5	-5.31	1.38	1.43
23	A	607	C	N1-C6	-5.29	1.33	1.37
23	A	2093	C	N1-C6	-5.29	1.33	1.37
23	A	720	A	N9-C4	-5.29	1.34	1.37
1	a	270	A	N7-C5	-5.29	1.36	1.39
23	A	627	C	N1-C6	-5.29	1.33	1.37
23	A	723	C	N1-C6	-5.28	1.33	1.37
23	A	876	G	N9-C4	-5.28	1.33	1.38
23	A	2536	G	N9-C4	-5.27	1.33	1.38
23	A	2288	C	C4-C5	-5.27	1.38	1.43
23	A	1829	A	N9-C4	-5.27	1.34	1.37
23	A	2026	C	N1-C6	-5.26	1.33	1.37
23	A	831	C	N1-C6	-5.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	844	G	N3-C4	-5.25	1.31	1.35
23	A	624	C	N1-C6	-5.24	1.34	1.37
23	A	2090	C	C4-C5	-5.24	1.38	1.43
23	A	670	G	C2-N3	-5.23	1.28	1.32
23	A	998	G	N9-C8	-5.23	1.34	1.37
23	A	1393	C	C4-C5	-5.23	1.38	1.43
23	A	1855	G	C2-N2	-5.22	1.29	1.34
23	A	2644	C	C4-C5	-5.21	1.38	1.43
23	A	2644	C	N1-C6	-5.19	1.34	1.37
23	A	1702	C	C4-C5	-5.19	1.38	1.43
23	A	1768	C	N1-C6	-5.18	1.34	1.37
23	A	1539	A	N9-C4	-5.17	1.34	1.37
23	A	1695	G	N7-C5	-5.17	1.36	1.39
23	A	2092	C	N1-C6	-5.16	1.34	1.37
23	A	2091	C	N1-C6	-5.16	1.34	1.37
23	A	2539	C	N1-C6	-5.16	1.34	1.37
23	A	116	G	N9-C8	-5.16	1.34	1.37
23	A	717	C	N1-C6	-5.16	1.34	1.37
25	D	223	VAL	CB-CG1	-5.16	1.42	1.52
23	A	2275	C	C4-C5	-5.15	1.38	1.43
23	A	1830	A	N9-C4	-5.14	1.34	1.37
23	A	1932	C	N1-C6	-5.14	1.34	1.37
1	a	911	A	N7-C5	-5.14	1.36	1.39
23	A	1855	G	N3-C4	-5.14	1.31	1.35
23	A	509	G	N9-C4	-5.13	1.33	1.38
23	A	2445	A	N9-C4	-5.13	1.34	1.37
23	A	2619	G	N9-C8	-5.12	1.34	1.37
23	A	1822	C	N1-C6	-5.11	1.34	1.37
23	A	2006	C	N1-C6	-5.11	1.34	1.37
23	A	854	G	N9-C4	-5.11	1.33	1.38
23	A	1336	G	N9-C8	-5.11	1.34	1.37
23	A	1814	A	N7-C5	-5.11	1.36	1.39
23	A	1391	A	N9-C4	-5.10	1.34	1.37
23	A	838	A	C6-N6	-5.10	1.29	1.33
23	A	230	A	N9-C4	-5.09	1.34	1.37
23	A	2100	C	N1-C6	-5.09	1.34	1.37
29	H	87	LEU	CA-CB	-5.09	1.42	1.53
23	A	2474	G	N9-C8	-5.08	1.34	1.37
23	A	1335	C	C4-C5	-5.08	1.38	1.43
23	A	2077	C	C4-C5	-5.08	1.38	1.43
23	A	1435	C	C4-C5	-5.07	1.38	1.43
23	A	1810	A	N9-C4	-5.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	79	C	C4-C5	-5.06	1.38	1.43
23	A	988	C	N1-C6	-5.06	1.34	1.37
23	A	1324	A	N9-C4	-5.06	1.34	1.37
23	A	2469	C	N3-C4	-5.06	1.30	1.33
23	A	806	A	N7-C5	-5.05	1.36	1.39
23	A	228	A	N9-C4	-5.04	1.34	1.37
23	A	1015	C	C4-C5	-5.04	1.39	1.43
23	A	1368	C	N1-C6	-5.03	1.34	1.37
23	A	864	A	N9-C4	-5.03	1.34	1.37
23	A	1292	A	N9-C4	-5.03	1.34	1.37
1	a	740	C	N1-C6	-5.03	1.34	1.37
23	A	844	G	N9-C8	-5.02	1.34	1.37
23	A	1857	C	C4-C5	-5.01	1.39	1.43
23	A	1039	C	N1-C6	-5.01	1.34	1.37
23	A	734	A	C6-N6	-5.00	1.29	1.33
23	A	1414	G	N1-C2	-5.00	1.33	1.37

