



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

Aug 24, 2017 – 05:58 AM EDT

PDB ID : 5LZE  
EMDB ID: : EMD-4125  
Title : Structure of the 70S ribosome with Sec-tRNA<sup>Sec</sup> in the classical pre-translocation state (C)  
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.  
Deposited on : unknown  
Resolution : 3.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
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

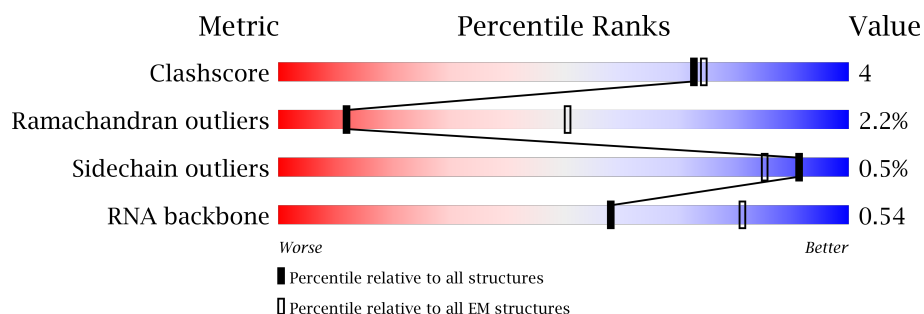
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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





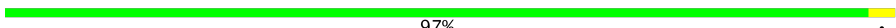










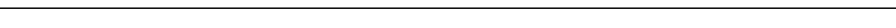











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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

Mol	Chain	Length	Quality of chain
1	a	1539	69% 28% .
2	b	218	97% .
3	c	206	99% .
4	d	205	99% .
5	e	157	94% . .
6	f	100	93% 5% .
7	g	151	98% .
8	h	129	98% .

























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Mol	Chain	Length	Quality of chain
9	i	127	 94% 5% .
10	j	98	 94% 5% .
11	k	116	 97% .
12	l	123	 95% . . .
13	m	114	 93% 6% .
14	n	100	 96% .
15	o	88	 92% 7% .
16	p	82	 94% . .
17	q	80	 96% . .
18	r	65	 94% 6%
19	s	79	 96% . .
20	t	85	 100%
21	u	65	 86% 12% .
22	v	77	 65% 31% .
23	x	48	 33% 46% 21%
24	y	95	 72% 26% .
25	A	2903	 62% 29% 8% .
26	B	120	 64% 26% 9% .
27	C	271	 78% 21%
28	D	209	 90% 10%
29	E	201	 88% 11%
30	F	177	 84% 16%
31	G	176	 86% 14% .
32	I	141	 83% 16% .
33	H	149	 81% 16% .

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Mol	Chain	Length	Quality of chain
34	J	142	 89% 11% .
35	K	122	 81% 17% .
36	L	143	 81% 17% ..
37	M	136	 90% 9% .
38	N	120	 88% 12%
39	O	116	 89% 11%
40	P	114	 82% 18%
41	Q	117	 90% 9% .
42	R	103	 82% 17% .
43	S	110	 86% 14%
44	T	93	 84% 16%
45	U	102	 84% 13% .
46	V	94	 82% 18%
47	W	75	 85% 13% .
48	X	77	 82% 18%
49	Y	63	 94% 6%
50	Z	58	 91% 9%
51	0	56	 89% 9% .
52	1	50	 88% 8% .
53	2	46	 83% 17%
54	3	64	 84% 16%
55	4	38	 55% 42% .
56	6	66	 64% 30% 6%
57	w	3	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
25	G7M	A	2069	X	-	-	-

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 148018 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	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- 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
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called tRNA<sup>f</sup>Met.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called fMetSec-tRNA<sup>Sec</sup>.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	95	Total	C	N	O	P	0	0
			2031	907	357	672	95		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2900	Total	C	N	O	P	0	0
			62274	27787	11459	20128	2900		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	U	102	Total	C	N	O	S	0	0
			780	492	146	142			

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 57 is a RNA chain called CCA 3' end of E-site tRNA<sup>Sec</sup> (low occupancy).

Mol	Chain	Residues	Atoms					AltConf	Trace
57	w	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

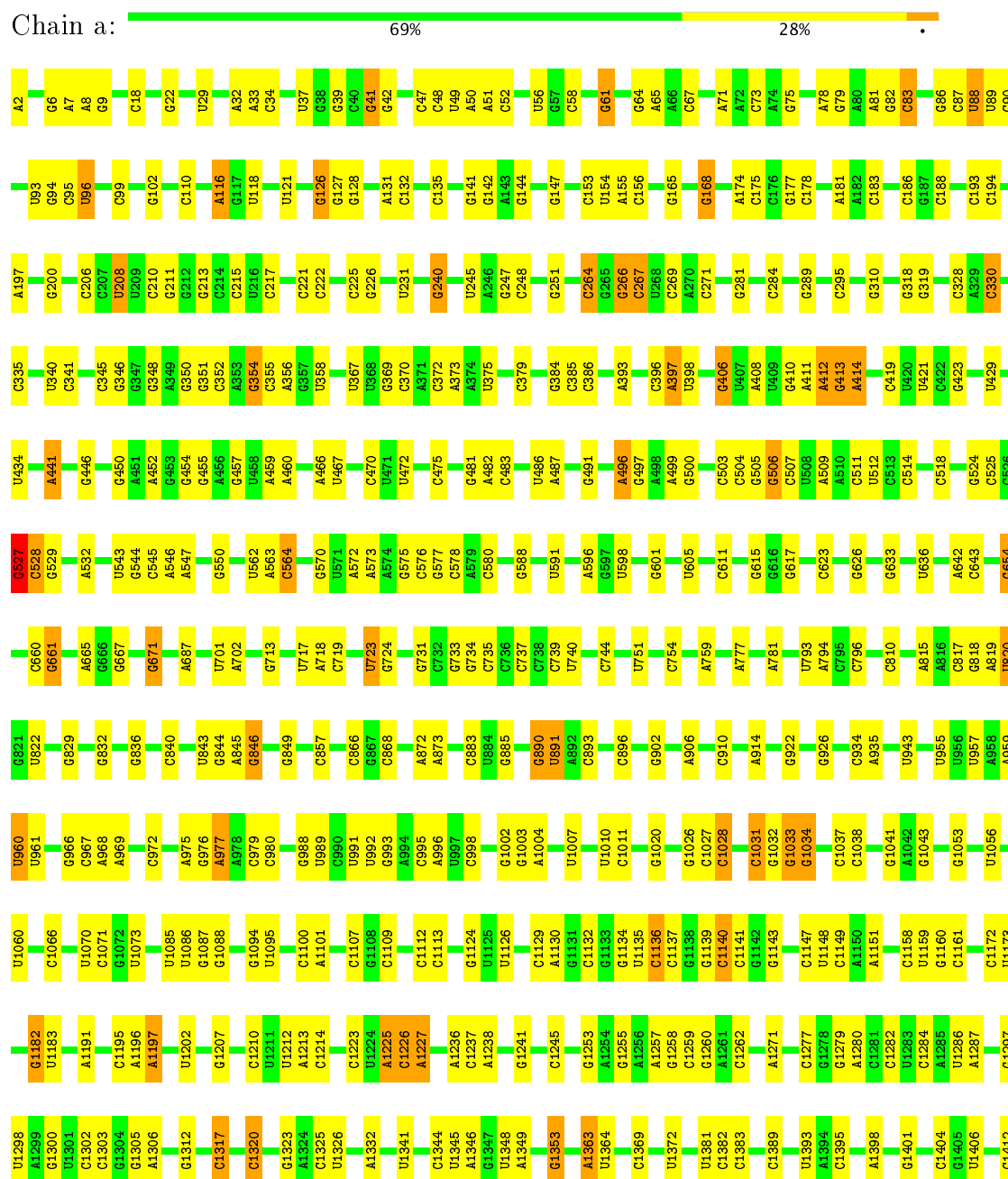
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

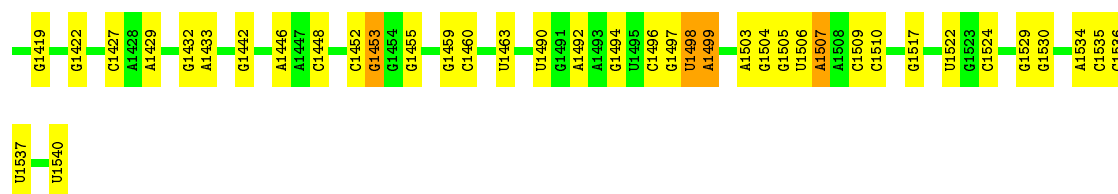
Mol	Chain	Residues	Atoms		AltConf
58	4	1	Total	Zn	0
			1	1	
58	6	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 97%



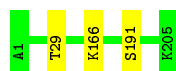
- Molecule 3: 30S ribosomal protein S3

Chain c: 99%



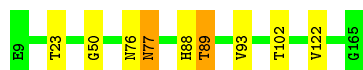
- Molecule 4: 30S ribosomal protein S4

Chain d: 99%



- Molecule 5: 30S ribosomal protein S5

Chain e: 94%



- Molecule 6: 30S ribosomal protein S6

Chain f: 93% 5%



- Molecule 7: 30S ribosomal protein S7

Chain g: 98%



- Molecule 8: 30S ribosomal protein S8



Chain h:  98% .



- Molecule 9: 30S ribosomal protein S9

Chain i:  94% 5% .



- Molecule 10: 30S ribosomal protein S10

Chain j:  94% 5% .



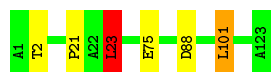
- Molecule 11: 30S ribosomal protein S11

Chain k:  97% .



- Molecule 12: 30S ribosomal protein S12

Chain l:  95% . .



- Molecule 13: 30S ribosomal protein S13

Chain m:  93% 6% .



- Molecule 14: 30S ribosomal protein S14

Chain n:  96% .



- Molecule 15: 30S ribosomal protein S15

Chain o:  92% 7% .



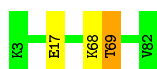
- Molecule 16: 30S ribosomal protein S16

Chain p: 94% ..



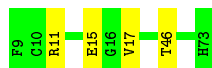
- Molecule 17: 30S ribosomal protein S17

Chain q: 96% ..



- Molecule 18: 30S ribosomal protein S18

Chain r: 94% 6%



- Molecule 19: 30S ribosomal protein S19

Chain s: 96% ..



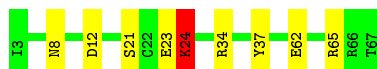
- Molecule 20: 30S ribosomal protein S20

Chain t: 100%

There are no outlier residues recorded for this chain.

- Molecule 21: 30S ribosomal protein S21

Chain u: 86% 12% .



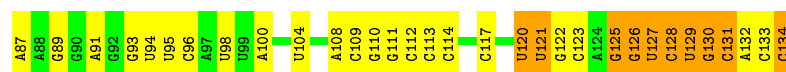
- Molecule 22: tRNAfMet

Chain v: 65% 31% .



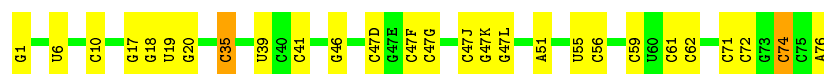
- Molecule 23: SECIS mRNA

Chain x:  33% 46% 21%



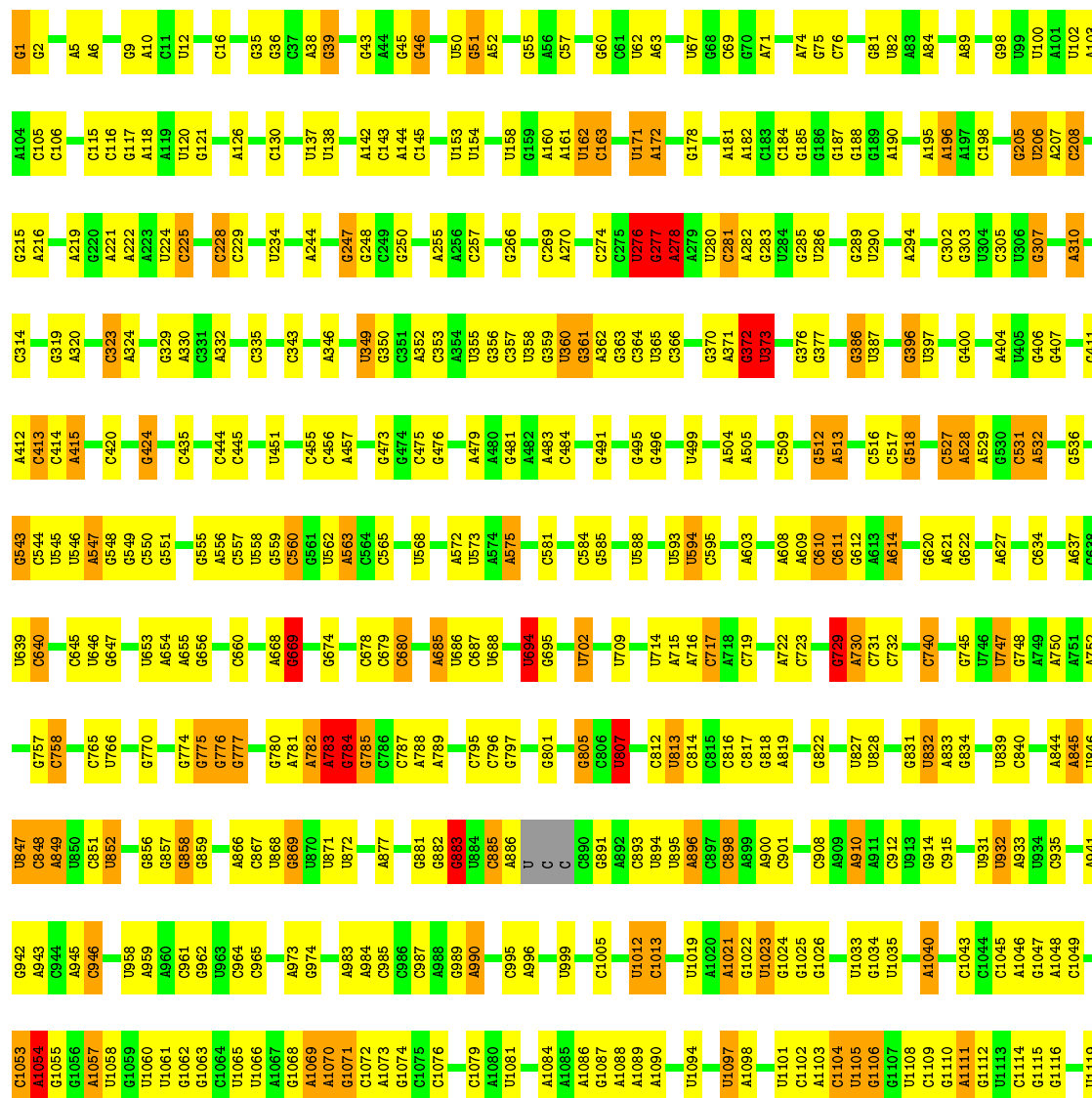
• Molecule 24: fMetSec-tRNA<sup>Sec</sup>

Chain y:  72% 26% .



• Molecule 25: 23S ribosomal RNA

Chain A:  62% 29% 8% .

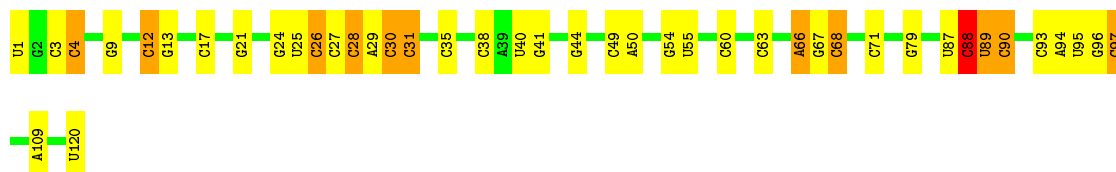


G2742	A2634	A2518	G2415	C2300	U2195	G2116	G2032	C1914	C1795	U1669	C1558	U1438	U1325	C1211	G1124
U2743	A2635	U2519	C2416	C2301	U2196	A2117	A2033	?1915	U1796	A1669	U1559	G1450	U1326	G1212	G1125
C2745	C2636	C2520	C2417	U2302	A2118	A2119	G2034	U1916	U1797	G1674	G1560	G1451	G1331	A1213	A1126
		G2535	A2418	U2305	A2199	G2120	G2035	U1917	U1798			A1452	G1332	G1223	A1127
A2748	C2646	A2542	C2424	C2306	C2200	G2121	C2036	A1918	C1800	U1680	C1564	G1453	U1340	G1227	U1132
C2782	C2651			G2307	G2204	U2122	G2040	A1919	A1801	G1681	U1567	G1454			
C2785	C2651			C2308	G2204		U2041	C1920		U1683	G1455				
C2785	C2651			A2309	G2204		A2042	G1929	C1804	U1683	G1455				
C2785	C2651			U2312	A2211	G2125	C2043	U1931	A1805	U1683	U1568	G1455			
A2757	G2663	U2554	A2430	U2321	U2213	G2128	C2044	U1931	A1808	U1683	U1568	U1458	G1344	A1237	G1136
A2758				C2321	U2214	C2129	C2047	A1932	A1809	U1683	U1568	U1459	C1345	G1238	G1137
G2759	C2686			A2322	C2215	U2130	G2047	G1933	A1809	U1683	U1568	U1460	C1348	G1238	G1138
							G2048					C1461		U1240	
C2762	G2669	A2566	U2438	G2325	C2222	U2131	G2049	A1936	U1812	U1715	U1578	C1462			U1141
G2763	C2676	C2567	C2428	C2326	G2223	U2132	C2050	A1937	U1813	U1716		C1463			A1142
A2764	C2676	U2568	U2441	A2327	G2224	G2133	C2055	U1939	C1816	U1716	G1581				U1148
A2765	C2677	G2569	C2442	C2328	A2225	U2137	G2056	U1940	C1817	G1723	U1584				A1151
A2766	C2678		C2443	U2329	C2226			A1941	A1829	G1724		G1475			A1155
U2768	A2682	C2572	G2444	G2330	C2238	G2140	A2059	C1942	C1830	U1729	G1588	G1478	A1365	A1253	A1156
U2768	C2683	C2573	G2445	G2331	G2239	G2141	A2060	G1945	C1833	C1730	U1589	G1478	G1368	G1256	G1157
U2769	C2683	C2574	G2446	C2332	G2239	A2142	A2061	U1946	C1833	C1731		G1482			C1158
	U2684	G2575	G2447	A2333			A2062	C1947	C1838	C1732	A1597	G1482	C1376	A1264	U1159
A2778	C2685	G2576	A2448	A2333	U2243	C2145	C2063		C1839	C1733	A1598				
U2779	G2686		U2449	C2347	U2244	C2146	C2064		C1839	C1734					
			A2450			A2147	C2065	U1955	C1843	A1735	G1601	U1487			
G2782	U2689	U2584	C2456	C2350	A2247			C1958	C1843	U1736		C1488	U1379	U1267	C1164
U2783	C2690	U2586		G2353	C2248	C2152	G2069		C1843	U1736		C1488	U1379	U1267	A1165
U2784	C2691			C2353	U2249	C2153	A2070	U1958	C1847	C1737	A1607	C1498	A1383	C1270	A1169
C2785				C2354	G2250	A2163	A2071	U1963	A1847	C1738	A1608	C1499		G1271	G1170
	U2698	G2591	G2464	C2359	G2251	A2158	C2072		G1857	A1744	A1504		C1386	A1272	G1171
C2788	C2698	G2592	C2465			G2159		A1966	A1858	A1745		A1387	A1388	U1273	C1172
C2789	C2699	C2599	C2467	C2364	C2258	C2160	U2076	C1967		A1746	C1507	U1394		U1273	U1173
G2791	C2704	C2601	A2468		U2262	C2161	U2086	A1970	C1868	U1747	C1615	A1395		C1278	U1174
A2792	U2707	A2602	A2469	G2375	C2263	A2163	G2087	U1971	C1869		A1616	A1509		G1279	A1175
C2793	G2708	G2603	G2470	A2376	C2264	C2164	A2088	G1972	C1870	C1752	G1617	G1510			U1176
C2794				A2377		C2165			A1871				C1398	A1287	G1177
				A2378	A2267	U2166	C2091	U1979	A1872	U1758	G1622	U1513		G1288	C1178
U2797		U2609	U2473	U2378	A2268	C2167	U2092	U1991	C1873	A1759	G1623	G1514	U1402	G1289	G1179
U2798	U2713	C2611	C2475	G2383	A2268	A2170	G2093	U1991	C1874	C1760	U1624	A1515		U1294	U1180
A2799	G2714	U2612	A2476	U2384	G2271	A2171	C2096	G1992	U1880	C1761	A1626	G1524		C1295	U1181
A2800	C2715	U2613	G2481	C2385	G2279	U2172	A2097	U1993	C1884	C1764	G1627		U1413	G1296	G1182
G2801	C2716	U2614	A2482	C2386	G2279	A2173	A2098	C1994				C1531	A1413	U1297	U1183
	C2717	U2615	C2483	C2387	G2282	C2177	U2099		G1891	A1773	A1630	C1532		G1300	G1186
C2805	G2718	U2616	G2484	C2388	G2283	A2178	G2100	C1997	C1892	C1774	A1533	C1533		G1300	G1190
	U2720	U2617	G2494	C2394	C2285	C2179	C2103	G2010	C1894	U1779	G1644	G1536		A1302	A1194
A2809	A2721	C2619		U2402	C2286	U2181	C2104	U2011	A1899	U1781	U1647	G1537		G1303	
	G2722	G2620	G2502	C2403	G2287	U2182	U2105	A2013	A1901	U1782	U1648	U1539		C1306	G1197
G2812	A2813	U2621	G2505	U2404	U2291	A2183	A2108	U2022	A1901	A1783	G1546	G1432		U1313	U1199
A2814		U2624	U2506	G2405	U2292	A2184	U2109	G2023	A1901	A1784	G1547	G1432		U1314	C1200
	U2818	G2625		A2406	U2292	U2185	G2110	G2024	A1901	A1787	C1548	G1433		C1315	A1204
U2819	G2731	C2626	C2512	A2407	G2293	G2186	U2111	G2025	G1906	A1787	A1549	A1434		G1316	A1205
A2820	G2732	C2627	A2513	U2408	G2294		U2112	C2025	G1907	A1791	A1556	G1436		G1317	
G2821	A2733	U2628	U2514	G2409	G2294	U2189	G2112		C1908						
		U2629	C2515	G2410	A2297	U2192	U2113	N2030		A1794	C1557				
G2822		G2630						A2031	A1913						



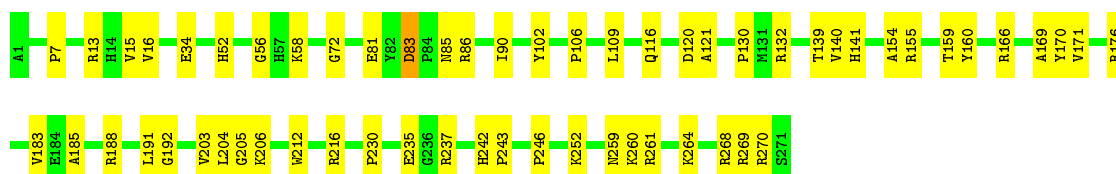
• Molecule 26: 5S ribosomal RNA

Chain B: 64% 26% 9%



• Molecule 27: 50S ribosomal protein L2

Chain C: 78% 21%



• Molecule 28: 50S ribosomal protein L3

Chain D: 90% 10%



• Molecule 29: 50S ribosomal protein L4

Chain E: 88% 11%



• Molecule 30: 50S ribosomal protein L5

Chain F: 84% 16%

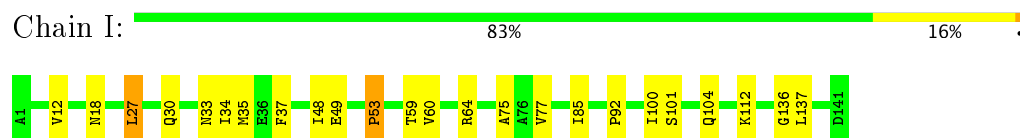


• Molecule 31: 50S ribosomal protein L6

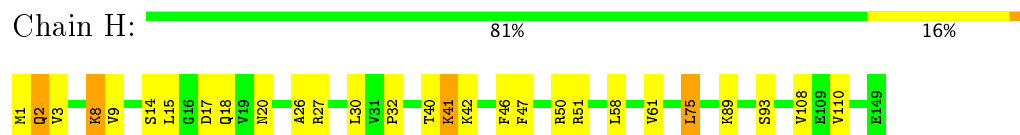
Chain G: 86% 14%



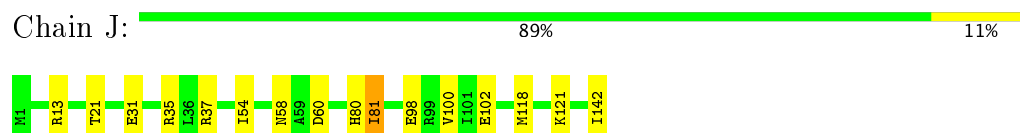
- Molecule 32: 50S ribosomal protein L11



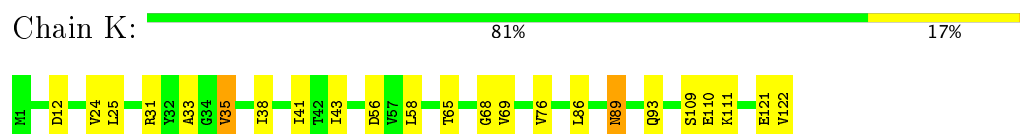
- Molecule 33: 50S ribosomal protein L9



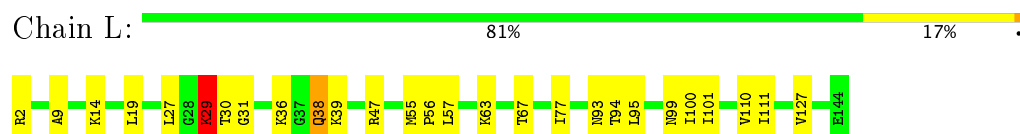
- Molecule 34: 50S ribosomal protein L13



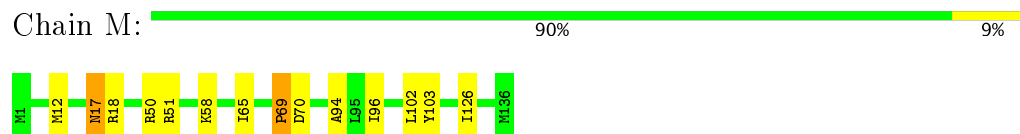
- Molecule 35: 50S ribosomal protein L14



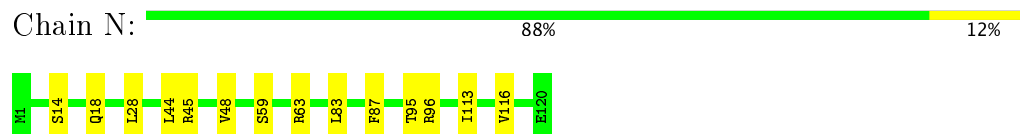
- Molecule 36: 50S ribosomal protein L15




- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17




- Molecule 39: 50S ribosomal protein L18

Chain O:  89% 11%




- Molecule 40: 50S ribosomal protein L19

Chain P:  82% 18%




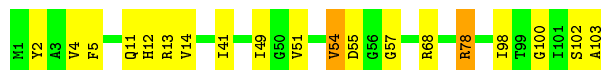
- Molecule 41: 50S ribosomal protein L20

Chain Q:  90% 9%




- Molecule 42: 50S ribosomal protein L21

Chain R:  82% 17%




- Molecule 43: 50S ribosomal protein L22

Chain S:  86% 14%




- Molecule 44: 50S ribosomal protein L23

Chain T:  84% 16%




- Molecule 45: 50S ribosomal protein L24

Chain U:  84% 13%



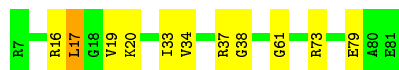
- Molecule 46: 50S ribosomal protein L25

Chain V:  82% 18%



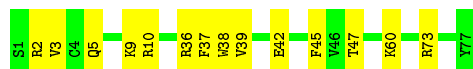
- Molecule 47: 50S ribosomal protein L27

Chain W: 85% 13%



- Molecule 48: 50S ribosomal protein L28

Chain X: 82% 18%



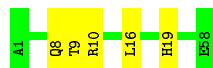
- Molecule 49: 50S ribosomal protein L29

Chain Y: 94% 6%



- Molecule 50: 50S ribosomal protein L30

Chain Z: 91% 9%



- Molecule 51: 50S ribosomal protein L32

Chain 0: 89% 9%



- Molecule 52: 50S ribosomal protein L33

Chain 1: 88% 8%



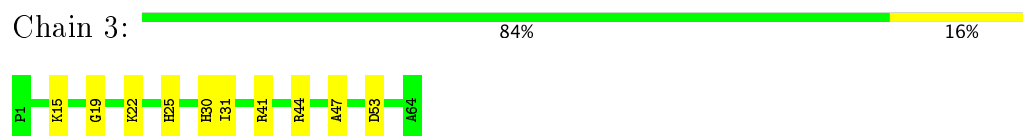
- Molecule 53: 50S ribosomal protein L34

Chain 2: 83% 17%

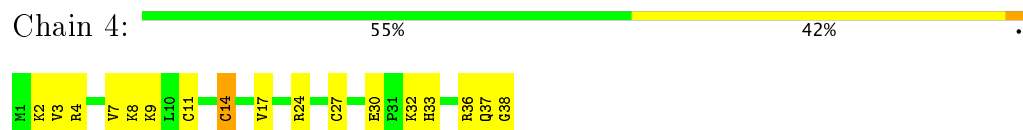




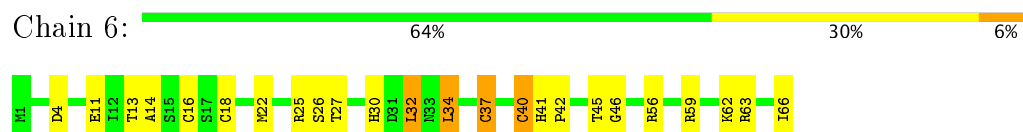
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L31



- Molecule 57: CCA 3' end of E-site tRNA<sup>Sec</sup> (low occupancy)



There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	130705	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 3TD, ZN, 6IA, OMG, 5MC, MA6, G7M, OMC, H2U, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, 4SU, 1MG, PSU

