



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 07:09 AM BST

PDB ID : 4U52
Title : Crystal structure of Nagilactone C bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

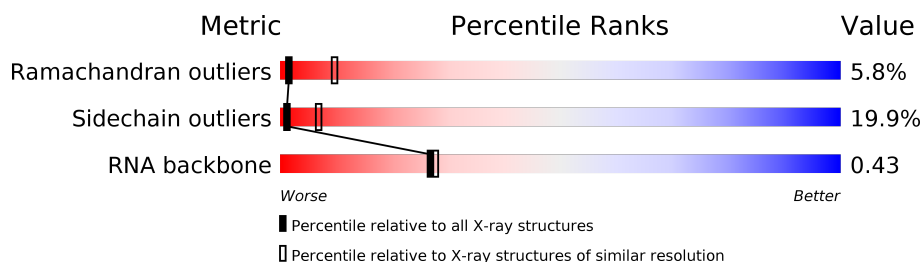
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)















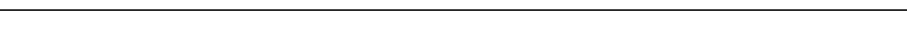




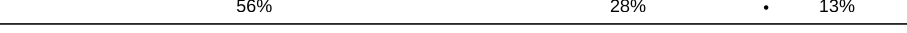





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	59% 32% 6% .
1	6	1800	59% 35% 6%
2	S0	251	61% 20% . 18%
2	s0	251	58% 20% . 18%
3	S1	254	59% 23% . 16%
3	s1	254	65% 18% . 15%
4	S2	253	69% 16% . 14%
4	s2	253	64% 19% . 14%




















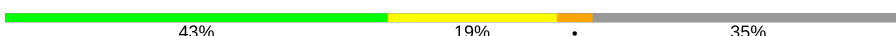





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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	
16	c4	136	
17	C5	141	

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Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	


























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Mol	Chain	Length	Quality of chain
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	















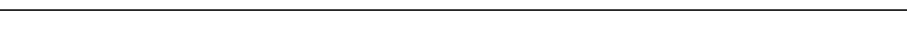




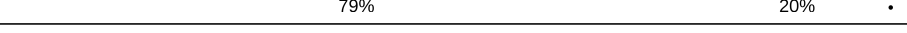





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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	















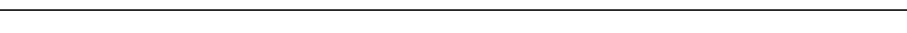




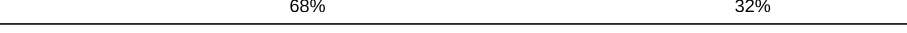





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Mol	Chain	Length	Quality of chain
55	m9	188	 84% 16% .
56	N0	172	 80% 19% .
56	n0	172	 81% 19% .
57	N1	159	 74% 23% .
57	n1	159	 79% 18% .
58	N2	120	 71% 13% 17%
58	n2	120	 71% 11% 18%
59	N3	136	 84% 15% .
59	n3	136	 88% 11% .
60	N4	155	 54% 9% 37%
60	n4	155	 71% 14% . 13%
61	N5	141	 67% 18% . 14%
61	n5	141	 67% 16% . 15%
62	N6	126	 74% 25% .
62	n6	126	 80% 18% .
63	N7	135	 73% 24% .
63	n7	135	 70% 27% .
64	N8	148	 81% 16% .
64	n8	148	 79% 20% .
65	N9	58	 79% 17% .
65	n9	58	 69% 24% 5% .
66	O0	104	 79% 13% . 7%
66	o0	104	 77% 19% .
67	O1	112	 73% 23% . .
67	o1	112	 72% 23% . .

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Mol	Chain	Length	Quality of chain
68	O2	129	 78% 21% .
68	o2	129	 77% 21% ..
69	O3	106	 86% 13% .
69	o3	106	 83% 17%
70	O4	119	 75% 18% . 6%
70	o4	119	 81% 12% . 6%
71	O5	119	 70% 29% .
71	o5	119	 78% 22%
72	O6	99	 72% 26% .
72	o6	99	 73% 27%
73	O7	87	 84% 11% 5%
73	o7	87	 84% 14% .
74	O8	77	 77% 22% .
74	o8	77	 73% 26% .
75	O9	50	 80% 18% .
75	o9	50	 72% 28%
76	Q0	52	 75% 21% .
76	q0	52	 79% 21%
77	Q1	25	 68% 32%
77	q1	25	 60% 32% 8%
78	Q2	105	 78% 17% 5%
78	q2	105	 84% 16%
79	Q3	91	 79% 20% .
79	q3	91	 82% 18%
80	e0	62	 74% 24% .

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Mol	Chain	Length	Quality of chain
81	m2	160	<div><div></div><div>94%6%</div></div>
82	p0	311	<div><div></div><div>38%8%54%</div></div>
83	p1	47	<div><div></div><div>100%</div></div>
84	p2	46	<div><div></div><div>100%</div></div>

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411206 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1750	Total	C	N	O	P	0	0	0
			37283	16668	6591	12274	1750			
1	6	1795	Total	C	N	O	P	0	0	0
			38238	17095	6758	12590	1795			

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S0	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S1	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
5	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
7	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	S6	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	s7	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	s8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			773	500	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745
c0	89	ALA	GLY	conflict	UNP Q08745

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	104	ALA	GLY	conflict	UNP P48589
C2	110	ALA	GLY	conflict	UNP P48589
c2	104	ALA	GLY	conflict	UNP P48589
c2	110	ALA	GLY	conflict	UNP P48589

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	C3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
15	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	C4	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
16	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
17	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C5	137	SER	ARG	conflict	UNP Q01855
c5	137	SER	ARG	conflict	UNP Q01855

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	C8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	C9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
21	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	D0	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
22	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	D1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
23	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	D2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
24	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	D3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
25	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	D4	134	Total	C	N	O	0	0	0
			1073	676	208	189			
26	d4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	D5	70	Total	C	N	O	0	0	0
			563	360	104	99			
27	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	D7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	D8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
30	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
31	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
33	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2441	1544	419	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			
35	sM	104	Total	C	N	O	0	0	0
			680	403	140	137			

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
37	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	l3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	l4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	l6	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	l7	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	l9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	M0	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
47	m0	213	Total	C	N	O	S	0	0	0
			1722	1094	325	297	6			

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	M1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
48	m1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	M3	193	Total	C	N	O	0	0	0
			1543	962	315	266			
49	m3	194	Total	C	N	O	0	0	0
			1548	965	316	267			

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	m5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
52	m6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	M7	183	Total	C	N	O		0	0	0
			1420	882	281	257				
53	m7	155	Total	C	N	O		0	0	0
			1227	764	238	225				

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	M8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
54	m8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O		0	0	0
			1521	935	326	260				
55	m9	188	Total	C	N	O		0	0	0
			1521	935	326	260				

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	N1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
57	n1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O	S	0	0	0
			796	516	131	149				
58	n2	98	Total	C	N	O	S	0	0	0
			778	505	127	146				

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	N3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
59	n3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
60	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	N6	126	Total	C	N	O	0	0	0
			993	625	192	176			
62	n6	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	N7	135	Total	C	N	O	0	0	0
			1092	710	202	180			
63	n7	135	Total	C	N	O	0	0	0
			1092	710	202	180			

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	N8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
64	n8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	N9	58	Total	C	N	O	0	0	0
			462	289	100	73			
65	n9	58	Total	C	N	O	0	0	0
			462	289	100	73			

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
66	o0	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	O1	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
67	o1	109	Total	C	N	O	S	0	0	0
			883	559	167	156	1			

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	O2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	o2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	O3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	o3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	O4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	o4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	110	GLU	-	expression tag	UNP P87262
O4	111	ALA	-	expression tag	UNP P87262
O4	112	ALA	-	expression tag	UNP P87262
O4	113	LYS	-	expression tag	UNP P87262
O4	114	SER	-	expression tag	UNP P87262
O4	115	GLU	-	expression tag	UNP P87262
O4	116	LYS	-	expression tag	UNP P87262
O4	117	LYS	-	expression tag	UNP P87262
O4	118	ALA	-	expression tag	UNP P87262
O4	119	LYS	-	expression tag	UNP P87262
O4	120	LYS	-	expression tag	UNP P87262

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Chain	Residue	Modelled	Actual	Comment	Reference
o4	110	GLU	-	expression tag	UNP P87262
o4	111	ALA	-	expression tag	UNP P87262
o4	112	ALA	-	expression tag	UNP P87262
o4	113	LYS	-	expression tag	UNP P87262
o4	114	SER	-	expression tag	UNP P87262
o4	115	GLU	-	expression tag	UNP P87262
o4	116	LYS	-	expression tag	UNP P87262
o4	117	LYS	-	expression tag	UNP P87262
o4	118	ALA	-	expression tag	UNP P87262
o4	119	LYS	-	expression tag	UNP P87262
o4	120	LYS	-	expression tag	UNP P87262

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	O5	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	o5	119	Total	C	N	O	S	0	0	0
			965	612	185	167	1			

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	o6	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	O7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
73	o7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O	0	0	0
			612	391	115	106			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	o8	77	Total	C	N	O	0	0	0
			608	388	114	106			

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	O9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
75	o9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	Q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
76	q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	Q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
78	q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	Q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
79	q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e0	62	VAL	-	expression tag	UNP P0CX33
e0	63	GLN	-	expression tag	UNP P0CX33

- Molecule 81 is a protein called Unknown Protein m2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
81	m2	150	Total	C	N	O	0	0	0
			750	450	150	150			

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

- Molecule 83 is a protein called Unknown Protein p1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
83	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			

- Molecule 84 is a protein called Unknown Protein p2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
84	p2	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	3	Total	Mg	0	0
			3	3		
85	N9	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	n8	5	Total 5	Mg 5	0	0
85	o1	1	Total 1	Mg 1	0	0
85	N5	1	Total 1	Mg 1	0	0
85	6	150	Total 150	Mg 150	0	0
85	sM	2	Total 2	Mg 2	0	0
85	O4	1	Total 1	Mg 1	0	0
85	m5	4	Total 4	Mg 4	0	0
85	l3	2	Total 2	Mg 2	0	0
85	M1	1	Total 1	Mg 1	0	0
85	n0	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	125	Total 125	Mg 125	0	0
85	O3	1	Total 1	Mg 1	0	0
85	L4	2	Total 2	Mg 2	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	3	Total 3	Mg 3	0	0
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	o4	2	Total 2	Mg 2	0	0
85	M9	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	SM	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	2	Total 2	Mg 2	0	0
85	5	502	Total 502	Mg 502	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	M4	1	Total 1	Mg 1	0	0
85	n9	1	Total 1	Mg 1	0	0
85	1	469	Total 469	Mg 469	0	0
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	3	Total 3	Mg 3	0	0
85	M8	1	Total 1	Mg 1	0	0
85	q3	1	Total 1	Mg 1	0	0
85	o3	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	3	Total 3	Mg 3	0	0
85	4	22	Total 22	Mg 22	0	0
85	n6	1	Total 1	Mg 1	0	0

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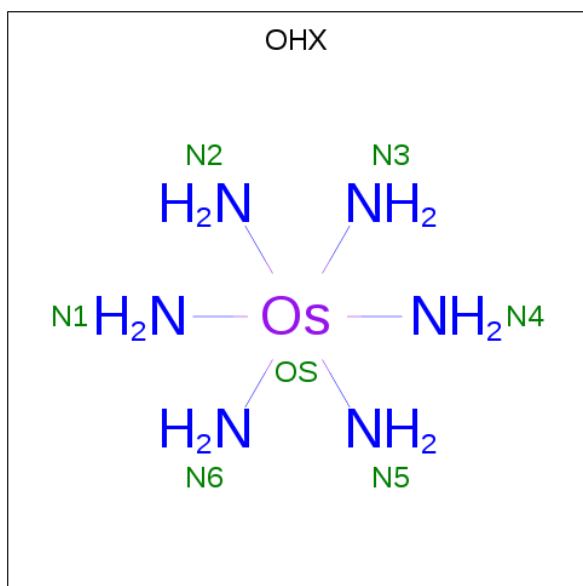
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L2	3	Total 3	Mg 3	0	0
85	m1	2	Total 2	Mg 2	0	0
85	l5	1	Total 1	Mg 1	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	3	Total 3	Mg 3	0	0
85	N8	5	Total 5	Mg 5	0	0
85	s1	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0
85	O1	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	l8	1	Total 1	Mg 1	0	0
85	c7	2	Total 2	Mg 2	0	0
85	7	17	Total 17	Mg 17	0	0
85	n3	1	Total 1	Mg 1	0	0
85	L3	2	Total 2	Mg 2	0	0
85	m6	1	Total 1	Mg 1	0	0
85	N6	1	Total 1	Mg 1	0	0
85	8	15	Total 15	Mg 15	0	0
85	m0	1	Total 1	Mg 1	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	3	14	Total	Mg	0	0
			14	14		

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	C3	1	Total	N	Os	0	0
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86	C5	1	Total	N	Os	0	0
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86	C8	1	Total	N	Os	0	0
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86	D9	1	Total	N	Os	0	0
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86	SR	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	L3	1	Total	N	Os	0	0
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86	L4	1	Total	N	Os	0	0
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86	M0	1	Total	N	Os	0	0
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86	M5	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M8	1	Total	N	Os	0	0
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86	M9	1	Total	N	Os	0	0
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86	N9	1	Total	N	Os	0	0
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86	O2	1	Total	N	Os	0	0
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86	O3	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	O9	1	Total	N	Os	0	0
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86	Q2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	19	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m9	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n6	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q1	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

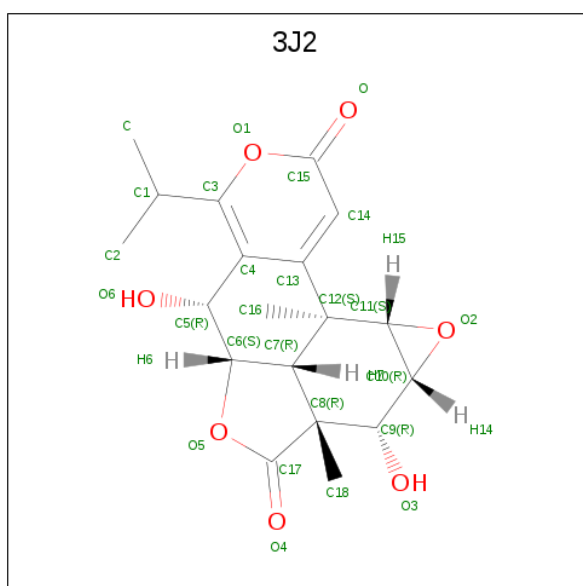
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0	0
			1	1		
87	q3	1	Total	Zn	0	0
			1	1		
87	d9	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	D7	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0	0
			1	1		
87	o7	1	Total	Zn	0	0
			1	1		
87	O7	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		

- Molecule 88 is Nagilactone C (three-letter code: 3J2) (formula: $C_{19}H_{22}O_7$).



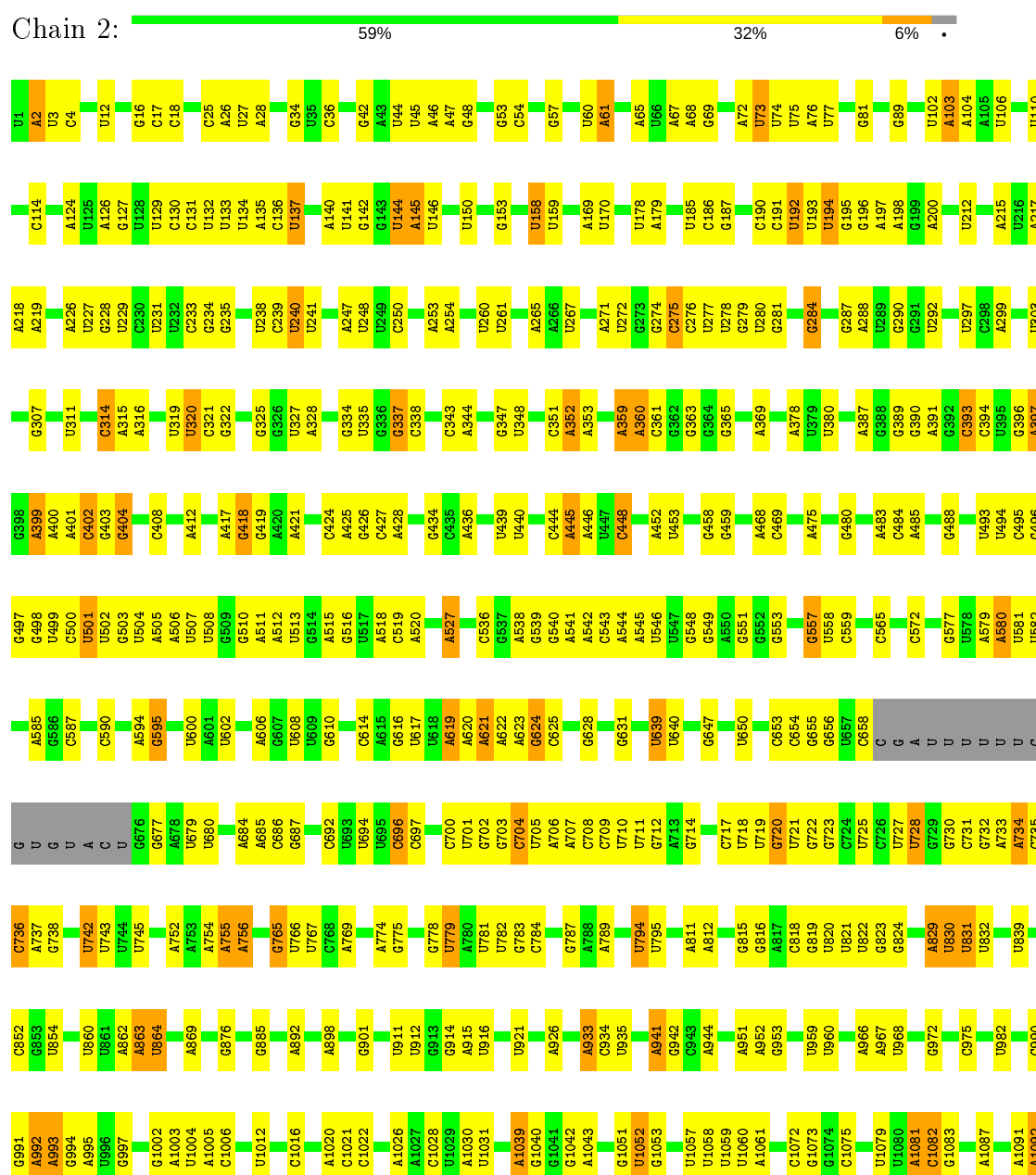
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	C	O	0	0
			26	19	7		
88	5	1	Total	C	O	0	0
			26	19	7		

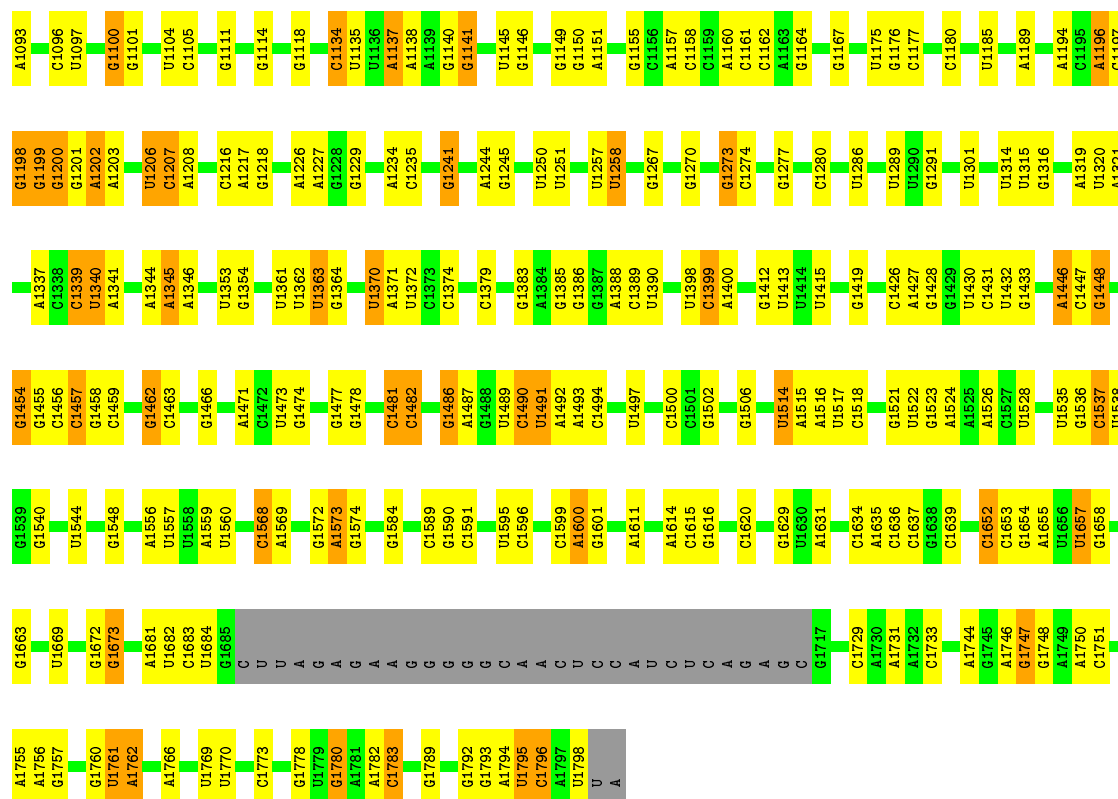
3 Residue-property plots

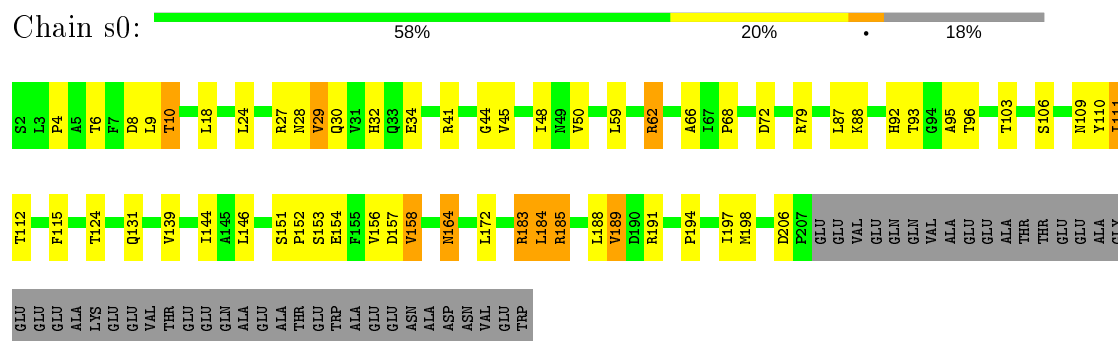
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

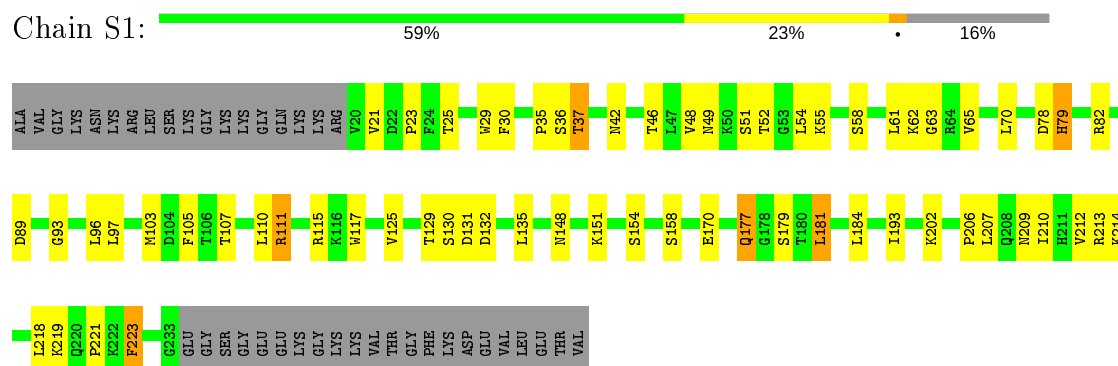
- Molecule 1: 18S ribosomal RNA



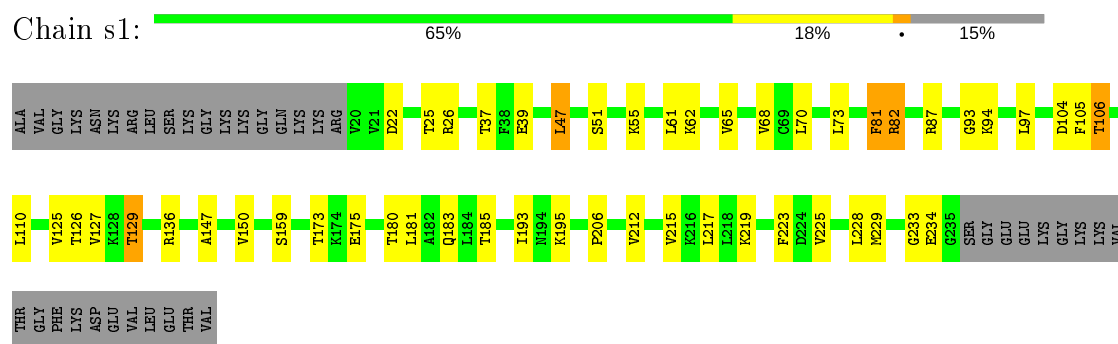




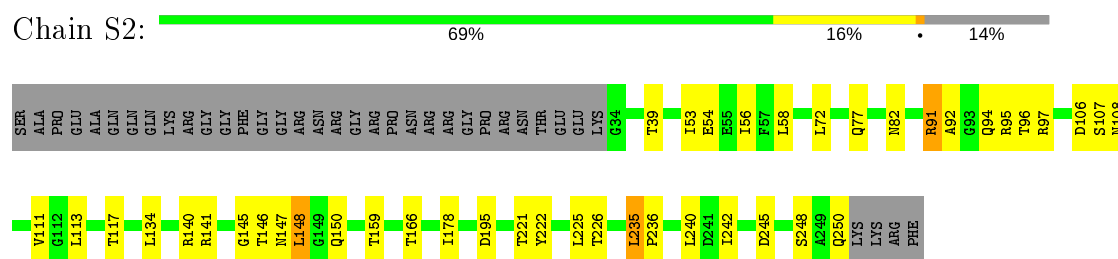
- Molecule 3: 40S ribosomal protein S1-A



- Molecule 3: 40S ribosomal protein S1-A

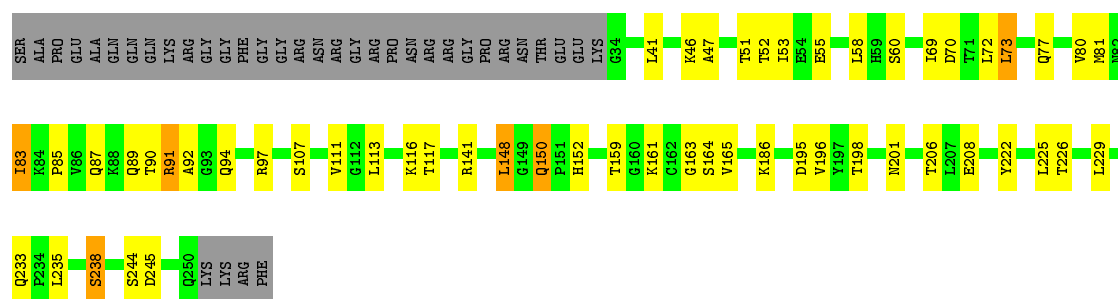


- Molecule 4: 40S ribosomal protein S2



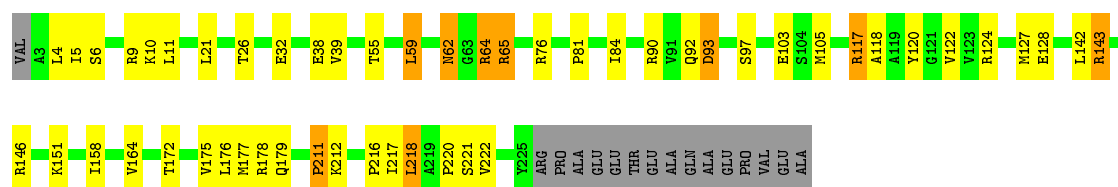
- Molecule 4: 40S ribosomal protein S2





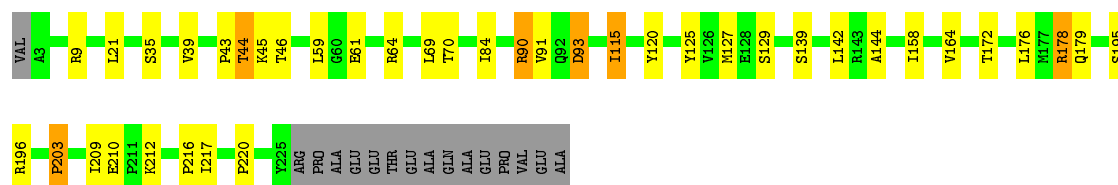
- Molecule 5: 40S ribosomal protein S3

Chain S3: 72% 18% 7%



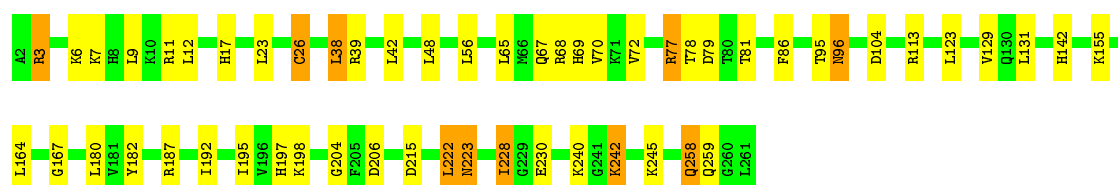
- Molecule 5: 40S ribosomal protein S3

Chain s3: 77% 14% 7%



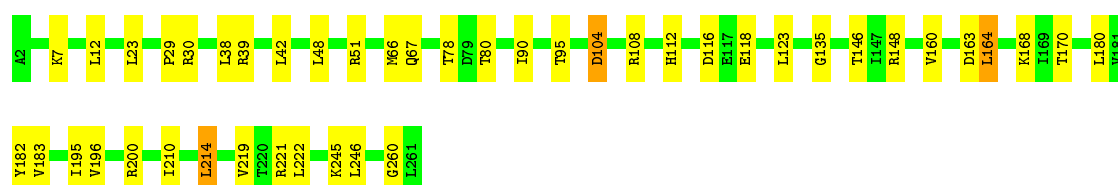
- Molecule 6: 40S ribosomal protein S4-A

Chain S4: 79% 17% 4%



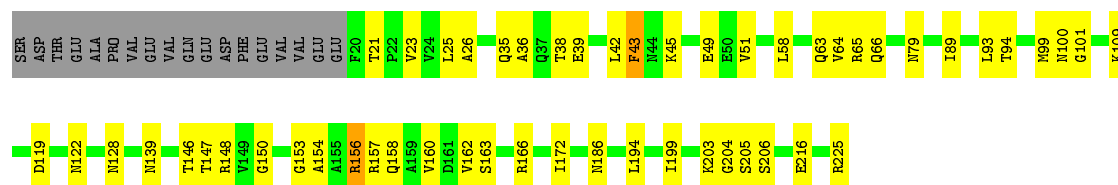
- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 83% 16% 1%



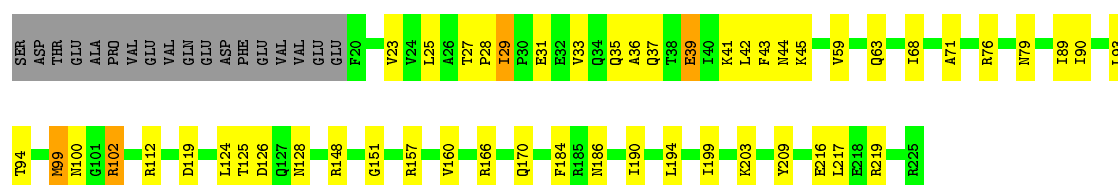
- Molecule 7: 40S ribosomal protein S5

Chain S5: 




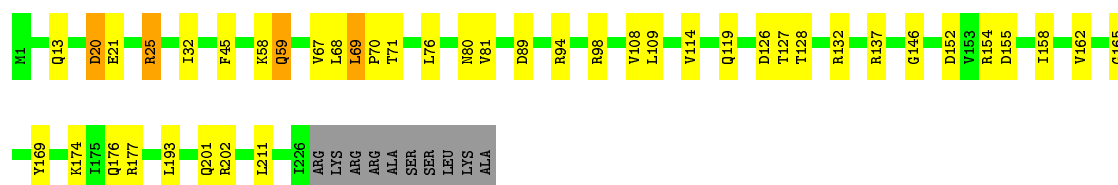
- Molecule 7: 40S ribosomal protein S5

Chain s5: 



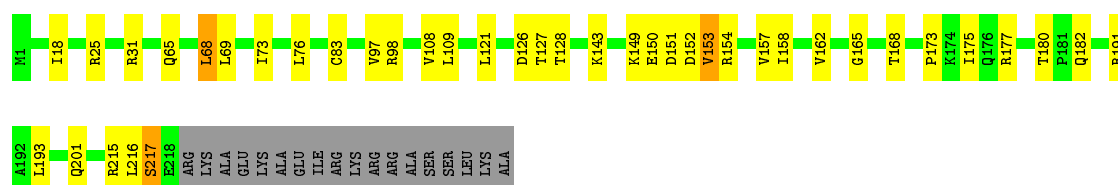
- Molecule 8: 40S ribosomal protein S6-A

Chain S6: 



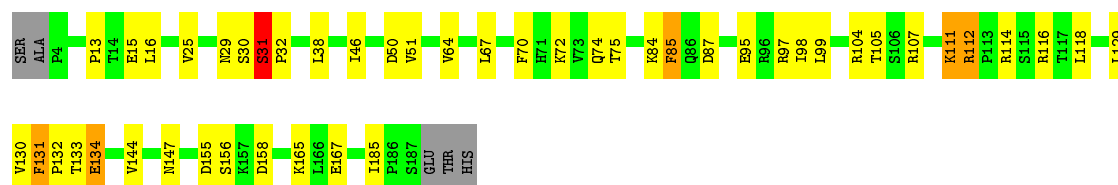
- Molecule 8: 40S ribosomal protein S6-A

Chain s6: 

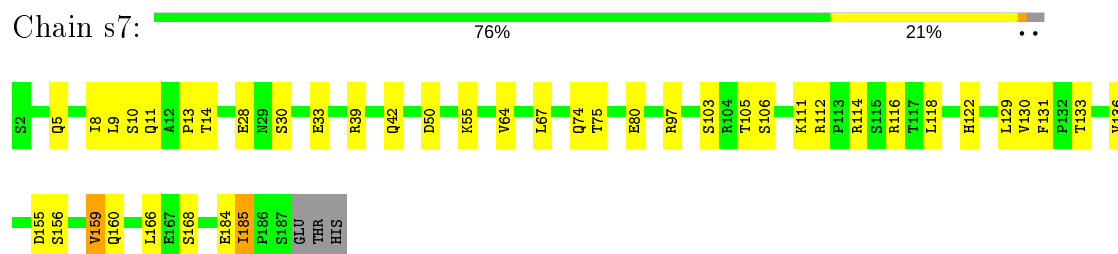


- Molecule 9: 40S ribosomal protein S7-A

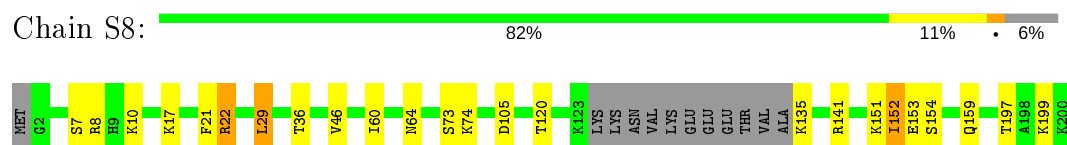
Chain S7: 



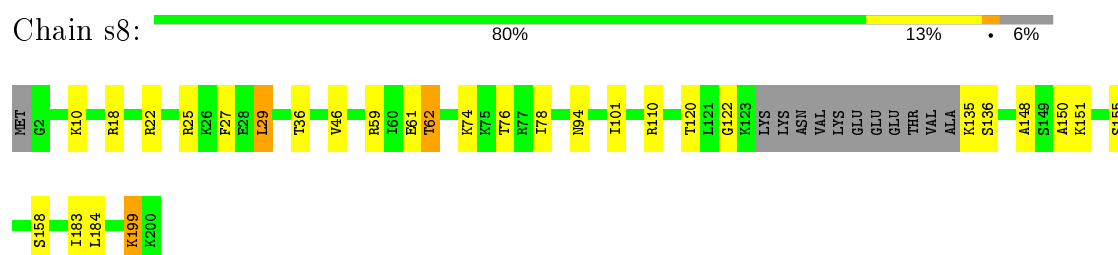
- Molecule 9: 40S ribosomal protein S7-A



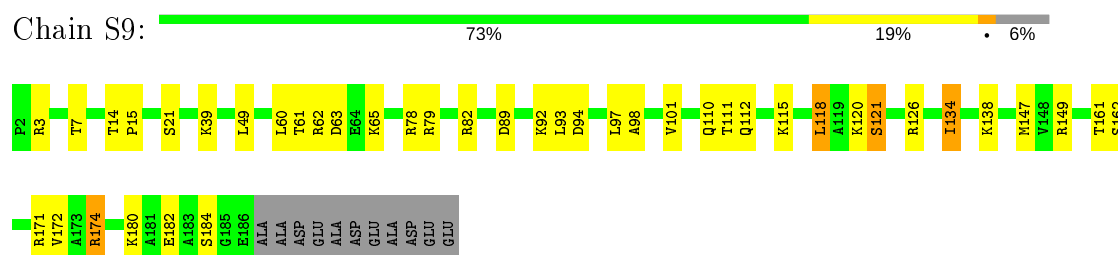
- Molecule 10: 40S ribosomal protein S8-A



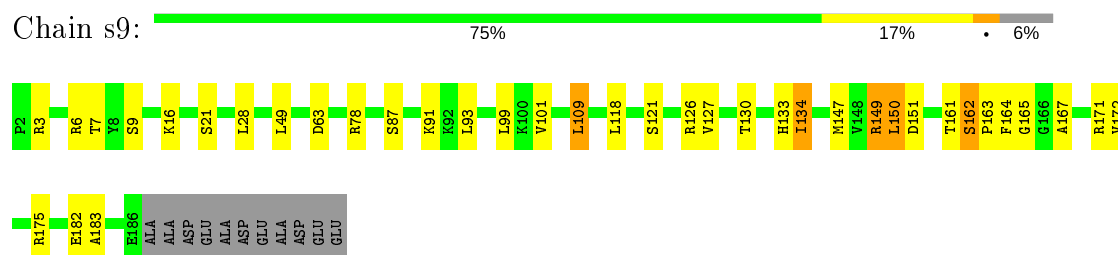
- Molecule 10: 40S ribosomal protein S8-A



- Molecule 11: 40S ribosomal protein S9-A

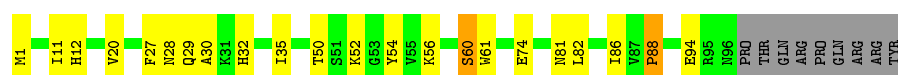


- Molecule 11: 40S ribosomal protein S9-A



- Molecule 12: 40S ribosomal protein S10-A

Chain C0:  70% 19% 9%




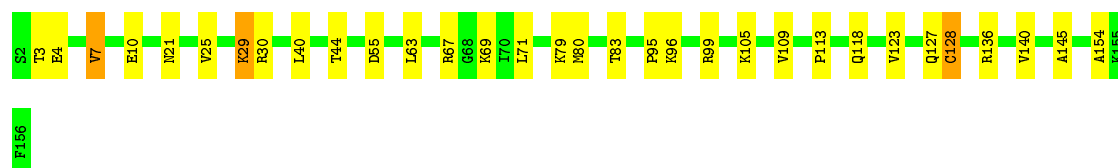
- Molecule 12: 40S ribosomal protein S10-A

Chain c0:  67% 21% 9%



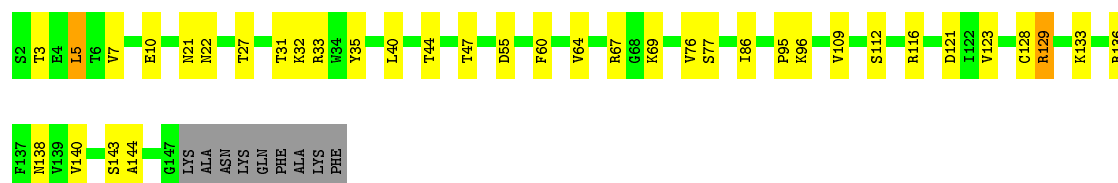
- Molecule 13: 40S ribosomal protein S11-A

Chain C1:  79% 19% 9%



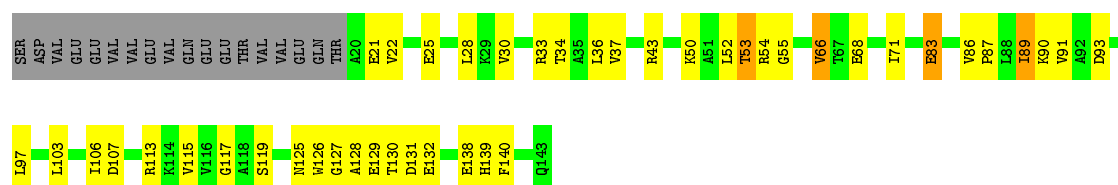
- Molecule 13: 40S ribosomal protein S11-A

Chain c1:  70% 23% 6%



- Molecule 14: 40S ribosomal protein S12

Chain C2:  56% 28% 13%



- Molecule 14: 40S ribosomal protein S12

Chain c2:  61% 25% 13%





- Molecule 15: 40S ribosomal protein S13

Chain C3: 84% 13%



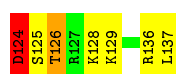
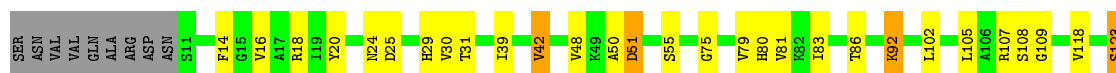
- Molecule 15: 40S ribosomal protein S13

Chain c3: 79% 19%



- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 67% 22% 7%



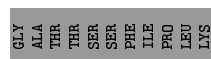
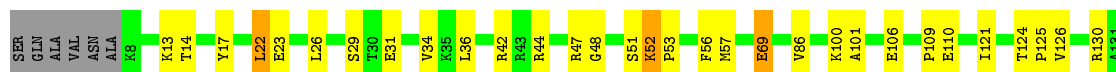
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 68% 24% 6%



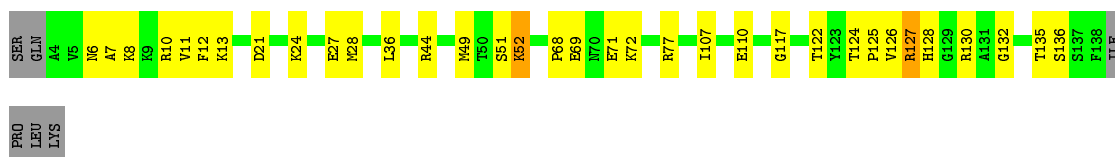
- Molecule 17: 40S ribosomal protein S15

Chain C5: 66% 20% 12%



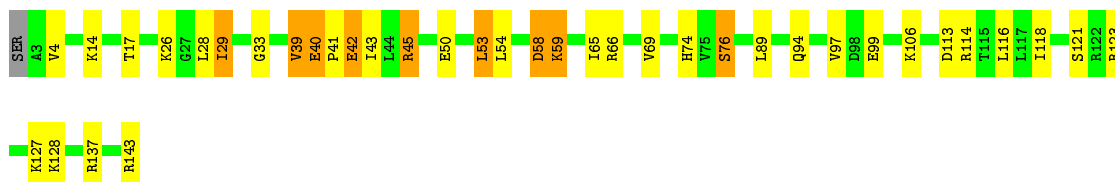
- Molecule 17: 40S ribosomal protein S15

Chain c5: 72% 23% 5%



- Molecule 18: 40S ribosomal protein S16-A

Chain C6: 73% 20% 6%



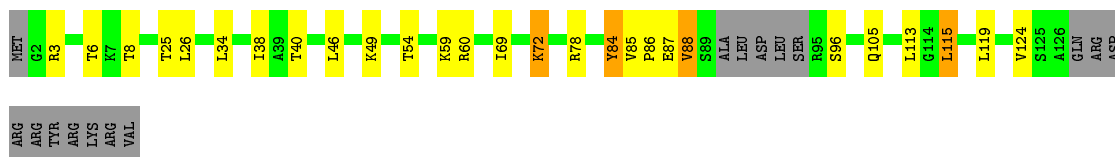
- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 75% 25%



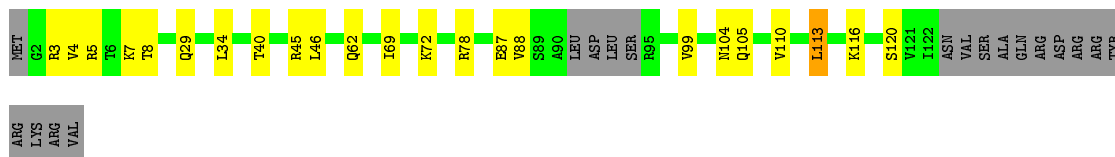
- Molecule 19: 40S ribosomal protein S17-A

Chain C7: 68% 17% 12%



- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 69% 16% 14%

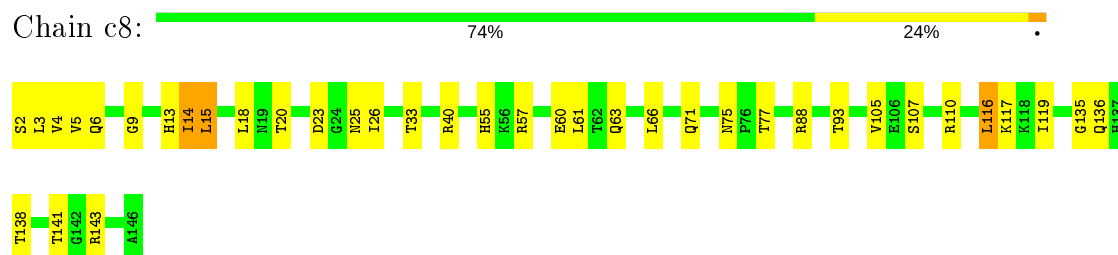


- Molecule 20: 40S ribosomal protein S18-A

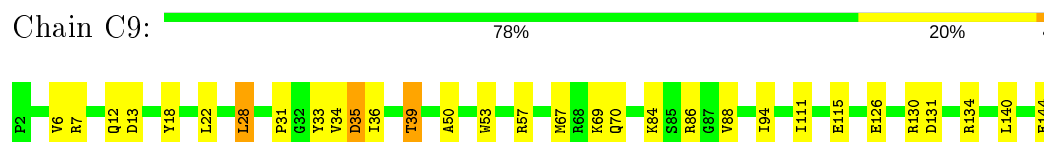
Chain C8: 74% 20% 6%



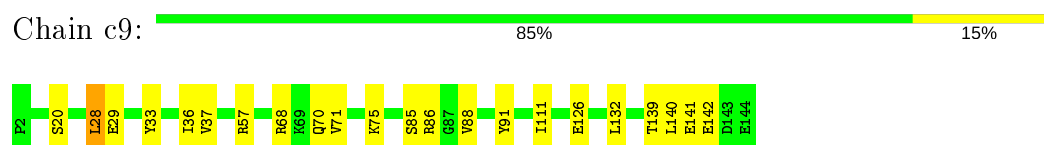
- Molecule 20: 40S ribosomal protein S18-A