All (935) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	Y	25	GLY	CA-C-N	-26.58	58.73	117.20
42	Y	25	GLY	O-C-N	25.46	163.44	122.70
42	Y	25	GLY	C-N-CA	-23.37	63.28	121.70
23	A	806	A	N1-C6-N6	18.77	129.86	118.60
23	A	2451	C	C6-N1-C2	-17.47	113.31	120.30
23	A	260	A	C5'-C4'-C3'	-14.85	92.23	116.00
23	A	2451	C	N3-C2-O2	-14.79	111.54	121.90
23	A	806	A	C5-C6-N6	-14.73	111.92	123.70
23	A	198	A	N1-C6-N6	13.88	126.93	118.60
23	A	806	A	C4-C5-N7	11.66	116.53	110.70
23	A	806	A	C6-C5-N7	-11.04	124.58	132.30
23	A	201	C	N1-C2-O2	10.90	125.44	118.90
23	A	806	A	C5-N7-C8	-10.64	98.58	103.90
23	A	1347	G	N1-C2-N2	-10.42	106.82	116.20
23	A	1714	C	C5-C4-N4	-10.16	113.08	120.20
23	A	806	A	N9-C4-C5	-9.89	101.84	105.80
23	A	2275	C	N1-C2-O2	9.63	124.68	118.90
23	A	2451	C	N1-C2-O2	9.47	124.58	118.90
23	A	732	C	C5-C4-N4	-9.40	113.62	120.20
1	a	136	C	N1-C2-O2	9.13	124.38	118.90
23	A	2090	C	C5-C4-N4	-9.00	113.90	120.20
23	A	1382	C	N1-C2-O2	8.95	124.27	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1857	C	N1-C2-O2	8.93	124.26	118.90
23	A	857	C	C5-C4-N4	-8.90	113.97	120.20
23	A	1347	G	N3-C2-N2	8.89	126.12	119.90
23	A	955	A	N1-C6-N6	-8.84	113.30	118.60
1	a	1541	G	N7-C8-N9	8.58	117.39	113.10
23	A	2033	C	N1-C2-O2	8.57	124.04	118.90
23	A	2290	C	C6-N1-C2	-8.55	116.88	120.30
23	A	840	C	N1-C2-O2	8.54	124.02	118.90
23	A	201	C	N3-C2-O2	-8.49	115.95	121.90
23	A	2451	C	C2-N1-C1'	8.49	128.14	118.80
23	A	198	A	C5-C6-N6	-8.41	116.97	123.70
24	B	79	C	N3-C4-N4	8.41	123.89	118.00
23	A	198	A	N9-C4-C5	-8.35	102.46	105.80
23	A	260	A	C5'-C4'-O4'	8.30	119.06	109.10
1	a	617	A	N1-C6-N6	8.24	123.55	118.60
23	A	1351	C	C6-N1-C2	-8.23	117.01	120.30
23	A	2452	A	N1-C6-N6	-8.22	113.67	118.60
23	A	1395	G	N1-C2-N2	-8.21	108.81	116.20
23	A	476	A	N1-C6-N6	-8.15	113.71	118.60
1	a	641	U	C2-N1-C1'	8.15	127.48	117.70
23	A	1248	U	C5-C4-O4	-8.13	121.02	125.90
1	a	1541	G	C8-N9-C4	-8.09	103.16	106.40
23	A	1604	C	N3-C2-O2	-8.09	116.24	121.90
24	B	79	C	C6-N1-C2	-8.08	117.07	120.30
23	A	1566	G	N3-C4-N9	-8.05	121.17	126.00
23	A	2052	C	C6-N1-C2	-8.05	117.08	120.30
23	A	1509	G	O4'-C1'-N9	8.02	114.62	108.20
23	A	1509	G	N3-C2-N2	7.98	125.48	119.90
1	a	1506	G	C4-C5-N7	7.95	113.98	110.80
23	A	2052	C	N1-C2-O2	7.91	123.64	118.90
23	A	1857	C	N3-C2-O2	-7.88	116.38	121.90
23	A	1395	G	N3-C2-N2	7.88	125.42	119.90
23	A	774	G	C6-C5-N7	-7.87	125.68	130.40
37	T	3	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	a	476	C	C6-N1-C2	-7.82	117.17	120.30
1	a	415	A	N1-C6-N6	7.82	123.29	118.60
23	A	1119	C	N1-C2-O2	7.80	123.58	118.90
23	A	806	A	N7-C8-N9	7.74	117.67	113.80
23	A	1197	C	N1-C2-O2	7.74	123.54	118.90
1	a	394	C	N1-C2-O2	7.73	123.54	118.90
23	A	1658	A	C5-C6-N6	-7.70	117.54	123.70
23	A	857	C	N3-C4-C5	7.63	124.95	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2058	A	C5-C6-N6	-7.59	117.63	123.70
23	A	2058	A	N1-C6-N6	7.58	123.15	118.60
23	A	623	C	N1-C2-O2	7.56	123.44	118.90
23	A	774	G	C4-C5-N7	7.55	113.82	110.80
23	A	1604	C	N1-C2-O2	7.54	123.42	118.90
23	A	1658	A	N1-C6-N6	7.54	123.12	118.60
23	A	2051	C	C6-N1-C2	-7.54	117.28	120.30
1	a	571	A	N1-C6-N6	-7.53	114.08	118.60
23	A	1920	C	N3-C2-O2	-7.52	116.64	121.90
23	A	2467	C	C2-N1-C1'	7.48	127.02	118.80
23	A	832	C	C6-N1-C2	-7.47	117.31	120.30
23	A	1008	C	N3-C2-O2	-7.43	116.70	121.90
23	A	2587	C	N3-C4-C5	7.41	124.86	121.90
1	a	572	U	N3-C2-O2	-7.41	117.02	122.20
23	A	2528	C	C6-N1-C2	-7.37	117.35	120.30
23	A	201	C	C6-N1-C2	-7.36	117.36	120.30
23	A	836	C	N3-C4-C5	7.36	124.84	121.90
23	A	841	C	N1-C2-O2	7.34	123.30	118.90
23	A	515	G	C8-N9-C1'	-7.34	117.46	127.00
23	A	1275	A	N1-C6-N6	7.31	122.99	118.60
1	a	1443	G	O4'-C1'-N9	7.31	114.05	108.20
23	A	2540	A	C5-C6-N6	-7.29	117.86	123.70
23	A	1382	C	N3-C2-O2	-7.28	116.81	121.90
23	A	774	G	N9-C4-C5	-7.25	102.50	105.40
36	S	94	VAL	CG1-CB-CG2	7.25	122.49	110.90
23	A	1857	C	C6-N1-C2	-7.23	117.41	120.30
23	A	1351	C	C2-N1-C1'	7.22	126.74	118.80
23	A	2409	G	C8-N9-C1'	-7.22	117.61	127.00
1	a	762	C	C2-N1-C1'	7.22	126.74	118.80
23	A	624	C	N1-C2-O2	7.21	123.22	118.90
23	A	2305	A	C5-C6-N6	-7.20	117.94	123.70
23	A	2051	C	C5-C4-N4	-7.19	115.17	120.20
23	A	1837	A	C5-C6-N6	-7.19	117.95	123.70
23	A	840	C	N3-C2-O2	-7.16	116.89	121.90
23	A	2057	A	C4-C5-C6	-7.12	113.44	117.00
24	B	79	C	C2-N1-C1'	7.12	126.63	118.80
23	A	2033	C	N3-C2-O2	-7.08	116.94	121.90
32	O	33	ARG	NE-CZ-NH1	7.08	123.84	120.30
23	A	2517	G	N1-C2-N2	-7.07	109.84	116.20
23	A	845	A	N1-C6-N6	7.07	122.84	118.60
23	A	2305	A	C5-C6-N1	7.06	121.23	117.70
23	A	491	C	N1-C2-O2	7.04	123.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1413	C	N1-C2-O2	7.04	123.12	118.90
1	a	1480	A	N1-C6-N6	7.03	122.81	118.60
23	A	2288	C	C5-C4-N4	-7.02	115.29	120.20
23	A	2569	A	C5-C6-N6	-7.02	118.08	123.70
23	A	1714	C	N3-C4-N4	7.02	122.91	118.00
1	a	894	U	C5-C6-N1	7.02	126.21	122.70
23	A	1119	C	N3-C2-O2	-7.01	116.99	121.90
23	A	1509	G	N1-C2-N2	-7.01	109.89	116.20
1	a	572	U	N1-C2-O2	7.00	127.70	122.80
23	A	198	A	C6-C5-N7	-7.00	127.40	132.30
1	a	1506	G	N9-C4-C5	-6.99	102.61	105.40
23	A	2504	C	C6-N1-C2	-6.99	117.50	120.30
23	A	1566	G	N3-C4-C5	6.98	132.09	128.60
23	A	2058	A	N9-C4-C5	-6.97	103.01	105.80
42	Y	82	LEU	CA-CB-CG	6.97	131.33	115.30
23	A	2275	C	C2-N1-C1'	6.93	126.42	118.80
1	a	211	A	N1-C6-N6	-6.90	114.46	118.60
1	a	196	A	N1-C6-N6	6.90	122.74	118.60
23	A	2017	C	N1-C2-O2	6.90	123.04	118.90
1	a	1408	C	C2-N1-C1'	6.89	126.38	118.80
23	A	2485	U	C5-C6-N1	6.88	126.14	122.70
23	A	2052	C	C5-C6-N1	6.88	124.44	121.00
23	A	1029	C	C2-N1-C1'	6.88	126.36	118.80
23	A	175	C	N3-C2-O2	-6.84	117.11	121.90
23	A	1347	G	N1-C6-O6	-6.84	115.80	119.90
23	A	1837	A	N1-C6-N6	6.82	122.69	118.60
23	A	1029	C	C6-N1-C2	-6.81	117.58	120.30
23	A	1920	C	N1-C2-O2	6.81	122.99	118.90
23	A	1004	A	C5-C6-N6	-6.80	118.26	123.70
23	A	2275	C	C6-N1-C2	-6.78	117.59	120.30
23	A	1029	C	N1-C2-O2	6.78	122.97	118.90
24	B	79	C	N1-C2-O2	6.78	122.97	118.90
23	A	2523	C	N3-C2-O2	-6.78	117.16	121.90
23	A	2004	A	C5-C6-N6	-6.78	118.28	123.70
23	A	2057	A	C5-C6-N1	6.77	121.09	117.70
1	a	86	G	N3-C4-N9	-6.76	121.94	126.00
23	A	1880	A	N1-C6-N6	6.75	122.65	118.60
23	A	1248	U	N3-C4-O4	6.75	124.13	119.40
23	A	2409	G	C4-N9-C1'	6.75	135.27	126.50
23	A	2628	C	N1-C2-O2	6.72	122.93	118.90
23	A	515	G	C4-N9-C1'	6.72	135.23	126.50
23	A	603	C	N1-C2-O2	6.72	122.93	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	3	80	LEU	CA-CB-CG	6.72	130.75	115.30
23	A	2078	A	N1-C6-N6	6.71	122.63	118.60
23	A	2052	C	N3-C2-O2	-6.71	117.20	121.90
23	A	2275	C	N3-C2-O2	-6.70	117.21	121.90
23	A	1004	A	C5-C6-N1	6.70	121.05	117.70
23	A	717	C	C2-N1-C1'	6.69	126.16	118.80
23	A	1148	C	C6-N1-C2	-6.67	117.63	120.30
23	A	2706	A	C5-C6-N6	-6.65	118.38	123.70
23	A	128	C	N1-C2-O2	6.64	122.89	118.90
23	A	1802	U	C5-C6-N1	6.61	126.00	122.70
23	A	136	A	C5-C6-N6	-6.60	118.42	123.70
23	A	1347	G	C5-C6-O6	6.60	132.56	128.60
24	B	79	C	C5-C4-N4	-6.60	115.58	120.20
23	A	1932	C	N3-C4-C5	6.59	124.54	121.90
23	A	1393	C	C6-N1-C2	-6.58	117.67	120.30
23	A	2619	G	C4-N9-C1'	6.58	135.05	126.50
23	A	832	C	C2-N1-C1'	6.57	126.02	118.80
23	A	2097	G	C2-N3-C4	-6.56	108.62	111.90
23	A	717	C	N1-C2-O2	6.56	122.83	118.90
23	A	994	A	C5-C6-N6	-6.55	118.46	123.70
23	A	1364	C	C5-C4-N4	-6.55	115.61	120.20
23	A	1393	C	N1-C2-O2	6.55	122.83	118.90
23	A	1798	C	C5-C4-N4	-6.55	115.61	120.20
23	A	2523	C	N1-C2-O2	6.53	122.82	118.90
23	A	2729	G	C4-N9-C1'	6.53	134.99	126.50
23	A	1695	G	C4-N9-C1'	6.53	134.99	126.50
23	A	178	A	N9-C4-C5	-6.52	103.19	105.80
23	A	1515	G	N3-C2-N2	6.51	124.46	119.90
23	A	1333	A	C5-N7-C8	-6.51	100.65	103.90
1	a	315	U	C6-N1-C2	-6.50	117.10	121.00
23	A	548	A	N1-C6-N6	6.50	122.50	118.60
1	a	1408	C	N1-C2-O2	6.50	122.80	118.90
23	A	2536	G	N3-C4-C5	6.49	131.84	128.60
23	A	515	G	O4'-C1'-N9	6.49	113.39	108.20
23	A	2456	G	C6-C5-N7	-6.49	126.51	130.40
23	A	2644	C	C5-C4-N4	-6.48	115.66	120.20
23	A	2873	C	N1-C2-O2	6.48	122.79	118.90
23	A	1289	A	C5-C6-N1	6.47	120.94	117.70
23	A	1695	G	C6-C5-N7	-6.47	126.52	130.40
23	A	491	C	C2-N1-C1'	6.47	125.91	118.80
23	A	1690	A	C5-C6-N6	-6.46	118.53	123.70
23	A	1202	C	N1-C2-O2	6.44	122.76	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	484	A	C5-C6-N6	-6.43	118.56	123.70
23	A	2051	C	N3-C4-N4	6.42	122.49	118.00
23	A	2517	G	C2-N3-C4	-6.37	108.72	111.90
1	a	641	U	N3-C2-O2	-6.36	117.75	122.20
23	A	1719	C	C5-C4-N4	-6.36	115.75	120.20
23	A	1274	G	N1-C2-N2	-6.35	110.48	116.20
23	A	1201	G	C4-N9-C1'	6.33	134.73	126.50
1	a	805	C	N1-C2-O2	6.32	122.69	118.90
23	A	718	C	N3-C4-C5	6.32	124.43	121.90
23	A	1880	A	C5-C6-N6	-6.32	118.64	123.70
32	O	47	ARG	NE-CZ-NH1	6.32	123.46	120.30
23	A	500	A	N1-C6-N6	6.32	122.39	118.60
23	A	1472	C	C5-C4-N4	-6.32	115.78	120.20
23	A	2569	A	N1-C6-N6	6.31	122.39	118.60
23	A	1831	A	C5-C6-N1	6.30	120.85	117.70
23	A	1855	G	N1-C2-N3	6.30	127.68	123.90
23	A	1380	G	C4-N9-C1'	6.30	134.69	126.50
23	A	876	G	N3-C4-C5	6.29	131.75	128.60
24	B	114	C	N1-C2-O2	6.28	122.67	118.90
23	A	436	A	C5-C6-N6	-6.27	118.68	123.70
23	A	1880	A	N9-C4-C5	-6.27	103.29	105.80
23	A	515	G	C2-N3-C4	-6.26	108.77	111.90
1	a	874	A	N1-C6-N6	-6.26	114.84	118.60
1	a	1452	G	N3-C2-N2	-6.26	115.52	119.90
23	A	548	A	C5-C6-N6	-6.25	118.70	123.70
1	a	412	G	C2-N3-C4	-6.25	108.78	111.90
23	A	732	C	N3-C4-N4	6.24	122.37	118.00
1	a	409	C	N1-C2-O2	6.24	122.64	118.90
23	A	2578	C	N1-C2-O2	6.23	122.64	118.90
23	A	558	A	C8-N9-C4	6.23	108.29	105.80
23	A	1607	A	N1-C6-N6	-6.23	114.86	118.60
23	A	2074	C	N1-C2-O2	6.22	122.63	118.90
23	A	2668	A	C5-C6-N1	6.22	120.81	117.70
23	A	1824	C	C5-C4-N4	-6.22	115.85	120.20
1	a	1160	C	C6-N1-C2	-6.20	117.82	120.30
1	a	1459	C	C6-N1-C2	-6.20	117.82	120.30
23	A	728	U	C5-C4-O4	-6.20	122.18	125.90
23	A	241	C	C6-N1-C2	-6.19	117.82	120.30
23	A	668	C	N1-C2-O2	6.19	122.61	118.90
23	A	436	A	N1-C6-N6	6.19	122.31	118.60
23	A	125	A	N1-C6-N6	6.19	122.31	118.60
23	A	2070	C	N1-C2-O2	6.18	122.61	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	O	47	ARG	NE-CZ-NH2	-6.18	117.21	120.30
23	A	1414	G	N1-C2-N2	-6.18	110.64	116.20
23	A	509	G	C2-N3-C4	-6.17	108.82	111.90
1	a	160	A	N1-C6-N6	6.17	122.30	118.60
23	A	2077	C	C6-N1-C2	-6.16	117.83	120.30
23	A	2528	C	C5-C4-N4	-6.16	115.89	120.20
23	A	2468	C	C5-C4-N4	-6.16	115.89	120.20
23	A	1031	C	N3-C4-C5	6.15	124.36	121.90
1	a	196	A	C6-C5-N7	-6.15	127.99	132.30
23	A	1956	G	C4-N9-C1'	6.15	134.50	126.50
1	a	168	G	C4-C5-N7	6.15	113.26	110.80
23	A	1393	C	C2-N1-C1'	6.14	125.56	118.80
23	A	2451	C	N1-C2-N3	6.14	123.50	119.20
23	A	1857	C	C2-N1-C1'	6.14	125.56	118.80
23	A	201	C	C2-N1-C1'	6.14	125.56	118.80
1	a	682	G	C2-N3-C4	-6.13	108.83	111.90
1	a	36	G	C4-N9-C1'	6.13	134.47	126.50
23	A	1798	C	C2-N1-C1'	6.13	125.54	118.80
1	a	725	C	N1-C2-O2	6.13	122.58	118.90
23	A	608	C	C5-C4-N4	-6.12	115.92	120.20
24	B	98	G	C6-C5-N7	-6.12	126.73	130.40
23	A	670	G	N3-C4-N9	-6.11	122.33	126.00
23	A	2479	C	C5-C4-N4	-6.11	115.92	120.20
1	a	762	C	C6-N1-C1'	-6.11	113.47	120.80
23	A	1685	A	N1-C6-N6	-6.11	114.94	118.60
23	A	153	G	C5-C6-O6	6.10	132.26	128.60
1	a	316	C	N1-C2-O2	6.09	122.55	118.90
1	a	315	U	C5-C6-N1	6.09	125.74	122.70
24	B	114	C	N3-C2-O2	-6.09	117.64	121.90
23	A	734	A	C5-C6-N1	6.08	120.74	117.70
23	A	789	C	C5-C4-N4	-6.08	115.94	120.20
23	A	1350	U	C2-N1-C1'	6.08	124.99	117.70
23	A	2707	C	C5-C4-N4	-6.08	115.95	120.20
23	A	1727	C	N3-C4-C5	6.08	124.33	121.90
23	A	2063	C	N1-C2-O2	6.08	122.55	118.90
1	a	932	G	C2-N3-C4	-6.07	108.86	111.90
23	A	656	G	N3-C4-C5	6.07	131.63	128.60
23	A	992	A	N9-C4-C5	-6.07	103.37	105.80
23	A	129	C	N1-C2-O2	6.07	122.54	118.90
23	A	198	A	C4-C5-N7	6.06	113.73	110.70
23	A	2028	A	C5-C6-N1	6.06	120.73	117.70
23	A	2456	G	N1-C6-O6	6.05	123.53	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	851	C	C6-N1-C2	-6.04	117.88	120.30
23	A	844	G	N3-C4-N9	-6.04	122.38	126.00
23	A	584	G	N3-C4-N9	-6.04	122.38	126.00
23	A	1148	C	C2-N1-C1'	6.04	125.44	118.80
23	A	2729	G	N3-C4-C5	-6.04	125.58	128.60
23	A	1049	C	C6-N1-C2	-6.03	117.89	120.30
23	A	1029	C	C5-C4-N4	-6.03	115.98	120.20
23	A	343	A	N1-C6-N6	6.03	122.22	118.60
23	A	1795	A	C5-C6-N1	6.03	120.71	117.70
23	A	2467	C	C6-N1-C1'	-6.03	113.57	120.80
1	a	621	C	N3-C4-C5	6.03	124.31	121.90
23	A	496	G	C2-N3-C4	-6.03	108.89	111.90
23	A	1768	C	C5-C6-N1	6.03	124.01	121.00
23	A	767	A	N9-C4-C5	-6.02	103.39	105.80
1	a	136	C	N3-C2-O2	-6.02	117.69	121.90
23	A	1658	A	N9-C4-C5	-6.02	103.39	105.80
23	A	2503	A	N3-C4-N9	-6.01	122.59	127.40
23	A	729	G	C2-N3-C4	-6.01	108.89	111.90
23	A	1336	G	C2-N3-C4	-6.01	108.89	111.90
23	A	1201	G	C6-C5-N7	-6.01	126.79	130.40
23	A	1338	U	C6-N1-C2	-6.00	117.40	121.00
23	A	2418	G	C5-C6-O6	-6.00	125.00	128.60
23	A	115	C	N1-C2-O2	5.99	122.49	118.90
23	A	419	U	N3-C2-O2	-5.99	118.01	122.20
23	A	728	U	N3-C4-O4	5.99	123.59	119.40
23	A	1333	A	C4-C5-N7	5.99	113.69	110.70
23	A	1369	G	C8-N9-C1'	-5.99	119.22	127.00
23	A	565	G	N3-C2-N2	5.98	124.09	119.90
1	a	641	U	N1-C2-O2	5.98	126.98	122.80
23	A	776	C	N1-C2-O2	5.98	122.49	118.90
23	A	2090	C	N3-C4-N4	5.98	122.19	118.00
23	A	1727	C	C5-C4-N4	-5.97	116.02	120.20
1	a	415	A	C5-C6-N6	-5.96	118.93	123.70
23	A	1980	A	N1-C6-N6	-5.96	115.03	118.60
23	A	2618	C	C5-C4-N4	-5.95	116.03	120.20
23	A	2077	C	C5-C4-N4	-5.95	116.03	120.20
1	a	911	A	C5-C6-N6	-5.95	118.94	123.70
23	A	994	A	C5-C6-N1	5.95	120.68	117.70
23	A	2063	C	C6-N1-C2	-5.95	117.92	120.30
1	a	394	C	N3-C2-O2	-5.95	117.74	121.90
23	A	777	C	C6-N1-C2	-5.95	117.92	120.30
1	a	196	A	N7-C8-N9	5.94	116.77	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	933	A	C5-C6-N6	-5.94	118.94	123.70
23	A	1289	A	N1-C6-N6	-5.94	115.03	118.60
23	A	2528	C	C5-C6-N1	5.94	123.97	121.00
1	a	911	A	N1-C6-N6	5.94	122.16	118.60
23	A	1295	C	N3-C4-C5	5.93	124.27	121.90
23	A	455	A	C5-C6-N6	-5.93	118.95	123.70
23	A	1475	A	C5-C6-N6	-5.93	118.95	123.70
1	a	1439	A	C5-C6-N6	-5.93	118.95	123.70
23	A	1713	A	C8-N9-C4	-5.93	103.43	105.80
23	A	2004	A	N1-C6-N6	5.93	122.16	118.60
38	U	26	ASP	CB-CG-OD1	5.93	123.64	118.30
23	A	960	C	C6-N1-C2	-5.93	117.93	120.30
23	A	2843	A	C5-C6-N6	-5.92	118.96	123.70
23	A	2488	C	N1-C2-O2	5.91	122.45	118.90
23	A	2704	A	C5-C6-N1	5.91	120.66	117.70
23	A	2706	A	C5-N7-C8	-5.91	100.95	103.90
1	a	1032	C	N3-C2-O2	-5.91	117.77	121.90
1	a	1522	C	N1-C2-O2	5.91	122.44	118.90
23	A	46	C	C6-N1-C2	-5.91	117.94	120.30
23	A	2517	G	N7-C8-N9	5.91	116.05	113.10
23	A	623	C	C2-N1-C1'	5.90	125.29	118.80
52	8	4	ARG	NE-CZ-NH1	5.90	123.25	120.30
23	A	863	G	C6-C5-N7	-5.90	126.86	130.40
23	A	1414	G	C4-C5-N7	5.90	113.16	110.80
23	A	271	C	N3-C4-C5	5.89	124.26	121.90
1	a	1408	C	C6-N1-C1'	-5.89	113.73	120.80
23	A	1393	C	C5-C4-N4	-5.89	116.08	120.20
25	D	181	ARG	NE-CZ-NH1	5.89	123.25	120.30
23	A	1370	C	N1-C2-O2	5.89	122.43	118.90
23	A	1956	G	C6-C5-N7	-5.88	126.87	130.40
23	A	168	A	N1-C6-N6	5.88	122.13	118.60
23	A	492	G	N1-C2-N2	-5.88	110.91	116.20
23	A	186	C	N1-C2-O2	5.88	122.43	118.90
23	A	824	A	C5-C6-N6	-5.88	119.00	123.70
23	A	2063	C	N3-C2-O2	-5.88	117.79	121.90
1	a	1539	C	N3-C2-O2	-5.87	117.79	121.90
1	a	476	C	C2-N1-C1'	5.86	125.24	118.80
23	A	509	G	N3-C4-C5	5.85	131.52	128.60
23	A	1291	A	C5-C6-N1	5.85	120.62	117.70
23	A	2359	C	N1-C2-O2	5.85	122.41	118.90
23	A	2661	A	C5-C6-N6	-5.84	119.03	123.70
23	A	2290	C	C2-N1-C1'	5.84	125.22	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1304	G	C4-C5-N7	5.84	113.14	110.80
23	A	250	G	N1-C2-N2	-5.84	110.95	116.20
23	A	2091	C	N3-C4-N4	5.83	122.08	118.00
1	a	1049	C	C6-N1-C2	-5.83	117.97	120.30
23	A	2587	C	N1-C2-O2	5.83	122.40	118.90
23	A	2360	A	N1-C6-N6	-5.82	115.11	118.60
23	A	2063	C	C2-N1-C1'	5.82	125.20	118.80
23	A	832	C	N3-C4-N4	5.82	122.07	118.00
23	A	2536	G	N3-C4-N9	-5.82	122.51	126.00
23	A	771	G	C2-N3-C4	-5.82	108.99	111.90
23	A	836	C	N1-C2-O2	5.82	122.39	118.90
1	a	1480	A	C5-C6-N6	-5.81	119.05	123.70
1	a	1506	G	C6-C5-N7	-5.81	126.91	130.40
1	a	1252	G	N7-C8-N9	5.81	116.00	113.10
23	A	2668	A	C5-C6-N6	-5.81	119.05	123.70
37	T	53	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	a	1418	C	N1-C2-O2	5.80	122.38	118.90
23	A	774	G	C8-N9-C1'	-5.80	119.46	127.00
24	B	104	C	N3-C4-C5	5.80	124.22	121.90
23	A	1253	G	N3-C2-N2	5.80	123.96	119.90
23	A	1369	G	C4-N9-C1'	5.80	134.04	126.50
23	A	2357	G	N3-C4-N9	-5.80	122.52	126.00
23	A	1855	G	C2-N3-C4	-5.79	109.00	111.90
23	A	2052	C	C2-N1-C1'	5.79	125.17	118.80
23	A	1811	A	N9-C4-C5	-5.79	103.48	105.80
1	a	1429	A	C5-C6-N6	-5.79	119.07	123.70
1	a	86	G	C8-N9-C1'	5.79	134.53	127.00
23	A	2017	C	N3-C2-O2	-5.79	117.85	121.90
23	A	876	G	N3-C4-N9	-5.79	122.53	126.00
23	A	128	C	N3-C2-O2	-5.79	117.85	121.90
23	A	1413	C	N3-C2-O2	-5.79	117.85	121.90
1	a	125	G	C2-N3-C4	-5.78	109.01	111.90
23	A	1308	C	C5-C4-N4	-5.78	116.15	120.20
1	a	1452	G	N3-C4-N9	-5.78	122.53	126.00
23	A	1453	G	N1-C2-N2	-5.78	111.00	116.20
23	A	1658	A	C4-C5-N7	5.78	113.59	110.70
1	a	725	C	N3-C2-O2	-5.78	117.86	121.90
23	A	1708	A	C5-C6-N6	-5.77	119.08	123.70
23	A	2288	C	N3-C4-N4	5.77	122.04	118.00
23	A	2816	C	N1-C2-O2	5.77	122.36	118.90
1	a	1487	G	N1-C2-N2	-5.77	111.01	116.20
23	A	2105	C	C2-N1-C1'	5.76	125.14	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2913	G	C5-C6-O6	5.76	132.06	128.60
1	a	221	U	N3-C2-O2	-5.76	118.17	122.20
23	A	624	C	N3-C2-O2	-5.75	117.87	121.90
23	A	1731	G	C2-N3-C4	-5.75	109.02	111.90
23	A	601	G	C4-C5-N7	5.75	113.10	110.80
1	a	34	A	C6-C5-N7	-5.75	128.28	132.30
23	A	824	A	C5-C6-N1	5.75	120.57	117.70
23	A	1798	C	N1-C2-O2	5.75	122.35	118.90
1	a	1428	G	C2-N3-C4	-5.75	109.03	111.90
23	A	2578	C	C2-N1-C1'	5.74	125.12	118.80
23	A	2528	C	N3-C4-N4	5.74	122.02	118.00
23	A	2706	A	C4-C5-N7	5.74	113.57	110.70
1	a	762	C	N1-C2-O2	5.73	122.34	118.90
1	a	903	C	C5-C4-N4	-5.73	116.19	120.20
1	a	1012	U	C2-N1-C1'	5.73	124.58	117.70
23	A	1029	C	N3-C2-O2	-5.73	117.89	121.90
23	A	1950	U	C5-C6-N1	5.73	125.56	122.70
23	A	2105	C	C6-N1-C2	-5.73	118.01	120.30
1	a	1155	G	N3-C2-N2	-5.73	115.89	119.90
23	A	1253	G	N1-C2-N2	-5.73	111.05	116.20
23	A	2409	G	N3-C4-N9	5.73	129.44	126.00
1	a	753	U	C5-C6-N1	5.72	125.56	122.70
1	a	1247	A	C5-C6-N6	-5.72	119.12	123.70
23	A	1956	G	C8-N9-C1'	-5.72	119.56	127.00
27	F	168	ARG	NE-CZ-NH2	5.72	123.16	120.30
23	A	2004	A	C4-C5-N7	5.72	113.56	110.70
23	A	623	C	C5-C4-N4	-5.72	116.20	120.20
1	a	536	C	N3-C2-O2	-5.71	117.90	121.90
23	A	1695	G	C8-N9-C1'	-5.71	119.57	127.00
23	A	188	C	C5-C4-N4	-5.71	116.20	120.20
23	A	1542	C	N3-C2-O2	-5.71	117.91	121.90
23	A	2919	A	N9-C4-C5	-5.71	103.52	105.80
23	A	175	C	C6-N1-C2	-5.70	118.02	120.30
1	a	315	U	N3-C2-O2	-5.70	118.21	122.20
23	A	1104	U	P-O3'-C3'	5.70	126.54	119.70
1	a	641	U	C6-N1-C1'	-5.70	113.23	121.20
23	A	1934	G	C6-C5-N7	-5.69	126.98	130.40
23	A	1108	C	C6-N1-C2	-5.69	118.02	120.30
1	a	34	A	C5-N7-C8	-5.69	101.06	103.90
1	a	493	G	N3-C4-C5	5.69	131.44	128.60
1	a	1252	G	C4-N9-C1'	5.69	133.89	126.50
23	A	1517	A	C5-C6-N6	-5.69	119.15	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2148	G	N3-C4-N9	5.69	129.41	126.00
23	A	2456	G	C4-N9-C1'	5.68	133.89	126.50
23	A	500	A	C5-C6-N6	-5.68	119.15	123.70
23	A	856	U	N3-C2-O2	-5.68	118.22	122.20
23	A	2021	C	C5-C4-N4	-5.68	116.22	120.20
23	A	2451	C	C5-C4-N4	5.68	124.18	120.20
51	7	13	ARG	NE-CZ-NH2	5.68	123.14	120.30
23	A	1822	C	N1-C2-O2	5.67	122.30	118.90
23	A	2635	G	C2-N3-C4	-5.67	109.06	111.90
24	B	98	G	C4-N9-C1'	5.67	133.87	126.50
23	A	2628	C	C2-N1-C1'	5.67	125.04	118.80
23	A	514	G	C8-N9-C1'	-5.67	119.64	127.00
23	A	876	G	C2-N3-C4	-5.67	109.07	111.90
23	A	1294	G	C4-N9-C1'	5.67	133.87	126.50
23	A	845	A	C5-C6-N6	-5.66	119.17	123.70
23	A	315	C	C6-N1-C2	-5.66	118.03	120.30
23	A	2798	C	N3-C4-C5	5.65	124.16	121.90
23	A	863	G	C2-N3-C4	-5.65	109.08	111.90
23	A	2091	C	C6-N1-C2	-5.65	118.04	120.30
23	A	2525	C	C6-N1-C2	-5.65	118.04	120.30
1	a	700	U	C5-C4-O4	-5.64	122.51	125.90
23	A	1811	A	C5-C6-N6	-5.64	119.19	123.70
23	A	828	A	C5-C6-N1	5.64	120.52	117.70
2	b	213	LEU	CA-CB-CG	5.63	128.25	115.30