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	0.84	6/36701 (0.0%)	1.37	537/57246 (0.9%)
10	j	0.44	0/797	0.78	0/1077
11	k	0.46	0/886	0.71	1/1195 (0.1%)
12	l	0.43	0/969	0.77	1/1300 (0.1%)
13	m	0.46	0/893	0.82	3/1193 (0.3%)
14	n	0.51	0/806	0.68	0/1074
15	o	0.45	0/722	0.73	2/964 (0.2%)
16	p	0.53	0/659	0.84	1/884 (0.1%)
17	q	0.49	0/658	0.78	1/881 (0.1%)
18	r	0.46	0/512	0.74	1/689 (0.1%)
19	s	0.50	0/653	0.87	3/877 (0.3%)
2	b	0.44	0/1736	0.69	1/2338 (0.0%)
20	t	0.44	0/671	0.64	0/888
21	u	0.53	0/501	0.98	2/668 (0.3%)
22	v	0.79	1/1747 (0.1%)	1.48	44/2721 (1.6%)
23	x	0.91	3/1145 (0.3%)	1.67	32/1781 (1.8%)
24	y	0.67	1/2162 (0.0%)	1.42	33/3351 (1.0%)
25	A	0.93	12/69171 (0.0%)	1.32	778/107904 (0.7%)
26	B	0.76	1/2873 (0.0%)	1.41	53/4478 (1.2%)
27	C	0.54	0/2122	0.74	2/2852 (0.1%)
28	D	0.48	0/1586	0.70	0/2134
29	E	0.49	0/1571	0.67	2/2113 (0.1%)
3	c	0.44	0/1652	0.63	0/2225
30	F	0.48	0/1435	0.74	1/1926 (0.1%)
31	G	0.45	0/1343	0.66	2/1816 (0.1%)
32	I	0.43	0/1046	0.71	1/1410 (0.1%)
33	H	0.40	0/1122	0.70	1/1515 (0.1%)
34	J	0.50	0/1152	0.64	0/1551
35	K	0.53	0/948	0.74	1/1268 (0.1%)
36	L	0.50	0/1054	0.78	1/1403 (0.1%)
37	M	0.47	0/1093	0.68	1/1460 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	N	0.49	0/974	0.68	0/1301
39	O	0.45	0/902	0.61	0/1209
4	d	0.42	0/1665	0.64	0/2227
40	P	0.50	0/929	0.70	1/1242 (0.1%)
41	Q	0.59	0/960	0.68	1/1278 (0.1%)
42	R	0.47	0/829	0.72	2/1107 (0.2%)
43	S	0.47	0/864	0.66	1/1156 (0.1%)
44	T	0.44	0/745	0.60	0/994
45	U	0.49	0/788	0.82	4/1051 (0.4%)
46	V	0.44	0/766	0.62	1/1025 (0.1%)
47	W	0.49	0/582	0.64	0/769
48	X	0.49	0/635	0.59	0/848
49	Y	0.42	0/510	0.61	0/677
5	e	0.49	0/1170	0.74	2/1573 (0.1%)
50	Z	0.39	0/453	0.65	0/605
51	0	0.51	0/450	0.75	0/599
52	1	0.47	0/417	0.78	1/554 (0.2%)
53	2	0.49	0/380	0.65	0/498
54	3	0.49	0/513	0.65	0/676
55	4	0.79	1/303 (0.3%)	1.05	1/397 (0.3%)
56	6	0.60	1/532 (0.2%)	1.09	4/709 (0.6%)
57	w	0.28	0/68	1.00	0/103
6	f	0.51	0/836	0.85	3/1128 (0.3%)
7	g	0.42	0/1196	0.62	0/1602
8	h	0.47	0/989	0.69	0/1326
9	i	0.49	1/1034 (0.1%)	0.78	1/1375 (0.1%)
All	All	0.79	27/159876 (0.0%)	1.22	1527/239211 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	2	0
10	j	0	3
12	l	0	2
13	m	0	2
15	o	0	1
16	p	0	1
17	q	0	1
19	s	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
21	u	0	2
25	A	2	0
27	C	0	1
28	D	0	1
29	E	0	1
30	F	0	1
33	H	0	3
35	K	0	1
36	L	0	1
45	U	0	2
5	e	0	3
51	0	0	1
52	1	0	1
54	3	0	1
6	f	0	2
9	i	0	2
All	All	4	35

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	1	G	OP3-P	-10.82	1.48	1.61
25	A	1	G	OP3-P	-10.72	1.48	1.61
22	v	1	C	OP3-P	-10.66	1.48	1.61
26	B	1	U	OP3-P	-10.62	1.48	1.61
1	a	2	A	OP3-P	-10.55	1.48	1.61
23	x	87	A	OP3-P	-10.53	1.48	1.61
55	4	27	CYS	CB-SG	8.23	1.96	1.82
1	a	1034	G	C6-O6	-7.96	1.17	1.24
25	A	1784	A	N7-C5	-7.30	1.34	1.39
25	A	984	A	N9-C4	-7.18	1.33	1.37
25	A	528	A	N9-C4	-6.99	1.33	1.37
25	A	783	A	N7-C5	-5.80	1.35	1.39
23	x	128	C	O3'-P	5.71	1.68	1.61
1	a	2	A	N7-C5	-5.68	1.35	1.39
25	A	360	U	C4-O4	-5.59	1.19	1.23
25	A	1105	U	C2-N3	-5.57	1.33	1.37
25	A	278	A	N9-C4	5.56	1.41	1.37
1	a	354	G	C6-N1	-5.48	1.35	1.39
25	A	787	C	O3'-P	-5.47	1.54	1.61
23	x	125	G	O3'-P	5.35	1.67	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1312	G	O3'-P	-5.34	1.54	1.61
25	A	1081	U	C4-O4	-5.33	1.19	1.23
1	a	1140	C	N3-C4	-5.32	1.30	1.33
56	6	40	CYS	CB-SG	5.19	1.91	1.82
25	A	1779	U	C5-C6	-5.16	1.29	1.34
9	i	90	ASP	CB-CG	5.07	1.62	1.51
25	A	528	A	N7-C5	-5.04	1.36	1.39