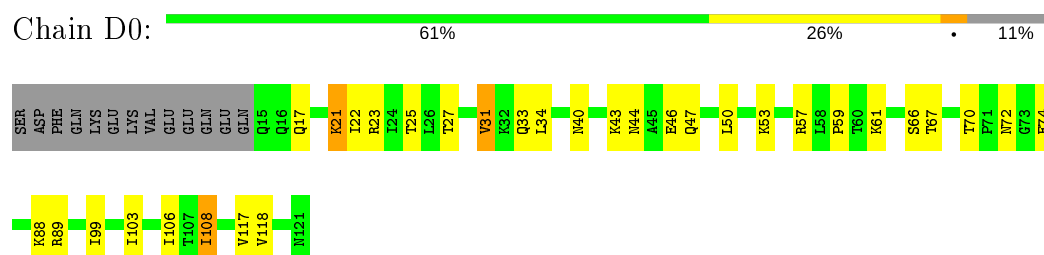
- Molecule 21: 40S ribosomal protein S19-A



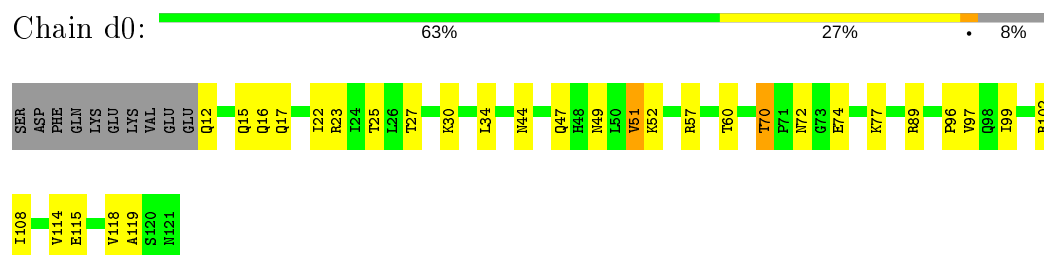
- Molecule 21: 40S ribosomal protein S19-A



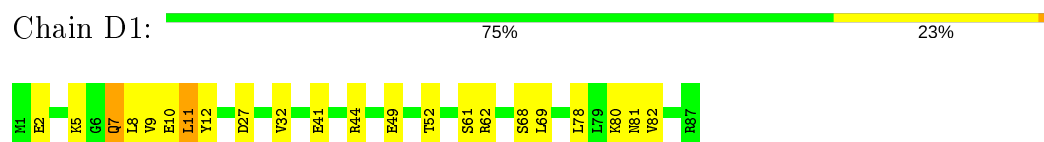
- Molecule 22: 40S ribosomal protein S20



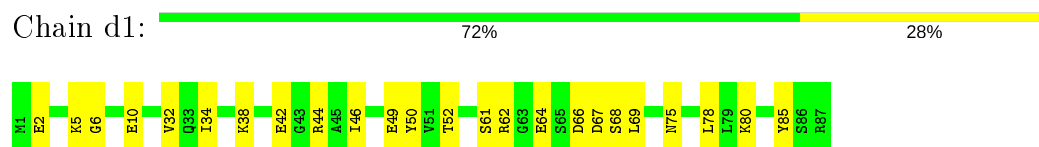
- Molecule 22: 40S ribosomal protein S20



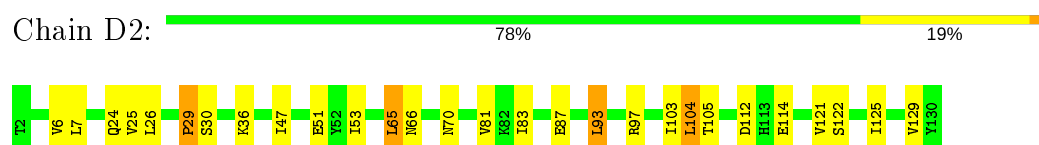
- Molecule 23: 40S ribosomal protein S21-A



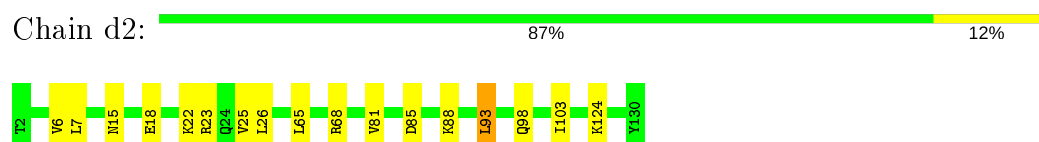
- Molecule 23: 40S ribosomal protein S21-A



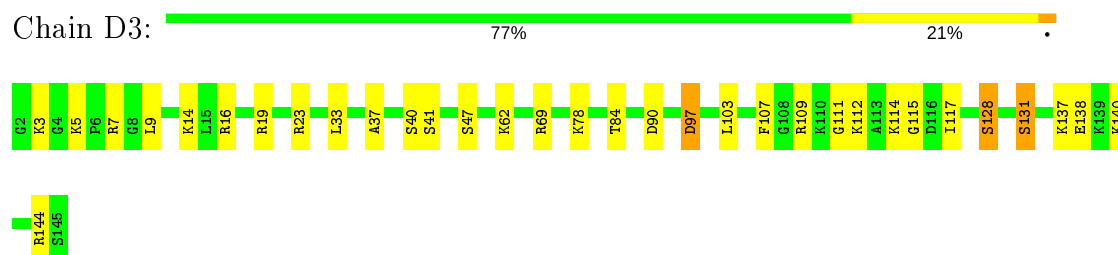
- Molecule 24: 40S ribosomal protein S22-A



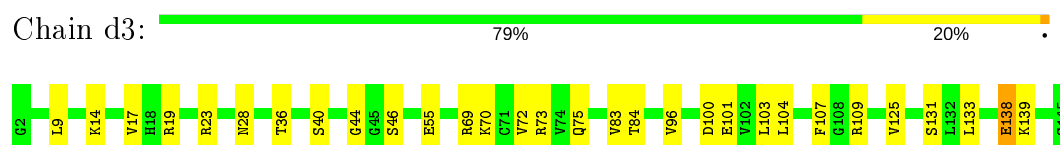
- Molecule 24: 40S ribosomal protein S22-A



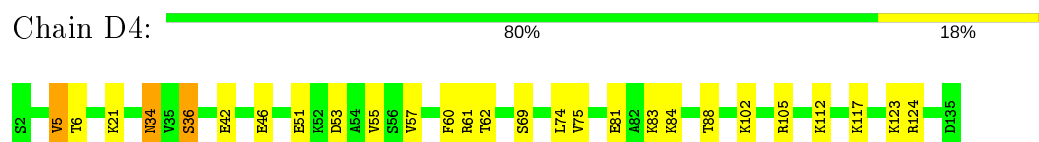
- Molecule 25: 40S ribosomal protein S23-A



- Molecule 25: 40S ribosomal protein S23-A

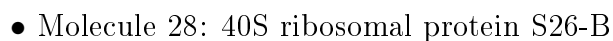
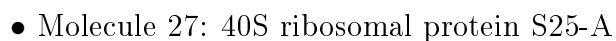
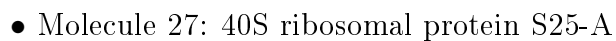


- Molecule 26: 40S ribosomal protein S24-A



- Molecule 26: 40S ribosomal protein S24-A







- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 71% 24% 5%



- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 80% 12% 5% • 5%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 75% 20% • •



- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 71% 22% • •



- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 72% 27% •



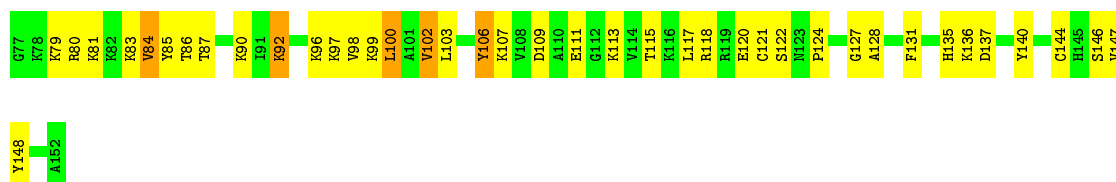
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 50% 33% 11% 7%



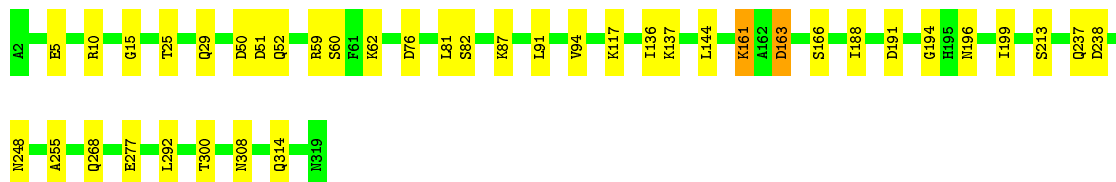
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 47% 46% 7% 7%



- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR: 87% 12% •



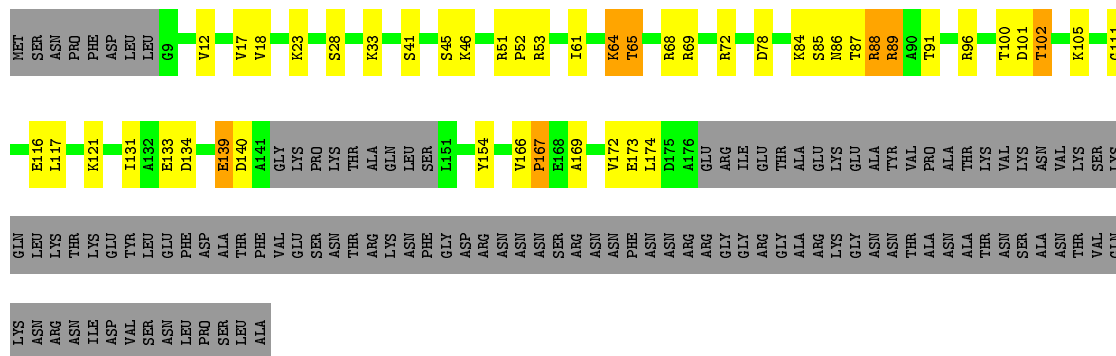
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 87% 13% •



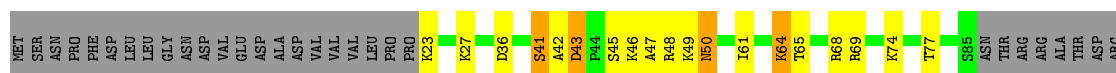
- Molecule 35: Suppressor protein STM1

Chain SM: 41% 15% • 42%



- Molecule 35: Suppressor protein STM1

Chain sM: 30% 7% • 62%

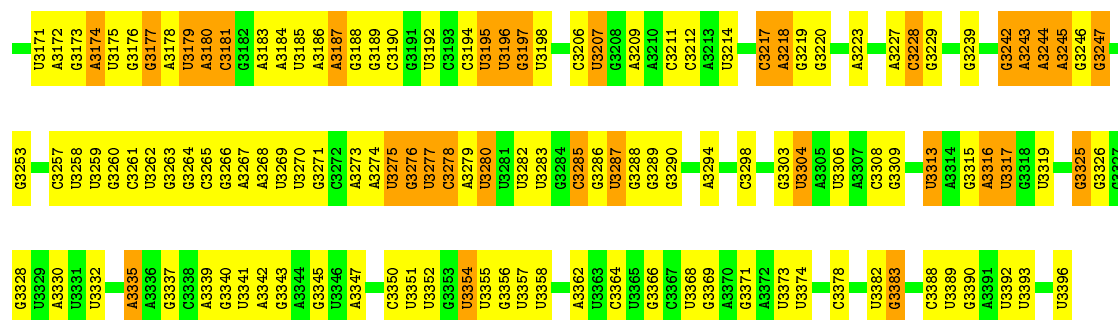


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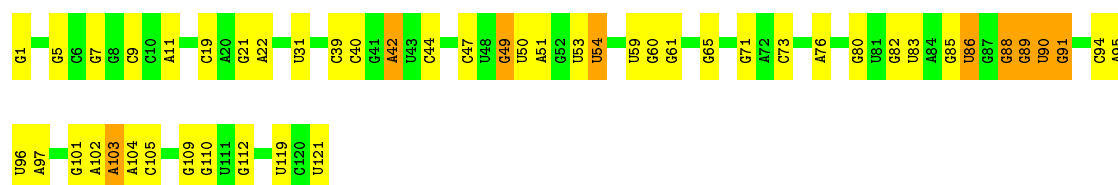
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				U2798	U2716	U2646	U	U2486	U2420	U2354	U2281	C	A2195
				U2799	U2717	U2647	U	U2487	U2421	U2355	U2282	C	A2196
				U2800	U2718	U2648	U	U2488	U2422	U2356	U2283	C	A2197
				U2801	U2719	U2649	U	U2489	U2423	U2357	U2284	C	A2198
				U2802	U2720	U2650	U	U2490	U2424	U2358	U2285	C	A2199
				U2803	U2721	U2651	U	U2491	U2425	U2359	U2286	C	A2200
				U2804	U2722	U2652	U	U2492	U2426	U2360	U2287	C	A2201
				U2805	U2723	U2653	U	U2493	U2427	U2361	U2288	C	A2202
				U2806	U2724	U2654	U	U2494	U2428	U2362	U2289	C	A2203
				U2807	U2725	U2655	U	U2495	U2429	U2363	U2290	C	A2204
				U2808	U2726	U2656	U	U2496	U2430	U2364	U2291	C	A2205
				U2809	U2727	U2657	U	U2497	U2431	U2365	U2292	C	A2206
				U2810	U2728	U2658	U	U2498	U2432	U2366	U2293	C	A2207
				U2811	U2729	U2659	U	U2499	U2433	U2367	U2294	C	A2208
				U2812	U2730	U2660	U	U2500	U2434	U2368	U2295	C	A2209
				U2813	U2731	U2661	U	U2501	U2435	U2369	U2296	C	A2210
				U2814	U2732	U2662	U	U2502	U2436	U2370	U2297	C	A2211
				U2815	U2733	U2663	U	U2503	U2437	U2371	U2298	C	A2212
				U2816	U2734	U2664	U	U2504	U2438	U2372	U2299	C	A2213
				U2817	U2735	U2665	U	U2505	U2439	U2373	U2300	C	A2214
				U2818	U2736	U2666	U	U2506	U2440	U2374	U2301	C	A2215
				U2819	U2737	U2667	U	U2507	U2441	U2375	U2302	C	A2216
				U2820	U2738	U2668	U	U2508	U2442	U2376	U2303	C	A2217
				U2821	U2739	U2669	U	U2509	U2443	U2377	U2304	C	A2218
				U2822	U2740	U2670	U	U2510	U2444	U2378	U2305	C	A2219
				U2823	U2741	U2671	U	U2511	U2445	U2379	U2306	C	A2220
				U2824	U2742	U2672	U	U2512	U2446	U2380	U2307	C	A2221



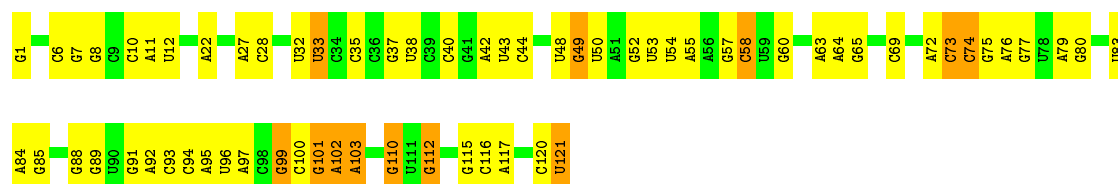
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G3102	A3032	G2960	U2826	G2753	C2685	A2609	U2509	A	A2384	A2313	A2243	G2157	G
G3103	G2962	G2961	U2827	G2754	G2686	G2610	G2510	G	G2385	G2314	A2244	A2158	U
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U3105	G3034	C2963	U2829	G2756	G2687	G2614	C2512	G	A2387	G2318	G2246	G2160	G
A3106	U3038	G2964	G2830	U2757	U2688	G2615	U2513	U	U2388	U	G2247	G2161	C
U3107	C3039	G2965	G2831	A2758	A2689	G2616	U2514	U	C2389	U2318	G2248	A2164	U
C3110	U3041	G2966	G2832	G2759	G2690	G2617	A2515	G	U2390	U	G2249	G2165	U
C3115	A2903	A2967	A2833	U2762	A2691	G2618	A2523	G	G2391	G2323	G2250	G2166	C
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A3123	U3047	U2975	G2842	U2771	A2697	G2623	C2531	U	A2397	G2334	A2255	A2173	A
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A3141	U3071	U2996	U2860	G2798	U2718	G2645	A2569	U	U2416	C2353	C2277	G2199	C
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C3081	G3081	A3006	A2872	U2806	G2730	C2653	G2585	C	U2424	A2363	G2285	U2208	C
G3082	C3082	U3007	U2873	U2807	U2731	C2654	G2586	C	U2425	G2364	G2286	C2135	C
C3083	G3083	G2942	U2874	A2808	G2732	U2655	G2587	C	U2426	U2365	U2287	G2210	C
G3084	A3008	G2943	U2875	C2810	G2733	C2656	G2588	C	A2430	C2366	C2289	U2211	C
G3085	G3085	U2944	C2876	A2811	A2734	A2657	A2593	U	G2431	A2367	G2290	A2138	C
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C3088	G3088	C2879	C2879	G2814	C2737	G2662	U2596	C	U2434	G2370	A2293	A2142	C
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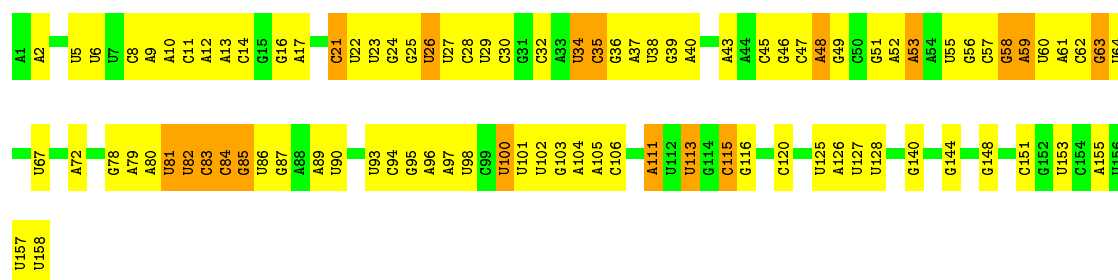
• Molecule 37: 5S ribosomal RNA



• Molecule 37: 5S ribosomal RNA



• Molecule 38: 5.8S ribosomal RNA



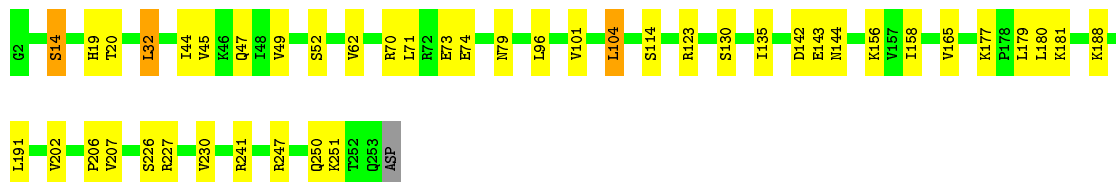
• Molecule 38: 5.8S ribosomal RNA





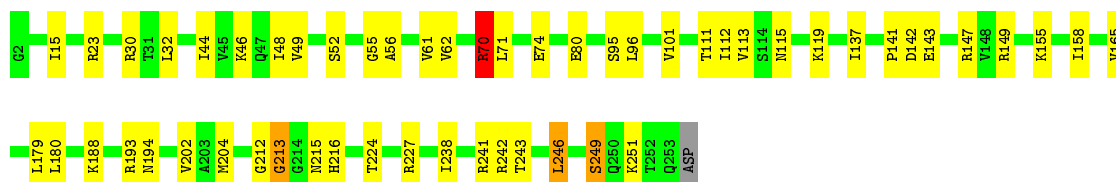
- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 82% 16%



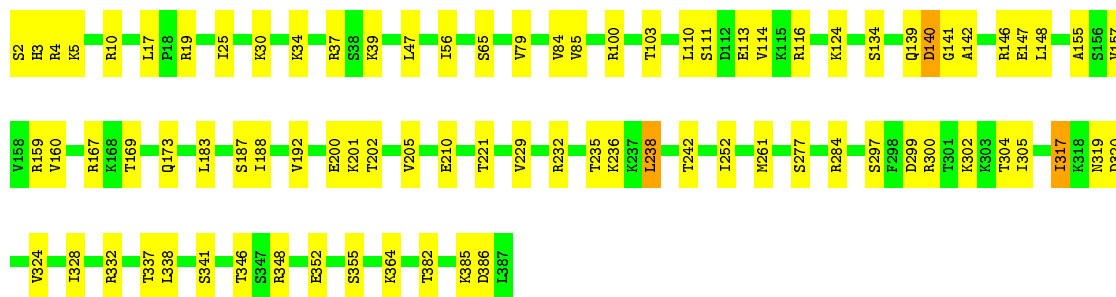
- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 78% 20%



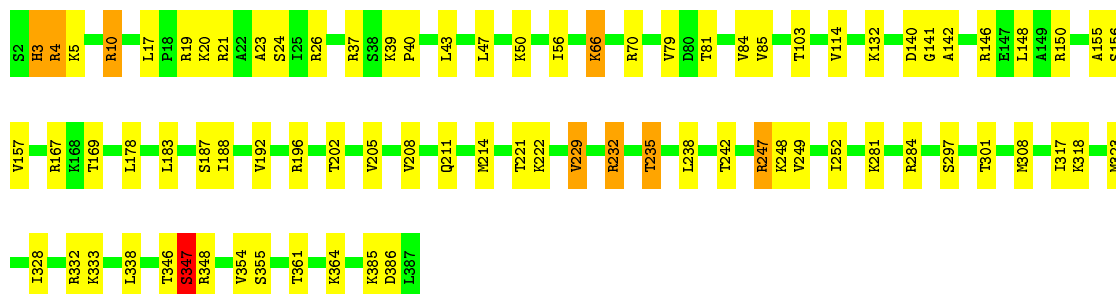
- Molecule 40: 60S ribosomal protein L3

Chain L3: 78% 21%

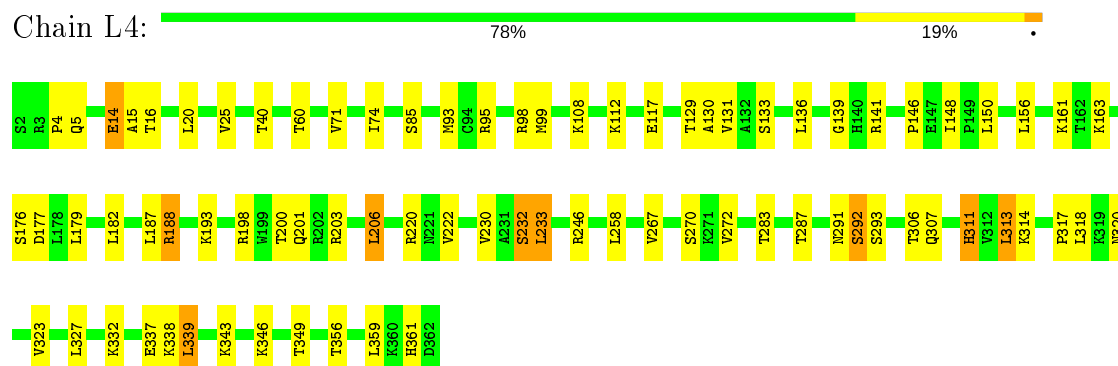


- Molecule 40: 60S ribosomal protein L3

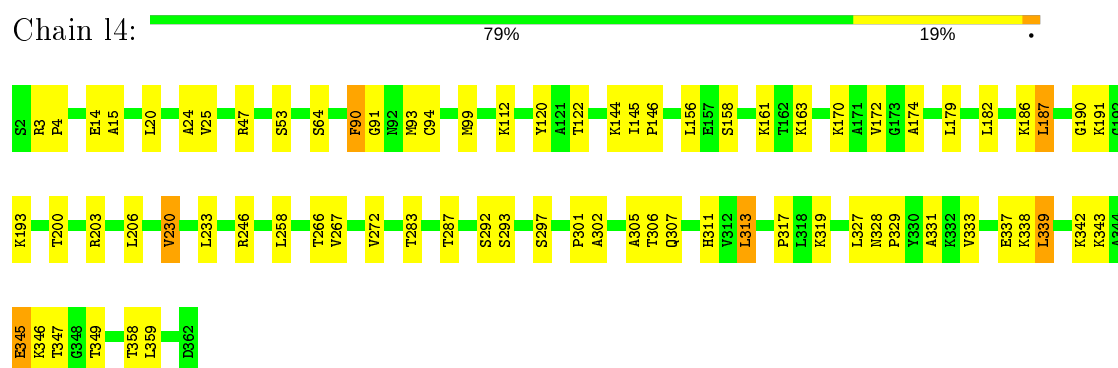
Chain L3: 79% 19%



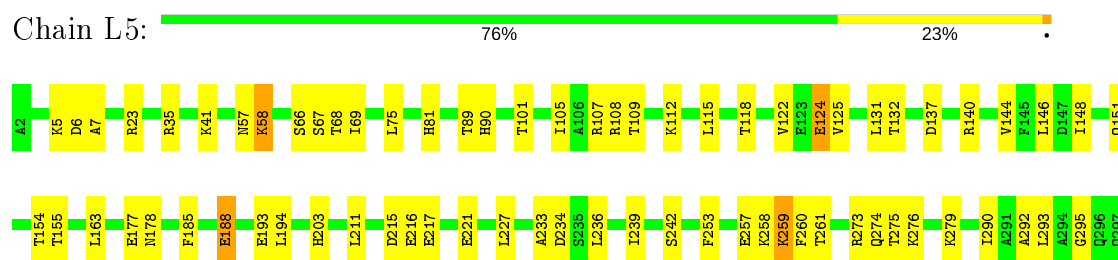
- Molecule 41: 60S ribosomal protein L4-A



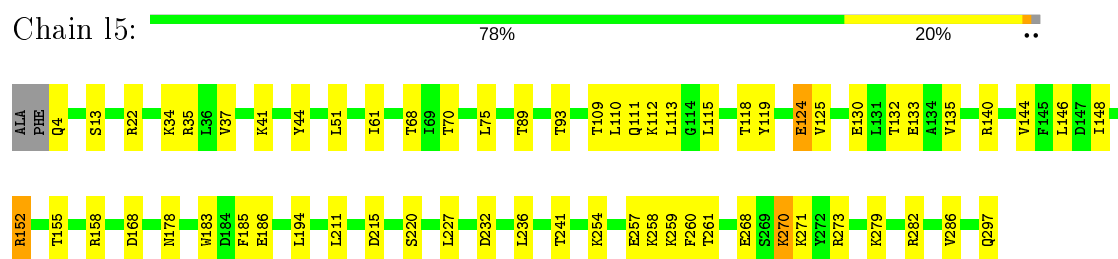
- Molecule 41: 60S ribosomal protein L4-A



- Molecule 42: 60S ribosomal protein L5



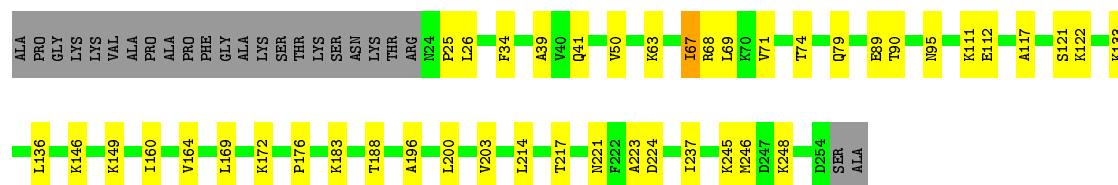
- Molecule 42: 60S ribosomal protein L5



- Molecule 43: 60S ribosomal protein L6-A

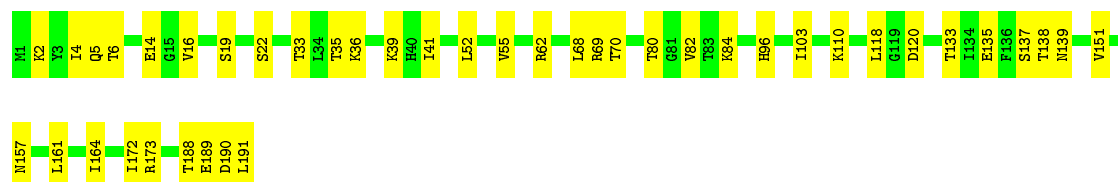






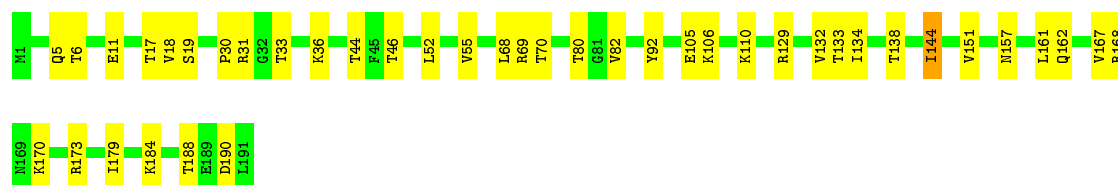
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 78% 22%



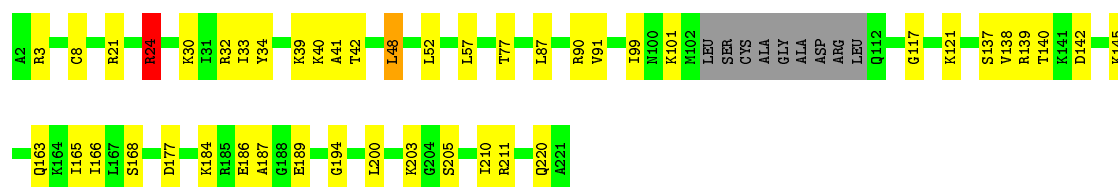
- Molecule 46: 60S ribosomal protein L9-A

Chain l9: 79% 21%



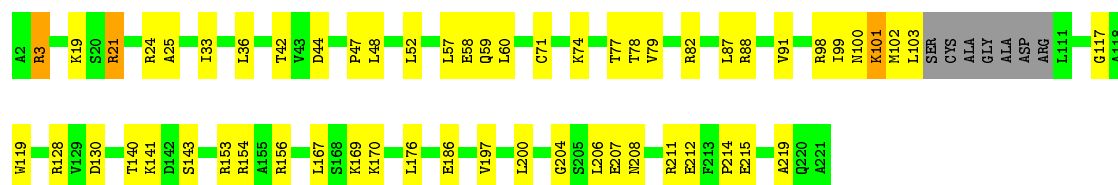
- Molecule 47: 60S ribosomal protein L10

Chain M0: 75% 20%



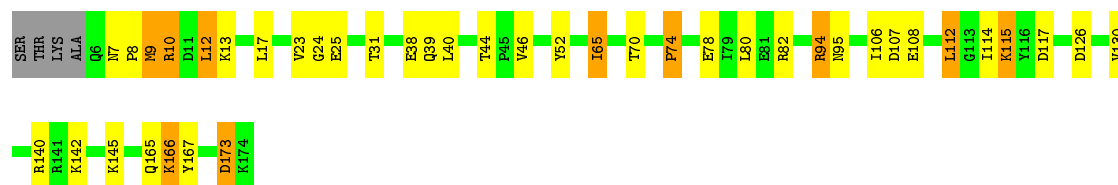
- Molecule 47: 60S ribosomal protein L10

Chain m0: 71% 25%



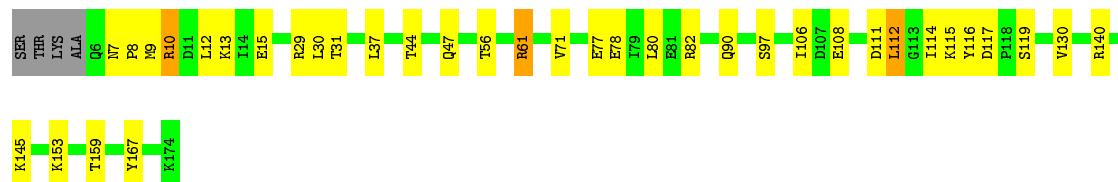
- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 74% 18% 6%



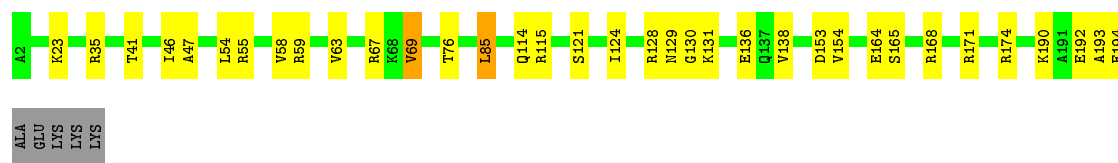
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 76% 20% ..



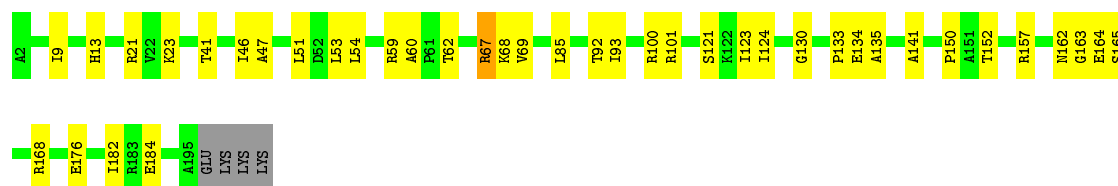
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 80% 17% ..



- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 78% 20% ..



- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 80% 18% ...

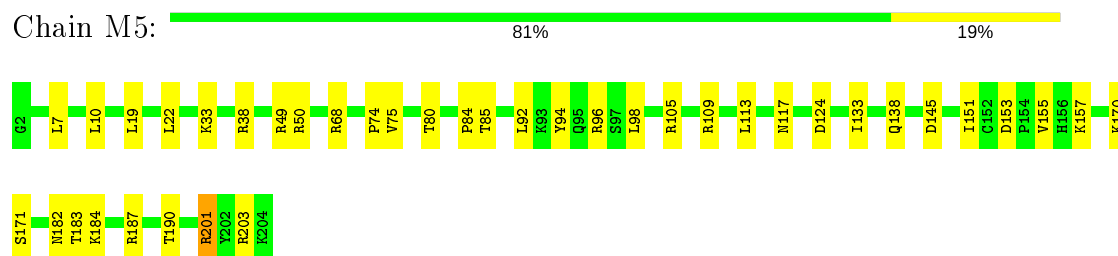


- Molecule 50: 60S ribosomal protein L14-A

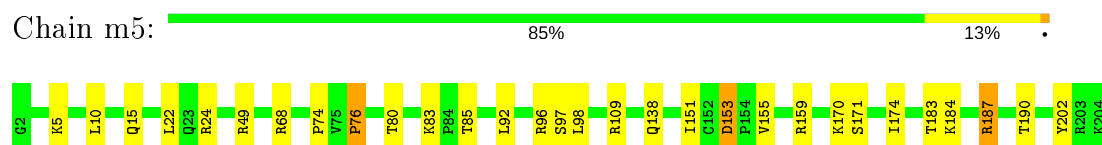
Chain m4: 85% 14% .



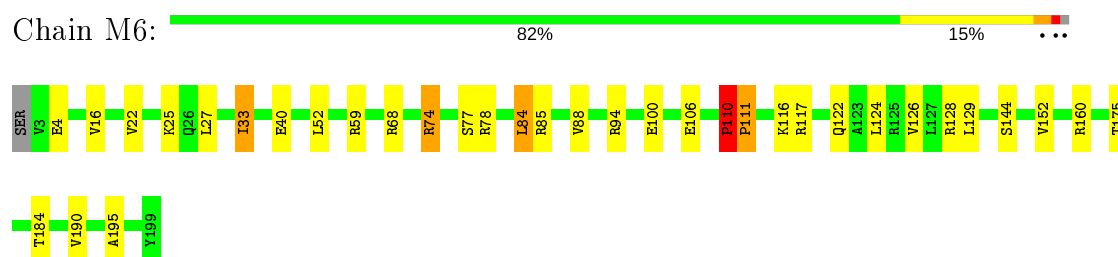
- Molecule 51: 60S ribosomal protein L15-A



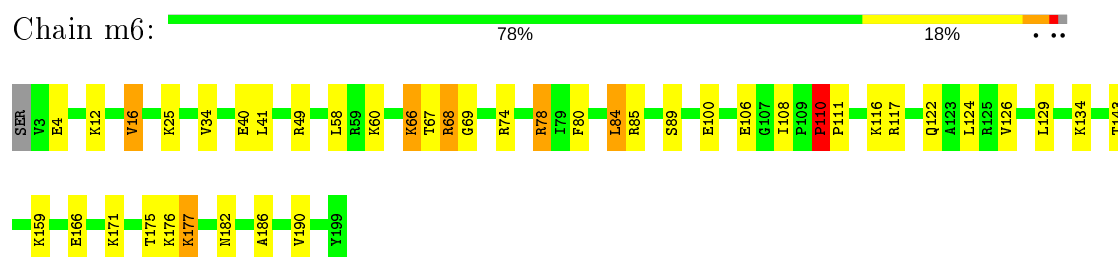
- Molecule 51: 60S ribosomal protein L15-A



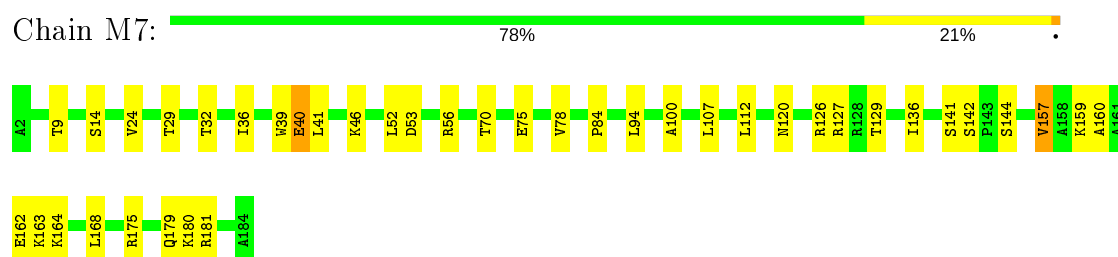
- Molecule 52: 60S ribosomal protein L16-A



- Molecule 52: 60S ribosomal protein L16-A

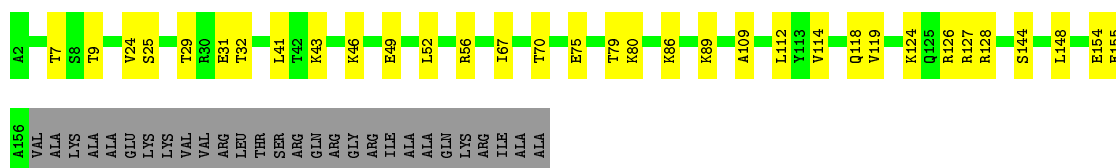


- Molecule 53: 60S ribosomal protein L17-A




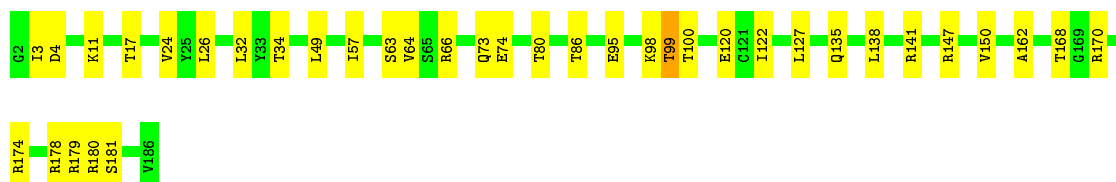
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:  67% 18% 15%




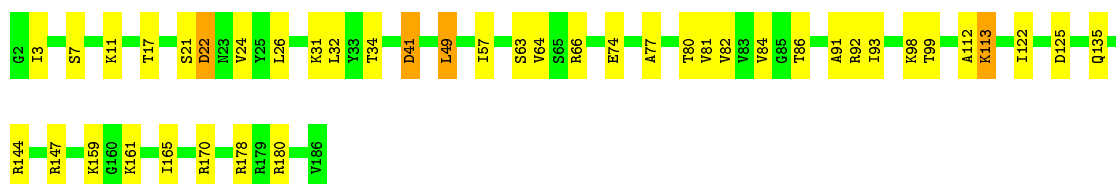
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:  80% 19% .




- Molecule 54: 60S ribosomal protein L18-A

Chain m8:  77% 21% .




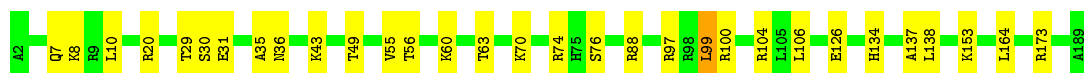
- Molecule 55: 60S ribosomal protein L19-A

Chain M9:  84% 15% .




- Molecule 55: 60S ribosomal protein L19-A

Chain m9:  84% 16% .




- Molecule 56: 60S ribosomal protein L20-A

Chain N0:  80% 19% .


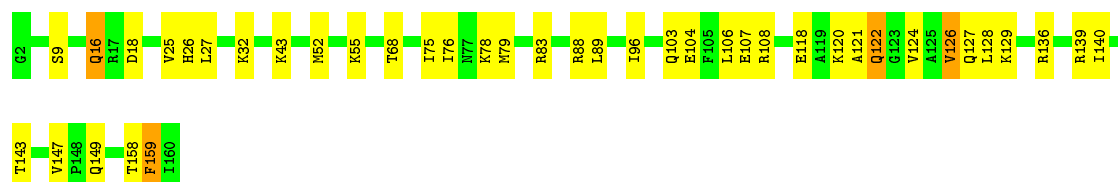


Y172


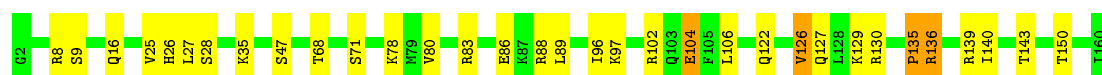
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:  81% 19%

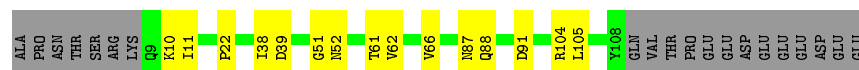
- Molecule 57: 60S ribosomal protein L21-A

Chain N1:  74% 23%

- Molecule 57: 60S ribosomal protein L21-A

Chain n1:  79% 18%

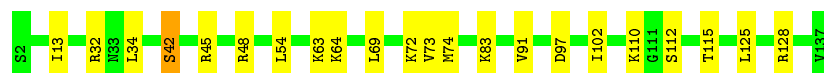
- Molecule 58: 60S ribosomal protein L22-A

Chain N2:  71% 13% 17%


- Molecule 58: 60S ribosomal protein L22-A

Chain n2:  71% 11% 18%

- Molecule 59: 60S ribosomal protein L23-A

Chain N3:  84% 15%

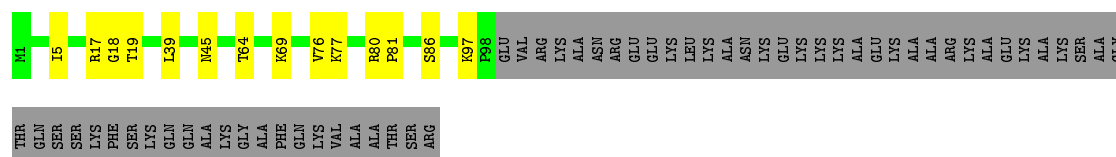
- Molecule 59: 60S ribosomal protein L23-A

Chain n3:  88% 11%



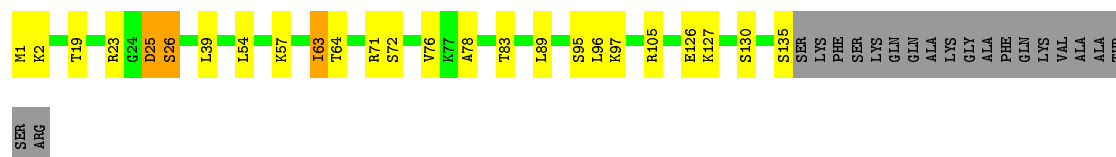
- Molecule 60: 60S ribosomal protein L24-A

Chain N4:  54% 9% 37%



- Molecule 60: 60S ribosomal protein L24-A

Chain n4:  71% 14% 13%



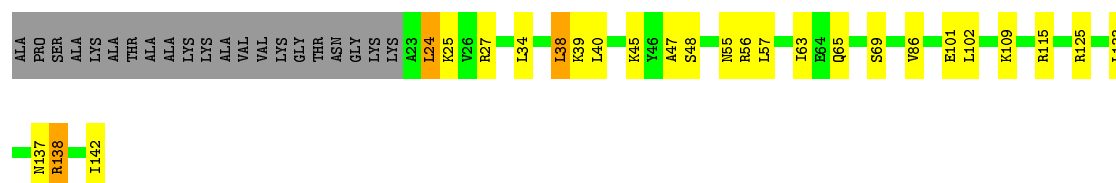
- Molecule 61: 60S ribosomal protein L25

Chain N5:  67% 18% 14%




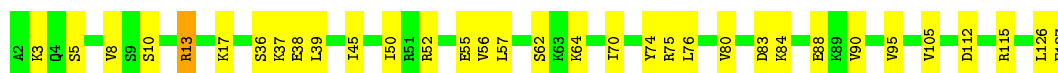
- Molecule 61: 60S ribosomal protein L25

Chain n5:  67% 16% 15%



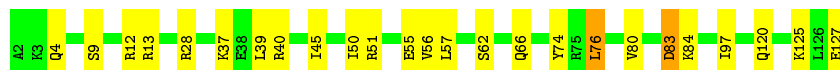
- Molecule 62: 60S ribosomal protein L26-A

Chain N6:  74% 25%



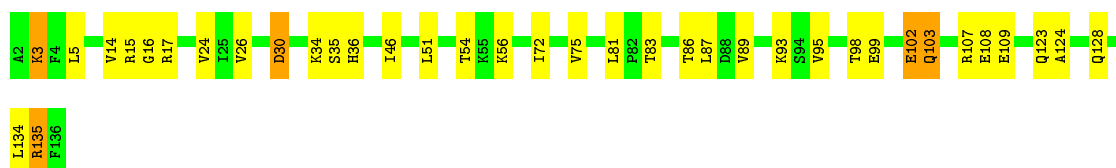
- Molecule 62: 60S ribosomal protein L26-A

Chain n6: 80% 18%



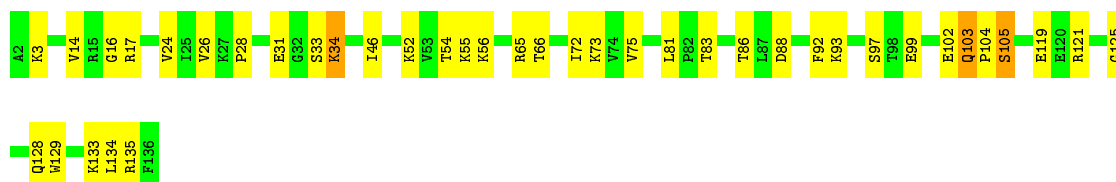
- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 73% 24%



- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 70% 27%



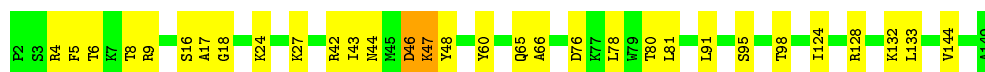
- Molecule 64: 60S ribosomal protein L28

Chain N8: 81% 16%



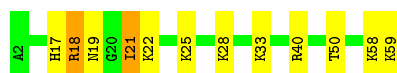
- Molecule 64: 60S ribosomal protein L28

Chain n8: 79% 20%



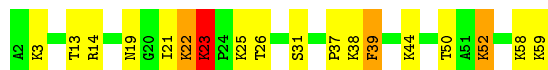
- Molecule 65: 60S ribosomal protein L29

Chain N9: 79% 17%



- Molecule 65: 60S ribosomal protein L29

Chain n9: 69% 24% 5%



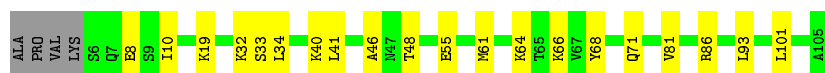
- Molecule 66: 60S ribosomal protein L30

Chain O0: 79% 13% 7%



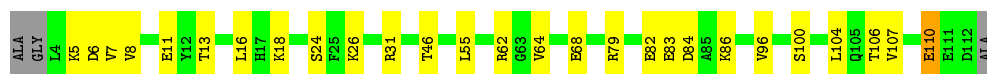
- Molecule 66: 60S ribosomal protein L30

Chain o0: 77% 19% 4%



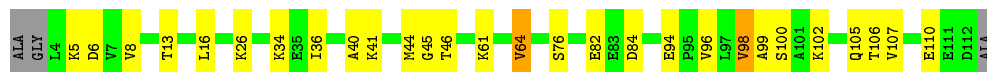
- Molecule 67: 60S ribosomal protein L31-A

Chain O1: 73% 23% 4%



- Molecule 67: 60S ribosomal protein L31-A

Chain o1: 72% 23% 5%



- Molecule 68: 60S ribosomal protein L32

Chain O2: 78% 21% 1%



- Molecule 68: 60S ribosomal protein L32

Chain o2: 77% 21% 2%



- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 86% 13%



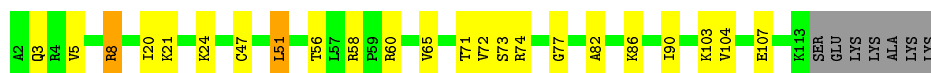
- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 83% 17%



- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 75% 18% 6%



- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 81% 12% 6%



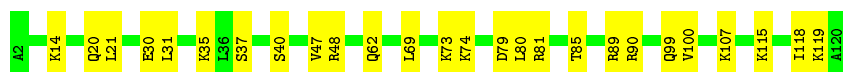
- Molecule 71: 60S ribosomal protein L35-A

Chain O5: 70% 29%



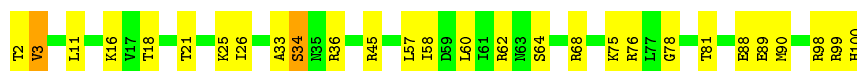
- Molecule 71: 60S ribosomal protein L35-A

Chain o5: 78% 22%



- Molecule 72: 60S ribosomal protein L36-A

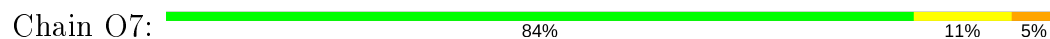
Chain O6: 72% 26%



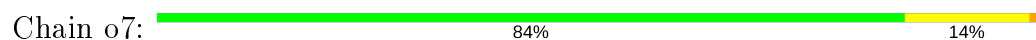
- Molecule 72: 60S ribosomal protein L36-A



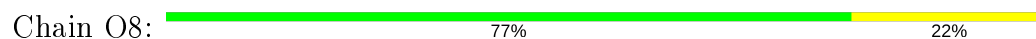
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 73: 60S ribosomal protein L37-A



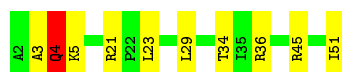
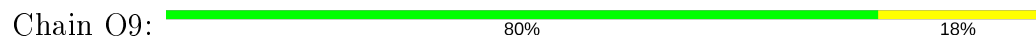
- Molecule 74: 60S ribosomal protein L38



- Molecule 74: 60S ribosomal protein L38

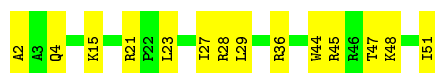


- Molecule 75: 60S ribosomal protein L39

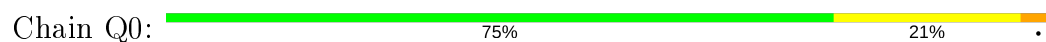


- Molecule 75: 60S ribosomal protein L39

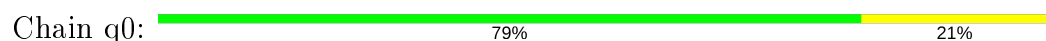




- Molecule 76: Ubiquitin-60S ribosomal protein L40



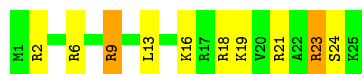
- Molecule 76: Ubiquitin-60S ribosomal protein L40



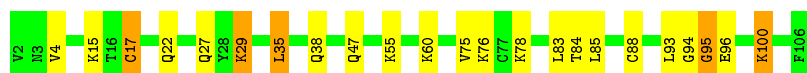
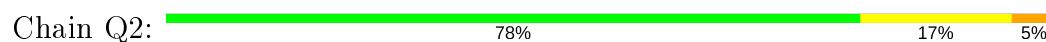
- Molecule 77: 60S ribosomal protein L41-A



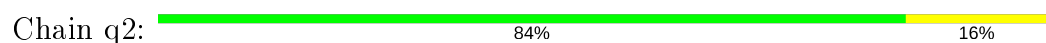
- Molecule 77: 60S ribosomal protein L41-A



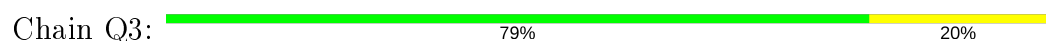
- Molecule 78: 60S ribosomal protein L42-A

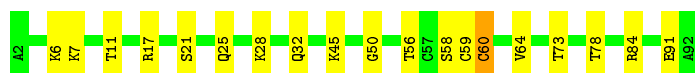


- Molecule 78: 60S ribosomal protein L42-A

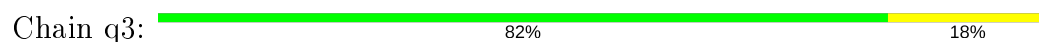


- Molecule 79: 60S ribosomal protein L43-A

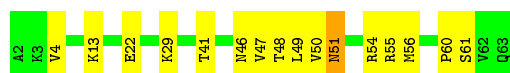




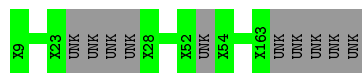
- Molecule 79: 60S ribosomal protein L43-A



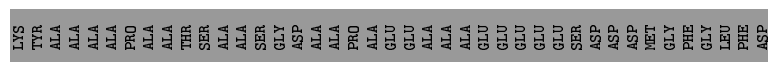
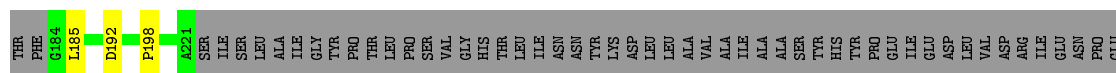
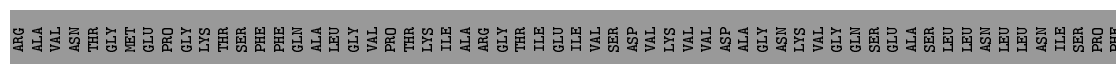
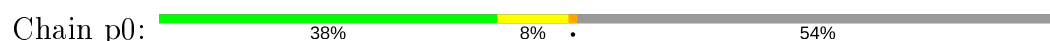
- Molecule 80: 40S ribosomal protein S30-A



- Molecule 81: Unknown Protein m2



- Molecule 82: 60S acidic ribosomal protein P0



- Molecule 83: Unknown Protein p1



There are no outlier residues recorded for this chain.