23	A	1484	G	C2-N3-C4	-5.63	109.08	111.90
23	A	2077	C	C2-N1-C1'	5.63	124.99	118.80
23	A	398	C	N3-C4-C5	5.63	124.15	121.90
23	A	654	C	C5-C4-N4	-5.62	116.26	120.20
1	a	409	C	N3-C2-O2	-5.62	117.97	121.90
23	A	2839	A	N9-C4-C5	-5.62	103.55	105.80
23	A	1274	G	N3-C2-N2	5.62	123.83	119.90
1	a	1482	G	C2-N3-C4	-5.62	109.09	111.90
1	a	772	C	C5-C4-N4	-5.61	116.27	120.20
23	A	260	A	O4'-C4'-C3'	-5.61	98.39	104.00
23	A	1008	C	N1-C2-O2	5.61	122.27	118.90
23	A	1380	G	C8-N9-C1'	-5.61	119.70	127.00
23	A	2021	C	N3-C4-C5	5.61	124.15	121.90
23	A	2603	G	N3-C2-N2	-5.61	115.97	119.90
23	A	2707	C	C2-N1-C1'	5.61	124.97	118.80
1	a	34	A	C4-C5-N7	5.61	113.50	110.70
23	A	2051	C	N1-C2-O2	5.61	122.27	118.90
23	A	2619	G	C8-N9-C1'	-5.61	119.71	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1547	C	N3-C2-O2	-5.61	117.97	121.90
1	a	86	G	C4-N9-C1'	-5.61	119.21	126.50
23	A	514	G	C4-N9-C1'	5.61	133.79	126.50
23	A	992	A	C4-C5-N7	5.61	113.50	110.70
23	A	838	A	C5-C6-N6	-5.60	119.22	123.70
23	A	1517	A	N3-C4-N9	5.60	131.88	127.40
23	A	757	G	N3-C4-C5	5.60	131.40	128.60
1	a	463	U	C2-N1-C1'	5.60	124.42	117.70
23	A	620	G	C4-N9-C1'	5.59	133.77	126.50
23	A	497	U	C5-C6-N1	5.59	125.50	122.70
23	A	555	C	C6-N1-C2	-5.59	118.06	120.30
23	A	565	G	N1-C2-N2	-5.59	111.17	116.20
23	A	1414	G	C5-N7-C8	-5.59	101.50	104.30
23	A	2059	G	N3-C4-N9	-5.59	122.65	126.00
1	a	484	A	N1-C6-N6	5.58	121.95	118.60
23	A	1490	G	N3-C2-N2	5.58	123.81	119.90
23	A	178	A	C4-C5-N7	5.58	113.49	110.70
23	A	1419	A	N1-C6-N6	5.58	121.95	118.60
23	A	718	C	C6-N1-C2	5.58	122.53	120.30
23	A	1542	C	N1-C2-O2	5.58	122.25	118.90
23	A	2057	A	N1-C6-N6	-5.58	115.25	118.60
23	A	1695	G	N3-C4-N9	5.58	129.35	126.00
23	A	865	A	C5-C6-N1	5.57	120.48	117.70
23	A	2848	G	N3-C4-N9	-5.57	122.66	126.00
23	A	2051	C	C2-N1-C1'	5.57	124.92	118.80
23	A	2729	G	C8-N9-C1'	-5.56	119.77	127.00
23	A	1803	G	C4-N9-C1'	5.56	133.73	126.50
23	A	2234	C	N1-C2-O2	5.56	122.24	118.90
23	A	288	C	C6-N1-C2	-5.56	118.08	120.30
23	A	2288	C	N1-C2-O2	5.56	122.23	118.90
23	A	1393	C	N3-C2-O2	-5.56	118.01	121.90
1	a	1183	C	C6-N1-C2	-5.55	118.08	120.30
23	A	955	A	C5-C6-N6	5.55	128.14	123.70
23	A	1414	G	N7-C8-N9	5.55	115.87	113.10
1	a	36	G	C8-N9-C1'	-5.54	119.80	127.00
23	A	272	C	C6-N1-C2	-5.54	118.08	120.30
23	A	2729	G	N1-C2-N2	-5.54	111.22	116.20
23	A	707	G	C2-N3-C4	-5.54	109.13	111.90
23	A	2540	A	C5-C6-N1	5.53	120.47	117.70
23	A	1696	C	C5-C4-N4	-5.53	116.33	120.20
23	A	2610	G	N3-C4-N9	-5.53	122.68	126.00
23	A	515	G	N1-C2-N2	-5.53	111.23	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2778	G	N3-C4-N9	-5.53	122.68	126.00
23	A	935	C	C2-N1-C1'	5.52	124.88	118.80
23	A	626	G	C4-N9-C1'	5.52	133.67	126.50
23	A	125	A	C5-C6-N6	-5.52	119.29	123.70
23	A	1286	G	N3-C4-C5	5.51	131.36	128.60
1	a	86	G	C6-C5-N7	5.51	133.71	130.40
23	A	1202	C	C2-N1-C1'	5.51	124.86	118.80
23	A	1547	C	N1-C2-O2	5.51	122.21	118.90
23	A	2503	A	N3-C4-C5	5.51	130.66	126.80
23	A	260	A	O4'-C1'-N9	5.51	112.61	108.20
23	A	1197	C	N3-C2-O2	-5.51	118.04	121.90
23	A	623	C	N3-C2-O2	-5.51	118.05	121.90
23	A	2059	G	N3-C4-C5	5.51	131.35	128.60
23	A	2409	G	N1-C2-N2	-5.51	111.24	116.20
23	A	1515	G	N1-C2-N2	-5.50	111.25	116.20
23	A	1333	A	N7-C8-N9	5.50	116.55	113.80
1	a	734	C	N1-C2-O2	5.50	122.20	118.90
23	A	2455	G	N3-C4-C5	5.50	131.35	128.60
23	A	1308	C	N3-C4-C5	5.49	124.10	121.90
23	A	2409	G	N3-C2-N2	5.49	123.75	119.90
23	A	1656	C	N1-C2-O2	5.49	122.19	118.90
23	A	1031	C	N1-C2-O2	5.48	122.19	118.90
1	a	564	C	N1-C2-O2	5.48	122.19	118.90
1	a	1367	G	C4-N9-C1'	5.48	133.62	126.50
23	A	584	G	N3-C4-C5	5.48	131.34	128.60
23	A	175	C	C6-N1-C1'	5.47	127.37	120.80
23	A	1472	C	N3-C4-N4	5.47	121.83	118.00
23	A	2409	G	N9-C4-C5	-5.47	103.21	105.40
23	A	1201	G	C8-N9-C1'	-5.47	119.89	127.00
23	A	2077	C	N1-C2-O2	5.47	122.18	118.90
23	A	85	G	N3-C4-C5	5.46	131.33	128.60
23	A	1811	A	N1-C6-N6	5.46	121.88	118.60
23	A	724	C	C5-C4-N4	-5.46	116.38	120.20
23	A	1880	A	C4-C5-N7	5.46	113.43	110.70
23	A	2900	C	N3-C2-O2	-5.46	118.08	121.90
23	A	1049	C	N1-C2-O2	5.46	122.17	118.90
1	a	1299	A	N1-C6-N6	5.45	121.87	118.60
23	A	2078	A	C5-N7-C8	-5.45	101.17	103.90
50	6	40	ARG	NE-CZ-NH2	5.45	123.03	120.30
52	8	4	ARG	NE-CZ-NH2	-5.45	117.57	120.30
23	A	1148	C	N3-C2-O2	-5.45	118.08	121.90
23	A	1213	C	N1-C2-O2	5.45	122.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	456	A	C2-N3-C4	5.45	113.33	110.60
1	a	593	G	C6-C5-N7	-5.45	127.13	130.40
24	B	98	G	C8-N9-C1'	-5.44	119.92	127.00
23	A	854	G	N3-C4-C5	5.44	131.32	128.60
23	A	2668	A	C6-N1-C2	-5.44	115.34	118.60
1	a	454	G	C4-N9-C1'	5.43	133.56	126.50
23	A	1302	G	C2-N3-C4	-5.43	109.18	111.90
23	A	2308	C	N3-C4-N4	-5.43	114.20	118.00
23	A	718	C	C5-C4-N4	-5.43	116.40	120.20
23	A	1393	C	N3-C4-N4	5.43	121.80	118.00
23	A	1956	G	N1-C2-N2	-5.43	111.31	116.20
23	A	2479	C	C2-N3-C4	-5.43	117.19	119.90
1	a	750	G	N3-C4-N9	-5.42	122.75	126.00
1	a	252	U	C2-N1-C1'	5.42	124.20	117.70
23	A	832	C	N3-C2-O2	-5.42	118.11	121.90
1	a	1156	C	N1-C2-O2	5.42	122.15	118.90
23	A	348	C	N1-C2-O2	5.42	122.15	118.90
23	A	1294	G	C5-C6-O6	5.41	131.85	128.60
23	A	1803	G	N7-C8-N9	5.41	115.81	113.10
23	A	2452	A	C8-N9-C4	-5.41	103.64	105.80
23	A	44	A	C5-N7-C8	-5.41	101.19	103.90
23	A	2778	G	N3-C2-N2	-5.41	116.11	119.90
36	S	94	VAL	CA-CB-CG2	5.41	119.01	110.90
23	A	113	U	C2-N1-C1'	5.40	124.19	117.70
23	A	2058	A	C4-C5-N7	5.40	113.40	110.70
23	A	2236	C	N1-C2-O2	5.40	122.14	118.90
23	A	2750	C	C5-C4-N4	-5.40	116.42	120.20
23	A	2621	C	C5-C4-N4	-5.40	116.42	120.20
23	A	476	A	C5-C6-N1	5.39	120.40	117.70
23	A	2082	C	C6-N1-C2	5.39	122.46	120.30
23	A	2503	A	C2-N3-C4	-5.39	107.90	110.60
1	a	1355	C	N3-C2-O2	-5.39	118.13	121.90
23	A	1435	C	C5-C4-N4	-5.39	116.43	120.20
23	A	1767	G	O4'-C1'-N9	5.39	112.51	108.20
23	A	2275	C	C5-C6-N1	5.39	123.69	121.00
23	A	1435	C	N1-C2-O2	5.39	122.13	118.90
1	a	196	A	C4-N9-C1'	5.38	135.99	126.30
1	a	415	A	C6-C5-N7	-5.38	128.53	132.30
1	a	1367	G	N7-C8-N9	5.38	115.79	113.10
23	A	574	A	N1-C6-N6	5.38	121.83	118.60
23	A	1395	G	C4-C5-N7	5.38	112.95	110.80
23	A	2176	C	N3-C4-N4	5.38	121.77	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1541	G	N3-C2-N2	5.38	123.66	119.90
23	A	2004	A	N9-C4-C5	-5.38	103.65	105.80
23	A	491	C	N3-C2-O2	-5.37	118.14	121.90
23	A	922	G	O4'-C1'-N9	5.37	112.50	108.20
23	A	1290	G	N1-C2-N2	-5.37	111.37	116.20
23	A	2456	G	N7-C8-N9	5.37	115.78	113.10
23	A	1669	C	N3-C4-C5	5.37	124.05	121.90
23	A	2083	G	C4-N9-C1'	5.37	133.47	126.50
23	A	627	C	C6-N1-C2	-5.36	118.15	120.30
23	A	1291	A	C5-C6-N6	-5.36	119.41	123.70
23	A	2059	G	C8-N9-C1'	5.36	133.97	127.00
34	Q	24	LEU	CA-CB-CG	5.36	127.63	115.30
23	A	1452	C	N3-C4-C5	5.36	124.04	121.90
23	A	319	G	N1-C2-N2	-5.35	111.38	116.20
23	A	2072	C	N1-C2-O2	5.35	122.11	118.90
23	A	1469	G	C2-N3-C4	-5.35	109.23	111.90
1	a	1156	C	N3-C2-O2	-5.35	118.16	121.90
51	7	44	LEU	CA-CB-CG	5.35	127.60	115.30
23	A	912	C	N3-C4-C5	5.34	124.04	121.90
23	A	1631	G	N1-C2-N2	5.34	121.01	116.20
23	A	2048	G	C4-N9-C1'	5.34	133.44	126.50
23	A	2082	C	N3-C4-C5	5.34	124.03	121.90
23	A	2654	G	C2-N3-C4	-5.34	109.23	111.90
23	A	1370	C	C5-C4-N4	-5.34	116.46	120.20
23	A	1917	A	N1-C6-N6	5.34	121.80	118.60
23	A	518	A	N1-C6-N6	5.33	121.80	118.60
23	A	2711	U	C5-C4-O4	-5.33	122.70	125.90
23	A	1347	G	C4-N9-C1'	5.33	133.44	126.50
23	A	2534	C	N1-C2-O2	5.33	122.10	118.90
23	A	774	G	C5-N7-C8	-5.33	101.63	104.30
23	A	914	G	N3-C4-N9	-5.33	122.80	126.00
23	A	1197	C	C2-N1-C1'	5.33	124.67	118.80
1	a	252	U	N3-C2-O2	-5.33	118.47	122.20
23	A	356	A	N9-C4-C5	-5.33	103.67	105.80
23	A	511	G	C2-N3-C4	-5.33	109.24	111.90
1	a	158	G	N3-C4-N9	-5.33	122.80	126.00
23	A	1490	G	N1-C6-O6	-5.33	116.70	119.90
23	A	1798	C	N3-C4-N4	5.32	121.73	118.00
23	A	2409	G	C6-C5-N7	-5.32	127.21	130.40
23	A	2919	A	C6-C5-N7	-5.32	128.57	132.30
1	a	100	A	N1-C6-N6	5.32	121.79	118.60
23	A	1226	G	C2-N3-C4	-5.31	109.24	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1295	C	N3-C2-O2	-5.31	118.18	121.90
23	A	181	G	N3-C4-N9	-5.31	122.81	126.00
23	A	1431	U	O4'-C1'-N1	-5.31	103.95	108.20
23	A	574	A	C5-N7-C8	-5.31	101.25	103.90
23	A	2302	C	C6-N1-C2	-5.31	118.18	120.30
23	A	767	A	C4-C5-N7	5.31	113.35	110.70
1	a	461	C	C5-C4-N4	-5.30	116.49	120.20
23	A	1663	G	C4-N9-C1'	5.30	133.40	126.50
23	A	2327	A	C5-C6-N6	-5.30	119.46	123.70
23	A	603	C	N3-C2-O2	-5.30	118.19	121.90
1	a	1304	G	N9-C4-C5	-5.30	103.28	105.40
23	A	178	A	C6-C5-N7	-5.30	128.59	132.30
23	A	186	C	N3-C2-O2	-5.30	118.19	121.90
23	A	685	C	N1-C2-O2	5.30	122.08	118.90
23	A	1934	G	C4-C5-N7	5.30	112.92	110.80
23	A	2456	G	C8-N9-C1'	-5.30	120.11	127.00
1	a	168	G	N3-C2-N2	5.30	123.61	119.90
23	A	656	G	N3-C4-N9	-5.30	122.82	126.00
23	A	1051	C	N3-C4-C5	5.29	124.02	121.90
23	A	1690	A	N1-C6-N6	5.29	121.77	118.60
23	A	548	A	C5-N7-C8	-5.29	101.25	103.90
1	a	905	A	C5-C6-N1	5.29	120.34	117.70
1	a	1353	C	N1-C2-O2	5.29	122.07	118.90
23	A	1950	U	C6-N1-C2	-5.29	117.83	121.00
23	A	2452	A	N9-C4-C5	5.29	107.91	105.80
1	a	168	G	C5-N7-C8	-5.28	101.66	104.30
23	A	1004	A	C6-N1-C2	-5.28	115.43	118.60
23	A	732	C	N3-C4-C5	5.28	124.01	121.90
1	a	1208	A	N9-C4-C5	-5.28	103.69	105.80
23	A	1274	G	C2-N3-C4	-5.28	109.26	111.90
1	a	493	G	N3-C4-N9	-5.28	122.83	126.00
1	a	614	G	N3-C4-N9	-5.28	122.83	126.00
23	A	436	A	N9-C4-C5	-5.28	103.69	105.80
23	A	2707	C	N1-C2-O2	5.27	122.06	118.90
23	A	1382	C	C2-N1-C1'	5.27	124.59	118.80
23	A	2385	A	N9-C4-C5	-5.27	103.69	105.80
23	A	2471	G	C8-N9-C1'	-5.27	120.16	127.00
1	a	1439	A	C4-C5-N7	5.26	113.33	110.70
23	A	1347	G	N1-C2-N3	5.26	127.06	123.90
24	B	114	C	C2-N1-C1'	5.26	124.59	118.80
1	a	415	A	C4-C5-N7	5.26	113.33	110.70
37	T	53	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2001	C	C5-C4-N4	-5.26	116.52	120.20
23	A	2275	C	N3-C4-N4	5.26	121.68	118.00
23	A	38	A	C6-N1-C2	-5.25	115.45	118.60
1	a	588	C	C5-C4-N4	-5.25	116.52	120.20
1	a	100	A	C5-N7-C8	-5.25	101.27	103.90
23	A	863	G	C4-N9-C1'	5.25	133.33	126.50
23	A	1815	C	N1-C2-O2	5.25	122.05	118.90
23	A	2706	A	C6-C5-N7	-5.25	128.63	132.30
23	A	567	G	C6-C5-N7	-5.24	127.25	130.40
23	A	862	C	C5-C4-N4	-5.24	116.53	120.20
1	a	355	G	C8-N9-C4	5.24	108.50	106.40
23	A	1932	C	C2-N3-C4	-5.24	117.28	119.90
23	A	2422	C	N1-C2-O2	5.24	122.05	118.90
23	A	1731	G	N3-C4-C5	5.24	131.22	128.60
23	A	729	G	N1-C2-N2	-5.24	111.48	116.20
23	A	872	U	C6-N1-C2	-5.24	117.86	121.00
46	2	10	ARG	NE-CZ-NH1	5.24	122.92	120.30
23	A	1919	C	N1-C2-O2	5.24	122.04	118.90
23	A	2654	G	N7-C8-N9	5.23	115.72	113.10
1	a	1099	G	C2-N3-C4	-5.23	109.28	111.90
23	A	341	G	N3-C4-C5	5.23	131.22	128.60
1	a	34	A	N7-C8-N9	5.23	116.42	113.80
23	A	908	A	C4-C5-N7	5.23	113.31	110.70
23	A	1453	G	N3-C2-N2	5.23	123.56	119.90
23	A	2064	A	C5-C6-N6	-5.23	119.52	123.70
23	A	1400	C	N1-C2-O2	5.22	122.03	118.90
23	A	2816	C	O4'-C1'-N1	5.22	112.38	108.20
1	a	1434	G	N3-C4-N9	-5.22	122.87	126.00
23	A	988	C	C5-C4-N4	-5.21	116.55	120.20
23	A	2788	A	C5-C6-N1	5.21	120.31	117.70
1	a	196	A	C5-C6-N6	-5.21	119.53	123.70
23	A	923	A	O4'-C1'-N9	5.21	112.37	108.20
23	A	2543	G	C4-N9-C1'	5.21	133.28	126.50
23	A	1035	C	N1-C2-O2	5.21	122.03	118.90
23	A	1202	C	C5-C4-N4	-5.21	116.55	120.20
23	A	1812	A	C5-C6-N1	5.21	120.30	117.70
23	A	2849	A	C5-C6-N6	-5.21	119.53	123.70
25	D	197	LEU	CB-CG-CD1	-5.21	102.15	111.00
23	A	1517	A	N9-C4-C5	-5.20	103.72	105.80
23	A	2074	C	C6-N1-C2	-5.20	118.22	120.30
23	A	2278	G	N3-C4-C5	5.20	131.20	128.60
1	a	876	C	N3-C4-C5	5.20	123.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	O	64	ARG	NE-CZ-NH2	5.20	122.90	120.30
23	A	777	C	N3-C2-O2	-5.20	118.26	121.90
23	A	1951	C	C6-N1-C2	-5.20	118.22	120.30
23	A	500	A	C5-N7-C8	-5.19	101.30	103.90
23	A	601	G	C5-N7-C8	-5.19	101.70	104.30
23	A	939	U	C5-C4-O4	5.19	129.01	125.90
23	A	136	A	N1-C6-N6	5.19	121.71	118.60
23	A	670	G	N3-C4-C5	5.19	131.19	128.60
23	A	2878	U	O4'-C1'-N1	-5.19	104.05	108.20
23	A	1695	G	N3-C2-N2	5.19	123.53	119.90
23	A	1735	C	N1-C2-O2	5.18	122.01	118.90
23	A	1352	C	N1-C2-O2	5.18	122.01	118.90
1	a	1513	C	N3-C2-O2	-5.18	118.27	121.90
23	A	727	G	C2-N3-C4	-5.18	109.31	111.90
23	A	1596	G	N3-C2-N2	-5.18	116.28	119.90
23	A	2715	G	N3-C4-C5	5.18	131.19	128.60
23	A	518	A	C5-C6-N6	-5.18	119.56	123.70
23	A	1148	C	N1-C2-O2	5.18	122.01	118.90
1	a	933	A	N1-C6-N6	5.18	121.71	118.60
23	A	241	C	C2-N1-C1'	5.18	124.49	118.80
23	A	2214	G	N9-C4-C5	-5.17	103.33	105.40
1	a	1439	A	N1-C6-N6	5.17	121.70	118.60
23	A	1361	G	C8-N9-C4	-5.17	104.33	106.40
23	A	1414	G	C6-C5-N7	-5.17	127.30	130.40
23	A	1328	C	C5-C4-N4	-5.17	116.58	120.20
23	A	1596	G	N3-C4-N9	-5.17	122.90	126.00
23	A	2104	A	C5-N7-C8	-5.17	101.32	103.90
23	A	668	C	N3-C2-O2	-5.17	118.28	121.90
23	A	2610	G	C2-N3-C4	-5.16	109.32	111.90
1	a	805	C	N3-C2-O2	-5.16	118.29	121.90
23	A	2706	A	N9-C4-C5	-5.16	103.74	105.80
23	A	1278	G	C8-N9-C4	-5.16	104.34	106.40
23	A	574	A	C5-C6-N6	-5.15	119.58	123.70
1	a	342	C	N1-C2-O2	5.15	121.99	118.90
23	A	548	A	N7-C8-N9	5.15	116.38	113.80
23	A	668	C	C2-N1-C1'	5.15	124.47	118.80
23	A	1802	U	C6-N1-C2	-5.15	117.91	121.00
23	A	2035	C	C5-C4-N4	-5.15	116.59	120.20
23	A	809	A	C6-N1-C2	-5.15	115.51	118.60
23	A	2493	C	C5-C4-N4	-5.15	116.60	120.20
1	a	316	C	N3-C2-O2	-5.14	118.30	121.90
23	A	448	A	C5-C6-N6	-5.14	119.58	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	547	A	C5-C6-N6	-5.14	119.58	123.70
23	A	593	U	P-O3'-C3'	5.14	125.87	119.70
23	A	624	C	C2-N1-C1'	5.14	124.46	118.80
23	A	1714	C	N3-C4-C5	5.14	123.96	121.90
23	A	2104	A	C4-C5-N7	5.14	113.27	110.70
23	A	1098	A	N1-C6-N6	-5.14	115.52	118.60
1	a	208	U	C2-N3-C4	5.14	130.08	127.00
1	a	1247	A	N1-C6-N6	5.13	121.68	118.60
1	a	955	G	N3-C2-N2	5.13	123.49	119.90
23	A	844	G	C2-N3-C4	-5.13	109.33	111.90
11	k	111	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	a	750	G	N3-C4-C5	5.13	131.16	128.60
2	b	214	THR	CA-CB-CG2	5.13	119.58	112.40
23	A	2578	C	N3-C2-O2	-5.12	118.31	121.90
23	A	809	A	C5-C6-N1	5.12	120.26	117.70
23	A	2729	G	N3-C4-N9	5.12	129.07	126.00
24	B	96	G	C4-N9-C1'	5.12	133.16	126.50
24	B	111	A	O4'-C1'-N9	5.12	112.30	108.20
23	A	1414	G	N3-C2-N2	5.12	123.48	119.90
23	A	2639	C	C2-N1-C1'	5.12	124.43	118.80
1	a	834	C	N1-C2-O2	5.11	121.97	118.90
23	A	1963	A	N1-C6-N6	5.11	121.67	118.60
23	A	2540	A	N1-C6-N6	5.11	121.67	118.60
23	A	2456	G	C5-C6-O6	-5.11	125.53	128.60
23	A	777	C	N1-C2-O2	5.11	121.97	118.90
24	B	81	A	C5-C6-N6	-5.11	119.61	123.70
1	a	235	G	N9-C4-C5	-5.11	103.36	105.40
23	A	967	C	N1-C2-O2	5.11	121.96	118.90
23	A	1282	A	C5-C6-N1	5.11	120.25	117.70
23	A	1632	A	O4'-C1'-N9	-5.11	104.11	108.20
23	A	1650	G	C2-N3-C4	-5.11	109.35	111.90
23	A	2698	A	C4-C5-N7	5.11	113.25	110.70
1	a	1439	A	N9-C4-C5	-5.11	103.76	105.80
23	A	2706	A	N1-C6-N6	5.11	121.66	118.60
23	A	674	C	N3-C4-C5	5.10	123.94	121.90
1	a	1544	U	C2-N1-C1'	5.10	123.82	117.70
23	A	44	A	C4-C5-N7	5.10	113.25	110.70
23	A	863	G	C8-N9-C1'	-5.10	120.37	127.00
23	A	2074	C	N3-C2-O2	-5.10	118.33	121.90
23	A	757	G	N3-C4-N9	-5.10	122.94	126.00
23	A	2539	C	N1-C2-O2	5.10	121.96	118.90
1	a	242	C	N1-C2-O2	5.10	121.96	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2069	A	N1-C6-N6	5.10	121.66	118.60
23	A	2718	C	N1-C2-O2	5.10	121.96	118.90
23	A	774	G	C4-N9-C1'	5.10	133.13	126.50
23	A	2887	G	O4'-C1'-N9	5.10	112.28	108.20
1	a	544	C	N1-C2-O2	5.09	121.96	118.90
23	A	37	C	C5-C4-N4	-5.09	116.63	120.20
23	A	868	A	C5-C6-N6	-5.09	119.62	123.70
23	A	1834	G	C2-N3-C4	-5.09	109.35	111.90
23	A	2633	C	N3-C4-C5	5.09	123.94	121.90
23	A	1310	A	C5-C6-N6	-5.09	119.63	123.70
23	A	725	A	C5-C6-N6	-5.09	119.63	123.70
23	A	724	C	N3-C4-N4	5.09	121.56	118.00
23	A	1408	G	C2-N3-C4	-5.09	109.36	111.90
23	A	1419	A	C5-N7-C8	-5.08	101.36	103.90
1	a	1101	G	N1-C6-O6	-5.08	116.85	119.90
1	a	1353	C	N3-C2-O2	-5.08	118.34	121.90
2	b	214	THR	OG1-CB-CG2	5.08	121.69	110.00
23	A	1294	G	N1-C6-O6	-5.08	116.85	119.90
23	A	1533	A	O4'-C1'-N9	5.08	112.27	108.20
23	A	1934	G	N9-C4-C5	-5.08	103.37	105.40
23	A	2900	C	N1-C2-O2	5.08	121.95	118.90
23	A	348	C	C2-N1-C1'	5.08	124.39	118.80
23	A	1880	A	C5-N7-C8	-5.08	101.36	103.90
23	A	2378	G	C2-N3-C4	-5.08	109.36	111.90
23	A	2048	G	C8-N9-C1'	-5.08	120.40	127.00
23	A	859	C	C5-C4-N4	-5.07	116.65	120.20
23	A	2816	C	N3-C2-O2	-5.07	118.35	121.90
23	A	574	A	N7-C8-N9	5.07	116.33	113.80
23	A	1399	C	N3-C4-C5	5.07	123.93	121.90
23	A	2214	G	C6-C5-N7	-5.07	127.36	130.40
23	A	2744	G	N1-C2-N2	-5.07	111.64	116.20
23	A	2839	A	C5-C6-N6	-5.07	119.64	123.70
1	a	837	A	C5-C6-N6	-5.07	119.64	123.70
23	A	250	G	C2-N3-C4	-5.07	109.36	111.90
23	A	1801	C	C5-C4-N4	-5.07	116.65	120.20
1	a	456	A	N1-C6-N6	-5.07	115.56	118.60
23	A	492	G	N3-C2-N2	5.07	123.45	119.90
23	A	2642	U	N3-C4-O4	5.07	122.95	119.40
1	a	234	A	N9-C4-C5	-5.07	103.77	105.80
23	A	461	A	N7-C8-N9	5.06	116.33	113.80
23	A	515	G	C6-C5-N7	-5.06	127.36	130.40
23	A	1118	G	N3-C4-N9	-5.06	122.96	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2056	G	N7-C8-N9	5.06	115.63	113.10
1	a	208	U	C2-N1-C1'	5.06	123.77	117.70
23	A	1708	A	N1-C6-N6	5.06	121.64	118.60
23	A	2087	A	O4'-C1'-N9	5.06	112.25	108.20
23	A	2452	A	C5-C6-N1	5.06	120.23	117.70
1	a	683	A	N1-C6-N6	5.06	121.63	118.60
23	A	6	A	C5-N7-C8	-5.06	101.37	103.90
23	A	555	C	C2-N1-C1'	5.06	124.36	118.80
23	A	862	C	N3-C4-N4	5.06	121.54	118.00
23	A	740	G	N3-C4-N9	-5.06	122.97	126.00
23	A	16	G	C2-N3-C4	-5.05	109.37	111.90
23	A	1826	G	N3-C4-N9	-5.05	122.97	126.00
23	A	2078	A	C5-C6-N6	-5.05	119.66	123.70
23	A	2317	G	C4-N9-C1'	5.05	133.07	126.50
23	A	20	C	N1-C2-O2	5.05	121.93	118.90
23	A	495	A	N9-C4-C5	-5.05	103.78	105.80
23	A	2475	A	C5-C6-N6	-5.05	119.66	123.70
23	A	136	A	N9-C4-C5	-5.05	103.78	105.80
23	A	436	A	C4-C5-N7	5.05	113.22	110.70
23	A	683	G	N7-C8-N9	5.05	115.62	113.10
1	a	406	C	N1-C2-O2	5.04	121.93	118.90
1	a	1541	G	C5-N7-C8	-5.04	101.78	104.30
23	A	767	A	C5-C6-N6	-5.04	119.67	123.70
23	A	1315	C	N1-C2-O2	5.04	121.92	118.90
23	A	2091	C	C2-N1-C1'	5.04	124.34	118.80
23	A	2264	G	C2-N3-C4	-5.04	109.38	111.90
23	A	2628	C	C6-N1-C1'	-5.04	114.75	120.80
23	A	1781	C	C5-C4-N4	-5.04	116.67	120.20
1	a	221	U	C6-N1-C2	-5.04	117.98	121.00
7	g	101	LEU	CA-CB-CG	5.04	126.88	115.30
23	A	1080	G	C2-N3-C4	-5.04	109.38	111.90
23	A	2097	G	N1-C2-N2	-5.04	111.67	116.20
23	A	2214	G	C4-C5-N7	5.04	112.81	110.80
24	B	86	C	C6-N1-C2	-5.03	118.29	120.30
23	A	1435	C	N3-C4-N4	5.03	121.52	118.00
1	a	1406	C	C5-C4-N4	-5.03	116.68	120.20
24	B	96	G	N1-C2-N2	-5.03	111.67	116.20
23	A	2823	G	C8-N9-C1'	5.03	133.54	127.00
23	A	875	G	N3-C2-N2	-5.03	116.38	119.90
23	A	2794	C	N1-C2-O2	5.03	121.92	118.90
23	A	2845	G	N3-C4-C5	5.03	131.11	128.60
23	A	1335	C	N1-C2-O2	5.03	121.92	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2540	A	C4-C5-N7	5.03	113.21	110.70
23	A	92	G	N3-C4-N9	-5.02	122.98	126.00
23	A	1414	G	C2-N3-C4	-5.02	109.39	111.90
23	A	2843	A	C5-C6-N1	5.02	120.21	117.70
1	a	252	U	N1-C2-O2	5.02	126.31	122.80
23	A	178	A	C5-C6-N6	-5.02	119.68	123.70
23	A	422	G	N7-C8-N9	5.02	115.61	113.10
23	A	2348	G	C4-N9-C1'	5.02	133.02	126.50
23	A	2815	C	C2-N1-C1'	5.02	124.32	118.80
23	A	1486	C	N3-C4-N4	-5.02	114.49	118.00
23	A	1658	A	C5-N7-C8	-5.01	101.39	103.90
23	A	2005	A	C5-N7-C8	-5.01	101.39	103.90
23	A	1386	U	O4'-C1'-N1	5.01	112.21	108.20
23	A	2610	G	N3-C4-C5	5.01	131.11	128.60
1	a	588	C	N1-C2-O2	5.01	121.91	118.90
1	a	1513	C	N1-C2-O2	5.01	121.91	118.90
23	A	1213	C	C6-N1-C2	-5.01	118.30	120.30
23	A	2698	A	C5-C6-N6	-5.01	119.69	123.70
7	g	95	ARG	NE-CZ-NH1	5.01	122.80	120.30
23	A	912	C	C5-C4-N4	-5.01	116.69	120.20
1	a	933	A	C4-C5-N7	5.01	113.20	110.70
23	A	545	G	C2-N3-C4	-5.01	109.40	111.90
23	A	1656	C	C2-N1-C1'	5.01	124.31	118.80
1	a	816	C	N1-C2-O2	5.00	121.90	118.90
23	A	37	C	N1-C2-O2	5.00	121.90	118.90
23	A	1370	C	N3-C4-N4	5.00	121.50	118.00
24	B	111	A	C4-C5-N7	5.00	113.20	110.70
23	A	2259	C	N1-C2-O2	5.00	121.90	118.90
23	A	2090	C	N3-C4-C5	5.00	123.90	121.90
23	A	2443	C	C5-C4-N4	-5.00	116.70	120.20
24	B	111	A	C5-N7-C8	-5.00	101.40	103.90