All (1527) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	529	G	C5-C6-O6	-14.39	119.96	128.60
24	y	35	C	C5-C6-N1	13.59	127.79	121.00
1	a	1027	C	C5-C6-N1	13.56	127.78	121.00
25	A	1313	U	N3-C2-O2	-12.91	113.16	122.20
24	y	35	C	C6-N1-C2	-12.72	115.21	120.30
25	A	1313	U	N1-C2-O2	12.61	131.63	122.80
1	a	215	C	N1-C2-O2	12.52	126.41	118.90
1	a	1003	G	N3-C2-N2	-12.32	111.27	119.90
25	A	278	A	C2-N3-C4	11.81	116.50	110.60
25	A	1081	U	N3-C2-O2	-11.45	114.19	122.20
1	a	1034	G	C5-C6-O6	-11.40	121.76	128.60
1	a	1034	G	C5-C6-N1	11.25	117.13	111.50
23	x	120	U	N1-C2-O2	11.08	130.56	122.80
56	6	32	LEU	CA-CB-CG	11.08	140.78	115.30
25	A	62	U	N1-C2-O2	11.04	130.53	122.80
25	A	1087	G	N3-C2-N2	-11.03	112.18	119.90
23	x	120	U	N3-C2-O2	-10.93	114.55	122.20
1	a	1134	G	N3-C2-N2	-10.81	112.33	119.90
25	A	2103	C	N1-C2-O2	-10.72	112.47	118.90
26	B	12	C	N1-C2-O2	10.70	125.32	118.90
25	A	783	A	N7-C8-N9	10.58	119.09	113.80
25	A	137	U	N3-C2-O2	-10.55	114.81	122.20
23	x	133	C	N1-C2-O2	10.54	125.23	118.90
26	B	4	C	C5-C6-N1	10.50	126.25	121.00
1	a	206	C	N1-C2-O2	-10.46	112.62	118.90
25	A	281	C	C6-N1-C2	-10.41	116.14	120.30
25	A	1101	U	N3-C2-O2	-10.38	114.94	122.20
1	a	1455	G	N1-C6-O6	10.36	126.11	119.90
25	A	1920	C	C6-N1-C2	-10.30	116.18	120.30
25	A	783	A	C8-N9-C4	-10.17	101.73	105.80
1	a	719	C	N1-C2-O2	10.16	125.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1507	C	C6-N1-C2	-10.16	116.24	120.30
1	a	355	C	N3-C2-O2	-10.13	114.81	121.90
1	a	355	C	N1-C2-O2	10.12	124.97	118.90
23	x	125	G	N9-C1'-C2'	-10.10	100.87	114.00
1	a	1395	C	N1-C2-O2	10.07	124.94	118.90
1	a	1349	A	O5'-P-OP1	-10.06	96.65	105.70
26	B	4	C	C6-N1-C2	-10.05	116.28	120.30
25	A	2072	C	C5-C6-N1	9.96	125.98	121.00
25	A	2072	C	C6-N1-C2	-9.94	116.32	120.30
1	a	719	C	N3-C2-O2	-9.88	114.99	121.90
25	A	1105	U	N3-C2-O2	-9.81	115.33	122.20
25	A	1180	U	C5-C4-O4	-9.79	120.03	125.90
25	A	2036	C	C6-N1-C2	-9.78	116.39	120.30
1	a	1141	C	N1-C2-O2	9.77	124.76	118.90
1	a	1027	C	C4-C5-C6	-9.76	112.52	117.40
1	a	1404	C	C6-N1-C2	-9.70	116.42	120.30
25	A	2036	C	C5-C6-N1	9.69	125.84	121.00
26	B	97	C	C2-N1-C1'	9.65	129.41	118.80
1	a	168	G	C5-C6-O6	-9.64	122.82	128.60
1	a	1317	C	N1-C2-O2	9.63	124.68	118.90
25	A	1081	U	N3-C4-C5	9.59	120.36	114.60
25	A	1314	C	C6-N1-C2	-9.59	116.46	120.30
25	A	283	G	N3-C2-N2	-9.55	113.21	119.90
25	A	546	U	N3-C2-O2	-9.55	115.51	122.20
25	A	1993	U	N1-C2-O2	9.54	129.47	122.80
1	a	1317	C	N3-C2-O2	-9.52	115.24	121.90
1	a	1140	C	N1-C2-O2	9.51	124.60	118.90
26	B	30	C	C6-N1-C2	-9.49	116.50	120.30
25	A	62	U	N3-C2-O2	-9.49	115.56	122.20
24	y	59	C	N1-C2-O2	9.47	124.58	118.90
1	a	529	G	N1-C6-O6	9.46	125.58	119.90
25	A	783	A	C5-N7-C8	-9.43	99.18	103.90
16	p	44	SER	N-CA-CB	-9.42	96.37	110.50
22	v	67	C	N1-C2-O2	9.42	124.55	118.90
1	a	1325	C	C6-N1-C2	-9.42	116.53	120.30
1	a	215	C	N3-C2-O2	-9.40	115.32	121.90
1	a	1034	G	C4-C5-N7	9.40	114.56	110.80
1	a	1395	C	N3-C2-O2	-9.39	115.33	121.90
1	a	186	C	N1-C2-O2	9.38	124.53	118.90
25	A	1081	U	N1-C2-O2	9.38	129.36	122.80
25	A	1313	U	C2-N1-C1'	9.37	128.95	117.70
1	a	503	C	C6-N1-C2	-9.35	116.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	120	U	N3-C2-O2	-9.33	115.67	122.20
25	A	1920	C	C5-C6-N1	9.33	125.66	121.00
25	A	2791	G	N3-C2-N2	-9.28	113.40	119.90
1	a	1455	G	C5-C6-O6	-9.26	123.04	128.60
1	a	221	C	N1-C2-O2	9.25	124.45	118.90
23	x	133	C	N3-C2-O2	-9.19	115.47	121.90
25	A	12	U	N3-C2-O2	-9.19	115.77	122.20
1	a	217	C	C6-N1-C2	-9.18	116.63	120.30
22	v	71	C	C6-N1-C2	-9.09	116.67	120.30
1	a	1149	C	N1-C2-O2	9.08	124.34	118.90
25	A	669	G	C2-N3-C4	9.06	116.43	111.90
25	A	1081	U	C2-N3-C4	-8.95	121.63	127.00
1	a	564	C	N1-C2-O2	8.95	124.27	118.90
1	a	457	G	N1-C6-O6	-8.92	114.55	119.90
25	A	1507	C	C5-C6-N1	8.87	125.44	121.00
25	A	962	G	O5'-P-OP1	-8.85	97.73	105.70
26	B	12	C	N3-C2-O2	-8.85	115.70	121.90
1	a	1027	C	C2-N3-C4	8.81	124.31	119.90
1	a	575	G	N3-C2-N2	-8.79	113.74	119.90
25	A	353	C	N1-C2-O2	8.76	124.16	118.90
25	A	557	C	N1-C2-O2	8.75	124.15	118.90
1	a	660	C	N1-C2-O2	8.73	124.14	118.90
25	A	2762	C	C6-N1-C2	-8.70	116.82	120.30
25	A	2409	G	C5-C6-O6	-8.70	123.38	128.60
25	A	2103	C	C2-N3-C4	-8.67	115.56	119.90
25	A	2473	U	N1-C2-O2	8.67	128.87	122.80
26	B	97	C	N1-C2-O2	8.67	124.10	118.90
25	A	1005	C	N1-C2-O2	8.65	124.09	118.90
25	A	2683	C	N1-C2-O2	8.65	124.09	118.90
22	v	51	C	N1-C2-O2	8.65	124.09	118.90
25	A	121	G	N1-C6-O6	8.63	125.08	119.90
25	A	281	C	C5-C6-N1	8.63	125.32	121.00
1	a	215	C	C6-N1-C2	-8.59	116.86	120.30
25	A	1102	C	N1-C2-O2	8.59	124.06	118.90
25	A	557	C	C6-N1-C2	-8.59	116.86	120.30
25	A	807	U	N3-C2-O2	-8.59	116.19	122.20
1	a	623	C	C6-N1-C2	-8.58	116.87	120.30
26	B	97	C	C6-N1-C2	-8.57	116.87	120.30
25	A	277	G	N7-C8-N9	8.55	117.38	113.10
1	a	500	G	N1-C6-O6	8.55	125.03	119.90
25	A	758	C	N3-C2-O2	-8.54	115.92	121.90
25	A	62	U	C2-N1-C1'	8.54	127.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	810	C	C5-C6-N1	8.53	125.26	121.00
22	v	41	C	N1-C2-O2	8.53	124.02	118.90
1	a	385	C	C6-N1-C2	-8.52	116.89	120.30
25	A	883	G	N7-C8-N9	8.51	117.36	113.10
1	a	1028	C	N1-C2-O2	-8.50	113.80	118.90
25	A	2410	G	N3-C2-N2	-8.48	113.96	119.90
25	A	1102	C	N3-C2-O2	-8.47	115.97	121.90
1	a	58	C	N1-C2-O2	-8.43	113.84	118.90
1	a	18	C	C5-C6-N1	8.43	125.21	121.00
26	B	38	C	N1-C2-O2	8.42	123.95	118.90
25	A	1993	U	N3-C2-O2	-8.39	116.33	122.20
25	A	1539	U	C5-C6-N1	8.38	126.89	122.70
22	v	56	C	N1-C2-O2	8.37	123.92	118.90
26	B	30	C	C5-C6-N1	8.37	125.18	121.00
13	m	65	GLU	N-CA-CB	-8.34	95.58	110.60
25	A	2834	G	N7-C8-N9	8.34	117.27	113.10
25	A	669	G	N3-C4-C5	-8.33	124.44	128.60
56	6	18	CYS	CA-CB-SG	-8.31	99.04	114.00
25	A	1498	C	N3-C4-N4	8.30	123.81	118.00
26	B	17	C	N1-C2-O2	8.30	123.88	118.90
23	x	133	C	N1-C1'-C2'	-8.29	102.88	112.00
25	A	2884	U	N3-C2-O2	-8.29	116.40	122.20
26	B	31	C	N1-C2-O2	8.29	123.87	118.90
1	a	102	G	C6-N1-C2	-8.29	120.13	125.10
1	a	544	G	N1-C6-O6	8.27	124.86	119.90
25	A	2226	C	N1-C2-O2	8.26	123.86	118.90
25	A	1087	G	C6-N1-C2	-8.26	120.14	125.10
25	A	1178	C	N1-C2-O2	8.25	123.85	118.90
25	A	2226	C	N3-C2-O2	-8.25	116.12	121.90
25	A	807	U	N1-C2-O2	8.24	128.57	122.80
1	a	1158	C	C2-N1-C1'	8.24	127.86	118.80
25	A	407	G	N1-C6-O6	-8.24	114.96	119.90
25	A	2011	U	N3-C2-O2	-8.22	116.45	122.20
1	a	998	C	N3-C2-O2	-8.21	116.15	121.90
25	A	2742	G	N1-C6-O6	-8.21	114.97	119.90
25	A	413	C	C6-N1-C2	-8.21	117.02	120.30
1	a	1149	C	C6-N1-C2	-8.16	117.03	120.30
22	v	19	G	N1-C6-O6	-8.16	115.00	119.90
1	a	626	G	N1-C6-O6	8.16	124.79	119.90
25	A	581	C	C6-N1-C2	-8.16	117.04	120.30
26	B	4	C	N1-C2-O2	8.15	123.79	118.90
25	A	105	C	C6-N1-C2	-8.14	117.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1716	U	C5-C6-N1	8.13	126.77	122.70
1	a	215	C	N3-C4-N4	8.12	123.69	118.00
25	A	1894	C	N1-C2-O2	8.12	123.77	118.90
25	A	2410	G	C6-N1-C2	-8.11	120.23	125.10
1	a	737	C	C6-N1-C2	-8.09	117.06	120.30
1	a	110	C	N1-C2-O2	8.09	123.75	118.90
25	A	2473	U	N3-C2-O2	-8.09	116.54	122.20
1	a	1003	G	C6-N1-C2	-8.08	120.25	125.10
25	A	1314	C	C5-C6-N1	8.08	125.04	121.00
25	A	1104	C	N1-C2-O2	8.08	123.75	118.90
2	b	73	ARG	N-CA-CB	-8.07	96.07	110.60
1	a	751	U	N3-C2-O2	-8.07	116.55	122.20
22	v	67	C	C6-N1-C2	-8.06	117.08	120.30
22	v	71	C	N3-C2-O2	-8.06	116.26	121.90
25	A	1451	C	N1-C2-O2	-8.04	114.07	118.90
1	a	450	G	N1-C6-O6	-8.04	115.08	119.90
25	A	2762	C	N1-C2-O2	8.03	123.72	118.90
1	a	1326	U	N3-C2-O2	-8.02	116.58	122.20
1	a	1149	C	N3-C2-O2	-8.02	116.29	121.90
25	A	2406	A	O5'-P-OP2	-8.01	98.49	105.70
1	a	102	G	N3-C2-N2	-8.01	114.30	119.90
24	y	47(D)	C	C2-N3-C4	-7.97	115.91	119.90
26	B	120	U	N1-C2-O2	7.96	128.38	122.80
19	s	5	LYS	CB-CA-C	-7.96	94.48	110.40
1	a	1056	U	N3-C2-O2	-7.95	116.63	122.20
1	a	355	C	C6-N1-C2	-7.93	117.13	120.30
25	A	1680	U	N3-C2-O2	-7.92	116.66	122.20
1	a	206	C	C2-N3-C4	-7.91	115.95	119.90
1	a	564	C	N3-C2-O2	-7.90	116.37	121.90
1	a	221	C	N3-C2-O2	-7.89	116.38	121.90
1	a	248	C	N1-C2-O2	7.88	123.62	118.90
25	A	866	A	C5-C6-N6	-7.86	117.41	123.70
25	A	1779	U	C4-C5-C6	7.84	124.41	119.70
1	a	529	G	C4-C5-N7	7.84	113.94	110.80
1	a	503	C	C5-C6-N1	7.83	124.92	121.00
25	A	1345	C	C6-N1-C2	-7.83	117.17	120.30
25	A	12	U	N1-C2-O2	7.83	128.28	122.80
26	B	26	C	N1-C2-O2	7.82	123.59	118.90
9	i	90	ASP	N-CA-CB	-7.82	96.53	110.60
25	A	1178	C	N3-C2-O2	-7.82	116.43	121.90
25	A	867	C	N1-C2-O2	7.82	123.59	118.90
25	A	2704	C	C5-C6-N1	7.80	124.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1027	C	C6-N1-C2	-7.79	117.19	120.30
22	v	34	C	C5-C6-N1	7.78	124.89	121.00
25	A	1402	U	N3-C2-O2	-7.78	116.76	122.20
1	a	1158	C	C6-N1-C2	-7.78	117.19	120.30
25	A	353	C	C6-N1-C2	-7.77	117.19	120.30
25	A	2125	G	N3-C4-C5	-7.77	124.72	128.60
25	A	547	A	C2-N3-C4	7.76	114.48	110.60
25	A	2794	C	N3-C4-N4	7.76	123.43	118.00
25	A	2262	U	C4-C5-C6	7.76	124.36	119.70
1	a	1383	C	N1-C2-O2	7.71	123.53	118.90
25	A	121	G	C6-C5-N7	-7.71	125.77	130.40
1	a	37	U	N3-C2-O2	-7.70	116.81	122.20
1	a	460	A	N1-C2-N3	-7.70	125.45	129.30
25	A	1816	C	N1-C2-O2	7.70	123.52	118.90
26	B	4	C	N3-C4-N4	7.68	123.38	118.00
23	x	126	G	P-O3'-C3'	7.68	128.91	119.70
1	a	998	C	N1-C2-O2	7.67	123.50	118.90
1	a	1262	C	N1-C2-O2	7.66	123.50	118.90
25	A	2416	C	C5-C6-N1	7.66	124.83	121.00
1	a	626	G	C5-C6-O6	-7.66	124.00	128.60
25	A	314	C	C6-N1-C2	-7.66	117.23	120.30
25	A	543	G	N1-C6-O6	7.65	124.49	119.90
1	a	528	C	C6-N1-C2	-7.65	117.24	120.30
1	a	385	C	C5-C6-N1	7.64	124.82	121.00
22	v	61	C	N1-C2-O2	7.64	123.49	118.90
25	A	2617	U	N3-C2-O2	-7.64	116.85	122.20
1	a	126	G	N1-C6-O6	7.63	124.48	119.90
25	A	2868	A	N7-C8-N9	7.63	117.62	113.80
25	A	1005	C	N3-C2-O2	-7.62	116.57	121.90
1	a	959	A	N7-C8-N9	7.60	117.60	113.80
43	S	62	ASP	C-N-CA	7.59	138.25	122.30
1	a	1262	C	N3-C2-O2	-7.59	116.59	121.90
1	a	1195	C	N1-C2-O2	7.59	123.45	118.90
1	a	168	G	N1-C6-O6	7.58	124.45	119.90
25	A	557	C	N3-C2-O2	-7.58	116.60	121.90
25	A	206	U	C5-C6-N1	7.58	126.49	122.70
1	a	177	G	C2-N3-C4	7.57	115.69	111.90
1	a	1034	G	N9-C4-C5	-7.56	102.38	105.40
1	a	1172	C	C6-N1-C2	-7.54	117.28	120.30
1	a	1140	C	N3-C2-O2	-7.53	116.63	121.90
25	A	2403	C	C6-N1-C2	-7.51	117.29	120.30
25	A	2409	G	N1-C6-O6	7.51	124.41	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2874	C	N1-C2-O2	7.50	123.40	118.90
22	v	67	C	C5-C6-N1	7.49	124.75	121.00
25	A	281	C	N1-C2-O2	7.49	123.39	118.90
25	A	2834	G	C8-N9-C4	-7.49	103.40	106.40
25	A	359	G	N1-C6-O6	-7.48	115.41	119.90
1	a	580	C	N1-C2-O2	7.48	123.39	118.90
25	A	1941	C	N1-C2-O2	7.48	123.39	118.90
22	v	56	C	C6-N1-C2	-7.47	117.31	120.30
25	A	722	A	N1-C2-N3	-7.47	125.57	129.30
25	A	1305	C	N1-C2-O2	7.46	123.38	118.90
25	A	2069	G7M	P-O3'-C3'	7.46	128.65	119.70
1	a	126	G	C6-C5-N7	-7.46	125.93	130.40
25	A	694	U	N3-C2-O2	-7.46	116.98	122.20
25	A	1461	C	C6-N1-C2	-7.45	117.32	120.30
1	a	1141	C	N3-C2-O2	-7.44	116.69	121.90
1	a	989	U	N3-C2-O2	-7.43	117.00	122.20
1	a	110	C	N3-C2-O2	-7.40	116.72	121.90
1	a	840	C	N3-C4-C5	7.40	124.86	121.90
1	a	661	G	N1-C6-O6	7.39	124.33	119.90
25	A	314	C	C5-C6-N1	7.38	124.69	121.00
1	a	1043	G	N1-C6-O6	-7.37	115.48	119.90
25	A	2793	C	N1-C2-O2	7.37	123.32	118.90
25	A	1348	C	N1-C2-O2	7.37	123.32	118.90
25	A	2669	G	N3-C2-N2	-7.37	114.74	119.90
1	a	943	U	N3-C2-O2	-7.37	117.04	122.20
25	A	1774	C	N3-C2-O2	-7.33	116.77	121.90
1	a	58	C	C2-N3-C4	-7.33	116.23	119.90
1	a	1448	C	N3-C2-O2	-7.32	116.77	121.90
23	x	111	G	N1-C6-O6	-7.32	115.51	119.90
29	E	82	GLY	CA-C-O	-7.32	107.43	120.60
25	A	1830	C	C6-N1-C2	-7.32	117.37	120.30
25	A	2192	U	C5-C6-N1	7.32	126.36	122.70
25	A	845	A	N1-C2-N3	-7.29	125.66	129.30
25	A	2769	U	N3-C2-O2	-7.29	117.10	122.20
1	a	116	A	O5'-P-OP2	-7.29	99.14	105.70
1	a	623	C	C5-C6-N1	7.29	124.64	121.00
1	a	89	U	C5-C4-O4	-7.28	121.53	125.90
1	a	215	C	C2-N1-C1'	7.28	126.81	118.80
25	A	2125	G	C2-N3-C4	7.28	115.54	111.90
25	A	2762	C	N3-C2-O2	-7.27	116.81	121.90
1	a	406	G	N1-C6-O6	7.27	124.26	119.90
25	A	2759	G	N1-C6-O6	-7.27	115.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	506	G	N1-C6-O6	7.26	124.26	119.90
25	A	784	G	OP1-P-O3'	7.26	121.18	105.20
1	a	840	C	N3-C4-N4	-7.26	112.92	118.00
1	a	93	U	C5-C6-N1	7.25	126.32	122.70
1	a	78	A	N1-C2-N3	-7.24	125.68	129.30
1	a	1448	C	N1-C2-O2	7.24	123.25	118.90
1	a	810	C	C6-N1-C2	-7.24	117.40	120.30
23	x	127	U	P-O3'-C3'	7.24	128.39	119.70
22	v	41	C	N3-C2-O2	-7.24	116.83	121.90
1	a	33	A	N7-C8-N9	7.23	117.42	113.80
25	A	1438	U	C5-C6-N1	7.22	126.31	122.70
25	A	758	C	C6-N1-C2	-7.21	117.42	120.30
1	a	1497	G	N1-C6-O6	-7.21	115.58	119.90
25	A	847	U	N1-C2-O2	7.20	127.84	122.80
1	a	413	G	N3-C4-N9	7.20	130.32	126.00
1	a	527	G7M	P-O3'-C3'	7.18	128.32	119.70
25	A	281	C	N3-C4-N4	7.17	123.02	118.00
25	A	984	A	C2-N3-C4	-7.16	107.02	110.60
24	y	47(L)	G	N3-C2-N2	-7.16	114.89	119.90
25	A	1947	C	C6-N1-C2	-7.16	117.44	120.30
25	A	2666	C	N1-C2-O2	7.16	123.19	118.90
25	A	1462	C	N1-C2-O2	7.15	123.19	118.90
25	A	1104	C	C2-N3-C4	7.15	123.47	119.90
25	A	1151	A	N1-C2-N3	-7.15	125.72	129.30
22	v	34	C	C6-N1-C2	-7.15	117.44	120.30
1	a	52	C	C6-N1-C2	-7.14	117.44	120.30
25	A	883	G	C8-N9-C4	-7.14	103.54	106.40
25	A	867	C	N3-C2-O2	-7.14	116.90	121.90
25	A	2742	G	C5-C6-N1	7.13	115.06	111.50
6	f	53	LYS	N-CA-CB	7.12	123.42	110.60
25	A	2326	C	C5-C6-N1	7.12	124.56	121.00
1	a	1195	C	N3-C2-O2	-7.12	116.92	121.90
25	A	1102	C	C6-N1-C2	-7.12	117.45	120.30
25	A	758	C	N1-C2-O2	7.10	123.16	118.90
25	A	2710	C	C6-N1-C2	-7.09	117.46	120.30
25	A	2805	C	C6-N1-C2	-7.09	117.47	120.30
1	a	126	G	N9-C4-C5	-7.09	102.56	105.40
25	A	847	U	N3-C2-O2	-7.09	117.24	122.20
25	A	1666	G	N1-C6-O6	-7.09	115.65	119.90
56	6	37	CYS	CA-CB-SG	7.08	126.75	114.00
1	a	723	U	C5-C6-N1	7.08	126.24	122.70
25	A	420	C	N1-C2-O2	7.08	123.15	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	34	C	N1-C2-O2	7.08	123.15	118.90
25	A	2456	C	C5-C6-N1	7.07	124.53	121.00
24	y	74	C	C6-N1-C2	-7.07	117.47	120.30
1	a	335	C	C6-N1-C2	-7.05	117.48	120.30
25	A	894	U	N3-C2-O2	-7.05	117.27	122.20
25	A	1578	U	N3-C2-O2	-7.05	117.27	122.20
24	y	74	C	C5-C6-N1	7.04	124.52	121.00
25	A	2791	G	C6-N1-C2	-7.04	120.88	125.10
25	A	2553	G	N1-C6-O6	7.04	124.12	119.90
25	A	281	C	C2-N3-C4	7.04	123.42	119.90
25	A	866	A	N1-C6-N6	7.04	122.82	118.60
26	B	4	C	C2-N3-C4	7.04	123.42	119.90
36	L	77	ILE	CG1-CB-CG2	-7.03	95.93	111.40
1	a	375	U	N3-C2-O2	-7.03	117.28	122.20
21	u	24	LYS	N-CA-CB	-7.02	97.96	110.60
25	A	2745	C	N1-C2-O2	7.02	123.11	118.90
26	B	97	C	C5-C6-N1	7.02	124.51	121.00
1	a	1003	G	N1-C2-N2	7.01	122.51	116.20
25	A	2063	C	C6-N1-C2	-7.01	117.50	120.30
25	A	2868	A	C8-N9-C4	-7.01	103.00	105.80
1	a	868	C	N1-C2-O2	7.01	123.11	118.90
25	A	1564	C	C5-C6-N1	7.00	124.50	121.00
25	A	1589	U	N3-C2-O2	-7.00	117.30	122.20
1	a	1134	G	N1-C2-N2	7.00	122.50	116.20
25	A	2884	U	N1-C2-O2	7.00	127.70	122.80
25	A	353	C	C5-C6-N1	6.99	124.50	121.00
1	a	719	C	C6-N1-C2	-6.99	117.50	120.30
25	A	2683	C	N3-C2-O2	-6.99	117.01	121.90
25	A	528	A	C5-N7-C8	-6.99	100.41	103.90
25	A	353	C	N3-C4-N4	6.98	122.89	118.00
25	A	1567	G	P-O3'-C3'	6.98	128.07	119.70
25	A	67	U	C5-C4-O4	-6.97	121.72	125.90
25	A	2424	C	N3-C4-C5	6.97	124.69	121.90
25	A	2610	C	P-O3'-C3'	6.97	128.07	119.70
25	A	1054	A	N1-C2-N3	-6.97	125.81	129.30
25	A	581	C	C5-C6-N1	6.97	124.48	121.00
25	A	359	G	N3-C2-N2	-6.96	115.03	119.90
25	A	1180	U	N3-C4-O4	6.96	124.27	119.40
1	a	1320	C	N1-C2-O2	6.96	123.08	118.90
26	B	31	C	N3-C2-O2	-6.96	117.03	121.90
25	A	278	A	N1-C6-N6	-6.95	114.43	118.60
25	A	2160	C	N3-C4-N4	-6.94	113.14	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	257	C	N1-C2-O2	6.94	123.06	118.90
25	A	1498	C	C2-N1-C1'	6.94	126.43	118.80
24	y	47(J)	C	N3-C4-C5	6.93	124.67	121.90
25	A	894	U	N1-C2-O2	6.93	127.65	122.80
1	a	455	G	N1-C6-O6	6.93	124.06	119.90
1	a	1011	C	C6-N1-C2	-6.92	117.53	120.30
25	A	528	A	N7-C8-N9	6.92	117.26	113.80
1	a	457	G	N3-C2-N2	-6.92	115.06	119.90
1	a	397	A	C2-N3-C4	6.91	114.06	110.60
1	a	1010	U	N3-C2-O2	-6.91	117.36	122.20
25	A	67	U	N3-C4-O4	6.90	124.23	119.40
1	a	960	U	P-O3'-C3'	6.90	127.97	119.70
25	A	278	A	N3-C4-C5	-6.89	121.97	126.80
1	a	957	U	N3-C2-O2	-6.89	117.38	122.20
1	a	1282	C	C6-N1-C2	-6.89	117.54	120.30
23	x	127	U	O4'-C1'-N1	6.88	113.70	108.20
25	A	2061	G	P-O3'-C3'	6.88	127.95	119.70
25	A	2128	G	C6-C5-N7	-6.88	126.27	130.40
1	a	99	C	C5-C6-N1	6.88	124.44	121.00
1	a	217	C	N3-C2-O2	-6.88	117.09	121.90
25	A	2308	G	N1-C6-O6	-6.88	115.77	119.90
45	U	88	ASP	N-CA-CB	6.87	122.97	110.60
25	A	1105	U	C2-N3-C4	-6.87	122.88	127.00
1	a	1109	C	C6-N1-C2	-6.87	117.55	120.30
1	a	1034	G	N3-C4-N9	6.87	130.12	126.00
25	A	1210	G	C2-N3-C4	6.87	115.33	111.90
25	A	1111	A	P-O3'-C3'	6.86	127.93	119.70
25	A	1331	G	N1-C6-O6	-6.86	115.78	119.90
25	A	694	U	N1-C2-O2	6.86	127.60	122.80
25	A	2769	U	N1-C2-O2	6.85	127.60	122.80
1	a	1143	G	N3-C2-N2	-6.85	115.11	119.90
25	A	1104	C	C6-N1-C2	-6.85	117.56	120.30
25	A	2785	C	C6-N1-C2	-6.85	117.56	120.30
25	A	1795	C	C5-C6-N1	6.85	124.42	121.00
25	A	1098	A	C5-C6-N6	-6.84	118.22	123.70
1	a	611	C	N1-C2-O2	6.84	123.00	118.90
25	A	1451	C	C2-N3-C4	-6.84	116.48	119.90
1	a	156	C	N1-C2-O2	-6.84	114.80	118.90
1	a	1277	C	N1-C2-O2	6.84	123.00	118.90
1	a	472	U	N3-C2-O2	-6.83	117.42	122.20
25	A	1005	C	C6-N1-C2	-6.83	117.57	120.30
1	a	998	C	C6-N1-C2	-6.83	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	240	G	N1-C6-O6	6.82	123.99	119.90
1	a	61	G	N1-C6-O6	6.82	123.99	119.90
25	A	912	C	N1-C2-O2	6.82	122.99	118.90
25	A	343	C	C6-N1-C2	-6.81	117.58	120.30
25	A	198	C	C5-C6-N1	6.81	124.41	121.00
25	A	1070	A	P-O3'-C3'	6.81	127.87	119.70
1	a	1326	U	N1-C2-O2	6.80	127.56	122.80
25	A	484	C	N1-C2-O2	6.80	122.98	118.90
1	a	545	C	N3-C4-C5	6.79	124.62	121.90
25	A	2553	G	C5-C6-O6	-6.79	124.53	128.60
25	A	2762	C	C2-N1-C1'	6.79	126.27	118.80
41	Q	27	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	a	1037	C	N3-C2-O2	-6.78	117.15	121.90
25	A	234	U	N3-C2-O2	-6.78	117.46	122.20
25	A	1021	A	C2-N3-C4	6.78	113.99	110.60
25	A	1900	A	P-O3'-C3'	6.78	127.83	119.70
22	v	51	C	C6-N1-C2	-6.77	117.59	120.30
25	A	2405	G	OP2-P-O3'	6.76	120.08	105.20
26	B	12	C	C2-N1-C1'	6.76	126.24	118.80
1	a	1389	C	N1-C2-O2	6.76	122.96	118.90
25	A	363	G	N1-C6-O6	6.76	123.95	119.90
25	A	1979	U	N3-C2-O2	-6.76	117.47	122.20
1	a	529	G	N9-C4-C5	-6.75	102.70	105.40
25	A	783	A	C4-C5-N7	6.75	114.07	110.70
1	a	545	C	C4-C5-C6	-6.74	114.03	117.40
25	A	2076	U	N3-C2-O2	-6.74	117.48	122.20
25	A	2666	C	N3-C2-O2	-6.74	117.18	121.90
1	a	89	U	C5-C6-N1	6.74	126.07	122.70
24	y	61	C	C6-N1-C2	-6.74	117.61	120.30
26	B	88	C	N1-C2-O2	6.73	122.94	118.90
22	v	56	C	N3-C2-O2	-6.72	117.19	121.90
25	A	373	U	N3-C2-O2	-6.72	117.49	122.20
1	a	972	C	C6-N1-C2	-6.72	117.61	120.30
1	a	1306	A	C8-N9-C4	-6.72	103.11	105.80
25	A	106	C	C6-N1-C2	-6.72	117.61	120.30
25	A	2870	C	C6-N1-C2	-6.72	117.61	120.30
1	a	89	U	N3-C4-O4	6.72	124.10	119.40
25	A	932	U	N1-C2-N3	6.72	118.93	114.90
1	a	142	G	N1-C6-O6	-6.71	115.87	119.90
25	A	1564	C	C6-N1-C2	-6.71	117.62	120.30
25	A	1737	G	C2-N3-C4	6.71	115.25	111.90
25	A	435	C	N1-C2-O2	6.70	122.92	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	845	A	C2-N3-C4	6.69	113.95	110.60
25	A	276	U	N1-C2-O2	6.69	127.48	122.80
1	a	213	G	C8-N9-C4	-6.69	103.72	106.40
1	a	737	C	C5-C6-N1	6.69	124.34	121.00
1	a	1383	C	N3-C2-O2	-6.69	117.22	121.90
1	a	1453	G	C2-N3-C4	6.69	115.24	111.90
25	A	2416	C	C6-N1-C2	-6.69	117.62	120.30
25	A	1159	U	N3-C2-O2	-6.68	117.52	122.20
17	q	69	THR	N-CA-CB	6.68	122.99	110.30
25	A	1119	U	N1-C2-O2	6.68	127.47	122.80
1	a	1284	C	C6-N1-C2	-6.67	117.63	120.30
25	A	2109	U	C5-C6-N1	6.67	126.03	122.70
22	v	71	C	N1-C2-O2	6.66	122.89	118.90
1	a	126	G	C4-C5-N7	6.65	113.46	110.80
25	A	445	C	N3-C2-O2	-6.65	117.25	121.90
25	A	528	A	C2-N3-C4	-6.65	107.28	110.60
25	A	1087	G	N9-C4-C5	6.63	108.05	105.40
25	A	528	A	C8-N9-C4	-6.62	103.15	105.80
1	a	1382	C	N1-C2-O2	6.61	122.87	118.90
25	A	869	G	N1-C6-O6	-6.61	115.93	119.90
1	a	1306	A	N7-C8-N9	6.61	117.11	113.80
1	a	29	U	N3-C2-O2	-6.60	117.58	122.20
1	a	857	C	N1-C2-O2	6.59	122.86	118.90
24	y	61	C	N1-C2-O2	6.59	122.86	118.90
25	A	2178	C	C6-N1-C2	-6.59	117.66	120.30
1	a	1259	C	N1-C2-O2	6.59	122.85	118.90
1	a	1033	G	N1-C6-O6	6.58	123.85	119.90
1	a	284	C	N1-C2-O2	6.58	122.85	118.90
25	A	2574	G	N1-C6-O6	6.58	123.85	119.90
25	A	2758	A	N1-C6-N6	-6.57	114.66	118.60
25	A	373	U	N1-C2-O2	6.56	127.39	122.80
25	A	2456	C	C6-N1-C2	-6.56	117.68	120.30
1	a	1282	C	N1-C2-O2	6.55	122.83	118.90
1	a	213	G	N7-C8-N9	6.55	116.38	113.10
25	A	1584	U	C5-C6-N1	6.55	125.97	122.70
25	A	2863	C	C5-C6-N1	6.54	124.27	121.00
1	a	99	C	C6-N1-C2	-6.54	117.68	120.30
1	a	1173	U	N3-C4-O4	6.54	123.98	119.40
1	a	318	G	N1-C6-O6	-6.54	115.98	119.90
1	a	475	C	C6-N1-C2	-6.54	117.69	120.30
25	A	1578	U	N1-C2-O2	6.53	127.37	122.80
25	A	2125	G	N3-C4-N9	6.53	129.92	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	310	G	N1-C6-O6	6.53	123.81	119.90
25	A	360	U	N3-C4-C5	6.53	118.52	114.60
25	A	1104	C	N3-C4-N4	6.53	122.57	118.00
26	B	26	C	N3-C2-O2	-6.52	117.33	121.90
26	B	31	C	C6-N1-C2	-6.52	117.69	120.30
1	a	1344	C	C6-N1-C2	-6.52	117.69	120.30
25	A	205	G	OP2-P-O3'	6.52	119.54	105.20
1	a	475	C	N1-C2-O2	6.52	122.81	118.90
1	a	1226	C	C2-N3-C4	-6.52	116.64	119.90
25	A	1114	C	C6-N1-C2	-6.52	117.69	120.30
25	A	1119	U	N3-C2-O2	-6.52	117.64	122.20
25	A	121	G	C4-C5-N7	6.52	113.41	110.80
1	a	284	C	C6-N1-C2	-6.51	117.70	120.30
25	A	783	A	C6-C5-N7	-6.51	127.74	132.30
1	a	623	C	N1-C2-O2	6.51	122.81	118.90
1	a	1320	C	N3-C2-O2	-6.51	117.34	121.90
1	a	1134	G	C6-N1-C2	-6.50	121.20	125.10
25	A	205	G	P-O3'-C3'	6.50	127.51	119.70
25	A	2248	C	N1-C2-O2	6.50	122.80	118.90
25	A	546	U	C6-N1-C2	-6.50	117.10	121.00
1	a	1011	C	C5-C6-N1	6.50	124.25	121.00
25	A	1297	C	C6-N1-C2	-6.50	117.70	120.30
1	a	739	C	C6-N1-C2	-6.50	117.70	120.30
25	A	1644	C	C6-N1-C2	-6.50	117.70	120.30
1	a	165	G	N1-C6-O6	6.49	123.80	119.90
1	a	450	G	N3-C2-N2	-6.49	115.36	119.90
24	y	35	C	N3-C4-N4	6.49	122.54	118.00
1	a	126	G	N3-C2-N2	6.49	124.44	119.90
25	A	274	C	N3-C4-N4	-6.49	113.46	118.00
26	B	38	C	N3-C2-O2	-6.48	117.36	121.90
25	A	81	G	N1-C6-O6	-6.48	116.01	119.90
25	A	282	A	N1-C2-N3	-6.48	126.06	129.30
25	A	1760	C	C6-N1-C2	-6.47	117.71	120.30
19	s	5	LYS	CB-CG-CD	6.47	128.42	111.60
22	v	34	C	C2-N1-C1'	6.47	125.91	118.80
1	a	660	C	N3-C2-O2	-6.46	117.38	121.90
25	A	357	C	C6-N1-C2	-6.46	117.71	120.30
25	A	228	C	P-O3'-C3'	6.46	127.45	119.70
1	a	528	C	C5-C6-N1	6.46	124.23	121.00
25	A	281	C	N3-C4-C5	-6.45	119.32	121.90
25	A	372	G	P-O3'-C3'	6.44	127.43	119.70
25	A	435	C	N3-C2-O2	-6.44	117.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1294	U	N3-C2-O2	-6.44	117.69	122.20
25	A	2658	C	N1-C2-O2	6.44	122.77	118.90
1	a	1510	C	N1-C2-O2	6.44	122.77	118.90
25	A	2325	G	N1-C6-O6	6.44	123.76	119.90
25	A	2863	C	C6-N1-C2	-6.44	117.72	120.30
25	A	847	U	C2-N1-C1'	6.44	125.42	117.70
25	A	868	U	N3-C2-O2	-6.44	117.69	122.20
23	x	125	G	C4'-C3'-O3'	6.43	125.87	113.00
1	a	1393	U	N3-C2-O2	-6.43	117.70	122.20
25	A	908	C	C6-N1-C2	-6.43	117.73	120.30
25	A	2056	G	N1-C6-O6	6.43	123.76	119.90
1	a	215	C	C2-N3-C4	6.42	123.11	119.90
13	m	57	ASP	CB-CG-OD1	6.42	124.08	118.30
25	A	1081	U	C5-C4-O4	-6.42	122.05	125.90
1	a	1389	C	C5-C6-N1	6.41	124.21	121.00
25	A	611	C	C6-N1-C2	-6.41	117.73	120.30
1	a	126	G	N3-C4-N9	6.41	129.85	126.00
25	A	121	G	C5-C6-O6	-6.41	124.76	128.60
1	a	193	C	N1-C2-O2	6.40	122.74	118.90
25	A	484	C	C5-C6-N1	6.40	124.20	121.00
25	A	1662	U	N3-C2-O2	-6.40	117.72	122.20
25	A	2407	A	O5'-P-OP2	-6.40	99.94	105.70
25	A	640	C	C6-N1-C2	-6.40	117.74	120.30
25	A	2799	A	N1-C6-N6	6.40	122.44	118.60
25	A	1804	C	C6-N1-C2	-6.39	117.75	120.30
25	A	121	G	N9-C4-C5	-6.38	102.85	105.40
25	A	2243	U	N3-C2-O2	-6.38	117.73	122.20
25	A	813	U	N3-C2-O2	-6.38	117.73	122.20
6	f	98	GLU	N-CA-CB	6.38	122.08	110.60
25	A	2767	C	C6-N1-C2	-6.38	117.75	120.30
25	A	1105	U	N1-C2-O2	6.37	127.26	122.80
25	A	1114	C	N1-C2-O2	6.37	122.72	118.90
1	a	414	A	O5'-P-OP2	-6.36	99.97	105.70
1	a	846	G	C6-C5-N7	-6.36	126.58	130.40
22	v	49	G	N1-C6-O6	6.36	123.72	119.90
25	A	2128	G	N1-C6-O6	6.36	123.72	119.90
1	a	1344	C	N3-C2-O2	-6.36	117.45	121.90
25	A	2164	C	N1-C2-O2	6.36	122.71	118.90
23	x	91	A	N1-C2-N3	-6.35	126.12	129.30
25	A	1267	U	N1-C2-O2	6.35	127.25	122.80
24	y	47(D)	C	N1-C2-N3	6.35	123.64	119.20
26	B	97	C	N3-C2-O2	-6.33	117.47	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	67	C	C2-N3-C4	6.33	123.07	119.90
23	x	134	C	C6-N1-C2	-6.33	117.77	120.30
25	A	281	C	C2-N1-C1'	6.33	125.76	118.80
1	a	660	C	C6-N1-C2	-6.32	117.77	120.30
25	A	2065	C	C6-N1-C2	-6.32	117.77	120.30
1	a	1037	C	C6-N1-C2	-6.32	117.77	120.30
1	a	1129	C	OP1-P-O3'	6.32	119.10	105.20
25	A	1894	C	N3-C2-O2	-6.32	117.48	121.90
24	y	71	C	N1-C2-O2	6.32	122.69	118.90
25	A	51	G	P-O3'-C3'	6.31	127.27	119.70
25	A	2720	U	N3-C2-O2	-6.31	117.78	122.20
25	A	1752	C	C6-N1-C2	-6.31	117.78	120.30
25	A	669	G	C4-N9-C1'	6.30	134.69	126.50
25	A	1114	C	C5-C6-N1	6.30	124.15	121.00
25	A	1498	C	C5-C4-N4	-6.30	115.79	120.20
26	B	28	C	C6-N1-C2	-6.30	117.78	120.30
25	A	932	U	C2-N3-C4	-6.29	123.22	127.00
25	A	1054	A	C6-N1-C2	6.29	122.38	118.60
1	a	896	C	C5-C6-N1	6.29	124.15	121.00
25	A	965	C	C6-N1-C2	-6.29	117.79	120.30
25	A	172	A	N1-C2-N3	-6.28	126.16	129.30
26	B	120	U	C2-N1-C1'	6.28	125.23	117.70
1	a	1173	U	C5-C6-N1	6.28	125.84	122.70
1	a	413	G	OP2-P-O3'	6.27	119.00	105.20
25	A	1574	C	C6-N1-C2	-6.27	117.79	120.30
1	a	52	C	C5-C6-N1	6.27	124.13	121.00
1	a	1303	C	N1-C2-O2	6.27	122.66	118.90
25	A	2669	G	C6-N1-C2	-6.26	121.34	125.10
25	A	2794	C	C5-C4-N4	-6.26	115.81	120.20
1	a	222	C	C6-N1-C2	-6.26	117.80	120.30
25	A	2704	C	C6-N1-C2	-6.26	117.80	120.30
25	A	2171	A	N1-C6-N6	6.25	122.35	118.60
1	a	221	C	C6-N1-C2	-6.25	117.80	120.30
1	a	1140	C	C6-N1-C2	-6.25	117.80	120.30
25	A	565	C	N1-C2-O2	6.25	122.65	118.90
24	y	41	C	C6-N1-C2	-6.25	117.80	120.30
25	A	1348	C	N3-C2-O2	-6.24	117.53	121.90
1	a	459	A	N1-C2-N3	-6.24	126.18	129.30
1	a	846	G	N1-C6-O6	6.24	123.64	119.90
25	A	1135	C	OP1-P-O3'	6.24	118.93	105.20
25	A	2767	C	C5-C6-N1	6.24	124.12	121.00
1	a	240	G	C5-C6-O6	-6.23	124.86	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	56	C	C2-N1-C1'	6.23	125.66	118.80
23	x	128	C	C3'-C2'-C1'	6.23	106.49	101.50
1	a	890	G	C8-N9-C4	6.23	108.89	106.40
25	A	1774	C	N1-C2-O2	6.23	122.64	118.90
1	a	1226	C	N1-C2-O2	-6.23	115.16	118.90
1	a	1463	U	C5-C6-N1	6.23	125.81	122.70
25	A	2214	C	N3-C2-O2	-6.23	117.54	121.90
1	a	1197	A	O5'-P-OP2	-6.22	100.10	105.70
1	a	1427	C	C6-N1-C2	-6.22	117.81	120.30
25	A	783	A	N1-C6-N6	6.22	122.33	118.60
25	A	1212	G	P-O3'-C3'	6.22	127.17	119.70
22	v	67	C	C2-N1-C1'	6.22	125.64	118.80
56	6	34	LEU	CA-CB-CG	6.22	129.61	115.30
24	y	6	U	N3-C2-O2	-6.22	117.85	122.20
1	a	487	A	C2-N3-C4	6.21	113.71	110.60
1	a	717	U	N3-C2-O2	-6.21	117.85	122.20
25	A	407	G	N3-C2-N2	-6.21	115.55	119.90
26	B	4	C	C2-N1-C1'	6.21	125.63	118.80
45	U	88	ASP	N-CA-C	-6.21	94.24	111.00
25	A	1958	C	C6-N1-C2	-6.21	117.82	120.30
1	a	193	C	N3-C2-O2	-6.20	117.56	121.90
25	A	57	C	C5-C6-N1	6.20	124.10	121.00
25	A	2576	G	N3-C4-N9	6.20	129.72	126.00
1	a	988	G	C6-N1-C2	-6.20	121.38	125.10
25	A	2200	C	C6-N1-C2	-6.20	117.82	120.30
26	B	68	C	C6-N1-C2	-6.19	117.82	120.30
1	a	1245	C	C5-C6-N1	6.19	124.09	121.00
25	A	2591	C	C6-N1-C2	-6.19	117.83	120.30
35	K	12	ASP	CB-CG-OD1	6.19	123.87	118.30
25	A	702	U	C5-C6-N1	6.19	125.79	122.70
1	a	231	U	N3-C2-O2	-6.18	117.87	122.20
5	e	77	ASN	N-CA-CB	-6.18	99.47	110.60
23	x	108	A	C2-N3-C4	6.18	113.69	110.60
25	A	1314	C	C2-N1-C1'	6.18	125.60	118.80
25	A	413	C	N1-C2-O2	6.18	122.61	118.90
25	A	669	G	N3-C4-N9	6.18	129.71	126.00
25	A	1567	G	OP2-P-O3'	6.18	118.79	105.20
1	a	1496	C	C6-N1-C2	-6.18	117.83	120.30
25	A	1345	C	C5-C6-N1	6.16	124.08	121.00
1	a	386	C	N3-C4-N4	6.16	122.31	118.00
1	a	988	G	N3-C2-N2	-6.16	115.59	119.90
22	v	51	C	N3-C2-O2	-6.16	117.59	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1182	G	OP2-P-O3'	6.16	118.75	105.20
25	A	1104	C	C5-C6-N1	6.16	124.08	121.00
25	A	2129	C	C6-N1-C2	-6.16	117.84	120.30
1	a	264	C	C6-N1-C2	-6.16	117.84	120.30
25	A	358	U	N3-C2-O2	-6.15	117.89	122.20
1	a	1353	G	N1-C6-O6	-6.14	116.21	119.90
26	B	60	C	C5-C6-N1	6.14	124.07	121.00
25	A	2076	U	N1-C2-O2	6.14	127.10	122.80
1	a	186	C	C5-C6-N1	6.14	124.07	121.00
25	A	1348	C	C6-N1-C2	-6.14	117.84	120.30
25	A	2226	C	C6-N1-C2	-6.14	117.84	120.30
25	A	2745	C	N3-C2-O2	-6.14	117.61	121.90
25	A	2128	G	N3-C4-N9	6.13	129.68	126.00
1	a	126	G	C5-C6-O6	-6.13	124.92	128.60
1	a	1277	C	C6-N1-C2	-6.13	117.85	120.30
26	B	68	C	C5-C6-N1	6.13	124.07	121.00
1	a	977	A	C2-N3-C4	6.13	113.66	110.60
1	a	67	C	C6-N1-C2	-6.13	117.85	120.30
25	A	611	C	C5-C6-N1	6.12	124.06	121.00
25	A	1994	C	N3-C2-O2	-6.12	117.61	121.90
25	A	206	U	C6-N1-C2	-6.12	117.33	121.00
1	a	266	G	O4'-C1'-N9	-6.12	103.30	108.20
1	a	1056	U	N1-C2-O2	6.12	127.09	122.80
1	a	1173	U	C5-C4-O4	-6.12	122.23	125.90
25	A	1267	U	N3-C2-O2	-6.12	117.91	122.20
25	A	2326	C	O4'-C1'-N1	6.12	113.10	108.20
22	v	67	C	N3-C4-N4	6.12	122.28	118.00
25	A	1200	C	C6-N1-C2	-6.12	117.85	120.30
25	A	1648	U	N3-C2-O2	-6.12	117.92	122.20
25	A	1656	C	C6-N1-C2	-6.11	117.86	120.30
1	a	1087	G	N1-C2-N3	6.11	127.56	123.90
25	A	1376	C	N1-C2-O2	6.11	122.56	118.90
1	a	896	C	C6-N1-C2	-6.11	117.86	120.30
22	v	3	C	C6-N1-C2	-6.11	117.86	120.30
23	x	125	G	C3'-C2'-C1'	6.10	106.38	101.50
25	A	2666	C	C6-N1-C2	-6.10	117.86	120.30
25	A	2326	C	C4-C5-C6	-6.10	114.35	117.40
1	a	1158	C	N3-C2-O2	-6.09	117.63	121.90
1	a	1282	C	N3-C2-O2	-6.09	117.64	121.90
1	a	544	G	C5-C6-O6	-6.09	124.95	128.60
25	A	353	C	C2-N1-C1'	6.09	125.50	118.80
25	A	557	C	C2-N1-C1'	6.09	125.50	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	144	G	N1-C6-O6	6.09	123.55	119.90
55	4	14	CYS	CA-CB-SG	6.09	124.96	114.00
25	A	2782	G	C6-C5-N7	-6.09	126.75	130.40
1	a	883	C	N1-C2-O2	6.08	122.55	118.90
1	a	419	C	N1-C2-O2	-6.08	115.25	118.90
25	A	137	U	N1-C2-O2	6.08	127.06	122.80
1	a	500	G	C6-C5-N7	-6.08	126.75	130.40
1	a	868	C	N3-C2-O2	-6.08	117.65	121.90
1	a	890	G	O4'-C1'-N9	6.07	113.06	108.20
25	A	353	C	C2-N3-C4	6.07	122.94	119.90
1	a	1382	C	N3-C2-O2	-6.07	117.65	121.90
1	a	1237	C	OP1-P-O3'	6.07	118.56	105.20
25	A	640	C	C5-C6-N1	6.07	124.03	121.00
18	r	15	GLU	C-N-CA	6.07	135.04	122.30
1	a	957	U	N1-C2-N3	6.06	118.54	114.90
1	a	356	A	N1-C2-N3	6.06	132.33	129.30
25	A	335	C	C6-N1-C2	-6.06	117.88	120.30
25	A	2691	C	C6-N1-C2	-6.06	117.88	120.30
25	A	1945	G	C5-C6-O6	-6.06	124.96	128.60
1	a	310	G	C5-C6-O6	-6.05	124.97	128.60
1	a	215	C	C5-C6-N1	6.05	124.03	121.00
1	a	506	G	C5-C6-O6	-6.05	124.97	128.60
1	a	840	C	C2-N3-C4	-6.05	116.88	119.90
25	A	2646	C	C6-N1-C2	-6.05	117.88	120.30
25	A	901	C	N1-C2-O2	6.04	122.53	118.90
22	v	34	C	C2-N3-C4	6.04	122.92	119.90
25	A	1048	A	N7-C8-N9	6.04	116.82	113.80
1	a	475	C	N3-C2-O2	-6.03	117.68	121.90
26	B	97	C	N3-C4-N4	6.03	122.22	118.00
1	a	1195	C	C6-N1-C2	-6.03	117.89	120.30
1	a	408	A	N1-C2-N3	-6.03	126.29	129.30
42	R	78	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	a	1277	C	N3-C2-O2	-6.01	117.69	121.90
1	a	1297	G	P-O3'-C3'	6.01	126.91	119.70
1	a	1383	C	C6-N1-C2	-6.01	117.90	120.30
1	a	186	C	N3-C2-O2	-6.00	117.70	121.90
25	A	1101	U	N1-C2-O2	6.00	127.00	122.80
1	a	1225	A	C2-N3-C4	6.00	113.60	110.60
5	e	89	THR	N-CA-CB	-6.00	98.90	110.30
25	A	435	C	C6-N1-C2	-6.00	117.90	120.30
25	A	1237	A	N7-C8-N9	6.00	116.80	113.80
1	a	717	U	N1-C2-O2	6.00	127.00	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2716	C	N1-C2-O2	6.00	122.50	118.90
13	m	78	ARG	NE-CZ-NH1	6.00	123.30	120.30
25	A	1313	U	C6-N1-C1'	-5.99	112.81	121.20
1	a	979	C	C6-N1-C2	-5.99	117.91	120.30
1	a	636	U	C5-C6-N1	5.99	125.69	122.70
25	A	866	A	C4-C5-N7	5.99	113.69	110.70
25	A	634	C	C5-C6-N1	5.98	123.99	121.00
25	A	2832	U	P-O3'-C3'	5.98	126.88	119.70
25	A	1413	A	N1-C2-N3	-5.98	126.31	129.30
25	A	2805	C	N1-C2-O2	5.98	122.49	118.90
25	A	2884	U	C2-N1-C1'	5.98	124.87	117.70
1	a	1363	A	C2-N3-C4	5.97	113.59	110.60
1	a	717	U	OP2-P-O3'	5.97	118.34	105.20
1	a	1182	G	P-O3'-C3'	5.97	126.87	119.70
25	A	1303	G	N1-C6-O6	5.97	123.48	119.90
25	A	2177	C	C6-N1-C2	-5.97	117.91	120.30
1	a	1507	A	N1-C2-N3	-5.97	126.31	129.30
24	y	35	C	N1-C2-O2	5.97	122.48	118.90
1	a	225	C	C6-N1-C2	-5.97	117.91	120.30