- Molecule 84: Unknown Protein p2



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.39Å 286.22Å 303.33Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	299.62 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (299.62-3.00)	Depositor
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.207 , 0.258	Depositor
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.193	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411206	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3J2, ZN, OHX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.87	13/41698 (0.0%)	1.42	462/64972 (0.7%)
1	6	0.97	33/42765 (0.1%)	1.48	645/66634 (1.0%)
2	S0	0.49	0/1617	0.69	0/2215
2	s0	0.52	0/1623	0.73	1/2222 (0.0%)
3	S1	0.42	0/1735	0.68	2/2335 (0.1%)
3	s1	0.54	0/1748	0.74	1/2352 (0.0%)
4	S2	0.54	0/1665	0.72	0/2263
4	s2	0.62	0/1665	0.81	2/2263 (0.1%)
5	S3	0.54	0/1759	0.72	1/2368 (0.0%)
5	s3	0.46	0/1759	0.65	0/2368
6	S4	0.56	0/2109	0.79	2/2839 (0.1%)
6	s4	0.56	0/2109	0.80	0/2839
7	S5	0.43	0/1629	0.63	0/2202
7	s5	0.47	0/1629	0.67	0/2202
8	S6	0.54	0/1823	0.72	0/2439
8	s6	0.64	1/1779 (0.1%)	0.74	0/2379
9	S7	0.48	0/1506	0.70	1/2028 (0.0%)
9	s7	0.52	0/1516	0.73	0/2043
10	S8	0.65	0/1514	0.82	1/2021 (0.0%)
10	s8	0.65	0/1514	0.79	1/2021 (0.0%)
11	S9	0.54	0/1519	0.74	1/2035 (0.0%)
11	s9	0.59	0/1519	0.80	4/2035 (0.2%)
12	C0	0.44	0/790	0.68	1/1069 (0.1%)
12	c0	0.39	0/777	0.66	3/1049 (0.3%)
13	C1	0.68	1/1239 (0.1%)	0.74	0/1673
13	c1	0.66	0/1194	0.82	1/1610 (0.1%)
14	C2	0.42	0/900	0.65	0/1224
14	c2	0.32	0/900	0.58	0/1224
15	C3	0.60	0/1215	0.73	2/1638 (0.1%)
15	c3	0.62	0/1215	0.82	2/1638 (0.1%)
16	C4	0.42	0/901	0.69	0/1217
16	c4	0.58	0/960	0.84	3/1290 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.54	0/998	0.78	1/1341 (0.1%)
17	c5	0.51	0/1060	0.69	0/1426
18	C6	0.50	0/1125	0.75	2/1510 (0.1%)
18	c6	0.52	0/1131	0.71	0/1518
19	C7	0.49	0/935	0.69	0/1254
19	c7	0.52	0/914	0.70	0/1224
20	C8	0.48	0/1211	0.72	1/1628 (0.1%)
20	c8	0.51	0/1211	0.73	2/1628 (0.1%)
21	C9	0.48	0/1130	0.69	0/1517
21	c9	0.52	0/1130	0.68	1/1517 (0.1%)
22	D0	0.51	0/865	0.70	0/1169
22	d0	0.53	0/892	0.69	0/1205
23	D1	0.55	0/693	0.70	0/935
23	d1	0.59	0/693	0.79	0/935
24	D2	0.58	0/1038	0.80	3/1395 (0.2%)
24	d2	0.66	0/1038	0.80	1/1395 (0.1%)
25	D3	0.73	0/1139	0.85	1/1518 (0.1%)
25	d3	0.74	0/1139	0.83	1/1518 (0.1%)
26	D4	0.53	0/1087	0.66	0/1449
26	d4	0.57	0/1087	0.78	0/1449
27	D5	0.43	0/571	0.75	0/768
27	d5	0.46	0/566	0.69	0/761
28	D6	0.48	0/782	0.72	0/1047
28	d6	0.60	0/782	0.75	0/1047
29	D7	0.50	0/620	0.70	0/838
29	d7	0.53	0/620	0.73	0/838
30	D8	0.43	0/499	0.62	0/670
30	d8	0.45	0/499	0.69	0/670
31	D9	0.63	0/452	0.85	1/600 (0.2%)
31	d9	0.57	0/452	0.75	1/600 (0.2%)
32	E0	0.54	0/483	0.68	0/643
33	E1	0.53	0/577	0.86	0/770
33	e1	0.42	0/619	0.72	0/822
34	SR	0.42	0/2494	0.63	1/3393 (0.0%)
34	sR	0.42	0/2495	0.59	0/3395
35	SM	0.58	0/1113	0.78	2/1502 (0.1%)
35	sM	0.55	0/683	0.78	2/923 (0.2%)
36	1	1.38	411/75394 (0.5%)	1.86	2927/117545 (2.5%)
36	5	1.40	457/75414 (0.6%)	1.87	2915/117575 (2.5%)
37	3	1.08	4/2883 (0.1%)	1.61	59/4491 (1.3%)
37	7	1.39	14/2883 (0.5%)	1.82	95/4491 (2.1%)
38	4	1.32	12/3746 (0.3%)	1.84	130/5832 (2.2%)
38	8	1.20	10/3746 (0.3%)	1.71	88/5832 (1.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.86	0/1948	0.93	2/2617 (0.1%)
39	l2	0.84	1/1946 (0.1%)	0.95	5/2614 (0.2%)
40	L3	0.87	1/3146 (0.0%)	0.93	2/4228 (0.0%)
40	l3	0.98	2/3146 (0.1%)	0.96	6/4228 (0.1%)
41	L4	0.93	0/2800	1.03	10/3790 (0.3%)
41	l4	0.90	1/2800 (0.0%)	0.95	5/3790 (0.1%)
42	L5	0.66	0/2425	0.75	0/3271
42	l5	0.87	2/2408 (0.1%)	0.89	2/3248 (0.1%)
43	L6	0.93	0/1260	0.91	1/1694 (0.1%)
43	l6	0.95	0/1269	0.97	4/1705 (0.2%)
44	L7	0.92	1/1821 (0.1%)	0.98	7/2451 (0.3%)
44	l7	1.01	4/1828 (0.2%)	0.98	3/2461 (0.1%)
45	L8	0.68	0/1836	0.76	1/2481 (0.0%)
45	l8	0.59	0/1795	0.71	0/2429
46	L9	0.77	0/1539	0.85	0/2073
46	l9	0.88	1/1539 (0.1%)	0.87	0/2073
47	M0	0.81	1/1741 (0.1%)	0.90	4/2335 (0.2%)
47	m0	0.88	1/1758 (0.1%)	0.98	6/2358 (0.3%)
48	M1	0.59	0/1374	0.80	1/1842 (0.1%)
48	m1	0.75	0/1374	0.85	2/1842 (0.1%)
49	M3	0.88	0/1568	0.93	1/2106 (0.0%)
49	m3	0.82	1/1573 (0.1%)	0.92	2/2113 (0.1%)
50	M4	0.88	0/1068	0.87	1/1438 (0.1%)
50	m4	0.96	0/1074	0.92	1/1446 (0.1%)
51	M5	0.90	0/1757	0.99	4/2354 (0.2%)
51	m5	0.78	1/1757 (0.1%)	0.91	2/2354 (0.1%)
52	M6	1.08	5/1585 (0.3%)	1.04	9/2128 (0.4%)
52	m6	1.18	4/1585 (0.3%)	1.08	6/2128 (0.3%)
53	M7	0.91	1/1443 (0.1%)	0.91	0/1944
53	m7	1.00	0/1250	0.97	0/1683
54	M8	0.90	0/1465	0.96	4/1965 (0.2%)
54	m8	0.90	0/1465	1.01	3/1965 (0.2%)
55	M9	0.69	0/1538	0.74	0/2050
55	m9	0.70	0/1538	0.77	0/2050
56	N0	0.89	0/1481	0.93	4/1990 (0.2%)
56	n0	1.01	0/1481	0.97	4/1990 (0.2%)
57	N1	0.87	0/1300	0.88	0/1743
57	n1	1.00	2/1300 (0.2%)	0.96	2/1743 (0.1%)
58	N2	0.49	0/812	0.66	0/1099
58	n2	0.54	0/794	0.72	0/1076
59	N3	0.87	0/1018	0.93	0/1369
59	n3	0.97	1/1018 (0.1%)	1.04	4/1369 (0.3%)
60	N4	0.70	0/712	0.77	1/958 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.75	0/1052	0.80	1/1398 (0.1%)
61	N5	0.80	0/979	0.91	1/1321 (0.1%)
61	n5	0.73	0/974	0.91	1/1314 (0.1%)
62	N6	0.83	0/1004	0.99	2/1341 (0.1%)
62	n6	0.87	1/1004 (0.1%)	0.98	2/1341 (0.1%)
63	N7	0.64	0/1118	0.78	1/1497 (0.1%)
63	n7	0.55	0/1118	0.71	0/1497
64	N8	0.93	0/1204	1.01	2/1612 (0.1%)
64	n8	0.90	1/1204 (0.1%)	0.95	2/1612 (0.1%)
65	N9	0.79	0/473	0.91	1/629 (0.2%)
65	n9	0.96	0/473	1.05	2/629 (0.3%)
66	O0	0.57	0/751	0.74	1/1008 (0.1%)
66	o0	0.55	0/775	0.69	0/1040
67	O1	0.75	0/890	0.80	1/1196 (0.1%)
67	o1	0.90	0/897	0.89	0/1205
68	O2	0.98	0/1041	1.04	4/1394 (0.3%)
68	o2	1.03	1/1041 (0.1%)	1.03	1/1394 (0.1%)
69	O3	1.14	3/868 (0.3%)	0.98	0/1168
69	o3	1.06	0/868	0.96	0/1168
70	O4	0.74	0/890	0.94	5/1189 (0.4%)
70	o4	0.69	0/890	0.82	1/1189 (0.1%)
71	O5	0.88	1/978 (0.1%)	0.91	2/1301 (0.2%)
71	o5	0.68	0/974	0.80	0/1297
72	O6	0.75	0/778	0.88	0/1034
72	o6	0.64	0/777	0.75	0/1033
73	O7	0.96	0/696	1.05	3/923 (0.3%)
73	o7	0.85	0/696	0.96	1/923 (0.1%)
74	O8	0.61	0/618	0.73	0/826
74	o8	0.53	0/614	0.76	1/822 (0.1%)
75	O9	0.91	0/443	0.93	0/588
75	o9	0.82	0/443	0.96	0/588
76	Q0	0.89	1/423 (0.2%)	0.95	1/562 (0.2%)
76	q0	1.00	0/423	1.01	0/562
77	Q1	0.75	0/234	0.96	1/300 (0.3%)
77	q1	0.92	0/234	1.15	3/300 (1.0%)
78	Q2	1.02	1/860 (0.1%)	0.94	1/1136 (0.1%)
78	q2	0.88	0/860	0.91	1/1136 (0.1%)
79	Q3	0.90	0/701	0.94	1/934 (0.1%)
79	q3	0.84	0/701	0.90	0/934
80	e0	0.60	0/499	0.78	0/665
82	p0	0.48	0/1092	0.61	0/1474
All	All	1.06	995/430073 (0.2%)	1.45	7522/631362 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	S1	0	1
3	s1	0	1
5	s3	0	1
6	S4	0	1
7	S5	0	1
7	s5	0	2
9	S7	0	2
9	s7	0	1
16	C4	0	1
16	c4	0	1
18	c6	0	2
19	c7	0	1
22	d0	0	1
26	d4	0	1
27	D5	0	2
28	D6	0	2
33	E1	0	1
33	e1	0	1
39	L2	0	1
39	l2	0	3
41	L4	0	1
41	l4	0	1
42	L5	0	2
42	l5	0	1
43	L6	0	1
44	L7	0	1
44	l7	0	1
45	l8	0	1
48	M1	0	1
49	M3	0	1
51	M5	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
56	N0	0	1
56	n0	0	1
57	N1	0	1
59	n3	0	1
60	n4	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	N7	0	1
64	N8	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	2
67	O1	0	2
67	o1	0	1
71	o5	0	1
72	O6	0	2
75	O9	0	1
75	o9	0	1
76	Q0	0	1
78	Q2	0	2
All	All	0	65