There are no chirality outliers.

All (65) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	2	17	GLU	Peptide
47	3	11	GLN	Peptide
47	3	13	ILE	Peptide
47	3	42	GLU	Peptide
50	6	15	LYS	Peptide
50	6	7	GLN	Peptide

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Mol	Chain	Res	Type	Group
51	7	28	PHE	Peptide
51	7	33	PHE	Peptide
25	D	120	GLU	Peptide
25	D	214	GLY	Peptide
26	E	140	PRO	Peptide
26	E	141	MET	Peptide
26	E	142	SER	Peptide
26	E	200	ASN	Peptide
26	E	9	LYS	Peptide
27	F	154	VAL	Peptide
27	F	155	VAL	Peptide
30	M	40	LYS	Peptide
31	N	23	LYS	Peptide
32	O	110	LYS	Peptide
32	O	35	HIS	Peptide
32	O	58	PHE	Peptide
32	O	65	GLY	Peptide
33	P	134	ARG	Sidechain
33	P	90	VAL	Peptide
33	P	98	LYS	Peptide
35	R	110	GLU	Peptide
35	R	29	PRO	Peptide
35	R	89	ILE	Peptide
36	S	103	ARG	Peptide
36	S	105	LEU	Peptide
37	T	85	LYS	Peptide
38	U	100	ILE	Peptide
41	X	77	GLU	Peptide
43	Z	82	ARG	Peptide
2	b	19	GLN	Peptide
2	b	21	ARG	Peptide
3	c	160	ASP	Peptide
4	d	160	PHE	Peptide
4	d	93	ARG	Peptide
5	e	108	GLY	Peptide
6	f	81	LYS	Peptide
7	g	13	LEU	Peptide
7	g	14	PRO	Peptide
7	g	146	GLU	Peptide
7	g	73	LEU	Peptide
7	g	8	PRO	Peptide
7	g	9	LYS	Peptide

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Mol	Chain	Res	Type	Group
11	k	53	LYS	Peptide
12	l	109	HIS	Peptide
12	l	23	ALA	Peptide
12	l	32	LYS	Peptide
13	m	44	ARG	Peptide
14	n	18	VAL	Peptide
14	n	54	PRO	Peptide
17	q	4	ARG	Peptide
17	q	72	THR	Peptide
19	s	40	ILE	Peptide
22	v	47	TYR	Peptide
22	v	49	ASN	Peptide
22	v	50	SER	Peptide
22	v	51	ALA	Peptide
22	v	66	ARG	Sidechain
22	v	87	ARG	Sidechain
22	v	98	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33006	0	16615	0	0
2	b	1788	0	1847	0	0
3	c	1600	0	1662	0	0
4	d	1600	0	1628	0	0
5	e	1194	0	1255	0	0
6	f	781	0	784	0	0
7	g	1142	0	1171	0	0
8	h	1032	0	1082	0	0
9	i	1017	0	1039	0	0
10	j	791	0	829	0	0
11	k	851	0	864	0	0
12	l	1058	0	1130	0	0
13	m	877	0	919	0	0
14	n	502	0	527	0	0
15	o	738	0	769	0	0
16	p	712	0	744	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	q	698	0	738	0	0
18	r	466	0	496	0	0
19	s	677	0	672	0	0
20	t	606	0	650	0	0
21	u	377	0	404	0	0
22	v	831	0	846	0	0
23	A	62480	0	31402	558	0
24	B	2430	0	1229	26	0
25	D	2103	0	2220	37	0
26	E	1649	0	1689	27	0
27	F	1524	0	1570	22	0
28	G	1311	0	1366	4	0
29	H	1284	0	1301	25	0
30	M	1151	0	1145	16	0
31	N	920	0	981	13	0
32	O	997	0	1044	10	0
33	P	1065	0	1122	24	0
34	Q	924	0	970	21	0
35	R	922	0	968	25	0
36	S	862	0	932	18	0
37	T	943	0	1014	16	0
38	U	799	0	836	12	0
39	V	862	0	920	14	0
40	W	725	0	761	11	0
41	X	668	0	725	8	0
42	Y	738	0	785	44	0
43	Z	591	0	602	29	0
44	0	373	0	407	5	0
45	1	536	0	567	9	0
46	2	441	0	478	5	0
47	3	663	0	644	17	0
48	4	360	0	385	11	0
49	5	229	0	224	12	0
50	6	373	0	420	13	0
51	7	487	0	548	11	0
52	8	297	0	342	7	0
All	All	141051	0	94268	929	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 9.