25	A	1301	A	C2-N3-C4	5.96	113.58	110.60
25	A	278	A	C8-N9-C4	-5.96	103.42	105.80
31	G	165	ASP	CB-CG-OD1	5.96	123.66	118.30
1	a	1100	C	C5-C6-N1	5.96	123.98	121.00
1	a	1460	C	C6-N1-C2	-5.95	117.92	120.30
1	a	1258	G	N1-C6-O6	-5.95	116.33	119.90
25	A	2691	C	C5-C6-N1	5.95	123.97	121.00
25	A	2867	G	C4-C5-N7	5.95	113.18	110.80
1	a	58	C	C5-C4-N4	-5.95	116.04	120.20
1	a	177	G	N3-C4-C5	-5.95	125.63	128.60
1	a	240	G	N9-C4-C5	-5.95	103.02	105.40
1	a	544	G	N9-C4-C5	-5.94	103.02	105.40
1	a	153	C	N1-C2-O2	5.94	122.46	118.90
25	A	1784	A	C5-N7-C8	5.94	106.87	103.90
25	A	1498	C	C6-N1-C2	-5.93	117.93	120.30
27	C	269	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	a	29	U	N1-C2-N3	5.93	118.46	114.90
25	A	2903	U	N1-C2-O2	5.93	126.95	122.80
1	a	483	C	C6-N1-C2	-5.93	117.93	120.30
25	A	2195	U	N3-C2-O2	-5.93	118.05	122.20
1	a	128	G	N1-C6-O6	5.92	123.45	119.90
1	a	141	G	N3-C2-N2	-5.92	115.76	119.90
25	A	413	C	N3-C2-O2	-5.91	117.76	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2542	A	N1-C6-N6	-5.91	115.05	118.60
26	B	97	C	C6-N1-C1'	-5.91	113.70	120.80
1	a	156	C	N3-C4-N4	-5.91	113.86	118.00
25	A	420	C	N3-C2-O2	-5.91	117.77	121.90
25	A	1450	G	N1-C6-O6	-5.90	116.36	119.90
25	A	2424	C	N1-C2-O2	5.90	122.44	118.90
1	a	248	C	N3-C2-O2	-5.90	117.77	121.90
25	A	314	C	N1-C2-O2	5.89	122.44	118.90
25	A	2147	A	C8-N9-C4	-5.89	103.44	105.80
25	A	2867	G	N9-C4-C5	-5.89	103.04	105.40
25	A	2793	C	N3-C2-O2	-5.89	117.78	121.90
25	A	1058	U	C2-N3-C4	5.88	130.53	127.00
25	A	2391	G	P-O3'-C3'	5.88	126.76	119.70
25	A	359	G	N1-C2-N2	5.88	121.49	116.20
25	A	2162	G	C4-N9-C1'	5.88	134.14	126.50
1	a	1007	U	N3-C2-O2	-5.88	118.09	122.20
25	A	898	C	C5-C6-N1	5.88	123.94	121.00
25	A	1624	U	N3-C2-O2	-5.88	118.09	122.20
1	a	64	G	OP2-P-O3'	5.88	118.12	105.20
1	a	611	C	N3-C2-O2	-5.88	117.79	121.90
25	A	281	C	N3-C2-O2	-5.87	117.79	121.90
25	A	610	C	N3-C2-O2	-5.87	117.79	121.90
25	A	1049	C	N1-C2-O2	5.87	122.42	118.90
25	A	1941	C	N3-C2-O2	-5.87	117.79	121.90
25	A	1804	C	C5-C6-N1	5.87	123.94	121.00
1	a	356	A	C6-N1-C2	-5.86	115.08	118.60
1	a	1210	C	C6-N1-C2	-5.86	117.95	120.30
24	y	59	C	N3-C2-O2	-5.86	117.80	121.90
25	A	2785	C	C5-C6-N1	5.86	123.93	121.00
1	a	591	U	N3-C2-O2	-5.85	118.10	122.20
1	a	601	G	N1-C6-O6	5.85	123.41	119.90
22	v	49	G	C6-C5-N7	-5.85	126.89	130.40
1	a	132	C	C6-N1-C2	-5.85	117.96	120.30
25	A	2840	C	C5-C6-N1	5.85	123.92	121.00
23	x	129	U	C5'-C4'-C3'	5.85	125.35	116.00
25	A	2484	G	N1-C6-O6	5.85	123.41	119.90
25	A	678	C	C6-N1-C2	-5.84	117.96	120.30
37	M	70	ASP	CB-CG-OD1	5.84	123.56	118.30
25	A	1731	G	N1-C6-O6	5.84	123.40	119.90
23	x	112	C	C6-N1-C2	-5.83	117.97	120.30
1	a	570	G	N1-C6-O6	-5.83	116.40	119.90
25	A	2164	C	N3-C4-C5	5.83	124.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	1	39	ASP	CB-CG-OD1	5.83	123.55	118.30
25	A	2181	U	C5-C6-N1	5.83	125.62	122.70
24	y	18	G	N1-C6-O6	5.83	123.40	119.90
1	a	660	C	C2-N1-C1'	5.83	125.21	118.80
32	I	27	LEU	CA-CB-CG	5.83	128.70	115.30
22	v	67	C	N3-C2-O2	-5.82	117.83	121.90
25	A	277	G	C8-N9-C4	-5.82	104.07	106.40
1	a	264	C	C5-C6-N1	5.81	123.91	121.00
25	A	610	C	N1-C2-O2	5.81	122.39	118.90
1	a	1112	C	C6-N1-C2	-5.81	117.98	120.30
1	a	491	G	N1-C6-O6	-5.80	116.42	119.90
25	A	2716	C	C6-N1-C2	-5.80	117.98	120.30
33	H	75	LEU	CA-CB-CG	-5.80	101.95	115.30
22	v	22	G	N1-C6-O6	5.80	123.38	119.90
24	y	59	C	C2-N3-C4	5.80	122.80	119.90
25	A	353	C	N3-C2-O2	-5.80	117.84	121.90
25	A	2300	C	C2-N1-C1'	5.80	125.17	118.80
1	a	200	G	N1-C6-O6	-5.79	116.42	119.90
1	a	529	G	C5-C6-N1	5.79	114.40	111.50
24	y	61	C	C5-C6-N1	5.79	123.90	121.00
25	A	1994	C	C6-N1-C2	-5.79	117.98	120.30
1	a	37	U	N1-C2-O2	5.79	126.85	122.80
25	A	1455	G	C6-C5-N7	-5.79	126.93	130.40
25	A	1784	A	N7-C8-N9	-5.79	110.90	113.80
25	A	1947	C	C5-C6-N1	5.79	123.89	121.00
1	a	350	G	N1-C6-O6	-5.79	116.43	119.90
25	A	1138	G	N1-C6-O6	-5.78	116.43	119.90
1	a	56	U	N3-C4-O4	5.78	123.45	119.40
1	a	1442	G	N1-C6-O6	-5.78	116.43	119.90
1	a	1147	C	N1-C2-O2	5.78	122.37	118.90
25	A	1180	U	C2-N1-C1'	5.78	124.64	117.70
1	a	1524	C	C5-C6-N1	5.78	123.89	121.00
25	A	2215	C	C5-C6-N1	5.78	123.89	121.00
1	a	525	C	N3-C4-C5	5.78	124.21	121.90
25	A	420	C	C2-N1-C1'	5.78	125.15	118.80
25	A	1057	A	N1-C2-N3	-5.78	126.41	129.30
25	A	1737	G	N3-C4-C5	-5.78	125.71	128.60
25	A	2805	C	N3-C2-O2	-5.78	117.86	121.90
25	A	1386	C	C6-N1-C2	-5.77	117.99	120.30
1	a	18	C	C6-N1-C2	-5.77	117.99	120.30
25	A	1622	G	N1-C6-O6	5.77	123.36	119.90
1	a	406	G	C5-C6-O6	-5.77	125.14	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	434	U	N3-C2-O2	-5.76	118.16	122.20
25	A	935	C	N1-C2-O2	5.76	122.36	118.90
25	A	2063	C	N3-C2-O2	-5.76	117.86	121.90
25	A	2566	A	O4'-C1'-N9	5.76	112.81	108.20
1	a	890	G	P-O3'-C3'	5.76	126.61	119.70
1	a	1510	C	N3-C4-N4	5.76	122.03	118.00
1	a	188	C	C6-N1-C2	-5.76	118.00	120.30
25	A	2385	C	N1-C2-O2	5.76	122.35	118.90
25	A	286	U	N3-C2-O2	-5.75	118.17	122.20
25	A	1455	G	C4-C5-N7	5.75	113.10	110.80
23	x	111	G	C5-C6-N1	5.75	114.37	111.50
1	a	413	G	N3-C4-C5	-5.75	125.73	128.60
1	a	1038	C	C6-N1-C2	-5.75	118.00	120.30
1	a	413	G	C4-N9-C1'	5.74	133.97	126.50
25	A	2214	C	N1-C2-O2	5.74	122.34	118.90
1	a	922	G	N1-C6-O6	-5.74	116.46	119.90
25	A	852	U	C5-C6-N1	5.73	125.57	122.70
1	a	660	C	N3-C4-N4	5.73	122.01	118.00
26	B	4	C	C5-C4-N4	-5.73	116.19	120.20
1	a	393	A	O5'-P-OP2	-5.72	100.55	105.70
1	a	1455	G	C6-C5-N7	-5.72	126.97	130.40
25	A	278	A	C5-C6-N1	5.72	120.56	117.70
25	A	1013	C	N1-C2-O2	5.72	122.33	118.90
24	y	46	G	N3-C2-N2	5.72	123.91	119.90
25	A	1787	A	N1-C2-N3	-5.72	126.44	129.30
1	a	1002	G	N1-C6-O6	-5.71	116.47	119.90
25	A	1669	A	C2-N3-C4	5.71	113.46	110.60
25	A	1169	A	C5-C6-N1	5.71	120.56	117.70
1	a	406	G	C6-C5-N7	-5.71	126.97	130.40
26	B	38	C	C6-N1-C2	-5.71	118.02	120.30
26	B	30	C	N1-C2-O2	5.71	122.33	118.90
25	A	1546	G	N1-C6-O6	-5.71	116.47	119.90
25	A	105	C	N1-C2-O2	5.71	122.32	118.90
25	A	512	G	P-O3'-C3'	5.70	126.54	119.70
1	a	186	C	C6-N1-C2	-5.70	118.02	120.30
1	a	193	C	C6-N1-C2	-5.70	118.02	120.30
25	A	984	A	N3-C4-C5	5.70	130.79	126.80
1	a	544	G	C8-N9-C4	5.70	108.68	106.40
25	A	1289	C	N1-C2-O2	5.70	122.32	118.90
1	a	719	C	C2-N1-C1'	5.69	125.06	118.80
1	a	1510	C	C6-N1-C2	-5.69	118.02	120.30
1	a	1031	C	C6-N1-C2	-5.69	118.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2047	C	N1-C2-O2	5.69	122.31	118.90
25	A	818	G	C6-C5-N7	-5.69	126.99	130.40
25	A	2264	C	N1-C2-O2	-5.68	115.49	118.90
25	A	352	A	N1-C2-N3	-5.68	126.46	129.30
25	A	543	G	C6-C5-N7	-5.68	126.99	130.40
1	a	61	G	C5-C6-O6	-5.68	125.19	128.60
25	A	550	C	C5-C6-N1	5.68	123.84	121.00
25	A	901	C	N3-C2-O2	-5.68	117.92	121.90
25	A	366	C	C6-N1-C2	-5.68	118.03	120.30
1	a	1034	G	C6-N1-C2	-5.67	121.69	125.10
25	A	1063	G	C5-C6-O6	-5.67	125.19	128.60
25	A	847	U	C6-N1-C2	-5.67	117.60	121.00
22	v	51	C	N3-C4-N4	5.67	121.97	118.00
26	B	38	C	N3-C4-N4	5.67	121.97	118.00
25	A	1148	U	C5-C6-N1	5.67	125.53	122.70
25	A	1945	G	N1-C6-O6	5.67	123.30	119.90
25	A	2867	G	P-O3'-C3'	5.67	126.50	119.70
1	a	1129	C	C6-N1-C2	-5.67	118.03	120.30
1	a	505	G	N1-C6-O6	5.67	123.30	119.90
25	A	286	U	N1-C2-O2	5.66	126.77	122.80
25	A	2730	C	C6-N1-C2	-5.66	118.04	120.30
1	a	524	G	N1-C6-O6	5.66	123.30	119.90
25	A	62	U	C5-C6-N1	5.66	125.53	122.70
25	A	2023	C	N1-C2-O2	5.66	122.29	118.90
26	B	27	C	N1-C2-O2	5.66	122.29	118.90
25	A	2716	C	C5-C6-N1	5.65	123.83	121.00
25	A	1463	C	C6-N1-C2	-5.65	118.04	120.30
25	A	2874	C	N3-C2-O2	-5.65	117.94	121.90
25	A	818	G	N3-C4-N9	5.65	129.39	126.00
25	A	130	C	N3-C4-C5	5.65	124.16	121.90
25	A	1157	G	N3-C4-N9	5.64	129.39	126.00
1	a	221	C	C2-N1-C1'	5.64	125.00	118.80
1	a	671	G	N1-C6-O6	5.64	123.28	119.90
1	a	1003	G	N9-C4-C5	5.64	107.65	105.40
25	A	484	C	C6-N1-C2	-5.64	118.05	120.30
25	A	1103	A	OP1-P-O3'	5.64	117.60	105.20
25	A	1295	C	N1-C2-O2	5.64	122.28	118.90
25	A	2354	C	C6-N1-C2	-5.63	118.05	120.30
1	a	215	C	N3-C4-C5	-5.63	119.65	121.90
1	a	626	G	C6-C5-N7	-5.63	127.02	130.40
25	A	1086	A	N1-C2-N3	5.63	132.12	129.30
26	B	3	C	N1-C2-O2	5.63	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	34	C	N3-C4-N4	5.63	121.94	118.00
25	A	277	G	C5-N7-C8	-5.63	101.49	104.30
1	a	737	C	N1-C2-O2	5.63	122.28	118.90
1	a	1134	G	C5-C6-O6	-5.63	125.22	128.60
1	a	1143	G	N1-C6-O6	-5.63	116.52	119.90
25	A	2752	C	N1-C2-O2	5.63	122.28	118.90
30	F	172	PHE	C-N-CA	5.63	135.76	121.70
1	a	1432	G	P-O3'-C3'	5.62	126.45	119.70
25	A	283	G	N1-C2-N2	5.62	121.26	116.20
25	A	171	U	N3-C2-O2	-5.62	118.27	122.20
25	A	2056	G	C6-C5-N7	-5.62	127.03	130.40
25	A	2403	C	C5-C6-N1	5.62	123.81	121.00
22	v	71	C	C5-C6-N1	5.62	123.81	121.00
25	A	1314	C	N1-C2-O2	5.61	122.27	118.90
25	A	1931	U	C5-C6-N1	5.61	125.51	122.70
1	a	413	G	C8-N9-C1'	-5.61	119.70	127.00
1	a	506	G	C6-C5-N7	-5.61	127.03	130.40
24	y	71	C	C6-N1-C2	-5.61	118.06	120.30
25	A	2410	G	C5-C6-O6	-5.61	125.23	128.60
25	A	2574	G	C5-C6-O6	-5.61	125.23	128.60
25	A	1317	G	N1-C6-O6	5.61	123.27	119.90
23	x	91	A	N9-C4-C5	-5.61	103.56	105.80
25	A	495	G	N1-C6-O6	5.61	123.26	119.90
25	A	2297	A	N1-C2-N3	-5.60	126.50	129.30
1	a	144	G	C6-C5-N7	-5.60	127.04	130.40
25	A	121	G	N3-C4-N9	5.60	129.36	126.00
25	A	1683	U	N3-C2-O2	-5.60	118.28	122.20
25	A	740	C	C5-C6-N1	5.60	123.80	121.00
1	a	543	U	N3-C2-O2	-5.59	118.28	122.20
1	a	1303	C	N3-C2-O2	-5.59	117.98	121.90
1	a	168	G	C4-C5-N7	5.59	113.04	110.80
1	a	1255	G	N1-C6-O6	-5.59	116.55	119.90
25	A	413	C	C5-C6-N1	5.59	123.79	121.00
25	A	849	A	N7-C8-N9	5.59	116.59	113.80
22	v	28	C	N1-C2-O2	5.59	122.25	118.90
25	A	896	A	N1-C6-N6	5.59	121.95	118.60
1	a	588	G	N3-C4-C5	-5.58	125.81	128.60
1	a	598	U	N3-C2-O2	-5.58	118.29	122.20
22	v	51	C	C5-C6-N1	5.58	123.79	121.00
1	a	906	A	C5-C6-N6	-5.58	119.24	123.70
25	A	2164	C	N3-C4-N4	-5.58	114.10	118.00
25	A	2103	C	C5-C4-N4	-5.58	116.30	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	234	U	N1-C2-O2	5.57	126.70	122.80
25	A	2566	A	P-O3'-C3'	5.57	126.38	119.70
25	A	513	A	N7-C8-N9	5.57	116.58	113.80
25	A	2108	A	N1-C2-N3	5.57	132.08	129.30
1	a	1404	C	C5-C6-N1	5.57	123.78	121.00
25	A	154	U	N3-C2-O2	-5.56	118.31	122.20
25	A	1352	U	N3-C2-O2	-5.56	118.31	122.20
1	a	194	C	C6-N1-C2	-5.56	118.08	120.30
1	a	626	G	N3-C2-N2	5.56	123.79	119.90
1	a	1041	G	N1-C6-O6	5.56	123.23	119.90
24	y	62	C	C6-N1-C2	-5.56	118.08	120.30
25	A	1533	C	N3-C4-N4	-5.56	114.11	118.00
22	v	56	C	N3-C4-C5	-5.55	119.68	121.90
23	x	133	C	C3'-C2'-C1'	5.55	105.94	101.50
25	A	1531	C	N3-C4-N4	-5.55	114.11	118.00
25	A	2889	C	N1-C2-O2	5.55	122.23	118.90
1	a	1088	G	C5-C6-O6	-5.55	125.27	128.60
25	A	420	C	C6-N1-C2	-5.55	118.08	120.30
1	a	41	G	N3-C4-C5	-5.55	125.83	128.60
1	a	507	C	N3-C4-C5	5.55	124.12	121.90
25	A	1795	C	C6-N1-C2	-5.55	118.08	120.30
1	a	441	A	C2-N3-C4	5.55	113.37	110.60
1	a	1262	C	C6-N1-C2	-5.55	118.08	120.30
25	A	2171	A	C5-C6-N6	-5.55	119.26	123.70
25	A	2870	C	C5-C6-N1	5.55	123.77	121.00
26	B	21	G	N1-C6-O6	-5.55	116.57	119.90
1	a	1459	G	N1-C6-O6	5.54	123.23	119.90
11	k	126	ARG	NE-CZ-NH2	-5.54	117.53	120.30
25	A	1940	U	P-O3'-C3'	5.54	126.35	119.70
25	A	2292	U	C5-C6-N1	5.54	125.47	122.70
25	A	1087	G	N1-C2-N3	5.54	127.22	123.90
25	A	2178	C	C5-C6-N1	5.54	123.77	121.00
1	a	1325	C	N3-C2-O2	-5.54	118.03	121.90
25	A	687	C	N1-C2-O2	5.54	122.22	118.90
25	A	444	C	C6-N1-C2	-5.53	118.09	120.30
25	A	2863	C	N1-C2-O2	5.53	122.22	118.90
25	A	2791	G	N1-C2-N2	5.53	121.18	116.20
1	a	93	U	C6-N1-C2	-5.53	117.68	121.00
25	A	276	U	N3-C2-O2	-5.53	118.33	122.20
25	A	1048	A	C8-N9-C4	-5.53	103.59	105.80
25	A	1499	C	N3-C4-N4	-5.53	114.13	118.00
25	A	1539	U	C5-C4-O4	-5.53	122.58	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1833	C	N3-C2-O2	-5.53	118.03	121.90
25	A	1993	U	C2-N1-C1'	5.53	124.33	117.70
25	A	2056	G	C5-C6-O6	-5.52	125.28	128.60
25	A	362	A	C8-N9-C4	-5.52	103.59	105.80
25	A	2466	C	O5'-P-OP1	-5.52	100.73	105.70
25	A	2636	C	C2-N1-C1'	5.52	124.87	118.80
25	A	2794	C	C2-N1-C1'	5.52	124.87	118.80
1	a	1369	C	N3-C2-O2	-5.52	118.04	121.90
1	a	960	U	N1-C2-O2	5.52	126.66	122.80
22	v	49	G	C4-C5-N7	5.52	113.01	110.80
1	a	980	C	N1-C2-O2	5.51	122.21	118.90
25	A	581	C	O5'-P-OP1	-5.51	100.74	105.70
25	A	2438	U	N3-C2-O2	-5.51	118.34	122.20
1	a	1460	C	N1-C2-O2	5.51	122.21	118.90
25	A	1395	A	O4'-C1'-N9	5.51	112.61	108.20
1	a	1147	C	N3-C2-O2	-5.51	118.05	121.90
25	A	360	U	C4-C5-C6	-5.51	116.40	119.70
25	A	565	C	N3-C2-O2	-5.51	118.05	121.90
1	a	643	C	C6-N1-C2	-5.50	118.10	120.30
1	a	1317	C	C6-N1-C2	-5.50	118.10	120.30
24	y	61	C	C2-N3-C4	5.50	122.65	119.90
25	A	965	C	C5-C6-N1	5.50	123.75	121.00
1	a	891	U	C5-C6-N1	5.50	125.45	122.70
25	A	2592	G	N3-C2-N2	5.50	123.75	119.90
23	x	126	G	N7-C8-N9	5.50	115.85	113.10
1	a	168	G	C6-C5-N7	-5.50	127.10	130.40
1	a	1522	U	C6-N1-C2	-5.50	117.70	121.00
1	a	96	U	N1-C2-O2	5.50	126.65	122.80
25	A	359	G	C2-N3-C4	5.50	114.65	111.90
25	A	445	C	C6-N1-C2	-5.50	118.10	120.30
1	a	623	C	C2-N1-C1'	5.49	124.84	118.80
1	a	910	C	N3-C2-O2	-5.49	118.06	121.90
25	A	208	C	C5-C6-N1	5.49	123.75	121.00
1	a	1348	U	N3-C2-O2	-5.49	118.36	122.20
1	a	206	C	N1-C2-N3	5.49	123.04	119.20
1	a	504	C	C5-C6-N1	5.49	123.74	121.00
25	A	1760	C	C5-C6-N1	5.49	123.74	121.00
23	x	93	G	N1-C6-O6	5.49	123.19	119.90
25	A	62	U	C2-N3-C4	5.49	130.29	127.00
25	A	396	G	N1-C6-O6	5.49	123.19	119.90
1	a	269	C	C6-N1-C2	-5.48	118.11	120.30
25	A	362	A	N7-C8-N9	5.48	116.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1462	C	N3-C2-O2	-5.48	118.06	121.90
1	a	67	C	N3-C2-O2	-5.48	118.06	121.90
1	a	575	G	C6-N1-C2	-5.48	121.81	125.10
1	a	671	G	C5-C6-O6	-5.48	125.31	128.60
25	A	717	C	C6-N1-C2	-5.48	118.11	120.30
25	A	2814	A	C8-N9-C4	-5.47	103.61	105.80
1	a	102	G	C4-C5-N7	-5.47	108.61	110.80
1	a	1124	G	N1-C6-O6	-5.47	116.62	119.90
26	B	27	C	N3-C2-O2	-5.47	118.07	121.90
1	a	1149	C	N3-C4-N4	5.47	121.83	118.00
25	A	2518	A	C2-N3-C4	5.46	113.33	110.60
6	f	53	LYS	N-CA-C	-5.46	96.25	111.00
25	A	1098	A	N1-C6-N6	5.46	121.88	118.60
1	a	959	A	C5-N7-C8	-5.46	101.17	103.90
25	A	1830	C	C5-C6-N1	5.46	123.73	121.00
1	a	33	A	C8-N9-C4	-5.46	103.62	105.80
1	a	1448	C	N3-C4-C5	5.45	124.08	121.90
25	A	1081	U	C4-C5-C6	-5.45	116.43	119.70
1	a	358	U	N3-C2-O2	-5.45	118.39	122.20
26	B	17	C	C6-N1-C2	-5.45	118.12	120.30
1	a	1073	U	N3-C2-O2	-5.44	118.39	122.20
1	a	284	C	C5-C6-N1	5.44	123.72	121.00
26	B	31	C	C2-N1-C1'	5.44	124.79	118.80
1	a	155	A	N1-C2-N3	-5.44	126.58	129.30
1	a	1499	A	OP2-P-O3'	5.44	117.17	105.20
22	v	6	G	N1-C6-O6	-5.44	116.64	119.90
25	A	1362	C	C6-N1-C2	-5.44	118.12	120.30
1	a	1071	C	N1-C2-O2	5.44	122.16	118.90
1	a	910	C	N1-C2-O2	5.43	122.16	118.90
25	A	1894	C	C2-N1-C1'	5.43	124.78	118.80
25	A	2416	C	N1-C2-O2	5.43	122.16	118.90
23	x	130	G	N9-C1'-C2'	-5.43	106.02	112.00
1	a	1369	C	C6-N1-C2	-5.43	118.13	120.30
23	x	125	G	C4-N9-C1'	-5.43	119.44	126.50
25	A	1499	C	N1-C2-O2	-5.43	115.64	118.90
25	A	2592	G	N1-C6-O6	5.43	123.16	119.90
1	a	73	C	N3-C4-N4	-5.43	114.20	118.00
1	a	866	C	C6-N1-C2	-5.43	118.13	120.30
25	A	816	C	C6-N1-C2	-5.43	118.13	120.30
1	a	330	C	N1-C2-O2	5.42	122.16	118.90
25	A	81	G	N3-C2-N2	-5.42	116.10	119.90
25	A	1930	G	P-O3'-C3'	5.42	126.21	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1816	C	N3-C2-O2	-5.42	118.11	121.90
25	A	1402	U	N1-C2-O2	5.42	126.59	122.80
25	A	536	G	N1-C6-O6	-5.42	116.65	119.90
25	A	1306	C	N3-C4-C5	5.42	124.07	121.90
25	A	16	C	C6-N1-C2	-5.42	118.13	120.30
25	A	2834	G	C5-N7-C8	-5.42	101.59	104.30
25	A	2628	C	C6-N1-C2	-5.42	118.13	120.30
1	a	412	A	OP2-P-O3'	5.41	117.11	105.20
1	a	667	G	N1-C6-O6	-5.41	116.65	119.90
25	A	283	G	C6-N1-C2	-5.41	121.85	125.10
1	a	2	A	C5-N7-C8	5.41	106.61	103.90
25	A	2056	G	C4-C5-N7	5.41	112.96	110.80
1	a	563	A	N3-C4-N9	5.41	131.73	127.40
25	A	775	G	O4'-C1'-N9	5.41	112.53	108.20
25	A	1994	C	N1-C2-O2	5.41	122.14	118.90
1	a	385	C	N1-C2-O2	5.40	122.14	118.90
25	A	1104	C	C2-N1-C1'	5.40	124.75	118.80
1	a	1043	G	C5-C6-N1	5.40	114.20	111.50
25	A	931	U	C5-C6-N1	5.40	125.40	122.70
25	A	1564	C	N1-C2-O2	5.40	122.14	118.90
25	A	2889	C	C6-N1-C2	-5.40	118.14	120.30
25	A	1461	C	N1-C2-O2	5.40	122.14	118.90
1	a	379	C	N3-C4-C5	5.40	124.06	121.90
1	a	578	C	C6-N1-C2	-5.40	118.14	120.30
25	A	407	G	C5-C6-O6	5.40	131.84	128.60
25	A	584	C	N1-C2-O2	5.40	122.14	118.90
25	A	1682	G	N3-C4-N9	5.40	129.24	126.00
21	u	24	LYS	CA-CB-CG	5.39	125.27	113.40
25	A	2720	U	N1-C2-O2	5.39	126.58	122.80
1	a	1498	UR3	OP1-P-O3'	5.39	117.06	105.20
25	A	2321	U	C4-C5-C6	5.39	122.94	119.70
1	a	528	C	N1-C2-O2	5.39	122.13	118.90
25	A	1761	C	N1-C2-O2	5.39	122.13	118.90
26	B	17	C	C5-C6-N1	5.38	123.69	121.00
26	B	120	U	C6-N1-C2	-5.38	117.77	121.00
1	a	1271	A	N1-C2-N3	-5.38	126.61	129.30
25	A	1507	C	C2-N3-C4	5.38	122.59	119.90
25	A	2117	A	N1-C2-N3	-5.38	126.61	129.30
1	a	1325	C	C5-C6-N1	5.38	123.69	121.00
25	A	2192	U	N3-C4-O4	5.38	123.17	119.40
23	x	132	A	P-O5'-C5'	5.38	129.50	120.90
26	B	4	C	OP1-P-OP2	-5.38	111.53	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2903	U	N3-C2-O2	-5.38	118.44	122.20
1	a	455	G	C6-C5-N7	-5.37	127.18	130.40
25	A	1680	U	N1-C2-O2	5.37	126.56	122.80
25	A	680	C	C5-C6-N1	5.37	123.69	121.00
25	A	1625	C	N3-C4-C5	5.37	124.05	121.90
1	a	186	C	C5-C4-N4	-5.37	116.44	120.20
1	a	1404	C	N3-C4-C5	-5.37	119.75	121.90
1	a	1113	C	C6-N1-C2	-5.37	118.15	120.30
25	A	1945	G	C4-C5-N7	5.37	112.95	110.80
1	a	341	C	N3-C4-N4	-5.37	114.24	118.00
1	a	1172	C	C5-C6-N1	5.37	123.68	121.00
29	E	82	GLY	N-CA-C	5.37	126.52	113.10
1	a	524	G	C5-C6-O6	-5.36	125.38	128.60
1	a	822	U	C6-N1-C2	-5.36	117.78	121.00
1	a	893	C	C6-N1-C2	-5.36	118.16	120.30
25	A	137	U	N1-C2-N3	5.36	118.12	114.90
23	x	131	C	C3'-C2'-C1'	5.36	105.79	101.50
45	U	38	ILE	CG1-CB-CG2	-5.36	99.61	111.40
1	a	890	G	OP2-P-O3'	5.36	116.99	105.20
25	A	188	G	N3-C2-N2	-5.36	116.15	119.90
25	A	278	A	N1-C2-N3	-5.36	126.62	129.30
25	A	1455	G	N1-C6-O6	5.36	123.11	119.90
1	a	1112	C	N3-C2-O2	-5.36	118.15	121.90
1	a	1459	G	C5-C6-O6	-5.35	125.39	128.60
25	A	2450	A	N1-C2-N3	-5.35	126.62	129.30
25	A	1843	C	N1-C2-O2	5.35	122.11	118.90
25	A	82	U	N1-C2-O2	5.35	126.54	122.80
1	a	820	U	P-O3'-C3'	5.35	126.12	119.70
25	A	82	U	N3-C2-O2	-5.35	118.46	122.20
25	A	1588	G	N1-C6-O6	5.35	123.11	119.90
15	o	88	ARG	N-CA-CB	5.35	120.22	110.60
1	a	208	U	N1-C2-O2	5.34	126.54	122.80
25	A	546	U	N1-C2-O2	5.34	126.54	122.80
1	a	154	U	N1-C2-O2	5.34	126.54	122.80
25	A	832	U	N1-C2-N3	5.34	118.11	114.90
25	A	2585	U	C5-C6-N1	5.34	125.37	122.70
25	A	2394	C	N1-C2-O2	5.34	122.11	118.90
25	A	1487	U	N3-C2-O2	-5.34	118.46	122.20
25	A	1908	C	C6-N1-C2	-5.34	118.16	120.30
25	A	2347	C	C6-N1-C2	-5.34	118.16	120.30
40	P	113	LEU	CA-CB-CG	5.34	127.58	115.30
1	a	75	G	N1-C6-O6	-5.34	116.70	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	500	G	C5-C6-O6	-5.34	125.40	128.60
25	A	12	U	C2-N1-C1'	5.34	124.10	117.70
25	A	528	A	C5-C6-N1	-5.34	115.03	117.70
25	A	2742	G	C6-N1-C2	-5.33	121.90	125.10
25	A	965	C	N1-C2-O2	5.33	122.10	118.90
25	A	1352	U	N1-C2-O2	5.33	126.53	122.80
25	A	307	G	N3-C2-N2	-5.33	116.17	119.90
1	a	605	U	N3-C2-O2	-5.33	118.47	122.20
1	a	355	C	C2-N1-C1'	5.33	124.66	118.80
25	A	2306	C	C5-C6-N1	5.33	123.66	121.00
25	A	2364	C	N1-C2-O2	-5.33	115.70	118.90
1	a	1148	U	N3-C2-O2	-5.32	118.47	122.20
25	A	943	A	O5'-P-OP1	-5.32	100.91	105.70
25	A	1315	C	N1-C2-O2	5.32	122.09	118.90
25	A	2069	G7M	OP2-P-O3'	5.32	116.90	105.20
25	A	2283	C	N3-C4-C5	5.32	124.03	121.90
25	A	215	G	OP1-P-O3'	5.32	116.90	105.20
19	s	54	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	a	1345	U	N1-C2-O2	-5.31	119.08	122.80
25	A	1104	C	N3-C4-C5	-5.31	119.77	121.90
25	A	740	C	N1-C2-O2	5.31	122.09	118.90
25	A	2745	C	C6-N1-C2	-5.31	118.17	120.30
25	A	2759	G	N3-C2-N2	-5.31	116.18	119.90
25	A	1963	U	C5-C6-N1	5.31	125.36	122.70
1	a	267	C	N1-C2-O2	5.31	122.09	118.90
23	x	121	U	N1-C2-O2	5.31	126.52	122.80
25	A	343	C	C5-C6-N1	5.31	123.66	121.00
1	a	1107	C	O5'-P-OP1	-5.31	100.92	105.70
1	a	1086	U	N3-C2-O2	-5.31	118.49	122.20
25	A	2043	C	C2-N1-C1'	5.31	124.64	118.80
1	a	601	G	C5-C6-O6	-5.30	125.42	128.60
25	A	1730	C	OP2-P-O3'	5.30	116.87	105.20
1	a	1406	U	N3-C2-O2	-5.30	118.49	122.20
25	A	2566	A	OP2-P-O3'	5.30	116.86	105.20
25	A	1317	G	C6-C5-N7	-5.30	127.22	130.40
25	A	278	A	N3-C4-N9	5.30	131.64	127.40
1	a	810	C	N1-C2-O2	5.30	122.08	118.90
25	A	363	G	C6-C5-N7	-5.29	127.22	130.40
1	a	661	G	C6-C5-N7	-5.29	127.22	130.40
1	a	1490	U	N3-C2-O2	-5.29	118.50	122.20
1	a	450	G	C5-C6-O6	5.29	131.78	128.60
25	A	1069	A	OP1-P-O3'	5.29	116.84	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	671	G	C4-C5-N7	5.29	112.92	110.80
25	A	1090	A	N1-C2-N3	-5.29	126.66	129.30
1	a	1497	G	N3-C2-N2	-5.29	116.20	119.90
25	A	1833	C	N1-C2-O2	5.29	122.07	118.90
25	A	2248	C	C5-C6-N1	5.29	123.64	121.00
1	a	735	C	N1-C2-O2	5.28	122.07	118.90
1	a	1253	G	N1-C6-O6	-5.28	116.73	119.90
1	a	514	C	C5-C6-N1	5.28	123.64	121.00
25	A	2043	C	C5-C6-N1	5.28	123.64	121.00
25	A	2059	A	OP2-P-O3'	5.28	116.82	105.20
25	A	2282	G	N1-C6-O6	-5.28	116.73	119.90
25	A	2474	U	N3-C2-O2	-5.28	118.50	122.20
25	A	415	A	N1-C2-N3	-5.28	126.66	129.30
25	A	1644	C	C5-C6-N1	5.28	123.64	121.00
1	a	671	G	N9-C4-C5	-5.28	103.29	105.40
25	A	2297	A	C6-N1-C2	5.28	121.77	118.60
1	a	240	G	C4-C5-N7	5.28	112.91	110.80
1	a	563	A	C2-N3-C4	5.28	113.24	110.60
1	a	737	C	N3-C4-N4	5.27	121.69	118.00
1	a	989	U	N1-C2-O2	5.27	126.49	122.80
23	x	114	C	N1-C2-O2	5.27	122.06	118.90
1	a	457	G	C6-C5-N7	5.27	133.56	130.40
25	A	12	U	C6-N1-C2	-5.27	117.84	121.00
25	A	62	U	C6-N1-C2	-5.26	117.84	121.00
25	A	776	G	N3-C4-C5	-5.26	125.97	128.60
25	A	2200	C	N1-C2-O2	5.26	122.06	118.90
26	B	71	C	N1-C2-O2	5.26	122.06	118.90
1	a	375	U	N1-C2-O2	5.26	126.48	122.80
25	A	2023	C	C6-N1-C2	-5.26	118.19	120.30
25	A	2417	C	C6-N1-C2	-5.26	118.20	120.30
25	A	2394	C	N3-C2-O2	-5.26	118.22	121.90
25	A	1054	A	N9-C4-C5	-5.26	103.70	105.80
1	a	910	C	C6-N1-C2	-5.26	118.20	120.30
1	a	1060	U	N3-C2-O2	-5.26	118.52	122.20
1	a	1172	C	N1-C2-O2	5.26	122.05	118.90
1	a	754	C	OP1-P-O3'	5.25	116.75	105.20
25	A	2678	C	C5-C6-N1	5.25	123.63	121.00
1	a	87	C	C5-C6-N1	5.25	123.62	121.00
25	A	1164	C	N1-C2-O2	5.24	122.05	118.90
25	A	2215	C	C6-N1-C2	-5.24	118.20	120.30
1	a	18	C	C4-C5-C6	-5.24	114.78	117.40
1	a	396	C	C6-N1-C2	-5.24	118.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	271	C	N1-C2-O2	5.24	122.04	118.90
1	a	661	G	C4-C5-N7	5.24	112.90	110.80
25	A	69	C	N1-C2-O2	5.24	122.04	118.90
1	a	225	C	C5-C6-N1	5.24	123.62	121.00
25	A	2329	U	C5-C6-N1	5.24	125.32	122.70
1	a	168	G	N3-C4-N9	5.24	129.14	126.00
1	a	1158	C	N1-C2-O2	5.24	122.04	118.90
25	A	1892	C	C5-C6-N1	5.24	123.62	121.00
25	A	1101	U	N1-C2-N3	5.23	118.04	114.90
1	a	754	C	C2-N1-C1'	5.23	124.56	118.80
25	A	933	A	C2-N3-C4	5.23	113.22	110.60
1	a	1537	U	C5-C6-N1	5.23	125.31	122.70
25	A	1105	U	N3-C4-O4	-5.23	115.74	119.40
1	a	995	C	N1-C2-O2	5.23	122.04	118.90
25	A	163	C	C6-N1-C2	-5.23	118.21	120.30
25	A	2164	C	N3-C2-O2	-5.22	118.24	121.90
25	A	2752	C	N3-C2-O2	-5.22	118.24	121.90
1	a	213	G	C4-N9-C1'	5.22	133.29	126.50
1	a	1100	C	C6-N1-C2	-5.22	118.21	120.30
1	a	496	A	C2-N3-C4	5.22	113.21	110.60
25	A	143	C	C6-N1-C2	-5.22	118.21	120.30
25	A	987	C	N3-C4-C5	5.22	123.99	121.90
25	A	484	C	C2-N1-C1'	5.22	124.54	118.80
25	A	1269	A	N1-C2-N3	-5.22	126.69	129.30
25	A	105	C	N3-C2-O2	-5.21	118.25	121.90
25	A	557	C	C5-C6-N1	5.21	123.61	121.00
25	A	396	G	C6-C5-N7	-5.21	127.27	130.40
1	a	623	C	N3-C2-O2	-5.21	118.25	121.90
1	a	1227	A	C2-N3-C4	5.21	113.21	110.60
25	A	777	G	N1-C6-O6	5.21	123.03	119.90
1	a	33	A	C5-N7-C8	-5.21	101.30	103.90
1	a	34	C	C5-C6-N1	5.21	123.60	121.00
22	v	49	G	N3-C2-N2	5.21	123.55	119.90
25	A	2306	C	C6-N1-C2	-5.21	118.22	120.30
15	o	86	LEU	CA-CB-CG	5.21	127.28	115.30
25	A	1559	U	P-O3'-C3'	5.21	125.94	119.70
24	y	72	C	C6-N1-C2	-5.20	118.22	120.30
25	A	777	G	C6-C5-N7	-5.20	127.28	130.40
25	A	1055	G	N3-C2-N2	-5.20	116.26	119.90
1	a	413	G	C2-N3-C4	5.20	114.50	111.90
25	A	894	U	C2-N1-C1'	5.20	123.94	117.70
25	A	2162	G	N3-C4-N9	5.20	129.12	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	776	G	C2-N3-C4	5.20	114.50	111.90
25	A	2651	C	C6-N1-C2	-5.20	118.22	120.30
1	a	840	C	N1-C2-O2	-5.20	115.78	118.90
25	A	274	C	N3-C4-C5	5.19	123.98	121.90
25	A	1101	U	C2-N3-C4	-5.19	123.89	127.00
1	a	240	G	C8-N9-C4	5.19	108.47	106.40
25	A	2162	G	N3-C4-C5	-5.18	126.01	128.60
46	V	92	VAL	CG1-CB-CG2	-5.18	102.60	110.90
25	A	2325	G	C5-C6-O6	-5.18	125.49	128.60
25	A	363	G	C5-C6-N1	-5.17	108.91	111.50
22	v	74	C	C5-C6-N1	5.17	123.59	121.00
24	y	35	C	C2-N1-C1'	5.17	124.49	118.80
1	a	1225	A	C4-N9-C1'	5.17	135.60	126.30
25	A	1035	U	N3-C2-O2	-5.17	118.58	122.20
25	A	2409	G	C6-C5-N7	-5.17	127.30	130.40
1	a	661	G	N9-C4-C5	-5.17	103.33	105.40
1	a	1136	C	C5-C6-N1	5.17	123.58	121.00
1	a	1225	A	N1-C2-N3	-5.17	126.72	129.30
25	A	560	C	C5-C6-N1	5.17	123.58	121.00
45	U	51	LEU	N-CA-CB	-5.17	100.07	110.40
1	a	1033	G	C6-C5-N7	-5.16	127.30	130.40
25	A	349	U	N1-C2-O2	5.16	126.41	122.80
25	A	848	C	N1-C2-O2	5.16	122.00	118.90
1	a	386	C	C5-C4-N4	-5.16	116.59	120.20
1	a	1536	C	C6-N1-C2	-5.16	118.24	120.30
22	v	49	G	N9-C4-C5	-5.16	103.34	105.40
24	y	39	U	N3-C4-O4	5.16	123.01	119.40
25	A	817	C	N1-C2-O2	5.16	122.00	118.90
25	A	2262	U	N3-C4-O4	5.16	123.01	119.40
26	B	63	C	C6-N1-C2	-5.16	118.24	120.30
25	A	1538	G	C2-N3-C4	-5.16	109.32	111.90
25	A	2799	A	C4-C5-N7	5.15	113.28	110.70
1	a	452	A	N1-C2-N3	-5.15	126.72	129.30
25	A	550	C	C4-C5-C6	-5.15	114.83	117.40
25	A	680	C	C6-N1-C2	-5.15	118.24	120.30
25	A	2105	U	C2-N3-C4	5.15	130.09	127.00
25	A	2797	U	N1-C2-O2	5.15	126.41	122.80
25	A	740	C	C6-N1-C2	-5.15	118.24	120.30
25	A	1945	G	N3-C4-N9	5.15	129.09	126.00
25	A	2222	C	N3-C2-O2	-5.15	118.30	121.90
1	a	457	G	C2-N3-C4	5.15	114.47	111.90
22	v	1	C	C6-N1-C2	-5.15	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2222	C	N1-C2-O2	5.15	121.99	118.90
1	a	88	U	C5-C6-N1	5.15	125.27	122.70
24	y	35	C	C2-N3-C4	5.14	122.47	119.90
25	A	1394	U	C5-C6-N1	5.14	125.27	122.70
25	A	1583	A	C2-N3-C4	5.14	113.17	110.60
25	A	1630	A	C6-N1-C2	-5.14	115.51	118.60
1	a	1031	C	C5-C6-N1	5.14	123.57	121.00
12	l	23	LEU	CA-CB-CG	5.14	127.12	115.30
25	A	516	C	N1-C2-O2	5.14	121.98	118.90
25	A	2056	G	N9-C4-C5	-5.14	103.34	105.40
25	A	2443	C	N1-C2-O2	5.14	121.98	118.90
42	R	78	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	a	1088	G	N9-C4-C5	-5.14	103.34	105.40
24	y	18	G	C2-N3-C4	-5.14	109.33	111.90
25	A	805	G	N9-C4-C5	-5.14	103.35	105.40
1	a	1412	C	N1-C2-O2	5.13	121.98	118.90
1	a	544	G	C4-C5-N7	5.13	112.85	110.80
1	a	781	A	C2-N3-C4	5.13	113.17	110.60
24	y	56	C	N1-C2-O2	-5.13	115.82	118.90
25	A	1611	C	N1-C2-O2	5.13	121.98	118.90
25	A	2624	G	N1-C6-O6	5.12	122.97	119.90
23	x	100	A	C2-N3-C4	5.12	113.16	110.60
25	A	143	C	N1-C2-O2	5.12	121.97	118.90
25	A	257	C	N3-C2-O2	-5.12	118.31	121.90
25	A	1398	C	C2-N1-C1'	5.12	124.43	118.80
25	A	594	U	C5-C6-N1	5.12	125.26	122.70
25	A	2215	C	N1-C2-O2	5.12	121.97	118.90
1	a	1341	U	N3-C2-O2	-5.12	118.62	122.20
25	A	1584	U	C6-N1-C2	-5.12	117.93	121.00
25	A	2011	U	N1-C2-O2	5.12	126.38	122.80
25	A	2515	C	C5-C6-N1	5.12	123.56	121.00
1	a	83	C	C5-C6-N1	5.12	123.56	121.00
26	B	66	A	OP1-P-O3'	5.12	116.46	105.20
25	A	1880	U	C2-N1-C1'	5.12	123.84	117.70
25	A	69	C	N3-C2-O2	-5.11	118.32	121.90
25	A	2861	U	C5-C6-N1	5.11	125.26	122.70
25	A	709	U	N3-C2-O2	-5.11	118.62	122.20
31	G	136	ASP	CB-CG-OD1	5.11	122.90	118.30
25	A	1967	C	N1-C2-O2	5.11	121.97	118.90
1	a	524	G	C6-C5-N7	-5.11	127.34	130.40
22	v	56	C	C2-N3-C4	5.11	122.45	119.90
25	A	1874	C	N1-C2-O2	5.11	121.96	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2601	C	C5-C6-N1	5.11	123.55	121.00
25	A	1723	G	C5-C6-N1	5.10	114.05	111.50
25	A	2739	U	N1-C2-O2	5.10	126.37	122.80
25	A	1212	G	OP2-P-O3'	5.10	116.42	105.20
25	A	1108	U	N3-C2-O2	-5.10	118.63	122.20
25	A	2561	U	C2-N3-C4	-5.10	123.94	127.00
1	a	154	U	N3-C2-O2	-5.10	118.63	122.20
27	C	83	ASP	CB-CG-OD1	5.09	122.89	118.30
1	a	217	C	N1-C2-O2	5.09	121.95	118.90
1	a	661	G	C5-C6-O6	-5.09	125.55	128.60
25	A	946	C	C6-N1-C2	-5.09	118.26	120.30
1	a	348	G	C6-C5-N7	-5.09	127.35	130.40
1	a	147	G	C5-C6-O6	-5.08	125.55	128.60
1	a	796	C	C6-N1-C2	-5.08	118.27	120.30
25	A	158	U	N3-C2-O2	-5.08	118.64	122.20
25	A	531	C	C6-N1-C2	5.08	122.33	120.30
1	a	213	G	N1-C2-N3	5.08	126.95	123.90
25	A	2592	G	C6-C5-N7	-5.08	127.35	130.40
1	a	454	G	N7-C8-N9	5.08	115.64	113.10
25	A	55	G	N1-C6-O6	-5.08	116.85	119.90
25	A	307	G	N3-C4-N9	-5.08	122.95	126.00
26	B	97	C	C5-C4-N4	-5.08	116.64	120.20
25	A	105	C	N3-C4-C5	-5.08	119.87	121.90
25	A	305	C	C5-C6-N1	5.08	123.54	121.00
1	a	744	C	N3-C4-C5	5.07	123.93	121.90
25	A	2109	U	C6-N1-C2	-5.07	117.96	121.00
25	A	2192	U	C5-C4-O4	-5.07	122.86	125.90
1	a	1225	A	N3-C4-N9	5.07	131.46	127.40
1	a	1509	C	C6-N1-C2	-5.07	118.27	120.30
23	x	121	U	N3-C2-O2	-5.07	118.65	122.20
25	A	1669	A	C4-N9-C1'	5.07	135.43	126.30
25	A	1761	C	N3-C2-O2	-5.07	118.35	121.90
25	A	2515	C	C6-N1-C2	-5.07	118.27	120.30
26	B	79	G	C5-C6-N1	5.07	114.03	111.50
25	A	2091	C	N1-C2-O2	-5.07	115.86	118.90
1	a	370	C	N1-C2-O2	5.07	121.94	118.90
1	a	457	G	N9-C4-C5	5.07	107.43	105.40
1	a	1202	U	N3-C2-O2	-5.07	118.65	122.20
25	A	832	U	N3-C2-O2	-5.07	118.66	122.20
25	A	1198	U	N3-C2-O2	-5.07	118.65	122.20
1	a	1141	C	N3-C4-N4	5.06	121.54	118.00
25	A	115	C	C6-N1-C2	-5.06	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	195	A	OP1-P-O3'	5.06	116.33	105.20
1	a	90	C	C6-N1-C2	-5.06	118.28	120.30
1	a	215	C	C5-C4-N4	-5.06	116.66	120.20
25	A	2798	U	N1-C2-O2	5.06	126.34	122.80
1	a	248	C	C2-N1-C1'	5.06	124.36	118.80
22	v	61	C	N3-C2-O2	-5.06	118.36	121.90
25	A	1891	G	C4-N9-C1'	5.06	133.07	126.50
25	A	2300	C	N1-C2-O2	5.06	121.94	118.90
1	a	955	U	C5-C6-N1	5.06	125.23	122.70
25	A	145	C	N1-C2-O2	5.06	121.93	118.90
25	A	795	C	C5-C6-N1	5.06	123.53	121.00
25	A	1581	G	N1-C6-O6	5.05	122.93	119.90
25	A	2152	G	N7-C8-N9	5.05	115.63	113.10
1	a	740	U	N3-C2-O2	-5.05	118.66	122.20
25	A	282	A	C6-N1-C2	5.05	121.63	118.60
25	A	719	C	C6-N1-C2	-5.05	118.28	120.30
25	A	964	C	C6-N1-C2	-5.05	118.28	120.30
25	A	1734	G	N1-C6-O6	5.05	122.93	119.90
25	A	2791	G	C5-C6-O6	-5.05	125.57	128.60
25	A	62	U	C6-N1-C1'	-5.05	114.13	121.20
25	A	495	G	C5-C6-O6	-5.05	125.57	128.60
1	a	1037	C	N1-C2-O2	5.04	121.93	118.90
1	a	452	A	C2-N3-C4	5.04	113.12	110.60
1	a	654	G	C6-C5-N7	-5.04	127.37	130.40
1	a	1279	G	C8-N9-C4	-5.04	104.38	106.40
25	A	732	C	N1-C2-O2	5.04	121.92	118.90
25	A	2302	U	C6-N1-C2	-5.04	117.98	121.00
25	A	363	G	C2-N3-C4	-5.04	109.38	111.90
24	y	59	C	C2-N1-C1'	5.03	124.34	118.80
26	B	3	C	P-O3'-C3'	5.03	125.74	119.70
1	a	102	G	C5-C6-N1	5.03	114.02	111.50
1	a	1113	C	N1-C2-O2	5.03	121.92	118.90
25	A	999	U	N3-C2-O2	-5.03	118.68	122.20
25	A	2840	C	C6-N1-C2	-5.03	118.29	120.30
25	A	2863	C	N3-C4-N4	5.03	121.52	118.00
1	a	943	U	N1-C2-O2	5.03	126.32	122.80
25	A	89	A	N1-C2-N3	-5.03	126.78	129.30
25	A	153	U	N3-C2-O2	-5.03	118.68	122.20
25	A	740	C	N3-C4-N4	5.03	121.52	118.00
25	A	1343	G	N3-C4-N9	5.03	129.02	126.00
1	a	175	C	O5'-P-OP2	-5.03	101.18	105.70
25	A	653	U	O5'-P-OP2	-5.02	101.18	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	x	129	U	O4'-C1'-N1	5.02	112.22	108.20
25	A	2419	U	C6-N1-C2	-5.02	117.99	121.00
1	a	135	C	C6-N1-C2	-5.02	118.29	120.30
25	A	731	C	N1-C2-O2	5.02	121.91	118.90
25	A	2065	C	C5-C6-N1	5.02	123.51	121.00
1	a	56	U	C5-C6-N1	5.02	125.21	122.70
1	a	470	C	C6-N1-C2	-5.02	118.29	120.30
25	A	208	C	C6-N1-C2	-5.02	118.29	120.30
25	A	867	C	C6-N1-C2	-5.02	118.29	120.30
25	A	1200	C	C5-C6-N1	5.02	123.51	121.00
1	a	1149	C	C5-C6-N1	5.02	123.51	121.00
1	a	1372	U	N3-C2-O2	-5.02	118.69	122.20
25	A	766	U	C6-N1-C2	-5.01	117.99	121.00
1	a	58	C	N3-C4-C5	5.01	123.90	121.90
1	a	450	G	C6-C5-N7	5.01	133.41	130.40
24	y	39	U	C5-C4-O4	-5.01	122.90	125.90
25	A	848	C	C6-N1-C2	-5.01	118.30	120.30
25	A	729	G	C6-C5-N7	-5.00	127.40	130.40
1	a	1510	C	C5-C4-N4	-5.00	116.70	120.20
24	y	56	C	N3-C4-C5	5.00	123.90	121.90
25	A	349	U	N3-C2-O2	-5.00	118.70	122.20
25	A	1539	U	N3-C4-O4	5.00	122.90	119.40
25	A	2128	G	C4-C5-C6	5.00	121.80	118.80
1	a	295	C	N1-C2-O2	5.00	121.90	118.90
25	A	1892	C	C6-N1-C2	-5.00	118.30	120.30
25	A	2025	C	N1-C2-O2	5.00	121.90	118.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4',C3'
25	A	2069	G7M	C4',C3'