All (995) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	16.46	2.10	1.82
36	5	1152	G	N9-C4	-12.28	1.28	1.38
36	5	2872	A	N9-C4	-12.03	1.30	1.37
57	n1	104	GLU	CB-CG	10.19	1.71	1.52
36	1	3181	C	N3-C4	-9.73	1.27	1.33
36	1	2406	C	N1-C6	-9.39	1.31	1.37
36	5	1152	G	C2-N3	-9.39	1.25	1.32
36	1	2142	A	N3-C4	-9.31	1.29	1.34
37	7	73	C	N1-C6	9.17	1.42	1.37
36	5	1432	C	N3-C4	-9.15	1.27	1.33
36	1	2404	A	N7-C5	9.12	1.44	1.39
36	5	1143	A	N9-C4	-9.11	1.32	1.37
36	1	2911	A	N9-C4	-9.03	1.32	1.37
36	1	1114	U	C2-N3	-8.93	1.31	1.37
36	5	2971	A	N7-C5	8.68	1.44	1.39
36	5	1159	A	N9-C4	-8.65	1.32	1.37
36	5	1103	A	N9-C4	8.62	1.43	1.37
36	5	941	G	C6-N1	-8.60	1.33	1.39
36	1	2333	C	N3-C4	-8.54	1.27	1.33
36	1	1433	A	N7-C5	-8.50	1.34	1.39
36	5	2899	C	N3-C4	-8.46	1.28	1.33
36	5	947	G	C6-N1	-8.41	1.33	1.39
36	1	1143	A	N9-C4	-8.41	1.32	1.37
36	5	970	A	N9-C4	-8.25	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	645	A	C8-N7	-8.23	1.25	1.31
52	M6	4	GLU	CG-CD	8.21	1.64	1.51
36	1	1394	A	N9-C4	-8.17	1.32	1.37
36	5	2377	G	C6-N1	-8.17	1.33	1.39
36	5	2364	G	N7-C5	-8.06	1.34	1.39
36	5	3106	A	N7-C5	-8.06	1.34	1.39
36	5	876	A	C6-N1	-8.04	1.29	1.35
36	1	2616	C	N1-C6	-8.03	1.32	1.37
36	5	877	C	C4-N4	-7.99	1.26	1.33
36	5	2703	A	N7-C5	-7.98	1.34	1.39
36	5	922	U	N1-C2	7.94	1.45	1.38
36	5	2872	A	N9-C8	7.92	1.44	1.37
36	5	922	U	N3-C4	-7.88	1.31	1.38
36	1	2376	G	C6-N1	-7.88	1.34	1.39
36	5	2411	U	C4-O4	-7.88	1.17	1.23
36	1	2987	A	C6-N1	-7.87	1.30	1.35
36	5	2872	A	N3-C4	-7.87	1.30	1.34
36	5	953	G	C5-C4	-7.85	1.32	1.38
36	5	2397	A	N3-C4	-7.85	1.30	1.34
36	5	1199	C	N1-C6	-7.79	1.32	1.37
36	5	2726	C	N3-C4	-7.77	1.28	1.33
36	5	2636	A	C6-N1	-7.76	1.30	1.35
36	5	1117	G	C5-C4	-7.75	1.32	1.38
36	5	1847	A	N9-C4	-7.75	1.33	1.37
36	1	1116	G	N7-C5	-7.74	1.34	1.39
36	1	2398	A	N7-C5	-7.73	1.34	1.39
52	m6	66	LYS	CE-NZ	7.73	1.68	1.49
36	5	1433	A	N7-C5	-7.70	1.34	1.39
36	1	909	G	C5-C4	-7.63	1.33	1.38
36	5	3039	C	N3-C4	-7.61	1.28	1.33
36	5	2971	A	N9-C4	7.61	1.42	1.37
36	5	3245	A	C5-C6	-7.61	1.34	1.41
36	1	3142	A	N3-C4	-7.59	1.30	1.34
13	C1	128	CYS	CB-SG	-7.56	1.69	1.82
36	5	1152	G	N9-C8	7.55	1.43	1.37
36	5	2386	A	N7-C5	-7.55	1.34	1.39
36	5	410	U	C4-O4	7.53	1.29	1.23
36	5	631	U	C2-N3	-7.52	1.32	1.37
36	1	887	G	N9-C8	-7.51	1.32	1.37
36	5	36	C	N1-C6	-7.49	1.32	1.37
36	1	367	A	N3-C4	-7.48	1.30	1.34
36	5	895	A	N9-C4	-7.47	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	970	A	N9-C4	-7.46	1.33	1.37
36	1	921	A	N7-C5	-7.46	1.34	1.39
36	5	2792	A	N3-C4	-7.45	1.30	1.34
36	5	980	A	N7-C5	7.44	1.43	1.39
36	5	2136	C	N1-C6	-7.43	1.32	1.37
36	5	802	C	N1-C6	-7.42	1.32	1.37
36	1	1103	A	N7-C5	7.41	1.43	1.39
36	1	2640	A	C6-N1	-7.41	1.30	1.35
36	5	1874	A	N9-C4	-7.41	1.33	1.37
36	5	804	C	N1-C6	-7.40	1.32	1.37
36	1	2411	U	C4-O4	-7.39	1.17	1.23
36	1	423	A	N7-C5	-7.39	1.34	1.39
36	1	2800	G	C5-C4	-7.37	1.33	1.38
36	1	1149	G	N3-C4	-7.35	1.30	1.35
36	1	1116	G	C5-C4	-7.34	1.33	1.38
36	5	711	A	N9-C4	-7.32	1.33	1.37
36	5	1432	C	C2-N3	-7.32	1.29	1.35
36	1	1103	A	N9-C4	7.32	1.42	1.37
36	5	404	G	N9-C8	-7.31	1.32	1.37
40	L3	200	GLU	CG-CD	7.30	1.62	1.51
36	1	1891	A	N9-C4	-7.30	1.33	1.37
36	1	92	G	C5-C4	-7.29	1.33	1.38
36	1	1133	A	C5-C4	-7.28	1.33	1.38
36	5	2335	G	N3-C4	-7.27	1.30	1.35
36	1	1589	A	N9-C4	-7.26	1.33	1.37
36	1	3209	A	C5-C4	7.26	1.43	1.38
36	1	85	A	C5-C6	-7.24	1.34	1.41
36	1	2820	A	N3-C4	-7.22	1.30	1.34
1	2	1657	U	N1-C2	7.21	1.45	1.38
36	1	40	A	N9-C8	-7.13	1.32	1.37
36	5	2980	U	C2-O2	-7.12	1.16	1.22
36	5	1103	A	C5-C4	7.11	1.43	1.38
36	1	36	C	N1-C6	-7.09	1.32	1.37
36	1	2983	C	N3-C4	-7.08	1.28	1.33
38	4	79	A	N9-C4	7.08	1.42	1.37
36	5	3052	G	C2-N3	-7.05	1.27	1.32
36	1	1156	C	N3-C4	-7.00	1.29	1.33
36	1	2143	A	N9-C4	-7.00	1.33	1.37
36	5	947	G	N1-C2	-6.99	1.32	1.37
36	5	2147	A	C5-C6	-6.98	1.34	1.41
36	1	1113	G	N3-C4	-6.98	1.30	1.35
36	1	931	C	N3-C4	-6.96	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2404	A	N3-C4	6.96	1.39	1.34
1	6	754	A	N9-C4	6.94	1.42	1.37
36	1	2648	G	N1-C2	-6.94	1.32	1.37
36	1	34	A	N9-C4	-6.94	1.33	1.37
36	1	906	A	N7-C5	-6.93	1.35	1.39
36	1	909	G	N9-C8	-6.93	1.32	1.37
36	1	2281	A	N9-C4	-6.93	1.33	1.37
36	5	3245	A	N9-C4	-6.92	1.33	1.37
52	m6	80	PHE	CB-CG	-6.90	1.39	1.51
36	5	3136	G	C6-N1	-6.89	1.34	1.39
36	1	61	A	C6-N1	-6.88	1.30	1.35
36	5	2813	A	N7-C5	-6.87	1.35	1.39
36	1	936	A	N9-C4	-6.86	1.33	1.37
36	1	907	G	N7-C5	-6.84	1.35	1.39
36	1	2356	A	N9-C4	-6.82	1.33	1.37
36	5	2903	A	N9-C4	-6.81	1.33	1.37
36	1	2143	A	C6-N1	-6.81	1.30	1.35
36	1	2139	A	C6-N1	-6.79	1.30	1.35
36	1	2812	C	N1-C6	-6.79	1.33	1.37
36	1	92	G	N1-C2	-6.79	1.32	1.37
36	5	1193	A	N7-C5	-6.78	1.35	1.39
36	5	2383	C	N1-C6	-6.77	1.33	1.37
36	1	865	U	N1-C2	-6.76	1.32	1.38
36	1	1047	A	N9-C4	-6.76	1.33	1.37
36	5	3362	A	N9-C4	-6.75	1.33	1.37
36	1	40	A	C8-N7	-6.75	1.26	1.31
36	1	2885	C	N1-C6	-6.75	1.33	1.37
36	1	931	C	N1-C6	-6.74	1.33	1.37
36	5	428	A	N3-C4	-6.74	1.30	1.34
36	5	40	A	N7-C5	-6.73	1.35	1.39
36	1	504	A	N3-C4	-6.72	1.30	1.34
36	1	895	A	N9-C4	-6.72	1.33	1.37
36	5	437	G	C5-C4	6.72	1.43	1.38
1	2	1599	C	N1-C6	-6.71	1.33	1.37
36	1	2372	A	N9-C4	6.68	1.41	1.37
36	5	1332	A	N3-C4	-6.67	1.30	1.34
36	1	2761	G	C5-C4	-6.67	1.33	1.38
36	5	1152	G	N3-C4	-6.67	1.30	1.35
36	5	2824	G	C6-N1	-6.66	1.34	1.39
36	5	404	G	N7-C5	-6.66	1.35	1.39
36	5	895	A	N3-C4	-6.65	1.30	1.34
36	1	1547	G	C5-C4	-6.64	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	1132	C	N3-C4	-6.64	1.29	1.33
36	5	1047	A	C5-C6	-6.63	1.35	1.41
36	5	3008	A	N9-C4	-6.62	1.33	1.37
36	1	36	C	N1-C2	-6.62	1.33	1.40
36	1	2714	G	N9-C8	6.62	1.42	1.37
36	1	2958	A	C5-C4	-6.61	1.34	1.38
36	5	889	U	C4-O4	-6.60	1.18	1.23
36	5	861	C	N1-C6	-6.60	1.33	1.37
1	6	163	G	N9-C4	-6.60	1.32	1.38
38	4	11	C	N1-C6	-6.59	1.33	1.37
36	5	2134	G	N1-C2	-6.59	1.32	1.37
36	1	1164	G	N7-C5	-6.58	1.35	1.39
36	1	1154	A	N7-C5	-6.58	1.35	1.39
36	5	1332	A	C5-C4	-6.57	1.34	1.38
1	2	1274	C	N3-C4	-6.56	1.29	1.33
69	O3	15	SER	CB-OG	6.55	1.50	1.42
36	5	924	G	N3-C4	-6.55	1.30	1.35
1	6	366	A	N9-C4	-6.54	1.33	1.37
36	5	934	G	C5-C4	-6.53	1.33	1.38
36	5	2639	G	N9-C8	-6.53	1.33	1.37
38	8	80	A	N9-C4	6.53	1.41	1.37
36	1	1452	A	N9-C4	-6.53	1.33	1.37
36	5	1103	A	N3-C4	6.52	1.38	1.34
36	1	34	A	N3-C4	-6.51	1.30	1.34
36	5	3209	A	C5-C4	6.51	1.43	1.38
36	5	2811	A	N9-C4	-6.50	1.33	1.37
36	1	49	A	N9-C4	-6.48	1.33	1.37
36	1	2138	A	N7-C5	-6.48	1.35	1.39
36	5	922	U	C4-O4	-6.47	1.18	1.23
36	5	61	A	N3-C4	-6.47	1.30	1.34
1	2	320	U	N1-C2	6.44	1.44	1.38
36	1	2643	A	N9-C4	-6.44	1.33	1.37
36	5	2894	C	C4-C5	-6.44	1.37	1.43
36	1	61	A	N3-C4	-6.43	1.30	1.34
36	1	1373	A	C6-N1	-6.43	1.31	1.35
36	5	417	A	C6-N1	-6.42	1.31	1.35
36	1	1507	G	N9-C8	-6.42	1.33	1.37
36	5	2138	A	N7-C5	-6.42	1.35	1.39
38	8	79	A	N9-C4	6.42	1.41	1.37
36	1	94	G	C5-C6	-6.41	1.35	1.42
36	5	643	U	C2-N3	-6.41	1.33	1.37
36	5	1149	G	N9-C8	-6.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1886	A	C5-C6	-6.41	1.35	1.41
36	1	92	G	P-O5'	-6.41	1.53	1.59
36	5	1901	A	N7-C5	-6.41	1.35	1.39
36	1	3091	A	N7-C5	-6.39	1.35	1.39
36	1	1370	G	N7-C5	-6.38	1.35	1.39
36	1	3107	U	C2-N3	-6.37	1.33	1.37
36	5	338	A	C5-C6	-6.36	1.35	1.41
36	1	2800	G	N9-C8	-6.35	1.33	1.37
36	1	1370	G	C5-C4	-6.34	1.33	1.38
36	5	3374	U	C4-O4	-6.34	1.18	1.23
36	5	980	A	C5-C6	6.34	1.46	1.41
36	1	2363	A	C6-N1	-6.34	1.31	1.35
36	5	1436	U	N1-C6	-6.34	1.32	1.38
36	5	2945	G	N7-C5	-6.34	1.35	1.39
36	5	647	A	N3-C4	-6.33	1.31	1.34
36	1	1428	A	N9-C4	-6.33	1.34	1.37
76	Q0	110	CYS	CB-SG	-6.32	1.71	1.82
42	l5	257	GLU	CG-CD	6.32	1.61	1.51
36	5	2609	A	C5-C4	-6.32	1.34	1.38
36	1	2748	A	N9-C4	-6.32	1.34	1.37
36	5	1885	U	N1-C2	-6.32	1.32	1.38
36	5	3046	A	C6-N1	-6.32	1.31	1.35
36	5	36	C	C4-C5	-6.31	1.38	1.43
36	1	658	G	C8-N7	-6.30	1.27	1.30
36	5	1379	G	C6-N1	-6.30	1.35	1.39
36	1	1143	A	N3-C4	-6.30	1.31	1.34
36	1	2945	G	N9-C8	-6.30	1.33	1.37
36	1	1459	C	N3-C4	-6.30	1.29	1.33
37	7	101	G	C5-C4	-6.30	1.33	1.38
36	1	28	C	N1-C6	-6.29	1.33	1.37
38	8	138	A	N3-C4	-6.29	1.31	1.34
36	5	1195	A	N7-C5	-6.29	1.35	1.39
36	5	3362	A	N3-C4	-6.28	1.31	1.34
36	5	3095	U	C2-N3	-6.28	1.33	1.37
36	5	3330	A	C5-C4	-6.28	1.34	1.38
36	1	661	G	N7-C5	-6.28	1.35	1.39
36	5	420	G	N9-C8	-6.27	1.33	1.37
36	1	3078	U	C4-O4	6.27	1.28	1.23
36	1	2823	G	N7-C5	-6.27	1.35	1.39
57	n1	104	GLU	CG-CD	6.27	1.61	1.51
36	1	3057	U	N3-C4	-6.26	1.32	1.38
36	5	645	A	C8-N7	-6.26	1.27	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	367	A	N3-C4	-6.26	1.31	1.34
36	5	1429	G	N9-C8	-6.25	1.33	1.37
36	5	2375	G	C6-N1	-6.25	1.35	1.39
36	5	909	G	N9-C8	-6.25	1.33	1.37
36	1	426	G	N1-C2	-6.24	1.32	1.37
36	1	2821	C	N1-C6	-6.24	1.33	1.37
36	1	878	G	N9-C8	-6.24	1.33	1.37
36	1	1370	G	C5-C6	-6.24	1.36	1.42
36	5	1340	G	C5-C4	-6.24	1.33	1.38
36	5	425	G	C5-C6	-6.23	1.36	1.42
44	17	234	GLU	CD-OE1	6.23	1.32	1.25
37	7	102	A	N9-C4	-6.22	1.34	1.37
36	1	984	G	N7-C5	-6.22	1.35	1.39
36	5	960	U	N1-C2	6.21	1.44	1.38
36	5	1406	A	N3-C4	-6.21	1.31	1.34
36	5	2919	A	C6-N1	-6.21	1.31	1.35
36	5	980	A	N3-C4	6.20	1.38	1.34
36	1	200	C	N1-C6	-6.20	1.33	1.37
36	1	1351	U	N1-C2	6.20	1.44	1.38
36	1	1399	A	N9-C4	-6.19	1.34	1.37
36	1	2617	U	N3-C4	-6.19	1.32	1.38
36	5	41	G	N9-C4	-6.19	1.32	1.38
36	5	653	A	N7-C5	-6.19	1.35	1.39
36	5	666	A	N3-C4	-6.18	1.31	1.34
36	5	1200	A	N3-C4	-6.18	1.31	1.34
36	1	2920	U	C2-N3	-6.18	1.33	1.37
36	5	651	G	N7-C5	-6.17	1.35	1.39
36	1	2169	G	N7-C5	6.17	1.43	1.39
36	1	440	A	N9-C4	6.16	1.41	1.37
1	2	1600	A	N9-C4	-6.16	1.34	1.37
36	1	805	G	N9-C8	-6.15	1.33	1.37
36	5	1370	G	C6-N1	-6.15	1.35	1.39
36	1	411	U	C2-N3	-6.15	1.33	1.37
1	6	616	G	N3-C4	-6.15	1.31	1.35
36	5	2970	C	N1-C6	-6.15	1.33	1.37
36	1	638	C	C2-N3	-6.14	1.30	1.35
36	5	704	U	N1-C2	-6.14	1.33	1.38
38	4	25	G	N7-C5	-6.14	1.35	1.39
36	1	659	G	N1-C2	-6.14	1.32	1.37
36	1	610	G	N9-C4	-6.13	1.33	1.38
36	1	1348	U	N1-C2	6.13	1.44	1.38
38	4	25	G	C6-N1	-6.13	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	3216	G	C5-C4	-6.12	1.34	1.38
36	5	983	A	C5-C4	-6.12	1.34	1.38
36	5	1174	G	C5-C4	-6.12	1.34	1.38
36	1	859	G	N7-C5	-6.12	1.35	1.39
36	1	3136	G	C6-N1	-6.12	1.35	1.39
36	5	969	C	N3-C4	-6.11	1.29	1.33
36	5	649	A	C5-C6	-6.10	1.35	1.41
36	1	895	A	C5-C6	-6.10	1.35	1.41
36	1	1847	A	C6-N6	-6.10	1.29	1.33
36	5	874	U	C4'-C3'	-6.10	1.46	1.53
36	1	3307	A	C6-N1	-6.09	1.31	1.35
36	5	2399	A	N9-C4	-6.09	1.34	1.37
36	5	2202	C	N1-C6	-6.09	1.33	1.37
36	1	2911	A	N3-C4	-6.08	1.31	1.34
36	5	2367	A	N7-C5	-6.08	1.35	1.39
36	5	2138	A	N3-C4	-6.08	1.31	1.34
36	1	1157	G	C6-N1	-6.08	1.35	1.39
36	5	1332	A	N7-C5	-6.07	1.35	1.39
36	1	2968	G	C6-N1	-6.07	1.35	1.39
36	5	3039	C	N1-C6	-6.07	1.33	1.37
38	8	25	G	N1-C2	-6.07	1.32	1.37
36	5	1205	A	N7-C5	-6.06	1.35	1.39
36	5	2957	G	C8-N7	-6.06	1.27	1.30
36	1	656	A	N7-C5	-6.05	1.35	1.39
36	5	2201	G	N1-C2	-6.05	1.32	1.37
36	5	2915	U	C2-N3	-6.05	1.33	1.37
36	1	3087	A	N3-C4	-6.04	1.31	1.34
36	5	636	C	N1-C6	-6.04	1.33	1.37
36	1	342	A	N3-C4	-6.04	1.31	1.34
36	1	635	G	C5-C4	-6.04	1.34	1.38
36	1	1119	C	N3-C4	-6.04	1.29	1.33
38	4	11	C	C4-C5	-6.04	1.38	1.43
1	6	397	A	N9-C4	-6.03	1.34	1.37
62	n6	55	GLU	CG-CD	6.03	1.60	1.51
36	5	3084	C	N1-C6	-6.03	1.33	1.37
36	1	874	U	C2-N3	-6.03	1.33	1.37
36	5	408	A	C5-C4	-6.03	1.34	1.38
36	1	345	G	N9-C8	-6.03	1.33	1.37
36	1	658	G	N9-C8	-6.03	1.33	1.37
36	5	1432	C	N1-C2	-6.03	1.34	1.40
36	5	2987	A	N7-C5	-6.02	1.35	1.39
36	5	2860	U	C2-O2	6.02	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	654	C	N1-C6	-6.02	1.33	1.37
36	5	1158	A	C5-C6	-6.01	1.35	1.41
36	5	3042	U	N3-C4	-6.01	1.33	1.38
36	1	1660	C	N1-C6	-6.01	1.33	1.37
36	1	3362	A	N7-C5	-6.01	1.35	1.39
36	5	1884	A	C5-C6	-6.00	1.35	1.41
36	5	1865	A	N9-C4	-6.00	1.34	1.37
38	8	14	C	N1-C2	-6.00	1.34	1.40
1	6	1027	A	N9-C4	-6.00	1.34	1.37
39	12	213	GLY	C-O	5.99	1.33	1.23
36	5	953	G	N9-C4	-5.99	1.33	1.38
36	5	668	G	C6-N1	-5.98	1.35	1.39
36	5	1301	A	N7-C5	-5.97	1.35	1.39
36	5	2937	G	C5-C4	-5.96	1.34	1.38
36	5	2848	G	N7-C5	-5.96	1.35	1.39
36	1	2404	A	C5-C6	5.95	1.46	1.41
36	5	513	G	C6-N1	-5.95	1.35	1.39
36	5	2334	U	C4-O4	-5.95	1.18	1.23
36	5	2728	G	C2-N3	-5.95	1.27	1.32
36	5	2987	A	N9-C8	-5.95	1.32	1.37
38	4	40	A	C5-C6	-5.94	1.35	1.41
36	1	636	C	N3-C4	-5.94	1.29	1.33
36	1	2833	A	N3-C4	-5.94	1.31	1.34
36	5	909	G	C8-N7	-5.94	1.27	1.30
36	5	1115	G	N1-C2	-5.94	1.33	1.37
36	5	1174	G	N3-C4	-5.94	1.31	1.35
36	5	2934	A	C6-N1	-5.94	1.31	1.35
36	1	1865	A	N9-C4	-5.93	1.34	1.37
1	6	337	G	C2-N3	5.93	1.37	1.32
36	5	2343	C	N1-C6	-5.93	1.33	1.37
38	8	104	A	N9-C4	-5.93	1.34	1.37
36	5	875	G	C6-N1	-5.93	1.35	1.39
36	5	3274	A	N9-C4	-5.93	1.34	1.37
36	5	3330	A	N9-C4	-5.93	1.34	1.37
36	5	2636	A	C5-C4	-5.92	1.34	1.38
1	6	1657	U	C2-O2	5.92	1.27	1.22
36	5	1436	U	C4-C5	-5.92	1.38	1.43
36	5	2830	G	N3-C4	-5.92	1.31	1.35
36	1	941	G	C6-N1	-5.91	1.35	1.39
36	1	1325	U	N1-C2	-5.91	1.33	1.38
1	6	1659	A	N9-C4	-5.91	1.34	1.37
36	5	2138	A	N9-C4	-5.91	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	971	G	C5-C4	-5.90	1.34	1.38
36	1	1846	C	N1-C2	-5.90	1.34	1.40
71	O5	64	GLU	CG-CD	5.90	1.60	1.51
36	1	1156	C	C2-N3	-5.90	1.31	1.35
36	1	2362	C	C4-C5	-5.89	1.38	1.43
36	5	876	A	N3-C4	-5.89	1.31	1.34
36	5	952	A	C5-C6	-5.89	1.35	1.41
36	5	1352	A	N9-C4	5.89	1.41	1.37
36	5	924	G	C2-N3	-5.88	1.28	1.32
36	5	2647	A	N9-C4	-5.88	1.34	1.37
36	1	1154	A	C6-N1	-5.88	1.31	1.35
36	1	406	G	C6-N1	-5.87	1.35	1.39
36	1	878	G	N3-C4	-5.87	1.31	1.35
36	5	924	G	C5-C4	-5.87	1.34	1.38
36	5	1843	C	N1-C6	-5.87	1.33	1.37
36	5	2874	G	N7-C5	-5.87	1.35	1.39
36	5	2899	C	C2-N3	-5.87	1.31	1.35
36	5	3139	A	N3-C4	-5.87	1.31	1.34
36	1	402	A	N3-C4	-5.87	1.31	1.34
36	1	1165	A	N3-C4	-5.87	1.31	1.34
36	5	794	U	N3-C4	-5.86	1.33	1.38
36	5	818	C	C2-O2	-5.86	1.19	1.24
36	5	36	C	N1-C2	-5.86	1.34	1.40
36	5	1134	G	N3-C4	-5.86	1.31	1.35
36	5	1157	G	N9-C8	-5.86	1.33	1.37
36	1	1305	U	C4-C5	-5.86	1.38	1.43
36	1	1103	A	N3-C4	5.86	1.38	1.34
36	5	1372	C	N1-C6	-5.86	1.33	1.37
36	1	2390	A	C6-N1	-5.85	1.31	1.35
36	1	99	A	N7-C5	-5.85	1.35	1.39
36	5	981	U	N1-C2	5.85	1.43	1.38
1	6	1537	C	C2-N3	5.85	1.40	1.35
36	5	2401	A	N9-C8	5.84	1.42	1.37
36	5	2899	C	C2-O2	-5.84	1.19	1.24
36	1	361	A	N3-C4	-5.84	1.31	1.34
1	6	1657	U	C2-N3	5.84	1.41	1.37
37	7	89	G	N9-C8	-5.83	1.33	1.37
36	1	2601	A	N9-C4	-5.83	1.34	1.37
36	5	1929	G	C6-N1	-5.83	1.35	1.39
36	1	1459	C	N1-C6	-5.83	1.33	1.37
36	5	711	A	N3-C4	-5.83	1.31	1.34
36	5	648	C	C4-C5	-5.83	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	804	C	N1-C6	-5.83	1.33	1.37
36	5	903	U	C2-N3	-5.82	1.33	1.37
36	5	832	G	N7-C5	-5.82	1.35	1.39
36	5	3330	A	N3-C4	-5.82	1.31	1.34
36	1	2814	G	C8-N7	-5.82	1.27	1.30
1	2	1200	G	N7-C5	-5.82	1.35	1.39
36	1	49	A	N9-C8	-5.82	1.33	1.37
36	5	3004	C	N1-C6	-5.81	1.33	1.37
36	1	890	C	N3-C4	-5.81	1.29	1.33
36	1	1134	G	C5-C6	-5.81	1.36	1.42
36	1	607	A	C6-N1	-5.81	1.31	1.35
36	5	1841	A	N7-C5	-5.81	1.35	1.39
52	M6	4	GLU	CD-OE2	5.81	1.32	1.25
36	1	653	A	C5-C6	-5.80	1.35	1.41
36	1	2986	U	N1-C6	-5.80	1.32	1.38
36	5	957	C	N3-C4	-5.80	1.29	1.33
36	1	206	G	C5-C4	-5.80	1.34	1.38
36	5	1849	C	N1-C6	-5.80	1.33	1.37
36	5	1195	A	N9-C4	-5.80	1.34	1.37
36	1	2984	C	N3-C4	-5.79	1.29	1.33
36	5	2335	G	N1-C2	-5.79	1.33	1.37
36	1	2800	G	N7-C5	-5.79	1.35	1.39
38	4	28	C	N1-C6	-5.79	1.33	1.37
36	1	36	C	C4-C5	-5.78	1.38	1.43
36	1	1606	U	N1-C2	-5.78	1.33	1.38
36	1	1522	U	N1-C6	-5.78	1.32	1.38
36	5	1114	U	C2-O2	-5.78	1.17	1.22
1	2	1291	G	N3-C4	-5.77	1.31	1.35
36	1	1405	U	C4-O4	-5.77	1.19	1.23
36	5	953	G	N7-C5	-5.76	1.35	1.39
36	1	963	G	N7-C5	-5.76	1.35	1.39
36	1	3277	U	N1-C2	5.76	1.43	1.38
36	1	2550	U	N3-C4	-5.76	1.33	1.38
1	2	1655	A	N3-C4	-5.76	1.31	1.34
36	1	1114	U	N3-C4	-5.75	1.33	1.38
36	1	1164	G	C8-N7	-5.75	1.27	1.30
36	5	3042	U	C2-N3	-5.75	1.33	1.37
37	3	88	G	C6-N1	-5.75	1.35	1.39
36	5	3008	A	N3-C4	-5.75	1.31	1.34
36	5	2996	U	N1-C2	5.75	1.43	1.38
36	1	805	G	C5-C4	-5.74	1.34	1.38
69	O3	3	GLU	CD-OE1	5.74	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1195	A	N3-C4	-5.74	1.31	1.34
36	1	1905	G	N3-C4	-5.74	1.31	1.35
36	5	3186	A	C6-N1	-5.74	1.31	1.35
36	1	432	G	N7-C5	-5.73	1.35	1.39
36	1	1845	G	C6-N1	-5.73	1.35	1.39
36	5	1318	A	N3-C4	-5.73	1.31	1.34
36	5	2336	U	N1-C2	-5.73	1.33	1.38
36	1	2362	C	N1-C6	-5.72	1.33	1.37
36	1	2648	G	C6-N1	-5.72	1.35	1.39
1	6	331	A	N9-C4	-5.72	1.34	1.37
36	1	908	G	C5-C6	-5.71	1.36	1.42
36	5	1121	U	N1-C2	-5.71	1.33	1.38
36	5	2816	G	N1-C2	-5.71	1.33	1.37
36	1	645	A	N7-C5	-5.71	1.35	1.39
36	1	3261	C	N1-C6	-5.71	1.33	1.37
36	5	3136	G	C2-N3	-5.71	1.28	1.32
36	5	2389	C	N3-C4	-5.70	1.29	1.33
36	5	3083	G	N1-C2	-5.70	1.33	1.37
36	1	2361	A	N9-C4	5.70	1.41	1.37
36	1	2733	A	N7-C5	-5.70	1.35	1.39
36	1	2368	A	N3-C4	-5.69	1.31	1.34
47	M0	8	CYS	CB-SG	-5.69	1.72	1.81
36	5	919	U	C4-O4	-5.68	1.19	1.23
36	1	2385	G	N9-C8	-5.68	1.33	1.37
36	5	645	A	C5-C6	5.68	1.46	1.41
36	5	2993	G	C5-C4	-5.68	1.34	1.38
36	1	2400	G	C5-C4	-5.68	1.34	1.38
36	1	2927	C	C2-O2	-5.67	1.19	1.24
36	5	3141	A	N9-C8	-5.67	1.33	1.37
36	1	1120	A	C6-N1	-5.67	1.31	1.35
36	1	2147	A	N3-C4	-5.67	1.31	1.34
36	5	3214	U	C2-N3	-5.67	1.33	1.37
36	5	868	C	N1-C6	-5.66	1.33	1.37
36	5	420	G	C5-C4	-5.66	1.34	1.38
36	5	981	U	C2-N3	5.66	1.41	1.37
36	5	1170	A	N7-C5	-5.66	1.35	1.39
36	1	651	G	N9-C8	-5.66	1.33	1.37
36	1	2614	G	N9-C8	-5.66	1.33	1.37
36	5	2342	U	C2-N3	-5.66	1.33	1.37
36	5	2945	G	C5-C6	-5.65	1.36	1.42
36	5	2399	A	N3-C4	-5.65	1.31	1.34
36	1	924	G	N1-C2	-5.65	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	951	A	C6-N1	-5.65	1.31	1.35
36	5	981	U	N1-C6	5.65	1.43	1.38
36	1	2631	U	N3-C4	-5.65	1.33	1.38
36	1	2640	A	C6-N6	-5.65	1.29	1.33
36	5	437	G	C6-N1	5.65	1.43	1.39
36	5	988	U	N3-C4	-5.64	1.33	1.38
36	1	2649	A	C5-C6	-5.64	1.35	1.41
36	5	2233	A	N7-C5	-5.64	1.35	1.39
36	5	2942	C	N1-C6	-5.64	1.33	1.37
36	1	2706	G	N7-C5	-5.64	1.35	1.39
36	5	1304	A	N3-C4	5.63	1.38	1.34
36	5	2887	A	N9-C8	-5.63	1.33	1.37
36	5	2625	C	N1-C6	-5.63	1.33	1.37
36	1	2719	U	C2-O2	-5.63	1.17	1.22
36	5	2280	A	N9-C4	-5.63	1.34	1.37
36	1	937	G	N9-C8	-5.62	1.33	1.37
36	1	2376	G	C6-O6	-5.62	1.19	1.24
36	1	1313	G	N7-C5	-5.62	1.35	1.39
36	5	3214	U	N3-C4	-5.62	1.33	1.38
36	5	706	A	N9-C4	-5.61	1.34	1.37
38	4	111	A	N7-C5	-5.61	1.35	1.39
37	7	73	C	N3-C4	5.61	1.37	1.33
36	5	2164	A	N7-C5	-5.60	1.35	1.39
36	1	1429	G	N9-C8	-5.60	1.33	1.37
38	8	79	A	C5-C4	5.60	1.42	1.38
36	5	1456	A	N9-C4	-5.59	1.34	1.37
36	1	1116	G	N1-C2	-5.59	1.33	1.37
36	1	2276	G	N7-C5	-5.59	1.35	1.39
36	5	3136	G	N1-C2	-5.59	1.33	1.37
36	5	2147	A	N7-C5	-5.59	1.35	1.39
36	1	2920	U	C4-O4	-5.59	1.19	1.23
36	5	981	U	N3-C4	5.59	1.43	1.38
36	5	1171	G	N7-C5	-5.58	1.35	1.39
36	5	2201	G	C5-C4	-5.58	1.34	1.38
36	5	3207	U	C2-N3	5.58	1.41	1.37
36	5	2639	G	N7-C5	-5.58	1.35	1.39
36	1	30	G	C6-N1	-5.58	1.35	1.39
36	5	645	A	N7-C5	-5.58	1.35	1.39
36	5	28	C	N1-C6	-5.57	1.33	1.37
36	5	431	U	C2-N3	-5.57	1.33	1.37
36	5	2758	A	N9-C4	5.57	1.41	1.37
36	1	3008	A	N9-C4	-5.57	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	l3	229	VAL	CB-CG2	-5.57	1.41	1.52
36	1	1430	U	N1-C6	-5.56	1.32	1.38
36	1	1436	U	N3-C4	-5.56	1.33	1.38
36	5	2425	G	N9-C4	-5.56	1.33	1.38
1	6	1746	A	N7-C5	-5.56	1.35	1.39
1	6	1023	A	C5-C4	-5.55	1.34	1.38
36	5	2851	A	C6-N1	-5.55	1.31	1.35
1	2	972	G	C6-N1	-5.55	1.35	1.39
38	4	79	A	O3'-P	5.55	1.67	1.61
36	5	1155	C	C4-N4	-5.55	1.28	1.33
36	1	2805	G	C8-N7	-5.55	1.27	1.30
36	5	2636	A	N3-C4	-5.54	1.31	1.34
36	1	2945	G	C5-C4	-5.54	1.34	1.38
36	5	947	G	N3-C4	-5.54	1.31	1.35
36	1	2878	G	C6-O6	-5.54	1.19	1.24
36	1	1806	A	N3-C4	-5.54	1.31	1.34
36	5	2953	U	C4-O4	5.54	1.28	1.23
36	1	2350	C	N1-C6	-5.54	1.33	1.37
52	m6	40	GLU	CG-CD	5.54	1.60	1.51
36	1	2762	A	N3-C4	-5.53	1.31	1.34
36	5	29	C	N1-C6	-5.53	1.33	1.37
36	1	878	G	C2-N3	-5.53	1.28	1.32
36	1	1416	C	N3-C4	-5.53	1.30	1.33
36	5	348	A	N9-C4	-5.53	1.34	1.37
36	1	652	G	N1-C2	-5.52	1.33	1.37
36	5	3197	G	N9-C8	5.52	1.41	1.37
36	5	21	G	C5-C6	-5.52	1.36	1.42
36	1	2714	G	N9-C4	-5.52	1.33	1.38
36	5	2389	C	N1-C6	-5.51	1.33	1.37
36	5	1174	G	N9-C8	-5.50	1.33	1.37
36	5	2637	A	N9-C4	-5.50	1.34	1.37
36	1	1155	C	N3-C4	-5.50	1.30	1.33
36	1	2980	U	C2-O2	-5.50	1.17	1.22
36	1	287	G	N9-C8	-5.50	1.34	1.37
36	1	1107	C	N1-C6	-5.50	1.33	1.37
1	6	126	A	N9-C4	-5.49	1.34	1.37
36	5	953	G	N3-C4	-5.49	1.31	1.35
36	5	1304	A	N7-C5	-5.49	1.35	1.39
36	1	2919	A	C6-N1	-5.49	1.31	1.35
69	O3	31	LYS	CD-CE	5.49	1.65	1.51
36	1	504	A	C6-N1	-5.49	1.31	1.35
36	1	3319	U	N1-C2	5.49	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N1-C2	5.49	1.42	1.37
36	1	508	U	N1-C2	-5.49	1.33	1.38
37	7	88	G	N7-C5	-5.49	1.35	1.39
36	1	402	A	C5-C4	-5.48	1.34	1.38
36	1	864	G	N3-C4	-5.48	1.31	1.35
36	1	910	G	N7-C5	-5.48	1.35	1.39
36	5	2411	U	C2-N3	-5.48	1.33	1.37
36	1	1116	G	N3-C4	-5.48	1.31	1.35
36	5	1429	G	N7-C5	-5.48	1.35	1.39
52	M6	40	GLU	CG-CD	5.48	1.60	1.51
36	5	2361	A	N3-C4	5.48	1.38	1.34
36	1	1192	C	N1-C6	5.47	1.40	1.37
36	5	3180	A	C5-C4	-5.47	1.34	1.38
36	1	404	G	N9-C8	-5.47	1.34	1.37
36	1	1178	G	C5-C4	-5.47	1.34	1.38
36	5	1164	G	N9-C8	-5.47	1.34	1.37
36	1	1392	G	C5-C4	-5.47	1.34	1.38
36	5	1403	C	N3-C4	-5.47	1.30	1.33
36	5	2609	A	C6-N1	-5.47	1.31	1.35
36	1	1404	G	N9-C8	-5.46	1.34	1.37
40	l3	66	LYS	CD-CE	5.46	1.65	1.51
36	1	900	G	N9-C8	-5.46	1.34	1.37
36	1	2943	G	N1-C2	-5.46	1.33	1.37
1	6	65	A	N9-C4	-5.46	1.34	1.37
36	5	586	C	N1-C6	-5.45	1.33	1.37
41	l4	94	CYS	CB-SG	-5.45	1.73	1.81
36	5	2891	U	C2-N3	-5.45	1.33	1.37
36	1	2820	A	N1-C2	-5.44	1.29	1.34
36	1	2130	G	C6-N1	-5.44	1.35	1.39
36	5	1843	C	C4-C5	-5.44	1.38	1.43
36	1	2950	G	N1-C2	-5.44	1.33	1.37
8	s6	83	CYS	CB-SG	-5.44	1.73	1.81
36	5	1148	G	N9-C8	-5.44	1.34	1.37
36	1	406	G	N7-C5	5.43	1.42	1.39
36	5	966	U	N3-C4	-5.43	1.33	1.38
36	5	2411	U	C2-O2	-5.43	1.17	1.22
36	5	794	U	C2-N3	-5.43	1.33	1.37
36	1	2382	G	N1-C2	-5.43	1.33	1.37
36	5	643	U	N3-C4	-5.43	1.33	1.38
36	1	1149	G	C2-N3	-5.42	1.28	1.32
36	5	307	A	N3-C4	-5.42	1.31	1.34
36	5	2636	A	C2-N3	-5.42	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2326	A	N9-C4	-5.42	1.34	1.37
52	M6	100	GLU	CD-OE2	5.42	1.31	1.25
36	5	16	A	N9-C4	-5.42	1.34	1.37
36	5	1613	A	N9-C8	-5.42	1.33	1.37
36	5	1373	A	N7-C5	-5.41	1.36	1.39
36	1	1133	A	N9-C4	-5.41	1.34	1.37
36	1	1137	C	N1-C6	-5.41	1.33	1.37
52	m6	78	ARG	CZ-NH1	5.41	1.40	1.33
36	1	1532	C	N1-C6	-5.41	1.33	1.37
36	1	2896	A	N9-C4	-5.40	1.34	1.37
36	5	1186	G	C6-N1	-5.40	1.35	1.39
36	5	691	A	C6-N1	-5.40	1.31	1.35
36	1	1446	A	N9-C8	-5.40	1.33	1.37
53	M7	129	THR	CB-CG2	-5.39	1.34	1.52
36	5	1429	G	N9-C4	-5.39	1.33	1.38
36	5	1207	G	N1-C2	-5.39	1.33	1.37
36	5	2145	A	C6-N1	-5.39	1.31	1.35
36	5	3330	A	N9-C8	-5.39	1.33	1.37
36	5	406	G	N1-C2	-5.39	1.33	1.37
36	1	2647	A	C5-C4	-5.38	1.34	1.38
36	5	2174	G	N7-C5	-5.38	1.36	1.39
36	5	3106	A	N9-C8	-5.38	1.33	1.37
36	1	1428	A	C5-C6	-5.38	1.36	1.41
36	1	2991	A	N3-C4	-5.38	1.31	1.34
36	1	3245	A	N9-C4	-5.38	1.34	1.37
36	5	3209	A	C6-N1	5.38	1.39	1.35
36	1	2761	G	N9-C8	-5.38	1.34	1.37
36	1	16	A	N3-C4	-5.38	1.31	1.34
49	m3	23	LYS	CD-CE	5.38	1.64	1.51
36	1	2761	G	N3-C4	-5.38	1.31	1.35
36	5	2727	A	C5-C4	-5.37	1.34	1.38
44	17	158	LYS	CG-CD	5.37	1.70	1.52
36	1	1476	G	C5-C4	-5.37	1.34	1.38
36	1	952	A	N3-C4	-5.37	1.31	1.34
36	5	2340	U	C4-O4	-5.37	1.19	1.23
36	1	716	A	C5-C6	-5.37	1.36	1.41
36	1	2762	A	N9-C4	-5.37	1.34	1.37
37	3	83	U	C4-O4	-5.36	1.19	1.23
36	5	53	G	N9-C8	-5.36	1.34	1.37
36	5	1902	G	N7-C5	-5.36	1.36	1.39
36	5	2818	U	C5-C6	-5.36	1.29	1.34
36	1	699	A	N9-C4	-5.36	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2189	U	C4-C5	-5.36	1.38	1.43
36	1	626	U	C2-N3	-5.36	1.33	1.37
36	5	3366	G	N7-C5	-5.36	1.36	1.39
36	5	2299	A	C5-C4	-5.36	1.35	1.38
36	1	2397	A	N9-C4	-5.36	1.34	1.37
36	5	2818	U	C2-N3	-5.36	1.34	1.37
36	5	2960	C	N3-C4	-5.36	1.30	1.33
38	4	53	A	N9-C4	5.35	1.41	1.37
36	5	2375	G	C5-C4	-5.35	1.34	1.38
36	5	2807	U	C4-O4	-5.35	1.19	1.23
37	7	77	G	N9-C8	-5.35	1.34	1.37
1	6	173	A	N9-C4	-5.35	1.34	1.37
1	6	428	A	N3-C4	-5.35	1.31	1.34
36	5	1061	A	N9-C4	-5.35	1.34	1.37
1	6	1022	C	N1-C6	-5.35	1.33	1.37
36	5	1053	A	C6-N6	-5.35	1.29	1.33
36	5	1348	U	N1-C2	5.35	1.43	1.38
36	5	3174	A	N9-C8	5.35	1.42	1.37
36	5	1152	G	C5-C6	-5.35	1.37	1.42
36	5	2411	U	N1-C2	-5.34	1.33	1.38
36	5	2845	A	N3-C4	5.34	1.38	1.34
38	8	20	U	C4-O4	-5.34	1.19	1.23
1	6	163	G	N3-C4	-5.34	1.31	1.35
36	5	1134	G	C6-N1	-5.34	1.35	1.39
36	5	2375	G	N9-C8	-5.34	1.34	1.37
36	1	1375	G	N7-C5	-5.33	1.36	1.39
36	1	3000	A	N9-C4	-5.33	1.34	1.37
36	1	1390	A	N3-C4	-5.33	1.31	1.34
36	1	2802	A	C8-N7	5.33	1.35	1.31
36	5	1851	G	C5-C4	-5.33	1.34	1.38
36	5	3206	C	N3-C4	-5.33	1.30	1.33
36	5	1796	G	N9-C8	-5.33	1.34	1.37
36	5	2373	A	C6-N6	-5.33	1.29	1.33
36	1	92	G	C6-O6	-5.33	1.19	1.24
36	5	2271	A	C5-C4	-5.32	1.35	1.38
36	5	3140	G	C5-C6	-5.32	1.37	1.42
36	1	92	G	C6-N1	-5.32	1.35	1.39
37	3	97	A	N3-C4	-5.32	1.31	1.34
36	5	2976	A	N9-C8	-5.32	1.33	1.37
36	5	1187	C	N1-C6	-5.32	1.33	1.37
36	5	1335	C	C4-N4	-5.32	1.29	1.33
36	1	1047	A	N3-C4	-5.32	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	345	G	N7-C5	-5.31	1.36	1.39
36	5	980	A	C5-C4	5.31	1.42	1.38
36	1	1858	A	N7-C5	-5.31	1.36	1.39
36	1	1395	G	C5-C4	-5.31	1.34	1.38
36	1	949	C	N1-C6	-5.30	1.33	1.37
1	6	1800	A	N9-C4	5.30	1.41	1.37
36	5	2832	C	N3-C4	-5.30	1.30	1.33
36	5	3245	A	N7-C5	-5.30	1.36	1.39
36	1	960	U	N1-C6	5.30	1.42	1.38
36	5	795	G	C5-C4	-5.30	1.34	1.38
36	5	2372	A	N3-C4	-5.30	1.31	1.34
36	5	3139	A	N9-C4	-5.30	1.34	1.37
36	1	1336	U	C2-N3	-5.30	1.34	1.37
36	5	2971	A	C6-N1	5.30	1.39	1.35
36	1	2867	C	C2-N3	-5.30	1.31	1.35
36	1	2816	G	C5-C4	-5.29	1.34	1.38
36	5	1582	C	N1-C6	5.29	1.40	1.37
36	1	2733	A	C5-C6	-5.29	1.36	1.41
36	5	2950	G	N1-C2	-5.29	1.33	1.37
36	5	942	U	C5-C6	-5.29	1.29	1.34
36	1	3207	U	C4-C5	5.29	1.48	1.43
36	5	3060	C	C4-C5	-5.29	1.38	1.43
36	1	785	G	N1-C2	-5.29	1.33	1.37
36	1	3052	G	N7-C5	-5.29	1.36	1.39
36	5	916	G	C2-N3	-5.29	1.28	1.32
36	5	2138	A	N9-C8	-5.29	1.33	1.37
36	5	2396	G	C6-N1	-5.29	1.35	1.39
36	5	2824	G	N7-C5	-5.29	1.36	1.39
36	5	2147	A	C6-N6	-5.28	1.29	1.33
36	5	2823	G	N7-C5	-5.28	1.36	1.39
36	1	673	U	C4-O4	-5.28	1.19	1.23
52	M6	195	ALA	CA-CB	-5.28	1.41	1.52
36	1	895	A	N7-C5	-5.28	1.36	1.39
36	1	2147	A	C5-C4	-5.28	1.35	1.38
36	5	1844	C	N3-C4	-5.28	1.30	1.33
36	5	2737	C	N1-C6	-5.28	1.33	1.37
36	1	1380	G	C6-N1	-5.28	1.35	1.39
36	1	2811	A	C6-N1	-5.28	1.31	1.35
36	1	421	G	C2-N3	-5.27	1.28	1.32
36	1	947	G	N1-C2	-5.27	1.33	1.37
36	1	2867	C	N1-C6	-5.27	1.33	1.37
1	6	1765	A	N9-C4	-5.27	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1051	U	C4-O4	-5.27	1.19	1.23
37	7	80	G	C6-N1	-5.27	1.35	1.39
44	17	234	GLU	CD-OE2	5.27	1.31	1.25
37	7	57	G	N7-C5	-5.27	1.36	1.39
1	6	1773	C	C2-N3	5.26	1.40	1.35
36	1	895	A	N9-C8	5.26	1.42	1.37
36	1	2628	A	N9-C8	-5.26	1.33	1.37
36	5	1476	G	N9-C4	-5.26	1.33	1.38
36	1	2996	U	N3-C4	5.25	1.43	1.38
36	5	3138	U	N1-C2	-5.25	1.33	1.38
36	1	1133	A	N9-C8	-5.25	1.33	1.37
36	5	2816	G	C5-C4	-5.25	1.34	1.38
37	7	96	U	N3-C4	-5.25	1.33	1.38
36	1	65	A	N9-C4	5.25	1.41	1.37
36	1	1364	C	N1-C6	-5.25	1.33	1.37
36	5	420	G	C6-N1	-5.25	1.35	1.39
36	5	2362	C	C2-N3	-5.25	1.31	1.35
1	2	320	U	C2-N3	5.25	1.41	1.37
36	5	1310	G	N3-C4	-5.25	1.31	1.35
36	5	2894	C	N1-C6	-5.25	1.34	1.37
36	5	3104	U	C4-C5	-5.25	1.38	1.43
59	n3	38	ALA	CA-CB	-5.25	1.41	1.52
36	5	2889	C	N1-C6	-5.25	1.34	1.37
1	6	1137	A	C5-C4	-5.24	1.35	1.38
36	5	425	G	C6-O6	-5.24	1.19	1.24
36	5	1302	A	N3-C4	-5.24	1.31	1.34
38	4	10	A	C6-N6	-5.24	1.29	1.33
36	5	1851	G	C8-N7	-5.24	1.27	1.30
36	5	2897	A	C5-C4	-5.24	1.35	1.38
36	1	2514	U	N1-C2	-5.24	1.33	1.38
36	1	343	U	N3-C4	-5.24	1.33	1.38
44	L7	234	GLU	CD-OE2	5.24	1.31	1.25
36	5	1443	G	C2-N3	-5.23	1.28	1.32
36	1	92	G	N7-C5	-5.23	1.36	1.39
36	5	934	G	C5-C6	-5.23	1.37	1.42
38	8	17	A	C5-C6	-5.23	1.36	1.41
36	1	629	U	C2-N3	-5.23	1.34	1.37
1	6	1653	C	N1-C2	-5.22	1.34	1.40
68	o2	29	ALA	CA-CB	-5.22	1.41	1.52
36	1	2814	G	N7-C5	-5.22	1.36	1.39
36	1	99	A	C5-C4	-5.22	1.35	1.38
36	5	1331	U	N1-C2	-5.22	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	799	G	C8-N7	-5.21	1.27	1.30
36	1	1308	A	C6-N1	-5.21	1.31	1.35
36	1	776	U	N3-C4	-5.21	1.33	1.38
36	1	43	A	N9-C4	-5.21	1.34	1.37
36	1	1002	A	N9-C4	-5.21	1.34	1.37
36	1	2732	G	C6-N1	-5.21	1.35	1.39
36	5	3223	A	N3-C4	-5.21	1.31	1.34
36	1	968	G	C6-N1	-5.21	1.35	1.39
36	1	1129	A	C5-C6	-5.21	1.36	1.41
36	1	1556	C	N1-C2	5.20	1.45	1.40
1	2	1560	U	N3-C4	-5.20	1.33	1.38
36	5	1796	G	N7-C5	-5.20	1.36	1.39
36	1	1336	U	N3-C4	-5.20	1.33	1.38
36	5	1144	U	N3-C4	-5.20	1.33	1.38
36	5	2908	G	N9-C8	-5.20	1.34	1.37
36	5	2395	G	C5-C4	-5.20	1.34	1.38
36	1	695	C	C2-N3	-5.19	1.31	1.35
36	5	1887	A	N7-C5	-5.19	1.36	1.39
36	1	2617	U	C4-C5	5.19	1.48	1.43
36	5	1187	C	N3-C4	-5.19	1.30	1.33
36	5	2949	U	C4-O4	-5.19	1.19	1.23
36	5	3052	G	N1-C2	-5.19	1.33	1.37
36	1	663	C	N1-C6	-5.19	1.34	1.37
36	1	2933	A	C5-C6	-5.19	1.36	1.41
36	1	196	G	C5-C6	-5.19	1.37	1.42
36	5	2893	C	C4-C5	-5.19	1.38	1.43
36	5	947	G	C5-C4	-5.19	1.34	1.38
36	5	969	C	N1-C6	-5.19	1.34	1.37
36	1	2207	A	N9-C4	5.18	1.41	1.37
36	1	2247	G	N7-C5	-5.18	1.36	1.39
36	1	1048	A	C5-C4	-5.18	1.35	1.38
36	5	2704	A	C5-C6	-5.18	1.36	1.41
36	5	1134	G	N1-C2	-5.18	1.33	1.37
36	5	2185	G	N9-C8	-5.18	1.34	1.37
36	5	3132	C	C4-C5	-5.18	1.38	1.43
1	6	1748	G	N9-C8	-5.18	1.34	1.37
36	1	1308	A	P-OP2	-5.18	1.40	1.49
36	1	2978	U	N1-C2	5.17	1.43	1.38
36	1	709	A	N9-C8	-5.17	1.33	1.37
44	17	158	LYS	CB-CG	5.17	1.66	1.52
1	6	1734	U	N1-C2	-5.17	1.33	1.38
1	2	992	A	N9-C4	-5.17	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	429	U	C2-N3	-5.16	1.34	1.37
36	5	639	G	N3-C4	-5.16	1.31	1.35
36	1	367	A	C6-N1	-5.16	1.31	1.35
36	5	909	G	C5-C4	-5.16	1.34	1.38
36	5	1851	G	N7-C5	-5.16	1.36	1.39
36	1	2281	A	C6-N1	-5.16	1.31	1.35
36	5	2310	U	C2-N3	-5.16	1.34	1.37
36	1	3273	A	N7-C5	-5.15	1.36	1.39
36	1	289	A	N3-C4	-5.15	1.31	1.34
36	5	2856	G	N7-C5	-5.15	1.36	1.39
36	5	3153	U	N1-C2	5.15	1.43	1.38
36	1	668	G	C6-N1	-5.15	1.35	1.39
36	1	1133	A	N7-C5	-5.15	1.36	1.39
36	1	2938	G	N9-C8	-5.15	1.34	1.37
36	5	523	A	N9-C4	-5.15	1.34	1.37
36	1	189	G	N7-C5	-5.15	1.36	1.39
36	1	504	A	N9-C4	-5.15	1.34	1.37
36	5	2949	U	C4-C5	-5.15	1.39	1.43
1	6	366	A	N3-C4	-5.15	1.31	1.34
36	1	635	G	C6-O6	-5.14	1.19	1.24
36	5	872	U	C4-C5	-5.14	1.39	1.43
36	5	1838	G	N3-C4	-5.14	1.31	1.35
36	5	1433	A	C5-C6	-5.14	1.36	1.41
36	5	2635	A	N3-C4	-5.14	1.31	1.34
36	5	1373	A	C5-C4	-5.14	1.35	1.38
36	1	974	G	C6-N1	-5.13	1.35	1.39
36	5	611	A	C5-C4	-5.13	1.35	1.38
36	5	2869	U	C2-N3	-5.13	1.34	1.37
36	1	718	G	N9-C8	5.13	1.41	1.37
36	5	45	A	N9-C4	-5.13	1.34	1.37
36	5	417	A	N3-C4	-5.13	1.31	1.34
36	5	2199	G	N7-C5	-5.13	1.36	1.39
36	5	407	A	N3-C4	5.13	1.38	1.34
36	1	2280	A	N3-C4	-5.13	1.31	1.34
36	5	800	G	N9-C8	-5.13	1.34	1.37
36	5	959	C	N1-C6	-5.13	1.34	1.37
36	1	2169	G	C5-C6	5.12	1.47	1.42
36	5	1514	G	N7-C5	-5.12	1.36	1.39
36	1	635	G	C6-N1	-5.12	1.35	1.39
36	1	659	G	N7-C5	-5.12	1.36	1.39
36	1	2180	G	N7-C5	-5.12	1.36	1.39
36	5	2336	U	C2-N3	-5.12	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	993	A	N3-C4	-5.12	1.31	1.34
36	5	2705	A	C5-C6	-5.12	1.36	1.41
36	1	1170	A	N7-C5	-5.12	1.36	1.39
36	1	2323	G	N1-C2	-5.12	1.33	1.37
36	1	645	A	N9-C8	-5.12	1.33	1.37
36	1	874	U	C2-O2	-5.12	1.17	1.22
36	1	2418	G	O3'-P	5.12	1.67	1.61
36	5	1462	A	C5-C6	-5.12	1.36	1.41
36	5	2609	A	N9-C8	-5.11	1.33	1.37
36	5	1117	G	C8-N7	-5.11	1.27	1.30
36	5	818	C	N1-C2	-5.11	1.35	1.40
36	1	627	U	N1-C2	-5.11	1.33	1.38
36	1	1164	G	N9-C8	-5.11	1.34	1.37
36	1	2726	C	N3-C4	-5.11	1.30	1.33
46	l9	11	GLU	CG-CD	5.11	1.59	1.51
51	m5	202	TYR	CD1-CE1	-5.11	1.31	1.39
36	1	657	A	N3-C4	-5.11	1.31	1.34
36	1	2910	A	N9-C4	-5.11	1.34	1.37
36	5	339	C	N3-C4	-5.11	1.30	1.33
36	1	952	A	N7-C5	-5.10	1.36	1.39
36	5	1113	G	N3-C4	-5.10	1.31	1.35
37	3	80	G	C6-N1	-5.10	1.35	1.39
36	1	2920	U	C2-O2	-5.10	1.17	1.22
38	4	46	G	N9-C8	-5.10	1.34	1.37
36	5	644	G	N3-C4	-5.10	1.31	1.35
37	7	92	A	C5-C6	-5.10	1.36	1.41
36	1	833	G	N1-C2	-5.10	1.33	1.37
36	5	2364	G	N3-C4	-5.10	1.31	1.35
36	5	642	U	N1-C2	-5.10	1.33	1.38
36	5	1438	U	N3-C4	-5.10	1.33	1.38
36	5	1586	G	C8-N7	-5.09	1.27	1.30
36	1	2994	A	C6-N1	-5.09	1.31	1.35
36	1	688	G	N9-C8	-5.09	1.34	1.37
36	1	1308	A	N7-C5	-5.09	1.36	1.39
36	1	2384	A	C6-N6	-5.09	1.29	1.33
36	5	367	A	N9-C4	-5.09	1.34	1.37
36	5	1332	A	N9-C8	-5.09	1.33	1.37
36	5	2276	G	N9-C8	-5.09	1.34	1.37
36	5	2985	C	C5-C6	-5.09	1.30	1.34
36	5	411	U	C2-O2	-5.09	1.17	1.22
36	5	1504	A	C6-N1	-5.09	1.31	1.35
36	5	1912	U	N1-C2	-5.09	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	579	A	N3-C4	5.09	1.38	1.34
36	5	3102	G	C6-N1	-5.09	1.35	1.39
36	1	808	A	N3-C4	-5.08	1.31	1.34
36	1	2945	G	N7-C5	-5.08	1.36	1.39
36	5	876	A	C6-N6	-5.08	1.29	1.33
36	5	1176	C	N1-C6	-5.08	1.34	1.37
36	1	1509	A	N9-C8	-5.08	1.33	1.37
36	1	2121	G	N1-C2	-5.08	1.33	1.37
36	1	343	U	N1-C6	-5.07	1.33	1.38
36	5	440	A	N9-C4	5.07	1.40	1.37
36	5	1847	A	C5-C6	-5.07	1.36	1.41
36	5	1432	C	C2-O2	-5.07	1.19	1.24
36	5	2825	C	N1-C6	-5.07	1.34	1.37
36	5	2897	A	N9-C8	-5.07	1.33	1.37
36	5	1301	A	C5-C6	-5.07	1.36	1.41
36	1	1915	A	C6-N6	-5.07	1.29	1.33
36	1	874	U	C4'-C3'	-5.06	1.47	1.52
1	6	623	A	N9-C4	-5.06	1.34	1.37
36	5	1145	G	N7-C5	-5.06	1.36	1.39
36	5	2968	G	N9-C8	-5.06	1.34	1.37
36	1	636	C	C4-N4	-5.06	1.29	1.33
36	5	2335	G	C6-N1	-5.06	1.36	1.39
36	5	3138	U	C4-C5	-5.06	1.39	1.43
36	1	2649	A	N9-C4	5.06	1.40	1.37
36	5	2703	A	N9-C8	-5.06	1.33	1.37
42	15	37	VAL	CB-CG2	-5.06	1.42	1.52
36	1	2413	A	C6-N1	-5.05	1.32	1.35
36	5	341	G	C5-C6	-5.05	1.37	1.42
36	1	406	G	N1-C2	-5.05	1.33	1.37
36	1	1374	G	N1-C2	-5.05	1.33	1.37
36	5	3211	C	N1-C6	-5.05	1.34	1.37
47	m0	119	TRP	CB-CG	-5.05	1.41	1.50
36	1	2116	G	N9-C8	-5.04	1.34	1.37
36	1	3377	G	C5-C4	-5.04	1.34	1.38
36	1	2867	C	N3-C4	-5.04	1.30	1.33
36	5	2550	U	N3-C4	-5.04	1.33	1.38
36	1	951	A	N9-C8	-5.04	1.33	1.37
36	5	2858	U	C4-O4	-5.04	1.19	1.23
36	5	2936	A	C5-C4	-5.04	1.35	1.38
36	5	2943	G	C6-N1	-5.04	1.36	1.39
36	5	2987	A	C5-C4	-5.04	1.35	1.38
36	1	2614	G	C5-C4	-5.04	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	616	G	C2-N3	-5.04	1.28	1.32
36	5	3337	G	C6-N1	-5.04	1.36	1.39
36	1	305	U	C2-N3	-5.03	1.34	1.37
36	1	2946	A	N9-C8	-5.03	1.33	1.37
36	1	677	A	C5-C6	-5.03	1.36	1.41
36	1	272	G	N7-C5	-5.03	1.36	1.39
36	1	677	A	C6-N6	-5.03	1.29	1.33
36	1	985	U	N1-C2	-5.03	1.34	1.38
36	1	1145	G	C5-C6	-5.03	1.37	1.42
36	1	2183	A	N3-C4	-5.03	1.31	1.34
36	1	2943	G	C6-N1	-5.03	1.36	1.39
37	7	95	A	N7-C5	-5.03	1.36	1.39
36	1	608	A	N9-C4	5.03	1.40	1.37
36	5	1834	U	C4-O4	5.03	1.27	1.23
36	5	2372	A	C6-N1	-5.03	1.32	1.35
37	7	95	A	C6-N1	-5.03	1.32	1.35
36	1	92	G	C5-C6	-5.03	1.37	1.42
36	1	408	A	N7-C5	-5.03	1.36	1.39
36	1	1120	A	C6-N6	-5.03	1.29	1.33
36	1	2143	A	N3-C4	-5.03	1.31	1.34
36	1	1144	U	C2-N3	-5.02	1.34	1.37
36	5	2936	A	C4'-C3'	-5.02	1.47	1.52
36	5	3309	G	N7-C5	-5.02	1.36	1.39
36	1	1062	A	N7-C5	-5.02	1.36	1.39
64	n8	5	PHE	CD2-CE2	-5.02	1.29	1.39
36	1	817	A	N9-C4	5.02	1.40	1.37
36	5	3050	U	N3-C4	-5.02	1.33	1.38
37	7	80	G	N1-C2	-5.02	1.33	1.37
36	1	64	G	N3-C4	-5.01	1.31	1.35
36	5	2270	A	N9-C4	-5.01	1.34	1.37
36	5	2945	G	C5-C4	-5.01	1.34	1.38
36	5	338	A	N7-C5	-5.01	1.36	1.39
36	5	421	G	C2-N3	-5.01	1.28	1.32
36	1	321	C	N1-C6	-5.01	1.34	1.37
36	1	613	G	C5-C6	-5.01	1.37	1.42
36	1	820	A	N9-C4	-5.01	1.34	1.37
36	1	1436	U	C4-C5	-5.01	1.39	1.43
36	1	584	G	C5-C4	-5.01	1.34	1.38
36	1	635	G	C5-C6	-5.01	1.37	1.42
36	1	2365	C	N3-C4	-5.01	1.30	1.33
36	1	2920	U	N3-C4	-5.01	1.33	1.38
1	6	794	U	N1-C2	5.01	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	1750	A	N7-C5	-5.01	1.36	1.39
38	8	57	C	N3-C4	-5.01	1.30	1.33
36	5	2941	A	N7-C5	-5.00	1.36	1.39
36	1	584	G	N9-C8	-5.00	1.34	1.37
36	5	790	U	C2-O2	-5.00	1.17	1.22