All (929) 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)
33:P:48:GLU:HG3	33:P:51:ARG:NH1	1.22	1.50
23:A:373:A:N7	23:A:1248:U:C4	2.00	1.30
42:Y:21:LEU:CD1	42:Y:42:LYS:HE3	1.60	1.28
42:Y:21:LEU:HD12	42:Y:42:LYS:CE	1.64	1.26
33:P:48:GLU:CG	33:P:51:ARG:NH1	2.01	1.22
42:Y:21:LEU:CD1	42:Y:42:LYS:CE	2.17	1.22
42:Y:22:ARG:NH2	42:Y:87:THR:HG23	1.60	1.15
33:P:48:GLU:CG	33:P:51:ARG:HH11	1.60	1.09
42:Y:21:LEU:CD1	42:Y:42:LYS:CD	2.32	1.08
23:A:2287:C:N4	43:Z:22:ARG:HD3	1.68	1.08
23:A:275:A:N6	23:A:296:G:C2	2.22	1.07
23:A:1583:G:OP1	23:A:1584:A:C8	2.09	1.05
49:5:35:PHE:CD1	49:5:36:CYS:N	2.25	1.04
23:A:1496:G:N7	23:A:1501:G:N1	2.06	1.03
23:A:1584:A:P	23:A:1585:G:H8	1.82	1.02
42:Y:21:LEU:HD11	42:Y:42:LYS:CD	1.87	1.02
43:Z:27:LYS:HG3	43:Z:29:LEU:HD11	1.43	1.01
42:Y:21:LEU:HD13	42:Y:42:LYS:HE3	1.38	1.01
42:Y:21:LEU:HD11	42:Y:42:LYS:CG	1.90	1.00
42:Y:25:GLY:O	42:Y:44:ASP:HA	1.62	0.99
42:Y:21:LEU:HD11	42:Y:42:LYS:HG2	1.42	0.99
49:5:35:PHE:HD1	49:5:36:CYS:H	0.99	0.93
33:P:48:GLU:HG3	33:P:51:ARG:HH11	1.12	0.92
23:A:1307:G:H1	23:A:2038:U:H3	1.15	0.92
23:A:2695:G:HO2'	29:H:111:HIS:HE2	1.01	0.92
23:A:1584:A:OP1	23:A:1585:G:H8	1.55	0.90
23:A:2288:C:OP2	43:Z:24:SER:OG	1.86	0.90
23:A:1584:A:OP1	23:A:1585:G:C8	2.25	0.90
43:Z:27:LYS:HG3	43:Z:29:LEU:CD1	2.02	0.89
33:P:48:GLU:HG3	33:P:51:ARG:HH12	1.31	0.89
23:A:1086:G:O6	23:A:1157:U:C4	2.28	0.87
23:A:1584:A:O5'	23:A:1585:G:C8	2.26	0.87
23:A:1121:A:O2'	23:A:1122:U:O4'	1.92	0.86
42:Y:21:LEU:HD12	42:Y:42:LYS:CD	2.02	0.86
23:A:373:A:N7	23:A:1248:U:O4	2.08	0.84
42:Y:21:LEU:HD12	42:Y:42:LYS:HE2	1.59	0.84
42:Y:21:LEU:CD1	42:Y:42:LYS:HD3	2.06	0.84
23:A:1302:G:OP1	48:4:16:ARG:NH1	2.11	0.83
23:A:2287:C:H42	43:Z:22:ARG:HD3	1.36	0.83
49:5:35:PHE:CE1	49:5:37:SER:N	2.46	0.83
23:A:1584:A:O5'	23:A:1585:G:H8	1.59	0.83
24:B:64:A:N6	24:B:105:G:O4'	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1851:G:OP2	25:D:52:HIS:NE2	2.11	0.82
23:A:2581:U:O2'	23:A:2582:U:O4'	1.97	0.82
23:A:263:G:C2	23:A:264:G:H1'	2.15	0.82
23:A:2868:G:H21	23:A:2888:A:H62	1.24	0.81
23:A:1591:G:O2'	23:A:1592:A:O4'	1.98	0.81
47:3:9:TYR:OH	47:3:24:LEU:O	1.99	0.81
23:A:1491:C:O2	23:A:1574:G:N2	2.14	0.80
23:A:1583:G:OP1	23:A:1584:A:H8	1.64	0.80
23:A:2332:U:O2'	23:A:2333:U:O4'	1.99	0.80
23:A:1806:U:OP2	23:A:1811:A:N6	2.15	0.80
23:A:1584:A:P	23:A:1585:G:C8	2.73	0.79
23:A:373:A:N7	23:A:1248:U:N3	2.31	0.79
23:A:84:A:N6	23:A:99:U:O4'	2.15	0.79
23:A:198:A:N6	23:A:201:C:OP2	2.16	0.79
23:A:955:A:N3	23:A:2291:C:O2'	2.15	0.79
23:A:1323:A:O2'	23:A:1325:U:OP2	2.01	0.79
24:B:7:G:OP1	35:R:19:ARG:NH1	2.15	0.79
23:A:1490:G:O6	23:A:1595:C:N4	2.15	0.79
23:A:1652:A:O2'	23:A:1654:A:OP2	1.99	0.79
23:A:2260:A:N6	23:A:2261:G:O6	2.16	0.79
23:A:1533:A:O2'	25:D:97:ASP:OD1	2.01	0.79
23:A:2127:G:O6	23:A:2216:U:O2	2.00	0.79
23:A:2060:A:O2'	23:A:2062:G:OP2	1.99	0.78
23:A:2260:A:H2'	23:A:2261:G:C8	2.18	0.78
23:A:674:C:O2	23:A:684:U:O2'	2.01	0.78
23:A:2442:G:O2'	32:O:60:ARG:NH1	2.17	0.78
42:Y:14:THR:O	42:Y:18:LEU:CD2	2.32	0.78
24:B:72:U:O2	42:Y:38:ASN:ND2	2.17	0.77
24:B:57:G:O2'	35:R:6:ASP:OD1	2.01	0.77
23:A:2682:G:O2'	23:A:2691:G:O6	2.03	0.77
23:A:1499:U:O4	23:A:2731:C:N4	2.17	0.77
43:Z:27:LYS:O	43:Z:28:ARG:HB2	1.83	0.77
26:E:9:LYS:NZ	26:E:201:VAL:O	2.16	0.77
23:A:1116:C:O2'	23:A:1138:U:O2	2.02	0.77
26:E:187:GLN:HB2	26:E:196:LEU:HD12	1.67	0.77
23:A:1051:C:OP1	30:M:38:ARG:NH1	2.18	0.77
23:A:1843:U:O4	25:D:34:LYS:NZ	2.18	0.76
23:A:273:A:OP2	23:A:297:G:N2	2.19	0.76
23:A:2649:U:O2'	23:A:2845:G:N2	2.16	0.76
23:A:59:U:O2'	23:A:74:U:OP2	2.02	0.76
24:B:53:U:O2	24:B:55:A:N6	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1079:U:N3	23:A:1164:G:O6	2.18	0.76
23:A:2287:C:N4	43:Z:22:ARG:CD	2.48	0.76
23:A:275:A:C6	23:A:296:G:N2	2.54	0.76
43:Z:27:LYS:CG	43:Z:29:LEU:HD11	2.16	0.76
23:A:2102:U:OP2	23:A:2265:G:O2'	2.04	0.76
23:A:2550:G:O2'	23:A:2791:A:O2'	2.04	0.76
24:B:9:C:O2'	24:B:13:A:N6	2.18	0.76
23:A:2146:A:N6	23:A:2197:G:O6	2.19	0.76
23:A:614:U:O5'	23:A:2057:A:N6	2.18	0.76
27:F:21:ASP:O	27:F:25:GLY:N	2.19	0.76
23:A:269:G:N2	23:A:323:C:O2	2.18	0.75
23:A:923:A:O2'	23:A:924:G:OP2	2.04	0.75
23:A:2187:G:N2	23:A:2200:A:O2'	2.19	0.75
23:A:373:A:C5	23:A:1248:U:C4	2.74	0.75
23:A:2404:A:O2'	35:R:119:PHE:OXT	2.03	0.75
23:A:328:G:N1	23:A:399:U:O2	2.18	0.75
23:A:373:A:C5	23:A:1248:U:N3	2.54	0.75
35:R:71:GLU:O	35:R:74:THR:OG1	2.04	0.75
23:A:2033:C:O2'	23:A:2843:A:N3	2.20	0.75
23:A:815:G:OP1	50:6:9:ASN:ND2	2.19	0.75
52:8:2:LYS:NZ	52:8:31:LYS:O	2.20	0.75
23:A:1265:G:N7	37:T:16:LYS:NZ	2.35	0.75
23:A:1379:A:O2'	23:A:1381:U:OP2	2.03	0.75
23:A:922:G:N2	23:A:945:A:N7	2.31	0.75
23:A:2673:C:OP2	23:A:2759:G:O2'	2.05	0.75
23:A:1880:A:N6	23:A:1916:A:N7	2.36	0.74
23:A:263:G:H5''	23:A:666:A:H1'	1.68	0.74
33:P:35:GLN:NE2	33:P:36:ALA:O	2.20	0.74
23:A:512:A:OP1	50:6:35:ARG:NH1	2.20	0.74
23:A:1101:A:N6	23:A:1131:G:OP2	2.21	0.74
23:A:1711:G:O2'	23:A:2018:U:O4	2.05	0.74
23:A:363:A:O2'	23:A:365:A:OP2	2.06	0.74
23:A:2124:U:O4	23:A:2219:C:N4	2.17	0.74
24:B:64:A:O2'	24:B:104:C:N4	2.20	0.74
23:A:2127:G:O6	23:A:2216:U:C2	2.41	0.74
23:A:608:C:N4	23:A:619:U:O4	2.20	0.74
23:A:1963:A:OP2	23:A:1989:C:N4	2.21	0.73
23:A:2530:A:O2'	23:A:2532:G:OP2	2.06	0.73
23:A:2821:U:OP2	23:A:2824:G:N2	2.21	0.73
24:B:100:A:HO2'	42:Y:32:TYR:HH	1.33	0.73
47:3:30:THR:OG1	47:3:33:GLU:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:116:G:OP2	23:A:118:A:O2'	2.04	0.73
23:A:1520:A:N6	23:A:1562:C:O2	2.20	0.73
23:A:2277:G:O2'	23:A:2523:C:OP1	2.06	0.73
23:A:865:A:N3	23:A:987:U:O2'	2.21	0.73
23:A:1546:A:O2'	23:A:1547:C:O4'	3.01	0.73
23:A:1306:C:O2	23:A:2040:A:C6	2.41	0.73
24:B:53:U:O2'	24:B:55:A:N7	2.21	0.73
36:S:16:ARG:NH2	36:S:80:THR:O	2.22	0.73
23:A:1423:C:O2'	23:A:1512:U:O2	2.04	0.72
23:A:2261:G:O2'	23:A:2262:G:H5'	1.88	0.72
23:A:2465:U:O2'	23:A:2467:C:OP1	2.06	0.72
23:A:2038:U:OP2	39:V:16:LYS:NZ	2.16	0.72
23:A:1306:C:C2	23:A:2040:A:C6	2.77	0.72
29:H:60:GLU:O	29:H:63:THR:OG1	2.06	0.72
23:A:418:G:O2'	23:A:446:G:O6	2.04	0.72
45:1:46:VAL:O	45:1:49:THR:OG1	2.08	0.72
47:3:33:GLU:O	47:3:51:SER:OG	2.07	0.72
23:A:261:U:O4'	23:A:283:G:N2	61.59	0.72
23:A:1891:U:OP1	23:A:2437:G:O2'	2.03	0.71
43:Z:41:GLY:N	43:Z:72:ASP:OD1	2.22	0.71
23:A:327:G:N7	23:A:400:C:O2'	2.23	0.71
23:A:1067:U:OP2	23:A:1069:G:O2'	2.08	0.71
23:A:1088:C:O2'	23:A:1155:A:N6	2.22	0.71
27:F:6:VAL:O	27:F:8:LYS:NZ	2.17	0.71
23:A:1131:G:N2	23:A:1134:U:O4'	2.24	0.71
42:Y:15:ARG:O	42:Y:18:LEU:HD23	1.91	0.71
51:7:34:ALA:O	51:7:38:THR:OG1	2.05	0.71
23:A:2647:C:O2'	26:E:170:PRO:O	2.09	0.71
42:Y:27:VAL:N	42:Y:43:VAL:O	2.23	0.71
23:A:1089:C:OP1	23:A:1090:A:O2'	2.05	0.70
42:Y:21:LEU:HD11	42:Y:42:LYS:HD3	1.68	0.70
23:A:1550:G:O2'	23:A:1551:U:O4'	2.09	0.70
23:A:2357:G:O3'	43:Z:52:LYS:NZ	2.24	0.70
42:Y:14:THR:HB	42:Y:18:LEU:HD22	1.72	0.70
45:1:17:GLN:O	45:1:20:SER:OG	2.10	0.70
23:A:1377:U:OP2	40:W:58:TYR:OH	2.08	0.70
23:A:1450:A:N6	23:A:1634:A:O2'	2.24	0.70
23:A:575:G:O2'	23:A:577:A:N7	2.22	0.70
23:A:1064:A:N1	23:A:1185:U:O2'	2.20	0.70
23:A:1357:G:OP2	23:A:1357:G:N2	2.20	0.70
23:A:2560:U:OP1	23:A:2692:A:O2'	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:263:G:N2	23:A:652:A:N3	2.38	0.69
49:5:35:PHE:CZ	49:5:37:SER:HA	2.27	0.69
23:A:1945:A:O2'	23:A:1946:A:OP2	2.07	0.69
30:M:28:ARG:O	30:M:31:SER:OG	2.10	0.69
23:A:1168:C:O2	52:8:36:GLN:NE2	2.25	0.69
23:A:1844:G:OP2	25:D:155:ARG:NH2	2.24	0.69
23:A:1306:C:C2	23:A:2040:A:N6	2.61	0.69
26:E:37:GLN:OE1	26:E:76:HIS:NE2	2.26	0.69
36:S:61:PHE:O	36:S:75:THR:OG1	2.05	0.69
23:A:1740:G:N2	23:A:2004:A:O2'	2.25	0.69
23:A:1835:U:O2'	23:A:1836:A:O5'	2.11	0.69
23:A:229:A:O2'	23:A:231:A:N1	2.23	0.69
23:A:790:G:O2'	23:A:793:G:O2'	2.08	0.69
23:A:1567:A:OP2	23:A:1568:U:O2'	2.07	0.69
37:T:48:ARG:NH2	37:T:49:ASP:OD1	2.24	0.69
23:A:1086:G:O2'	23:A:1113:A:N1	40.51	0.69
25:D:68:ARG:O	25:D:188:ARG:NH1	2.26	0.69
23:A:1892:U:O2'	23:A:1902:G:N2	2.26	0.68
23:A:1110:U:O2'	23:A:1113:A:N7	2.23	0.68
23:A:163:U:O2'	23:A:166:A:N6	2.26	0.68
23:A:2589:U:O2'	31:N:23:LYS:NZ	2.25	0.68
37:T:26:GLY:O	37:T:29:HIS:ND1	2.27	0.68
23:A:672:A:O4'	23:A:682:A:N6	2.27	0.68
38:U:22:VAL:O	38:U:93:THR:N	2.26	0.68
23:A:1134:U:O4	23:A:1145:U:O2'	2.11	0.68
23:A:1491:C:C2	23:A:1574:G:N2	2.60	0.68
23:A:2229:C:O2'	23:A:2231:C:OP1	2.11	0.68
23:A:263:G:C2'	23:A:264:G:O5'	2.41	0.68
23:A:2287:C:H41	43:Z:22:ARG:HD3	1.57	0.68
23:A:373:A:C8	23:A:1248:U:C4	2.79	0.68
23:A:643:G:N2	23:A:648:G:O2'	2.26	0.68
34:Q:24:LEU:O	34:Q:28:GLU:HA	1.92	0.68
23:A:1135:G:N2	23:A:1143:G:O2'	2.20	0.68
23:A:1885:G:O2'	23:A:1911:A:N6	2.27	0.67
23:A:572:C:O2'	23:A:573:A:OP2	2.10	0.67
23:A:242:U:O2'	23:A:667:G:O2'	2.12	0.67
23:A:275:A:N6	23:A:296:G:N2	2.41	0.67
23:A:606:G:OP1	38:U:78:ARG:NH2	2.27	0.67
23:A:2302:C:O2	43:Z:18:THR:HG22	1.94	0.67
23:A:2333:U:OP2	23:A:2334:G:N1	2.27	0.67
33:P:27:VAL:CG1	33:P:134:ARG:HD2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Y:3:SER:O	42:Y:62:GLU:N	2.27	0.67
23:A:1053:A:OP2	30:M:40:LYS:NZ	2.27	0.67
23:A:1631:G:O2'	23:A:1632:A:N1	2.26	0.67
27:F:152:VAL:HG12	27:F:190:ASP:OD2	1.95	0.67
49:5:36:CYS:SG	49:5:43:THR:OG1	2.51	0.67
23:A:246:U:OP2	51:7:8:ARG:NH1	2.28	0.67
23:A:2260:A:C6	23:A:2261:G:O6	2.48	0.67
23:A:2362:A:O2'	23:A:2364:G:N7	2.22	0.67
24:B:40:C:OP2	47:3:2:LYS:NZ	2.23	0.67
39:V:25:ARG:NH2	39:V:74:ALA:O	2.27	0.67
23:A:729:G:O6	23:A:819:A:O2'	2.06	0.67
42:Y:10:GLN:HE21	42:Y:14:THR:HG21	1.59	0.67
34:Q:32:THR:OG1	34:Q:33:THR:O	2.11	0.67
23:A:1452:C:H42	23:A:1632:A:H62	1.43	0.67
35:R:84:ALA:O	35:R:88:GLY:N	2.27	0.66
49:5:35:PHE:HD1	49:5:36:CYS:N	1.72	0.66
23:A:99:U:OP1	23:A:100:U:O2'	2.13	0.66
49:5:32:MET:SD	49:5:46:ARG:NH1	2.68	0.66
23:A:1086:G:O6	23:A:1157:U:O4	2.14	0.66
23:A:1518:G:O2'	23:A:1519:U:O5'	2.13	0.66
45:1:42:ARG:O	45:1:45:THR:OG1	2.12	0.66
23:A:1215:U:O2'	23:A:1217:U:O5'	2.08	0.66
23:A:1018:A:O4'	23:A:1225:G:N2	2.29	0.66
23:A:224:A:N1	23:A:268:A:O2'	2.27	0.66
23:A:731:U:O5'	50:6:12:LYS:NZ	2.29	0.66
23:A:263:G:N2	23:A:264:G:H1'	2.11	0.66
23:A:1138:U:N3	23:A:1291:A:OP1	106.84	0.65
48:4:28:THR:N	48:4:37:TYR:O	2.28	0.65
23:A:590:U:OP1	23:A:1257:G:O2'	2.13	0.65
33:P:48:GLU:HG2	33:P:51:ARG:HH11	1.54	0.65
23:A:2260:A:H2'	23:A:2261:G:H8	1.62	0.65
23:A:2869:G:OP1	36:S:95:ARG:NH2	2.29	0.65
41:X:24:ILE:HG22	41:X:25:ALA:H	1.61	0.65
37:T:18:ILE:O	37:T:21:ALA:N	2.30	0.65
40:W:13:THR:O	40:W:17:SER:OG	2.06	0.65
23:A:2161:A:N6	23:A:2184:G:C2	2.65	0.65
23:A:2822:C:O2'	23:A:2823:G:O4'	2.15	0.65
23:A:1039:C:O2'	37:T:93:LYS:NZ	2.30	0.65
23:A:1583:G:P	23:A:1584:A:H8	2.19	0.65
23:A:1651:C:N4	23:A:1666:A:OP2	2.30	0.65
23:A:1767:G:O2'	23:A:1768:C:O5'	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Y:25:GLY:O	42:Y:44:ASP:CA	2.42	0.64
23:A:1360:G:O2'	23:A:1361:G:O5'	2.13	0.64
23:A:319:G:N2	23:A:400:C:O2	2.30	0.64
42:Y:14:THR:O	42:Y:18:LEU:HD23	1.96	0.64
23:A:1135:G:O2'	23:A:1146:C:N3	2.30	0.64
23:A:2058:A:O2'	23:A:2481:G:N2	2.31	0.64
23:A:250:G:OP2	23:A:252:C:N4	2.29	0.64
23:A:312:A:O2'	23:A:313:U:O4'	2.11	0.64
42:Y:25:GLY:C	42:Y:44:ASP:OD1	2.36	0.64
45:1:10:THR:O	45:1:11:THR:OG1	2.12	0.64
23:A:1492:G:N3	23:A:1574:G:N2	2.46	0.64
23:A:616:G:N2	23:A:2058:A:OP1	2.28	0.64
23:A:618:A:OP2	23:A:2526:C:O2'	2.15	0.64
23:A:2715:G:OP1	23:A:2740:A:N6	2.31	0.64
42:Y:21:LEU:HD12	42:Y:42:LYS:HD3	1.73	0.64
23:A:2695:G:O2'	29:H:111:HIS:NE2	2.16	0.64
31:N:24:VAL:CG1	31:N:33:ALA:HB2	2.26	0.64
23:A:1288:G:OP2	32:O:21:ARG:NH1	2.30	0.64
23:A:1305:U:H5"	23:A:1306:C:OP2	1.98	0.64
23:A:1450:A:OP2	23:A:1634:A:N6	2.30	0.64
34:Q:18:ARG:NE	34:Q:65:THR:O	2.28	0.64
23:A:1733:A:OP2	23:A:1742:A:N6	2.31	0.64
23:A:2842:G:O2'	23:A:2844:U:OP2	2.14	0.64
23:A:925:G:N2	23:A:926:G:N7	2.46	0.64
23:A:107:G:OP2	23:A:107:G:N2	10.05	0.64
23:A:1018:A:O5'	23:A:1225:G:N2	2.31	0.64
23:A:674:C:O3'	23:A:694:G:N2	2.31	0.64
23:A:1320:G:N2	23:A:1366:U:O4	2.28	0.63
23:A:325:A:N6	23:A:402:C:O4'	2.31	0.63
23:A:562:C:OP1	48:4:13:LYS:NZ	2.30	0.63
23:A:1453:G:O3'	23:A:1455:U:N3	2.31	0.63
23:A:1128:A:N3	23:A:1149:U:O2'	2.23	0.63
23:A:2811:U:O2'	26:E:39:LYS:NZ	2.32	0.63
39:V:96:ILE:O	39:V:97:ASN:CB	3.77	0.63
23:A:1153:C:O2'	23:A:1154:G:O4'	2.15	0.63
39:V:96:ILE:O	39:V:97:ASN:HB2	4.40	0.63
23:A:1472:C:N4	23:A:1617:A:OP2	2.27	0.63
26:E:9:LYS:HZ3	26:E:201:VAL:HG23	1.64	0.62
23:A:582:G:O2'	23:A:599:A:N6	2.31	0.62
23:A:904:G:N2	23:A:962:A:OP2	2.32	0.62
29:H:99:GLN:O	29:H:102:ASP:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:315:C:N4	23:A:404:U:OP2	2.33	0.62
25:D:81:GLN:NE2	25:D:82:TYR:O	2.31	0.62
33:P:31:GLU:HA	33:P:134:ARG:HD3	1.80	0.62
34:Q:47:LEU:O	34:Q:51:GLY:N	2.31	0.62
27:F:112:SER:O	27:F:115:SER:OG	2.12	0.62
23:A:1938:U:O2'	23:A:1946:A:N6	2.32	0.62
23:A:2349:A:N6	23:A:2360:A:N7	2.47	0.62
23:A:2024:A:OP2	26:E:138:ARG:NH1	2.33	0.62
23:A:287:G:N2	23:A:288:C:O3'	2.33	0.62
42:Y:25:GLY:HA3	42:Y:44:ASP:OD1	2.00	0.62
23:A:275:A:C5	23:A:296:G:N2	2.68	0.62
23:A:1810:A:O2'	23:A:2634:G:O2'	2.16	0.62
23:A:2372:G:O6	23:A:2398:G:N2	2.29	0.62
26:E:2:THR:OG1	26:E:93:ASN:O	2.18	0.62
25:D:29:GLU:N	25:D:29:GLU:OE1	2.33	0.62
26:E:38:LYS:NZ	26:E:98:ALA:O	2.25	0.62
23:A:160:G:N2	23:A:167:U:OP2	2.33	0.61
39:V:31:GLU:O	39:V:34:ALA:N	2.33	0.61
23:A:263:G:H2'	23:A:264:G:O5'	1.99	0.61
23:A:545:G:N1	23:A:548:A:OP2	2.33	0.61
23:A:927:G:O6	23:A:939:U:N3	2.32	0.61
23:A:1979:A:N3	23:A:2587:C:O2'	2.24	0.61
23:A:1145:U:O2'	23:A:1147:A:OP2	2.19	0.61
23:A:661:U:OP1	27:F:106:ARG:NE	2.34	0.61
33:P:48:GLU:HG2	33:P:51:ARG:NH1	2.08	0.61
23:A:1401:G:N2	23:A:1404:A:OP2	2.33	0.61
23:A:2703:C:O2	23:A:2759:G:N2	2.33	0.61
23:A:1135:G:H21	23:A:1146:C:H41	1.49	0.61
23:A:2039:G:O2'	23:A:2040:A:O5'	2.14	0.61
23:A:1777:G:O2'	23:A:2880:A:N6	2.33	0.61
33:P:34:LEU:HD23	33:P:35:GLN:N	2.16	0.61
23:A:234:C:O2'	23:A:235:G:O4'	2.19	0.61
23:A:797:A:OP1	50:6:4:ARG:NH2	2.33	0.61
50:6:19:PHE:O	50:6:22:ARG:N	2.34	0.61
23:A:1091:G:N2	23:A:1154:G:O2'	2.33	0.61
23:A:614:U:O4'	23:A:2057:A:N6	2.34	0.61
23:A:1091:G:OP1	26:E:138:ARG:NH1	98.78	0.61
39:V:96:ILE:HG13	39:V:97:ASN:H	4.49	0.61
23:A:1952:C:O2'	23:A:1953:U:O4'	2.17	0.60
36:S:55:GLY:N	36:S:58:SER:OG	2.34	0.60
47:3:28:THR:HG22	47:3:30:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:P:75:THR:OG1	33:P:89:ALA:O	2.09	0.60
30:M:38:ARG:NH2	30:M:45:TYR:OH	2.35	0.60
30:M:65:PHE:O	30:M:66:THR:OG1	2.17	0.60
42:Y:14:THR:C	42:Y:18:LEU:HD23	2.22	0.60
23:A:902:A:OP1	43:Z:85:LYS:NZ	2.25	0.60
27:F:60:GLY:O	27:F:77:THR:OG1	2.19	0.60
23:A:1487:G:N2	23:A:1597:U:O2	2.35	0.60
33:P:48:GLU:CG	33:P:51:ARG:HH12	1.98	0.60
25:D:44:ASN:OD1	25:D:45:GLN:N	2.35	0.59
31:N:24:VAL:HG13	31:N:33:ALA:HB2	1.84	0.59
23:A:1306:C:O2	23:A:2040:A:N1	2.34	0.59
23:A:115:C:O2'	23:A:125:A:N3	2.32	0.59
23:A:161:A:N1	23:A:355:G:O2'	111.33	0.59
23:A:1462:G:H21	23:A:1626:A:H62	1.48	0.59
50:6:25:THR:O	50:6:28:GLY:N	2.35	0.59
23:A:1896:U:N3	23:A:1898:C:OP2	2.35	0.59
23:A:2260:A:C6	23:A:2261:G:C6	2.91	0.59
23:A:313:U:O2'	23:A:314:A:O4'	2.16	0.59
34:Q:18:ARG:O	34:Q:22:THR:HG22	2.03	0.59
23:A:1578:A:N6	23:A:1591:G:O6	2.34	0.59
23:A:1109:U:O2'	23:A:1117:A:N6	2.30	0.59
24:B:82:C:O2'	24:B:83:U:O5'	2.20	0.59
23:A:588:G:N2	23:A:589:U:O4	2.35	0.58
26:E:17:GLY:N	26:E:21:GLU:O	2.36	0.58
29:H:94:TYR:OH	29:H:160:LYS:O	2.21	0.58
35:R:55:GLN:O	35:R:83:LYS:NZ	2.21	0.58
23:A:2868:G:H8	36:S:97:ALA:HB2	1.68	0.58
47:3:1:MET:SD	47:3:2:LYS:N	2.77	0.58
36:S:7:ILE:O	36:S:11:THR:HG23	2.04	0.58
23:A:1038:C:OP2	37:T:54:LYS:NZ	2.36	0.58
43:Z:51:THR:HG21	43:Z:54:TYR:CD1	2.38	0.58
23:A:1250:G:O2'	23:A:1274:G:N1	2.35	0.58
23:A:1183:G:O2'	23:A:1187:A:N1	2.36	0.58
23:A:675:G:N2	23:A:678:A:OP2	2.30	0.58
23:A:138:U:N3	23:A:141:U:OP2	2.35	0.58
23:A:330:C:H42	23:A:337:A:H62	23.81	0.58
29:H:58:SER:O	29:H:62:ARG:NH1	2.37	0.57
31:N:71:ARG:NH1	31:N:72:ASN:OD1	2.37	0.57
38:U:88:HIS:NE2	38:U:90:GLN:OE1	2.34	0.57
40:W:51:ALA:HB1	40:W:81:THR:HG23	1.87	0.57
30:M:6:MET:SD	30:M:48:HIS:NE2	2.71	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1397:G:N2	23:A:2241:C:H42	2.03	0.57
23:A:2693:C:N4	29:H:108:GLY:O	2.37	0.57
26:E:158:SER:O	26:E:161:SER:OG	2.07	0.57
23:A:2112:C:H42	23:A:2261:G:H1	1.51	0.57
34:Q:100:TYR:O	34:Q:101:THR:OG1	2.21	0.57
50:6:3:LYS:HZ3	50:6:3:LYS:HB3	1.69	0.57
23:A:925:G:N1	23:A:941:A:C2	2.73	0.57
24:B:82:C:O2'	24:B:83:U:O4'	2.20	0.57
34:Q:52:LYS:NZ	34:Q:96:ARG:O	2.37	0.57
23:A:2772:C:O2'	29:H:139:GLU:O	2.16	0.57
23:A:677:A:O4'	32:O:60:ARG:NH2	2.37	0.57
42:Y:22:ARG:HH22	42:Y:87:THR:HG23	1.63	0.57
23:A:2683:U:O2	23:A:2692:A:N7	2.38	0.56
23:A:2302:C:O2	43:Z:18:THR:CG2	2.53	0.56
23:A:1518:G:HO2'	23:A:1519:U:P	2.28	0.56
23:A:510:U:O2'	23:A:511:G:O5'	2.23	0.56
33:P:54:MET:HG3	33:P:117:ALA:HB1	1.86	0.56
23:A:1927:A:O2'	23:A:1928:A:OP1	2.21	0.56
24:B:95:A:O2'	24:B:96:G:O4'	2.17	0.56
23:A:1360:G:HO2'	23:A:1361:G:P	2.28	0.56
26:E:9:LYS:O	26:E:11:GLY:N	2.39	0.56
23:A:272:C:O2'	34:Q:67:ARG:NH1	121.07	0.56
23:A:1063:U:O2'	23:A:1065:A:N7	2.35	0.56
23:A:2347:A:N6	23:A:2360:A:O2'	2.39	0.56
23:A:2860:U:H5''	34:Q:49:THR:HG21	1.88	0.56
23:A:329:A:O2'	23:A:330:C:O4'	4.46	0.56
47:3:12:VAL:HG22	47:3:13:ILE:H	1.70	0.56
23:A:2261:G:O5'	23:A:2261:G:H8	1.89	0.56
23:A:2777:A:O2'	23:A:2780:A:N6	2.39	0.56
36:S:55:GLY:O	36:S:58:SER:OG	2.22	0.56
23:A:1003:A:N3	23:A:2484:U:O2'	2.29	0.56
23:A:373:A:N6	23:A:1248:U:O4	2.38	0.56
23:A:1885:G:H2'	23:A:1910:G:H22	1.71	0.56
23:A:528:C:O2'	23:A:542:A:N1	2.39	0.56
23:A:510:U:O4	23:A:729:G:O2'	2.23	0.56
24:B:49:G:H5'	35:R:67:ALA:HB1	1.87	0.56
25:D:124:LYS:HB2	25:D:127:ASN:HD22	1.70	0.56
33:P:13:HIS:NE2	33:P:88:GLY:O	2.39	0.55
40:W:49:LYS:HD3	40:W:51:ALA:HB2	1.87	0.55
23:A:2905:C:H42	48:4:39:LEU:HD22	1.72	0.55
23:A:1306:C:H2'	23:A:1307:G:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1307:G:O5'	23:A:1307:G:H8	1.88	0.55
23:A:1450:A:HO2'	23:A:1451:U:C4'	2.18	0.55
23:A:27:G:O2'	23:A:557:G:N2	2.38	0.55
25:D:208:GLY:O	25:D:212:TRP:N	2.39	0.55
23:A:2362:A:OP1	35:R:17:ARG:NH1	2.40	0.55
23:A:1479:G:O2'	23:A:1480:G:OP2	2.18	0.55
23:A:192:G:OP2	44:O:28:ARG:NH1	2.39	0.55
23:A:2142:G:N2	23:A:2189:G:OP1	2.39	0.55
23:A:592:A:O2'	23:A:593:U:O5'	2.23	0.55
24:B:46:A:OP1	35:R:35:ARG:NH2	2.40	0.55
23:A:1865:C:N4	23:A:1926:A:O4'	2.39	0.55
23:A:241:C:C4	23:A:263:G:O6	2.59	0.55
23:A:437:A:O2'	23:A:438:U:OP1	2.23	0.55
23:A:61:A:OP2	23:A:395:U:O2'	53.72	0.55
35:R:68:THR:OG1	35:R:104:ARG:NH1	2.39	0.55
23:A:346:A:OP2	31:N:97:ARG:NH2	154.79	0.55
23:A:1583:G:OP1	23:A:1584:A:N7	2.39	0.55
23:A:1452:C:N4	23:A:1632:A:N7	2.55	0.55
23:A:1712:A:O2'	23:A:1718:G:N7	2.32	0.55
23:A:659:A:O2'	27:F:43:SER:OG	2.22	0.55
24:B:50:A:N6	35:R:37:ASN:O	2.38	0.55
23:A:446:G:N2	23:A:504:G:O6	61.00	0.55
23:A:261:U:C1'	23:A:283:G:H21	62.85	0.55
23:A:614:U:O2'	23:A:616:G:OP2	2.10	0.55
48:4:43:VAL:O	48:4:44:CYS:HB2	2.06	0.55
50:6:3:LYS:NZ	50:6:7:GLN:OE1	2.32	0.55
23:A:1845:U:OP2	25:D:155:ARG:NE	2.40	0.55
48:4:18:THR:OG1	48:4:19:HIS:ND1	2.37	0.54
23:A:1036:C:O2	23:A:1046:G:N1	29.19	0.54
47:3:24:LEU:O	47:3:24:LEU:HD13	2.06	0.54
23:A:1400:C:O2'	23:A:1836:A:O2'	2.12	0.54
23:A:1306:C:OP1	23:A:2033:C:OP1	2.25	0.54
28:G:89:VAL:O	28:G:92:ARG:N	2.40	0.54
36:S:33:ARG:N	36:S:82:LYS:O	2.34	0.54
23:A:1033:G:O2'	23:A:1034:A:OP2	2.23	0.54
28:G:90:THR:O	28:G:93:GLY:N	2.40	0.54
23:A:1124:A:O2'	23:A:1125:U:O5'	2.25	0.54
23:A:1597:U:O2'	23:A:1598:U:O4'	2.18	0.54
23:A:49:A:H61	23:A:179:A:H2'	1.73	0.54
23:A:2112:C:N4	23:A:2261:G:H1	2.06	0.54
23:A:275:A:C6	23:A:296:G:C2	2.94	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:37:ASN:N	28:G:145:LYS:O	2.41	0.54
47:3:30:THR:HG1	47:3:51:SER:HG	1.49	0.54
23:A:1397:G:H22	23:A:2241:C:H42	1.56	0.54
23:A:1037:A:OP2	37:T:51:ARG:NH1	2.39	0.54
23:A:162:A:O2'	23:A:163:U:OP1	2.20	0.54
23:A:632:U:OP1	32:O:16:ARG:NH1	2.41	0.54
51:7:34:ALA:HB3	51:7:37:SER:HB2	1.89	0.54
23:A:1582:U:O2'	23:A:1585:G:O6	2.17	0.54
23:A:2418:G:N2	23:A:2449:C:N3	2.55	0.54
23:A:2495:A:N1	23:A:2508:G:O2'	2.39	0.54
42:Y:14:THR:O	42:Y:18:LEU:HD21	2.05	0.54
23:A:1306:C:C5	23:A:2039:G:N2	2.76	0.54
23:A:373:A:C8	23:A:1248:U:N3	2.75	0.54
23:A:178:A:OP2	23:A:179:A:N6	2.41	0.54
23:A:1363:U:HO2'	23:A:2037:G:HO2'	1.53	0.54
32:O:83:ASN:OD1	32:O:84:LYS:N	2.41	0.54
23:A:10:A:O2'	23:A:11:U:O4'	2.25	0.53
26:E:74:GLU:O	26:E:78:LYS:N	2.40	0.53
23:A:2869:G:H22	23:A:2887:G:P	2.31	0.53
47:3:8:GLU:OE1	47:3:24:LEU:HD11	2.08	0.53
50:6:20:ARG:O	50:6:24:SER:OG	2.16	0.53
23:A:2161:A:C6	23:A:2184:G:C2	2.97	0.53
23:A:1397:G:H22	23:A:2241:C:N4	2.07	0.53
36:S:102:LEU:O	36:S:103:ARG:NE	2.41	0.53
23:A:687:G:N2	23:A:690:U:OP2	2.32	0.53
50:6:15:LYS:O	50:6:17:HIS:N	2.42	0.52
23:A:2860:U:O2'	34:Q:97:GLN:OE1	2.19	0.52
42:Y:25:GLY:CA	42:Y:44:ASP:OD1	2.57	0.52
52:8:27:CYS:SG	52:8:32:HIS:ND1	2.75	0.52
23:A:2419:A:N6	23:A:2456:G:O2'	2.42	0.52
23:A:516:A:OP1	27:F:79:ARG:NH2	2.42	0.52
23:A:319:G:N2	23:A:321:U:O4	2.41	0.52
23:A:961:G:O2'	23:A:962:A:O5'	2.19	0.52
23:A:2119:U:N3	23:A:2253:C:OP2	2.39	0.52
23:A:2287:C:H41	43:Z:22:ARG:CG	2.23	0.52
23:A:522:G:N1	23:A:525:A:OP2	2.42	0.52
23:A:488:G:O4'	27:F:46:GLN:NE2	2.42	0.52
42:Y:21:LEU:CD1	42:Y:42:LYS:CG	2.74	0.52
23:A:955:A:H62	33:P:15:PRO:HD3	1.73	0.52
45:1:24:GLU:OE2	45:1:42:ARG:NH2	2.40	0.52
23:A:419:U:OP2	44:0:52:ARG:NH1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R:31:LEU:HD12	35:R:43:GLN:O	2.10	0.52