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	0	1	ALA	Mainchain
52	1	3	GLY	Mainchain
54	3	30	HIS	Peptide
27	C	120	ASP	Peptide
28	D	166	GLY	Peptide
29	E	82	GLY	Mainchain

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Mol	Chain	Res	Type	Group
30	F	173	ASP	Mainchain
33	H	2	GLN	Peptide
33	H	41	LYS	Mainchain
33	H	8	LYS	Peptide
35	K	89	ASN	Mainchain
36	L	29	LYS	Mainchain
45	U	50	ALA	Peptide
45	U	87	GLU	Mainchain
2	b	72	LYS	Peptide
5	e	76	ASN	Mainchain,Peptide
5	e	88	HIS	Peptide
6	f	52	ASN	Mainchain
6	f	97	THR	Mainchain
9	i	56	MET	Mainchain,Peptide
10	j	33	GLY	Mainchain,Peptide
10	j	34	ALA	Mainchain
12	l	101	LEU	Mainchain
12	l	23	LEU	Mainchain
13	m	3	ILE	Peptide
13	m	64	VAL	Peptide
15	o	87	ARG	Mainchain
16	p	43	ALA	Peptide
17	q	68	LYS	Mainchain
19	s	4	LEU	Mainchain
21	u	23	GLU	Mainchain
21	u	24	LYS	Mainchain