All (7522) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	27.54	142.37	128.60
36	5	1152	G	N3-C4-N9	-26.81	109.91	126.00
36	1	2945	G	O5'-P-OP2	-22.04	84.25	110.70
36	5	1152	G	C2-N3-C4	-21.23	101.28	111.90
36	5	922	U	N3-C2-O2	-21.19	107.37	122.20
36	5	2403	G	O5'-P-OP2	-18.28	88.77	110.70
36	5	2923	U	O5'-P-OP1	-17.79	89.35	110.70
36	1	339	C	O5'-P-OP1	-17.48	89.73	110.70
36	5	1152	G	N3-C2-N2	-17.14	107.90	119.90
36	5	806	A	O5'-P-OP1	-16.93	90.38	110.70
36	5	877	C	N3-C4-C5	16.37	128.45	121.90
1	6	1657	U	O5'-P-OP2	-16.09	91.22	105.70
36	1	1495	U	C5-C6-N1	-16.05	114.67	122.70
36	1	2617	U	N1-C2-N3	15.96	124.47	114.90
36	5	2334	U	O5'-P-OP2	-15.83	91.45	105.70
36	5	2376	G	O5'-P-OP2	-15.61	91.65	105.70
36	1	2617	U	C5-C6-N1	-15.50	114.95	122.70
36	5	776	U	C5-C6-N1	-15.40	115.00	122.70
36	5	2385	G	O5'-P-OP1	-15.36	91.87	105.70
36	5	1152	G	C8-N9-C1'	15.12	146.65	127.00
36	5	2872	A	C2-N3-C4	-15.10	103.05	110.60
1	6	1773	C	N3-C4-C5	-15.01	115.90	121.90
36	1	1450	G	O5'-P-OP1	-14.80	92.38	105.70
36	5	2872	A	N3-C4-N9	-14.66	115.67	127.40
36	5	641	C	N1-C2-O2	-14.65	110.11	118.90
36	1	2281	A	O5'-P-OP2	-14.65	92.52	105.70
36	5	922	U	N3-C4-O4	-14.53	109.23	119.40
36	1	895	A	C5-N7-C8	-14.44	96.68	103.90
36	5	3245	A	C5-N7-C8	-14.38	96.71	103.90
36	5	1313	G	O5'-P-OP2	-14.38	92.76	105.70
36	1	1846	C	N1-C2-O2	-14.17	110.40	118.90
36	5	2872	A	N3-C4-C5	13.93	136.55	126.80
36	5	3245	A	C2-N3-C4	-13.82	103.69	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	C4-N9-C1'	-13.76	108.61	126.50
36	1	2923	U	O5'-P-OP1	-13.66	93.41	105.70
36	1	2621	G	N3-C2-N2	-13.56	110.41	119.90
36	1	2139	A	N1-C6-N6	-13.51	110.50	118.60
36	5	922	U	C5-C6-N1	-13.44	115.98	122.70
36	1	406	G	O4'-C1'-N9	13.32	118.85	108.20
36	5	922	U	C2-N3-C4	-13.26	119.04	127.00
36	1	3306	U	N3-C4-O4	-13.24	110.13	119.40
36	1	439	C	N1-C2-O2	13.19	126.81	118.90
36	5	398	A	O5'-P-OP2	-13.16	93.85	105.70
36	1	1196	C	C6-N1-C2	12.98	125.49	120.30
36	5	2872	A	C5-N7-C8	-12.97	97.42	103.90
36	1	2945	G	O5'-P-OP1	12.96	126.25	110.70
37	7	92	A	N1-C6-N6	12.92	126.35	118.60
1	2	553	G	N1-C6-O6	12.90	127.64	119.90
36	1	2617	U	C5-C4-O4	12.89	133.63	125.90
36	5	922	U	N1-C2-O2	12.85	131.79	122.80
36	5	2871	G	O5'-P-OP2	-12.78	94.20	105.70
36	1	1117	G	O5'-P-OP1	-12.75	94.23	105.70
36	1	2621	G	N1-C6-O6	12.68	127.51	119.90
36	5	1885	U	N1-C2-O2	-12.63	113.96	122.80
1	6	163	G	N3-C4-N9	-12.59	118.44	126.00
36	1	1495	U	N1-C2-N3	12.52	122.41	114.90
36	1	2373	A	O5'-P-OP1	-12.51	94.44	105.70
36	5	960	U	N3-C4-O4	-12.50	110.65	119.40
36	1	2714	G	N3-C4-C5	12.48	134.84	128.60
36	1	1495	U	C2-N3-C4	-12.47	119.52	127.00
36	1	2617	U	C2-N3-C4	-12.43	119.54	127.00
36	1	918	C	O5'-P-OP2	-12.38	94.56	105.70
36	1	2371	G	O5'-P-OP2	-12.37	94.57	105.70
36	1	802	C	O5'-P-OP1	-12.26	94.66	105.70
36	5	805	G	C8-N9-C4	12.24	111.30	106.40
36	5	1371	G	N1-C6-O6	-12.22	112.57	119.90
36	1	1495	U	C4-C5-C6	12.20	127.02	119.70
36	1	1899	G	C8-N9-C4	-12.18	101.53	106.40
36	5	1301	A	N1-C6-N6	12.13	125.88	118.60
36	1	2996	U	C2-N1-C1'	12.11	132.23	117.70
36	5	2726	C	C6-N1-C2	-12.10	115.46	120.30
36	1	2996	U	C6-N1-C1'	-12.07	104.30	121.20
36	1	3306	U	C5-C4-O4	12.01	133.11	125.90
36	5	3245	A	C4-C5-N7	12.00	116.70	110.70
38	4	51	G	C5-C6-O6	-11.98	121.41	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	718	G	N3-C4-C5	11.98	134.59	128.60
36	1	2400	G	C5-C6-O6	-11.98	121.41	128.60
36	1	3057	U	N3-C2-O2	-11.97	113.82	122.20
36	5	1158	A	N1-C6-N6	11.96	125.78	118.60
36	1	2362	C	O5'-P-OP2	-11.91	94.98	105.70
36	1	969	C	N3-C4-C5	11.91	126.66	121.90
36	1	86	G	O5'-P-OP2	-11.90	94.99	105.70
36	1	3181	C	N3-C2-O2	-11.88	113.58	121.90
36	5	204	A	N1-C6-N6	-11.83	111.50	118.60
36	5	1047	A	N1-C6-N6	11.82	125.69	118.60
36	1	1049	C	O5'-P-OP2	-11.82	95.07	105.70
36	5	2843	U	N3-C2-O2	-11.81	113.93	122.20
36	5	1047	A	C5-C6-N6	-11.77	114.28	123.70
36	1	2142	A	C6-N1-C2	-11.71	111.58	118.60
36	1	895	A	C4-C5-N7	11.68	116.54	110.70
36	5	1152	G	C5-N7-C8	-11.67	98.46	104.30
1	2	639	U	N3-C2-O2	-11.62	114.06	122.20
36	5	2634	U	C2-N3-C4	-11.61	120.03	127.00
36	1	2363	A	N1-C6-N6	-11.60	111.64	118.60
36	5	2726	C	C5-C4-N4	11.59	128.31	120.20
36	1	3181	C	N3-C4-N4	-11.55	109.92	118.00
36	5	1419	A	O5'-P-OP2	-11.54	95.32	105.70
1	6	1654	G	O5'-P-OP2	-11.53	95.33	105.70
36	1	111	C	C6-N1-C2	11.51	124.90	120.30
1	6	542	A	O5'-P-OP1	-11.50	95.35	105.70
36	1	895	A	N7-C8-N9	11.42	119.51	113.80
1	6	163	G	C2-N3-C4	-11.42	106.19	111.90
38	4	79	A	C8-N9-C4	-11.41	101.24	105.80
36	1	2209	U	C5-C6-N1	11.39	128.40	122.70
36	1	2818	U	O5'-P-OP1	-11.33	95.50	105.70
36	5	1869	C	C6-N1-C2	11.32	124.83	120.30
36	1	3181	C	C5-C4-N4	11.31	128.12	120.20
36	1	1308	A	O5'-P-OP2	-11.31	95.52	105.70
36	1	2870	C	N3-C4-N4	-11.31	110.08	118.00
36	1	805	G	C8-N9-C4	11.29	110.92	106.40
38	4	94	C	N3-C4-C5	11.29	126.42	121.90
37	7	73	C	C6-N1-C2	-11.25	115.80	120.30
36	5	1155	C	N3-C4-C5	11.24	126.40	121.90
36	1	806	A	O5'-P-OP2	-11.23	95.59	105.70
36	1	2385	G	O5'-P-OP1	-11.19	95.63	105.70
36	1	2411	U	N3-C4-O4	-11.19	111.57	119.40
1	2	1200	G	N1-C6-O6	11.15	126.59	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2827	U	N3-C2-O2	-11.15	114.40	122.20
36	1	1414	G	C5-C6-O6	-11.14	121.92	128.60
36	5	585	A	O5'-P-OP2	-11.13	95.69	105.70
36	1	3122	A	O5'-P-OP1	-11.10	95.71	105.70
36	5	946	U	N3-C4-O4	-11.09	111.64	119.40
36	5	2403	G	O5'-P-OP1	11.08	124.00	110.70
37	7	73	C	C5-C6-N1	11.03	126.52	121.00
36	5	437	G	C8-N9-C4	-11.03	101.99	106.40
36	5	3154	C	N1-C2-O2	10.99	125.49	118.90
36	5	3245	A	N1-C6-N6	10.99	125.19	118.60
36	1	2714	G	N3-C4-N9	-10.97	119.42	126.00
36	5	1001	G	O5'-P-OP1	-10.97	95.83	105.70
36	1	895	A	C2-N3-C4	-10.97	105.12	110.60
36	1	2617	U	N3-C4-O4	-10.96	111.72	119.40
36	1	2977	G	C5-C6-N1	10.95	116.97	111.50
36	1	3207	U	C2-N1-C1'	-10.94	104.57	117.70
36	5	805	G	N9-C4-C5	-10.92	101.03	105.40
36	1	1507	G	O5'-P-OP1	-10.91	95.88	105.70
36	1	2768	U	O5'-P-OP2	-10.91	95.88	105.70
36	1	2404	A	N1-C6-N6	-10.87	112.08	118.60
36	1	2621	G	N1-C2-N2	10.85	125.97	116.20
36	1	3306	U	N3-C2-O2	-10.83	114.62	122.20
36	5	2300	G	C5-C6-N1	10.82	116.91	111.50
36	1	1400	G	O5'-P-OP2	-10.80	95.98	105.70
36	5	1047	A	C4-C5-N7	10.80	116.10	110.70
36	5	3115	C	N1-C2-O2	-10.76	112.44	118.90
36	1	939	U	N1-C2-O2	-10.75	115.27	122.80
36	1	2314	U	C5-C4-O4	-10.75	119.45	125.90
1	6	973	A	O5'-P-OP2	-10.75	96.03	105.70
36	5	1193	A	C8-N9-C4	-10.74	101.50	105.80
36	1	635	G	C5-C6-N1	10.74	116.87	111.50
36	1	2983	C	N3-C2-O2	-10.73	114.39	121.90
36	1	2400	G	N3-C2-N2	-10.72	112.39	119.90
36	1	1381	A	O5'-P-OP2	10.71	123.56	110.70
36	5	662	U	O5'-P-OP1	-10.71	96.06	105.70
36	1	2836	C	C4-C5-C6	10.69	122.75	117.40
36	5	2617	U	O5'-P-OP2	-10.69	96.08	105.70
36	1	2983	C	C4-C5-C6	10.69	122.74	117.40
36	5	715	A	N1-C6-N6	-10.66	112.20	118.60
1	6	163	G	N3-C4-C5	10.64	133.92	128.60
36	1	1414	G	N1-C6-O6	10.63	126.28	119.90
36	5	2980	U	N3-C2-O2	-10.62	114.77	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2392	C	N3-C4-C5	10.62	126.15	121.90
36	5	422	A	O5'-P-OP1	-10.61	96.15	105.70
36	5	2899	C	N3-C2-O2	-10.61	114.48	121.90
36	1	3140	G	C5-C6-O6	-10.57	122.25	128.60
36	5	3245	A	N7-C8-N9	10.57	119.08	113.80
36	5	3245	A	C6-C5-N7	-10.53	124.93	132.30
36	5	2362	C	N1-C2-O2	10.51	125.21	118.90
36	1	1114	U	N3-C4-O4	-10.51	112.05	119.40
1	6	1596	C	N3-C2-O2	-10.47	114.57	121.90
36	5	2687	G	O5'-P-OP2	-10.47	96.28	105.70
36	1	304	G	N9-C4-C5	10.46	109.58	105.40
36	5	2618	G	C5-C6-N1	10.45	116.72	111.50
36	1	651	G	N3-C4-N9	10.44	132.26	126.00
36	1	2812	C	C4-C5-C6	10.42	122.61	117.40
36	5	3188	G	N1-C6-O6	-10.40	113.66	119.90
36	5	2899	C	N1-C2-N3	10.39	126.48	119.20
36	5	2375	G	N9-C4-C5	10.38	109.55	105.40
36	1	2617	U	C4-C5-C6	10.38	125.93	119.70
36	1	716	A	N9-C4-C5	-10.37	101.65	105.80
36	1	959	C	N3-C4-C5	10.36	126.04	121.90
36	5	2362	C	N3-C2-O2	-10.35	114.65	121.90
36	5	1124	U	O5'-P-OP1	-10.34	96.40	105.70
36	5	960	U	N3-C4-C5	10.33	120.80	114.60
1	6	337	G	N3-C4-N9	10.33	132.20	126.00
36	1	1419	A	O5'-P-OP2	-10.32	96.41	105.70
36	1	2884	C	N3-C4-C5	10.31	126.02	121.90
36	5	2372	A	C8-N9-C4	-10.31	101.67	105.80
36	1	651	G	N3-C4-C5	-10.29	123.46	128.60
36	5	2550	U	C5-C4-O4	10.28	132.07	125.90
36	1	2846	U	N3-C2-O2	-10.28	115.01	122.20
36	5	2860	U	C6-N1-C2	10.25	127.15	121.00
36	1	2945	G	OP1-P-OP2	-10.23	104.25	119.60
36	5	2889	C	C2-N3-C4	-10.23	114.79	119.90
36	5	1208	U	O5'-P-OP1	-10.21	96.51	105.70
36	1	2298	U	C5-C4-O4	10.15	131.99	125.90
36	1	2819	A	O5'-P-OP2	-10.14	96.57	105.70
36	1	2719	U	N1-C2-N3	10.13	120.98	114.90
36	1	2983	C	N1-C2-N3	10.12	126.28	119.20
36	1	2983	C	C5-C4-N4	10.10	127.27	120.20
36	5	2397	A	N1-C2-N3	10.09	134.35	129.30
36	1	2875	U	N1-C2-O2	-10.09	115.74	122.80
1	6	402	C	O5'-P-OP2	-10.08	96.63	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1773	C	N3-C4-N4	10.07	125.05	118.00
36	5	2618	G	C6-N1-C2	-10.06	119.06	125.10
36	1	718	G	N3-C4-N9	-10.06	119.97	126.00
36	5	2401	A	C8-N9-C4	-10.05	101.78	105.80
36	5	644	G	C5-C6-O6	10.04	134.63	128.60
36	1	2983	C	N3-C4-N4	-10.04	110.97	118.00
36	5	2816	G	C5-C6-N1	10.04	116.52	111.50
36	5	1312	C	N3-C4-C5	-10.02	117.89	121.90
1	6	1653	C	N1-C2-O2	-10.01	112.89	118.90
36	1	1421	G	O5'-P-OP2	-10.01	96.69	105.70
36	5	417	A	N1-C6-N6	-9.98	112.61	118.60
36	5	776	U	C2-N3-C4	-9.96	121.03	127.00
36	1	92	G	C5-C6-N1	9.95	116.47	111.50
36	5	645	A	C6-N1-C2	-9.94	112.64	118.60
36	5	92	G	N1-C6-O6	-9.94	113.94	119.90
36	1	648	C	C5-C4-N4	-9.93	113.25	120.20
36	5	1879	A	N1-C6-N6	9.91	124.55	118.60
37	7	92	A	N9-C4-C5	-9.91	101.83	105.80
36	5	2364	G	C8-N9-C4	-9.91	102.44	106.40
36	1	1101	G	C5-C6-O6	9.90	134.54	128.60
36	1	1307	G	N1-C6-O6	-9.90	113.96	119.90
36	1	608	A	N1-C6-N6	9.89	124.53	118.60
36	5	922	U	N1-C2-N3	9.87	120.82	114.90
36	5	205	C	O5'-P-OP1	-9.87	96.82	105.70
38	8	79	A	C8-N9-C4	-9.86	101.86	105.80
36	5	1149	G	O5'-P-OP2	-9.86	96.83	105.70
36	1	979	U	N1-C2-N3	9.85	120.81	114.90
36	5	1462	A	N1-C6-N6	9.85	124.51	118.60
36	1	3140	G	N1-C6-O6	9.84	125.80	119.90
36	5	877	C	N3-C4-N4	-9.84	111.11	118.00
36	1	3207	U	C5-C4-O4	9.83	131.80	125.90
36	5	348	A	O5'-P-OP1	-9.83	96.86	105.70
36	5	437	G	N7-C8-N9	9.82	118.01	113.10
36	1	25	U	N1-C2-O2	-9.80	115.94	122.80
36	1	969	C	C2-N3-C4	-9.80	115.00	119.90
36	5	993	G	O5'-P-OP2	-9.79	96.89	105.70
36	1	979	U	O4'-C1'-N1	9.79	116.03	108.20
36	1	1556	C	C2-N1-C1'	9.78	129.55	118.80
36	1	2302	G	C5-C6-O6	9.77	134.46	128.60
36	1	2343	C	N3-C4-C5	9.76	125.80	121.90
36	5	941	G	N1-C6-O6	-9.76	114.05	119.90
36	1	2763	U	C5-C4-O4	-9.75	120.05	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2395	G	C5-C6-O6	-9.75	122.75	128.60
36	5	2234	G	C5-C6-O6	-9.75	122.75	128.60
36	1	3362	A	O4'-C1'-N9	9.74	116.00	108.20
36	5	2278	C	N3-C4-C5	9.74	125.80	121.90
36	5	2953	U	N3-C4-O4	9.74	126.22	119.40
36	1	957	C	N1-C2-O2	-9.73	113.06	118.90
36	5	3050	U	C5-C4-O4	9.72	131.73	125.90
36	5	2393	G	O5'-P-OP2	-9.71	96.96	105.70
36	1	954	U	O5'-P-OP2	-9.70	96.97	105.70
36	1	3057	U	N3-C4-O4	-9.70	112.61	119.40
36	5	2816	G	N1-C6-O6	-9.69	114.08	119.90
38	4	120	C	N1-C2-O2	-9.69	113.09	118.90
36	5	969	C	N3-C4-N4	-9.69	111.22	118.00
1	6	1773	C	N1-C2-O2	-9.67	113.10	118.90
36	1	2279	A	C8-N9-C4	9.67	109.67	105.80
36	1	1196	C	C5-C6-N1	-9.66	116.17	121.00
36	1	2298	U	N1-C2-N3	9.66	120.70	114.90
36	1	1419	A	O5'-P-OP1	9.66	122.29	110.70
36	1	609	G	O5'-P-OP2	-9.65	97.02	105.70
36	1	1450	G	O5'-P-OP2	9.65	122.28	110.70
36	5	2935	U	O5'-P-OP2	-9.63	97.03	105.70
36	1	787	G	O5'-P-OP2	-9.63	97.03	105.70
36	5	2619	G	C5-C6-O6	-9.63	122.82	128.60
36	1	1303	A	C8-N9-C4	9.62	109.65	105.80
36	1	2609	A	N1-C6-N6	-9.62	112.83	118.60
36	5	217	U	C5-C6-N1	-9.61	117.89	122.70
36	1	1389	G	C5-C6-O6	-9.61	122.84	128.60
36	5	1152	G	N1-C6-O6	9.60	125.66	119.90
1	2	553	G	C6-C5-N7	-9.60	124.64	130.40
36	5	2255	A	O5'-P-OP1	-9.60	97.06	105.70
36	5	2290	C	C6-N1-C2	9.59	124.14	120.30
36	1	2983	C	C2-N3-C4	-9.57	115.11	119.90
36	1	2410	U	N1-C2-O2	-9.56	116.11	122.80
36	1	2889	C	C6-N1-C2	-9.55	116.48	120.30
36	5	2726	C	N3-C2-O2	-9.55	115.22	121.90
36	5	218	G	O5'-P-OP2	-9.54	97.11	105.70
36	1	2134	G	N1-C6-O6	-9.54	114.18	119.90
37	3	88	G	N1-C6-O6	-9.53	114.18	119.90
36	5	345	G	C5-C6-O6	-9.52	122.89	128.60
36	1	6	A	O5'-P-OP2	-9.51	97.14	105.70
36	1	665	A	N1-C6-N6	-9.51	112.90	118.60
36	5	1152	G	N1-C2-N2	9.50	124.75	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2192	C	O5'-P-OP2	-9.49	97.16	105.70
36	1	1858	A	C2-N3-C4	9.48	115.34	110.60
36	5	1051	U	N3-C4-C5	9.48	120.29	114.60
1	6	1670	G	O5'-P-OP2	-9.47	97.17	105.70
36	1	3362	A	N7-C8-N9	9.47	118.54	113.80
36	5	2763	U	C5-C4-O4	-9.47	120.22	125.90
36	5	343	U	O5'-P-OP1	-9.45	97.20	105.70
36	1	229	G	N3-C2-N2	-9.44	113.29	119.90
36	1	1371	G	C8-N9-C4	9.44	110.18	106.40
36	1	2617	U	N3-C2-O2	-9.44	115.59	122.20
36	5	2873	U	C2-N3-C4	-9.43	121.34	127.00
36	5	2375	G	C4-C5-N7	-9.43	107.03	110.80
36	5	2919	A	N1-C6-N6	-9.43	112.94	118.60
36	1	2871	G	O5'-P-OP2	-9.42	97.22	105.70
36	1	3362	A	C6-C5-N7	-9.42	125.70	132.30
36	1	1160	C	O5'-P-OP1	-9.42	97.22	105.70
36	5	2375	G	N1-C6-O6	-9.42	114.25	119.90
36	1	646	A	O5'-P-OP2	-9.42	97.23	105.70
36	1	895	A	C6-C5-N7	-9.42	125.71	132.30
36	1	2936	A	O5'-P-OP1	-9.41	97.23	105.70
36	1	3207	U	C6-N1-C1'	9.39	134.34	121.20
36	5	934	G	C5-C6-O6	-9.38	122.97	128.60
36	5	1899	G	C5-C6-O6	9.38	134.23	128.60
36	5	2813	A	C8-N9-C4	-9.38	102.05	105.80
36	5	2821	C	O5'-P-OP1	9.37	121.95	110.70
36	5	2379	U	C5-C6-N1	-9.36	118.02	122.70
1	2	1082	C	C2-N1-C1'	9.36	129.09	118.80
36	5	1548	C	N1-C2-O2	-9.35	113.29	118.90
36	5	2992	U	O5'-P-OP1	9.35	121.92	110.70
36	1	817	A	C8-N9-C4	-9.35	102.06	105.80
36	1	2870	C	C6-N1-C1'	9.35	132.01	120.80
1	6	144	U	N3-C2-O2	-9.32	115.68	122.20
36	1	645	A	C6-N1-C2	-9.31	113.01	118.60
36	5	2728	G	O5'-P-OP2	-9.31	97.32	105.70
36	5	960	U	C2-N3-C4	-9.30	121.42	127.00
36	5	1130	A	C2-N3-C4	9.29	115.25	110.60
36	5	372	A	N1-C6-N6	9.29	124.17	118.60
36	5	776	U	C4-C5-C6	9.28	125.27	119.70
36	1	2406	C	C6-N1-C2	9.28	124.01	120.30
36	1	2983	C	C5-C6-N1	-9.28	116.36	121.00
36	1	2800	G	C6-N1-C2	-9.27	119.54	125.10
36	5	2249	G	C8-N9-C4	-9.27	102.69	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	M6	74	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	6	448	C	C6-N1-C2	-9.26	116.60	120.30
36	1	3055	U	C5-C4-O4	-9.25	120.35	125.90
1	2	453	U	N3-C2-O2	-9.25	115.72	122.20
36	1	1389	G	C4-C5-N7	9.25	114.50	110.80
36	5	903	U	N3-C2-O2	-9.24	115.73	122.20
36	5	1047	A	N9-C4-C5	-9.24	102.11	105.80
36	5	3098	G	O5'-P-OP2	-9.23	97.39	105.70
36	1	2279	A	N9-C4-C5	-9.23	102.11	105.80
36	5	2389	C	O5'-P-OP1	-9.23	97.39	105.70
36	1	979	U	C6-N1-C2	-9.23	115.46	121.00
36	5	2411	U	N3-C4-C5	9.22	120.13	114.60
36	1	2650	U	N1-C2-N3	9.22	120.43	114.90
36	5	608	A	N1-C6-N6	9.22	124.13	118.60
36	5	2927	C	C6-N1-C2	-9.22	116.61	120.30
36	1	2406	C	C2-N3-C4	-9.21	115.29	119.90
36	5	1879	A	C4-C5-N7	9.21	115.31	110.70
36	5	338	A	N1-C6-N6	9.21	124.12	118.60
36	5	2908	G	N3-C2-N2	-9.21	113.45	119.90
36	5	2400	G	N1-C6-O6	9.19	125.42	119.90
36	1	2147	A	O5'-P-OP1	-9.19	97.43	105.70
36	1	1445	U	C2-N3-C4	-9.18	121.49	127.00
36	1	2953	U	N1-C2-O2	-9.18	116.37	122.80
36	1	2400	G	N1-C6-O6	9.17	125.40	119.90
36	5	1149	G	N3-C4-C5	-9.16	124.02	128.60
36	1	2827	U	N3-C4-O4	-9.15	112.99	119.40
36	5	2996	U	N1-C2-O2	9.15	129.21	122.80
36	1	2286	U	O5'-P-OP2	-9.15	97.47	105.70
24	d2	93	LEU	CA-CB-CG	9.14	136.33	115.30
1	2	1773	C	N3-C4-N4	9.13	124.39	118.00
1	2	73	U	O4'-C1'-N1	9.13	115.50	108.20
36	1	1899	G	N9-C4-C5	9.13	109.05	105.40
36	5	922	U	C5-C4-O4	9.13	131.38	125.90
36	1	1374	G	N3-C2-N2	9.13	126.29	119.90
36	1	1405	U	N3-C4-C5	9.13	120.08	114.60
36	1	2411	U	N3-C4-C5	9.12	120.07	114.60
1	6	337	G	C6-C5-N7	-9.10	124.94	130.40
1	2	639	U	N1-C2-O2	9.10	129.17	122.80
36	1	3362	A	C5-N7-C8	-9.09	99.36	103.90
36	1	681	U	C5-C4-O4	-9.09	120.45	125.90
36	5	927	C	N1-C2-O2	-9.08	113.45	118.90
36	1	284	A	C8-N9-C4	-9.07	102.17	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1902	G	O5'-P-OP1	-9.07	97.54	105.70
36	1	716	A	N1-C6-N6	9.06	124.04	118.60
36	5	805	G	C5-C6-O6	-9.06	123.16	128.60
36	5	1372	C	C6-N1-C2	9.06	123.92	120.30
36	5	1200	A	C8-N9-C4	-9.06	102.18	105.80
36	1	2712	U	C5-C4-O4	9.04	131.33	125.90
36	1	1556	C	N3-C2-O2	-9.04	115.57	121.90
36	5	2392	C	C2-N3-C4	-9.03	115.38	119.90
36	5	3187	A	N1-C6-N6	-9.03	113.18	118.60
38	8	80	A	N7-C8-N9	9.03	118.32	113.80
47	M0	24	ARG	NE-CZ-NH1	9.03	124.81	120.30
36	5	2872	A	N7-C8-N9	9.03	118.31	113.80
36	1	3005	A	N1-C2-N3	-9.02	124.79	129.30
36	5	57	A	C8-N9-C4	9.02	109.41	105.80
36	1	704	U	O5'-P-OP2	-9.01	97.59	105.70
36	1	2424	A	N1-C6-N6	9.01	124.00	118.60
36	5	410	U	N3-C4-C5	-9.01	109.19	114.60
36	5	2899	C	C6-N1-C2	-9.01	116.70	120.30
1	6	928	U	O5'-P-OP1	-9.01	97.59	105.70
36	1	3209	A	N1-C6-N6	9.00	124.00	118.60
36	5	1496	C	N1-C2-O2	9.00	124.30	118.90
36	5	645	A	N1-C2-N3	8.99	133.80	129.30
36	5	2375	G	C5-C6-O6	8.99	133.99	128.60
36	5	1181	U	O5'-P-OP1	-8.98	97.61	105.70
36	1	1893	A	C2-N3-C4	-8.98	106.11	110.60
36	1	2177	G	N3-C4-N9	8.98	131.39	126.00
36	1	2726	C	C2-N3-C4	-8.98	115.41	119.90
36	1	2872	A	O5'-P-OP2	-8.98	97.62	105.70
36	1	792	G	O5'-P-OP1	-8.97	97.62	105.70
36	1	2875	U	N1-C2-N3	8.97	120.28	114.90
36	1	1904	C	C6-N1-C2	-8.97	116.71	120.30
36	1	2177	G	N3-C2-N2	8.97	126.18	119.90
1	2	1600	A	C2-N3-C4	-8.97	106.12	110.60
36	1	1114	U	N1-C2-O2	8.97	129.08	122.80
36	1	1373	A	N1-C6-N6	-8.96	113.22	118.60
36	1	639	G	C8-N9-C4	8.96	109.98	106.40
36	1	2176	U	N3-C2-O2	-8.95	115.93	122.20
36	1	2870	C	C5-C4-N4	8.95	126.46	120.20
36	5	21	G	N9-C4-C5	-8.95	101.82	105.40
36	5	1884	A	C2-N3-C4	-8.95	106.13	110.60
36	5	1879	A	C5-N7-C8	-8.94	99.43	103.90
36	5	2694	A	C8-N9-C4	-8.94	102.23	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1000	C	C6-N1-C2	8.93	123.87	120.30
36	1	2983	C	O5'-P-OP2	-8.93	97.67	105.70
36	5	3247	G	O5'-P-OP2	-8.92	97.67	105.70
36	5	1445	U	C2-N3-C4	-8.91	121.65	127.00
36	5	2870	C	C6-N1-C1'	8.90	131.49	120.80
36	1	2899	C	C2-N3-C4	-8.90	115.45	119.90
36	5	958	C	N1-C2-O2	8.90	124.24	118.90
36	5	668	G	N1-C6-O6	-8.88	114.57	119.90
36	5	822	G	O5'-P-OP1	-8.88	97.70	105.70
36	5	3186	A	N1-C6-N6	-8.88	113.27	118.60
36	1	644	G	C8-N9-C4	-8.87	102.85	106.40
36	1	1101	G	N1-C6-O6	-8.87	114.58	119.90
36	1	346	C	C2-N3-C4	-8.87	115.47	119.90
36	1	2714	G	C2-N3-C4	-8.87	107.47	111.90
36	5	2820	A	C8-N9-C4	-8.86	102.25	105.80
37	3	88	G	C5-C6-O6	8.86	133.92	128.60
36	1	2984	C	N1-C2-O2	-8.86	113.58	118.90
36	5	1117	G	C8-N9-C4	8.86	109.94	106.40
36	1	1114	U	C4-C5-C6	-8.86	114.39	119.70
36	5	3183	A	N1-C6-N6	8.86	123.91	118.60
36	5	2899	C	C5-C4-N4	8.85	126.39	120.20
1	6	609	U	C5-C4-O4	8.85	131.21	125.90
36	1	3005	A	C2-N3-C4	8.84	115.02	110.60
36	1	1517	G	O5'-P-OP2	-8.84	97.75	105.70
36	5	3178	A	O5'-P-OP1	-8.84	97.75	105.70
36	1	2815	G	C8-N9-C4	8.83	109.93	106.40
36	5	590	G	C5-C6-O6	-8.83	123.30	128.60
36	5	2872	A	C8-N9-C4	-8.83	102.27	105.80
1	6	1731	A	O5'-P-OP2	-8.83	97.76	105.70
36	5	1110	U	N1-C2-O2	8.82	128.98	122.80
36	5	2410	U	N3-C2-O2	8.81	128.37	122.20
36	5	2973	G	O5'-P-OP1	-8.81	97.77	105.70
36	1	2870	C	C2-N1-C1'	-8.81	109.11	118.80
36	1	1177	G	N3-C2-N2	-8.80	113.74	119.90
37	7	92	A	C5-C6-N6	-8.80	116.66	123.70
36	1	895	A	C8-N9-C4	-8.80	102.28	105.80
36	5	1336	U	O5'-P-OP2	-8.80	97.78	105.70
36	1	611	A	O5'-P-OP2	-8.79	97.79	105.70
36	5	2405	C	N3-C2-O2	-8.78	115.75	121.90
36	5	3188	G	C5-C6-O6	8.78	133.87	128.60
36	5	1178	G	C8-N9-C4	-8.78	102.89	106.40
36	1	28	C	N1-C2-O2	8.77	124.16	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	895	A	N1-C6-N6	8.77	123.86	118.60
36	5	2802	A	N9-C4-C5	8.77	109.31	105.80
36	1	2419	A	OP1-P-OP2	-8.76	106.46	119.60
36	5	929	A	N1-C6-N6	-8.76	113.34	118.60
37	7	92	A	C6-C5-N7	-8.76	126.17	132.30
36	1	3190	C	N3-C4-C5	8.74	125.40	121.90
38	4	47	C	N3-C2-O2	-8.74	115.78	121.90
1	6	65	A	C2-N3-C4	-8.74	106.23	110.60
36	5	874	U	O5'-P-OP1	-8.74	97.84	105.70
36	5	1430	U	C6-N1-C2	8.74	126.24	121.00
36	5	1856	C	C6-N1-C2	-8.73	116.81	120.30
36	5	2971	A	C2-N3-C4	8.73	114.97	110.60
1	6	48	G	O5'-P-OP2	-8.73	97.85	105.70
1	2	1486	G	C8-N9-C4	-8.72	102.91	106.40
36	1	2812	C	C5-C6-N1	-8.72	116.64	121.00
36	5	2281	A	C8-N9-C4	8.71	109.28	105.80
36	1	2602	G	C5-C6-O6	8.71	133.82	128.60
36	1	267	G	N1-C6-O6	8.70	125.12	119.90
36	5	716	A	O5'-P-OP1	-8.70	97.87	105.70
1	6	314	C	C6-N1-C2	-8.69	116.82	120.30
36	5	2821	C	O5'-P-OP2	-8.69	97.88	105.70
36	1	62	A	O5'-P-OP2	-8.69	97.88	105.70
1	6	337	G	C4-N9-C1'	8.68	137.79	126.50
36	5	2199	G	C6-C5-N7	-8.68	125.19	130.40
36	1	112	U	C2-N1-C1'	8.68	128.11	117.70
36	1	1127	G	C5-C6-O6	-8.67	123.40	128.60
36	1	1152	G	OP1-P-OP2	8.67	132.61	119.60
36	1	649	A	OP1-P-OP2	-8.67	106.59	119.60
36	5	640	U	N1-C2-O2	-8.67	116.73	122.80
36	1	1380	G	O5'-P-OP2	-8.66	97.90	105.70
36	1	2726	C	N3-C4-N4	-8.66	111.94	118.00
36	1	2758	A	C2-N3-C4	8.66	114.93	110.60
36	1	922	U	C5-C6-N1	8.66	127.03	122.70
36	5	1300	G	C5-C6-O6	-8.66	123.40	128.60
36	5	2634	U	N1-C2-N3	8.65	120.09	114.90
36	1	2142	A	N1-C2-N3	8.65	133.63	129.30
36	5	3092	C	N1-C2-O2	8.65	124.09	118.90
36	1	3174	A	C5-N7-C8	-8.65	99.58	103.90
36	1	2621	G	C5-C6-O6	-8.64	123.42	128.60
36	5	1868	G	C6-C5-N7	-8.64	125.22	130.40
1	6	87	C	C6-N1-C2	-8.64	116.84	120.30
36	1	361	A	N1-C6-N6	-8.63	113.42	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	908	G	N1-C6-O6	8.63	125.08	119.90
36	5	2873	U	N1-C2-N3	8.63	120.08	114.90
36	1	2642	A	C5-C6-N1	-8.63	113.39	117.70
36	5	1401	A	O5'-P-OP2	-8.63	97.94	105.70
36	5	2797	C	O5'-P-OP2	-8.62	97.94	105.70
36	5	1060	U	C5-C6-N1	-8.61	118.39	122.70
36	1	3344	A	O4'-C1'-N9	8.61	115.09	108.20
36	5	1123	U	O5'-P-OP2	-8.61	97.95	105.70
1	6	1481	C	N3-C2-O2	-8.61	115.87	121.90
36	5	1371	G	C4-C5-N7	-8.61	107.36	110.80
36	1	1130	A	C2-N3-C4	8.61	114.90	110.60
36	5	644	G	C4-C5-N7	-8.61	107.36	110.80
36	5	871	U	C5-C4-O4	8.60	131.06	125.90
36	5	1158	A	C4-C5-N7	8.60	115.00	110.70
36	1	648	C	O5'-P-OP1	-8.60	97.96	105.70
36	5	3260	G	C5-C6-O6	8.60	133.76	128.60
36	5	2383	C	N3-C4-N4	8.60	124.02	118.00
36	5	909	G	C5-N7-C8	8.59	108.60	104.30
36	1	1741	A	C2-N3-C4	-8.59	106.31	110.60
36	5	828	A	O5'-P-OP2	-8.59	97.97	105.70
36	5	2191	U	N3-C4-O4	-8.58	113.39	119.40
1	2	1043	A	O5'-P-OP2	-8.58	97.98	105.70
36	1	2323	G	N3-C4-N9	8.58	131.15	126.00
36	5	1427	U	N3-C4-O4	-8.58	113.40	119.40
36	1	1855	U	O5'-P-OP2	-8.57	97.99	105.70
38	4	29	U	C5-C4-O4	-8.57	120.76	125.90
36	1	3000	A	C8-N9-C4	8.57	109.23	105.80
36	1	3214	U	N3-C2-O2	-8.57	116.20	122.20
1	6	18	C	C6-N1-C2	-8.57	116.87	120.30
36	1	949	C	C4-C5-C6	8.56	121.68	117.40
36	5	3209	A	O4'-C1'-N9	8.56	115.05	108.20
36	1	2622	C	C6-N1-C2	-8.55	116.88	120.30
36	1	2706	G	C6-C5-N7	-8.56	125.27	130.40
36	5	2211	U	C4-C5-C6	8.55	124.83	119.70
36	5	2758	A	C2-N3-C4	8.55	114.88	110.60
1	6	1481	C	C6-N1-C2	-8.55	116.88	120.30
36	5	2572	C	N1-C2-O2	8.55	124.03	118.90
1	2	144	U	N3-C2-O2	-8.55	116.22	122.20
36	1	2679	A	C2-N3-C4	-8.55	106.33	110.60
36	1	2550	U	C5-C4-O4	8.54	131.03	125.90
36	1	3143	C	O5'-P-OP2	-8.54	98.02	105.70
36	1	2314	U	C6-N1-C1'	-8.53	109.26	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2310	U	N3-C2-O2	-8.53	116.23	122.20
1	6	1596	C	N1-C2-O2	8.52	124.01	118.90
36	5	295	A	O5'-P-OP1	-8.52	98.03	105.70
36	5	412	G	N3-C4-C5	-8.52	124.34	128.60
36	5	229	G	N3-C2-N2	-8.52	113.94	119.90
36	5	2300	G	N1-C6-O6	-8.51	114.79	119.90
36	5	878	G	C8-N9-C4	-8.51	103.00	106.40
38	4	40	A	N1-C6-N6	8.50	123.70	118.60
37	7	101	G	C5-C6-O6	-8.49	123.50	128.60
36	1	369	A	C8-N9-C4	-8.49	102.40	105.80
36	5	1743	G	C5-C6-O6	-8.49	123.51	128.60
36	5	2726	C	N3-C4-C5	-8.49	118.51	121.90
36	1	1370	G	C4-C5-N7	8.48	114.19	110.80
36	1	2620	G	C8-N9-C4	8.48	109.79	106.40
1	2	830	U	N3-C2-O2	-8.48	116.26	122.20
1	2	1596	C	N3-C2-O2	-8.48	115.96	121.90
36	1	2978	U	N1-C2-O2	8.48	128.74	122.80
36	5	1879	A	C6-C5-N7	-8.48	126.36	132.30
36	5	2308	C	N1-C2-O2	-8.48	113.81	118.90
36	5	406	G	N1-C6-O6	-8.48	114.81	119.90
36	5	3214	U	N3-C2-O2	-8.48	116.27	122.20
36	1	1133	A	C6-N1-C2	-8.47	113.52	118.60
1	2	1796	C	C4-C5-C6	8.47	121.63	117.40
36	1	1837	U	N3-C2-O2	8.47	128.13	122.20
36	1	2978	U	N3-C2-O2	-8.47	116.27	122.20
36	1	2121	G	N1-C6-O6	-8.46	114.82	119.90
36	1	2814	G	C5-C6-O6	-8.46	123.52	128.60
1	2	1039	A	O4'-C1'-N9	8.46	114.97	108.20
36	5	283	G	O4'-C1'-N9	-8.46	101.43	108.20
36	5	947	G	N1-C6-O6	-8.46	114.83	119.90
36	1	658	G	N1-C6-O6	8.46	124.97	119.90
36	5	2611	U	C5-C6-N1	-8.46	118.47	122.70
36	1	3214	U	C5-C4-O4	8.45	130.97	125.90
36	1	1495	U	N1-C2-O2	-8.45	116.88	122.80
36	1	1729	A	O5'-P-OP2	-8.45	98.09	105.70
37	7	100	C	C6-N1-C2	8.45	123.68	120.30
36	5	780	A	N1-C2-N3	-8.45	125.07	129.30
36	1	942	U	N1-C2-O2	-8.45	116.89	122.80
36	5	661	G	C5-N7-C8	-8.45	100.08	104.30
36	5	645	A	C4-C5-N7	-8.44	106.48	110.70
36	5	2838	A	N1-C6-N6	8.43	123.66	118.60
36	1	346	C	C5-C6-N1	-8.43	116.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L3	159	ARG	NE-CZ-NH2	-8.43	116.08	120.30
36	1	94	G	C4-C5-N7	8.43	114.17	110.80
36	1	938	C	C5-C4-N4	-8.43	114.30	120.20
36	5	861	C	O5'-P-OP2	-8.43	98.11	105.70
36	5	1301	A	C6-C5-N7	-8.42	126.41	132.30
36	1	2889	C	N3-C2-O2	-8.41	116.01	121.90
36	5	776	U	N1-C2-N3	8.41	119.95	114.90
36	1	716	A	C8-N9-C4	8.41	109.17	105.80
36	1	770	G	O4'-C1'-N9	8.41	114.93	108.20
36	1	1606	U	N1-C2-O2	-8.41	116.92	122.80
1	2	830	U	N1-C2-O2	8.40	128.68	122.80
36	5	1370	G	N1-C6-O6	-8.40	114.86	119.90
36	1	2154	U	C5-C4-O4	-8.40	120.86	125.90
1	6	434	G	O5'-P-OP2	-8.40	98.14	105.70
36	1	2343	C	C2-N3-C4	-8.40	115.70	119.90
36	1	340	C	C2-N3-C4	-8.39	115.70	119.90
36	1	1405	U	C2-N3-C4	-8.39	121.97	127.00
52	m6	68	ARG	NE-CZ-NH2	8.39	124.50	120.30
36	1	3344	A	N7-C8-N9	8.38	117.99	113.80
36	1	2176	U	N1-C2-O2	8.38	128.66	122.80
36	1	2602	G	N1-C6-O6	-8.38	114.87	119.90
36	1	3319	U	N3-C2-O2	-8.38	116.34	122.20
1	2	1200	G	C6-C5-N7	-8.38	125.37	130.40
1	6	102	U	O5'-P-OP1	-8.38	98.16	105.70
36	5	1482	A	O5'-P-OP2	-8.38	98.16	105.70
1	2	1773	C	C6-N1-C2	-8.37	116.95	120.30
36	1	942	U	C2-N3-C4	-8.37	121.98	127.00
1	2	1672	G	O5'-P-OP2	-8.37	98.17	105.70
36	1	2827	U	C5-C6-N1	-8.36	118.52	122.70
36	5	2843	U	N1-C2-O2	8.36	128.65	122.80
36	5	421	G	C5-C6-O6	-8.36	123.58	128.60
36	5	715	A	N9-C4-C5	8.36	109.14	105.80
36	5	835	G	O4'-C1'-N9	8.35	114.88	108.20
36	1	2148	U	N3-C2-O2	8.35	128.04	122.20
38	8	4	C	C2-N3-C4	-8.35	115.73	119.90
36	1	1331	U	O4'-C1'-N1	-8.34	101.53	108.20
36	5	1340	G	N7-C8-N9	-8.34	108.93	113.10
1	2	1486	G	N7-C8-N9	8.34	117.27	113.10
36	1	2816	G	C5-C6-O6	-8.34	123.60	128.60
36	5	2287	C	O5'-P-OP2	-8.34	98.20	105.70
36	5	2278	C	C4-C5-C6	-8.33	113.23	117.40
36	1	3278	C	N3-C2-O2	-8.32	116.07	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	75	G	C5-C6-O6	-8.32	123.61	128.60
36	1	1301	A	O5'-P-OP1	-8.32	98.21	105.70
36	5	1907	C	N1-C2-O2	-8.32	113.91	118.90
36	1	1351	U	N1-C2-O2	8.31	128.62	122.80
36	5	2851	A	O5'-P-OP1	-8.31	98.22	105.70
36	5	2362	C	C6-N1-C2	-8.31	116.98	120.30
36	1	1316	C	N1-C2-O2	-8.30	113.92	118.90
1	6	60	U	C5-C6-N1	8.30	126.85	122.70
36	1	1556	C	N1-C2-O2	8.30	123.88	118.90
36	5	1311	G	N1-C6-O6	-8.30	114.92	119.90
36	1	3278	C	N1-C2-O2	8.30	123.88	118.90
36	1	1132	C	O5'-P-OP1	-8.29	98.24	105.70
36	1	2710	C	N1-C2-O2	-8.29	113.93	118.90
1	6	1123	C	N3-C4-C5	8.29	125.22	121.90
36	5	1160	C	C5-C4-N4	8.29	126.00	120.20
36	1	2923	U	O5'-P-OP2	8.28	120.64	110.70
36	1	2941	A	N9-C4-C5	-8.28	102.49	105.80
36	1	1113	G	N3-C2-N2	-8.28	114.10	119.90
36	1	2732	G	N3-C2-N2	8.28	125.70	119.90
36	5	1844	C	C6-N1-C2	-8.28	116.99	120.30
36	5	1239	C	C5-C6-N1	8.28	125.14	121.00
41	14	339	LEU	CA-CB-CG	8.28	134.34	115.30
1	6	163	G	C5-N7-C8	-8.28	100.16	104.30
36	5	2398	A	N1-C6-N6	-8.28	113.63	118.60
36	5	3166	C	C5-C6-N1	8.27	125.14	121.00
36	1	1507	G	N3-C2-N2	-8.27	114.11	119.90
1	2	1761	U	P-O3'-C3'	8.26	129.62	119.70
36	1	968	G	C8-N9-C4	-8.26	103.09	106.40
36	1	681	U	N3-C4-O4	8.26	125.18	119.40
36	5	345	G	N1-C6-O6	8.26	124.85	119.90
36	5	1190	A	C8-N9-C4	-8.26	102.50	105.80
52	m6	84	LEU	CA-CB-CG	-8.26	96.31	115.30
36	5	2830	G	C4-C5-N7	-8.25	107.50	110.80
36	5	1054	A	C8-N9-C4	8.25	109.10	105.80
36	5	3197	G	N3-C4-N9	-8.25	121.05	126.00
36	5	1305	U	O5'-P-OP1	-8.24	98.28	105.70
36	5	2550	U	N1-C2-N3	8.24	119.85	114.90
36	5	645	A	C5-N7-C8	8.24	108.02	103.90
36	1	1547	G	N7-C8-N9	-8.24	108.98	113.10
1	6	1123	C	C6-N1-C2	8.23	123.59	120.30
36	1	86	G	N1-C6-O6	-8.23	114.96	119.90
36	5	2991	A	C8-N9-C4	-8.23	102.51	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1121	C	O5'-P-OP2	-8.22	98.30	105.70
36	1	2977	G	C6-N1-C2	-8.22	120.17	125.10
36	5	2531	C	C2-N1-C1'	8.22	127.84	118.80
36	1	1403	C	C6-N1-C2	8.22	123.59	120.30
36	5	116	A	O4'-C1'-N9	8.22	114.78	108.20
36	5	200	C	N3-C4-C5	-8.22	118.61	121.90
1	6	1137	A	C8-N9-C4	8.21	109.09	105.80
36	1	859	G	N3-C2-N2	8.21	125.65	119.90
36	1	2417	U	C2-N3-C4	-8.21	122.07	127.00
36	5	877	C	C4-C5-C6	-8.21	113.29	117.40
36	1	3306	U	N1-C2-O2	8.21	128.55	122.80
36	1	2130	G	N1-C6-O6	-8.21	114.98	119.90
1	6	1560	U	N3-C2-O2	-8.21	116.45	122.20
36	5	2899	C	N3-C4-N4	-8.21	112.25	118.00
36	1	2941	A	C8-N9-C4	8.21	109.08	105.80
36	1	1157	G	N1-C6-O6	-8.20	114.98	119.90
36	1	1713	G	C8-N9-C4	8.20	109.68	106.40
38	8	26	U	N1-C2-O2	8.21	128.54	122.80
36	5	661	G	C4-C5-N7	8.20	114.08	110.80
36	1	2362	C	N1-C2-O2	8.20	123.82	118.90
36	1	2412	G	C5-C6-O6	-8.20	123.68	128.60
36	5	805	G	N1-C6-O6	8.20	124.82	119.90
36	5	1416	C	N1-C2-O2	8.20	123.82	118.90
36	5	1882	G	O5'-P-OP1	-8.20	98.33	105.70
36	1	1081	U	C5-C6-N1	8.19	126.80	122.70
36	1	2996	U	C5-C4-O4	-8.19	120.98	125.90
1	6	980	G	N1-C6-O6	-8.19	114.98	119.90
36	1	1445	U	C5-C4-O4	-8.19	120.99	125.90
36	1	2412	G	C6-N1-C2	-8.19	120.19	125.10
36	1	1507	G	N1-C6-O6	8.18	124.81	119.90
36	1	2405	C	N3-C4-C5	-8.18	118.63	121.90
36	5	1301	A	C5-C6-N6	-8.18	117.15	123.70
36	1	640	U	N1-C2-O2	-8.18	117.08	122.80
36	1	104	G	N1-C6-O6	8.18	124.81	119.90
1	6	57	G	O5'-P-OP2	-8.18	98.34	105.70
38	8	80	A	C8-N9-C4	-8.17	102.53	105.80
36	1	2899	C	N3-C2-O2	-8.17	116.18	121.90
36	5	2744	U	N3-C2-O2	-8.17	116.48	122.20
36	5	1122	U	N1-C2-N3	8.17	119.80	114.90
1	6	426	G	N3-C4-C5	-8.17	124.52	128.60