44:0:29:TRP:CZ2	44:0:31:ALA:HB2	2.43	0.52
23:A:2804:G:OP2	23:A:2808:A:O2'	2.25	0.52
23:A:2806:U:OP1	23:A:2807:G:N2	2.43	0.52
23:A:446:G:N1	23:A:504:G:N7	61.00	0.52
23:A:825:G:N1	25:D:228:ASP:OD2	2.40	0.52
33:P:31:GLU:OE1	33:P:31:GLU:N	2.42	0.52
23:A:2137:G:O2'	23:A:2138:U:O5'	2.25	0.52
23:A:863:G:O2'	23:A:864:A:O5'	2.17	0.52
42:Y:25:GLY:O	42:Y:45:GLU:N	2.42	0.52
23:A:1708:A:H61	23:A:2023:C:H42	1.57	0.52
23:A:1991:G:O2'	23:A:1994:C:OP1	2.19	0.52
23:A:2683:U:C2	23:A:2692:A:N7	2.77	0.52
23:A:349:U:H3	23:A:353:A:H62	1.58	0.52
23:A:527:G:O2'	23:A:552:A:N6	2.43	0.52
24:B:37:A:O2'	24:B:38:U:O4'	2.22	0.52
36:S:42:ILE:HD12	36:S:43:GLN:N	2.25	0.52
24:B:100:A:O2'	42:Y:32:TYR:OH	2.09	0.52
23:A:1712:A:H61	23:A:1720:A:H61	1.58	0.51
25:D:172:LEU:O	25:D:173:ILE:HD13	2.08	0.51
27:F:173:VAL:HG21	27:F:196:GLU:OE2	2.10	0.51
23:A:2711:U:OP2	36:S:53:ARG:NH1	2.42	0.51
23:A:2361:U:H3	35:R:16:ALA:HB1	1.75	0.51
23:A:1031:C:O2'	23:A:1044:A:N3	2.40	0.51
23:A:1520:A:HO2'	23:A:1561:G:H22	1.59	0.51
23:A:275:A:N6	23:A:297:G:N3	2.58	0.51
23:A:1583:G:P	23:A:1584:A:C8	2.99	0.51
23:A:1968:C:N4	23:A:1992:C:O4'	2.43	0.51
27:F:177:THR:O	27:F:180:GLY:N	2.44	0.51
35:R:70:VAL:HG12	35:R:104:ARG:HB3	1.93	0.51
23:A:2287:C:H42	43:Z:22:ARG:CD	2.15	0.51
33:P:35:GLN:HE21	33:P:100:GLY:HA2	1.75	0.51
43:Z:27:LYS:CG	43:Z:29:LEU:CD1	2.80	0.51
23:A:2192:G:OP1	23:A:2193:G:N2	2.43	0.51
23:A:2649:U:C2'	23:A:2845:G:H22	2.23	0.51
47:3:63:LYS:HD2	47:3:66:ALA:HB3	1.93	0.51
23:A:2152:G:N2	23:A:2200:A:H62	2.08	0.51
23:A:1825:U:O2'	23:A:1829:A:N3	2.43	0.51
43:Z:18:THR:O	43:Z:18:THR:HG23	2.10	0.51
49:5:35:PHE:CZ	49:5:40:ASN:HA	2.46	0.50
23:A:1320:G:N1	23:A:1323:A:OP2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R:44:ILE:HD12	35:R:54:ALA:HB3	1.93	0.50
23:A:1092:A:OP2	23:A:1154:G:N2	2.39	0.50
23:A:2527:U:O2'	23:A:2531:U:OP1	2.12	0.50
23:A:481:C:O2	23:A:481:C:O2'	3.67	0.50
33:P:27:VAL:HG11	33:P:134:ARG:HD2	1.94	0.50
23:A:321:U:O2'	23:A:322:A:OP1	2.28	0.50
23:A:1306:C:O2	23:A:2040:A:N6	2.43	0.50
23:A:2287:C:N4	43:Z:22:ARG:CG	2.75	0.50
23:A:63:U:O3'	40:W:63:LYS:NZ	2.35	0.50
23:A:788:A:O2'	23:A:1703:U:OP1	2.28	0.50
23:A:460:C:O2	23:A:1891:U:O2'	2.27	0.50
23:A:677:A:O2'	23:A:678:A:O4'	2.18	0.50
29:H:10:ASP:OD1	29:H:11:ILE:N	2.44	0.50
23:A:2432:G:N2	23:A:2439:A:H62	2.10	0.50
25:D:227:ASN:OD1	25:D:228:ASP:N	2.45	0.50
23:A:1884:G:N2	23:A:1913:U:O4	2.44	0.50
23:A:2603:G:N2	23:A:2603:G:OP2	2.39	0.50
23:A:517:A:N6	23:A:518:A:N1	2.85	0.50
25:D:9:THR:HG23	25:D:11:GLY:H	1.76	0.50
33:P:14:ARG:O	33:P:87:LYS:NZ	2.45	0.50
43:Z:27:LYS:O	43:Z:28:ARG:CB	2.56	0.50
23:A:2432:G:OP1	32:O:63:LYS:NZ	2.44	0.49
29:H:155:GLU:O	29:H:159:GLY:N	2.44	0.49
23:A:1290:G:OP2	37:T:13:ARG:NH2	2.45	0.49
23:A:227:G:O6	23:A:465:C:O2'	2.30	0.49
23:A:2231:C:OP2	25:D:149:LYS:NZ	2.45	0.49
25:D:83:ASP:OD2	25:D:86:ARG:NH2	2.46	0.49
23:A:1805:U:H3	23:A:1812:A:H62	1.60	0.49
29:H:44:LYS:O	29:H:50:ILE:HG23	2.11	0.49
23:A:2039:G:OP1	39:V:11:ARG:NH1	2.45	0.49
23:A:1123:C:O2'	23:A:1124:A:O4'	2.26	0.49
23:A:994:A:H4'	24:B:85:A:H61	1.77	0.49
23:A:1496:G:N7	23:A:1501:G:C6	2.80	0.49
23:A:2516:G:O2'	23:A:2545:A:N6	2.40	0.49
23:A:590:U:OP2	23:A:766:G:N1	136.57	0.49
40:W:49:LYS:CD	40:W:51:ALA:HB2	2.42	0.49
44:O:19:SER:N	44:O:27:ARG:O	2.38	0.49
25:D:69:ASN:ND2	25:D:69:ASN:O	2.43	0.49
27:F:173:VAL:HG11	27:F:196:GLU:OE2	2.13	0.49
31:N:114:ILE:O	31:N:118:ALA:HB2	2.13	0.49
36:S:38:THR:O	36:S:38:THR:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1303:A:C1'	23:A:1305:U:C4	2.96	0.49
23:A:1496:G:H22	23:A:2729:G:H3'	1.77	0.49
23:A:969:A:O2'	23:A:971:U:OP2	2.10	0.49
24:B:73:G:N3	42:Y:88:HIS:NE2	2.61	0.49
48:4:18:THR:HG1	48:4:19:HIS:HD1	1.57	0.49
23:A:2868:G:N2	23:A:2888:A:H62	2.03	0.49
27:F:39:LEU:O	27:F:42:ALA:N	2.45	0.49
31:N:14:SER:O	31:N:51:VAL:N	2.46	0.49
23:A:1726:A:OP2	23:A:1743:G:N2	2.30	0.49
26:E:49:ILE:HG22	26:E:50:GLN:N	2.28	0.49
23:A:2302:C:C2	43:Z:18:THR:HG21	2.47	0.49
36:S:66:ILE:O	36:S:66:ILE:HG22	2.13	0.48
23:A:113:U:O2'	40:W:32:ARG:NH1	2.46	0.48
23:A:1515:G:N2	23:A:1565:U:O2	2.45	0.48
23:A:260:A:N6	23:A:261:U:N3	2.61	0.48
25:D:171:VAL:O	25:D:183:ILE:N	2.45	0.48
23:A:1319:U:H3	23:A:1323:A:H62	1.60	0.48
23:A:1458:A:N6	23:A:1459:A:H62	2.11	0.48
23:A:904:G:O2'	23:A:961:G:O6	2.31	0.48
28:G:9:ASN:O	28:G:13:THR:CB	2.62	0.48
38:U:34:THR:HG22	38:U:59:THR:HG22	1.94	0.48
29:H:99:GLN:N	29:H:102:ASP:O	2.47	0.48
45:1:45:THR:O	45:1:49:THR:HG23	2.14	0.48
49:5:35:PHE:O	49:5:45:HIS:ND1	2.46	0.48
23:A:373:A:C5	23:A:1248:U:O4	2.62	0.48
23:A:1290:G:H21	37:T:33:LYS:HB3	1.77	0.48
23:A:342:A:OP1	41:X:80:ARG:NH1	2.46	0.48
27:F:80:ALA:HB1	27:F:81:PRO:HD2	1.94	0.48
32:O:119:LYS:O	32:O:123:VAL:HG12	2.14	0.48
41:X:93:ILE:HD13	41:X:102:LYS:HB2	1.96	0.48
23:A:2662:U:O2'	26:E:50:GLN:NE2	2.46	0.48
36:S:80:THR:HG22	36:S:82:LYS:H	1.79	0.48
43:Z:26:SER:OG	43:Z:28:ARG:NH1	2.38	0.48
44:0:32:ASN:HD22	44:0:33:LEU:N	2.11	0.48
23:A:1261:G:N7	38:U:70:LYS:NZ	2.61	0.48
23:A:1261:G:N2	23:A:1264:A:OP2	2.39	0.48
23:A:263:G:H5''	23:A:666:A:C1'	2.41	0.48
23:A:936:G:O2'	23:A:937:G:OP1	4.41	0.48
23:A:2502:C:O2'	23:A:2504:C:OP2	2.29	0.48
24:B:107:U:H3'	24:B:108:G:H21	1.79	0.48
23:A:2287:C:H41	43:Z:22:ARG:CD	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:2452:A:N3	23:A:2454:C:N4	2.61	0.48
38:U:61:THR:OG1	38:U:98:ASP:OD2	2.18	0.48
23:A:1939:A:N7	23:A:1944:U:O4	2.47	0.48
30:M:59:ASN:N	30:M:128:GLY:O	2.45	0.47
42:Y:25:GLY:C	42:Y:44:ASP:HA	2.33	0.47
23:A:2868:G:C8	36:S:97:ALA:HB2	2.48	0.47
23:A:1396:A:OP2	23:A:1408:G:N1	2.42	0.47
23:A:75:G:O2'	45:1:48:LYS:NZ	2.46	0.47
25:D:52:HIS:ND1	25:D:52:HIS:O	2.47	0.47
47:3:61:ARG:NH2	47:3:66:ALA:HB1	2.28	0.47
23:A:942:C:O2'	23:A:943:C:O5'	2.32	0.47
30:M:18:VAL:N	30:M:139:GLU:O	2.48	0.47
42:Y:27:VAL:O	42:Y:43:VAL:N	2.46	0.47
23:A:248:G:N7	51:7:8:ARG:NH2	2.62	0.47
37:T:115:ASP:OD1	37:T:116:ALA:N	2.48	0.47
38:U:7:THR:HG21	38:U:22:VAL:HG21	1.96	0.47
36:S:48:VAL:HG12	36:S:49:VAL:O	2.15	0.47
23:A:2432:G:H21	23:A:2439:A:H62	1.63	0.47
23:A:2905:C:N3	48:4:39:LEU:HD22	2.30	0.47
23:A:722:A:O2'	23:A:2097:G:O2'	2.05	0.47
23:A:595:G:N2	23:A:762:C:OP2	143.54	0.47
23:A:2380:G:N2	43:Z:42:GLY:O	2.41	0.47
23:A:1892:U:C2'	23:A:1902:G:H22	2.27	0.47
23:A:1631:G:OP1	23:A:1631:G:N2	2.48	0.47
23:A:1732:U:O2'	23:A:1744:A:N7	2.42	0.47
23:A:1836:A:O2'	23:A:1837:A:O4'	2.32	0.47
47:3:9:TYR:OH	47:3:41:LYS:O	2.32	0.47
23:A:1826:G:N2	23:A:1846:A:OP2	2.40	0.47
38:U:59:THR:OG1	38:U:98:ASP:O	2.22	0.47
51:7:34:ALA:HB3	51:7:37:SER:CB	2.45	0.46
23:A:2276:U:N3	23:A:2280:G:OP2	2.48	0.46
23:A:2085:A:N6	23:A:2086:A:N1	2.64	0.46
23:A:1576:A:N6	23:A:1589:U:O4	2.49	0.46
23:A:1708:A:H61	23:A:2023:C:N4	2.14	0.46
33:P:27:VAL:HG12	33:P:134:ARG:HD2	1.98	0.46
49:5:39:GLU:N	49:5:39:GLU:OE1	2.48	0.46
23:A:1361:G:O2'	23:A:1363:U:OP2	2.22	0.46
23:A:1311:A:N6	23:A:1690:A:N3	2.63	0.46
23:A:2152:G:C2	23:A:2200:A:N6	2.84	0.46
23:A:2127:G:C6	23:A:2216:U:O2	2.69	0.46
23:A:330:C:N4	23:A:337:A:N7	25.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:809:A:N3	25:D:211:ARG:NH1	2.63	0.46
33:P:110:SER:OG	33:P:111:GLU:N	2.49	0.46
43:Z:57:GLU:N	43:Z:57:GLU:OE1	2.48	0.46
23:A:1215:U:HO2'	23:A:1217:U:C5'	2.23	0.46
23:A:1491:C:O2	23:A:1574:G:C2	2.67	0.46
23:A:318:A:N6	23:A:402:C:H42	2.14	0.46
29:H:35:ARG:HB3	29:H:37:LEU:HD21	1.98	0.46
23:A:491:C:H5	23:A:492:G:HO2'	8.49	0.46
29:H:86:VAL:HG11	29:H:165:GLN:HE21	1.81	0.46
30:M:117:GLU:O	30:M:120:GLY:N	2.44	0.46
47:3:5:ILE:O	47:3:5:ILE:HD12	2.16	0.46
23:A:1487:G:H22	23:A:1596:G:N2	2.14	0.46
23:A:1786:A:O2'	23:A:2741:G:O2'	2.31	0.46
23:A:2172:C:O2'	23:A:2173:U:OP1	2.28	0.46
23:A:2152:G:N2	23:A:2199:U:OP1	2.48	0.46
23:A:2860:U:C5'	34:Q:49:THR:HG21	2.46	0.46
25:D:215:ILE:HG22	25:D:216:ARG:N	2.31	0.46
23:A:1058:U:N3	23:A:1059:A:N7	2.64	0.46
26:E:35:VAL:C	26:E:36:LEU:HD12	2.37	0.46
35:R:74:THR:HB	35:R:111:ALA:HB2	1.98	0.46
40:W:52:SER:O	40:W:81:THR:HG22	2.15	0.46
23:A:1078:G:OP2	52:8:18:LYS:NZ	2.40	0.46
23:A:1576:A:H61	23:A:1587:C:H41	1.64	0.46
25:D:194:VAL:HG12	25:D:195:GLY:H	1.81	0.46
23:A:1452:C:H42	23:A:1632:A:N6	2.11	0.46
23:A:1693:G:N2	34:Q:112:ASP:O	2.49	0.46
37:T:96:SER:O	37:T:99:ALA:HB3	2.15	0.46
23:A:1099:G:H1	23:A:1148:C:H42	1.64	0.45
23:A:2432:G:O2'	23:A:2433:C:OP2	2.15	0.45
23:A:2869:G:O2'	23:A:2886:G:N2	2.49	0.45
23:A:864:A:OP2	23:A:1226:G:N2	2.47	0.45
29:H:64:ASN:O	29:H:68:THR:OG1	2.23	0.45
39:V:23:LEU:HB2	39:V:24:ILE:HG23	1.97	0.45
46:2:11:SER:O	46:2:15:ARG:NH1	2.49	0.45
47:3:28:THR:HG22	47:3:30:THR:CG2	2.46	0.45
47:3:75:ASN:O	47:3:75:ASN:ND2	2.49	0.45
23:A:467:U:O4	23:A:483:C:N4	55.13	0.45
23:A:684:U:C2	23:A:694:G:O6	2.69	0.45
51:7:32:LEU:HD11	51:7:33:PHE:CE1	2.52	0.45
23:A:283:G:N7	23:A:284:C:O2'	2.44	0.45
41:X:70:LEU:HD23	41:X:76:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1505:G:N7	23:A:1506:C:N4	2.65	0.45
23:A:1569:G:H21	23:A:1570:G:C4'	2.30	0.45
23:A:2161:A:C6	23:A:2184:G:N3	2.84	0.45
25:D:207:ALA:O	25:D:210:SER:N	2.48	0.45
26:E:195:ILE:N	26:E:195:ILE:HD12	2.32	0.45
29:H:11:ILE:HG23	29:H:15:VAL:HG11	1.98	0.45
23:A:1042:C:OP2	37:T:58:ARG:NH2	2.49	0.45
40:W:56:MET:SD	40:W:56:MET:N	2.89	0.45
23:A:2778:G:O2'	23:A:2778:G:N3	2.44	0.45
23:A:513:G:O2'	23:A:841:C:O2'	2.09	0.45
24:B:82:C:HO2'	24:B:83:U:C4'	2.26	0.45
23:A:1001:A:N6	23:A:1003:A:N1	2.64	0.45
25:D:20:PHE:HB3	25:D:23:ILE:HD12	1.99	0.45
23:A:160:G:O2'	23:A:167:U:O4	2.25	0.45
23:A:1767:G:HO2'	23:A:1768:C:P	2.40	0.45
23:A:903:G:OP2	43:Z:85:LYS:NZ	2.50	0.45
23:A:300:G:HO2'	23:A:467:U:H5	1.65	0.45
23:A:921:C:O2	23:A:945:A:N6	2.50	0.45
27:F:88:ILE:HG22	27:F:89:VAL:N	2.32	0.45
29:H:151:VAL:HG12	29:H:152:ARG:HG2	1.99	0.45
29:H:61:ASP:OD1	29:H:62:ARG:N	2.50	0.45
46:2:17:GLU:N	46:2:17:GLU:OE1	2.50	0.44
23:A:1039:C:H42	30:M:4:THR:HG22	1.81	0.44
23:A:2289:U:O2'	23:A:2355:A:N3	2.44	0.44
23:A:2501:U:OP2	23:A:2502:C:N4	2.43	0.44
31:N:2:ILE:HG22	31:N:3:GLN:N	2.32	0.44
24:B:21:G:N1	24:B:59:U:C2	2.85	0.44
23:A:1250:G:N2	23:A:1274:G:O2'	2.51	0.44
23:A:1902:G:HO2'	23:A:1903:A:H8	1.64	0.44
23:A:2710:C:O2	31:N:76:TYR:OH	2.33	0.44
34:Q:40:VAL:O	34:Q:44:VAL:HG22	2.17	0.44
23:A:1124:A:O2'	23:A:1125:U:O4'	2.36	0.44
23:A:1726:A:P	23:A:1743:G:H22	2.38	0.44
23:A:572:C:HO2'	23:A:573:A:P	2.38	0.44
23:A:590:U:H3	23:A:767:A:H62	132.86	0.44
26:E:5:ILE:O	26:E:211:ILE:N	2.42	0.44
27:F:144:SER:OG	27:F:186:ILE:HG21	2.17	0.44
42:Y:14:THR:HB	42:Y:18:LEU:CD2	2.44	0.44
23:A:634:C:HO2'	51:7:2:PRO:N	2.16	0.44
52:8:17:ILE:HD12	52:8:18:LYS:N	2.33	0.44
23:A:6:A:HO2'	30:M:133:HIS:HD1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R:86:ASP:OD1	35:R:87:LYS:N	2.50	0.44
23:A:1506:C:O2'	23:A:1507:A:O4'	2.26	0.44
35:R:46:ASP:O	35:R:50:GLY:N	2.50	0.44
38:U:22:VAL:HG22	38:U:23:GLU:H	1.83	0.44
23:A:2048:G:OP1	48:4:9:SER:OG	2.32	0.44
23:A:2150:A:OP2	23:A:2197:G:O2'	2.35	0.44
23:A:32:C:N4	23:A:493:A:OP2	2.50	0.44
23:A:901:G:H2'	23:A:902:A:C8	2.53	0.44
39:V:108:SER:OG	39:V:110:GLY:N	2.51	0.44
23:A:744:A:N3	23:A:1677:G:O2'	2.45	0.44
30:M:74:VAL:HG11	30:M:76:TYR:CE1	2.53	0.44
35:R:95:ASP:OD1	35:R:96:ARG:N	2.47	0.44
40:W:14:GLU:O	40:W:17:SER:N	2.51	0.44
42:Y:24:SER:OG	42:Y:26:LYS:HG2	2.17	0.44
23:A:1698:A:N6	23:A:2033:C:O4'	2.51	0.43
23:A:2261:G:O2'	23:A:2262:G:C5'	2.64	0.43
23:A:263:G:C2	23:A:264:G:C1'	2.96	0.43
23:A:660:A:C3'	23:A:661:U:H5'	2.48	0.43
23:A:2757:U:O2'	26:E:181:GLN:O	2.34	0.43
31:N:65:THR:HG22	31:N:67:SER:N	2.32	0.43
23:A:2302:C:C2	43:Z:18:THR:CG2	3.01	0.43
23:A:577:A:O2'	23:A:2048:G:N2	2.42	0.43
27:F:7:LEU:HD12	27:F:8:LYS:H	1.82	0.43
34:Q:24:LEU:O	34:Q:28:GLU:CA	2.64	0.43
39:V:32:ALA:HA	39:V:35:ILE:HD13	2.00	0.43
45:1:10:THR:OG1	45:1:13:GLU:N	2.48	0.43
46:2:57:GLU:N	46:2:57:GLU:OE1	2.51	0.43
23:A:2854:A:N6	23:A:2899:A:O2'	2.50	0.43
23:A:2733:A:O2'	34:Q:60:ARG:NH1	2.51	0.43
47:3:12:VAL:HG12	47:3:45:VAL:HB	1.99	0.43
23:A:261:U:H3'	23:A:262:G:H8	1.82	0.43
38:U:94:LYS:C	38:U:95:LEU:HD12	2.39	0.43
50:6:20:ARG:O	50:6:24:SER:CB	2.66	0.43
25:D:138:THR:N	25:D:162:GLN:OE1	2.51	0.43
31:N:24:VAL:HG11	31:N:33:ALA:HB2	2.01	0.43
23:A:2285:C:O2'	23:A:2453:A:O3'	2.35	0.43
23:A:720:A:N3	23:A:2470:C:O2'	2.39	0.43
23:A:774:G:OP2	25:D:206:LYS:NZ	2.49	0.43
23:A:1099:G:N2	23:A:1148:C:N3	2.67	0.43
23:A:628:G:H2'	23:A:1289:A:H62	1.84	0.43
23:A:260:A:N6	23:A:261:U:H3	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:H:9:ILE:HD11	29:H:69:ARG:HA	2.00	0.43
36:S:106:ARG:NE	36:S:106:ARG:HA	2.34	0.43
45:1:38:GLU:N	45:1:38:GLU:OE1	2.52	0.43
23:A:1033:G:C8	46:2:13:ILE:HD11	2.54	0.43
25:D:159:ALA:HA	25:D:193:GLN:HE21	1.84	0.43
49:5:35:PHE:CE1	49:5:37:SER:CA	3.02	0.43
51:7:49:LEU:HD12	51:7:49:LEU:N	2.34	0.43
23:A:628:G:H2'	23:A:1289:A:N6	2.34	0.43
23:A:263:G:O2'	23:A:264:G:O5'	2.35	0.43
23:A:2869:G:N2	23:A:2886:G:O2'	2.50	0.43
24:B:22:G:O6	24:B:54:U:O2'	2.35	0.43
23:A:1305:U:H2'	23:A:1305:U:O2	2.18	0.43
23:A:297:G:O2'	23:A:304:G:O2'	2.26	0.43
23:A:9:U:O4	23:A:2656:A:N7	2.52	0.43
25:D:107:LYS:N	25:D:193:GLN:O	2.43	0.43
29:H:8:ILE:C	29:H:9:ILE:HD12	2.39	0.43
41:X:34:VAL:HG22	41:X:62:ALA:HB2	2.01	0.43
48:4:43:VAL:O	48:4:44:CYS:CB	2.67	0.42
51:7:32:LEU:HD11	51:7:33:PHE:CZ	2.54	0.42
23:A:1885:G:C2'	23:A:1910:G:H22	2.32	0.42
29:H:128:ASN:OD1	29:H:129:THR:N	2.52	0.42
41:X:81:VAL:HG22	41:X:82:GLY:H	1.84	0.42
50:6:35:ARG:HE	50:6:43:LEU:HA	1.85	0.42
51:7:18:ALA:O	51:7:19:SER:OG	2.25	0.42
23:A:1591:G:O2'	23:A:1592:A:O5'	2.37	0.42
23:A:590:U:O4	23:A:767:A:N7	130.77	0.42
24:B:74:G:H22	24:B:97:A:N6	2.16	0.42
34:Q:26:ILE:HD12	34:Q:26:ILE:N	2.34	0.42
39:V:28:ASN:OD1	39:V:29:ALA:N	2.49	0.42
41:X:8:ASN:OD1	41:X:9:VAL:N	2.51	0.42
23:A:1550:G:O2'	23:A:1551:U:O5'	2.37	0.42
23:A:13:A:O2'	23:A:15:G:N7	2.52	0.42
23:A:2231:C:H2'	23:A:2232:A:C8	2.55	0.42
23:A:2272:U:O2'	23:A:2463:G:OP2	2.18	0.42
23:A:921:C:H1'	23:A:946:A:H61	1.84	0.42
25:D:17:SER:OG	25:D:18:LEU:N	2.51	0.42
33:P:43:THR:OG1	33:P:44:SER:N	2.50	0.42
35:R:92:ILE:HD12	35:R:93:VAL:O	2.19	0.42
23:A:99:U:O2	23:A:101:G:N1	2.51	0.42
31:N:65:THR:HG22	31:N:67:SER:H	1.84	0.42
34:Q:107:GLY:O	34:Q:116:SER:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:T:65:ILE:HD11	37:T:95:LEU:HB2	2.01	0.42
23:A:1079:U:C4	23:A:1164:G:O6	2.71	0.42
23:A:1281:U:O4	23:A:1282:A:N6	2.53	0.42
23:A:1470:G:O2'	23:A:1619:A:N6	2.45	0.42
23:A:1822:C:H2'	23:A:1823:U:O4'	2.20	0.42
25:D:50:VAL:O	25:D:50:VAL:HG23	2.20	0.42
42:Y:21:LEU:CD1	42:Y:42:LYS:HG2	2.29	0.42
23:A:1893:A:H2'	23:A:1894:G:O4'	2.20	0.42
25:D:223:VAL:HG23	25:D:224:MET:N	2.34	0.42
26:E:138:ARG:HE	26:E:141:MET:CE	2.33	0.42
42:Y:25:GLY:O	42:Y:27:VAL:HG23	2.20	0.42
23:A:2147:G:N2	23:A:2206:C:N3	2.68	0.42
25:D:190:THR:OG1	25:D:191:ILE:N	2.50	0.42
26:E:118:VAL:HG12	26:E:211:ILE:HG12	2.01	0.42
35:R:16:ALA:O	35:R:20:THR:N	2.52	0.42
23:A:1455:U:O4	23:A:1631:G:N1	2.53	0.42
23:A:749:G:O2'	23:A:771:G:N2	2.47	0.42
46:2:8:LEU:HD23	46:2:31:THR:HA	2.01	0.42
50:6:27:ASN:O	50:6:31:VAL:HG23	2.20	0.42
23:A:1392:G:O6	23:A:1414:G:N2	2.53	0.42
23:A:1668:U:O4	23:A:1669:C:N4	2.52	0.42
23:A:2516:G:O6	23:A:2517:G:N2	2.53	0.42
23:A:2680:U:OP2	23:A:2681:A:O2'	2.30	0.42
23:A:592:A:O2'	23:A:592:A:N3	2.52	0.42
23:A:1495:C:N3	23:A:1504:U:N3	2.67	0.42
23:A:341:G:O2'	23:A:383:A:N6	2.53	0.42
29:H:77:GLN:O	29:H:82:GLY:N	2.46	0.42
30:M:72:ASP:OD1	30:M:73:LYS:N	2.53	0.42
42:Y:22:ARG:HH21	42:Y:87:THR:HG23	1.68	0.42
23:A:1099:G:H21	23:A:1128:A:H2	1.68	0.41
23:A:2467:C:HO2'	23:A:2468:C:C1'	2.29	0.41
23:A:1094:A:H2	23:A:2778:G:H22	1.68	0.41
39:V:80:PRO:HD3	39:V:102:HIS:HE2	1.85	0.41
42:Y:14:THR:C	42:Y:18:LEU:CD2	2.85	0.41
42:Y:70:ILE:HG22	42:Y:71:LYS:O	2.19	0.41
23:A:1175:G:O6	30:M:80:ASN:ND2	2.53	0.41
23:A:1945:A:HO2'	23:A:1946:A:P	2.36	0.41
23:A:2358:G:HO2'	23:A:2363:A:N6	2.18	0.41
23:A:672:A:N7	32:O:70:ASN:ND2	2.63	0.41
26:E:9:LYS:NZ	26:E:201:VAL:HG23	2.32	0.41
30:M:46:THR:OG1	30:M:49:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:856:U:O2	32:O:21:ARG:HG2	2.20	0.41
23:A:2342:U:H4'	35:R:2:ILE:HD11	2.01	0.41
37:T:35:ALA:O	37:T:39:VAL:HG23	2.20	0.41
48:4:37:TYR:CE1	48:4:43:VAL:HG22	2.55	0.41
23:A:1303:A:H1'	23:A:1305:U:C4	2.55	0.41
23:A:139:U:O4	23:A:140:A:N6	4.77	0.41
26:E:9:LYS:HG2	26:E:9:LYS:O	2.20	0.41
29:H:105:LEU:O	29:H:106:ASN:ND2	2.54	0.41
34:Q:26:ILE:H	34:Q:26:ILE:HD12	1.86	0.41
52:8:11:CYS:N	52:8:14:CYS:SG	2.88	0.41
23:A:1081:G:H22	23:A:1163:U:H1'	1.85	0.41
23:A:1382:C:N4	23:A:1383:G:O6	2.53	0.41
23:A:1798:C:H2'	23:A:1799:G:O4'	2.19	0.41
23:A:2657:G:N2	23:A:2911:A:N3	2.69	0.41
29:H:80:SER:OG	29:H:81:GLN:N	2.54	0.41
39:V:3:ALA:N	39:V:107:VAL:O	2.53	0.41
39:V:19:LEU:O	39:V:22:ASP:N	2.54	0.41
49:5:35:PHE:CE1	49:5:37:SER:HA	2.54	0.41
23:A:2137:G:HO2'	23:A:2138:U:C5'	2.33	0.41
23:A:2533:U:HO2'	23:A:2534:C:C5'	2.34	0.41
23:A:459:C:HO2'	23:A:1907:U:HO2'	1.68	0.41
25:D:126:GLY:O	25:D:128:ALA:N	2.54	0.41
36:S:72:VAL:HG22	36:S:73:GLU:H	1.85	0.41
23:A:2161:A:C5	23:A:2184:G:N2	2.88	0.41
23:A:2679:U:H2'	23:A:2680:U:O4'	2.20	0.41
29:H:96:ALA:HA	29:H:105:LEU:HD23	2.03	0.41
35:R:68:THR:O	35:R:68:THR:HG23	2.20	0.41
23:A:1206:G:H21	38:U:90:GLN:HE22	1.67	0.41
23:A:1390:A:OP2	23:A:1414:G:N1	2.41	0.41
27:F:136:THR:O	27:F:140:LYS:NZ	2.43	0.41
27:F:155:VAL:HG22	27:F:156:THR:O	2.20	0.41
52:8:7:VAL:HG21	52:8:36:GLN:HB2	2.03	0.41
25:D:194:VAL:HG12	25:D:195:GLY:N	2.35	0.41
30:M:53:ASP:N	30:M:53:ASP:OD1	2.53	0.41
32:O:30:THR:HG22	32:O:30:THR:O	2.21	0.41
33:P:38:THR:OG1	33:P:39:THR:N	2.54	0.41
34:Q:37:ALA:HA	34:Q:40:VAL:HG12	2.03	0.41
23:A:2380:G:O2'	43:Z:41:GLY:O	2.39	0.41
23:A:2162:A:H61	23:A:2183:G:C2'	2.34	0.41
24:B:46:A:O3'	35:R:102:HIS:NE2	2.50	0.41
26:E:169:MET:HB2	26:E:170:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:U:29:GLU:OE1	38:U:30:GLY:N	2.54	0.41
23:A:2152:G:N2	23:A:2200:A:N6	2.69	0.41
23:A:318:A:H61	23:A:402:C:H42	1.69	0.41
25:D:92:LEU:HD22	25:D:93:VAL:H	1.86	0.41
31:N:102:VAL:CG2	31:N:121:VAL:HG22	2.51	0.41
23:A:1199:A:O3'	37:T:55:ARG:NH2	2.53	0.40
23:A:1584:A:H4'	23:A:1585:G:H5'	2.03	0.40
35:R:108:LEU:O	35:R:111:ALA:N	2.54	0.40
37:T:79:LEU:O	37:T:82:GLY:N	2.54	0.40
23:A:85:G:OP1	41:X:26:THR:OG1	2.39	0.40
26:E:158:SER:O	26:E:161:SER:N	2.55	0.40
27:F:187:THR:OG1	27:F:188:ASN:N	2.54	0.40
27:F:38:ASN:OD1	27:F:39:LEU:N	2.54	0.40
23:A:1241:A:O4'	27:F:41:ARG:NH2	2.53	0.40
23:A:1265:G:N1	23:A:1295:C:N3	32.49	0.40
23:A:198:A:H2'	23:A:201:C:H41	1.86	0.40
23:A:942:C:O2'	23:A:943:C:O4'	2.28	0.40
25:D:247:SER:HB2	25:D:248:PRO:HD2	2.03	0.40
23:A:2599:A:OP2	26:E:157:ALA:HB3	2.21	0.40
51:7:31:HIS:O	51:7:33:PHE:N	2.54	0.40
23:A:1583:G:H3'	23:A:1584:A:C5'	2.50	0.40
34:Q:52:LYS:HG2	34:Q:90:ALA:HB1	2.03	0.40
40:W:18:GLU:O	40:W:21:ALA:HB3	2.21	0.40
23:A:2501:U:O2'	23:A:2502:C:OP1	2.36	0.40
23:A:510:U:H2'	23:A:511:G:C8	2.57	0.40
34:Q:33:THR:HB	34:Q:36:ARG:HE	1.86	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	220/255 (86%)	192 (87%)	27 (12%)	1 (0%)	32	73
3	c	201/217 (93%)	166 (83%)	34 (17%)	1 (0%)	32	73
4	d	193/200 (96%)	163 (84%)	30 (16%)	0	100	100
5	e	158/166 (95%)	124 (78%)	34 (22%)	0	100	100
6	f	92/98 (94%)	73 (79%)	18 (20%)	1 (1%)	17	61
7	g	139/156 (89%)	117 (84%)	20 (14%)	2 (1%)	13	55
8	h	129/132 (98%)	107 (83%)	21 (16%)	1 (1%)	22	66
9	i	126/132 (96%)	107 (85%)	19 (15%)	0	100	100
10	j	97/102 (95%)	87 (90%)	10 (10%)	0	100	100
11	k	113/129 (88%)	89 (79%)	24 (21%)	0	100	100
12	l	133/137 (97%)	98 (74%)	33 (25%)	2 (2%)	12	55
13	m	108/121 (89%)	87 (81%)	21 (19%)	0	100	100
14	n	58/61 (95%)	40 (69%)	18 (31%)	0	100	100
15	o	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
16	p	88/91 (97%)	69 (78%)	19 (22%)	0	100	100
17	q	83/87 (95%)	64 (77%)	19 (23%)	0	100	100
18	r	54/80 (68%)	41 (76%)	13 (24%)	0	100	100
19	s	82/92 (89%)	63 (77%)	19 (23%)	0	100	100
20	t	78/83 (94%)	73 (94%)	5 (6%)	0	100	100
21	u	43/58 (74%)	31 (72%)	9 (21%)	3 (7%)	1	20
22	v	99/190 (52%)	70 (71%)	21 (21%)	8 (8%)	1	16
25	D	273/277 (99%)	228 (84%)	44 (16%)	1 (0%)	38	77
26	E	216/220 (98%)	172 (80%)	41 (19%)	3 (1%)	13	55
27	F	197/207 (95%)	157 (80%)	40 (20%)	0	100	100
28	G	164/179 (92%)	123 (75%)	40 (24%)	1 (1%)	28	70
29	H	162/178 (91%)	140 (86%)	22 (14%)	0	100	100
30	M	143/145 (99%)	117 (82%)	25 (18%)	1 (1%)	25	68
31	N	120/122 (98%)	83 (69%)	37 (31%)	0	100	100
32	O	129/146 (88%)	90 (70%)	39 (30%)	0	100	100
33	P	131/144 (91%)	101 (77%)	30 (23%)	0	100	100
34	Q	115/122 (94%)	89 (77%)	26 (23%)	0	100	100
35	R	117/119 (98%)	95 (81%)	22 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	S	105/116 (90%)	86 (82%)	17 (16%)	2 (2%)	9	51
37	T	114/118 (97%)	102 (90%)	12 (10%)	0	100	100
38	U	100/102 (98%)	79 (79%)	20 (20%)	1 (1%)	18	62
39	V	110/117 (94%)	98 (89%)	12 (11%)	0	100	100
40	W	87/91 (96%)	68 (78%)	19 (22%)	0	100	100
41	X	81/105 (77%)	50 (62%)	31 (38%)	0	100	100
42	Y	92/217 (42%)	68 (74%)	24 (26%)	0	100	100
43	Z	75/94 (80%)	65 (87%)	9 (12%)	1 (1%)	14	57
44	0	44/62 (71%)	33 (75%)	11 (25%)	0	100	100
45	1	63/69 (91%)	56 (89%)	7 (11%)	0	100	100
46	2	55/59 (93%)	48 (87%)	6 (11%)	1 (2%)	10	52
47	3	79/84 (94%)	47 (60%)	31 (39%)	1 (1%)	14	57
48	4	42/58 (72%)	36 (86%)	5 (12%)	1 (2%)	7	46
49	5	24/49 (49%)	19 (79%)	5 (21%)	0	100	100
50	6	42/45 (93%)	34 (81%)	6 (14%)	2 (5%)	2	29
51	7	58/66 (88%)	38 (66%)	20 (34%)	0	100	100
52	8	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
All	All	5353/6024 (89%)	4288 (80%)	1031 (19%)	34 (1%)	33	70