## 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	33029	0	16644	0	0
2	b	1705	0	1732	0	0
3	c	1625	0	1699	0	0
4	d	1643	0	1710	0	0
5	e	1157	0	1199	0	0
6	f	818	0	808	0	0
7	g	1182	0	1240	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	h	979	0	1034	0	0
9	i	1022	0	1070	0	0
10	j	787	0	828	0	0
11	k	870	0	878	0	0
12	l	955	0	1019	0	0
13	m	884	0	944	0	0
14	n	794	0	836	0	0
15	o	714	0	737	0	0
16	p	649	0	666	0	0
17	q	649	0	691	0	0
18	r	505	0	502	0	0
19	s	638	0	665	0	0
20	t	665	0	714	0	0
21	u	496	0	486	0	0
22	v	1644	0	840	0	0
23	x	1025	0	518	0	0
24	y	2031	0	1046	0	0
25	A	62274	0	31342	279	0
26	B	2570	0	1301	8	0
27	C	2083	0	2157	34	0
28	D	1565	0	1616	11	0
29	E	1552	0	1619	17	0
30	F	1411	0	1447	16	0
31	G	1323	0	1374	13	0
32	I	1032	0	1088	10	0
33	H	1111	0	1148	14	0
34	J	1129	0	1162	12	0
35	K	939	0	1012	11	0
36	L	1045	0	1117	18	0
37	M	1074	0	1157	10	0
38	N	961	0	1000	8	0
39	O	892	0	923	7	0
40	P	917	0	965	12	0
41	Q	947	0	1022	9	0
42	R	816	0	839	11	0
43	S	857	0	922	9	0
44	T	739	0	807	8	0
45	U	780	0	834	5	0
46	V	753	0	780	8	0
47	W	575	0	592	8	0
48	X	625	0	655	11	0
49	Y	509	0	543	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	Z	449	0	491	3	0
51	0	444	0	461	3	0
52	1	410	0	440	3	0
53	2	377	0	418	6	0
54	3	504	0	574	6	0
55	4	302	0	340	11	0
56	6	523	0	521	9	0
57	w	62	0	34	0	0
58	4	1	0	0	0	0
58	6	1	0	0	0	0
All	All	148018	0	99207	514	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (514) 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)
25:A:2164:C:H41	25:A:2171:A:H61	1.23	0.85
25:A:1171:G:H1	25:A:1177:G:H1	1.26	0.82
25:A:1171:G:N2	25:A:1178:C:O2	2.18	0.77
55:4:2:LYS:HD2	55:4:4:ARG:HH12	1.50	0.76
25:A:585:G:N7	41:Q:5:ARG:NH1	2.32	0.76
25:A:1270:C:H5''	25:A:1271:G:H5'	1.68	0.74
53:2:24:THR:HG23	53:2:27:GLY:H	1.53	0.73
25:A:1053:C:H42	25:A:1106:G:H1	1.37	0.73
25:A:1798:U:OP2	27:C:270:ARG:NH2	2.23	0.72
30:F:62:GLN:OE1	30:F:94:ARG:NH2	2.23	0.71
25:A:621:A:OP2	36:L:99:ASN:ND2	2.25	0.69
25:A:2691:C:HO2'	25:A:2871:U:HO2'	1.40	0.69
43:S:4:ILE:HG22	43:S:106:VAL:HG22	1.74	0.69
25:A:187:G:N2	25:A:190:A:N7	13.25	0.68
25:A:910:A:H62	37:M:12:MET:HA	1.57	0.68
25:A:1601:G:OP1	44:T:64:LYS:NZ	2.27	0.67
34:J:21:THR:OG1	34:J:58:ASN:ND2	2.27	0.67
27:C:141:HIS:ND1	27:C:192:GLY:O	2.26	0.67
47:W:33:ILE:HG22	47:W:34:VAL:HG23	1.77	0.67
31:G:83:THR:HA	31:G:132:LEU:O	1.95	0.66
25:A:2483:C:O2'	37:M:51:ARG:NH2	2.29	0.66
56:6:14:ALA:HB3	56:6:22:MET:HB2	1.78	0.66
36:L:100:ILE:HG13	36:L:101:ILE:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:88:ARG:HE	40:P:112:ARG:HH21	1.44	0.66
25:A:881:G:H21	25:A:896:A:H62	1.42	0.65
55:4:2:LYS:NZ	55:4:32:LYS:O	2.31	0.64
25:A:307:G:N2	25:A:310:A:OP2	2.29	0.64
40:P:59:THR:HG22	40:P:72:VAL:HG12	1.80	0.64
42:R:14:VAL:HG21	42:R:98:ILE:HG13	1.80	0.63
46:V:45:ASP:O	46:V:49:ASN:ND2	2.32	0.63
31:G:132:LEU:HB3	31:G:140:ILE:HD11	1.81	0.63
25:A:885:C:O2'	25:A:891:G:N2	2.28	0.63
29:E:146:VAL:HG12	29:E:185:LYS:HB2	1.80	0.63
25:A:1019:U:H3	25:A:1142:A:H62	1.47	0.62
27:C:169:ALA:O	27:C:185:ALA:N	2.29	0.62
25:A:2514:U:H4'	34:J:81:ILE:HD11	1.81	0.62
52:1:36:LYS:HD2	52:1:47:ILE:HG13	1.82	0.61
35:K:121:GLU:HG2	35:K:122:VAL:HG23	1.82	0.61
53:2:12:ARG:HE	53:2:44:VAL:HG21	1.65	0.61
25:A:1040:A:H61	25:A:1115:G:H1	1.46	0.61
48:X:5:GLN:O	48:X:73:ARG:NH2	2.33	0.61
34:J:98:GLU:O	34:J:102:GLU:HB2	2.01	0.60
30:F:43:ILE:HG21	30:F:78:ILE:HG22	1.84	0.59
25:A:1386:C:H2'	25:A:1387:A:C8	2.37	0.59
25:A:196:A:OP2	36:L:47:ARG:NH1	2.36	0.59
25:A:2199:A:OP1	48:X:36:ARG:NH2	2.35	0.59
25:A:1478:G:H1	25:A:1513:U:H3	1.50	0.59
43:S:3:THR:HG21	43:S:58:ALA:HB2	1.83	0.59
27:C:106:PRO:HD2	27:C:109:LEU:HD22	1.84	0.59
25:A:320:A:N3	29:E:163:ASN:ND2	2.51	0.59
29:E:119:ILE:O	29:E:187:VAL:HA	2.03	0.59
35:K:24:VAL:HG13	35:K:33:ALA:HB2	1.84	0.59
25:A:1264:A:H5'	51:0:7:PRO:HG2	1.85	0.59
25:A:750:A:OP1	25:A:1615:C:N4	2.36	0.59
25:A:680:C:O2'	27:C:268:ARG:NH2	60.50	0.59
27:C:7:PRO:HB3	27:C:13:ARG:HG3	1.85	0.58
42:R:4:VAL:HA	42:R:12:HIS:O	2.03	0.58
25:A:2394:C:H5''	36:L:63:LYS:HE3	1.85	0.58
41:Q:99:VAL:O	41:Q:102:LYS:NZ	2.36	0.58
54:3:41:ARG:HG2	54:3:44:ARG:HH21	1.67	0.58
25:A:848:C:H2'	25:A:849:A:C8	2.38	0.58
34:J:21:THR:HG1	34:J:58:ASN:ND2	2.00	0.58
46:V:64:VAL:HA	46:V:68:LYS:O	2.03	0.58
44:T:5:GLU:HA	44:T:8:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2676:C:OP1	35:K:31:ARG:NH2	2.37	0.57
47:W:17:LEU:O	47:W:20:LYS:NZ	2.36	0.57
25:A:1515:A:HO2'	25:A:1556:C:HO2'	1.53	0.57
25:A:1173:U:O2'	25:A:1177:G:N2	2.36	0.57
27:C:16:VAL:HB	27:C:203:VAL:HG22	1.87	0.57
33:H:14:SER:OG	33:H:17:ASP:OD2	2.22	0.57
30:F:28:PRO:HB3	30:F:159:ALA:HB2	1.86	0.57
35:K:109:SER:O	35:K:111:LYS:N	2.38	0.57
52:1:3:GLY:O	52:1:5:ARG:N	2.38	0.57
25:A:126:A:H5'	53:2:19:ARG:HG3	1.86	0.57
25:A:413:C:HO2'	25:A:1880:U:HO2'	1.52	0.57
34:J:60:ASP:N	34:J:60:ASP:OD1	2.39	0.56
27:C:170:TYR:HA	27:C:183:VAL:O	2.06	0.56
55:4:3:VAL:HG12	55:4:36:ARG:HD3	1.87	0.56
56:6:11:GLU:OE1	56:6:25:ARG:NH1	2.36	0.56
25:A:2377:A:O2'	39:O:117:PHE:O	2.23	0.56
36:L:95:LEU:HD22	36:L:100:ILE:HD11	1.88	0.56
49:Y:24:GLU:HB3	49:Y:46:VAL:HG21	1.86	0.56
32:I:75:ALA:HB2	32:I:112:LYS:HE3	1.87	0.55
25:A:2375:G:N2	25:A:2378:A:OP2	2.37	0.55
27:C:72:GLY:HA2	27:C:116:GLN:HE21	1.70	0.55
30:F:28:PRO:HB2	30:F:168:LEU:HD22	1.88	0.55
39:O:66:GLY:O	39:O:102:ARG:NH2	2.38	0.55
42:R:57:GLY:HA2	42:R:102:SER:O	2.06	0.55
39:O:30:ARG:HA	39:O:35:ILE:HD12	1.89	0.55
25:A:1326:U:O2'	25:A:2010:G:O2'	2.23	0.55
25:A:2271:G:H5'	47:W:16:ARG:HG2	1.89	0.55
25:A:1094:U:N3	25:A:1097:U:OP2	2.39	0.55
27:C:15:VAL:HG22	27:C:205:GLY:HA3	1.89	0.55
45:U:49:PRO:O	45:U:53:GLN:NE2	2.40	0.55
25:A:2133:G:H21	25:A:2158:A:H61	1.55	0.54
31:G:51:PHE:HZ	31:G:71:LEU:HD22	1.71	0.54
32:I:53:PRO:HD2	32:I:77:VAL:HG21	1.88	0.54
25:A:1012:U:OP2	41:Q:69:ARG:NH1	2.39	0.54
47:W:61:GLY:HA3	47:W:79:GLU:O	2.07	0.54
25:A:376:G:H2'	25:A:377:G:H8	1.73	0.54
27:C:86:ARG:HH12	27:C:155:ARG:HH21	1.54	0.54
35:K:35:VAL:HG22	35:K:69:VAL:HG12	1.90	0.54
25:A:2127:G:N2	25:A:2161:C:O2'	2.40	0.54
25:A:2506:U:H3	25:A:2585:U:H3	1.54	0.54
25:A:747:5MU:H5''	25:A:748:G:H5''	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:563:A:N3	41:Q:36:GLN:NE2	2.56	0.53
25:A:1223:G:OP1	42:R:68:ARG:NH2	2.42	0.53
25:A:290:U:O2	25:A:350:G:O6	2.27	0.53
31:G:82:PHE:O	31:G:133:LYS:HA	2.08	0.53
33:H:40:THR:O	33:H:42:LYS:N	2.42	0.53
25:A:848:C:H2'	25:A:849:A:H8	1.74	0.53
46:V:58:SER:OG	46:V:59:GLU:OE1	2.25	0.53
25:A:2327:A:H2'	25:A:2328:A:C8	2.44	0.53
25:A:2690:U:OP1	38:N:14:SER:OG	2.26	0.53
25:A:610:C:H2'	25:A:611:C:H6	1.74	0.53
25:A:2469:A:N6	25:A:2481:G:O2'	2.42	0.53
29:E:49:ARG:HE	29:E:75:SER:HA	1.74	0.53
33:H:26:ALA:HA	33:H:30:LEU:HB2	1.91	0.53
25:A:160:A:H2'	25:A:161:A:O4'	3.06	0.53
25:A:414:C:H2'	25:A:415:A:C8	2.43	0.53
25:A:269:C:H2'	25:A:270:A:C8	2.83	0.53
25:A:518:G:OP1	43:S:18:ARG:NH1	2.42	0.53
30:F:9:ASP:N	30:F:9:ASP:OD1	2.38	0.53
25:A:2130:U:H4'	25:A:2159:G:H22	1.73	0.52
25:A:276:U:O2'	25:A:278:A:N6	2.42	0.52
26:B:90:C:OP2	37:M:18:ARG:NH2	2.42	0.52
31:G:23:ILE:HD11	31:G:42:VAL:HG11	1.91	0.52
37:M:50:ARG:HD3	37:M:65:ILE:HD11	1.92	0.52
42:R:49:ILE:HG22	42:R:54:VAL:HA	1.90	0.52
27:C:140:VAL:HG12	27:C:191:LEU:HD23	1.91	0.52
25:A:1386:C:H2'	25:A:1387:A:H8	1.74	0.52
25:A:2359:C:O2'	54:3:53:ASP:OD2	2.27	0.52
30:F:72:SER:OG	30:F:80:GLN:N	2.43	0.52
38:N:45:ARG:HG2	38:N:95:THR:HG21	1.90	0.52
25:A:1340:U:OP1	44:T:19:LYS:NZ	2.33	0.52
25:A:1868:C:H2'	25:A:1869:G:O4'	2.09	0.52
25:A:2330:G:H21	47:W:38:GLY:HA2	1.75	0.52
40:P:91:VAL:HG21	40:P:96:LEU:HD21	1.92	0.52
50:Z:8:GLN:NE2	50:Z:10:ARG:O	2.39	0.52
25:A:1972:G:OP2	27:C:237:ARG:NH1	2.43	0.52
25:A:1794:A:H2'	25:A:1795:C:C6	2.45	0.51
25:A:9:G:O2'	25:A:2800:A:N6	2.43	0.51
40:P:26:GLU:HG2	40:P:43:GLU:HB2	1.91	0.51
25:A:560:C:O2'	41:Q:47:ARG:NH2	2.44	0.51
29:E:94:GLN:OE1	29:E:94:GLN:N	2.43	0.51
39:O:71:ALA:HB2	39:O:102:ARG:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:121:THR:HG21	28:D:143:PRO:HB3	1.93	0.51
44:T:58:VAL:HG22	44:T:85:VAL:HG13	1.93	0.51
25:A:558:U:H2'	25:A:559:G:C8	2.46	0.51
25:A:1124:G:H5''	34:J:37:ARG:HG3	41.59	0.51
32:I:100:ILE:HG22	32:I:101:SER:H	1.76	0.51
33:H:2:GLN:HB3	33:H:18:GLN:HB3	1.93	0.51
25:A:780:G:H21	25:A:783:A:H62	1.58	0.50
25:A:1779:U:H5	25:A:1784:A:N7	2.10	0.50
25:A:2267:A:H5''	25:A:2268:A:H5''	1.92	0.50
25:A:881:G:N2	25:A:896:A:H62	2.10	0.50
36:L:93:ASN:O	36:L:95:LEU:N	2.45	0.50
42:R:2:TYR:HA	42:R:14:VAL:O	2.11	0.50
25:A:796:C:H2'	25:A:797:G:C8	2.47	0.50
25:A:1040:A:N6	25:A:1115:G:H1	2.09	0.50
27:C:203:VAL:O	27:C:205:GLY:N	2.43	0.50
25:A:2512:C:O2'	28:D:159:LYS:NZ	2.36	0.50
41:Q:93:ILE:HD12	42:R:13:ARG:HB2	1.92	0.50
47:W:19:VAL:HG22	47:W:34:VAL:HG22	1.93	0.50
25:A:1194:A:OP2	36:L:14:LYS:NZ	2.45	0.50
37:M:69:PRO:HA	37:M:94:ALA:HB2	1.94	0.50
25:A:1918:A:O2'	25:A:1919:A:N7	2.43	0.50
25:A:2618:G:O2'	28:D:155:VAL:O	2.29	0.50
38:N:44:LEU:HD23	38:N:113:ILE:HD13	1.93	0.50
25:A:247:G:O2'	25:A:386:G:N1	2.44	0.49
25:A:277:G:H1'	25:A:361:G:H1	1.78	0.49
42:R:49:ILE:HB	42:R:51:VAL:O	2.13	0.49
43:S:82:MET:HB2	43:S:98:LYS:HB2	1.93	0.49
25:A:1469:A:H2'	25:A:1470:A:C8	2.46	0.49
25:A:2291:U:H2'	25:A:2292:U:C6	2.47	0.49
25:A:355:U:H2'	25:A:356:G:H8	1.78	0.49
55:4:11:CYS:SG	55:4:14:CYS:N	2.86	0.49
40:P:29:VAL:HG12	40:P:80:VAL:HG12	1.94	0.49
45:U:17:ASP:HB3	45:U:20:LYS:HD2	1.94	0.49
25:A:1816:C:N4	27:C:34:GLU:OE2	2.44	0.49
25:A:84:A:N1	25:A:98:G:O2'	2.36	0.49
34:J:35:ARG:HB2	34:J:54:ILE:HD11	1.94	0.49
27:C:130:PRO:HD3	27:C:188:ARG:NH1	2.28	0.49
46:V:20:LEU:HD21	46:V:41:GLU:HG3	1.95	0.49
36:L:19:LEU:HA	36:L:27:LEU:HD13	1.95	0.49
25:A:1858:A:N6	25:A:1884:G:O2'	2.45	0.48
25:A:269:C:H2'	25:A:270:A:H8	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:R:5:PHE:O	42:R:11:GLN:HA	2.13	0.48
25:A:770:G:H5''	53:2:10:LEU:HD23	1.94	0.48
25:A:639:U:H2'	25:A:640:C:C6	2.49	0.48
28:D:37:VAL:HG22	28:D:48:ILE:HG22	1.94	0.48
33:H:108:VAL:HG12	33:H:110:VAL:H	1.78	0.48
40:P:20:ARG:HH12	40:P:112:ARG:HD3	1.78	0.48
36:L:57:LEU:HD22	54:3:53:ASP:HB3	1.96	0.48
29:E:106:LYS:HG3	29:E:200:LEU:HD23	1.94	0.48
25:A:1278:C:H2'	25:A:1279:G:H8	1.78	0.48
25:A:2391:G:H2'	25:A:2424:C:N4	2.29	0.48
25:A:2832:U:H4'	25:A:2833:U:H5'	1.95	0.48
25:A:856:G:H2'	25:A:857:G:C8	2.48	0.48
54:3:22:LYS:HA	54:3:47:ALA:O	2.14	0.48
25:A:1073:A:H2'	25:A:1074:G:O4'	2.14	0.48
25:A:2514:U:H2'	25:A:2515:C:C6	2.49	0.48
25:A:2813:A:H2'	25:A:2814:A:C8	2.49	0.48
25:A:414:C:H2'	25:A:415:A:H8	1.78	0.48
25:A:558:U:H2'	25:A:559:G:H8	1.79	0.48
25:A:181:A:H2'	25:A:182:A:C8	2.48	0.48
25:A:2065:C:H4'	25:A:2251:OMG:HM23	1.94	0.48
31:G:94:ARG:HB2	31:G:105:SER:HB3	1.96	0.48
34:J:80:HIS:CE1	34:J:81:ILE:HG22	2.49	0.48
38:N:96:ARG:HH22	38:N:116:VAL:HG13	1.78	0.48
35:K:76:VAL:H	40:P:72:VAL:HG22	1.79	0.48
25:A:1326:U:HO2'	25:A:2010:G:HO2'	1.59	0.48
34:J:31:GLU:HG2	34:J:142:ILE:HG12	1.95	0.48
25:A:5:A:H2'	25:A:6:A:C8	2.49	0.47
28:D:25:THR:HG21	28:D:193:VAL:HG22	1.96	0.47
25:A:694:U:OP1	27:C:58:LYS:NZ	2.43	0.47
25:A:184:C:H2'	25:A:185:G:H8	1.79	0.47
25:A:2040:G:H2'	25:A:2041:U:O4'	2.14	0.47
25:A:2333:A:OP2	47:W:73:ARG:NH2	2.43	0.47
25:A:1723:G:H2'	25:A:1724:G:O4'	2.15	0.47
29:E:15:SER:HB2	29:E:18:THR:HB	1.97	0.47
25:A:2087:G:H2'	25:A:2088:A:C8	2.50	0.47
35:K:43:ILE:HD13	35:K:56:ASP:HB2	1.95	0.47
25:A:2013:A:H4'	43:S:96:ILE:HG22	1.97	0.47
55:4:9:LYS:HG3	55:4:14:CYS:HB2	1.96	0.47
25:A:1054:A:H61	25:A:1105:U:H3	1.60	0.47
25:A:2813:A:H2'	25:A:2814:A:H8	1.80	0.47
33:H:47:PHE:HA	33:H:51:ARG:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:U:61:GLU:N	45:U:61:GLU:OE1	2.47	0.47
25:A:1109:C:N3	25:A:1110:G:N2	2.62	0.47
25:A:277:G:H8	25:A:360:U:O4	1.97	0.47
47:W:37:ARG:HA	47:W:37:ARG:HD3	1.58	0.47
25:A:373:U:OP2	25:A:400:G:N1	2.47	0.47
25:A:2626:C:H2'	25:A:2627:G:C8	2.50	0.47
25:A:612:G:N2	25:A:614:A:O2'	2.48	0.47
25:A:839:U:H2'	25:A:840:C:C6	2.50	0.47
25:A:877:A:O2'	25:A:900:A:N6	2.48	0.47
55:4:17:VAL:HG23	55:4:24:ARG:HB2	1.97	0.46
25:A:1071:G:N2	25:A:1089:A:O2'	2.44	0.46
25:A:370:G:O2'	25:A:424:G:OP1	2.32	0.46
25:A:2092:U:OP2	33:H:27:ARG:NH2	2.31	0.46
32:I:85:ILE:HD11	32:I:137:LEU:HD21	1.96	0.46
34:J:13:ARG:HE	34:J:121:LYS:HZ1	1.63	0.46
48:X:37:PHE:O	48:X:45:PHE:HA	2.16	0.46
25:A:688:U:P	53:2:2:LYS:HZ1	2.37	0.46
54:3:25:HIS:CE1	54:3:47:ALA:HB2	2.50	0.46
25:A:1251:C:O2'	25:A:1253:A:OP2	2.34	0.46
25:A:1387:A:H2'	25:A:1388:G:H8	1.80	0.46
25:A:1548:A:H2'	25:A:1549:A:C8	2.51	0.46
25:A:2183:A:H2'	25:A:2184:A:C8	2.50	0.46
25:A:910:A:N3	25:A:2264:C:O2'	2.41	0.46
25:A:1715:G:HO2'	25:A:1716:U:H6	1.63	0.46
25:A:2626:C:H2'	25:A:2627:G:H8	1.81	0.46
25:A:2713:U:H3'	25:A:2714:G:H5''	1.97	0.46
25:A:280:U:H2'	25:A:281:C:C6	2.51	0.46
27:C:56:GLY:HA2	27:C:212:TRP:HA	1.98	0.46
25:A:2709:G:OP1	38:N:18:GLN:NE2	2.48	0.46
31:G:174:LYS:HG2	31:G:175:LYS:H	1.81	0.46
25:A:76:C:OP1	49:Y:48:ARG:NH1	2.49	0.46
27:C:230:PRO:HD2	27:C:246:PRO:HA	1.97	0.46
30:F:62:GLN:HE21	30:F:88:VAL:HG13	1.80	0.46
25:A:532:A:H5'	41:Q:27:ARG:HH12	1.81	0.46
33:H:46:PHE:HB3	33:H:50:ARG:HD2	1.97	0.46
33:H:75:LEU:HA	33:H:75:LEU:HD23	1.57	0.46
32:I:18:ASN:HD21	32:I:34:ILE:HG22	1.81	0.46
39:O:40:ILE:HG12	39:O:47:VAL:HG12	1.98	0.46
25:A:1746:A:H2'	25:A:1747:U:C6	2.52	0.45
25:A:2415:G:H2'	25:A:2416:C:C6	2.52	0.45
46:V:58:SER:O	46:V:73:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:3:ARG:HD3	53:2:3:ARG:HA	1.63	0.45
25:A:1434:A:H2'	25:A:1435:G:C8	2.51	0.45
25:A:1736:U:H2'	25:A:1737:G:O4'	2.16	0.45
25:A:729:G:H5''	25:A:730:A:O5'	2.16	0.45
25:A:882:G:O2'	25:A:883:G:H8	1.99	0.45
27:C:132:ARG:NH1	33:H:93:SER:OG	2.49	0.45
33:H:58:LEU:HA	33:H:61:VAL:HG22	1.98	0.45
35:K:58:LEU:HD11	35:K:86:LEU:HD13	1.98	0.45
25:A:1432:G:H2'	25:A:1433:A:C8	2.50	0.45
25:A:2584:U:H2'	25:A:2585:U:H5''	1.99	0.45
55:4:11:CYS:HB3	55:4:33:HIS:CE1	2.52	0.45
25:A:1597:A:H5''	25:A:1598:A:H5'	1.98	0.45
25:A:2467:C:OP1	55:4:8:LYS:NZ	2.39	0.45
25:A:729:G:C5	27:C:206:LYS:HB2	2.51	0.45
30:F:5:ASP:OD1	30:F:6:TYR:N	2.49	0.45
25:A:1023:U:H2'	25:A:1024:G:C8	3.90	0.45
25:A:171:U:H2'	25:A:172:A:H8	1.81	0.45
25:A:851:C:H2'	25:A:852:U:C6	2.52	0.45
27:C:166:ARG:HG3	27:C:171:VAL:HG22	1.99	0.45
25:A:2285:C:OP2	52:1:5:ARG:NH1	2.50	0.45
25:A:1817:G:OP1	27:C:86:ARG:NH2	2.49	0.45
32:I:30:GLN:HB3	32:I:60:VAL:HG11	1.99	0.45
55:4:7:VAL:HG13	55:4:38:GLY:HA3	1.99	0.45
25:A:1365:A:OP1	48:X:2:ARG:NH1	2.47	0.45
25:A:1744:A:H3'	25:A:1745:A:H8	1.82	0.45
25:A:1796:U:H2'	25:A:1797:G:H8	1.81	0.45
25:A:1:G:H2'	25:A:2:G:C8	2.52	0.45
27:C:259:ASN:O	27:C:261:ARG:N	2.44	0.45
25:A:2830:C:H5''	28:D:56:LYS:NZ	2.32	0.45
37:M:96:ILE:HG21	37:M:126:ILE:HD13	1.98	0.45
25:A:224:U:H2'	25:A:225:C:C6	4.03	0.45
29:E:7:ASP:OD1	29:E:7:ASP:N	2.48	0.45
44:T:63:VAL:HB	44:T:80:TRP:O	2.17	0.45
25:A:1023:U:OP2	25:A:1025:G:O2'	2.35	0.44
25:A:1:G:H2'	25:A:2:G:H8	1.81	0.44
25:A:499:U:H5''	45:U:42:LYS:HE2	1.99	0.44
25:A:871:U:H2'	25:A:872:U:C6	2.53	0.44
30:F:113:PHE:HD2	56:6:41:HIS:HE1	1.64	0.44
25:A:289:G:H2'	25:A:290:U:O4'	2.17	0.44
25:A:674:G:H1'	29:E:69:ARG:HH12	1.81	0.44
25:A:781:A:OP1	27:C:216:ARG:NH2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:942:G:OP2	36:L:39:LYS:NZ	2.45	0.44
25:A:832:U:H5'	36:L:38:GLN:HB3	1.99	0.44
25:A:1915:3TD:H10B	25:A:1916:A:C6	2.52	0.44
25:A:278:A:N1	25:A:361:G:C6	2.85	0.44
51:O:37:HIS:ND1	51:O:38:LEU:O	2.35	0.44
25:A:483:A:O4'	45:U:44:HIS:HB3	2.17	0.44
27:C:83:ASP:HB2	27:C:90:ILE:HG12	2.00	0.44
31:G:53:PRO:HG3	31:G:61:TRP:CE2	2.52	0.44
30:F:108:PRO:HB3	56:6:41:HIS:CD2	2.53	0.44
25:A:1278:C:H2'	25:A:1279:G:C8	2.52	0.44
25:A:1838:C:H4'	25:A:1839:G:H5''	2.00	0.44
31:G:53:PRO:HG3	31:G:61:TRP:CD2	2.53	0.44
39:O:25:ARG:HA	39:O:91:SER:O	2.18	0.44
25:A:1434:A:H2'	25:A:1435:G:O4'	2.63	0.44
27:C:252:LYS:HE2	27:C:252:LYS:HB2	1.84	0.44
29:E:154:ASP:OD1	29:E:154:ASP:N	2.49	0.44
25:A:568:U:H1'	25:A:2030:6MZ:H9C1	1.98	0.44
25:A:2098:U:H2'	25:A:2099:U:O4'	2.18	0.44
25:A:2788:C:H2'	25:A:2789:C:C6	2.52	0.44
25:A:610:C:H2'	25:A:611:C:C6	2.52	0.44
30:F:92:GLY:O	30:F:95:MET:HG2	2.17	0.44
35:K:65:THR:HG23	35:K:68:GLY:H	1.82	0.44
38:N:83:LEU:HD22	38:N:87:PHE:HE2	1.83	0.44
25:A:2328:A:H2'	25:A:2329:U:C6	2.53	0.44
30:F:30:VAL:HG23	30:F:155:ILE:HG23	2.00	0.44
37:M:102:LEU:HD11	37:M:126:ILE:HD11	2.00	0.44
40:P:21:PRO:HD3	40:P:49:ILE:HD12	1.99	0.44
25:A:1646:C:H5''	25:A:1647:U:H5''	2.00	0.43
35:K:41:ILE:HG13	35:K:58:LEU:O	2.18	0.43
54:3:15:LYS:HE2	54:3:19:GLY:HA2	2.00	0.43
25:A:1607:C:N4	25:A:1622:G:OP2	2.41	0.43
25:A:528:A:N1	25:A:2042:A:H2'	2.33	0.43
25:A:2834:G:H2'	25:A:2879:A:H61	1.83	0.43
25:A:1804:C:H2'	25:A:1805:A:H8	1.82	0.43
25:A:1869:G:N2	25:A:1872:A:OP2	2.49	0.43
25:A:2243:U:H2'	25:A:2244:U:C6	2.54	0.43
25:A:679:C:H2'	25:A:680:C:C6	2.53	0.43
27:C:86:ARG:NH1	27:C:155:ARG:HH21	2.16	0.43
32:I:104:GLN:OE1	32:I:104:GLN:N	2.49	0.43
46:V:77:VAL:HG23	46:V:89:ILE:HG12	2.00	0.43
25:A:161:A:H3'	25:A:162:U:H5''	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2812:G:H2'	25:A:2813:A:C8	2.54	0.43
25:A:2867:G:O2'	25:A:2868:A:H8	2.01	0.43
33:H:1:MET:O	33:H:20:ASN:ND2	2.51	0.43
55:4:30:GLU:O	55:4:33:HIS:HB2	2.19	0.43
25:A:1023:U:H2'	25:A:1024:G:H8	3.36	0.43
25:A:1509:A:H2'	25:A:1510:G:C8	2.52	0.43
25:A:2036:C:H6	25:A:2036:C:H5'	1.83	0.43
25:A:2899:A:H2'	25:A:2900:A:C8	2.53	0.43
25:A:319:G:H1	25:A:323:C:H5	1.67	0.43
40:P:24:THR:O	40:P:86:LYS:HB2	2.18	0.43
25:A:1932:A:H2'	25:A:1933:G:O4'	2.18	0.43
25:A:302:C:H2'	25:A:303:G:H8	1.83	0.43
25:A:2024:G:O3'	28:D:154:LYS:NZ	2.48	0.43
55:4:36:ARG:HG2	55:4:37:GLN:HB3	2.00	0.43
56:6:42:PRO:O	56:6:46:GLY:N	2.48	0.43
25:A:1437:C:H2'	25:A:1438:U:C6	2.54	0.43
25:A:2258:C:O2'	25:A:2427:C:OP2	2.37	0.43
25:A:2104:C:H2'	25:A:2105:U:H6	1.84	0.43
25:A:476:G:N1	25:A:479:A:OP2	2.48	0.43
25:A:883:G:H1	25:A:893:C:H42	1.67	0.43
31:G:37:ASN:OD1	31:G:38:ASP:N	2.52	0.43
48:X:39:VAL:HG12	48:X:42:GLU:H	1.84	0.43
25:A:1487:U:H2'	25:A:1488:C:C6	2.54	0.43
25:A:882:G:H22	25:A:895:U:H1'	1.84	0.43
33:H:32:PRO:HA	48:X:38:TRP:CD1	2.54	0.43
32:I:30:GLN:HG2	32:I:60:VAL:HB	2.00	0.43
41:Q:59:LEU:HD21	41:Q:63:ARG:HH12	1.84	0.43
42:R:41:ILE:HD13	42:R:103:ALA:HA	2.01	0.43
25:A:1614:A:H61	43:S:88:ARG:H	1.66	0.43
25:A:2140:G:H2'	25:A:2141:G:C8	2.53	0.42
25:A:2141:G:H2'	25:A:2142:A:H8	1.83	0.42
30:F:30:VAL:HG22	30:F:95:MET:HE1	2.00	0.42
39:O:2:ASP:O	39:O:5:SER:OG	2.34	0.42
25:A:38:A:H2'	25:A:39:G:O4'	2.18	0.42
25:A:715:A:H2'	25:A:716:A:C8	3.10	0.42
25:A:2599:G:C8	27:C:235:GLU:HG2	2.54	0.42
25:A:1126:A:H4'	25:A:1127:A:H5''	2.01	0.42
25:A:1469:A:H2'	25:A:1470:A:H8	1.84	0.42
26:B:30:C:H2'	26:B:31:C:H5'	2.00	0.42
26:B:93:C:H2'	26:B:94:A:C8	2.55	0.42
40:P:12:MET:O	40:P:14:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:6:62:LYS:HG2	56:6:63:ARG:NH1	2.34	0.42
25:A:1197:G:H2'	25:A:1198:U:H6	1.84	0.42
25:A:608:A:H2'	25:A:609:A:C8	2.54	0.42
28:D:184:ARG:HH12	40:P:6:GLN:HG2	1.84	0.42
25:A:2843:G:H2'	25:A:2844:G:O4'	2.20	0.42
56:6:56:ARG:O	56:6:59:ARG:HG2	2.20	0.42
25:A:116:C:H2'	25:A:117:G:O4'	2.18	0.42
26:B:28:C:H2'	26:B:29:A:C8	2.55	0.42
25:A:990:A:N1	42:R:78:ARG:NH1	2.67	0.42
43:S:17:VAL:HB	43:S:76:VAL:HG11	2.01	0.42
25:A:1387:A:H2'	25:A:1388:G:C8	2.54	0.42
25:A:685:A:H5''	25:A:788:A:H62	1.84	0.42
34:J:118:MET:HA	34:J:121:LYS:HG2	2.02	0.42
41:Q:97:ILE:HG22	41:Q:105:PHE:HB2	2.02	0.42
25:A:1353:A:H2'	25:A:1354:A:C8	2.54	0.42
25:A:745:1MG:HM11	25:A:745:1MG:HN21	1.69	0.42
31:G:94:ARG:HD2	31:G:127:GLN:HE21	1.85	0.42
25:A:144:A:H4'	44:T:2:ILE:HD11	2.02	0.42
25:A:2086:U:H2'	25:A:2087:G:C8	2.55	0.42
25:A:2301:C:H2'	25:A:2302:U:C6	2.55	0.42
35:K:25:LEU:HD12	35:K:38:ILE:HG22	2.02	0.42
25:A:2821:A:H2'	25:A:2822:G:O4'	2.20	0.42
26:B:95:U:H2'	26:B:96:G:H8	1.85	0.42
38:N:28:LEU:HD23	38:N:48:VAL:HG21	2.02	0.42
48:X:36:ARG:HA	48:X:47:THR:HA	2.01	0.42
56:6:37:CYS:O	56:6:41:HIS:HB2	2.20	0.41
25:A:2087:G:H2'	25:A:2088:A:H8	1.83	0.41
25:A:207:A:H2'	25:A:208:C:O4'	2.20	0.41
26:B:88:C:O2'	26:B:89:U:O5'	2.28	0.41
36:L:29:LYS:O	36:L:30:THR:OG1	2.38	0.41
50:Z:9:THR:OG1	50:Z:10:ARG:N	2.53	0.41
25:A:2376:A:H2'	25:A:2377:A:O4'	2.19	0.41
25:A:562:U:H5''	25:A:563:A:C5	11.89	0.41
25:A:660:C:H5''	29:E:94:GLN:HG3	2.01	0.41
25:A:782:A:H4'	25:A:783:A:H5'	2.01	0.41
26:B:49:C:H2'	26:B:50:A:C8	2.56	0.41
29:E:117:ARG:NH1	36:L:2:ARG:HG2	2.35	0.41
29:E:52:VAL:HG21	29:E:82:GLY:H	1.85	0.41
30:F:5:ASP:O	30:F:8:LYS:HB2	2.19	0.41
31:G:153:PRO:HA	31:G:159:LYS:O	2.20	0.41
25:A:1213:A:H1'	25:A:1237:A:C2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:527:C:C4	25:A:2779:U:H2'	2.55	0.41
25:A:45:G:H2'	25:A:46:G:C8	6.06	0.41
25:A:5:A:H2'	25:A:6:A:H8	1.84	0.41
25:A:2572:A:N7	28:D:150:GLN:HG2	2.35	0.41
34:J:37:ARG:HD3	34:J:37:ARG:HA	4.44	0.41
25:A:2757:A:N1	31:G:66:THR:OG1	2.47	0.41
25:A:397:U:OP2	48:X:9:LYS:NZ	2.36	0.41
25:A:801:G:O4'	29:E:49:ARG:NH2	2.54	0.41
25:A:833:A:H2'	25:A:834:G:C8	2.55	0.41
27:C:242:HIS:HA	27:C:243:PRO:HD3	1.90	0.41
25:A:364:C:H2'	25:A:365:U:C6	2.55	0.41
28:D:35:THR:OG1	28:D:49:GLN:HG3	2.20	0.41
40:P:46:VAL:HG22	40:P:60:VAL:HG22	2.01	0.41
43:S:17:VAL:HA	43:S:43:ALA:HB1	2.03	0.41
25:A:2800:A:C2	25:A:2895:G:H1'	2.56	0.41
25:A:517:C:OP1	51:O:12:ARG:NH2	2.54	0.41
25:A:669:G:H2'	25:A:669:G:N3	2.35	0.41
36:L:110:VAL:HG21	36:L:127:VAL:HG22	2.01	0.41
37:M:65:ILE:HG12	37:M:103:TYR:CE1	2.56	0.41
25:A:171:U:H2'	25:A:172:A:C8	2.56	0.41
25:A:2141:G:H2'	25:A:2142:A:C8	2.56	0.41
25:A:2784:U:H2'	25:A:2785:C:C6	2.55	0.41
25:A:620:G:H4'	25:A:621:A:O5'	2.21	0.41
32:I:92:PRO:HG3	32:I:136:GLY:HA2	2.03	0.41
25:A:475:C:O2	25:A:479:A:N6	2.53	0.41
25:A:593:U:H2'	25:A:594:U:C6	2.56	0.41
33:H:8:LYS:HE3	33:H:8:LYS:HB3	1.90	0.41
25:A:2247:A:H2'	25:A:2248:C:H6	1.86	0.41
25:A:2698:U:H2'	25:A:2699:C:C6	2.56	0.41
28:D:2:ILE:HG21	28:D:84:LEU:HD23	2.03	0.41
29:E:49:ARG:HH21	29:E:49:ARG:HD3	1.74	0.41
37:M:96:ILE:HA	37:M:96:ILE:HD12	1.93	0.41
25:A:1538:G:H2'	25:A:1539:U:C6	2.56	0.41
32:I:48:ILE:HG13	32:I:49:GLU:H	1.86	0.41
43:S:59:GLU:HA	43:S:64:ALA:HB2	2.03	0.41
44:T:57:VAL:O	44:T:86:THR:OG1	2.29	0.41
25:A:244:A:H5''	36:L:67:THR:HG21	2.03	0.41
25:A:594:U:H2'	25:A:595:C:C6	2.55	0.41
27:C:159:THR:HG23	27:C:176:ARG:HG2	2.03	0.41
30:F:60:SER:OG	30:F:61:GLY:N	2.54	0.41
56:6:26:SER:OG	56:6:27:THR:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2297:A:N1	25:A:2321:U:H5	2.18	0.40
25:A:807:U:H1'	25:A:2445:2MG:H5'	2.02	0.40
25:A:2610:C:H4'	25:A:2611:C:H5'	2.02	0.40
25:A:575:A:OP2	25:A:2055:C:N4	2.51	0.40
25:A:857:G:H2'	25:A:858:G:O4'	2.21	0.40
36:L:29:LYS:O	36:L:31:GLY:N	2.54	0.40
36:L:55:MET:HA	36:L:56:PRO:HD3	1.97	0.40
25:A:1170:C:H2'	25:A:1171:G:C8	2.56	0.40
37:M:17:ASN:ND2	37:M:17:ASN:O	2.55	0.40
38:N:59:SER:O	38:N:63:ARG:HG2	2.21	0.40
44:T:29:THR:O	44:T:33:LYS:HB2	13.65	0.40
48:X:3:VAL:HG22	48:X:10:ARG:HB3	2.03	0.40
25:A:1141:U:H4'	25:A:1142:A:O4'	2.20	0.40
25:A:1158:C:H2'	25:A:1159:U:H6	1.86	0.40
25:A:1178:C:H2'	25:A:1179:G:C8	2.56	0.40
25:A:1565:C:O2'	25:A:1566:A:H2'	2.20	0.40
25:A:2353:G:H2'	25:A:2354:C:O4'	2.21	0.40
25:A:2620:C:H2'	25:A:2621:G:O4'	2.22	0.40
25:A:372:G:H5''	48:X:60:LYS:HZ1	1.86	0.40
27:C:81:GLU:HG3	27:C:102:TYR:HE1	1.87	0.40
27:C:264:LYS:HE3	27:C:264:LYS:HB2	1.87	0.40
30:F:123:GLY:HA2	30:F:162:ASP:HB3	2.03	0.40
29:E:26:ALA:HB2	36:L:9:ALA:HB2	2.03	0.40
46:V:56:PHE:CE1	46:V:61:LEU:HD21	2.57	0.40
25:A:1410:G:H2'	25:A:1411:U:H6	1.87	0.40
25:A:1779:U:H5''	25:A:1780:A:H5''	2.03	0.40
25:A:2685:G:H2'	25:A:2686:G:H8	1.87	0.40
25:A:2836:U:H2'	25:A:2837:A:C8	2.56	0.40
25:A:2859:G:H2'	25:A:2860:A:C8	2.57	0.40
25:A:679:C:H2'	25:A:680:C:H6	1.86	0.40
26:B:54:G:H2'	26:B:55:U:H6	1.86	0.40
46:V:72:VAL:HG12	46:V:93:ARG:HA	2.02	0.40
50:Z:16:LEU:HB2	50:Z:19:HIS:ND1	2.37	0.40
25:A:2185:U:H2'	25:A:2186:G:C8	2.57	0.40
25:A:2834:G:H2'	25:A:2879:A:N6	2.36	0.40
25:A:372:G:H5''	48:X:60:LYS:NZ	2.36	0.40
25:A:784:G:H5'	25:A:785:G:OP1	2.21	0.40
25:A:813:U:H2'	25:A:814:C:C6	2.57	0.40
27:C:139:THR:HG23	27:C:160:TYR:HB2	2.03	0.40
29:E:149:ILE:HD11	29:E:172:ALA:HA	2.04	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	216/218 (99%)	190 (88%)	23 (11%)	3 (1%)	13	53
3	c	204/206 (99%)	191 (94%)	10 (5%)	3 (2%)	12	52
4	d	203/205 (99%)	181 (89%)	19 (9%)	3 (2%)	12	52
5	e	155/157 (99%)	139 (90%)	9 (6%)	7 (4%)	3	27
6	f	98/100 (98%)	83 (85%)	10 (10%)	5 (5%)	2	23
7	g	149/151 (99%)	136 (91%)	10 (7%)	3 (2%)	9	46
8	h	127/129 (98%)	115 (91%)	10 (8%)	2 (2%)	11	50
9	i	125/127 (98%)	105 (84%)	14 (11%)	6 (5%)	2	25
10	j	96/98 (98%)	83 (86%)	8 (8%)	5 (5%)	2	23
11	k	114/116 (98%)	102 (90%)	10 (9%)	2 (2%)	10	48
12	l	121/123 (98%)	101 (84%)	14 (12%)	6 (5%)	2	24
13	m	112/114 (98%)	100 (89%)	8 (7%)	4 (4%)	4	33
14	n	98/100 (98%)	86 (88%)	8 (8%)	4 (4%)	3	29
15	o	86/88 (98%)	73 (85%)	9 (10%)	4 (5%)	3	26
16	p	80/82 (98%)	69 (86%)	7 (9%)	4 (5%)	2	24
17	q	78/80 (98%)	65 (83%)	11 (14%)	2 (3%)	6	40
18	r	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	2	25
19	s	77/79 (98%)	71 (92%)	5 (6%)	1 (1%)	14	55
20	t	83/85 (98%)	76 (92%)	7 (8%)	0	100	100
21	u	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	12
27	C	269/271 (99%)	245 (91%)	19 (7%)	5 (2%)	9	47
28	D	207/209 (99%)	191 (92%)	13 (6%)	3 (1%)	13	53
29	E	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	12	52
30	F	175/177 (99%)	160 (91%)	13 (7%)	2 (1%)	17	59
31	G	174/176 (99%)	159 (91%)	12 (7%)	3 (2%)	11	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	I	139/141 (99%)	120 (86%)	15 (11%)	4 (3%)	5	38
33	H	147/149 (99%)	125 (85%)	17 (12%)	5 (3%)	4	35
34	J	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	13	53
35	K	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	4	35
36	L	141/143 (99%)	127 (90%)	10 (7%)	4 (3%)	6	39
37	M	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	12	52
38	N	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
39	O	114/116 (98%)	104 (91%)	9 (8%)	1 (1%)	20	63
40	P	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
41	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
42	R	101/103 (98%)	89 (88%)	9 (9%)	3 (3%)	5	37
43	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
44	T	91/93 (98%)	78 (86%)	11 (12%)	2 (2%)	8	44
45	U	100/102 (98%)	87 (87%)	7 (7%)	6 (6%)	2	19
46	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
47	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	13	53
48	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
49	Y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	11	50
50	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
51	0	54/56 (96%)	51 (94%)	2 (4%)	1 (2%)	9	47
52	1	48/50 (96%)	47 (98%)	0	1 (2%)	8	45
53	2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
54	3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	11	50
55	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
56	6	64/66 (97%)	58 (91%)	5 (8%)	1 (2%)	11	50
All	All	5717/5817 (98%)	5151 (90%)	439 (8%)	127 (2%)	12	44