36	1	2825	C	N1-C2-O2	8.16	123.80	118.90
1	6	421	A	C8-N9-C4	8.16	109.07	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	359	U	OP1-P-OP2	-8.16	107.36	119.60
36	5	2964	G	N1-C6-O6	-8.16	115.00	119.90
38	8	79	A	N7-C8-N9	8.16	117.88	113.80
36	5	1481	A	N7-C8-N9	8.16	117.88	113.80
36	1	653	A	N1-C6-N6	8.16	123.49	118.60
36	1	1904	C	C5-C6-N1	8.16	125.08	121.00
36	5	3214	U	C5-C4-O4	8.16	130.79	125.90
36	1	1192	C	C6-N1-C2	-8.15	117.04	120.30
36	1	776	U	C5-C6-N1	-8.15	118.62	122.70
36	1	2374	C	N1-C2-N3	8.14	124.90	119.20
36	5	3136	G	N1-C2-N3	8.14	128.79	123.90
36	1	325	A	C2-N3-C4	8.14	114.67	110.60
36	5	410	U	N3-C4-O4	8.14	125.10	119.40
36	1	2846	U	N1-C2-N3	8.14	119.78	114.90
36	1	1177	G	C5-C6-O6	-8.12	123.73	128.60
36	1	2823	G	C5-N7-C8	8.12	108.36	104.30
1	6	101	U	N3-C2-O2	-8.12	116.51	122.20
1	2	1773	C	N3-C4-C5	-8.12	118.65	121.90
36	1	1307	G	C6-C5-N7	8.12	135.27	130.40
36	1	776	U	C4-C5-C6	8.12	124.57	119.70
36	5	2925	C	O5'-P-OP1	-8.11	98.40	105.70
36	5	890	C	N3-C4-C5	8.11	125.14	121.90
36	5	3092	C	N3-C2-O2	-8.11	116.22	121.90
1	6	1644	C	O5'-P-OP2	-8.11	98.40	105.70
36	5	3093	C	N1-C2-O2	-8.10	114.04	118.90
36	1	2314	U	C2-N1-C1'	8.10	127.42	117.70
36	1	3277	U	N3-C2-O2	-8.10	116.53	122.20
36	5	2142	A	C6-N1-C2	-8.10	113.74	118.60
36	5	3154	C	C2-N1-C1'	8.10	127.71	118.80
36	1	1133	A	C5-C6-N6	-8.10	117.22	123.70
36	5	204	A	C5-C6-N6	8.10	130.18	123.70
36	5	617	G	C4-C5-N7	8.09	114.04	110.80
1	6	337	G	C8-N9-C1'	-8.09	116.49	127.00
36	5	2300	G	N3-C4-C5	-8.09	124.56	128.60
38	8	63	G	N1-C6-O6	-8.09	115.05	119.90
36	5	941	G	C5-C6-N1	8.08	115.54	111.50
36	1	2808	A	N1-C6-N6	8.08	123.45	118.60
1	6	609	U	C5-C6-N1	-8.08	118.66	122.70
36	1	805	G	N7-C8-N9	-8.08	109.06	113.10
36	5	931	C	N3-C4-C5	8.07	125.13	121.90
36	5	2618	G	C2-N3-C4	8.07	115.93	111.90
37	7	121	U	C2-N1-C1'	8.07	127.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	287	G	C4-C5-N7	-8.06	107.58	110.80
36	1	785	G	C2-N3-C4	8.06	115.93	111.90
37	7	7	G	O5'-P-OP1	8.06	120.37	110.70
36	1	30	G	O5'-P-OP2	-8.05	98.45	105.70
36	1	859	G	C6-C5-N7	-8.05	125.57	130.40
36	5	3144	G	N3-C4-C5	-8.05	124.57	128.60
36	5	3183	A	C5-C6-N6	-8.05	117.26	123.70
36	1	776	U	N1-C2-N3	8.04	119.73	114.90
36	1	2836	C	N3-C4-C5	-8.05	118.68	121.90
36	1	3228	C	P-O3'-C3'	8.04	129.35	119.70
36	5	2663	G	O5'-P-OP2	-8.04	98.46	105.70
36	5	3136	G	C2-N3-C4	-8.04	107.88	111.90
36	1	699	A	C2-N3-C4	-8.04	106.58	110.60
36	1	1443	G	N7-C8-N9	8.04	117.12	113.10
1	6	539	G	C8-N9-C4	-8.04	103.18	106.40
36	5	987	U	O5'-P-OP1	-8.04	98.47	105.70
37	7	40	C	C6-N1-C2	8.04	123.52	120.30
51	m5	187	ARG	NE-CZ-NH1	-8.04	116.28	120.30
36	1	339	C	O5'-P-OP2	8.03	120.34	110.70
70	O4	51	LEU	CA-CB-CG	8.03	133.78	115.30
36	1	1435	A	OP1-P-OP2	-8.03	107.55	119.60
36	1	1582	C	C6-N1-C2	-8.03	117.09	120.30
44	17	229	PHE	CB-CG-CD1	8.03	126.42	120.80
36	1	2189	U	C5-C4-O4	-8.03	121.08	125.90
36	5	2867	C	C2-N3-C4	8.03	123.91	119.90
36	1	663	C	C5-C4-N4	-8.02	114.58	120.20
36	1	2385	G	C8-N9-C4	8.02	109.61	106.40
36	1	2996	U	N1-C2-N3	-8.02	110.09	114.90
36	5	2347	U	N3-C4-C5	8.02	119.41	114.60
1	2	254	A	C8-N9-C4	8.02	109.01	105.80
36	1	896	A	C8-N9-C4	-8.02	102.59	105.80
36	5	2925	C	N1-C2-O2	-8.02	114.09	118.90
36	1	1114	U	N3-C4-C5	8.02	119.41	114.60
1	6	609	U	N1-C2-N3	8.02	119.71	114.90
36	1	979	U	N3-C2-O2	-8.01	116.59	122.20
36	5	2272	G	O4'-C1'-N9	8.01	114.61	108.20
36	1	2400	G	C6-N1-C2	-8.01	120.30	125.10
36	5	908	G	C5-C6-O6	-8.01	123.80	128.60
36	5	959	C	O5'-P-OP1	-8.01	98.50	105.70
36	1	2714	G	C5-N7-C8	-8.00	100.30	104.30
36	5	372	A	C5-C6-N6	-8.00	117.30	123.70
36	5	1117	G	O5'-P-OP1	-8.00	98.50	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	47	C	N3-C4-C5	-8.00	118.70	121.90
36	1	66	A	O5'-P-OP1	-8.00	98.50	105.70
36	1	2413	A	N1-C6-N6	-8.00	113.80	118.60
36	1	2614	G	C8-N9-C4	8.00	109.60	106.40
36	1	78	U	N1-C2-O2	-8.00	117.20	122.80
36	5	939	U	O5'-P-OP2	-8.00	98.50	105.70
36	5	2375	G	N3-C4-C5	-7.99	124.60	128.60
36	1	2820	A	N9-C4-C5	7.99	109.00	105.80
36	1	2118	C	O5'-P-OP2	-7.99	98.51	105.70
36	1	2920	U	C2-N3-C4	-7.98	122.21	127.00
36	1	2959	C	C6-N1-C2	-7.98	117.11	120.30
36	5	411	U	N1-C2-N3	7.98	119.69	114.90
36	5	922	U	N3-C4-C5	7.98	119.39	114.60
36	5	3012	A	C8-N9-C4	7.98	108.99	105.80
39	12	242	ARG	NE-CZ-NH1	-7.98	116.31	120.30
36	5	2601	A	N1-C6-N6	-7.97	113.82	118.60
36	5	909	G	C4-C5-N7	-7.97	107.61	110.80
36	5	2572	C	C2-N1-C1'	7.97	127.56	118.80
36	5	189	G	N1-C6-O6	-7.96	115.12	119.90
36	1	2897	A	C8-N9-C4	7.96	108.98	105.80
36	5	2928	C	C4-C5-C6	7.96	121.38	117.40
36	1	946	U	O5'-P-OP2	-7.96	98.54	105.70
36	5	2156	C	N3-C2-O2	7.96	127.47	121.90
36	1	922	U	N1-C2-O2	7.95	128.36	122.80
1	2	1291	G	N3-C4-N9	-7.95	121.23	126.00
36	5	224	C	OP1-P-O3'	7.95	122.68	105.20
36	5	1378	U	C6-N1-C2	7.94	125.77	121.00
36	1	1160	C	C6-N1-C2	7.94	123.47	120.30
36	1	1334	U	N3-C4-C5	-7.94	109.84	114.60
36	5	2664	C	O5'-P-OP1	-7.94	98.56	105.70
36	1	611	A	O5'-P-OP1	7.93	120.22	110.70
36	5	1926	C	N1-C2-O2	-7.93	114.14	118.90
36	5	220	G	O5'-P-OP2	-7.93	98.56	105.70
36	5	1189	C	N3-C4-C5	-7.93	118.73	121.90
36	5	1331	U	O4'-C1'-N1	-7.93	101.86	108.20
36	5	21	G	C4-C5-N7	7.93	113.97	110.80
36	5	72	C	C6-N1-C2	7.93	123.47	120.30
36	5	651	G	N3-C4-C5	-7.92	124.64	128.60
36	5	1113	G	C5-C6-N1	-7.92	107.54	111.50
36	1	1049	C	O5'-P-OP1	7.92	120.20	110.70
1	6	679	U	C5-C6-N1	7.92	126.66	122.70
36	5	641	C	C6-N1-C1'	7.92	130.30	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1741	A	N1-C2-N3	7.91	133.26	129.30
36	1	908	G	C5-C6-O6	-7.91	123.85	128.60
36	5	750	G	C8-N9-C4	-7.91	103.23	106.40
36	1	3362	A	N1-C6-N6	7.90	123.34	118.60
36	1	335	G	O5'-P-OP2	7.90	120.18	110.70
36	5	2950	G	O4'-C1'-N9	7.90	114.52	108.20
36	1	2374	C	N1-C2-O2	-7.90	114.16	118.90
36	5	437	G	N3-C2-N2	-7.90	114.37	119.90
36	5	729	C	C5-C4-N4	-7.89	114.67	120.20
36	5	1101	G	N3-C2-N2	7.89	125.43	119.90
36	5	2726	C	N1-C2-N3	7.89	124.72	119.20
36	1	1445	U	N1-C2-O2	-7.89	117.28	122.80
36	1	2878	G	O5'-P-OP2	-7.89	98.60	105.70
36	1	346	C	N1-C2-O2	-7.89	114.17	118.90
36	1	1180	A	O4'-C1'-N9	-7.89	101.89	108.20
36	1	2758	A	N1-C2-N3	-7.89	125.36	129.30
38	4	40	A	C5-C6-N6	-7.89	117.39	123.70
36	5	1885	U	N3-C2-O2	7.88	127.72	122.20
36	5	1118	C	O5'-P-OP1	-7.88	98.61	105.70
36	5	1108	U	O5'-P-OP2	-7.88	98.61	105.70
37	7	92	A	C4-C5-N7	7.88	114.64	110.70
1	6	538	A	N1-C6-N6	-7.88	113.87	118.60
38	4	51	G	N1-C6-O6	7.87	124.62	119.90
1	6	337	G	N3-C4-C5	-7.87	124.66	128.60
36	5	1483	G	O4'-C1'-N9	7.87	114.50	108.20
1	2	1596	C	N1-C2-O2	7.87	123.62	118.90
36	1	1492	G	N3-C4-C5	-7.87	124.67	128.60
36	1	1899	G	N7-C8-N9	7.86	117.03	113.10
38	4	63	G	N1-C6-O6	-7.86	115.18	119.90
36	1	143	G	N1-C6-O6	-7.86	115.18	119.90
36	1	2823	G	C4-C5-N7	-7.86	107.66	110.80
36	5	406	G	O4'-C1'-N9	7.86	114.49	108.20
36	5	3103	A	C5-C6-N1	7.86	121.63	117.70
36	5	1884	A	N1-C6-N6	7.85	123.31	118.60
36	1	1313	G	C5-C6-O6	-7.84	123.89	128.60
36	5	1115	G	P-O3'-C3'	7.84	129.11	119.70
36	1	2836	C	C5-C4-N4	7.84	125.69	120.20
36	5	1191	U	N1-C2-O2	-7.84	117.31	122.80
36	5	2364	G	N9-C4-C5	7.84	108.54	105.40
1	2	1560	U	N3-C2-O2	-7.84	116.71	122.20
36	1	92	G	N1-C6-O6	-7.84	115.20	119.90
36	1	610	G	C2-N3-C4	-7.84	107.98	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2941	A	N1-C6-N6	7.84	123.30	118.60
36	5	2719	U	N1-C2-N3	7.84	119.60	114.90
36	5	513	G	N1-C6-O6	-7.83	115.20	119.90
39	12	246	LEU	CA-CB-CG	7.83	133.31	115.30
36	1	2850	G	N1-C6-O6	7.83	124.60	119.90
48	M1	112	LEU	CA-CB-CG	7.83	133.30	115.30
36	5	699	A	C2-N3-C4	-7.83	106.69	110.60
36	5	1926	C	C6-N1-C2	7.82	123.43	120.30
36	5	2240	G	N1-C6-O6	-7.82	115.21	119.90
36	5	1169	A	OP1-P-OP2	-7.82	107.87	119.60
36	5	2870	C	C2-N1-C1'	-7.82	110.20	118.80
36	5	2888	U	C5-C4-O4	-7.82	121.21	125.90
36	5	1390	A	C8-N9-C4	-7.82	102.67	105.80
36	5	1890	U	O5'-P-OP2	-7.82	98.67	105.70
36	1	2359	C	O5'-P-OP2	-7.82	98.67	105.70
36	1	2980	U	N1-C2-N3	7.81	119.59	114.90
37	7	80	G	N3-C4-C5	-7.81	124.69	128.60
36	5	813	G	C6-N1-C2	-7.81	120.42	125.10
36	5	1134	G	O5'-P-OP2	-7.81	98.67	105.70
36	1	2411	U	C2-N3-C4	-7.81	122.32	127.00
36	1	1134	G	C5-C6-O6	-7.80	123.92	128.60
36	5	1047	A	C5-N7-C8	-7.80	100.00	103.90
36	1	325	A	C5-C6-N1	7.80	121.60	117.70
36	1	3107	U	N3-C2-O2	-7.80	116.74	122.20
1	6	1700	C	C2-N1-C1'	7.80	127.38	118.80
36	1	2827	U	C5-C4-O4	7.80	130.58	125.90
36	5	1103	A	C8-N9-C4	-7.80	102.68	105.80
36	1	691	A	N1-C2-N3	-7.80	125.40	129.30
36	5	27	C	N1-C2-O2	-7.79	114.22	118.90
36	1	328	U	N1-C2-O2	7.79	128.25	122.80
36	1	2424	A	C4-C5-N7	7.79	114.59	110.70
36	5	889	U	N3-C4-C5	7.79	119.27	114.60
36	1	637	C	N3-C4-N4	-7.79	112.55	118.00
52	m6	78	ARG	NE-CZ-NH2	-7.78	116.41	120.30
36	5	1743	G	N1-C6-O6	7.78	124.57	119.90
36	1	1383	G	C5-C6-O6	-7.78	123.93	128.60
36	1	3048	A	O5'-P-OP2	-7.78	98.70	105.70
1	2	453	U	C2-N1-C1'	7.78	127.03	117.70
36	1	1503	A	C2-N3-C4	-7.78	106.71	110.60
36	5	1116	G	N9-C4-C5	7.78	108.51	105.40
36	5	946	U	C5-C4-O4	7.77	130.56	125.90
36	1	635	G	N3-C4-N9	7.77	130.66	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1082	C	N1-C2-O2	7.77	123.56	118.90
36	1	1194	G	N1-C6-O6	-7.77	115.24	119.90
1	6	696	C	O4'-C1'-N1	7.77	114.41	108.20
36	5	2861	U	C5-C6-N1	-7.77	118.82	122.70
36	5	2873	U	N1-C2-O2	-7.77	117.36	122.80
36	1	439	C	N3-C2-O2	-7.77	116.46	121.90
36	1	2712	U	N3-C2-O2	-7.77	116.76	122.20
36	5	1402	C	C4-C5-C6	7.76	121.28	117.40
36	5	2797	C	C6-N1-C2	-7.76	117.19	120.30
36	1	2362	C	C5-C6-N1	7.76	124.88	121.00
36	1	3079	U	C5-C6-N1	-7.76	118.82	122.70
38	4	60	U	N1-C2-N3	7.76	119.55	114.90
36	5	513	G	C5-C6-N1	7.76	115.38	111.50
36	5	3362	A	C5-N7-C8	-7.76	100.02	103.90
36	5	1899	G	C5-C6-N1	-7.75	107.62	111.50
36	1	3326	G	C8-N9-C4	7.75	109.50	106.40
36	5	3154	C	N3-C2-O2	-7.75	116.47	121.90
1	2	553	G	C5-C6-N1	-7.75	107.62	111.50
36	1	983	A	C8-N9-C4	7.74	108.90	105.80
36	5	1155	C	C5-C4-N4	-7.74	114.78	120.20
36	5	2392	C	N3-C4-N4	-7.74	112.58	118.00
36	5	2897	A	C6-N1-C2	-7.74	113.96	118.60
1	2	359	A	C8-N9-C4	7.74	108.90	105.80
36	1	1319	G	N1-C6-O6	-7.74	115.26	119.90
36	5	2375	G	C2-N3-C4	7.74	115.77	111.90
36	5	217	U	C6-N1-C2	7.74	125.64	121.00
36	5	1015	U	O4'-C1'-N1	7.74	114.39	108.20
36	5	2400	G	C5-C6-O6	-7.74	123.96	128.60
36	1	2614	G	O5'-P-OP2	-7.73	98.74	105.70
36	1	407	A	OP1-P-OP2	-7.73	108.00	119.60
36	1	1156	C	C5-C6-N1	-7.73	117.14	121.00
36	5	95	A	N7-C8-N9	-7.73	109.94	113.80
36	1	2281	A	C2-N3-C4	-7.72	106.74	110.60
36	5	3245	A	N1-C2-N3	7.72	133.16	129.30
36	5	1445	U	N1-C2-O2	-7.72	117.39	122.80
36	1	2169	G	C6-C5-N7	7.72	135.03	130.40
36	1	2883	U	O5'-P-OP2	-7.72	98.75	105.70
36	1	908	G	O4'-C1'-N9	-7.72	102.03	108.20
36	5	95	A	C8-N9-C4	7.71	108.89	105.80
36	5	661	G	C5-C6-O6	-7.71	123.97	128.60
36	1	2944	U	N1-C2-O2	7.71	128.20	122.80
36	5	644	G	N9-C4-C5	7.71	108.48	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2349	U	O5'-P-OP2	-7.71	98.76	105.70
1	6	1036	A	O5'-P-OP2	-7.71	98.76	105.70
36	5	1331	U	C5-C4-O4	-7.71	121.27	125.90
36	5	2818	U	N3-C4-C5	7.71	119.23	114.60
36	1	2603	G	N1-C6-O6	-7.71	115.27	119.90
36	1	2842	U	N1-C2-O2	7.71	128.20	122.80
36	1	3217	C	C2-N1-C1'	7.71	127.28	118.80
36	5	86	G	N1-C6-O6	-7.71	115.28	119.90
36	5	691	A	N1-C6-N6	-7.71	113.97	118.60
36	5	1390	A	N1-C6-N6	-7.70	113.98	118.60
1	6	1600	A	N9-C1'-C2'	7.70	124.01	114.00
1	6	543	C	N3-C2-O2	-7.70	116.51	121.90
36	5	2618	G	N3-C4-C5	-7.70	124.75	128.60
1	6	25	C	P-O3'-C3'	7.70	128.94	119.70
36	1	645	A	N3-C4-N9	7.69	133.56	127.40
36	5	229	G	N1-C2-N2	7.69	123.12	116.20
1	6	1600	A	C2-N3-C4	-7.69	106.76	110.60
36	5	1371	G	C6-C5-N7	7.69	135.01	130.40
36	1	1481	A	O4'-C1'-N9	7.69	114.35	108.20
36	5	1481	A	P-O3'-C3'	7.68	128.92	119.70
36	1	877	C	N1-C2-O2	-7.68	114.29	118.90
36	1	2549	G	N3-C2-N2	7.68	125.28	119.90
36	1	3057	U	C5-C4-O4	7.68	130.51	125.90
1	6	815	G	C6-C5-N7	-7.68	125.79	130.40
36	5	1152	G	C4-C5-C6	-7.68	114.19	118.80
36	1	1314	C	C6-N1-C2	-7.67	117.23	120.30
36	1	2726	C	N3-C2-O2	-7.67	116.53	121.90
1	6	1537	C	C6-N1-C2	-7.67	117.23	120.30
36	1	859	G	N1-C2-N2	-7.67	109.30	116.20
36	1	1156	C	N3-C2-O2	-7.67	116.53	121.90
36	1	44	U	N3-C4-O4	-7.67	114.03	119.40
36	1	1556	C	C6-N1-C2	-7.67	117.23	120.30
36	5	639	G	C5-C6-N1	-7.67	107.67	111.50
36	1	2719	U	N1-C2-O2	-7.66	117.44	122.80
36	5	649	A	C4-C5-N7	7.66	114.53	110.70
36	5	1182	A	O5'-P-OP2	7.66	119.89	110.70
36	5	2139	A	O5'-P-OP1	-7.66	98.81	105.70
36	5	2401	A	N7-C8-N9	7.66	117.63	113.80
36	1	2942	C	N3-C4-C5	7.66	124.96	121.90
36	1	2180	G	C2-N3-C4	-7.66	108.07	111.90
36	1	2941	A	C5-C6-N6	-7.66	117.58	123.70
36	1	1555	U	C5-C6-N1	-7.65	118.87	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2867	C	O5'-P-OP1	-7.65	98.81	105.70
36	1	1365	G	C8-N9-C4	-7.65	103.34	106.40
38	4	28	C	N1-C2-O2	7.65	123.49	118.90
36	5	3166	C	C6-N1-C2	-7.65	117.24	120.30
36	5	966	U	N3-C2-O2	-7.64	116.85	122.20
36	1	63	A	C5-N7-C8	-7.64	100.08	103.90
36	1	2649	A	C5-C6-N6	-7.64	117.59	123.70
1	6	1300	A	O5'-P-OP1	-7.64	98.82	105.70
36	5	1160	C	C2-N1-C1'	-7.64	110.40	118.80
36	5	2889	C	N3-C2-O2	-7.64	116.55	121.90
36	5	1121	U	N1-C2-O2	-7.64	117.45	122.80
36	1	648	C	N3-C4-N4	7.64	123.35	118.00
36	1	817	A	C2-N3-C4	7.64	114.42	110.60
36	5	2406	C	C6-N1-C2	7.64	123.36	120.30
36	1	86	G	C4-C5-N7	-7.63	107.75	110.80
36	1	2607	G	O5'-P-OP2	-7.63	98.83	105.70
36	5	806	A	C8-N9-C4	7.63	108.85	105.80
36	5	3054	U	N1-C2-O2	-7.63	117.46	122.80
36	1	1848	G	C5-C6-N1	7.63	115.31	111.50
36	1	2363	A	C5-C6-N6	7.63	129.80	123.70
36	5	578	A	O5'-P-OP2	7.63	119.86	110.70
36	5	2735	U	C6-N1-C2	-7.63	116.42	121.00
36	1	2658	G	O5'-P-OP2	-7.63	98.83	105.70
36	1	410	U	N1-C2-O2	-7.62	117.46	122.80
36	5	2931	C	N1-C2-O2	-7.62	114.33	118.90
36	1	22	G	C6-N1-C2	-7.62	120.53	125.10
36	1	410	U	C6-N1-C2	-7.62	116.43	121.00
37	7	37	G	C5-C6-O6	-7.62	124.03	128.60
1	2	1490	C	C6-N1-C2	-7.62	117.25	120.30
36	1	1154	A	C8-N9-C4	-7.62	102.75	105.80
36	5	1937	U	C5-C6-N1	-7.62	118.89	122.70
36	1	2949	U	O5'-P-OP2	-7.62	98.84	105.70
1	6	75	U	O4'-C1'-N1	7.61	114.29	108.20
36	1	801	A	N1-C2-N3	-7.61	125.49	129.30
1	6	557	G	N1-C6-O6	-7.61	115.33	119.90
1	6	1700	C	N1-C2-O2	7.61	123.47	118.90
36	5	2164	A	C8-N9-C4	-7.61	102.76	105.80
36	1	809	G	C5-C6-O6	-7.61	124.03	128.60
36	5	825	U	N3-C2-O2	-7.61	116.87	122.20
36	1	3043	C	N3-C4-N4	-7.61	112.68	118.00
1	6	1614	A	C4-C5-N7	7.61	114.50	110.70
36	5	2357	A	C8-N9-C4	7.60	108.84	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3362	A	C2-N3-C4	-7.60	106.80	110.60
36	1	1640	G	O5'-P-OP2	-7.60	98.86	105.70
36	5	97	U	O5'-P-OP2	-7.60	98.86	105.70
36	1	1139	G	C2-N3-C4	-7.60	108.10	111.90
1	6	889	U	N1-C2-O2	-7.60	117.48	122.80
36	1	1450	G	N1-C6-O6	-7.59	115.34	119.90
36	1	2397	A	N1-C6-N6	7.59	123.16	118.60
36	5	2692	A	N1-C6-N6	-7.59	114.04	118.60
1	6	794	U	N1-C2-O2	7.59	128.11	122.80
1	2	1455	G	C4-C5-N7	-7.59	107.76	110.80
36	5	2873	U	O5'-P-OP2	-7.59	98.87	105.70
36	1	949	C	C6-N1-C2	-7.59	117.27	120.30
36	1	2958	A	C5-C6-N1	7.59	121.49	117.70
36	5	2310	U	N1-C2-O2	7.59	128.11	122.80
36	5	3174	A	C5-N7-C8	-7.59	100.11	103.90
36	1	782	U	N3-C4-O4	-7.58	114.09	119.40
36	5	56	G	O5'-P-OP2	-7.58	98.88	105.70
36	5	3046	A	N1-C6-N6	-7.58	114.05	118.60
36	1	1454	A	O5'-P-OP1	-7.58	98.88	105.70
36	5	1194	G	N1-C6-O6	-7.58	115.35	119.90
1	2	553	G	C4-C5-C6	7.58	123.34	118.80
36	1	702	C	N1-C2-O2	-7.58	114.36	118.90
36	5	3084	C	O5'-P-OP1	-7.58	98.88	105.70
36	1	424	G	C4-C5-N7	-7.57	107.77	110.80
36	1	351	A	C8-N9-C4	7.57	108.83	105.80
36	5	641	C	C2-N1-C1'	-7.57	110.47	118.80
36	1	931	C	N3-C4-C5	7.57	124.93	121.90
36	1	2834	G	N1-C6-O6	7.57	124.44	119.90
36	5	1416	C	C6-N1-C2	-7.57	117.27	120.30
36	5	3209	A	C8-N9-C4	-7.57	102.77	105.80
36	1	2874	G	C5-C6-N1	-7.57	107.72	111.50
38	4	14	C	O5'-P-OP2	-7.56	98.89	105.70
1	2	608	U	N3-C2-O2	-7.56	116.91	122.20
36	1	2944	U	N3-C4-C5	7.56	119.14	114.60
1	2	863	A	N1-C6-N6	7.56	123.14	118.60
36	5	2888	U	N3-C4-O4	7.56	124.69	119.40
36	5	2199	G	C4-C5-N7	7.56	113.82	110.80
36	5	2656	A	O5'-P-OP2	-7.56	98.90	105.70
36	5	2736	A	O5'-P-OP2	-7.56	98.90	105.70
36	1	61	A	N1-C2-N3	7.55	133.08	129.30
36	1	663	C	N3-C4-N4	7.55	123.29	118.00
36	1	2513	U	O4'-C1'-N1	7.55	114.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1747	G	C8-N9-C4	7.55	109.42	106.40
1	2	61	A	N7-C8-N9	7.55	117.57	113.80
36	1	942	U	C5-C4-O4	-7.55	121.37	125.90
36	1	2886	U	C5-C4-O4	-7.55	121.37	125.90
36	5	1902	G	C5-C6-O6	-7.55	124.07	128.60
36	5	2136	C	C2-N3-C4	-7.55	116.13	119.90
36	1	229	G	N1-C6-O6	7.54	124.43	119.90
36	1	410	U	N1-C2-N3	7.54	119.43	114.90
36	1	420	G	O5'-P-OP2	-7.54	98.91	105.70
36	1	1660	C	O5'-P-OP2	-7.54	98.91	105.70
36	5	2623	G	N3-C4-N9	7.54	130.53	126.00
36	5	1373	A	N1-C6-N6	7.54	123.12	118.60
36	1	2302	G	N1-C6-O6	-7.54	115.38	119.90
36	1	2402	A	C8-N9-C4	-7.54	102.78	105.80
36	5	2753	G	N3-C2-N2	-7.54	114.62	119.90
36	5	1117	G	N7-C8-N9	-7.54	109.33	113.10
1	2	1145	U	N1-C2-O2	-7.54	117.53	122.80
36	1	1790	G	N1-C6-O6	7.54	124.42	119.90
37	3	83	U	N3-C4-C5	7.54	119.12	114.60
36	5	2249	G	N9-C4-C5	7.54	108.41	105.40
1	2	647	G	N3-C4-N9	-7.53	121.48	126.00
37	7	93	C	C6-N1-C2	-7.53	117.29	120.30
37	3	73	C	N1-C2-O2	7.53	123.42	118.90
36	5	1433	A	C5-C6-N6	-7.53	117.68	123.70
36	5	3003	G	C8-N9-C4	-7.53	103.39	106.40
36	1	3088	G	C5-C6-O6	7.52	133.11	128.60
36	5	338	A	C5-C6-N6	-7.52	117.68	123.70
36	1	2962	U	C5-C4-O4	-7.52	121.39	125.90
36	5	683	U	O5'-P-OP2	-7.52	98.93	105.70
36	5	1378	U	C5-C6-N1	-7.52	118.94	122.70
36	1	3269	U	C5-C4-O4	7.52	130.41	125.90
36	5	639	G	N1-C6-O6	7.52	124.41	119.90
36	1	817	A	O5'-P-OP1	-7.52	98.94	105.70
36	1	1547	G	C8-N9-C4	7.52	109.41	106.40
73	O7	65	ARG	NE-CZ-NH1	7.51	124.06	120.30
36	5	3243	A	C4-C5-C6	7.51	120.76	117.00
36	1	2688	U	N1-C2-N3	-7.51	110.39	114.90
36	1	44	U	C5-C6-N1	-7.51	118.95	122.70
1	6	1773	C	C4-C5-C6	7.51	121.15	117.40
36	1	2374	C	C2-N3-C4	-7.51	116.15	119.90
1	6	163	G	C8-N9-C4	-7.51	103.40	106.40
36	5	200	C	N3-C4-N4	7.50	123.25	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2864	A	O5'-P-OP1	-7.50	98.95	105.70
36	5	412	G	C8-N9-C4	-7.50	103.40	106.40
1	2	303	U	N3-C2-O2	-7.50	116.95	122.20
36	1	406	G	N1-C6-O6	-7.50	115.40	119.90
36	1	932	U	N1-C2-N3	7.50	119.40	114.90
36	1	2378	C	C5-C4-N4	-7.50	114.95	120.20
1	6	334	G	N1-C6-O6	-7.50	115.40	119.90
36	5	2849	C	N3-C4-C5	-7.50	118.90	121.90
36	5	3047	U	C5-C6-N1	-7.50	118.95	122.70
36	1	748	U	C5-C4-O4	-7.49	121.40	125.90
36	5	1304	A	O5'-P-OP1	-7.49	98.96	105.70
36	5	1306	G	C5-C6-O6	-7.49	124.10	128.60
36	5	2891	U	N3-C2-O2	-7.49	116.95	122.20
38	8	100	U	C2-N1-C1'	7.49	126.69	117.70
36	1	2973	G	N1-C6-O6	7.49	124.39	119.90
36	1	2142	A	C4-C5-C6	7.49	120.74	117.00
36	1	2296	A	O5'-P-OP1	-7.49	98.96	105.70
1	2	1145	U	N3-C4-O4	7.49	124.64	119.40
36	1	2850	G	C5-C6-O6	-7.49	124.11	128.60
1	6	941	A	N1-C6-N6	-7.49	114.11	118.60
36	5	2385	G	N1-C6-O6	7.49	124.39	119.90
36	1	2944	U	C4-C5-C6	-7.48	115.21	119.70
36	5	309	U	N1-C2-O2	-7.48	117.56	122.80
36	5	1481	A	C8-N9-C4	-7.48	102.81	105.80
12	C0	88	PRO	N-CA-CB	7.48	112.27	103.30
36	1	857	G	O5'-P-OP1	-7.48	98.97	105.70
36	1	3265	C	C6-N1-C2	7.48	123.29	120.30
36	5	1160	C	N3-C4-N4	-7.48	112.77	118.00
36	1	2827	U	C2-N3-C4	-7.48	122.51	127.00
36	1	1509	A	C8-N9-C4	7.47	108.79	105.80
36	5	1133	A	C5-C6-N1	7.47	121.44	117.70
36	5	1152	G	C4-C5-N7	7.47	113.79	110.80
36	5	1830	G	O5'-P-OP2	-7.47	98.97	105.70
1	2	934	C	C2-N1-C1'	7.47	127.02	118.80
1	6	1535	U	N3-C2-O2	-7.47	116.97	122.20
36	1	968	G	N7-C8-N9	7.47	116.83	113.10
36	5	612	U	O5'-P-OP1	-7.47	98.98	105.70
1	2	1363	U	N3-C2-O2	-7.47	116.97	122.20
36	1	648	C	C2-N1-C1'	7.47	127.01	118.80
36	1	2404	A	C5-C6-N1	7.47	121.43	117.70
36	1	2996	U	N1-C2-O2	7.46	128.02	122.80
36	5	617	G	N9-C4-C5	-7.46	102.42	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	776	U	C5-C4-O4	7.46	130.38	125.90
36	1	1351	U	N3-C2-O2	-7.46	116.98	122.20
36	1	2279	A	N1-C6-N6	7.46	123.08	118.60
36	1	3270	U	O5'-P-OP1	-7.46	98.98	105.70
36	5	2747	A	N1-C6-N6	-7.46	114.12	118.60
36	1	2314	U	N1-C2-N3	-7.46	110.42	114.90
1	6	453	U	C2-N1-C1'	7.46	126.65	117.70
36	5	1060	U	C6-N1-C2	7.46	125.47	121.00
36	5	3197	G	N3-C2-N2	-7.46	114.68	119.90
38	8	84	C	C6-N1-C2	-7.45	117.32	120.30
36	1	2653	C	C6-N1-C2	-7.45	117.32	120.30
36	5	358	G	N1-C6-O6	7.45	124.37	119.90
36	5	1598	G	N1-C6-O6	-7.45	115.43	119.90
37	7	49	G	O4'-C1'-N9	7.45	114.16	108.20
36	1	1377	G	N9-C4-C5	-7.45	102.42	105.40
36	1	2293	C	N1-C2-O2	7.45	123.37	118.90
36	5	804	C	N3-C4-C5	-7.45	118.92	121.90
36	1	1141	C	N1-C2-O2	-7.45	114.43	118.90
36	1	2973	G	C5-C6-O6	-7.45	124.13	128.60
36	1	3132	C	C6-N1-C2	-7.45	117.32	120.30
36	1	3344	A	C5-N7-C8	-7.45	100.18	103.90
36	1	42	C	C6-N1-C2	-7.44	117.32	120.30
36	1	2891	U	C2-N3-C4	-7.44	122.54	127.00
36	5	1128	U	C5-C6-N1	-7.44	118.98	122.70
36	1	584	G	C5-C6-O6	7.44	133.06	128.60
36	5	2838	A	C5-C6-N6	-7.44	117.75	123.70
36	1	2658	G	C8-N9-C4	7.44	109.37	106.40
1	6	1137	A	N7-C8-N9	-7.43	110.08	113.80
36	5	2996	U	N3-C2-O2	-7.43	117.00	122.20
36	5	190	U	N3-C2-O2	-7.43	117.00	122.20
36	5	2941	A	O4'-C1'-N9	-7.43	102.25	108.20
36	1	304	G	C8-N9-C4	-7.43	103.43	106.40
36	5	2870	C	N3-C4-N4	-7.43	112.80	118.00
36	1	1846	C	N1-C2-N3	7.43	124.40	119.20
36	5	1330	A	O5'-P-OP1	-7.43	99.02	105.70
36	1	2298	U	N3-C4-O4	-7.43	114.20	119.40
1	6	646	C	C6-N1-C2	-7.43	117.33	120.30
36	5	350	C	C6-N1-C2	-7.43	117.33	120.30
36	1	661	G	C5-C6-O6	-7.42	124.15	128.60
36	1	2323	G	N3-C4-C5	-7.42	124.89	128.60
36	1	29	C	C6-N1-C2	7.42	123.27	120.30
36	5	1343	A	C2-N3-C4	-7.42	106.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1762	A	C8-N9-C4	7.42	108.77	105.80
36	1	614	C	C6-N1-C2	7.42	123.27	120.30
36	1	661	G	C4-C5-N7	7.42	113.77	110.80
36	5	3245	A	C8-N9-C4	-7.42	102.83	105.80
36	1	2763	U	N3-C2-O2	7.41	127.39	122.20
36	1	646	A	N1-C2-N3	7.41	133.01	129.30
36	1	1421	G	C8-N9-C4	7.41	109.36	106.40
36	1	1366	A	C8-N9-C4	-7.41	102.84	105.80
36	1	3143	C	N1-C2-O2	-7.41	114.46	118.90
38	4	79	A	N7-C8-N9	7.41	117.50	113.80
1	6	1614	A	C5-N7-C8	-7.41	100.20	103.90
36	1	27	C	C2-N3-C4	-7.40	116.20	119.90
36	1	1374	G	N1-C2-N2	-7.40	109.54	116.20
36	1	2827	U	N1-C2-N3	7.40	119.34	114.90
1	6	380	U	N3-C2-O2	-7.40	117.02	122.20
36	1	635	G	C5-C6-O6	-7.39	124.16	128.60
36	1	3362	A	C4-C5-N7	7.39	114.40	110.70
36	1	2620	G	C5-C6-N1	7.39	115.19	111.50
36	1	2424	A	N1-C2-N3	-7.39	125.61	129.30
36	1	3135	U	C5-C6-N1	-7.39	119.01	122.70
1	6	426	G	O5'-P-OP2	-7.39	99.05	105.70
36	5	85	A	C8-N9-C4	7.39	108.76	105.80
36	5	1331	U	N3-C2-O2	7.39	127.37	122.20
36	1	53	G	C8-N9-C4	7.38	109.35	106.40
36	1	938	C	N1-C2-O2	-7.38	114.47	118.90
36	5	634	C	N3-C4-C5	7.38	124.85	121.90
1	2	1657	U	O4'-C1'-N1	7.38	114.11	108.20
36	5	2338	C	N1-C2-O2	-7.38	114.47	118.90
36	1	1660	C	N1-C2-O2	-7.38	114.47	118.90
64	N8	4	ARG	NE-CZ-NH1	-7.38	116.61	120.30
36	1	1399	A	C8-N9-C4	7.38	108.75	105.80
36	1	2640	A	N1-C6-N6	-7.38	114.17	118.60
36	5	1158	A	C6-C5-N7	-7.37	127.14	132.30
36	5	2401	A	C5-N7-C8	-7.37	100.21	103.90
36	1	2317	A	O5'-P-OP1	-7.37	99.07	105.70
37	3	88	G	N1-C2-N2	-7.37	109.56	116.20
36	5	3214	U	N3-C4-O4	-7.37	114.24	119.40
36	1	43	A	C8-N9-C4	7.37	108.75	105.80
36	1	2954	U	O5'-P-OP1	7.37	119.54	110.70
36	5	969	C	C5-C6-N1	-7.37	117.32	121.00
36	5	1160	C	C6-N1-C1'	7.37	129.64	120.80
36	5	2619	G	C5-C6-N1	7.37	115.19	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1114	U	N1-C2-N3	-7.37	110.48	114.90
36	1	1144	U	N1-C2-N3	7.37	119.32	114.90
36	5	2314	U	C2-N1-C1'	7.36	126.54	117.70
38	4	38	U	N3-C2-O2	-7.36	117.05	122.20
1	2	1104	U	O5'-P-OP2	-7.36	99.08	105.70
36	1	1318	A	N7-C8-N9	7.36	117.48	113.80
36	5	2735	U	C5-C6-N1	7.36	126.38	122.70
36	1	111	C	C2-N1-C1'	-7.35	110.71	118.80
36	1	295	A	O5'-P-OP1	-7.35	99.08	105.70
36	1	329	U	N1-C2-N3	7.35	119.31	114.90
36	1	1399	A	C2-N3-C4	-7.35	106.92	110.60
36	1	2143	A	C5-N7-C8	-7.35	100.22	103.90
36	1	78	U	N3-C4-O4	7.35	124.54	119.40
1	6	1127	G	N1-C2-N3	7.35	128.31	123.90
36	5	411	U	C2-N3-C4	-7.35	122.59	127.00
36	1	2614	G	N7-C8-N9	-7.35	109.43	113.10
38	4	97	A	C8-N9-C4	-7.35	102.86	105.80
36	1	642	U	C5-C6-N1	-7.34	119.03	122.70
36	1	897	U	O5'-P-OP1	-7.34	99.09	105.70
36	1	2978	U	O4'-C1'-N1	7.34	114.08	108.20
36	1	1145	G	C5-C6-O6	-7.34	124.19	128.60
36	5	2693	C	N3-C4-C5	7.34	124.84	121.90
36	1	2797	C	O5'-P-OP1	-7.34	99.09	105.70
36	5	38	U	O5'-P-OP1	7.34	119.51	110.70
36	5	2660	G	C8-N9-C4	7.34	109.34	106.40
36	1	347	G	C4-C5-N7	7.34	113.73	110.80
1	6	331	A	C2-N3-C4	-7.34	106.93	110.60
36	5	1870	C	C2-N3-C4	-7.33	116.23	119.90
36	5	3008	A	N1-C2-N3	7.33	132.97	129.30
36	1	1509	A	N9-C4-C5	-7.33	102.87	105.80
36	5	969	C	N3-C4-C5	7.33	124.83	121.90
36	1	1119	C	N3-C4-N4	-7.33	112.87	118.00
36	1	2169	G	N1-C6-O6	-7.33	115.50	119.90
1	6	119	A	C2-N3-C4	-7.33	106.94	110.60
36	5	2211	U	C5-C4-O4	7.33	130.29	125.90
36	5	2817	A	C2-N3-C4	7.33	114.26	110.60
36	1	1405	U	C5-C6-N1	-7.32	119.04	122.70
42	15	152	ARG	NE-CZ-NH1	7.32	123.96	120.30
36	1	878	G	OP1-P-O3'	7.32	121.31	105.20
36	1	1307	G	N9-C4-C5	7.32	108.33	105.40
36	1	2618	G	N1-C6-O6	-7.32	115.51	119.90
1	2	16	G	N3-C4-C5	-7.32	124.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	645	A	N3-C4-C5	-7.32	121.68	126.80
36	1	1144	U	C2-N3-C4	-7.32	122.61	127.00
36	5	928	C	O5'-P-OP2	-7.32	99.12	105.70
38	4	93	U	OP1-P-OP2	7.31	130.57	119.60
1	6	1537	C	N3-C4-C5	-7.31	118.97	121.90
36	1	2726	C	N1-C2-N3	7.31	124.32	119.20
36	1	2697	A	N1-C6-N6	-7.31	114.21	118.60
36	1	2247	G	N1-C6-O6	7.31	124.28	119.90
36	1	2602	G	C4-C5-N7	-7.31	107.88	110.80
36	1	2942	C	N1-C2-O2	-7.31	114.51	118.90
36	1	890	C	O5'-P-OP2	-7.31	99.12	105.70
36	1	1531	C	N3-C2-O2	-7.31	116.79	121.90
36	1	805	G	N9-C4-C5	-7.30	102.48	105.40
36	1	2619	G	O5'-P-OP1	-7.30	99.12	105.70
36	1	2773	C	O5'-P-OP2	-7.30	99.12	105.70
38	4	51	G	C8-N9-C4	7.30	109.32	106.40
1	6	93	A	N1-C6-N6	7.30	122.98	118.60
36	5	1372	C	C5-C6-N1	-7.30	117.35	121.00
36	5	3142	A	N1-C6-N6	7.30	122.98	118.60
36	1	1898	G	C5-C6-O6	-7.30	124.22	128.60
54	M8	174	ARG	NE-CZ-NH1	-7.30	116.65	120.30
36	5	2350	C	O5'-P-OP2	-7.30	99.13	105.70
36	5	3214	U	C5-C6-N1	-7.30	119.05	122.70
36	5	339	C	C6-N1-C1'	7.30	129.56	120.80
36	1	2777	G	C8-N9-C4	-7.30	103.48	106.40
37	3	88	G	N3-C2-N2	7.30	125.01	119.90
36	5	1208	U	C5-C4-O4	7.30	130.28	125.90
36	5	1838	G	N3-C2-N2	-7.30	114.79	119.90
1	2	453	U	N1-C2-O2	7.29	127.91	122.80
36	1	1368	U	C5-C4-O4	-7.29	121.52	125.90
36	1	55	G	C8-N9-C4	7.29	109.32	106.40
36	5	92	G	C5-C6-N1	7.29	115.15	111.50
36	5	1462	A	C4-C5-N7	7.29	114.35	110.70
36	1	2898	G	O4'-C1'-N9	-7.29	102.37	108.20
36	5	2707	C	N3-C4-C5	7.29	124.82	121.90
36	1	949	C	N3-C4-C5	-7.29	118.98	121.90
36	1	2550	U	N3-C2-O2	-7.29	117.10	122.20
1	6	351	C	N3-C4-N4	7.29	123.10	118.00
36	5	37	U	N1-C2-N3	7.29	119.27	114.90
36	5	3309	G	C6-C5-N7	-7.29	126.03	130.40
36	5	1416	C	C5-C6-N1	7.29	124.64	121.00
36	5	3209	A	N7-C8-N9	7.29	117.44	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	410	U	N3-C4-C5	-7.29	110.23	114.60
36	1	1141	C	C4-C5-C6	7.29	121.04	117.40
36	5	3392	U	C5-C4-O4	7.29	130.27	125.90
1	6	450	U	O5'-P-OP1	-7.28	99.14	105.70
36	5	920	A	OP1-P-OP2	-7.28	108.67	119.60
36	1	968	G	C5-N7-C8	-7.28	100.66	104.30
36	1	2942	C	N3-C2-O2	7.28	127.00	121.90
36	1	1390	A	C8-N9-C4	-7.28	102.89	105.80
36	5	2351	U	C5-C4-O4	7.28	130.27	125.90
1	2	1486	G	C5-N7-C8	-7.28	100.66	104.30
36	1	509	U	N3-C2-O2	-7.28	117.11	122.20
36	5	2820	A	N7-C8-N9	7.28	117.44	113.80
36	5	1292	C	C6-N1-C2	7.28	123.21	120.30
36	5	1906	G	C2-N3-C4	-7.28	108.26	111.90
38	4	67	U	N1-C2-N3	7.27	119.26	114.90
36	5	47	C	C6-N1-C2	7.27	123.21	120.30
36	1	55	G	N7-C8-N9	-7.27	109.47	113.10
36	1	970	A	C5-N7-C8	-7.27	100.27	103.90
36	1	3181	C	N1-C2-N3	7.27	124.29	119.20
36	5	2211	U	N3-C2-O2	-7.27	117.11	122.20
1	6	558	U	N1-C2-O2	7.26	127.89	122.80
36	5	2948	C	O5'-P-OP1	7.26	119.42	110.70
36	5	3060	C	N3-C4-N4	7.26	123.09	118.00
36	1	2129	U	C5-C6-N1	7.26	126.33	122.70
36	1	44	U	C5-C4-O4	7.26	130.25	125.90
36	5	2908	G	N9-C4-C5	7.26	108.30	105.40
36	5	1175	C	N3-C4-C5	7.26	124.80	121.90
36	5	1657	C	N1-C2-O2	7.26	123.25	118.90
36	1	786	A	N1-C6-N6	-7.25	114.25	118.60
36	1	2833	A	C8-N9-C4	7.25	108.70	105.80
36	1	3022	G	C8-N9-C4	-7.25	103.50	106.40
37	3	21	G	C8-N9-C4	7.25	109.30	106.40
38	8	63	G	C5-C6-O6	7.25	132.95	128.60
36	5	1373	A	C5-C6-N6	-7.25	117.90	123.70
1	2	581	U	C2-N1-C1'	7.25	126.40	117.70
36	1	159	A	N1-C6-N6	7.25	122.95	118.60
36	5	1396	C	N3-C4-C5	7.25	124.80	121.90
36	1	918	C	C6-N1-C2	-7.25	117.40	120.30
1	6	1783	C	O5'-P-OP2	-7.25	99.18	105.70
36	1	835	G	O4'-C1'-N9	7.25	114.00	108.20
36	5	2831	G	N3-C4-N9	7.25	130.35	126.00
36	1	2936	A	N1-C6-N6	-7.24	114.25	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	795	U	N3-C2-O2	-7.24	117.13	122.20
36	5	2772	C	P-O3'-C3'	7.24	128.39	119.70
36	5	3212	C	N1-C2-O2	-7.24	114.56	118.90
1	2	1198	G	C8-N9-C4	-7.24	103.50	106.40
38	4	89	A	C8-N9-C4	7.24	108.69	105.80
36	1	939	U	C2-N3-C4	-7.24	122.66	127.00
36	5	1060	U	N3-C4-C5	7.24	118.94	114.60
36	1	112	U	C6-N1-C1'	-7.23	111.07	121.20
36	1	651	G	C8-N9-C1'	-7.23	117.60	127.00
36	1	802	C	O5'-P-OP2	7.23	119.38	110.70
36	1	2634	U	C2-N3-C4	-7.23	122.66	127.00
36	5	2602	G	O5'-P-OP2	-7.23	99.19	105.70
1	2	602	U	O5'-P-OP1	-7.23	99.19	105.70
36	1	3309	G	N1-C6-O6	7.23	124.24	119.90
36	5	3096	C	N1-C2-O2	-7.23	114.56	118.90
36	1	435	C	C6-N1-C2	7.22	123.19	120.30
38	4	32	C	N3-C4-C5	7.22	124.79	121.90
38	4	61	A	C5-C6-N6	-7.22	117.92	123.70
36	5	1111	U	C5-C4-O4	-7.22	121.57	125.90
36	5	410	U	N1-C2-O2	-7.22	117.75	122.80
36	5	3197	G	N3-C4-C5	7.22	132.21	128.60
36	1	515	C	N3-C4-C5	-7.22	119.01	121.90
36	1	1307	G	C5-C6-O6	7.22	132.93	128.60
36	5	404	G	O5'-P-OP2	-7.22	99.21	105.70
36	5	1462	A	C5-C6-N6	-7.22	117.93	123.70
36	5	2936	A	O5'-P-OP2	7.21	119.36	110.70
1	6	433	C	O5'-P-OP1	-7.21	99.21	105.70
36	5	3179	U	N1-C2-O2	7.21	127.85	122.80
36	1	786	A	N9-C4-C5	7.21	108.68	105.80
36	5	1869	C	N3-C4-C5	7.21	124.78	121.90
36	1	824	C	C6-N1-C2	-7.21	117.42	120.30
36	1	1383	G	N1-C6-O6	7.21	124.22	119.90
36	5	610	G	C8-N9-C4	-7.21	103.52	106.40
36	5	1170	A	N1-C6-N6	7.21	122.92	118.60
36	1	283	G	C5-N7-C8	-7.20	100.70	104.30
36	1	716	A	C2-N3-C4	-7.20	107.00	110.60