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	u	13	GLU
21	u	50	GLU
22	v	97	ASN
22	v	99	LYS
22	v	100	SER
22	v	102	ASP
2	b	104	TYR
21	u	51	ALA
22	v	51	ALA
22	v	79	ASP
22	v	83	ASN
22	v	101	ARG
26	E	10	ILE
26	E	142	SER

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Mol	Chain	Res	Type
36	S	105	LEU
43	Z	28	ARG
47	3	12	VAL
50	6	16	VAL
7	g	14	PRO
50	6	15	LYS
7	g	13	LEU
36	S	106	ARG
48	4	44	CYS
3	c	203	ARG
12	l	57	LYS
28	G	99	PHE
30	M	66	THR
38	U	23	GLU
8	h	100	GLY
46	2	30	LYS
12	l	41	PRO
6	f	12	PRO
25	D	252	PRO
26	E	154	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	192/221 (87%)	188 (98%)	4 (2%)	59	84
3	c	164/175 (94%)	160 (98%)	4 (2%)	54	82
4	d	172/175 (98%)	171 (99%)	1 (1%)	89	95
5	e	126/131 (96%)	120 (95%)	6 (5%)	30	67
6	f	82/86 (95%)	81 (99%)	1 (1%)	75	90
7	g	122/132 (92%)	118 (97%)	4 (3%)	43	76
8	h	112/113 (99%)	110 (98%)	2 (2%)	64	86
9	i	106/109 (97%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	j	89/91 (98%)	86 (97%)	3 (3%)	42	75
11	k	91/104 (88%)	90 (99%)	1 (1%)	78	90
12	l	117/119 (98%)	114 (97%)	3 (3%)	51	80
13	m	94/104 (90%)	93 (99%)	1 (1%)	78	90
14	n	52/53 (98%)	51 (98%)	1 (2%)	62	85
15	o	80/81 (99%)	77 (96%)	3 (4%)	38	73
16	p	76/77 (99%)	74 (97%)	2 (3%)	51	80
17	q	80/82 (98%)	80 (100%)	0	100	100
18	r	51/68 (75%)	50 (98%)	1 (2%)	60	84
19	s	73/80 (91%)	73 (100%)	0	100	100
20	t	67/69 (97%)	66 (98%)	1 (2%)	70	88
21	u	41/54 (76%)	33 (80%)	8 (20%)	1	11
22	v	91/173 (53%)	66 (72%)	25 (28%)	0	4
25	D	222/224 (99%)	219 (99%)	3 (1%)	71	89
26	E	175/177 (99%)	174 (99%)	1 (1%)	89	95
27	F	163/169 (96%)	162 (99%)	1 (1%)	89	95
28	G	147/158 (93%)	146 (99%)	1 (1%)	87	94
29	H	144/155 (93%)	143 (99%)	1 (1%)	87	94
30	M	123/123 (100%)	123 (100%)	0	100	100
31	N	100/100 (100%)	100 (100%)	0	100	100
32	O	104/112 (93%)	102 (98%)	2 (2%)	62	85
33	P	110/119 (92%)	104 (94%)	6 (6%)	25	64
34	Q	98/102 (96%)	98 (100%)	0	100	100
35	R	95/95 (100%)	95 (100%)	0	100	100
36	S	93/102 (91%)	93 (100%)	0	100	100
37	T	96/98 (98%)	96 (100%)	0	100	100
38	U	86/86 (100%)	86 (100%)	0	100	100
39	V	91/94 (97%)	91 (100%)	0	100	100
40	W	80/82 (98%)	80 (100%)	0	100	100
41	X	73/90 (81%)	73 (100%)	0	100	100
42	Y	83/190 (44%)	82 (99%)	1 (1%)	75	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	Z	60/75 (80%)	59 (98%)	1 (2%)	66	87
44	0	39/52 (75%)	37 (95%)	2 (5%)	28	66
45	1	59/62 (95%)	59 (100%)	0	100	100
46	2	51/53 (96%)	50 (98%)	1 (2%)	60	84
47	3	72/75 (96%)	70 (97%)	2 (3%)	49	79
48	4	41/51 (80%)	39 (95%)	2 (5%)	29	66
49	5	26/47 (55%)	25 (96%)	1 (4%)	38	73
50	6	39/40 (98%)	39 (100%)	0	100	100
51	7	52/57 (91%)	50 (96%)	2 (4%)	38	73
52	8	35/35 (100%)	35 (100%)	0	100	100
All	All	4635/5120 (90%)	4537 (98%)	98 (2%)	62	84

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	35	ARG
2	b	36	ASN
2	b	55	ASN
2	b	159	GLN
3	c	61	ASN
3	c	85	LYS
3	c	88	ASN
3	c	141	MET
4	d	178	ARG
5	e	8	THR
5	e	9	LYS
5	e	32	ARG
5	e	43	ASN
5	e	146	ASN
5	e	149	ASN
6	f	53	ASN
7	g	19	ASN
7	g	109	ARG
7	g	137	LYS
7	g	148	ASN
8	h	96	LYS
8	h	99	ASN
10	j	4	GLN

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Mol	Chain	Res	Type
10	j	5	LYS
10	j	16	ARG
11	k	14	LYS
12	l	43	LYS
12	l	56	LYS
12	l	73	ASN
13	m	3	ARG
14	n	57	ARG
15	o	40	ASN
15	o	59	MET
15	o	71	ARG
16	p	15	ASN
16	p	81	MET
18	r	40	GLU
20	t	45	ASN
21	u	11	SER
21	u	12	LEU
21	u	16	LEU
21	u	24	SER
21	u	25	LYS
21	u	44	LYS
21	u	53	ARG
21	u	54	LYS
22	v	19	ASN
22	v	20	TYR
22	v	22	GLU
22	v	30	ARG
22	v	41	HIS
22	v	45	LYS
22	v	47	TYR
22	v	66	ARG
22	v	70	ARG
22	v	74	LEU
22	v	75	TYR
22	v	78	ILE
22	v	80	LEU
22	v	82	ASN
22	v	83	ASN
22	v	88	GLN
22	v	90	ARG
22	v	91	LYS
22	v	92	TYR

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Mol	Chain	Res	Type
22	v	93	LYS
22	v	94	THR
22	v	96	ILE
22	v	99	LYS
22	v	101	ARG
22	v	103	ARG
25	D	69	ASN
25	D	81	GLN
25	D	254	LEU
26	E	212	ARG
27	F	135	LYS
28	G	96	MET
29	H	132	LYS
32	O	59	ARG
32	O	84	LYS
33	P	6	ARG
33	P	51	ARG
33	P	60	ARG
33	P	133	LYS
33	P	135	GLU
33	P	136	GLU
42	Y	21	LEU
43	Z	19	LYS
44	0	23	ASN
44	0	32	ASN
46	2	3	LYS
47	3	75	ASN
47	3	77	LYS
48	4	44	CYS
48	4	45	LYS
49	5	46	ARG
51	7	26	ARG
51	7	45	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	19	GLN
2	b	36	ASN
2	b	55	ASN
2	b	77	GLN
2	b	159	GLN

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Mol	Chain	Res	Type
3	c	6	ASN
3	c	44	ASN
3	c	88	ASN
4	d	159	ASN
5	e	43	ASN
5	e	146	ASN
5	e	149	ASN
6	f	53	ASN
7	g	19	ASN
7	g	40	GLN
8	h	31	ASN
8	h	68	GLN
9	i	33	ASN
12	l	25	ASN
12	l	73	ASN
13	m	76	ASN
16	p	15	ASN
20	t	21	ASN
20	t	62	GLN
22	v	19	ASN
22	v	41	HIS
22	v	71	ASN
22	v	82	ASN
22	v	88	GLN
22	v	97	ASN
25	D	43	ASN
25	D	193	GLN
26	E	50	GLN
26	E	103	GLN
27	F	75	GLN
27	F	148	GLN
29	H	23	HIS
29	H	106	ASN
29	H	120	ASN
29	H	165	GLN
31	N	82	ASN
32	O	114	ASN
33	P	35	GLN
34	Q	61	ASN
35	R	37	ASN
39	V	90	GLN
41	X	76	ASN

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Mol	Chain	Res	Type
42	Y	10	GLN
43	Z	20	ASN
44	0	32	ASN
44	0	34	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1540/1556 (98%)	373 (24%)	0
23	A	2909/2923 (99%)	727 (24%)	18 (0%)
24	B	113/114 (99%)	23 (20%)	0
All	All	4562/4593 (99%)	1123 (24%)	18 (0%)

All (1123) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	8	G
1	a	9	A
1	a	10	G
1	a	11	A
1	a	15	U
1	a	28	G
1	a	31	U
1	a	32	G
1	a	33	A
1	a	40	G
1	a	44	C
1	a	48	C
1	a	49	C
1	a	51	A
1	a	52	A
1	a	53	U
1	a	58	G
1	a	61	A
1	a	62	G
1	a	67	G
1	a	69	G
1	a	74	G
1	a	82	G
1	a	83	C
1	a	84	U

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Mol	Chain	Res	Type
1	a	85	U
1	a	86	G
1	a	88	U
1	a	89	U
1	a	90	C
1	a	92	C
1	a	94	G
1	a	95	A
1	a	120	C
1	a	129	A
1	a	130	A
1	a	138	A
1	a	142	G
1	a	144	C
1	a	148	G
1	a	149	A
1	a	154	U
1	a	159	G
1	a	163	C
1	a	165	G
1	a	168	G
1	a	169	C
1	a	170	U
1	a	171	A
1	a	173	U
1	a	182	A
1	a	183	U
1	a	191	A
1	a	196	A
1	a	205	A
1	a	211	A
1	a	212	A
1	a	213	G
1	a	214	A
1	a	218	U
1	a	221	U
1	a	234	A
1	a	247	C
1	a	248	U
1	a	252	U
1	a	255	G
1	a	259	G