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	73	ARG
5	e	77	ASN
5	e	89	THR

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Mol	Chain	Res	Type
5	e	93	VAL
6	f	53	LYS
6	f	54	LEU
6	f	98	GLU
9	i	57	VAL
9	i	90	ASP
10	j	34	ALA
11	k	88	PRO
12	l	23	LEU
12	l	75	GLU
13	m	4	ALA
13	m	65	GLU
16	p	44	SER
16	p	79	ASN
16	p	80	LYS
17	q	69	THR
18	r	11	ARG
19	s	4	LEU
21	u	24	LYS
27	C	121	ALA
28	D	167	ASN
29	E	83	VAL
30	F	174	PHE
31	G	108	PHE
33	H	3	VAL
33	H	9	VAL
33	H	41	LYS
35	K	35	VAL
35	K	110	GLU
36	L	36	LYS
45	U	6	ARG
45	U	38	ILE
45	U	51	LEU
45	U	88	ASP
51	0	2	VAL
52	1	4	ILE
54	3	31	ILE
2	b	18	GLN
3	c	156	LEU
6	f	92	THR
7	g	145	GLU
10	j	57	VAL

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Mol	Chain	Res	Type
13	m	6	ILE
14	n	34	ASN
15	o	46	LYS
18	r	17	VAL
18	r	46	THR
21	u	62	GLU
27	C	204	LEU
28	D	153	GLY
30	F	20	ASN
31	G	174	LYS
36	L	29	LYS
36	L	111	ILE
39	O	63	LYS
42	R	100	GLY
49	Y	22	LEU
56	6	4	ASP
4	d	191	SER
5	e	23	THR
5	e	50	GLY
5	e	102	THR
5	e	122	VAL
6	f	86	ARG
7	g	29	LEU
7	g	83	THR
8	h	47	ASP
9	i	12	LYS
9	i	107	ALA
9	i	125	GLN
10	j	42	LEU
10	j	93	ALA
11	k	92	ARG
13	m	104	ASN
14	n	2	LYS
14	n	53	ASP
15	o	2	LEU
16	p	43	ALA
21	u	8	ASN
29	E	80	SER
29	E	122	GLU
32	I	53	PRO
32	I	59	THR
42	R	55	ASP

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Mol	Chain	Res	Type
45	U	54	PRO
45	U	97	SER
3	c	96	VAL
3	c	205	GLU
4	d	29	THR
9	i	31	GLN
10	j	89	ARG
17	q	17	GLU
27	C	52	HIS
28	D	139	SER
31	G	47	ASN
32	I	64	ARG
33	H	15	LEU
35	K	89	ASN
44	T	38	ALA
8	h	2	MET
12	l	2	THR
12	l	21	PRO
12	l	88	ASP
12	l	101	LEU
15	o	27	GLN
15	o	45	HIS
27	C	154	ALA
33	H	89	LYS
36	L	94	THR
37	M	58	LYS
44	T	52	GLU
47	W	17	LEU
4	d	166	LYS
14	n	54	SER
21	u	34	ARG
21	u	65	ARG
27	C	260	LYS
35	K	93	GLN
37	M	69	PRO
2	b	27	LYS
42	R	54	VAL
32	I	12	VAL
34	J	81	ILE
34	J	100	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	180/180 (100%)	178 (99%)	2 (1%)	78	91
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	172 (100%)	0	100	100
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	103 (100%)	0	100	100
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	75 (99%)	1 (1%)	73	90
16	p	65/65 (100%)	64 (98%)	1 (2%)	70	88
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	41 (93%)	3 (7%)	18	56
27	C	216/216 (100%)	215 (100%)	1 (0%)	91	96
28	D	164/164 (100%)	164 (100%)	0	100	100
29	E	165/165 (100%)	165 (100%)	0	100	100
30	F	148/148 (100%)	148 (100%)	0	100	100
31	G	137/137 (100%)	137 (100%)	0	100	100
32	I	109/109 (100%)	105 (96%)	4 (4%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	H	114/114 (100%)	114 (100%)	0	100	100
34	J	116/116 (100%)	116 (100%)	0	100	100
35	K	103/103 (100%)	103 (100%)	0	100	100
36	L	102/102 (100%)	101 (99%)	1 (1%)	80	91
37	M	109/109 (100%)	108 (99%)	1 (1%)	82	93
38	N	100/100 (100%)	100 (100%)	0	100	100
39	O	86/86 (100%)	86 (100%)	0	100	100
40	P	99/99 (100%)	99 (100%)	0	100	100
41	Q	89/89 (100%)	89 (100%)	0	100	100
42	R	84/84 (100%)	84 (100%)	0	100	100
43	S	93/93 (100%)	93 (100%)	0	100	100
44	T	80/80 (100%)	80 (100%)	0	100	100
45	U	83/83 (100%)	82 (99%)	1 (1%)	75	90
46	V	78/78 (100%)	77 (99%)	1 (1%)	73	90
47	W	57/57 (100%)	57 (100%)	0	100	100
48	X	67/67 (100%)	67 (100%)	0	100	100
49	Y	55/55 (100%)	55 (100%)	0	100	100
50	Z	48/48 (100%)	48 (100%)	0	100	100
51	0	47/47 (100%)	46 (98%)	1 (2%)	59	84
52	1	45/45 (100%)	44 (98%)	1 (2%)	57	83
53	2	38/38 (100%)	38 (100%)	0	100	100
54	3	51/51 (100%)	51 (100%)	0	100	100
55	4	34/34 (100%)	34 (100%)	0	100	100
56	6	59/59 (100%)	51 (86%)	8 (14%)	4	23
All	All	4728/4751 (100%)	4702 (100%)	26 (0%)	91	96

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	86	CYS
2	b	122	ASP
15	o	87	ARG
16	p	19	VAL
21	u	12	ASP

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Mol	Chain	Res	Type
21	u	21	SER
21	u	37	TYR
27	C	85	ASN
32	I	27	LEU
32	I	33	ASN
32	I	35	MET
32	I	37	PHE
36	L	38	GLN
37	M	17	ASN
45	U	39	ASN
46	V	42	LEU
51	0	2	VAL
52	1	36	LYS
56	6	13	THR
56	6	16	CYS
56	6	30	HIS
56	6	32	LEU
56	6	34	LEU
56	6	40	CYS
56	6	45	THR
56	6	66	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	40	GLN
7	g	147	ASN
11	k	80	ASN
15	o	34	GLN
16	p	79	ASN
27	C	44	ASN
27	C	52	HIS
27	C	116	GLN
29	E	41	GLN
31	G	127	GLN
32	I	42	ASN
33	H	20	ASN
34	J	58	ASN
45	U	39	ASN
46	V	78	GLN
48	X	15	ASN
52	1	44	GLN

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Mol	Chain	Res	Type
56	6	41	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	247 (16%)	0
22	v	76/77 (98%)	15 (19%)	0
23	x	47/48 (97%)	22 (46%)	0
24	y	87/95 (91%)	12 (13%)	0
25	A	2894/2903 (99%)	513 (17%)	34 (1%)
26	B	119/120 (99%)	19 (15%)	3 (2%)
57	w	2/3 (66%)	0	0
All	All	4760/4785 (99%)	828 (17%)	37 (0%)

All (828) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	G
1	a	7	A
1	a	8	A
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	41	G
1	a	42	G
1	a	47	C
1	a	48	C
1	a	49	U
1	a	50	A
1	a	51	A
1	a	61	G
1	a	65	A
1	a	71	A
1	a	79	G
1	a	81	A
1	a	82	G
1	a	83	C
1	a	86	G
1	a	88	U
1	a	94	G

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Mol	Chain	Res	Type
1	a	95	C
1	a	96	U
1	a	116	A
1	a	118	U
1	a	121	U
1	a	126	G
1	a	127	G
1	a	131	A
1	a	168	G
1	a	174	A
1	a	178	C
1	a	181	A
1	a	183	C
1	a	197	A
1	a	208	U
1	a	210	C
1	a	211	G
1	a	226	G
1	a	240	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	264	C
1	a	266	G
1	a	267	C
1	a	281	G
1	a	289	G
1	a	319	G
1	a	328	C
1	a	330	C
1	a	340	U
1	a	345	C
1	a	346	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	367	U
1	a	369	G
1	a	372	C
1	a	373	A
1	a	384	G
1	a	397	A

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Mol	Chain	Res	Type
1	a	398	U
1	a	406	G
1	a	410	G
1	a	411	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	421	U
1	a	423	G
1	a	429	U
1	a	441	A
1	a	446	G
1	a	466	A
1	a	467	U
1	a	481	G
1	a	482	A
1	a	486	U
1	a	496	A
1	a	497	G
1	a	499	A
1	a	506	G
1	a	509	A
1	a	511	C
1	a	512	U
1	a	518	C
1	a	527	G7M
1	a	528	C
1	a	532	A
1	a	546	A
1	a	547	A
1	a	550	G
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	596	A
1	a	615	G
1	a	617	G
1	a	633	G
1	a	642	A

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Mol	Chain	Res	Type
1	a	654	G
1	a	661	G
1	a	665	A
1	a	671	G
1	a	687	A
1	a	701	U
1	a	702	A
1	a	713	G
1	a	718	A
1	a	723	U
1	a	724	G
1	a	731	G
1	a	733	G
1	a	734	G
1	a	759	A
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	829	G
1	a	832	G
1	a	836	G
1	a	843	U
1	a	844	G
1	a	845	A
1	a	846	G
1	a	849	G
1	a	872	A
1	a	873	A
1	a	885	G
1	a	890	G
1	a	891	U
1	a	902	G
1	a	914	A
1	a	926	G
1	a	934	C
1	a	935	A
1	a	960	U

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Mol	Chain	Res	Type
1	a	961	U
1	a	966	2MG
1	a	967	5MC
1	a	968	A
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	991	U
1	a	992	U
1	a	993	G
1	a	996	A
1	a	1004	A
1	a	1020	G
1	a	1026	G
1	a	1028	C
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1053	G
1	a	1066	C
1	a	1070	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1126	U
1	a	1130	A
1	a	1132	C
1	a	1135	U
1	a	1136	C
1	a	1137	C
1	a	1139	G
1	a	1140	C
1	a	1151	A
1	a	1159	U
1	a	1160	G
1	a	1161	C
1	a	1182	G
1	a	1183	U
1	a	1191	A

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Mol	Chain	Res	Type
1	a	1196	A
1	a	1197	A
1	a	1207	2MG
1	a	1212	U
1	a	1213	A
1	a	1214	C
1	a	1223	C
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1236	A
1	a	1238	A
1	a	1241	G
1	a	1257	A
1	a	1260	G
1	a	1280	A
1	a	1286	U
1	a	1287	A
1	a	1298	U
1	a	1300	G
1	a	1302	C
1	a	1305	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1332	A
1	a	1346	A
1	a	1353	G
1	a	1363	A
1	a	1364	U
1	a	1381	U
1	a	1398	A
1	a	1401	G
1	a	1419	G
1	a	1422	G
1	a	1429	A
1	a	1433	A
1	a	1446	A
1	a	1452	C
1	a	1453	G
1	a	1492	A
1	a	1494	G

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Mol	Chain	Res	Type
1	a	1498	UR3
1	a	1499	A
1	a	1503	A
1	a	1504	G
1	a	1505	G
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1534	A
1	a	1535	C
1	a	1540	U
22	v	8	4SU
22	v	9	G
22	v	14	A
22	v	17	C
22	v	17(A)	U
22	v	18	G
22	v	19	G
22	v	20	H2U
22	v	22	G
22	v	47	U
22	v	49	G
22	v	59	A
22	v	60	U
22	v	75	C
22	v	76	A
23	x	89	G
23	x	94	U
23	x	95	U
23	x	96	C
23	x	98	U
23	x	104	U
23	x	109	C
23	x	110	G
23	x	113	C
23	x	117	C
23	x	120	U
23	x	121	U
23	x	122	G
23	x	123	C

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Mol	Chain	Res	Type
23	x	125	G
23	x	126	G
23	x	127	U
23	x	128	C
23	x	129	U
23	x	130	G
23	x	131	C
23	x	134	C
24	y	10	C
24	y	17	G
24	y	19	H2U
24	y	20	G
24	y	35	C
24	y	47(F)	C
24	y	47(G)	C
24	y	47(K)	G
24	y	51	A
24	y	55	PSU
24	y	74	C
24	y	76	A
25	A	10	A
25	A	35	G
25	A	36	G
25	A	39	G
25	A	43	G
25	A	46	G
25	A	50	U
25	A	51	G
25	A	52	A
25	A	60	G
25	A	63	A
25	A	71	A
25	A	74	A
25	A	75	G
25	A	100	U
25	A	102	U
25	A	103	A
25	A	118	A
25	A	120	U
25	A	138	U
25	A	142	A
25	A	162	U

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Mol	Chain	Res	Type
25	A	163	C
25	A	178	G
25	A	196	A
25	A	205	G
25	A	206	U
25	A	216	A
25	A	219	A
25	A	221	A
25	A	222	A
25	A	225	C
25	A	228	C
25	A	229	C
25	A	247	G
25	A	248	G
25	A	250	G
25	A	255	A
25	A	266	G
25	A	276	U
25	A	277	G
25	A	278	A
25	A	285	G
25	A	294	A
25	A	310	A
25	A	323	C
25	A	324	A
25	A	329	G
25	A	330	A
25	A	332	A
25	A	346	A
25	A	349	U
25	A	361	G
25	A	371	A
25	A	372	G
25	A	373	U
25	A	386	G
25	A	387	U
25	A	396	G
25	A	404	A
25	A	406	G
25	A	411	G
25	A	412	A
25	A	424	G

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Mol	Chain	Res	Type
25	A	451	U
25	A	455	C
25	A	456	C
25	A	457	A
25	A	473	G
25	A	481	G
25	A	491	G
25	A	496	G
25	A	504	A
25	A	505	A
25	A	509	C
25	A	513	A
25	A	518	G
25	A	527	C
25	A	529	A
25	A	531	C
25	A	532	A
25	A	543	G
25	A	544	C
25	A	545	U
25	A	547	A
25	A	548	G
25	A	549	G
25	A	551	G
25	A	556	A
25	A	563	A
25	A	572	A
25	A	573	U
25	A	575	A
25	A	588	U
25	A	603	A
25	A	614	A
25	A	622	G
25	A	627	A
25	A	637	A
25	A	645	C
25	A	646	U
25	A	647	G
25	A	654	A
25	A	655	A
25	A	656	G
25	A	668	A

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Mol	Chain	Res	Type
25	A	669	G
25	A	685	A
25	A	686	U
25	A	694	U
25	A	695	G
25	A	702	U
25	A	714	U
25	A	717	C
25	A	723	C
25	A	729	G
25	A	730	A
25	A	740	C
25	A	747	5MU
25	A	752	A
25	A	757	G
25	A	765	C
25	A	775	G
25	A	776	G
25	A	777	G
25	A	782	A
25	A	783	A
25	A	784	G
25	A	785	G
25	A	789	A
25	A	805	G
25	A	807	U
25	A	812	C
25	A	819	A
25	A	822	G
25	A	827	U
25	A	828	U
25	A	831	G
25	A	844	A
25	A	845	A
25	A	846	U
25	A	847	U
25	A	858	G
25	A	859	G
25	A	869	G
25	A	883	G
25	A	885	C
25	A	886	A

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Mol	Chain	Res	Type
25	A	898	C
25	A	910	A
25	A	914	G
25	A	915	C
25	A	932	U
25	A	941	A
25	A	945	A
25	A	946	C
25	A	958	U
25	A	959	A
25	A	961	C
25	A	973	A
25	A	974	G
25	A	983	A
25	A	985	C
25	A	990	A
25	A	995	C
25	A	996	A
25	A	1012	U
25	A	1013	C
25	A	1021	A
25	A	1022	G
25	A	1023	U
25	A	1026	G
25	A	1033	U
25	A	1034	G
25	A	1040	A
25	A	1043	C
25	A	1045	C
25	A	1046	A
25	A	1047	G
25	A	1053	C
25	A	1054	A
25	A	1057	A
25	A	1060	U
25	A	1061	U
25	A	1062	G
25	A	1065	U
25	A	1066	U
25	A	1068	G
25	A	1069	A
25	A	1070	A

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Mol	Chain	Res	Type
25	A	1071	G
25	A	1072	C
25	A	1076	C
25	A	1079	C
25	A	1084	A
25	A	1088	A
25	A	1097	U
25	A	1104	C
25	A	1106	G
25	A	1112	G
25	A	1116	G
25	A	1132	U
25	A	1135	C
25	A	1136	G
25	A	1137	G
25	A	1142	A
25	A	1148	U
25	A	1155	A
25	A	1165	A
25	A	1172	C
25	A	1174	U
25	A	1175	A
25	A	1178	C
25	A	1179	G
25	A	1180	U
25	A	1183	U
25	A	1186	G
25	A	1204	A
25	A	1205	A
25	A	1210	G
25	A	1211	C
25	A	1212	G
25	A	1213	A
25	A	1227	G
25	A	1237	A
25	A	1238	G
25	A	1247	A
25	A	1248	G
25	A	1250	G
25	A	1251	C
25	A	1253	A
25	A	1256	G

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Mol	Chain	Res	Type
25	A	1271	G
25	A	1272	A
25	A	1273	U
25	A	1287	A
25	A	1300	G
25	A	1301	A
25	A	1306	C
25	A	1314	C
25	A	1325	U
25	A	1326	U
25	A	1332	G
25	A	1345	C
25	A	1352	U
25	A	1365	A
25	A	1368	G
25	A	1379	U
25	A	1383	A
25	A	1386	C
25	A	1395	A
25	A	1416	G
25	A	1417	C
25	A	1421	G
25	A	1428	C
25	A	1429	G
25	A	1453	A
25	A	1454	C
25	A	1458	U
25	A	1459	G
25	A	1475	G
25	A	1482	G
25	A	1498	C
25	A	1504	A
25	A	1515	A
25	A	1524	G
25	A	1533	C
25	A	1536	C
25	A	1558	C
25	A	1559	U
25	A	1560	G
25	A	1567	G
25	A	1568	G
25	A	1569	A

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Mol	Chain	Res	Type
25	A	1578	U
25	A	1581	G
25	A	1583	A
25	A	1584	U
25	A	1608	A
25	A	1617	C
25	A	1627	G
25	A	1646	C
25	A	1647	U
25	A	1648	U
25	A	1649	G
25	A	1665	A
25	A	1669	A
25	A	1674	G
25	A	1682	G
25	A	1695	G
25	A	1698	A
25	A	1715	G
25	A	1716	U
25	A	1729	U
25	A	1730	C
25	A	1732	C
25	A	1733	G
25	A	1738	G
25	A	1758	U
25	A	1764	C
25	A	1773	A
25	A	1781	U
25	A	1782	U
25	A	1784	A
25	A	1791	A
25	A	1800	C
25	A	1801	A
25	A	1808	A
25	A	1809	A
25	A	1812	U
25	A	1816	C
25	A	1829	A
25	A	1833	C
25	A	1847	A
25	A	1857	G
25	A	1870	C

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Mol	Chain	Res	Type
25	A	1873	G
25	A	1884	G
25	A	1899	A
25	A	1901	A
25	A	1906	G
25	A	1913	A
25	A	1919	A
25	A	1929	G
25	A	1930	G
25	A	1931	U
25	A	1936	A
25	A	1937	A
25	A	1938	A
25	A	1941	C
25	A	1942	C
25	A	1955	U
25	A	1966	A
25	A	1967	C
25	A	1970	A
25	A	1971	U
25	A	1972	G
25	A	1991	U
25	A	1993	U
25	A	1997	C
25	A	2022	U
25	A	2023	C
25	A	2031	A
25	A	2032	G
25	A	2034	U
25	A	2036	C
25	A	2043	C
25	A	2044	C
25	A	2049	G
25	A	2050	C
25	A	2055	C
25	A	2056	G
25	A	2060	A
25	A	2061	G
25	A	2062	A
25	A	2069	G7M
25	A	2070	A
25	A	2072	C

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Mol	Chain	Res	Type
25	A	2093	G
25	A	2096	C
25	A	2100	G
25	A	2108	A
25	A	2111	U
25	A	2112	G
25	A	2113	U
25	A	2116	G
25	A	2118	U
25	A	2119	A
25	A	2120	G
25	A	2121	G
25	A	2122	U
25	A	2125	G
25	A	2127	G
25	A	2129	C
25	A	2131	U
25	A	2132	U
25	A	2133	G
25	A	2137	U
25	A	2145	C
25	A	2147	A
25	A	2152	G
25	A	2153	C
25	A	2159	G
25	A	2160	C
25	A	2166	U
25	A	2169	A
25	A	2170	A
25	A	2172	U
25	A	2173	A
25	A	2178	C
25	A	2182	U
25	A	2183	A
25	A	2189	U
25	A	2192	U
25	A	2198	A
25	A	2199	A
25	A	2204	G
25	A	2211	A
25	A	2213	U
25	A	2223	G

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Mol	Chain	Res	Type
25	A	2225	A
25	A	2238	G
25	A	2239	G
25	A	2250	G
25	A	2268	A
25	A	2279	G
25	A	2283	C
25	A	2287	A
25	A	2294	G
25	A	2305	U
25	A	2309	A
25	A	2312	U
25	A	2321	U
25	A	2322	A
25	A	2325	G
25	A	2327	A
25	A	2331	G
25	A	2333	A
25	A	2347	C
25	A	2350	C
25	A	2354	C
25	A	2383	G
25	A	2385	C
25	A	2392	A
25	A	2402	U
25	A	2403	C
25	A	2406	A
25	A	2429	G
25	A	2430	A
25	A	2435	A
25	A	2441	U
25	A	2445	2MG
25	A	2448	A
25	A	2464	G
25	A	2470	G
25	A	2476	A
25	A	2484	G
25	A	2494	G
25	A	2502	G
25	A	2505	G
25	A	2506	U
25	A	2513	A

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Mol	Chain	Res	Type
25	A	2518	A
25	A	2519	U
25	A	2520	C
25	A	2535	G
25	A	2542	A
25	A	2547	A
25	A	2554	U
25	A	2567	G
25	A	2569	G
25	A	2572	A
25	A	2573	C
25	A	2585	U
25	A	2586	U
25	A	2602	A
25	A	2603	G
25	A	2609	U
25	A	2610	C
25	A	2611	C
25	A	2613	U
25	A	2615	U
25	A	2621	G
25	A	2629	U
25	A	2630	G
25	A	2634	A
25	A	2646	C
25	A	2663	G
25	A	2682	A
25	A	2689	U
25	A	2690	U
25	A	2707	U
25	A	2713	U
25	A	2714	G
25	A	2716	C
25	A	2718	G
25	A	2720	U
25	A	2722	G
25	A	2729	G
25	A	2732	G
25	A	2733	A
25	A	2744	G
25	A	2748	A
25	A	2755	C

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Mol	Chain	Res	Type
25	A	2764	A
25	A	2765	A
25	A	2766	A
25	A	2769	U
25	A	2778	A
25	A	2791	G
25	A	2793	C
25	A	2794	C
25	A	2798	U
25	A	2800	A
25	A	2801	G
25	A	2809	A
25	A	2818	U
25	A	2820	A
25	A	2821	A
25	A	2832	U
25	A	2833	U
25	A	2834	G
25	A	2849	U
25	A	2867	G
25	A	2868	A
25	A	2872	A
25	A	2873	A
25	A	2880	C
25	A	2883	A
25	A	2887	A
25	A	2891	U
25	A	2894	G
25	A	2902	C
26	B	4	C
26	B	9	G
26	B	12	C
26	B	13	G
26	B	24	G
26	B	25	U
26	B	26	C
26	B	35	C
26	B	40	U
26	B	41	G
26	B	44	G
26	B	67	G
26	B	68	C