36	5	3364	C	C6-N1-C2	-7.20	117.42	120.30
36	1	3319	U	N1-C2-O2	7.20	127.84	122.80
36	1	104	G	C6-C5-N7	-7.20	126.08	130.40
36	5	2300	G	C6-N1-C2	-7.20	120.78	125.10
36	5	2872	A	C5-C6-N1	-7.20	114.10	117.70
36	1	1896	A	O5'-P-OP1	-7.20	99.22	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	543	C	N1-C2-O2	7.20	123.22	118.90
1	6	1000	C	C2-N1-C1'	7.20	126.71	118.80
36	1	2944	U	C5-C6-N1	7.19	126.30	122.70
1	6	453	U	N3-C2-O2	-7.19	117.17	122.20
36	5	1054	A	N9-C4-C5	-7.19	102.92	105.80
1	2	192	U	C2-N1-C1'	7.19	126.33	117.70
36	5	2395	G	N1-C6-O6	7.19	124.21	119.90
37	7	120	C	C6-N1-C2	7.19	123.18	120.30
36	1	1269	U	C2-N1-C1'	7.19	126.32	117.70
36	5	2725	U	N1-C2-O2	-7.19	117.77	122.80
36	5	1113	G	C2-N3-C4	-7.19	108.31	111.90
36	5	2824	G	C6-N1-C2	-7.19	120.79	125.10
36	5	2880	U	O5'-P-OP1	-7.19	99.23	105.70
36	5	3161	C	C6-N1-C2	-7.19	117.43	120.30
36	1	338	A	OP2-P-O3'	7.18	121.00	105.20
36	1	2128	C	C6-N1-C2	-7.18	117.43	120.30
36	1	3272	C	C6-N1-C2	-7.18	117.43	120.30
36	5	640	U	OP1-P-OP2	-7.18	108.82	119.60
36	5	989	A	OP2-P-O3'	7.18	121.00	105.20
36	5	1852	G	N1-C6-O6	-7.18	115.59	119.90
36	5	1899	G	C8-N9-C4	-7.18	103.53	106.40
36	1	1541	G	C5-C6-O6	-7.18	124.29	128.60
38	8	25	G	N3-C2-N2	7.18	124.93	119.90
37	7	101	G	N1-C6-O6	7.18	124.21	119.90
36	5	2249	G	N3-C4-C5	-7.18	125.01	128.60
36	1	2847	A	O5'-P-OP1	-7.18	99.24	105.70
36	5	1514	G	C5-C6-O6	-7.18	124.29	128.60
36	5	3177	G	C2-N3-C4	-7.18	108.31	111.90
36	5	1902	G	O5'-P-OP2	7.18	119.31	110.70
1	2	1636	C	C6-N1-C2	-7.17	117.43	120.30
36	1	931	C	N3-C4-N4	-7.17	112.98	118.00
36	1	1433	A	C5-C6-N6	-7.17	117.96	123.70
36	1	2817	A	C5-C6-N1	7.17	121.29	117.70
36	1	2875	U	C6-N1-C2	-7.17	116.69	121.00
36	5	637	C	OP2-P-O3'	7.17	120.98	105.20
36	5	2411	U	N3-C4-O4	-7.17	114.38	119.40
36	1	1443	G	C8-N9-C4	-7.17	103.53	106.40
1	6	1122	G	O5'-P-OP1	-7.17	99.25	105.70
36	5	1140	G	C5-C6-O6	7.17	132.90	128.60
1	6	1117	U	C6-N1-C2	-7.17	116.70	121.00
36	5	2824	G	C5-C6-N1	7.17	115.08	111.50
36	5	3218	A	C4-C5-N7	7.17	114.28	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1136	A	C8-N9-C4	7.17	108.67	105.80
36	1	120	G	C8-N9-C4	7.17	109.27	106.40
36	1	905	U	C5-C6-N1	-7.17	119.12	122.70
36	5	2156	C	C6-N1-C2	7.17	123.17	120.30
36	5	2349	U	OP1-P-O3'	7.16	120.96	105.20
36	5	111	C	C6-N1-C2	7.16	123.17	120.30
36	5	2121	G	O5'-P-OP2	-7.16	99.25	105.70
36	5	2851	A	OP1-P-OP2	7.16	130.34	119.60
1	6	1629	G	OP2-P-O3'	7.16	120.95	105.20
36	5	1412	G	C8-N9-C4	-7.16	103.54	106.40
36	1	2416	U	O5'-P-OP2	-7.16	99.26	105.70
36	1	1445	U	C5-C6-N1	-7.16	119.12	122.70
1	2	1537	C	N3-C4-N4	7.15	123.01	118.00
36	1	2705	A	O5'-P-OP2	-7.15	99.26	105.70
36	1	52	A	C8-N9-C4	7.15	108.66	105.80
1	6	1031	U	C6-N1-C2	7.15	125.29	121.00
36	5	1301	A	C4-C5-N7	7.15	114.28	110.70
36	1	859	G	N3-C4-N9	7.15	130.29	126.00
1	6	794	U	C2-N1-C1'	7.15	126.28	117.70
15	C3	22	ALA	C-N-CD	-7.14	104.88	120.60
36	1	2334	U	O5'-P-OP2	-7.14	99.27	105.70
1	6	1145	U	N3-C4-C5	-7.14	110.31	114.60
36	5	937	G	C4-C5-N7	-7.14	107.94	110.80
36	5	2830	G	N3-C2-N2	-7.14	114.90	119.90
36	5	3217	C	C2-N1-C1'	-7.14	110.94	118.80
36	1	190	U	O5'-P-OP2	-7.14	99.27	105.70
36	5	2621	G	N3-C2-N2	-7.14	114.90	119.90
36	1	2873	U	N1-C2-O2	-7.14	117.80	122.80
36	1	3181	C	C5-C6-N1	-7.14	117.43	121.00
56	N0	40	ARG	NE-CZ-NH2	7.14	123.87	120.30
36	5	2234	G	C5-C6-N1	7.14	115.07	111.50
1	2	1733	C	N3-C4-N4	7.14	123.00	118.00
1	6	163	G	N7-C8-N9	7.14	116.67	113.10
1	6	901	G	C4-C5-N7	7.14	113.66	110.80
36	5	1158	A	C5-C6-N6	-7.14	117.99	123.70
36	5	1522	U	O5'-P-OP2	-7.14	99.28	105.70
36	1	2387	A	N1-C6-N6	7.13	122.88	118.60
1	6	1125	A	O5'-P-OP1	-7.13	99.28	105.70
36	1	895	A	C5-C6-N1	-7.13	114.13	117.70
36	5	3133	C	N3-C4-C5	-7.13	119.05	121.90
36	1	628	A	C8-N9-C4	7.13	108.65	105.80
36	1	2629	U	O5'-P-OP2	-7.13	99.28	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	794	U	N1-C2-O2	7.13	127.79	122.80
36	1	3209	A	C6-C5-N7	-7.13	127.31	132.30
1	6	943	C	O5'-P-OP1	-7.13	99.28	105.70
36	5	1662	G	O5'-P-OP1	-7.13	99.28	105.70
1	2	1274	C	N3-C4-N4	-7.13	113.01	118.00
36	1	958	C	C2-N3-C4	-7.13	116.34	119.90
36	1	2920	U	C5-C6-N1	-7.12	119.14	122.70
36	5	1402	C	C5-C6-N1	-7.12	117.44	121.00
36	5	969	C	C2-N3-C4	-7.12	116.34	119.90
36	5	2199	G	C5-C6-O6	-7.12	124.33	128.60
36	5	2350	C	O5'-P-OP1	7.12	119.24	110.70
37	7	10	C	C6-N1-C2	7.12	123.15	120.30
36	1	878	G	C4-C5-N7	-7.12	107.95	110.80
36	5	334	A	N7-C8-N9	-7.12	110.24	113.80
36	5	1665	C	N3-C4-C5	7.12	124.75	121.90
36	1	635	G	C6-N1-C2	-7.12	120.83	125.10
36	5	1379	G	C2-N3-C4	-7.12	108.34	111.90
1	6	402	C	C5-C4-N4	-7.11	115.22	120.20
36	1	968	G	C5-C6-N1	7.11	115.06	111.50
1	2	1798	U	C2-N1-C1'	7.10	126.22	117.70
36	5	3140	G	C5-C6-O6	-7.10	124.34	128.60
1	2	959	U	C2-N1-C1'	7.10	126.22	117.70
36	1	2811	A	N1-C6-N6	-7.10	114.34	118.60
36	1	28	C	N3-C2-O2	-7.10	116.93	121.90
36	1	1510	G	C6-C5-N7	-7.10	126.14	130.40
1	6	1796	C	C5-C6-N1	-7.10	117.45	121.00
10	S8	29	LEU	CA-CB-CG	7.10	131.62	115.30
36	1	2634	U	C5-C6-N1	-7.10	119.15	122.70
1	6	957	G	N1-C6-O6	7.10	124.16	119.90
36	1	939	U	N1-C2-N3	7.10	119.16	114.90
36	1	1192	C	N3-C4-C5	-7.09	119.06	121.90
36	1	2554	A	P-O3'-C3'	7.09	128.21	119.70
36	1	2762	A	C8-N9-C4	7.09	108.64	105.80
1	6	610	G	C8-N9-C1'	-7.09	117.78	127.00
36	5	1348	U	C6-N1-C2	-7.09	116.75	121.00
36	1	809	G	N9-C4-C5	-7.09	102.56	105.40
36	1	639	G	N1-C6-O6	7.09	124.15	119.90
36	5	287	G	O5'-P-OP1	-7.09	99.32	105.70
36	5	1340	G	C8-N9-C4	7.09	109.23	106.40
1	6	163	G	N3-C2-N2	-7.08	114.94	119.90
36	5	395	A	N1-C6-N6	7.08	122.85	118.60
1	2	1426	C	C4-C5-C6	-7.08	113.86	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	328	U	N3-C2-O2	-7.08	117.25	122.20
36	1	1153	A	O5'-P-OP1	-7.08	99.33	105.70
36	1	1292	C	C6-N1-C2	7.08	123.13	120.30
36	1	2175	U	C5-C6-N1	-7.08	119.16	122.70
36	1	2331	C	C2-N3-C4	-7.08	116.36	119.90
36	5	2402	A	C5-C6-N6	7.08	129.36	123.70
36	5	1918	C	O5'-P-OP2	-7.08	99.33	105.70
1	2	831	U	C5-C6-N1	7.07	126.23	122.70
36	5	369	A	N7-C8-N9	7.07	117.33	113.80
36	5	1155	C	C4-C5-C6	-7.07	113.86	117.40
36	1	931	C	C2-N3-C4	-7.07	116.37	119.90
36	1	963	G	O5'-P-OP2	-7.07	99.34	105.70
36	5	37	U	C6-N1-C2	-7.07	116.76	121.00
36	5	2732	G	O5'-P-OP2	-7.07	99.34	105.70
36	5	2872	A	C4-C5-N7	7.07	114.23	110.70
36	1	650	C	N1-C2-O2	-7.07	114.66	118.90
36	5	61	A	N1-C2-N3	7.07	132.83	129.30
36	5	341	G	C5-C6-O6	-7.07	124.36	128.60
36	5	1879	A	O5'-P-OP1	7.07	119.18	110.70
36	5	2397	A	C6-N1-C2	-7.07	114.36	118.60
36	1	702	C	C2-N3-C4	-7.06	116.37	119.90
36	5	96	G	O5'-P-OP2	-7.06	99.35	105.70
36	5	638	C	C6-N1-C2	-7.06	117.48	120.30
36	5	2334	U	O5'-P-OP1	7.06	119.17	110.70
36	5	35	A	O5'-P-OP2	-7.06	99.35	105.70
36	5	1387	G	O5'-P-OP1	-7.06	99.35	105.70
36	1	610	G	C8-N9-C4	7.05	109.22	106.40
36	1	1496	C	C5-C6-N1	7.05	124.53	121.00
36	5	1846	C	P-O3'-C3'	-7.05	111.24	119.70
36	1	2891	U	N1-C2-N3	7.05	119.13	114.90
36	1	333	G	C5-C6-O6	7.05	132.83	128.60
36	5	338	A	C4-C5-N7	7.05	114.22	110.70
36	5	661	G	N7-C8-N9	7.05	116.62	113.10
36	1	1493	G	O4'-C1'-N9	7.05	113.84	108.20
36	1	1386	A	N1-C2-N3	7.04	132.82	129.30
36	1	2123	G	C8-N9-C4	7.04	109.22	106.40
36	1	3045	G	C2-N3-C4	7.04	115.42	111.90
36	5	2848	G	C8-N9-C4	-7.04	103.58	106.40
36	1	2121	G	O5'-P-OP2	-7.04	99.36	105.70
36	1	1151	U	OP1-P-OP2	-7.04	109.04	119.60
36	1	1394	A	OP2-P-O3'	7.04	120.68	105.20
36	5	2860	U	P-O3'-C3'	-7.04	111.25	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2366	C	C5-C6-N1	7.04	124.52	121.00
36	5	370	U	N1-C2-O2	7.03	127.72	122.80
1	2	402	C	N3-C2-O2	7.03	126.82	121.90
1	2	1200	G	C8-N9-C4	-7.03	103.59	106.40
36	5	995	U	O5'-P-OP2	-7.03	99.38	105.70
36	1	1911	A	N1-C6-N6	7.03	122.81	118.60
36	5	75	G	C8-N9-C4	7.03	109.21	106.40
36	5	2372	A	P-O3'-C3'	7.03	128.13	119.70
36	5	436	A	OP1-P-OP2	-7.02	109.06	119.60
36	1	2413	A	C5-C6-N1	7.02	121.21	117.70
1	6	965	U	C5-C4-O4	-7.02	121.69	125.90
36	5	2412	G	C8-N9-C4	-7.02	103.59	106.40
1	2	1657	U	O5'-P-OP2	-7.02	99.38	105.70
36	1	1505	C	N3-C4-C5	7.02	124.71	121.90
1	6	337	G	C5-C6-O6	-7.02	124.39	128.60
36	5	339	C	C6-N1-C2	-7.02	117.49	120.30
36	5	2135	U	C5-C4-O4	-7.02	121.69	125.90
36	5	325	A	C6-N1-C2	-7.02	114.39	118.60
36	5	758	C	O5'-P-OP2	-7.02	99.39	105.70
36	1	644	G	N7-C8-N9	7.01	116.61	113.10
36	1	3362	A	N1-C2-N3	7.01	132.81	129.30
36	5	328	U	N3-C2-O2	-7.01	117.29	122.20
36	5	388	G	C4-C5-N7	7.01	113.61	110.80
36	1	86	G	N9-C4-C5	7.01	108.20	105.40
36	5	56	G	N1-C6-O6	-7.01	115.69	119.90
36	5	3362	A	O4'-C1'-N9	7.01	113.81	108.20
36	1	1048	A	N7-C8-N9	-7.01	110.30	113.80
1	6	1642	G	C5-C6-O6	-7.01	124.39	128.60
36	5	813	G	C5-C6-O6	-7.01	124.39	128.60
36	1	189	G	N3-C4-N9	7.01	130.20	126.00
38	8	104	A	C8-N9-C4	7.01	108.60	105.80
1	2	1082	C	N3-C2-O2	-7.00	117.00	121.90
36	1	1469	C	N1-C2-O2	7.00	123.10	118.90
38	8	100	U	N3-C2-O2	-7.00	117.30	122.20
36	5	875	G	N1-C6-O6	-7.00	115.70	119.90
77	q1	9	ARG	NE-CZ-NH1	7.00	123.80	120.30
36	1	1114	U	O5'-P-OP2	-7.00	99.40	105.70
36	1	1125	U	C5-C6-N1	-7.00	119.20	122.70
36	1	1468	A	N1-C2-N3	7.00	132.80	129.30
36	1	1943	C	C6-N1-C2	-7.00	117.50	120.30
1	2	287	G	O4'-C1'-N9	7.00	113.80	108.20
36	1	2387	A	N9-C4-C5	-7.00	103.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	876	A	N1-C6-N6	-7.00	114.40	118.60
36	1	1452	A	C2-N3-C4	-7.00	107.10	110.60
1	2	779	U	O4'-C1'-N1	6.99	113.80	108.20
36	5	2949	U	C2-N1-C1'	6.99	126.09	117.70
36	5	3130	A	N7-C8-N9	-6.99	110.30	113.80
36	5	1367	G	C4-C5-C6	6.99	122.99	118.80
36	1	810	A	N1-C6-N6	-6.99	114.41	118.60
36	1	2867	C	C5'-C4'-O4'	-6.99	100.71	109.10
36	5	704	U	N1-C2-O2	-6.99	117.91	122.80
36	1	304	G	C2-N3-C4	6.99	115.39	111.90
36	1	2814	G	O5'-P-OP1	-6.99	99.41	105.70
1	6	444	C	C6-N1-C2	6.99	123.09	120.30
36	5	2323	G	O5'-P-OP2	6.99	119.08	110.70
36	5	2945	G	C5-C6-O6	-6.99	124.41	128.60
36	5	697	A	N1-C6-N6	6.98	122.79	118.60
36	5	364	G	C4-C5-N7	6.98	113.59	110.80
36	5	903	U	N1-C2-O2	6.98	127.69	122.80
36	5	2747	A	N9-C4-C5	6.98	108.59	105.80
36	1	2343	C	C6-N1-C2	6.98	123.09	120.30
36	1	2623	G	N9-C4-C5	-6.98	102.61	105.40
36	1	3135	U	C6-N1-C2	6.98	125.19	121.00
36	5	358	G	N3-C4-C5	6.98	132.09	128.60
36	5	2964	G	C5-C6-O6	6.98	132.79	128.60
36	1	62	A	O5'-P-OP1	6.98	119.07	110.70
36	1	639	G	C5-C6-O6	-6.98	124.41	128.60
36	5	2985	C	C5-C6-N1	6.98	124.49	121.00
59	n3	45	ARG	NE-CZ-NH1	-6.98	116.81	120.30
36	1	25	U	N3-C4-O4	6.98	124.28	119.40
36	1	1843	C	C6-N1-C2	-6.97	117.51	120.30
36	5	350	C	N1-C2-O2	-6.97	114.72	118.90
36	5	1152	G	C5-C6-N1	-6.97	108.01	111.50
36	1	422	A	N1-C6-N6	-6.97	114.42	118.60
36	1	2182	A	N1-C6-N6	-6.97	114.42	118.60
36	5	646	A	O5'-P-OP2	-6.97	99.42	105.70
36	1	2848	G	O5'-P-OP2	-6.97	99.43	105.70
36	1	1820	U	P-O3'-C3'	6.97	128.06	119.70
36	5	1313	G	O5'-P-OP1	6.97	119.06	110.70
36	5	2158	A	C5-C6-N1	6.97	121.19	117.70
36	5	2704	A	O5'-P-OP1	-6.97	99.43	105.70
36	5	2820	A	C2'-C3'-O3'	6.97	124.85	113.70
36	1	575	G	N1-C6-O6	-6.97	115.72	119.90
36	1	801	A	O5'-P-OP1	6.97	119.06	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2142	A	OP1-P-O3'	6.97	120.53	105.20
36	5	194	U	N1-C2-N3	6.97	119.08	114.90
36	5	617	G	C6-C5-N7	-6.97	126.22	130.40
36	1	921	A	C8-N9-C4	-6.96	103.01	105.80
36	5	617	G	N1-C6-O6	6.96	124.08	119.90
38	8	82	U	O4'-C1'-N1	6.96	113.77	108.20
36	1	905	U	N1-C2-N3	6.96	119.08	114.90
10	s8	29	LEU	CA-CB-CG	6.96	131.31	115.30
36	1	1581	C	N1-C2-O2	6.96	123.08	118.90
36	5	2661	G	N1-C6-O6	-6.96	115.72	119.90
36	5	342	A	O5'-P-OP2	-6.96	99.44	105.70
36	1	1082	U	C6-N1-C2	-6.96	116.82	121.00
36	1	1351	U	C2-N1-C1'	6.96	126.05	117.70
36	1	2956	A	C8-N9-C4	-6.96	103.02	105.80
37	7	92	A	C8-N9-C4	6.96	108.58	105.80
1	2	1280	C	N3-C4-C5	-6.96	119.12	121.90
1	6	1658	G	C5-C6-O6	6.96	132.77	128.60
36	5	2631	U	OP1-P-O3'	6.96	120.50	105.20
36	5	3218	A	C5-N7-C8	-6.96	100.42	103.90
36	1	2130	G	C5-C6-O6	6.95	132.77	128.60
36	5	3090	U	C2-N3-C4	-6.95	122.83	127.00
36	1	586	C	N1-C2-O2	-6.95	114.73	118.90
36	5	2889	C	N1-C2-N3	6.95	124.06	119.20
36	1	974	G	N3-C4-C5	-6.95	125.13	128.60
36	5	985	U	O5'-P-OP2	-6.95	99.44	105.70
36	5	2849	C	C6-N1-C2	-6.95	117.52	120.30
36	1	696	C	N3-C4-C5	6.94	124.68	121.90
1	2	704	C	N1-C2-O2	6.94	123.07	118.90
36	1	1160	C	N1-C2-N3	-6.94	114.34	119.20
36	1	2383	C	C5-C6-N1	-6.94	117.53	121.00
36	5	2632	G	N1-C6-O6	-6.94	115.73	119.90
36	1	906	A	C6-N1-C2	-6.94	114.44	118.60
36	1	975	C	N1-C2-O2	-6.94	114.74	118.90
36	5	1371	G	C5-C6-N1	6.94	114.97	111.50
36	5	1331	U	N1-C2-O2	-6.94	117.94	122.80
36	5	2770	G	O5'-P-OP2	6.94	119.02	110.70
38	8	90	U	N1-C2-N3	-6.94	110.74	114.90
36	1	2176	U	N3-C4-O4	-6.93	114.55	119.40
36	5	3076	C	N1-C2-O2	6.93	123.06	118.90
36	5	2184	U	N1-C2-O2	6.93	127.65	122.80
36	1	801	A	C2-N3-C4	6.93	114.06	110.60
36	1	3316	A	C2-N3-C4	-6.93	107.14	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1154	A	N1-C2-N3	-6.93	125.84	129.30
36	5	1879	A	N7-C8-N9	6.93	117.26	113.80
36	5	2358	A	C8-N9-C4	6.93	108.57	105.80
36	1	608	A	N3-C4-N9	6.92	132.94	127.40
36	1	645	A	C5-C6-N6	-6.92	118.16	123.70
38	4	8	C	C5-C4-N4	-6.92	115.35	120.20
36	5	44	U	N1-C2-O2	-6.92	117.95	122.80
36	5	369	A	C8-N9-C4	-6.92	103.03	105.80
37	3	88	G	C5-N7-C8	6.92	107.76	104.30
1	2	767	U	N3-C2-O2	-6.92	117.36	122.20
36	1	981	U	O5'-P-OP2	-6.92	99.47	105.70
1	6	1581	C	C6-N1-C2	6.92	123.07	120.30
36	5	2400	G	C2-N3-C4	-6.92	108.44	111.90
59	n3	87	ARG	NE-CZ-NH2	-6.92	116.84	120.30
36	1	663	C	C6-N1-C2	6.92	123.07	120.30
1	6	1658	G	N1-C6-O6	-6.92	115.75	119.90
36	5	704	U	N3-C2-O2	6.92	127.04	122.20
36	5	3058	U	C2-N1-C1'	6.92	126.00	117.70
36	1	371	G	C4-C5-N7	6.91	113.57	110.80
36	1	1841	A	O5'-P-OP2	-6.91	99.48	105.70
1	6	978	A	C8-N9-C4	-6.91	103.04	105.80
36	5	2606	G	C8-N9-C4	-6.91	103.64	106.40
36	5	2946	A	N1-C6-N6	-6.91	114.45	118.60
36	1	1891	A	C2-N3-C4	-6.91	107.14	110.60
36	1	283	G	O4'-C1'-N9	-6.91	102.68	108.20
36	5	339	C	N1-C2-O2	-6.91	114.76	118.90
36	5	1868	G	C4-C5-N7	6.91	113.56	110.80
36	1	2950	G	N1-C6-O6	-6.90	115.76	119.90
36	1	1117	G	OP1-P-OP2	6.90	129.95	119.60
36	1	2874	G	C8-N9-C4	-6.90	103.64	106.40
36	5	2300	G	C2-N3-C4	6.90	115.35	111.90
36	1	2355	G	N1-C6-O6	6.90	124.04	119.90
36	5	2344	U	C2-N3-C4	-6.90	122.86	127.00
36	1	142	C	C6-N1-C2	-6.89	117.54	120.30
36	5	1838	G	OP1-P-O3'	6.89	120.36	105.20
36	5	1852	G	C5-C6-N1	6.89	114.95	111.50
36	5	2169	G	N1-C6-O6	-6.89	115.77	119.90
36	1	2396	G	N7-C8-N9	-6.89	109.66	113.10
16	c4	35	GLY	N-CA-C	6.89	130.32	113.10
36	5	3128	G	C5-C6-N1	6.89	114.94	111.50
1	2	1537	C	C5-C4-N4	-6.89	115.38	120.20
1	2	1568	C	P-O3'-C3'	6.89	127.97	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	391	A	N7-C8-N9	-6.89	110.36	113.80
36	1	304	G	N3-C2-N2	-6.89	115.08	119.90
36	1	2244	A	O5'-P-OP1	6.88	118.96	110.70
36	5	2726	C	N3-C4-N4	-6.88	113.18	118.00
36	5	645	A	O5'-P-OP2	6.88	118.96	110.70
36	5	2335	G	N1-C6-O6	-6.88	115.77	119.90
36	1	2714	G	C4-C5-N7	6.88	113.55	110.80
36	5	2886	U	O4'-C1'-N1	6.88	113.70	108.20
36	1	334	A	C8-N9-C4	-6.88	103.05	105.80
36	5	2274	U	N1-C2-O2	6.88	127.61	122.80
1	2	1241	G	O4'-C1'-N9	6.88	113.70	108.20
36	1	1339	C	N1-C2-O2	-6.88	114.77	118.90
36	1	2922	G	N1-C2-N2	-6.88	110.01	116.20
1	6	1774	G	N1-C6-O6	-6.88	115.77	119.90
36	5	2395	G	O5'-P-OP2	-6.88	99.51	105.70
36	5	3081	C	O5'-P-OP2	-6.88	99.51	105.70
38	8	90	U	C6-N1-C2	6.88	125.13	121.00
36	1	81	C	O5'-P-OP1	-6.88	99.51	105.70
36	1	155	G	N3-C4-N9	6.88	130.12	126.00
36	5	933	A	C4-C5-C6	6.88	120.44	117.00
36	1	3309	G	C5-C6-O6	-6.87	124.48	128.60
36	5	941	G	N3-C4-C5	-6.87	125.16	128.60
36	5	2983	C	C4-C5-C6	6.87	120.84	117.40
38	4	153	U	C6-N1-C2	6.87	125.12	121.00
1	6	1104	U	O5'-P-OP2	-6.87	99.52	105.70
36	5	3309	G	C4-N9-C1'	6.87	135.43	126.50
36	1	2314	U	P-O3'-C3'	-6.87	111.46	119.70
36	5	1926	C	N3-C2-O2	6.87	126.71	121.90
36	1	798	G	N3-C2-N2	-6.87	115.09	119.90
36	5	2913	C	O5'-P-OP1	-6.87	99.52	105.70
36	1	1386	A	C6-N1-C2	-6.87	114.48	118.60
49	M3	85	LEU	CA-CB-CG	6.87	131.09	115.30
1	6	1389	C	N3-C4-C5	6.87	124.65	121.90
36	5	900	G	N9-C4-C5	6.87	108.15	105.40
36	5	2756	C	OP2-P-O3'	6.87	120.30	105.20
36	1	85	A	N1-C6-N6	6.86	122.72	118.60
1	6	864	U	O4'-C1'-N1	6.86	113.69	108.20
36	5	750	G	N9-C4-C5	6.86	108.14	105.40
1	6	1773	C	C6-N1-C2	-6.86	117.56	120.30
36	1	2257	C	C6-N1-C2	-6.86	117.56	120.30
37	3	86	U	C2-N3-C4	-6.86	122.88	127.00
36	5	1116	G	O5'-P-OP1	-6.86	99.53	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	664	U	C5-C6-N1	-6.86	119.27	122.70
1	6	974	A	C8-N9-C4	6.86	108.54	105.80
36	5	1159	A	C8-N9-C4	6.86	108.54	105.80
1	6	350	U	N1-C2-O2	-6.86	118.00	122.80
36	5	2343	C	C6-N1-C2	6.86	123.04	120.30
36	1	1660	C	N3-C4-N4	6.86	122.80	118.00
36	5	817	A	C8-N9-C4	-6.86	103.06	105.80
36	5	2400	G	C6-C5-N7	-6.86	126.29	130.40
36	1	716	A	C4-C5-N7	6.85	114.13	110.70
36	1	808	A	N1-C6-N6	-6.85	114.49	118.60
36	1	2899	C	N1-C2-N3	6.85	124.00	119.20
36	5	968	G	N3-C2-N2	6.85	124.70	119.90
36	5	2142	A	C5-C6-N1	6.85	121.13	117.70
36	5	2385	G	C2-N3-C4	-6.85	108.47	111.90
36	1	1468	A	C2-N3-C4	-6.85	107.18	110.60
36	1	3031	G	O5'-P-OP2	-6.85	99.54	105.70
36	5	222	A	O5'-P-OP2	-6.85	99.54	105.70
36	5	1841	A	O5'-P-OP2	-6.85	99.53	105.70
1	2	1634	C	C6-N1-C2	6.85	123.04	120.30
36	1	1113	G	N9-C4-C5	6.85	108.14	105.40
36	1	2324	A	N9-C4-C5	6.85	108.54	105.80
1	6	1775	U	C5-C4-O4	6.84	130.01	125.90
36	5	2938	G	C5-C6-N1	6.84	114.92	111.50
36	1	614	C	N3-C4-C5	6.84	124.64	121.90
36	5	1051	U	C5-C4-O4	-6.84	121.79	125.90
36	5	3049	A	C5-C6-N1	-6.84	114.28	117.70
1	2	1345	A	O5'-P-OP2	-6.84	99.54	105.70
36	1	1098	A	C8-N9-C4	-6.84	103.06	105.80
36	5	2411	U	C4-C5-C6	-6.84	115.59	119.70
36	5	1833	G	N1-C6-O6	-6.84	115.80	119.90
36	1	1879	A	O4'-C1'-N9	6.84	113.67	108.20
36	1	2549	G	N1-C2-N2	-6.84	110.05	116.20
36	5	197	G	C4-N9-C1'	6.84	135.39	126.50
36	5	1885	U	C2-N1-C1'	-6.84	109.50	117.70
36	5	2385	G	N3-C4-C5	6.84	132.02	128.60
1	2	1454	G	N1-C6-O6	-6.83	115.80	119.90
36	1	1370	G	N3-C2-N2	6.83	124.68	119.90
36	1	1411	C	N3-C2-O2	-6.83	117.11	121.90
36	1	3057	U	N1-C2-O2	6.83	127.58	122.80
36	5	2932	U	N3-C4-C5	6.83	118.70	114.60
36	5	3025	C	N3-C2-O2	-6.83	117.12	121.90
36	5	2648	G	C5-C6-N1	6.83	114.92	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1200	G	C5-C6-O6	-6.83	124.50	128.60
36	1	1520	G	C5-N7-C8	6.83	107.72	104.30
36	1	2884	C	C6-N1-C2	6.83	123.03	120.30
36	5	2954	U	O4'-C1'-N1	6.83	113.66	108.20
36	1	826	G	O5'-P-OP1	-6.83	99.56	105.70
36	1	1324	U	O5'-P-OP1	6.83	118.89	110.70
36	5	930	U	N3-C4-O4	-6.83	114.62	119.40
36	5	1879	A	C5-C6-N6	-6.83	118.24	123.70
36	5	2376	G	C2-N3-C4	6.83	115.31	111.90
1	6	314	C	N3-C2-O2	-6.83	117.12	121.90
36	5	57	A	N9-C4-C5	-6.83	103.07	105.80
36	5	2327	U	C5-C6-N1	-6.83	119.29	122.70
1	2	1795	U	N1-C2-O2	-6.82	118.03	122.80
36	5	2310	U	C5-C4-O4	6.82	129.99	125.90
36	1	1488	G	C8-N9-C4	6.82	109.13	106.40
36	5	670	C	N1-C2-O2	-6.82	114.81	118.90
36	5	1880	U	N1-C2-N3	-6.82	110.81	114.90
38	8	113	U	C2-N1-C1'	6.82	125.89	117.70
36	1	2387	A	C8-N9-C4	6.82	108.53	105.80
36	5	1392	G	N1-C6-O6	6.82	123.99	119.90
36	1	704	U	N1-C2-N3	6.82	118.99	114.90
36	1	1507	G	C5-C6-O6	-6.82	124.51	128.60
36	5	1012	G	C4-N9-C1'	-6.82	117.64	126.50
36	1	1137	C	C5-C4-N4	-6.82	115.43	120.20
1	2	1030	A	N1-C6-N6	6.81	122.69	118.60
36	1	2682	C	O5'-P-OP2	-6.81	99.57	105.70
36	5	1239	C	C6-N1-C2	-6.81	117.58	120.30
36	5	3218	A	N1-C6-N6	6.81	122.69	118.60
61	n5	138	ARG	NE-CZ-NH2	6.81	123.71	120.30
36	5	2997	G	N3-C4-C5	6.81	132.01	128.60
38	4	113	U	C5-C6-N1	-6.81	119.30	122.70
36	5	204	A	C6-C5-N7	6.81	137.07	132.30
36	5	1116	G	C8-N9-C4	-6.81	103.68	106.40
36	5	290	G	O5'-P-OP1	-6.80	99.58	105.70
36	5	437	G	N9-C4-C5	6.80	108.12	105.40
36	5	2314	U	C5-C6-N1	6.80	126.10	122.70
36	5	1147	G	O4'-C1'-N9	6.80	113.64	108.20
36	1	397	A	C5-C6-N1	6.80	121.10	117.70
36	1	2282	U	N3-C4-C5	6.80	118.68	114.60
38	4	51	G	N9-C4-C5	-6.80	102.68	105.40
1	6	539	G	N7-C8-N9	6.80	116.50	113.10
36	5	883	A	O5'-P-OP2	6.80	118.86	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	351	A	N7-C8-N9	-6.80	110.40	113.80
36	1	2802	A	N9-C4-C5	6.80	108.52	105.80
36	5	1830	G	O5'-P-OP1	6.80	118.86	110.70
36	5	2826	U	N3-C2-O2	-6.80	117.44	122.20
36	5	3018	C	C6-N1-C2	-6.80	117.58	120.30
36	1	104	G	C5-C6-O6	-6.80	124.52	128.60
36	5	1161	G	C8-N9-C4	6.80	109.12	106.40
36	1	578	A	O5'-P-OP1	-6.79	99.58	105.70
1	2	73	U	N3-C2-O2	-6.79	117.44	122.20
1	2	158	U	N3-C2-O2	-6.79	117.44	122.20
36	1	1308	A	N7-C8-N9	6.79	117.20	113.80
36	1	817	A	N9-C1'-C2'	6.79	122.83	114.00
36	5	2397	A	N1-C6-N6	-6.79	114.53	118.60
36	5	2411	U	C6-N1-C2	6.79	125.08	121.00
38	8	58	G	C5-C6-N1	-6.79	108.10	111.50
36	1	646	A	O5'-P-OP1	6.79	118.85	110.70
36	1	2198	A	N7-C8-N9	-6.79	110.41	113.80
1	6	815	G	C4-C5-N7	6.79	113.52	110.80
36	5	2980	U	C6-N1-C2	-6.79	116.93	121.00
36	1	1199	C	C2-N3-C4	-6.79	116.51	119.90
36	5	741	U	O5'-P-OP1	-6.79	99.59	105.70
36	1	2730	G	N3-C2-N2	-6.79	115.15	119.90
36	1	2825	C	N3-C2-O2	-6.78	117.15	121.90
36	1	3362	A	C8-N9-C4	-6.78	103.09	105.80
1	6	158	U	P-O3'-C3'	6.78	127.84	119.70
36	5	2199	G	N1-C6-O6	6.78	123.97	119.90
36	5	2402	A	C6-N1-C2	6.78	122.67	118.60
37	7	6	C	N1-C2-O2	-6.78	114.83	118.90
1	2	794	U	N3-C2-O2	-6.78	117.45	122.20
36	1	2830	G	N3-C2-N2	-6.78	115.15	119.90
1	6	323	A	C8-N9-C4	-6.78	103.09	105.80
36	5	805	G	O5'-P-OP1	6.78	118.84	110.70
36	5	3060	C	N1-C2-O2	-6.78	114.83	118.90
36	1	2649	A	N9-C4-C5	-6.78	103.09	105.80
36	5	2983	C	O5'-P-OP1	-6.78	99.60	105.70
1	2	412	A	C5-C6-N1	-6.78	114.31	117.70
1	2	1363	U	N1-C2-O2	6.78	127.54	122.80
36	5	2626	A	O4'-C1'-N9	-6.78	102.78	108.20
1	2	1426	C	N3-C2-O2	6.78	126.64	121.90
36	1	3256	G	N1-C6-O6	6.78	123.97	119.90
36	5	2410	U	N1-C2-O2	-6.78	118.06	122.80
36	5	2832	C	O5'-P-OP2	-6.78	99.60	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1392	G	C5-C6-O6	-6.77	124.53	128.60
36	5	3154	C	C5-C6-N1	6.77	124.39	121.00
36	1	999	G	C5-C6-N1	6.77	114.89	111.50
36	1	2142	A	N3-C4-C5	-6.77	122.06	126.80
1	2	1455	G	N9-C4-C5	6.77	108.11	105.40
1	2	448	C	C6-N1-C2	-6.77	117.59	120.30
1	2	1748	G	C5-C6-O6	6.77	132.66	128.60
36	1	635	G	C4-C5-N7	6.77	113.51	110.80
36	1	2121	G	C5-C6-O6	6.77	132.66	128.60
1	2	1653	C	N3-C4-C5	-6.77	119.19	121.90
36	1	32	U	O5'-P-OP2	-6.77	99.61	105.70
36	1	396	A	O5'-P-OP1	-6.77	99.61	105.70
36	5	21	G	C8-N9-C4	6.77	109.11	106.40
1	2	610	G	C8-N9-C1'	-6.76	118.21	127.00
36	1	2549	G	N3-C4-N9	6.76	130.06	126.00
1	6	1280	C	N1-C2-O2	-6.76	114.84	118.90
36	5	3130	A	C5-N7-C8	6.76	107.28	103.90
36	1	281	G	N3-C2-N2	-6.76	115.17	119.90
1	6	44	U	N1-C2-O2	-6.76	118.07	122.80
36	5	2820	A	P-O3'-C3'	6.76	127.81	119.70
36	1	2763	U	C6-N1-C2	6.76	125.06	121.00
36	1	2814	G	N3-C4-N9	6.76	130.06	126.00
1	6	1747	G	O5'-P-OP2	-6.76	99.62	105.70
36	5	1906	G	O5'-P-OP1	-6.76	99.62	105.70
36	1	709	A	N7-C8-N9	-6.76	110.42	113.80
36	1	2143	A	C2-N3-C4	-6.76	107.22	110.60
36	5	2772	C	C2-N1-C1'	-6.76	111.37	118.80
36	1	2143	A	N1-C2-N3	6.75	132.68	129.30
36	1	948	C	N1-C2-O2	-6.75	114.85	118.90
36	1	1050	U	O5'-P-OP1	-6.75	99.62	105.70
36	1	651	G	C4-N9-C1'	6.75	135.28	126.50
36	5	1119	C	N3-C4-C5	6.75	124.60	121.90
36	1	2298	U	C5-C6-N1	-6.75	119.33	122.70
36	5	857	G	N1-C6-O6	6.75	123.95	119.90
36	1	2120	A	O5'-P-OP2	-6.75	99.63	105.70
36	1	2177	G	N1-C2-N2	-6.75	110.13	116.20
36	5	3392	U	C5-C6-N1	-6.75	119.33	122.70
37	7	38	U	C5-C4-O4	-6.75	121.85	125.90
36	1	1906	G	C5-C6-O6	-6.74	124.55	128.60
36	1	2947	G	N1-C2-N3	6.74	127.95	123.90
1	6	1361	U	C2-N1-C1'	6.74	125.79	117.70
36	5	2425	G	N3-C4-N9	-6.74	121.95	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1884	A	C4-C5-N7	6.74	114.07	110.70
1	6	923	A	O5'-P-OP2	-6.74	99.63	105.70
36	5	2351	U	C6-N1-C2	-6.74	116.96	121.00
36	1	1300	G	C4-C5-N7	6.74	113.50	110.80
36	1	3088	G	N1-C6-O6	-6.74	115.86	119.90
36	5	922	U	C4-C5-C6	6.74	123.74	119.70
36	5	1207	G	N1-C6-O6	-6.74	115.86	119.90
38	8	3	A	N1-C6-N6	-6.74	114.56	118.60
36	1	585	A	O5'-P-OP2	-6.74	99.64	105.70
36	5	875	G	N3-C4-C5	-6.74	125.23	128.60
36	1	2896	A	N1-C2-N3	6.73	132.67	129.30
36	5	1140	G	N1-C6-O6	-6.73	115.86	119.90
1	6	1731	A	N1-C6-N6	-6.73	114.56	118.60
36	5	1513	G	C8-N9-C4	-6.73	103.71	106.40
36	1	795	G	O5'-P-OP1	-6.73	99.64	105.70
36	1	2349	U	C2-N3-C4	-6.73	122.96	127.00
36	1	2982	A	C8-N9-C4	6.73	108.49	105.80
36	5	83	U	OP1-P-OP2	6.73	129.70	119.60
36	5	805	G	C2-N3-C4	-6.73	108.53	111.90
36	5	2913	C	N1-C2-O2	-6.73	114.86	118.90
36	1	2846	U	C5-C4-O4	6.73	129.94	125.90
36	5	1523	U	C5-C4-O4	6.73	129.94	125.90
36	1	1177	G	C6-N1-C2	-6.73	121.06	125.10
36	1	1428	A	N1-C6-N6	6.73	122.64	118.60
36	1	205	C	N3-C4-C5	6.72	124.59	121.90
36	1	1139	G	C5-C6-O6	6.72	132.63	128.60
36	5	2199	G	N7-C8-N9	6.72	116.46	113.10
36	1	1204	A	C8-N9-C4	6.72	108.49	105.80
36	1	1733	G	N3-C4-C5	-6.72	125.24	128.60
1	2	1773	C	N1-C2-O2	-6.72	114.87	118.90
36	1	767	U	O4'-C1'-N1	6.72	113.57	108.20
36	5	596	C	C6-N1-C2	-6.72	117.61	120.30
36	5	1409	G	N1-C6-O6	-6.72	115.87	119.90
36	5	3048	A	O5'-P-OP2	-6.71	99.66	105.70
1	2	18	C	C5-C6-N1	6.71	124.36	121.00
36	5	2353	G	N3-C4-N9	6.71	130.03	126.00
36	1	2343	C	C5-C6-N1	-6.71	117.64	121.00
1	6	1607	G	C4-C5-N7	-6.71	108.12	110.80
36	5	2434	U	N1-C2-N3	6.71	118.92	114.90
36	5	2871	G	C2-N3-C4	6.71	115.25	111.90
36	1	229	G	N1-C2-N2	6.71	122.24	116.20
36	1	1891	A	N3-C4-C5	6.71	131.50	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2887	A	N1-C6-N6	6.71	122.62	118.60
36	1	2899	C	P-O3'-C3'	6.71	127.75	119.70
36	5	1205	A	N9-C4-C5	6.71	108.48	105.80
36	5	2838	A	O5'-P-OP2	-6.71	99.66	105.70
36	5	2953	U	C5-C4-O4	-6.71	121.88	125.90
36	5	3166	C	C2-N1-C1'	6.71	126.18	118.80
36	1	1375	G	C6-C5-N7	-6.71	126.38	130.40
1	2	404	G	C8-N9-C4	6.70	109.08	106.40
36	1	653	A	C4-C5-N7	6.70	114.05	110.70
36	1	3368	U	C2-N1-C1'	-6.70	109.66	117.70
36	1	1307	G	N3-C4-N9	-6.70	121.98	126.00
36	5	2754	G	N1-C6-O6	-6.70	115.88	119.90
36	5	2835	U	C5-C6-N1	6.70	126.05	122.70
36	1	2623	G	C2-N3-C4	-6.70	108.55	111.90
38	4	81	U	N3-C2-O2	-6.70	117.51	122.20
36	5	76	G	N1-C6-O6	6.70	123.92	119.90
36	1	2522	G	N9-C4-C5	-6.70	102.72	105.40
36	5	1167	U	OP2-P-O3'	6.70	119.94	105.20
36	5	2915	U	C5-C6-N1	-6.70	119.35	122.70
36	1	2996	U	C4-C5-C6	-6.70	115.68	119.70
1	6	1615	C	N3-C4-C5	6.70	124.58	121.90
36	5	934	G	C5-C6-N1	6.70	114.85	111.50
1	2	1432	U	C6-N1-C2	6.70	125.02	121.00
36	5	660	A	O5'-P-OP2	-6.70	99.67	105.70
36	5	1587	A	C8-N9-C4	6.70	108.48	105.80
36	5	3161	C	C5-C6-N1	6.69	124.35	121.00
38	8	14	C	N1-C2-O2	-6.69	114.88	118.90
36	1	419	G	N1-C2-N2	-6.69	110.18	116.20
36	1	877	C	N3-C4-C5	6.69	124.58	121.90
36	5	877	C	C2-N3-C4	-6.69	116.55	119.90
36	1	297	G	O4'-C1'-N9	6.69	113.55	108.20
36	1	397	A	C2-N3-C4	6.69	113.94	110.60
36	1	2372	A	C2-N3-C4	6.69	113.95	110.60
36	5	820	A	O5'-P-OP1	-6.69	99.68	105.70
36	5	1155	C	C6-N1-C2	6.69	122.98	120.30
38	4	24	G	C5-C6-O6	-6.69	124.59	128.60
36	5	2347	U	C2-N3-C4	-6.69	122.99	127.00
36	5	2707	C	C6-N1-C2	6.69	122.98	120.30
36	1	1448	U	N1-C2-N3	6.69	118.91	114.90
36	1	704	U	N1-C2-O2	-6.69	118.12	122.80
36	5	1514	G	N1-C6-O6	6.69	123.91	119.90
36	5	1842	A	N9-C4-C5	-6.69	103.13	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1301	A	C5-N7-C8	-6.68	100.56	103.90
36	1	97	U	C5-C6-N1	-6.68	119.36	122.70
1	6	426	G	C4-N9-C1'	6.68	135.19	126.50
36	5	420	G	C5-C6-N1	6.68	114.84	111.50
36	5	793	C	N1-C2-O2	-6.68	114.89	118.90
36	5	2139	A	C5-C6-N6	6.68	129.05	123.70
36	1	1148	G	C8-N9-C4	6.68	109.07	106.40
36	1	104	G	C4-C5-N7	6.68	113.47	110.80
36	1	2420	C	C4-C5-C6	6.68	120.74	117.40
36	5	1158	A	C5-N7-C8	-6.68	100.56	103.90
1	2	380	U	N1-C2-O2	6.68	127.47	122.80
36	5	895	A	O5'-P-OP1	6.68	118.71	110.70
1	2	1280	C	N1-C2-O2	-6.67	114.90	118.90
36	1	2980	U	N1-C2-O2	-6.67	118.13	122.80
37	7	6	C	C2-N1-C1'	-6.67	111.46	118.80
36	1	2165	G	O5'-P-OP2	-6.67	99.69	105.70
36	1	3311	C	C6-N1-C2	6.67	122.97	120.30
36	5	1200	A	N9-C4-C5	6.67	108.47	105.80
1	6	1744	A	C5-C6-N6	-6.67	118.36	123.70
36	5	439	C	C6-N1-C2	-6.67	117.63	120.30
36	5	1928	G	N1-C6-O6	6.67	123.90	119.90
36	5	3374	U	N3-C4-C5	6.67	118.60	114.60
36	1	496	C	O5'-P-OP1	-6.67	99.70	105.70
1	6	1048	G	N9-C4-C5	-6.67	102.73	105.40
57	n1	136	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	2	106	U	C6-N1-C2	-6.67	117.00	121.00
1	6	1135	U	N3-C2-O2	-6.67	117.53	122.20
36	1	325	A	N1-C6-N6	-6.67	114.60	118.60
36	1	1156	C	N3-C4-N4	-6.67	113.33	118.00
38	8	42	G	C5-C6-O6	6.67	132.60	128.60
36	1	3108	G	C4-C5-N7	-6.67	108.13	110.80
36	5	2944	U	OP2-P-O3'	6.67	119.86	105.20
36	1	653	A	O5'-P-OP1	-6.66	99.70	105.70
36	1	1858	A	N3-C4-N9	6.66	132.73	127.40
36	5	2816	G	C8-N9-C4	6.66	109.06	106.40
36	1	1060	U	C6-N1-C2	6.66	125.00	121.00
36	1	2756	C	C6-N1-C2	-6.66	117.64	120.30
36	5	2824	G	N1-C2-N2	-6.66	110.21	116.20
36	5	2908	G	C4-C5-N7	-6.66	108.14	110.80
36	1	3183	A	N1-C6-N6	6.66	122.59	118.60
36	5	909	G	N7-C8-N9	-6.66	109.77	113.10
36	5	2375	G	C8-N9-C4	-6.66	103.74	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2679	A	O4'-C1'-N9	6.66	113.53	108.20
41	L4	327	LEU	CA-CB-CG	6.66	130.61	115.30
36	5	2660	G	N9-C4-C5	-6.66	102.74	105.40
36	1	1447	G	O5'-P-OP2	-6.65	99.71	105.70
38	4	58	G	O5'-P-OP1	6.65	118.68	110.70
36	5	633	C	N3-C4-C5	-6.65	119.24	121.90
36	5	1389	G	C5-C6-O6	-6.65	124.61	128.60
36	1	1318	A	C8-N9-C4	-6.65	103.14	105.80
36	5	740	G	O5'-P-OP1	-6.65	99.72	105.70
1	2	1600	A	C5-C6-N1	-6.65	114.38	117.70
36	5	2197	C	C2-N1-C1'	-6.65	111.49	118.80
36	1	2947	G	N3-C2-N2	-6.65	115.25	119.90
36	1	426	G	N3-C2-N2	6.64	124.55	119.90
1	6	1600	A	O4'-C1'-N9	6.64	113.52	108.20
36	1	1157	G	C5-C6-O6	6.64	132.59	128.60
36	1	934	G	C4-N9-C1'	6.64	135.13	126.50
36	1	1440	G	C5-C6-O6	6.64	132.59	128.60
36	1	1834	U	C4-C5-C6	6.64	123.68	119.70
36	1	3143	C	O5'-P-OP1	6.64	118.67	110.70
45	L8	189	LEU	CA-CB-CG	6.64	130.57	115.30
36	5	1499	C	C6-N1-C2	-6.64	117.64	120.30
1	6	351	C	C5-C4-N4	-6.64	115.55	120.20
1	6	815	G	N7-C8-N9	6.64	116.42	113.10
36	5	2141	U	N1-C2-N3	6.64	118.88	114.90
36	5	2353	G	N3-C4-C5	-6.64	125.28	128.60
36	5	3154	C	C6-N1-C2	-6.64	117.64	120.30
1	2	1092	A	N1-C6-N6	6.64	122.58	118.60
36	1	608	A	C6-C5-N7	-6.64	127.65	132.30
36	1	1367	G	C5-C6-O6	-6.64	124.62	128.60
36	5	2345	A	N1-C6-N6	6.64	122.58	118.60
36	1	1377	G	C8-N9-C4	6.63	109.05	106.40