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Mol	Chain	Res	Type
1	a	260	U
1	a	269	U
1	a	274	G
1	a	275	C
1	a	287	A
1	a	297	G
1	a	301	A
1	a	307	G
1	a	314	A
1	a	315	U
1	a	333	A
1	a	334	G
1	a	336	C
1	a	354	G
1	a	355	G
1	a	356	G
1	a	360	C
1	a	361	A
1	a	362	G
1	a	364	A
1	a	373	U
1	a	375	U
1	a	380	C
1	a	402	G
1	a	405	A
1	a	406	C
1	a	414	G
1	a	419	A
1	a	420	U
1	a	421	G
1	a	422	A
1	a	429	U
1	a	431	G
1	a	432	G
1	a	436	G
1	a	437	U
1	a	438	A
1	a	444	C
1	a	447	U
1	a	449	A
1	a	454	G
1	a	455	G

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Mol	Chain	Res	Type
1	a	456	A
1	a	457	A
1	a	459	A
1	a	462	A
1	a	466	G
1	a	467	U
1	a	470	A
1	a	476	C
1	a	477	U
1	a	478	G
1	a	480	G
1	a	481	C
1	a	482	A
1	a	483	C
1	a	484	A
1	a	492	G
1	a	494	U
1	a	503	A
1	a	504	G
1	a	505	A
1	a	508	G
1	a	513	G
1	a	516	U
1	a	519	C
1	a	520	U
1	a	526	C
1	a	528	A
1	a	529	G
1	a	532	G
1	a	535	G
1	a	539	U
1	a	540	A
1	a	541	A
1	a	555	A
1	a	556	G
1	a	557	C
1	a	558	G
1	a	567	A
1	a	569	U
1	a	570	U
1	a	572	U
1	a	575	G

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Mol	Chain	Res	Type
1	a	576	G
1	a	580	A
1	a	581	A
1	a	583	G
1	a	584	C
1	a	585	G
1	a	587	G
1	a	588	C
1	a	604	A
1	a	613	U
1	a	615	A
1	a	634	U
1	a	635	G
1	a	640	G
1	a	641	U
1	a	647	G
1	a	650	A
1	a	661	U
1	a	669	G
1	a	673	A
1	a	693	G
1	a	695	A
1	a	701	G
1	a	710	A
1	a	711	G
1	a	725	C
1	a	726	A
1	a	731	U
1	a	736	A
1	a	741	G
1	a	742	A
1	a	756	A
1	a	757	A
1	a	758	C
1	a	763	G
1	a	774	A
1	a	781	G
1	a	789	A
1	a	802	A
1	a	807	G
1	a	811	G
1	a	817	G

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Mol	Chain	Res	Type
1	a	819	C
1	a	820	G
1	a	825	C
1	a	828	U
1	a	829	G
1	a	836	A
1	a	850	U
1	a	851	U
1	a	854	C
1	a	855	G
1	a	856	C
1	a	865	G
1	a	868	G
1	a	869	C
1	a	881	U
1	a	882	A
1	a	883	A
1	a	886	A
1	a	900	G
1	a	924	A
1	a	932	G
1	a	936	G
1	a	937	G
1	a	944	C
1	a	945	A
1	a	946	C
1	a	949	G
1	a	955	G
1	a	957	G
1	a	958	C
1	a	968	A
1	a	970	U
1	a	971	U
1	a	975	A
1	a	976	G
1	a	979	A
1	a	981	G
1	a	985	A
1	a	986	G
1	a	992	U
1	a	993	A
1	a	994	C

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Mol	Chain	Res	Type
1	a	999	U
1	a	1002	U
1	a	1003	G
1	a	1012	U
1	a	1014	A
1	a	1024	A
1	a	1027	U
1	a	1028	A
1	a	1030	A
1	a	1034	U
1	a	1036	C
1	a	1037	C
1	a	1038	C
1	a	1039	C
1	a	1040	U
1	a	1041	U
1	a	1042	C
1	a	1044	G
1	a	1049	C
1	a	1050	A
1	a	1057	C
1	a	1065	G
1	a	1067	A
1	a	1068	U
1	a	1076	G
1	a	1078	C
1	a	1083	C
1	a	1087	U
1	a	1091	G
1	a	1092	A
1	a	1097	U
1	a	1106	G
1	a	1107	U
1	a	1113	A
1	a	1117	A
1	a	1130	A
1	a	1139	G
1	a	1141	C
1	a	1142	A
1	a	1144	C
1	a	1150	G
1	a	1151	U

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Mol	Chain	Res	Type
1	a	1154	G
1	a	1157	A
1	a	1162	A
1	a	1163	A
1	a	1164	G
1	a	1165	U
1	a	1168	A
1	a	1169	C
1	a	1170	U
1	a	1171	G
1	a	1172	C
1	a	1179	C
1	a	1190	A
1	a	1195	G
1	a	1207	A
1	a	1208	A
1	a	1223	U
1	a	1225	U
1	a	1226	G
1	a	1232	G
1	a	1237	C
1	a	1239	C
1	a	1244	G
1	a	1249	A
1	a	1251	U
1	a	1261	A
1	a	1264	G
1	a	1271	G
1	a	1272	A
1	a	1273	A
1	a	1279	G
1	a	1281	G
1	a	1289	A
1	a	1291	A
1	a	1293	C
1	a	1296	A
1	a	1297	U
1	a	1298	A
1	a	1304	G
1	a	1309	C
1	a	1310	A
1	a	1311	G

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Mol	Chain	Res	Type
1	a	1313	U
1	a	1316	G
1	a	1323	G
1	a	1328	C
1	a	1330	A
1	a	1331	C
1	a	1333	C
1	a	1334	G
1	a	1335	A
1	a	1338	A
1	a	1346	C
1	a	1347	U
1	a	1356	U
1	a	1357	A
1	a	1358	G
1	a	1371	A
1	a	1375	U
1	a	1381	G
1	a	1386	A
1	a	1389	C
1	a	1390	G
1	a	1392	U
1	a	1406	C
1	a	1408	C
1	a	1410	C
1	a	1430	G
1	a	1437	A
1	a	1442	C
1	a	1443	G
1	a	1453	G
1	a	1454	A
1	a	1457	A
1	a	1459	C
1	a	1462	U
1	a	1463	U
1	a	1464	U
1	a	1465	A
1	a	1478	C
1	a	1487	G
1	a	1492	A
1	a	1503	G
1	a	1505	A

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Mol	Chain	Res	Type
1	a	1514	A
1	a	1515	A
1	a	1516	G
1	a	1517	G
1	a	1518	U
1	a	1519	A
1	a	1529	G
1	a	1532	G
1	a	1536	C
1	a	1541	G
1	a	1542	G
1	a	1546	A
23	A	15	G
23	A	23	G
23	A	28	A
23	A	34	U
23	A	39	C
23	A	46	C
23	A	52	A
23	A	61	A
23	A	63	U
23	A	64	A
23	A	71	A
23	A	75	G
23	A	76	C
23	A	80	G
23	A	82	G
23	A	85	G
23	A	90	A
23	A	100	U
23	A	102	A
23	A	104	C
23	A	108	A
23	A	117	A
23	A	118	A
23	A	119	U
23	A	121	G
23	A	130	A
23	A	135	G
23	A	150	A
23	A	161	A
23	A	162	A

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Mol	Chain	Res	Type
23	A	163	U
23	A	164	A
23	A	166	A
23	A	168	A
23	A	173	A
23	A	177	G
23	A	180	G
23	A	182	C
23	A	183	A
23	A	184	C
23	A	185	A
23	A	199	A
23	A	201	C
23	A	202	A
23	A	204	C
23	A	207	A
23	A	218	G
23	A	219	A
23	A	225	A
23	A	229	A
23	A	231	A
23	A	233	U
23	A	236	A
23	A	244	A
23	A	251	G
23	A	255	G
23	A	263	G
23	A	267	G
23	A	282	A
23	A	284	C
23	A	285	U
23	A	286	U
23	A	287	G
23	A	288	C
23	A	289	U
23	A	298	U
23	A	300	G
23	A	301	U
23	A	305	A
23	A	312	A
23	A	314	A
23	A	316	G

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Mol	Chain	Res	Type
23	A	317	G
23	A	318	A
23	A	319	G
23	A	320	U
23	A	321	U
23	A	329	A
23	A	330	C
23	A	331	G
23	A	337	A
23	A	338	G
23	A	342	A
23	A	345	C
23	A	353	A
23	A	354	A
23	A	355	G
23	A	364	A
23	A	365	A
23	A	373	A
23	A	374	U
23	A	389	A
23	A	393	G
23	A	398	C
23	A	401	U
23	A	404	U
23	A	411	A
23	A	418	G
23	A	432	G
23	A	438	U
23	A	451	U
23	A	457	G
23	A	464	U
23	A	468	A
23	A	482	U
23	A	489	A
23	A	490	C
23	A	502	C
23	A	503	A
23	A	504	G
23	A	510	U
23	A	511	G
23	A	525	A
23	A	526	A

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Mol	Chain	Res	Type
23	A	527	G
23	A	530	C
23	A	536	A
23	A	538	G
23	A	543	G
23	A	550	A
23	A	551	G
23	A	553	A
23	A	554	C
23	A	555	C
23	A	572	C
23	A	574	A
23	A	575	G
23	A	576	U
23	A	577	A
23	A	578	G
23	A	588	G
23	A	589	U
23	A	591	A
23	A	593	U
23	A	594	G
23	A	599	A
23	A	605	U
23	A	606	G
23	A	611	U
23	A	613	G
23	A	618	A
23	A	628	G
23	A	629	A
23	A	630	G
23	A	631	U
23	A	646	A
23	A	650	U
23	A	657	U
23	A	658	A
23	A	659	A
23	A	660	A
23	A	661	U
23	A	663	U
23	A	665	G
23	A	682	A
23	A	683	G

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Mol	Chain	Res	Type
23	A	690	U
23	A	693	G
23	A	698	U
23	A	713	A
23	A	715	A
23	A	716	C
23	A	727	G
23	A	731	U
23	A	732	C
23	A	733	U
23	A	760	A
23	A	762	C
23	A	763	A
23	A	771	G
23	A	774	G
23	A	775	A
23	A	777	C
23	A	785	C
23	A	792	U
23	A	793	G
23	A	795	A
23	A	797	A
23	A	806	A
23	A	807	U
23	A	809	A
23	A	820	G
23	A	827	A
23	A	828	A
23	A	829	U
23	A	834	A
23	A	835	U
23	A	837	G
23	A	838	A
23	A	845	A
23	A	847	A
23	A	848	U
23	A	850	G
23	A	852	U
23	A	864	A
23	A	872	U
23	A	873	U
23	A	875	G

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Mol	Chain	Res	Type
23	A	876	G
23	A	887	A
23	A	891	A
23	A	904	G
23	A	905	U
23	A	911	A
23	A	912	C
23	A	913	U
23	A	921	C
23	A	922	G
23	A	923	A
23	A	924	G
23	A	925	G
23	A	926	G
23	A	929	C
23	A	930	C
23	A	932	U
23	A	936	G
23	A	938	G
23	A	944	G
23	A	945	A
23	A	955	A
23	A	959	C
23	A	962	A
23	A	963	A
23	A	968	A
23	A	970	U
23	A	985	A
23	A	987	U
23	A	989	A
23	A	990	G
23	A	1001	A
23	A	1002	U
23	A	1003	A
23	A	1005	G
23	A	1006	G
23	A	1017	A
23	A	1018	A
23	A	1033	G
23	A	1040	A
23	A	1041	G
23	A	1052	A

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Mol	Chain	Res	Type
23	A	1053	A
23	A	1055	A
23	A	1056	U
23	A	1057	A
23	A	1066	G
23	A	1067	U
23	A	1069	G
23	A	1070	A
23	A	1073	A
23	A	1077	U
23	A	1079	U
23	A	1083	G
23	A	1085	U
23	A	1088	C
23	A	1091	G
23	A	1097	U
23	A	1098	A
23	A	1101	A
23	A	1104	U
23	A	1105	U
23	A	1106	G
23	A	1107	G
23	A	1108	C
23	A	1110	U
23	A	1112	G
23	A	1113	A
23	A	1114	A
23	A	1115	G
23	A	1116	C
23	A	1119	C
23	A	1120	C
23	A	1121	A
23	A	1122	U
23	A	1123	C
23	A	1124	A
23	A	1125	U
23	A	1126	U
23	A	1128	A
23	A	1131	G
23	A	1132	A
23	A	1133	G
23	A	1134	U

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Mol	Chain	Res	Type
23	A	1135	G
23	A	1138	U
23	A	1139	A
23	A	1140	A
23	A	1143	G
23	A	1145	U
23	A	1146	C
23	A	1149	U
23	A	1150	A
23	A	1154	G
23	A	1156	G
23	A	1158	G
23	A	1160	C
23	A	1163	U
23	A	1170	A
23	A	1172	A
23	A	1177	A
23	A	1178	C
23	A	1179	C
23	A	1185	U
23	A	1199	A
23	A	1213	C
23	A	1216	U
23	A	1217	U
23	A	1218	G
23	A	1225	G
23	A	1226	G
23	A	1234	G
23	A	1244	G
23	A	1245	G
23	A	1248	U
23	A	1250	G
23	A	1252	A
23	A	1258	A
23	A	1265	G
23	A	1267	A
23	A	1273	G
23	A	1276	G
23	A	1278	G
23	A	1286	G
23	A	1287	U
23	A	1288	G

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Mol	Chain	Res	Type
23	A	1289	A
23	A	1291	A
23	A	1293	U
23	A	1294	G
23	A	1300	G
23	A	1303	A
23	A	1305	U
23	A	1306	C
23	A	1308	C
23	A	1309	G
23	A	1310	A
23	A	1312	A
23	A	1323	A
23	A	1337	A
23	A	1338	U
23	A	1339	U
23	A	1345	A
23	A	1350	U
23	A	1358	A
23	A	1359	A
23	A	1361	G
23	A	1363	U
23	A	1369	G
23	A	1378	U
23	A	1379	A
23	A	1398	G
23	A	1404	A
23	A	1405	G
23	A	1416	U
23	A	1417	G
23	A	1421	A
23	A	1423	C
23	A	1429	G
23	A	1432	A
23	A	1435	C
23	A	1451	U
23	A	1452	C
23	A	1454	U
23	A	1455	U
23	A	1458	A
23	A	1459	A
23	A	1463	A

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Mol	Chain	Res	Type
23	A	1464	U
23	A	1471	A
23	A	1472	C
23	A	1473	G
23	A	1479	G
23	A	1480	G
23	A	1489	A
23	A	1490	G
23	A	1491	C
23	A	1494	G
23	A	1495	C
23	A	1496	G
23	A	1498	U
23	A	1499	U
23	A	1503	U
23	A	1504	U
23	A	1510	U
23	A	1511	C
23	A	1512	U
23	A	1519	U
23	A	1520	A
23	A	1522	G
23	A	1526	G
23	A	1533	A
23	A	1534	G
23	A	1536	C
23	A	1537	A
23	A	1550	G
23	A	1551	U
23	A	1552	U
23	A	1553	A
23	A	1555	G
23	A	1559	G
23	A	1561	G
23	A	1568	U
23	A	1576	A
23	A	1577	G
23	A	1578	A
23	A	1579	C
23	A	1580	A
23	A	1582	U
23	A	1583	G

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Mol	Chain	Res	Type
23	A	1584	A
23	A	1586	U
23	A	1587	C
23	A	1590	C
23	A	1592	A
23	A	1593	G
23	A	1594	U
23	A	1605	A
23	A	1606	C
23	A	1614	A
23	A	1616	A
23	A	1625	U
23	A	1630	A
23	A	1631	G
23	A	1632	A
23	A	1633	A
23	A	1635	A
23	A	1636	U
23	A	1651	C
23	A	1652	A
23	A	1653	A
23	A	1655	C
23	A	1659	C
23	A	1660	A
23	A	1661	C
23	A	1662	A
23	A	1670	A
23	A	1678	A
23	A	1690	A
23	A	1691	G
23	A	1692	C
23	A	1697	G
23	A	1698	A
23	A	1704	C
23	A	1709	A
23	A	1717	G
23	A	1718	G
23	A	1722	A
23	A	1738	C
23	A	1739	G
23	A	1742	A
23	A	1743	G

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Mol	Chain	Res	Type
23	A	1751	G
23	A	1759	G
23	A	1768	C
23	A	1772	G
23	A	1784	U
23	A	1785	G
23	A	1790	G
23	A	1791	G
23	A	1800	A
23	A	1801	C
23	A	1808	U
23	A	1811	A
23	A	1827	C
23	A	1828	U
23	A	1829	A
23	A	1835	U
23	A	1836	A
23	A	1842	A
23	A	1843	U
23	A	1844	G
23	A	1846	A
23	A	1855	G
23	A	1856	A
23	A	1857	C
23	A	1885	G
23	A	1891	U
23	A	1893	A
23	A	1897	U
23	A	1898	C
23	A	1900	G
23	A	1902	G
23	A	1908	A
23	A	1930	G
23	A	1933	G
23	A	1939	A
23	A	1943	A
23	A	1949	G
23	A	1952	C
23	A	1954	A
23	A	1956	G
23	A	1957	G
23	A	1958	U

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Mol	Chain	Res	Type
23	A	1965	A
23	A	1967	U
23	A	1970	U
23	A	1979	A
23	A	1982	U
23	A	1989	C
23	A	1992	C
23	A	1993	A
23	A	1994	C
23	A	1997	A
23	A	1998	A
23	A	1999	G
23	A	2009	U
23	A	2018	U
23	A	2020	U
23	A	2023	C
23	A	2040	A
23	A	2047	A
23	A	2057	A
23	A	2058	A
23	A	2059	G
23	A	2060	A
23	A	2061	U
23	A	2063	C
23	A	2070	C
23	A	2073	G
23	A	2082	C
23	A	2083	G
23	A	2086	A
23	A	2087	A
23	A	2088	G
23	A	2089	A
23	A	2096	G
23	A	2103	U
23	A	2104	A
23	A	2107	G
23	A	2120	G
23	A	2133	G
23	A	2135	U
23	A	2138	U
23	A	2139	A
23	A	2140	C

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Mol	Chain	Res	Type
23	A	2141	A
23	A	2143	G
23	A	2144	A
23	A	2145	U
23	A	2146	A
23	A	2147	G
23	A	2148	G
23	A	2153	A
23	A	2155	C
23	A	2159	U
23	A	2160	G
23	A	2162	A
23	A	2163	A
23	A	2170	C
23	A	2172	C
23	A	2173	U
23	A	2175	G
23	A	2176	C
23	A	2178	U
23	A	2180	C
23	A	2184	G
23	A	2185	A
23	A	2188	C
23	A	2191	U
23	A	2193	G
23	A	2194	U
23	A	2195	G
23	A	2197	G
23	A	2200	A
23	A	2203	A
23	A	2206	C
23	A	2208	A
23	A	2209	G
23	A	2217	G
23	A	2221	U
23	A	2225	A
23	A	2226	A
23	A	2230	G
23	A	2231	C
23	A	2240	U
23	A	2241	C
23	A	2252	A

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Mol	Chain	Res	Type
23	A	2254	A
23	A	2265	G
23	A	2266	G
23	A	2270	U
23	A	2286	G
23	A	2290	C
23	A	2293	A
23	A	2294	A
23	A	2295	A
23	A	2305	A
23	A	2310	C
23	A	2314	A
23	A	2326	G
23	A	2331	G
23	A	2332	U
23	A	2335	G
23	A	2336	A
23	A	2337	A
23	A	2339	U
23	A	2347	A
23	A	2354	A
23	A	2360	A
23	A	2361	U
23	A	2362	A
23	A	2372	G
23	A	2374	C
23	A	2377	C
23	A	2380	G
23	A	2381	A
23	A	2402	G
23	A	2410	G
23	A	2412	C
23	A	2417	U
23	A	2418	G
23	A	2419	A
23	A	2429	U
23	A	2430	C
23	A	2433	C
23	A	2447	C
23	A	2450	U
23	A	2451	C
23	A	2452	A

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Mol	Chain	Res	Type
23	A	2454	C
23	A	2455	G
23	A	2456	G
23	A	2457	A
23	A	2458	U
23	A	2461	A
23	A	2462	A
23	A	2468	C
23	A	2472	G
23	A	2475	A
23	A	2486	A
23	A	2492	C
23	A	2495	A
23	A	2496	A
23	A	2502	C
23	A	2505	A
23	A	2511	G
23	A	2516	G
23	A	2518	U
23	A	2525	C
23	A	2529	G
23	A	2530	A
23	A	2531	U
23	A	2532	G
23	A	2533	U
23	A	2545	A
23	A	2546	U
23	A	2547	C
23	A	2552	G
23	A	2561	C
23	A	2576	G
23	A	2579	U
23	A	2583	C
23	A	2589	U
23	A	2593	A
23	A	2594	G
23	A	2599	A
23	A	2600	C
23	A	2601	G
23	A	2603	G
23	A	2604	A
23	A	2605	G

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Mol	Chain	Res	Type
23	A	2612	U
23	A	2613	C
23	A	2623	U
23	A	2624	G
23	A	2629	A
23	A	2630	G
23	A	2636	U
23	A	2637	C
23	A	2638	C
23	A	2640	U
23	A	2641	A
23	A	2657	G
23	A	2667	G
23	A	2668	A
23	A	2681	A
23	A	2683	U
23	A	2688	G
23	A	2690	G
23	A	2704	A
23	A	2708	C
23	A	2716	U
23	A	2717	A
23	A	2739	U
23	A	2741	G
23	A	2753	U
23	A	2756	G
23	A	2760	A
23	A	2771	G
23	A	2775	A
23	A	2777	A
23	A	2778	G
23	A	2791	A
23	A	2792	A
23	A	2793	G
23	A	2794	C
23	A	2798	C
23	A	2803	A
23	A	2805	A
23	A	2806	U
23	A	2807	G
23	A	2817	A
23	A	2820	U

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Mol	Chain	Res	Type
23	A	2821	U
23	A	2822	C
23	A	2823	G
23	A	2824	G
23	A	2827	A
23	A	2828	U
23	A	2838	C
23	A	2840	A
23	A	2850	G
23	A	2853	U
23	A	2868	G
23	A	2869	G
23	A	2880	A
23	A	2881	C
23	A	2886	G
23	A	2887	G
23	A	2892	G
23	A	2896	A
23	A	2899	A
23	A	2900	C
23	A	2903	A
23	A	2906	G
23	A	2911	A
23	A	2913	G
23	A	2920	U
24	B	8	A
24	B	10	U
24	B	13	A
24	B	23	U
24	B	24	C
24	B	33	U
24	B	35	C
24	B	38	U
24	B	39	G
24	B	40	C
24	B	42	G
24	B	49	G
24	B	51	A
24	B	55	A
24	B	60	C
24	B	67	G
24	B	84	U

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Mol	Chain	Res	Type
24	B	87	G
24	B	88	U
24	B	92	G
24	B	93	C
24	B	106	U
24	B	113	G

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	A	162	A
23	A	179	A
23	A	300	G
23	A	311	U
23	A	437	A
23	A	593	U
23	A	863	G
23	A	961	G
23	A	1104	U
23	A	1288	G
23	A	1478	A
23	A	1532	U
23	A	2039	G
23	A	2360	A
23	A	2418	G
23	A	2432	G
23	A	2467	C
23	A	2501	U

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	A	1
25	D	1
42	Y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1569:G	O3'	1570:G	P	3.00
1	Y	25:GLY	C	26:LYS	N	1.74
1	D	5:TYR	C	6:LYS	N	1.17