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Mol	Chain	Res	Type
26	B	87	U
26	B	88	C
26	B	89	U
26	B	90	C
26	B	97	C
26	B	109	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	51	G
25	A	205	G
25	A	228	C
25	A	372	G
25	A	512	G
25	A	555	G
25	A	758	C
25	A	774	G
25	A	989	G
25	A	1070	A
25	A	1111	A
25	A	1182	G
25	A	1190	G
25	A	1212	G
25	A	1236	G
25	A	1240	U
25	A	1432	G
25	A	1458	U
25	A	1567	G
25	A	1715	G
25	A	1900	A
25	A	1930	G
25	A	1940	U
25	A	2061	G
25	A	2128	G
25	A	2326	C
25	A	2391	G
25	A	2447	G
25	A	2566	A
25	A	2610	C
25	A	2800	A
25	A	2820	A

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Mol	Chain	Res	Type
25	A	2832	U
25	A	2867	G
26	B	24	G
26	B	66	A
26	B	88	C

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

43 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	6MZ	A	1618	25	18,25,26	1.10	1 (5%)	16,36,39	3.02	4 (25%)
25	2MG	A	1835	25	19,26,27	0.96	2 (10%)	20,38,41	2.25	7 (35%)
25	PSU	A	1911	25	16,21,22	1.55	4 (25%)	20,30,33	3.38	6 (30%)
25	3TD	A	1915	25	16,22,23	3.01	5 (31%)	19,32,35	1.97	5 (26%)
25	PSU	A	1917	25	16,21,22	1.54	4 (25%)	20,30,33	3.29	6 (30%)
25	5MU	A	1939	25	14,22,23	1.04	1 (7%)	16,32,35	2.01	3 (18%)
25	5MC	A	1962	25	15,22,23	1.22	1 (6%)	17,32,35	1.49	3 (17%)
25	6MZ	A	2030	25	18,25,26	1.15	2 (11%)	16,36,39	3.31	4 (25%)
25	G7M	A	2069	25	19,26,27	1.33	3 (15%)	19,39,42	2.43	7 (36%)
25	OMG	A	2251	25,22	18,26,27	1.10	2 (11%)	22,38,41	2.07	6 (27%)
25	2MG	A	2445	25	19,26,27	1.06	2 (10%)	20,38,41	2.23	6 (30%)
25	H2U	A	2449	25	17,21,22	1.44	4 (23%)	21,30,33	2.18	3 (14%)
25	PSU	A	2457	25	16,21,22	2.12	4 (25%)	20,30,33	3.30	7 (35%)
25	OMC	A	2498	25	15,22,23	1.13	3 (20%)	19,31,34	0.84	0
25	2MA	A	2503	25	18,25,26	1.48	3 (16%)	17,37,40	2.23	2 (11%)
25	PSU	A	2504	25	16,21,22	1.71	5 (31%)	20,30,33	3.47	6 (30%)
25	OMU	A	2552	25	14,22,23	0.91	2 (14%)	18,31,34	1.94	1 (5%)
25	PSU	A	2580	25	16,21,22	1.73	5 (31%)	20,30,33	3.44	6 (30%)
25	PSU	A	2604	25	16,21,22	1.59	3 (18%)	20,30,33	3.87	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	PSU	A	2605	25	16,21,22	1.45	4 (25%)	20,30,33	3.16	5 (25%)
25	1MG	A	745	25	18,26,27	1.53	2 (11%)	18,39,42	1.75	3 (16%)
25	PSU	A	746	25	16,21,22	1.77	5 (31%)	20,30,33	3.55	6 (30%)
25	5MU	A	747	25	14,22,23	0.93	2 (14%)	16,32,35	2.35	3 (18%)
25	PSU	A	955	25	16,21,22	1.62	5 (31%)	20,30,33	3.47	6 (30%)
1	2MG	a	1207	1	19,26,27	1.24	3 (15%)	20,38,41	2.20	8 (40%)
1	4OC	a	1402	1	16,23,24	0.99	2 (12%)	19,32,35	1.27	1 (5%)
1	5MC	a	1407	1	15,22,23	1.28	1 (6%)	17,32,35	1.11	1 (5%)
1	UR3	a	1498	1	14,22,23	1.06	1 (7%)	16,32,35	0.96	1 (6%)
1	2MG	a	1516	1	19,26,27	1.19	2 (10%)	20,38,41	2.32	6 (30%)
1	MA6	a	1518	1	16,26,27	1.08	1 (6%)	18,38,41	2.48	7 (38%)
1	MA6	a	1519	1	16,26,27	0.87	1 (6%)	18,38,41	2.56	7 (38%)
1	PSU	a	516	1	16,21,22	1.49	3 (18%)	20,30,33	3.57	6 (30%)
1	G7M	a	527	1	19,26,27	1.22	2 (10%)	19,39,42	2.61	8 (42%)
1	2MG	a	966	1	19,26,27	1.21	2 (10%)	20,38,41	2.42	8 (40%)
1	5MC	a	967	1	15,22,23	1.40	2 (13%)	17,32,35	1.14	2 (11%)
22	H2U	v	20	22	17,21,22	1.07	2 (11%)	21,30,33	1.76	3 (14%)
22	5MU	v	54	22	14,22,23	0.73	1 (7%)	16,32,35	2.50	2 (12%)
22	PSU	v	55	22	16,21,22	1.32	2 (12%)	20,30,33	3.49	8 (40%)
22	4SU	v	8	22	14,21,22	1.42	1 (7%)	15,30,33	1.30	2 (13%)
24	H2U	y	19	24	17,21,22	1.11	2 (11%)	21,30,33	1.24	3 (14%)
24	6IA	y	37	24	21,29,30	1.06	2 (9%)	21,41,44	2.28	4 (19%)
24	5MU	y	54	24	14,22,23	0.73	0	16,32,35	2.55	2 (12%)
24	PSU	y	55	24	16,21,22	1.61	3 (18%)	20,30,33	3.65	7 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	6MZ	A	1618	25	-	0/5/27/28	0/3/3/3
25	2MG	A	1835	25	-	0/5/27/28	0/3/3/3
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	3TD	A	1915	25	-	0/7/25/26	0/2/2/2
25	PSU	A	1917	25	-	0/7/25/26	0/2/2/2
25	5MU	A	1939	25	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	5MC	A	1962	25	-	0/3/25/26	0/2/2/2
25	6MZ	A	2030	25	-	0/5/27/28	0/3/3/3
25	G7M	A	2069	25	2/2/5/5	0/3/25/26	0/3/3/3
25	OMG	A	2251	25,22	-	0/5/27/28	0/3/3/3
25	2MG	A	2445	25	-	0/5/27/28	0/3/3/3
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
25	OMC	A	2498	25	-	0/5/27/28	0/2/2/2
25	2MA	A	2503	25	-	0/3/25/26	0/3/3/3
25	PSU	A	2504	25	-	0/7/25/26	0/2/2/2
25	OMU	A	2552	25	-	0/5/27/28	0/2/2/2
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
25	1MG	A	745	25	-	0/3/25/26	0/3/3/3
25	PSU	A	746	25	-	0/7/25/26	0/2/2/2
25	5MU	A	747	25	-	0/3/25/26	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	a	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	a	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	a	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	0/3/25/26	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
1	5MC	a	967	1	-	0/3/25/26	0/2/2/2
22	H2U	v	20	22	-	0/7/38/39	0/2/2/2
22	5MU	v	54	22	-	0/3/25/26	0/2/2/2
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2
22	4SU	v	8	22	-	0/3/25/26	0/2/2/2
24	H2U	y	19	24	-	0/7/38/39	0/2/2/2
24	6IA	y	37	24	-	0/9/31/32	0/3/3/3
24	5MU	y	54	24	-	0/3/25/26	0/2/2/2
24	PSU	y	55	24	-	0/7/25/26	0/2/2/2

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2457	PSU	C5-C1'	-6.71	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	746	PSU	C5-C1'	-5.23	1.47	1.52
25	A	2504	PSU	C5-C1'	-5.16	1.47	1.52
24	y	55	PSU	C5-C1'	-4.93	1.48	1.52
25	A	2604	PSU	C5-C1'	-4.62	1.48	1.52
25	A	2580	PSU	C5-C1'	-4.60	1.48	1.52
25	A	1911	PSU	C5-C1'	-4.49	1.48	1.52
22	v	8	4SU	C4-S4	-4.28	1.59	1.67
25	A	1917	PSU	C5-C1'	-4.23	1.48	1.52
1	a	516	PSU	C5-C1'	-4.09	1.48	1.52
25	A	955	PSU	C5-C1'	-3.70	1.49	1.52
25	A	2605	PSU	C5-C1'	-3.64	1.49	1.52
25	A	2449	H2U	C4-N3	-3.31	1.32	1.37
22	v	55	PSU	C5-C1'	-3.18	1.49	1.52
1	a	1498	UR3	O5'-C5'	-3.05	1.40	1.44
25	A	1915	3TD	O4-C4	-3.05	1.16	1.24
25	A	1939	5MU	C2-N3	-2.90	1.32	1.38
25	A	2449	H2U	C2-N3	-2.89	1.32	1.38
25	A	2457	PSU	C2-N3	-2.85	1.32	1.38
25	A	2069	G7M	O5'-C5'	-2.78	1.40	1.44
24	y	19	H2U	C4-N3	-2.71	1.33	1.37
25	A	955	PSU	C2-N1	-2.66	1.32	1.38
22	v	55	PSU	C2-N3	-2.66	1.32	1.38
25	A	2069	G7M	O2'-C2'	-2.65	1.36	1.43
25	A	2580	PSU	O4'-C1'	-2.61	1.40	1.44
22	v	20	H2U	C2-N3	-2.59	1.33	1.38
25	A	2580	PSU	C2-N1	-2.58	1.33	1.38
25	A	955	PSU	C2-N3	-2.57	1.33	1.38
24	y	19	H2U	C2-N3	-2.56	1.33	1.38
25	A	2605	PSU	C2-N3	-2.55	1.33	1.38
1	a	527	G7M	O2'-C2'	-2.47	1.37	1.43
1	a	1402	4OC	O5'-C5'	-2.46	1.41	1.44
25	A	746	PSU	O4'-C1'	-2.45	1.40	1.44
25	A	2449	H2U	C2-N1	-2.45	1.32	1.35
25	A	2604	PSU	C2-N3	-2.39	1.33	1.38
25	A	2580	PSU	C2-N3	-2.39	1.33	1.38
25	A	2504	PSU	C2-N3	-2.38	1.33	1.38
25	A	747	5MU	C2-N3	-2.38	1.33	1.38
25	A	1917	PSU	C2-N1	-2.37	1.33	1.38
1	a	967	5MC	O5'-C5'	-2.36	1.41	1.44
25	A	1917	PSU	O4'-C1'	-2.34	1.40	1.44
1	a	1207	2MG	O5'-C5'	-2.33	1.41	1.44
25	A	2457	PSU	O4'-C1'	-2.32	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2580	PSU	O5'-C5'	-2.32	1.41	1.44
25	A	2457	PSU	C2-N1	-2.32	1.33	1.38
25	A	2605	PSU	O4'-C1'	-2.29	1.41	1.44
1	a	516	PSU	C2-N3	-2.29	1.33	1.38
25	A	1911	PSU	O4'-C1'	-2.28	1.41	1.44
25	A	2604	PSU	C2-N1	-2.24	1.33	1.38
25	A	1917	PSU	C2-N3	-2.24	1.33	1.38
25	A	2449	H2U	C6-N1	-2.24	1.44	1.47
25	A	2498	OMC	O5'-C5'	-2.23	1.41	1.44
25	A	746	PSU	O5'-C5'	-2.23	1.41	1.44
25	A	747	5MU	O5'-C5'	-2.22	1.41	1.44
25	A	955	PSU	O4'-C1'	-2.21	1.41	1.44
25	A	1911	PSU	C2-N3	-2.21	1.33	1.38
25	A	746	PSU	C2-N1	-2.21	1.33	1.38
25	A	1911	PSU	C2-N1	-2.21	1.33	1.38
25	A	2030	6MZ	O5'-C5'	-2.18	1.41	1.44
22	v	20	H2U	C4-N3	-2.17	1.34	1.37
24	y	55	PSU	C2-N3	-2.16	1.33	1.38
25	A	2605	PSU	C2-N1	-2.15	1.33	1.38
25	A	2498	OMC	C2-N3	-2.15	1.33	1.38
1	a	516	PSU	C2-N1	-2.14	1.33	1.38
25	A	2498	OMC	C6-N1	-2.11	1.32	1.35
22	v	54	5MU	C2-N3	-2.10	1.34	1.38
25	A	2552	OMU	C2-N3	-2.10	1.34	1.38
24	y	37	6IA	C2'-C1'	-2.10	1.50	1.53
24	y	55	PSU	O4'-C1'	-2.09	1.41	1.44
25	A	955	PSU	O5'-C5'	-2.07	1.41	1.44
25	A	2504	PSU	O4'-C1'	-2.06	1.41	1.44
1	a	1402	4OC	C2-N3	-2.05	1.34	1.38
25	A	2504	PSU	C2-N1	-2.05	1.34	1.38
25	A	2504	PSU	O5'-C5'	-2.05	1.41	1.44
25	A	2552	OMU	O5'-C5'	-2.04	1.41	1.44
25	A	746	PSU	C2-N3	-2.01	1.34	1.38
25	A	1835	2MG	C5-C4	2.31	1.45	1.40
25	A	2445	2MG	C5-C4	2.40	1.45	1.40
1	a	1519	MA6	C5-C4	2.47	1.46	1.40
25	A	2251	OMG	C5-C4	2.48	1.46	1.40
1	a	966	2MG	C5-C4	2.59	1.46	1.40
25	A	2503	2MA	C5-C4	2.66	1.46	1.40
1	a	1516	2MG	C5-C4	2.72	1.46	1.40
25	A	1835	2MG	C6-C5	2.73	1.46	1.41
24	y	37	6IA	C5-C4	2.81	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1518	MA6	C5-C4	2.90	1.47	1.40
1	a	1207	2MG	C5-C4	2.99	1.47	1.40
25	A	2069	G7M	C6-C5	3.09	1.47	1.41
25	A	2445	2MG	C6-C5	3.21	1.47	1.41
25	A	2251	OMG	C6-C5	3.24	1.47	1.41
25	A	2503	2MA	C6-N6	3.32	1.35	1.27
1	a	1207	2MG	C6-C5	3.35	1.47	1.41
1	a	966	2MG	C6-C5	3.41	1.47	1.41
1	a	527	G7M	C6-C5	3.52	1.48	1.41
25	A	2030	6MZ	C5-C4	3.57	1.48	1.40
25	A	1618	6MZ	C5-C4	3.63	1.48	1.40
25	A	745	1MG	C5-C4	3.65	1.48	1.40
1	a	1516	2MG	C6-C5	3.66	1.48	1.41
25	A	1962	5MC	C5-C4	3.89	1.47	1.41
1	a	1407	5MC	C5-C4	3.93	1.47	1.41
25	A	2503	2MA	C6-C5	3.94	1.47	1.41
25	A	745	1MG	C6-C5	4.37	1.49	1.41
1	a	967	5MC	C5-C4	4.42	1.47	1.41
25	A	1915	3TD	C4-N3	4.74	1.45	1.38
25	A	1915	3TD	C6-N1	5.03	1.45	1.34
25	A	1915	3TD	C2-N1	5.18	1.48	1.38
25	A	1915	3TD	C6-C5	7.20	1.48	1.38

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	955	PSU	N1-C2-N3	-10.07	121.16	128.40
25	A	2604	PSU	N1-C2-N3	-9.59	121.50	128.40
25	A	746	PSU	N1-C2-N3	-9.39	121.64	128.40
1	a	516	PSU	N1-C2-N3	-9.36	121.67	128.40
25	A	2605	PSU	N1-C2-N3	-9.31	121.70	128.40
22	v	55	PSU	N1-C2-N3	-9.29	121.72	128.40
25	A	2604	PSU	C5-C4-N3	-9.12	117.95	125.43
25	A	2580	PSU	N1-C2-N3	-9.09	121.86	128.40
25	A	1911	PSU	N1-C2-N3	-9.09	121.86	128.40
24	y	55	PSU	N1-C2-N3	-8.97	121.95	128.40
24	y	55	PSU	C5-C4-N3	-8.83	118.19	125.43
1	a	516	PSU	C5-C4-N3	-8.81	118.20	125.43
25	A	1917	PSU	N1-C2-N3	-8.78	122.09	128.40
25	A	2457	PSU	C5-C4-N3	-8.55	118.41	125.43
25	A	2504	PSU	C5-C4-N3	-8.53	118.43	125.43
25	A	2580	PSU	C5-C4-N3	-8.39	118.54	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2504	PSU	N1-C2-N3	-8.36	122.38	128.40
25	A	746	PSU	C5-C4-N3	-8.23	118.68	125.43
25	A	1911	PSU	C5-C4-N3	-8.02	118.85	125.43
25	A	1917	PSU	C5-C4-N3	-7.98	118.88	125.43
25	A	2449	H2U	C5-C6-N1	-7.58	102.83	110.70
25	A	955	PSU	C5-C4-N3	-7.44	119.33	125.43
22	v	55	PSU	C5-C4-N3	-7.37	119.39	125.43
25	A	2030	6MZ	C9-N6-C6	-7.29	116.61	122.85
25	A	1618	6MZ	N3-C2-N1	-6.63	123.08	128.86
25	A	2457	PSU	N1-C2-N3	-6.51	123.72	128.40
24	y	54	5MU	C5-C4-N3	-6.49	118.08	125.24
1	a	1519	MA6	N3-C2-N1	-6.42	123.27	128.86
22	v	54	5MU	C5-C4-N3	-6.28	118.32	125.24
1	a	1518	MA6	N3-C2-N1	-6.19	123.47	128.86
25	A	2605	PSU	C5-C4-N3	-6.04	120.47	125.43
22	v	20	H2U	C5-C6-N1	-5.97	104.50	110.70
25	A	747	5MU	C5-C4-N3	-5.69	118.97	125.24
24	y	37	6IA	N3-C2-N1	-5.64	123.95	128.86
25	A	2030	6MZ	N3-C2-N1	-5.64	123.95	128.86
25	A	2069	G7M	C5-C6-N1	-5.37	115.84	123.48
25	A	2457	PSU	C5-C1'-C2'	-5.36	106.30	115.55
25	A	2604	PSU	C5-C1'-C2'	-5.36	106.30	115.55
25	A	1915	3TD	C5-C1'-C2'	-5.35	106.32	115.55
1	a	527	G7M	C5-C6-N1	-4.68	116.81	123.48
25	A	2457	PSU	C5-C6-N1	-4.66	118.35	124.39
25	A	1939	5MU	C5-C4-N3	-4.56	120.22	125.24
25	A	2449	H2U	C4-N3-C2	-4.55	121.92	125.81
25	A	1835	2MG	C6-C5-C4	-4.45	116.42	120.84
1	a	1402	4OC	CM4-N4-C4	-4.34	119.19	122.94
24	y	55	PSU	C5-C1'-C2'	-4.34	108.07	115.55
25	A	2504	PSU	C5-C1'-C2'	-4.33	108.08	115.55
25	A	1618	6MZ	C9-N6-C6	-4.31	119.17	122.85
25	A	746	PSU	C5-C6-N1	-4.26	118.87	124.39
24	y	55	PSU	C5-C6-N1	-4.23	118.90	124.39
25	A	2504	PSU	C5-C6-N1	-4.12	119.04	124.39
25	A	2030	6MZ	C4-C5-N7	-4.12	105.43	109.41
25	A	1939	5MU	C5-C6-N1	-4.07	117.75	122.15
1	a	966	2MG	C6-C5-C4	-4.02	116.84	120.84
25	A	2251	OMG	C5-C6-N1	-4.00	117.79	123.48
1	a	1518	MA6	C10-N6-C6	-3.93	107.61	119.51
25	A	2605	PSU	C5-C6-N1	-3.85	119.39	124.39
25	A	746	PSU	C5-C1'-C2'	-3.85	108.91	115.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1519	MA6	C4-C5-N7	-3.83	105.71	109.41
1	a	1516	2MG	C6-C5-C4	-3.81	117.05	120.84
25	A	1911	PSU	C5-C6-N1	-3.78	119.49	124.39
25	A	2445	2MG	CM2-N2-C2	-3.75	119.06	123.63
1	a	1207	2MG	C5-C6-N1	-3.73	118.17	123.48
1	a	1516	2MG	C5-C6-N1	-3.70	118.22	123.48
1	a	1516	2MG	C4-C5-N7	-3.63	105.90	109.41
22	v	55	PSU	C5-C6-N1	-3.62	119.70	124.39
22	v	20	H2U	C4-N3-C2	-3.60	122.73	125.81
25	A	2445	2MG	C5-C6-N1	-3.58	118.38	123.48
25	A	1917	PSU	C5-C6-N1	-3.54	119.79	124.39
1	a	1518	MA6	C10-N6-C9	-3.49	104.74	116.03
1	a	1207	2MG	C6-C5-C4	-3.46	117.41	120.84
25	A	2445	2MG	C6-C5-C4	-3.43	117.43	120.84
25	A	745	1MG	C4-C5-N7	-3.42	106.10	109.41
1	a	1516	2MG	CM2-N2-C2	-3.41	119.48	123.63
1	a	516	PSU	C5-C6-N1	-3.39	120.00	124.39
25	A	2580	PSU	C5-C6-N1	-3.32	120.08	124.39
25	A	1618	6MZ	C4-C5-N7	-3.28	106.24	109.41
1	a	966	2MG	C5-C6-N1	-3.28	118.82	123.48
25	A	2604	PSU	C5-C6-N1	-3.24	120.19	124.39
25	A	1915	3TD	C5-C6-N1	-3.21	120.23	124.39
25	A	2251	OMG	C6-C5-C4	-3.21	117.65	120.84
25	A	2251	OMG	C4-C5-N7	-3.19	106.33	109.41
1	a	1518	MA6	C4-C5-N7	-3.12	106.39	109.41
1	a	966	2MG	N3-C2-N1	-3.06	121.61	126.23
25	A	1962	5MC	CM5-C5-C4	-3.05	118.52	121.65
24	y	37	6IA	C12-N6-C6	-3.00	119.39	123.26
25	A	1835	2MG	CM2-N2-C2	-2.97	120.02	123.63
1	a	1519	MA6	C10-N6-C9	-2.96	106.43	116.03
25	A	745	1MG	C6-C5-C4	-2.88	117.93	119.92
24	y	37	6IA	C4-C5-N7	-2.88	106.63	109.41
25	A	955	PSU	C5-C6-N1	-2.87	120.67	124.39
24	y	19	H2U	C4-N3-C2	-2.83	123.38	125.81
25	A	2251	OMG	N3-C2-N1	-2.83	123.32	127.46
25	A	2503	2MA	C4-C5-N7	-2.83	106.68	109.41
1	a	527	G7M	N3-C2-N1	-2.82	123.35	127.46
25	A	1835	2MG	C5-C6-N1	-2.79	119.51	123.48
22	v	8	4SU	C5-C4-N3	-2.77	120.23	123.73
1	a	1519	MA6	C9-N6-C6	-2.77	111.13	119.51
1	a	1207	2MG	CM2-N2-C2	-2.65	120.41	123.63
1	a	967	5MC	C5-C6-N1	-2.61	119.33	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2445	2MG	C4-C5-N7	-2.53	106.96	109.41
25	A	1835	2MG	N3-C2-N1	-2.49	122.46	126.23
25	A	2069	G7M	N3-C2-N1	-2.47	123.85	127.46
1	a	527	G7M	C4'-O4'-C1'	-2.46	107.16	109.77
22	v	55	PSU	C5-C1'-C2'	-2.39	111.43	115.55
25	A	1962	5MC	C5-C6-N1	-2.36	119.59	122.15
1	a	1519	MA6	C10-N6-C6	-2.35	112.39	119.51
1	a	1518	MA6	C9-N6-C6	-2.33	112.46	119.51
25	A	955	PSU	O2'-C2'-C1'	-2.30	107.00	112.21
24	y	19	H2U	C5-C6-N1	-2.29	108.33	110.70
1	a	966	2MG	C4-C5-N7	-2.19	107.29	109.41
1	a	1207	2MG	C4-C5-N7	-2.14	107.34	109.41
1	a	1207	2MG	N3-C2-N1	-2.09	123.07	126.23
25	A	2449	H2U	O2-C2-N1	-2.06	120.54	123.12
25	A	747	5MU	C5-C6-N1	-2.03	119.95	122.15
25	A	1911	PSU	O2'-C2'-C1'	-2.03	107.62	112.21
1	a	966	2MG	N2-C2-N1	2.01	118.90	116.95
25	A	2580	PSU	O4'-C1'-C2'	2.02	107.69	104.45
25	A	2457	PSU	O4'-C1'-C2'	2.02	107.70	104.45
24	y	55	PSU	O4'-C1'-C2'	2.03	107.71	104.45
25	A	1915	3TD	O4'-C1'-C2'	2.03	107.72	104.45
25	A	1917	PSU	O4'-C1'-C2'	2.08	107.78	104.45
25	A	2069	G7M	C1'-N9-C4	2.11	130.28	126.64
22	v	55	PSU	O4'-C1'-C2'	2.22	108.01	104.45
1	a	516	PSU	O4'-C1'-C2'	2.22	108.01	104.45
1	a	1518	MA6	N1-C6-N6	2.25	119.38	117.00
1	a	967	5MC	N4-C4-N3	2.36	120.48	117.00
1	a	1498	UR3	C3U-N3-C4	2.51	121.48	118.15
22	v	20	H2U	C5-C4-N3	2.55	119.26	116.72
1	a	966	2MG	N2-C2-N3	2.59	119.47	116.95
1	a	527	G7M	C1'-N9-C4	2.61	131.14	126.64
24	y	19	H2U	N3-C2-N1	2.63	119.35	116.73
25	A	1915	3TD	C6-N1-C2	2.68	119.65	115.36
25	A	2069	G7M	O3'-C3'-C2'	2.68	120.41	111.83
25	A	1835	2MG	N2-C2-N3	2.76	119.64	116.95
1	a	1407	5MC	N4-C4-N3	2.78	121.11	117.00
1	a	1207	2MG	N2-C2-N3	2.86	119.73	116.95
25	A	1962	5MC	N4-C4-N3	3.10	121.58	117.00
1	a	527	G7M	O3'-C3'-C2'	3.29	122.36	111.83
22	v	55	PSU	O4'-C1'-C5	3.32	115.07	109.93
25	A	2069	G7M	O3'-C3'-C4'	3.43	121.11	111.09
1	a	527	G7M	O3'-C3'-C4'	3.50	121.30	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	8	4SU	C2-N3-C4	3.51	120.29	115.11
25	A	1915	3TD	O4'-C1'-C5	3.54	115.41	109.93
25	A	2445	2MG	C6-N1-C2	3.62	121.66	115.18
25	A	1835	2MG	C6-N1-C2	3.66	121.73	115.18
25	A	2457	PSU	C6-N1-C2	3.69	121.27	115.36
1	a	1516	2MG	C6-N1-C2	3.71	121.83	115.18
25	A	1917	PSU	C6-N1-C2	3.93	121.65	115.36
1	a	1207	2MG	C6-N1-C2	3.93	122.22	115.18
25	A	2580	PSU	C6-N1-C2	3.95	121.68	115.36
1	a	966	2MG	C6-N1-C2	3.96	122.26	115.18
1	a	516	PSU	C6-N1-C2	3.97	121.72	115.36
1	a	1519	MA6	N1-C6-N6	4.02	121.27	117.00
24	y	55	PSU	C6-N1-C2	4.03	121.82	115.36
25	A	2604	PSU	C6-N1-C2	4.04	121.83	115.36
25	A	955	PSU	C6-N1-C2	4.11	121.94	115.36
25	A	2069	G7M	C2-N3-C4	4.12	119.97	115.16
25	A	2504	PSU	C6-N1-C2	4.16	122.03	115.36
25	A	2251	OMG	C6-N1-C2	4.20	122.11	116.06
25	A	1911	PSU	C6-N1-C2	4.21	122.09	115.36
22	v	55	PSU	C6-N1-C2	4.22	122.11	115.36
1	a	1519	MA6	C2-N1-C6	4.24	122.24	111.82
1	a	527	G7M	C6-N1-C2	4.27	122.21	116.06
1	a	1518	MA6	C2-N1-C6	4.30	122.38	111.82
25	A	746	PSU	C6-N1-C2	4.34	122.31	115.36
25	A	2605	PSU	C6-N1-C2	4.46	122.50	115.36
25	A	1939	5MU	C4-N3-C2	4.60	119.19	115.16
25	A	2251	OMG	C2-N3-C4	4.75	120.70	115.16
25	A	2069	G7M	C6-N1-C2	4.78	122.93	116.06
1	a	1207	2MG	C2-N3-C4	5.09	120.92	115.11
25	A	745	1MG	C2-N3-C4	5.12	121.13	115.16
25	A	2457	PSU	C4-N3-C2	5.19	119.70	115.16
1	a	527	G7M	C2-N3-C4	5.27	121.32	115.16
25	A	2605	PSU	C4-N3-C2	5.31	119.81	115.16
1	a	1516	2MG	C2-N3-C4	5.39	121.26	115.11
25	A	2445	2MG	C2-N3-C4	5.43	121.31	115.11
25	A	1835	2MG	C2-N3-C4	5.63	121.53	115.11
25	A	2504	PSU	C4-N3-C2	5.97	120.38	115.16
25	A	1917	PSU	C4-N3-C2	6.05	120.45	115.16
25	A	746	PSU	C4-N3-C2	6.13	120.52	115.16
25	A	1911	PSU	C4-N3-C2	6.14	120.53	115.16
22	v	55	PSU	C4-N3-C2	6.54	120.88	115.16
24	y	55	PSU	C4-N3-C2	6.55	120.88	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	966	2MG	C2-N3-C4	6.63	122.67	115.11
25	A	2580	PSU	C4-N3-C2	6.71	121.03	115.16
25	A	955	PSU	C4-N3-C2	6.80	121.10	115.16
25	A	747	5MU	C4-N3-C2	6.91	121.20	115.16
1	a	516	PSU	C4-N3-C2	7.10	121.37	115.16
22	v	54	5MU	C4-N3-C2	7.18	121.44	115.16
24	y	54	5MU	C4-N3-C2	7.27	121.52	115.16
24	y	37	6IA	C2-N1-C6	7.40	121.35	116.53
25	A	2604	PSU	C4-N3-C2	7.53	121.74	115.16
25	A	2552	OMU	C4-N3-C2	7.68	120.72	114.13
25	A	2030	6MZ	C2-N1-C6	8.09	121.80	116.53
25	A	2503	2MA	C2-N3-C4	8.11	122.42	115.41
25	A	1618	6MZ	C2-N1-C6	8.34	121.97	116.53

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4'
1	a	527	G7M	C3'
25	A	2069	G7M	C4'
25	A	2069	G7M	C3'

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1915	3TD	1	0
25	A	2030	6MZ	1	0
25	A	2251	OMG	1	0
25	A	2445	2MG	1	0
25	A	745	1MG	1	0
25	A	747	5MU	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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
24	y	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	y	5(A):A	O3'	6:U	P	3.00
1	y	47(Q):G	O3'	48:G	P	3.00
1	y	67(A):U	O3'	68:C	P	3.00
1	y	5:G	O3'	5(A):A	P	2.99
1	y	67:A	O3'	67(A):U	P	2.99
1	y	47:G	O3'	47(A):G	P	2.97