36	5	2893	C	N3-C2-O2	6.63	126.54	121.90
1	2	600	U	N3-C2-O2	-6.63	117.56	122.20
36	1	339	C	OP1-P-OP2	-6.63	109.65	119.60
36	5	2290	C	C2-N3-C4	-6.63	116.58	119.90
36	1	2850	G	C4-C5-N7	6.63	113.45	110.80
36	5	1904	C	C5-C4-N4	-6.63	115.56	120.20
36	5	2133	U	N3-C4-C5	6.63	118.58	114.60
36	1	2831	G	C5-C6-O6	-6.63	124.62	128.60
38	4	102	U	N1-C2-N3	6.63	118.88	114.90
70	O4	8	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	6	371	G	C6-C5-N7	-6.63	126.42	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	579	G	N1-C6-O6	-6.63	115.92	119.90
36	5	2735	U	N3-C4-C5	-6.63	110.62	114.60
38	8	12	A	C5-C6-N1	6.63	121.01	117.70
1	6	572	C	C5-C4-N4	-6.63	115.56	120.20
1	6	1791	A	N1-C6-N6	6.63	122.58	118.60
36	5	421	G	N3-C2-N2	-6.63	115.26	119.90
36	5	1208	U	N3-C2-O2	-6.63	117.56	122.20
36	5	1939	G	OP2-P-O3'	6.63	119.78	105.20
38	8	82	U	C2-N1-C1'	-6.63	109.75	117.70
36	1	677	A	O5'-P-OP1	-6.62	99.74	105.70
36	1	2726	C	C5-C4-N4	6.62	124.84	120.20
1	6	101	U	N1-C2-O2	6.62	127.44	122.80
36	5	372	A	N9-C4-C5	-6.62	103.15	105.80
1	6	25	C	OP2-P-O3'	6.62	119.77	105.20
36	5	3020	U	N3-C4-O4	6.62	124.03	119.40
36	1	1858	A	N1-C2-N3	-6.62	125.99	129.30
36	1	645	A	C2-N3-C4	6.62	113.91	110.60
38	8	100	U	C6-N1-C2	-6.62	117.03	121.00
36	1	628	A	C2-N3-C4	-6.62	107.29	110.60
1	6	1775	U	N3-C4-O4	-6.62	114.77	119.40
36	5	908	G	C4-C5-N7	6.62	113.45	110.80
36	5	908	G	O4'-C1'-N9	-6.62	102.91	108.20
1	2	704	C	C2-N1-C1'	6.62	126.08	118.80
36	1	342	A	O5'-P-OP2	-6.62	99.75	105.70
36	1	1365	G	N3-C4-C5	-6.62	125.29	128.60
36	1	2402	A	N9-C4-C5	6.62	108.45	105.80
36	5	1792	C	C5-C6-N1	-6.62	117.69	121.00
36	5	2377	G	N1-C6-O6	-6.62	115.93	119.90
36	5	3174	A	N7-C8-N9	6.62	117.11	113.80
36	1	65	A	P-O3'-C3'	6.61	127.64	119.70
36	5	1407	A	C8-N9-C4	6.61	108.45	105.80
36	5	3026	G	C5-C6-O6	-6.61	124.63	128.60
38	8	54	A	C5-N7-C8	-6.61	100.59	103.90
1	2	421	A	N1-C6-N6	6.61	122.57	118.60
36	1	640	U	N3-C4-O4	6.61	124.03	119.40
36	1	1116	G	N3-C4-C5	-6.61	125.29	128.60
36	5	960	U	C5-C6-N1	-6.61	119.39	122.70
36	5	2372	A	N9-C4-C5	6.61	108.44	105.80
36	5	2603	G	N1-C6-O6	-6.61	115.93	119.90
44	17	232	ARG	NE-CZ-NH1	-6.61	116.99	120.30
36	1	347	G	N9-C4-C5	-6.61	102.75	105.40
36	1	1329	U	O4'-C1'-N1	6.61	113.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1426	C	N3-C4-C5	6.61	124.54	121.90
1	2	110	U	C6-N1-C2	-6.61	117.03	121.00
36	1	2642	A	C6-N1-C2	6.61	122.56	118.60
56	N0	155	ARG	NE-CZ-NH2	6.61	123.60	120.30
36	5	1012	G	N3-C4-N9	-6.61	122.03	126.00
36	5	2199	G	C5-N7-C8	-6.61	101.00	104.30
1	2	389	G	N1-C6-O6	-6.61	115.94	119.90
36	1	33	G	O5'-P-OP1	-6.61	99.75	105.70
36	1	2522	G	C8-N9-C1'	-6.60	118.42	127.00
36	1	2842	U	N3-C2-O2	-6.60	117.58	122.20
36	1	3123	A	C8-N9-C4	-6.60	103.16	105.80
77	q1	9	ARG	NE-CZ-NH2	-6.60	117.00	120.30
36	5	2376	G	N1-C6-O6	-6.60	115.94	119.90
36	1	81	C	N3-C4-C5	6.60	124.54	121.90
36	1	2160	G	N1-C6-O6	-6.60	115.94	119.90
1	2	1100	G	C6-C5-N7	-6.60	126.44	130.40
1	6	1280	C	N3-C4-C5	-6.60	119.26	121.90
36	5	2584	G	O5'-P-OP1	-6.60	99.76	105.70
1	2	240	U	OP2-P-O3'	6.59	119.71	105.20
36	1	1507	G	OP1-P-OP2	6.59	129.49	119.60
36	1	2977	G	N1-C6-O6	-6.59	115.94	119.90
11	s9	149	ARG	NE-CZ-NH1	6.59	123.60	120.30
36	5	3042	U	C5-C6-N1	-6.59	119.40	122.70
36	5	3140	G	C4-C5-N7	6.59	113.44	110.80
36	5	3330	A	N7-C8-N9	-6.59	110.50	113.80
36	5	3078	U	C2-N1-C1'	6.59	125.61	117.70
77	q1	23	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	2	1399	C	C5-C6-N1	6.59	124.30	121.00
36	1	2688	U	C6-N1-C2	6.59	124.95	121.00
36	5	1188	U	OP2-P-O3'	6.59	119.70	105.20
36	5	1791	C	N3-C2-O2	-6.59	117.29	121.90
36	5	2407	C	N3-C4-C5	-6.59	119.27	121.90
36	1	1492	G	C4-C5-N7	-6.59	108.17	110.80
36	1	1492	G	C5-N7-C8	6.59	107.59	104.30
36	1	2603	G	N3-C2-N2	6.59	124.51	119.90
36	1	3055	U	C2-N1-C1'	6.59	125.61	117.70
36	5	3308	C	N1-C2-O2	-6.59	114.95	118.90
36	1	2323	G	N3-C2-N2	6.59	124.51	119.90
36	1	2984	C	C4-C5-C6	6.59	120.69	117.40
36	1	3091	A	N1-C6-N6	6.59	122.55	118.60
36	5	3217	C	C5-C4-N4	6.59	124.81	120.20
36	5	1136	A	N7-C8-N9	-6.58	110.51	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	349	A	OP2-P-O3'	6.58	119.68	105.20
41	L4	313	LEU	CA-CB-CG	6.58	130.44	115.30
15	c3	64	ARG	NE-CZ-NH1	6.58	123.59	120.30
36	5	658	G	N3-C2-N2	-6.58	115.29	119.90
36	1	964	G	OP2-P-O3'	6.58	119.68	105.20
36	1	2828	G	O5'-P-OP1	-6.58	99.78	105.70
38	4	63	G	C5-C6-O6	6.58	132.55	128.60
36	5	349	A	OP2-P-O3'	6.58	119.68	105.20
36	5	1379	G	N9-C4-C5	-6.58	102.77	105.40
36	1	1307	G	P-O3'-C3'	6.58	127.59	119.70
52	M6	74	ARG	NE-CZ-NH2	-6.58	117.01	120.30
63	N7	135	ARG	NE-CZ-NH2	6.58	123.59	120.30
36	1	653	A	N9-C4-C5	-6.58	103.17	105.80
36	1	895	A	N3-C4-C5	6.58	131.40	126.80
36	5	804	C	N1-C2-O2	-6.58	114.95	118.90
36	5	1158	A	N9-C4-C5	-6.58	103.17	105.80
74	o8	31	LEU	CA-CB-CG	6.58	130.42	115.30
1	2	1267	G	C8-N9-C4	-6.57	103.77	106.40
36	1	1398	U	OP2-P-O3'	6.57	119.66	105.20
36	1	3055	U	C6-N1-C1'	-6.57	112.00	121.20
52	M6	110	PRO	C-N-CD	-6.57	106.14	120.60
1	2	1634	C	N1-C2-O2	-6.57	114.96	118.90
36	5	41	G	N1-C6-O6	6.57	123.84	119.90
36	1	2161	G	N1-C6-O6	-6.57	115.96	119.90
36	1	2810	C	C2-N3-C4	-6.57	116.61	119.90
36	5	2383	C	C4-C5-C6	6.57	120.69	117.40
36	5	2641	U	C5-C6-N1	-6.57	119.42	122.70
36	1	942	U	OP1-P-OP2	-6.57	109.75	119.60
36	1	2614	G	C5-N7-C8	6.57	107.58	104.30
36	1	3109	G	OP1-P-OP2	-6.57	109.75	119.60
36	1	53	G	N9-C4-C5	-6.57	102.77	105.40
36	1	72	C	C2-N1-C1'	-6.57	111.58	118.80
36	1	2821	C	N3-C2-O2	-6.57	117.30	121.90
36	1	2897	A	N7-C8-N9	-6.57	110.52	113.80
36	1	3135	U	N3-C4-C5	6.57	118.54	114.60
36	5	1205	A	C8-N9-C4	-6.57	103.17	105.80
36	5	3328	G	N1-C6-O6	-6.57	115.96	119.90
36	1	439	C	C2-N1-C1'	6.57	126.02	118.80
37	3	86	U	C5-C4-O4	-6.57	121.96	125.90
36	5	1852	G	C8-N9-C4	-6.57	103.77	106.40
36	5	2843	U	C6-N1-C2	-6.57	117.06	121.00
36	1	2585	G	N3-C4-N9	6.56	129.94	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	987	U	C5-C4-O4	6.56	129.84	125.90
36	5	3153	U	N1-C2-O2	6.56	127.39	122.80
36	1	1377	G	C4-C5-N7	6.56	113.42	110.80
36	5	2728	G	N9-C4-C5	6.56	108.03	105.40
36	1	2792	A	C8-N9-C4	-6.56	103.18	105.80
38	4	13	A	O5'-P-OP1	-6.56	99.80	105.70
12	c0	97	PRO	N-CA-CB	6.56	111.17	103.30
36	5	803	C	N3-C4-C5	-6.56	119.28	121.90
36	1	2833	A	N7-C8-N9	-6.56	110.52	113.80
36	5	1127	G	N3-C4-N9	6.56	129.93	126.00
1	2	767	U	C4-C5-C6	6.55	123.63	119.70
36	1	1434	G	N7-C8-N9	6.55	116.38	113.10
36	5	2828	G	OP2-P-O3'	6.55	119.62	105.20
36	1	65	A	N1-C6-N6	-6.55	114.67	118.60
36	1	1429	G	N3-C2-N2	6.55	124.49	119.90
36	5	1133	A	C6-N1-C2	-6.55	114.67	118.60
36	1	339	C	C2-N3-C4	-6.55	116.62	119.90
36	1	1309	U	N1-C2-O2	-6.55	118.22	122.80
36	1	1858	A	N3-C4-C5	-6.55	122.21	126.80
36	5	2212	C	C6-N1-C2	-6.55	117.68	120.30
1	6	331	A	C8-N9-C4	6.55	108.42	105.80
36	1	1381	A	C8-N9-C4	6.55	108.42	105.80
1	6	1164	G	C5-C6-O6	-6.55	124.67	128.60
1	6	1340	U	N3-C2-O2	-6.55	117.62	122.20
36	5	2572	C	N3-C2-O2	-6.55	117.32	121.90
36	1	85	A	C2-N3-C4	-6.54	107.33	110.60
36	5	2300	G	N3-C4-N9	6.54	129.93	126.00
1	2	1030	A	N9-C4-C5	-6.54	103.18	105.80
36	5	388	G	N1-C6-O6	6.54	123.83	119.90
36	5	813	G	N3-C4-C5	-6.54	125.33	128.60
36	1	3022	G	O4'-C1'-N9	6.54	113.43	108.20
36	5	326	U	C5-C4-O4	-6.54	121.97	125.90
36	1	1216	C	C6-N1-C2	-6.54	117.68	120.30
36	1	2706	G	C4-C5-N7	6.54	113.42	110.80
1	6	791	A	N1-C6-N6	6.54	122.52	118.60
36	1	84	U	C5-C6-N1	6.54	125.97	122.70
36	1	2571	U	C2-N1-C1'	6.54	125.55	117.70
36	5	1379	G	C8-N9-C4	6.54	109.02	106.40
36	1	2142	A	O5'-P-OP2	6.54	118.54	110.70
36	5	424	G	C5-C6-N1	6.54	114.77	111.50
36	1	936	A	C5-N7-C8	-6.54	100.63	103.90
36	1	143	G	N3-C4-C5	-6.53	125.33	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1198	C	C6-N1-C2	-6.53	117.69	120.30
36	5	911	C	N1-C2-O2	-6.53	114.98	118.90
36	1	2983	C	C6-N1-C2	-6.53	117.69	120.30
1	6	1539	G	O4'-C1'-N9	-6.53	102.97	108.20
56	n0	147	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	2	1162	C	C6-N1-C2	-6.53	117.69	120.30
36	1	3209	A	N7-C8-N9	6.53	117.06	113.80
36	5	861	C	O5'-P-OP1	6.53	118.53	110.70
36	1	2816	G	C8-N9-C4	6.53	109.01	106.40
36	5	2362	C	O5'-P-OP2	-6.53	99.83	105.70
36	5	2634	U	N1-C2-O2	-6.53	118.23	122.80
36	1	607	A	N1-C6-N6	-6.52	114.69	118.60
1	6	1145	U	N1-C2-O2	-6.52	118.23	122.80
36	1	48	A	N1-C6-N6	6.52	122.51	118.60
36	1	613	G	C4-C5-N7	6.52	113.41	110.80
36	1	2139	A	C6-N1-C2	-6.52	114.69	118.60
36	1	3143	C	N3-C2-O2	6.52	126.46	121.90
36	1	3264	G	C8-N9-C4	6.52	109.01	106.40
36	5	506	U	C5-C6-N1	-6.52	119.44	122.70
36	5	1520	G	C5-C6-O6	-6.52	124.69	128.60
36	1	189	G	N3-C2-N2	6.51	124.46	119.90
36	1	2940	A	C6-N1-C2	-6.51	114.69	118.60
36	5	948	C	C6-N1-C2	6.51	122.91	120.30
36	5	1343	A	N1-C2-N3	6.51	132.56	129.30
36	5	2293	C	C5-C4-N4	-6.51	115.64	120.20
36	5	201	A	C8-N9-C4	-6.51	103.19	105.80
1	2	941	A	C8-N9-C4	-6.51	103.20	105.80
36	1	340	C	N3-C2-O2	-6.51	117.34	121.90
36	1	2679	A	N1-C2-N3	6.51	132.56	129.30
1	6	1767	G	C8-N9-C4	6.51	109.00	106.40
36	5	408	A	C6-N1-C2	-6.51	114.69	118.60
56	n0	106	LEU	CA-CB-CG	6.51	130.28	115.30
1	2	1241	G	C4-C5-N7	6.51	113.40	110.80
36	1	2427	U	N1-C2-O2	6.51	127.36	122.80
36	5	1060	U	N3-C4-O4	-6.51	114.84	119.40
36	5	2836	C	C2-N3-C4	-6.51	116.64	119.90
36	1	963	G	O5'-P-OP1	6.51	118.51	110.70
1	6	28	A	OP1-P-O3'	6.51	119.52	105.20
36	1	507	U	N1-C2-O2	-6.51	118.25	122.80
36	1	2912	G	N1-C6-O6	-6.51	116.00	119.90
36	5	2234	G	C8-N9-C4	6.51	109.00	106.40
36	5	2849	C	OP2-P-O3'	6.51	119.51	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	941	G	C5-C6-N1	6.50	114.75	111.50
36	5	834	U	N3-C4-C5	6.50	118.50	114.60
1	6	426	G	C2-N3-C4	6.50	115.15	111.90
36	5	2246	G	O5'-P-OP1	-6.50	99.85	105.70
36	1	3265	C	N3-C4-C5	6.50	124.50	121.90
1	6	538	A	C8-N9-C4	-6.50	103.20	105.80
36	5	2208	A	O4'-C1'-N9	6.50	113.40	108.20
36	5	2283	G	C5-C6-O6	-6.50	124.70	128.60
36	5	2772	C	OP2-P-O3'	6.50	119.50	105.20
36	5	3092	C	O4'-C1'-N1	6.50	113.40	108.20
36	5	1060	U	C2-N3-C4	-6.50	123.10	127.00
36	1	2299	A	C4-C5-C6	6.50	120.25	117.00
68	O2	27	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	6	47	A	O5'-P-OP1	-6.50	99.85	105.70
36	1	2360	C	OP1-P-OP2	-6.50	109.86	119.60
36	5	613	G	C4-C5-N7	-6.50	108.20	110.80
36	1	3000	A	N7-C8-N9	-6.50	110.55	113.80
36	5	1365	G	N3-C2-N2	6.50	124.45	119.90
36	5	2290	C	C5-C6-N1	-6.50	117.75	121.00
36	1	1148	G	N9-C4-C5	-6.49	102.80	105.40
36	1	2282	U	C5-C4-O4	-6.49	122.00	125.90
36	5	1462	A	C5-N7-C8	-6.49	100.65	103.90
47	m0	21	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	2	1454	G	O5'-P-OP2	-6.49	99.86	105.70
36	1	2194	G	C6-C5-N7	-6.49	126.51	130.40
36	5	260	C	O5'-P-OP1	-6.49	99.86	105.70
36	5	1115	G	C8-N9-C4	-6.49	103.80	106.40
36	1	297	G	C8-N9-C4	-6.49	103.81	106.40
36	1	2896	A	C2-N3-C4	-6.49	107.36	110.60
36	5	968	G	N1-C2-N2	-6.49	110.36	116.20
36	5	2297	U	C2-N1-C1'	-6.49	109.92	117.70
1	2	736	C	C5-C6-N1	6.49	124.24	121.00
36	1	512	U	C5-C6-N1	-6.49	119.46	122.70
36	1	1367	G	N9-C4-C5	-6.49	102.81	105.40
36	1	2602	G	C5-N7-C8	6.49	107.54	104.30
36	5	2434	U	N3-C2-O2	-6.49	117.66	122.20
36	5	2827	U	O4'-C1'-N1	6.49	113.39	108.20
36	5	3276	G	C2-N3-C4	6.49	115.14	111.90
36	1	1295	G	N1-C6-O6	-6.48	116.01	119.90
36	1	2962	U	N3-C4-C5	6.48	118.49	114.60
36	5	2775	U	C5-C4-O4	6.48	129.79	125.90
36	1	412	G	N3-C2-N2	-6.48	115.36	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	43	A	O5'-P-OP1	-6.48	99.87	105.70
36	5	21	G	N3-C2-N2	6.48	124.44	119.90
36	5	88	A	C8-N9-C4	6.48	108.39	105.80
36	1	282	G	C8-N9-C4	-6.48	103.81	106.40
36	5	1628	C	C6-N1-C2	-6.48	117.71	120.30
36	5	2818	U	O5'-P-OP1	-6.48	99.87	105.70
1	2	44	U	N1-C2-O2	-6.48	118.27	122.80
36	1	922	U	C5-C4-O4	6.48	129.79	125.90
36	1	2124	G	C5-C6-O6	-6.48	124.71	128.60
36	5	1349	G	C8-N9-C4	6.48	108.99	106.40
36	5	3013	U	N3-C2-O2	-6.48	117.67	122.20
1	2	16	G	N3-C4-N9	6.47	129.88	126.00
36	1	3272	C	C5-C6-N1	6.47	124.24	121.00
36	1	2393	G	C2-N3-C4	6.47	115.14	111.90
36	1	2855	U	N3-C4-O4	-6.47	114.87	119.40
36	1	3344	A	C8-N9-C4	-6.47	103.21	105.80
36	5	1184	A	C5-C6-N1	6.47	120.94	117.70
36	1	72	C	C6-N1-C1'	6.47	128.56	120.80
1	2	1611	A	N7-C8-N9	6.47	117.03	113.80
44	L7	163	LEU	CA-CB-CG	-6.47	100.42	115.30
52	M6	94	ARG	NE-CZ-NH1	-6.47	117.06	120.30
36	5	810	A	N1-C2-N3	-6.47	126.07	129.30
36	5	1299	U	N3-C4-C5	6.47	118.48	114.60
36	1	2142	A	N9-C4-C5	6.47	108.39	105.80
36	1	2648	G	C5-C6-N1	6.47	114.73	111.50
36	5	190	U	N1-C2-O2	6.47	127.33	122.80
36	5	810	A	C2-N3-C4	6.47	113.83	110.60
36	5	2719	U	N1-C2-O2	-6.47	118.27	122.80
1	2	1199	G	O5'-P-OP2	-6.46	99.88	105.70
36	1	2813	A	C5-C6-N1	-6.46	114.47	117.70
36	1	2850	G	C6-C5-N7	-6.46	126.52	130.40
36	5	2623	G	C5-C6-O6	-6.46	124.72	128.60
36	5	3192	U	O5'-P-OP1	-6.46	99.88	105.70
36	5	933	A	C6-N1-C2	-6.46	114.72	118.60
36	1	836	A	C6-N1-C2	-6.46	114.72	118.60
36	1	1546	A	N1-C2-N3	-6.46	126.07	129.30
36	1	3174	A	C4-C5-N7	6.46	113.93	110.70
36	5	1327	C	N3-C4-C5	6.46	124.48	121.90
36	5	1488	G	OP1-P-O3'	6.46	119.41	105.20
36	5	3304	U	OP1-P-OP2	6.46	129.29	119.60
36	5	58	G	N1-C6-O6	6.46	123.78	119.90
36	5	1910	A	C8-N9-C4	6.46	108.38	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3371	G	N3-C4-N9	-6.46	122.12	126.00
38	8	91	C	N3-C4-C5	-6.46	119.32	121.90
1	2	553	G	C5-C6-O6	-6.46	124.72	128.60
36	5	2813	A	C4-C5-C6	6.46	120.23	117.00
1	2	427	C	N3-C2-O2	-6.46	117.38	121.90
36	1	2883	U	C5-C6-N1	6.46	125.93	122.70
36	1	2980	U	C2-N3-C4	-6.46	123.13	127.00
1	6	603	U	O5'-P-OP1	-6.46	99.89	105.70
36	5	1869	C	C5-C6-N1	-6.46	117.77	121.00
1	2	248	U	N1-C2-O2	-6.45	118.28	122.80
1	2	1796	C	N3-C4-C5	-6.45	119.32	121.90
36	1	2249	G	N1-C6-O6	-6.45	116.03	119.90
36	1	2424	A	C5-C6-N6	-6.45	118.54	123.70
36	1	2766	U	OP1-P-O3'	6.45	119.40	105.20
36	1	2139	A	C5-C6-N1	6.45	120.93	117.70
1	6	362	G	N3-C4-C5	-6.45	125.37	128.60
36	5	1407	A	C2-N3-C4	-6.45	107.38	110.60
36	5	1419	A	N1-C6-N6	-6.45	114.73	118.60
36	1	847	A	N1-C6-N6	6.45	122.47	118.60
1	6	1489	U	C2-N1-C1'	6.45	125.44	117.70
36	1	2620	G	C5-C6-O6	-6.45	124.73	128.60
36	5	3362	A	C2-N3-C4	-6.45	107.38	110.60
1	2	1082	C	C6-N1-C1'	-6.45	113.06	120.80
36	1	347	G	N3-C2-N2	6.45	124.41	119.90
36	1	960	U	C5-C6-N1	6.45	125.92	122.70
36	1	1420	C	C5-C4-N4	6.45	124.71	120.20
38	4	111	A	N1-C6-N6	6.45	122.47	118.60
70	O4	60	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	6	1584	G	C5-C6-O6	-6.45	124.73	128.60
36	5	2158	A	C6-N1-C2	-6.45	114.73	118.60
36	1	628	A	C5-C6-N1	-6.44	114.48	117.70
36	1	1464	G	O5'-P-OP2	-6.44	99.90	105.70
1	2	1177	C	O5'-P-OP1	-6.44	99.90	105.70
36	1	610	G	N3-C4-C5	6.44	131.82	128.60
36	1	1430	U	C2-N3-C4	-6.44	123.13	127.00
36	1	1835	A	C6-N1-C2	6.44	122.47	118.60
36	1	2134	G	C5-C6-O6	6.44	132.47	128.60
36	5	1126	G	C5-C6-N1	-6.44	108.28	111.50
36	5	1371	G	C5-C6-O6	6.44	132.47	128.60
36	5	2295	A	C5-C6-N1	6.44	120.92	117.70
36	1	2401	A	C5-C6-N1	-6.44	114.48	117.70
37	3	44	C	N1-C2-O2	6.44	122.76	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3220	G	O5'-P-OP1	-6.44	99.90	105.70
36	1	635	G	N9-C4-C5	-6.44	102.82	105.40
36	1	887	G	C4-C5-N7	-6.44	108.22	110.80
1	6	1753	A	C8-N9-C4	-6.44	103.22	105.80
36	5	2287	C	C6-N1-C2	-6.44	117.72	120.30
1	2	1200	G	C4-C5-C6	6.44	122.66	118.80
36	1	829	U	N1-C2-N3	6.44	118.76	114.90
36	1	1300	G	C5-C6-O6	-6.44	124.74	128.60
36	1	2715	A	O5'-P-OP1	-6.44	99.91	105.70
36	1	2883	U	O5'-P-OP1	6.44	118.42	110.70
36	5	1130	A	N3-C4-C5	-6.44	122.29	126.80
36	5	3303	G	N3-C2-N2	6.44	124.41	119.90
1	2	1537	C	C5-C6-N1	6.44	124.22	121.00
36	5	364	G	N9-C4-C5	-6.44	102.83	105.40
36	5	2603	G	N3-C2-N2	6.44	124.41	119.90
36	1	233	C	C6-N1-C2	6.43	122.87	120.30
36	1	3079	U	O5'-P-OP2	6.43	118.42	110.70
36	1	3182	G	C2-N3-C4	-6.43	108.68	111.90
36	5	1416	C	N3-C2-O2	-6.43	117.39	121.90
36	5	2650	U	N1-C2-N3	6.43	118.76	114.90
36	1	2379	U	O5'-P-OP2	-6.43	99.91	105.70
36	5	1680	G	N1-C6-O6	-6.43	116.04	119.90
36	5	2372	A	N7-C8-N9	6.43	117.02	113.80
37	3	89	G	C5-C6-N1	6.43	114.72	111.50
36	1	660	A	C2-N3-C4	6.43	113.81	110.60
36	1	783	A	C2-N3-C4	-6.43	107.39	110.60
1	6	758	U	N3-C2-O2	-6.43	117.70	122.20
36	5	662	U	C5-C4-O4	6.43	129.76	125.90
36	1	637	C	C5-C4-N4	6.43	124.70	120.20
36	5	99	A	C8-N9-C4	6.43	108.37	105.80
36	5	873	C	P-O3'-C3'	6.43	127.41	119.70
36	5	3044	G	N1-C2-N2	-6.43	110.41	116.20
36	1	287	G	C5-N7-C8	6.43	107.51	104.30
36	5	41	G	C8-N9-C4	6.43	108.97	106.40
36	5	329	U	C5-C6-N1	-6.43	119.49	122.70
36	5	1716	U	P-O3'-C3'	6.43	127.41	119.70
36	5	2383	C	N1-C2-O2	-6.43	115.04	118.90
36	1	2850	G	N9-C4-C5	-6.42	102.83	105.40
1	6	1009	U	C5-C6-N1	-6.42	119.49	122.70
36	5	1200	A	N7-C8-N9	6.42	117.01	113.80
36	5	2184	U	N3-C2-O2	-6.42	117.70	122.20
1	2	1258	U	N3-C2-O2	-6.42	117.70	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2314	U	N1-C2-O2	6.42	127.30	122.80
36	5	561	C	C6-N1-C2	-6.42	117.73	120.30
36	1	416	A	OP2-P-O3'	6.42	119.33	105.20
36	1	1353	U	N1-C2-O2	6.42	127.30	122.80
36	5	948	C	O5'-P-OP1	6.42	118.41	110.70
36	1	1371	G	N7-C8-N9	-6.42	109.89	113.10
36	1	1556	C	C6-N1-C1'	-6.42	113.10	120.80
36	5	1379	G	N1-C2-N2	-6.42	110.42	116.20
36	5	1884	A	C5-N7-C8	-6.42	100.69	103.90
36	1	1125	U	C2-N3-C4	-6.42	123.15	127.00
36	1	1589	A	O4'-C1'-N9	-6.42	103.06	108.20
36	1	2169	G	C4-C5-N7	-6.42	108.23	110.80
36	1	2396	G	C4-C5-N7	-6.42	108.23	110.80
36	1	2647	A	C2-N3-C4	6.42	113.81	110.60
36	5	2385	G	C4-C5-N7	6.42	113.37	110.80
36	1	2624	G	N1-C6-O6	6.42	123.75	119.90
36	5	706	A	C8-N9-C4	6.42	108.37	105.80
36	1	985	U	N3-C2-O2	6.41	126.69	122.20
36	1	2627	C	C6-N1-C2	6.41	122.86	120.30
1	6	1190	C	C6-N1-C2	6.41	122.86	120.30
35	sM	167	PRO	N-CA-CB	6.41	111.00	103.30
36	5	425	G	N9-C4-C5	-6.41	102.83	105.40
36	5	1103	A	N7-C8-N9	6.41	117.01	113.80
36	5	1487	G	N1-C6-O6	-6.41	116.05	119.90
36	1	2406	C	C5-C6-N1	-6.41	117.80	121.00
36	5	2134	G	C8-N9-C4	6.41	108.96	106.40
36	1	662	U	N3-C4-O4	-6.41	114.92	119.40
66	O0	84	LEU	CA-CB-CG	6.41	130.04	115.30
36	5	1002	A	O5'-P-OP2	-6.41	99.93	105.70
36	5	2661	G	C5-C6-N1	6.41	114.70	111.50
36	1	345	G	N1-C6-O6	-6.41	116.06	119.90
36	1	1661	G	N1-C2-N2	-6.41	110.43	116.20
1	6	933	A	O5'-P-OP2	-6.41	99.93	105.70
36	1	1477	A	O5'-P-OP1	-6.41	99.94	105.70
36	1	2802	A	C8-N9-C4	-6.41	103.24	105.80
36	1	1380	G	C2-N3-C4	-6.40	108.70	111.90
36	5	358	G	C5-C6-N1	-6.40	108.30	111.50
36	5	1323	G	N3-C2-N2	6.40	124.38	119.90
36	1	663	C	N3-C2-O2	6.40	126.38	121.90
36	5	326	U	N3-C2-O2	6.40	126.68	122.20
36	5	622	A	N1-C6-N6	6.40	122.44	118.60
36	5	2869	U	C2-N3-C4	-6.40	123.16	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	37	G	C4-C5-N7	6.40	113.36	110.80
36	1	364	G	O5'-P-OP2	6.40	118.38	110.70
36	5	2280	A	N1-C6-N6	6.40	122.44	118.60
36	1	267	G	C5-C6-O6	-6.40	124.76	128.60
36	1	1381	A	O5'-P-OP1	-6.40	99.94	105.70
36	1	2382	G	C5-C6-O6	6.40	132.44	128.60
36	5	668	G	N3-C2-N2	6.40	124.38	119.90
36	5	933	A	N1-C2-N3	6.40	132.50	129.30
36	5	2898	G	O4'-C1'-N9	-6.40	103.08	108.20
36	1	37	U	O5'-P-OP2	-6.40	99.94	105.70
36	1	412	G	C4-C5-N7	-6.40	108.24	110.80
36	1	1414	G	C4-C5-N7	6.40	113.36	110.80
36	5	636	C	C5-C4-N4	-6.40	115.72	120.20
36	5	2344	U	C5-C6-N1	-6.40	119.50	122.70
35	SM	167	PRO	N-CA-CB	6.39	110.97	103.30
36	1	2306	C	C5-C6-N1	6.39	124.20	121.00
36	1	2938	G	OP1-P-OP2	6.39	129.19	119.60
1	6	337	G	C4-C5-N7	6.39	113.36	110.80
36	5	579	G	C6-C5-N7	6.39	134.24	130.40
36	5	1186	G	C8-N9-C4	-6.39	103.84	106.40
36	5	1207	G	O5'-P-OP1	-6.39	99.94	105.70
36	5	2171	G	N3-C2-N2	-6.39	115.42	119.90
36	1	659	G	N3-C4-C5	-6.39	125.40	128.60
36	1	2636	A	C8-N9-C4	-6.39	103.24	105.80
1	6	308	C	N3-C4-N4	-6.39	113.53	118.00
1	2	1750	A	C8-N9-C4	-6.39	103.24	105.80
36	5	1180	A	O4'-C1'-N9	-6.39	103.09	108.20
36	1	47	C	C4-C5-C6	6.39	120.59	117.40
36	5	2747	A	C5-C6-N6	6.39	128.81	123.70
1	2	137	U	N3-C2-O2	-6.39	117.73	122.20
36	1	957	C	O5'-P-OP2	-6.39	99.95	105.70
36	1	1330	A	C5-C6-N1	-6.39	114.51	117.70
38	4	30	C	N1-C2-O2	-6.39	115.07	118.90
1	2	142	G	N3-C4-C5	6.39	131.79	128.60
36	1	1145	G	N1-C2-N3	-6.39	120.07	123.90
36	1	1309	U	C2-N3-C4	-6.39	123.17	127.00
36	1	1329	U	N1-C1'-C2'	-6.39	104.98	112.00
36	1	2808	A	C2-N3-C4	-6.39	107.41	110.60
36	5	2980	U	N1-C2-N3	6.39	118.73	114.90
41	14	90	PHE	C-N-CA	-6.39	108.89	122.30
36	1	54	C	N3-C4-N4	-6.38	113.53	118.00
1	6	21	U	N3-C4-O4	6.38	123.87	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	647	G	N3-C4-N9	-6.38	122.17	126.00
36	5	653	A	O5'-P-OP2	6.38	118.36	110.70
36	5	1888	U	C2-N3-C4	-6.38	123.17	127.00
36	5	3092	C	N3-C4-C5	6.38	124.45	121.90
47	m0	128	ARG	NE-CZ-NH2	-6.38	117.11	120.30
36	5	3242	G	N9-C4-C5	6.38	107.95	105.40
36	1	631	U	O5'-P-OP2	-6.38	99.96	105.70
36	1	2515	A	N1-C6-N6	-6.38	114.77	118.60
36	5	2725	U	C2-N3-C4	-6.38	123.17	127.00
37	3	91	G	C5-C6-O6	-6.38	124.77	128.60
36	5	2882	U	C2-N3-C4	-6.38	123.17	127.00
1	2	553	G	N7-C8-N9	6.38	116.29	113.10
1	2	941	A	N9-C4-C5	6.38	108.35	105.80
36	1	205	C	N3-C4-N4	-6.38	113.53	118.00
36	1	663	C	N1-C2-O2	-6.38	115.07	118.90
36	1	2116	G	C8-N9-C4	6.38	108.95	106.40
1	6	1551	U	N1-C2-O2	6.38	127.27	122.80
36	5	608	A	C5-C6-N6	-6.38	118.60	123.70
36	5	2109	U	N3-C2-O2	-6.38	117.73	122.20
36	1	2192	C	C5-C6-N1	-6.38	117.81	121.00
36	1	1390	A	N9-C4-C5	6.38	108.35	105.80
36	1	2607	G	N1-C6-O6	-6.38	116.08	119.90
36	1	1313	G	C6-C5-N7	-6.37	126.58	130.40
54	M8	178	ARG	NE-CZ-NH1	-6.37	117.11	120.30
36	1	715	A	N1-C6-N6	6.37	122.42	118.60
36	1	2619	G	C4-C5-N7	-6.37	108.25	110.80
1	6	1048	G	C5-C6-O6	-6.37	124.78	128.60
36	5	434	U	O5'-P-OP1	6.37	118.35	110.70
36	1	351	A	C2-N3-C4	-6.37	107.42	110.60
36	1	1319	G	N3-C2-N2	6.37	124.36	119.90
36	1	400	G	O5'-P-OP2	-6.37	99.97	105.70
11	s9	149	ARG	NE-CZ-NH2	-6.37	117.12	120.30
36	5	908	G	N1-C6-O6	6.37	123.72	119.90
36	5	1556	C	C6-N1-C2	-6.37	117.75	120.30
36	5	2794	G	C5-C6-N1	6.37	114.69	111.50
38	4	40	A	C4-C5-N7	6.37	113.88	110.70
1	6	609	U	C4-C5-C6	6.37	123.52	119.70
36	5	1363	A	N1-C6-N6	-6.37	114.78	118.60
36	5	1419	A	O5'-P-OP1	6.37	118.34	110.70
1	2	1200	G	N3-C2-N2	-6.37	115.44	119.90
36	5	792	G	O5'-P-OP1	-6.37	99.97	105.70
1	2	311	U	N3-C2-O2	-6.36	117.75	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	586	C	C6-N1-C2	6.36	122.85	120.30
36	5	2906	C	N1-C2-O2	-6.36	115.08	118.90
36	5	2912	G	OP1-P-OP2	6.36	129.15	119.60
36	1	959	C	C2-N3-C4	-6.36	116.72	119.90
36	1	1046	A	OP1-P-OP2	-6.36	110.06	119.60
1	6	813	U	N1-C2-O2	6.36	127.25	122.80
36	1	3344	A	C6-C5-N7	-6.36	127.85	132.30
1	6	603	U	N1-C2-O2	-6.36	118.35	122.80
36	5	649	A	C5-C6-N6	-6.36	118.61	123.70
36	5	2421	U	N1-C2-O2	-6.36	118.35	122.80
36	5	3328	G	O5'-P-OP2	-6.36	99.98	105.70
38	8	139	U	N3-C2-O2	-6.36	117.75	122.20
47	M0	48	LEU	CA-CB-CG	6.36	129.93	115.30
36	5	840	C	C6-N1-C2	-6.36	117.76	120.30
1	6	371	G	N1-C6-O6	6.36	123.72	119.90
1	6	965	U	N3-C4-C5	6.36	118.42	114.60
36	5	890	C	O5'-P-OP2	-6.36	99.98	105.70
36	5	2797	C	N1-C2-O2	-6.36	115.08	118.90
36	5	2816	G	N3-C2-N2	6.36	124.35	119.90
1	2	1241	G	C5-N7-C8	-6.36	101.12	104.30
36	1	873	C	P-O3'-C3'	6.36	127.33	119.70
36	1	1850	A	OP1-P-OP2	-6.36	110.07	119.60
36	1	2618	G	N9-C4-C5	6.36	107.94	105.40
38	4	61	A	N9-C4-C5	-6.36	103.26	105.80
36	5	645	A	C4-C5-C6	6.36	120.18	117.00
36	5	2719	U	O4'-C1'-N1	6.36	113.28	108.20
36	5	2922	G	N3-C2-N2	6.36	124.35	119.90
36	5	2953	U	N3-C2-O2	6.36	126.65	122.20
1	2	334	G	C2-N3-C4	-6.35	108.72	111.90
36	1	70	A	C8-N9-C4	6.35	108.34	105.80
36	1	2609	A	C5-C6-N6	6.35	128.78	123.70
35	sM	68	ARG	NE-CZ-NH2	-6.35	117.12	120.30
36	5	36	C	N3-C4-C5	-6.35	119.36	121.90
36	5	813	G	N3-C4-N9	6.35	129.81	126.00
40	l3	10	ARG	NE-CZ-NH2	-6.35	117.12	120.30
36	5	1132	C	O5'-P-OP1	-6.35	99.98	105.70
36	1	304	G	C4-C5-N7	-6.35	108.26	110.80
36	1	2773	C	C5-C4-N4	-6.35	115.76	120.20
36	1	3154	C	C2-N1-C1'	6.35	125.78	118.80
1	6	687	G	N3-C4-N9	-6.35	122.19	126.00
38	8	82	U	C6-N1-C1'	6.35	130.09	121.20
36	1	2130	G	N1-C2-N2	-6.35	110.49	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2953	U	N1-C2-N3	6.35	118.71	114.90
1	6	1091	A	N1-C6-N6	6.35	122.41	118.60
36	5	949	C	N1-C2-O2	-6.35	115.09	118.90
38	4	103	G	N3-C4-C5	-6.35	125.43	128.60
1	6	795	U	C6-N1-C2	-6.35	117.19	121.00
36	1	345	G	N3-C4-C5	-6.34	125.43	128.60
36	1	1495	U	C2-N1-C1'	-6.34	110.09	117.70
36	1	1898	G	N1-C6-O6	6.34	123.71	119.90
36	1	2622	C	N3-C4-N4	6.34	122.44	118.00
36	1	152	U	N1-C2-O2	-6.34	118.36	122.80
36	1	584	G	C4-C5-N7	-6.34	108.26	110.80
1	6	934	C	N1-C2-O2	6.34	122.71	118.90
1	6	1026	A	O5'-P-OP1	-6.34	99.99	105.70
36	5	1845	G	C8-N9-C4	-6.34	103.86	106.40
38	4	46	G	C8-N9-C1'	-6.34	118.76	127.00
36	5	649	A	N1-C6-N6	6.34	122.41	118.60
36	1	52	A	OP1-P-OP2	6.34	129.11	119.60
36	1	1858	A	C4-N9-C1'	6.34	137.71	126.30
36	1	2322	C	OP2-P-O3'	6.34	119.14	105.20
36	1	947	G	N3-C4-C5	-6.34	125.43	128.60
36	1	947	G	O5'-P-OP2	-6.34	100.00	105.70
36	5	370	U	N3-C2-O2	-6.34	117.76	122.20
36	5	971	G	N7-C8-N9	-6.34	109.93	113.10
36	5	1291	A	O5'-P-OP1	-6.34	100.00	105.70
36	1	509	U	N1-C2-N3	6.33	118.70	114.90
36	5	2362	C	C5-C6-N1	6.33	124.17	121.00
36	5	3245	A	N3-C4-C5	6.33	131.23	126.80
36	1	345	G	C5-C6-N1	6.33	114.67	111.50
36	5	608	A	C6-C5-N7	-6.33	127.87	132.30
36	1	397	A	O4'-C1'-N9	6.33	113.26	108.20
36	1	2585	G	N3-C4-C5	-6.33	125.44	128.60
13	c1	5	LEU	CA-CB-CG	6.33	129.86	115.30
36	5	282	G	O5'-P-OP1	-6.33	100.00	105.70
36	5	1157	G	C4-C5-N7	-6.33	108.27	110.80
36	5	1487	G	C5-N7-C8	6.33	107.46	104.30
36	5	2763	U	N1-C2-O2	-6.33	118.37	122.80
36	5	2809	C	C6-N1-C2	6.33	122.83	120.30
36	1	151	A	N1-C2-N3	6.33	132.46	129.30
1	6	308	C	C2-N1-C1'	-6.33	111.84	118.80
36	5	2361	A	C5-C6-N1	6.33	120.86	117.70
36	5	3048	A	OP1-P-OP2	6.33	129.09	119.60
36	5	631	U	N3-C4-C5	6.32	118.39	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1192	C	N1-C2-O2	6.32	122.69	118.90
36	5	1403	C	N3-C4-N4	-6.32	113.57	118.00
36	5	2927	C	OP2-P-O3'	6.32	119.11	105.20
36	5	3368	U	C2-N1-C1'	-6.32	110.11	117.70
36	1	3005	A	N1-C6-N6	-6.32	114.81	118.60
36	1	3182	G	C8-N9-C4	6.32	108.93	106.40
1	6	988	A	O5'-P-OP2	-6.32	100.01	105.70
36	5	3041	U	N3-C4-C5	6.32	118.39	114.60
36	1	1365	G	N3-C2-N2	6.32	124.33	119.90
36	1	2966	G	C5-C6-N1	6.32	114.66	111.50
36	5	585	A	OP1-P-OP2	6.32	129.08	119.60
36	5	1239	C	C2-N1-C1'	6.32	125.75	118.80
36	5	2770	G	O5'-P-OP1	-6.32	100.01	105.70
1	2	391	A	C4-C5-C6	-6.32	113.84	117.00
36	1	582	G	C6-C5-N7	6.32	134.19	130.40
1	2	959	U	N1-C2-O2	6.32	127.22	122.80
1	2	1291	G	C2-N3-C4	-6.32	108.74	111.90
36	1	660	A	N1-C2-N3	-6.32	126.14	129.30
36	5	2872	A	C4-C5-C6	-6.32	113.84	117.00
36	1	3109	G	O5'-P-OP2	6.31	118.28	110.70
36	5	1513	G	N3-C4-C5	-6.31	125.44	128.60
59	n3	12	ARG	NE-CZ-NH1	6.31	123.46	120.30
68	o2	105	ARG	NE-CZ-NH2	-6.31	117.14	120.30
36	1	608	A	C4-C5-C6	6.31	120.16	117.00
36	1	1903	U	C5-C4-O4	-6.31	122.11	125.90
36	5	75	G	N1-C6-O6	6.31	123.69	119.90
36	5	2294	U	N1-C2-N3	6.31	118.69	114.90
36	5	2861	U	N1-C2-N3	6.31	118.69	114.90
1	2	794	U	P-O3'-C3'	6.31	127.27	119.70
36	1	282	G	O5'-P-OP1	-6.31	100.02	105.70
38	4	9	A	C5-C6-N1	6.31	120.86	117.70
1	6	18	C	N3-C4-C5	-6.31	119.38	121.90
43	l6	46	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	2	1280	C	N3-C4-N4	6.31	122.42	118.00
36	5	414	U	C5-C6-N1	-6.31	119.55	122.70
36	5	570	A	O5'-P-OP1	-6.31	100.02	105.70
36	5	3123	A	C8-N9-C4	6.31	108.32	105.80
36	1	2685	C	C6-N1-C2	-6.31	117.78	120.30
1	2	992	A	C2-N3-C4	-6.30	107.45	110.60
36	1	782	U	N3-C4-C5	6.30	118.38	114.60
36	1	817	A	O5'-P-OP2	6.30	118.27	110.70
1	6	386	G	C8-N9-C4	6.30	108.92	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	14	187	LEU	CA-CB-CG	6.30	129.80	115.30
36	1	2403	G	O5'-P-OP2	-6.30	100.03	105.70
36	5	94	G	C5-C6-N1	6.30	114.65	111.50
36	5	990	U	C5-C6-N1	6.30	125.85	122.70
36	5	1115	G	OP1-P-O3'	6.30	119.07	105.20
36	1	907	G	C6-C5-N7	-6.30	126.62	130.40
38	8	83	C	N1-C2-O2	-6.30	115.12	118.90
36	1	709	A	C8-N9-C4	6.30	108.32	105.80
36	1	2802	A	OP2-P-O3'	6.30	119.06	105.20
1	6	29	U	C5-C4-O4	6.30	129.68	125.90
36	5	871	U	N3-C2-O2	-6.30	117.79	122.20
1	2	1761	U	C5-C4-O4	6.30	129.68	125.90
36	1	208	C	C6-N1-C2	-6.30	117.78	120.30
36	1	1414	G	C6-C5-N7	-6.30	126.62	130.40
36	5	31	C	N3-C4-C5	6.30	124.42	121.90
36	5	900	G	N1-C6-O6	-6.30	116.12	119.90
36	5	1405	U	O5'-P-OP2	-6.30	100.03	105.70
36	5	812	G	N1-C2-N2	-6.29	110.53	116.20
36	5	2631	U	N1-C2-O2	-6.29	118.39	122.80
36	1	718	G	C4-C5-C6	-6.29	115.02	118.80
36	1	3043	C	O5'-P-OP2	-6.29	100.04	105.70
36	5	204	A	N9-C4-C5	6.29	108.32	105.80
36	5	1865	A	C8-N9-C4	6.29	108.32	105.80
36	5	2928	C	N1-C2-N3	6.29	123.61	119.20
36	5	3177	G	N3-C4-N9	-6.29	122.22	126.00
36	1	351	A	OP1-P-OP2	6.29	129.04	119.60
36	1	2522	G	C4-C5-N7	6.29	113.32	110.80
36	1	3105	U	C5-C4-O4	-6.29	122.13	125.90
36	5	1150	A	C5-N7-C8	-6.29	100.75	103.90
36	5	1300	G	C4-C5-N7	6.29	113.32	110.80
36	5	1473	G	N3-C2-N2	-6.29	115.50	119.90
1	2	829	A	P-O3'-C3'	6.29	127.25	119.70
36	1	2404	A	C2-N3-C4	6.29	113.74	110.60
36	1	3044	G	N3-C2-N2	6.29	124.30	119.90
36	1	3302	U	N3-C4-O4	-6.29	115.00	119.40
36	5	351	A	N1-C6-N6	6.29	122.37	118.60
36	1	1506	A	O5'-P-OP2	-6.29	100.04	105.70
36	1	2993	G	C6-N1-C2	-6.29	121.33	125.10
36	5	364	G	C5-C6-O6	-6.29	124.83	128.60
36	5	938	C	C2-N3-C4	-6.29	116.76	119.90
36	5	2199	G	C8-N9-C4	-6.29	103.89	106.40
36	1	2616	C	N1-C2-O2	6.29	122.67	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1461	A	N7-C8-N9	-6.29	110.66	113.80
36	5	2158	A	N1-C6-N6	-6.29	114.83	118.60
36	5	3309	G	N3-C4-C5	-6.29	125.46	128.60
36	5	410	U	N3-C2-O2	6.28	126.60	122.20
36	5	1157	G	OP2-P-O3'	6.28	119.03	105.20
36	5	1604	G	N3-C4-N9	6.28	129.77	126.00
36	1	2920	U	N1-C2-N3	6.28	118.67	114.90
36	1	228	U	N3-C2-O2	-6.28	117.80	122.20
36	1	2706	G	C4-N9-C1'	6.28	134.66	126.50
36	5	2852	C	N1-C2-O2	-6.28	115.13	118.90
1	2	647	G	N3-C2-N2	-6.28	115.50	119.90
1	6	616	G	N9-C4-C5	6.28	107.91	105.40
36	1	627	U	N3-C2-O2	6.28	126.59	122.20
36	1	948	C	N3-C2-O2	6.28	126.30	121.90
36	1	3275	U	OP1-P-O3'	6.28	119.01	105.20
36	1	3107	U	N1-C2-O2	6.28	127.19	122.80
36	5	127	G	N1-C6-O6	6.28	123.67	119.90
1	2	48	G	OP2-P-O3'	6.27	119.00	105.20
36	1	1334	U	N3-C4-O4	6.27	123.79	119.40
37	7	35	C	C5-C6-N1	-6.27	117.86	121.00
36	1	645	A	C5-C6-N1	6.27	120.84	117.70
36	1	974	G	N3-C4-N9	6.27	129.76	126.00
36	1	1620	U	C2-N1-C1'	6.27	125.23	117.70
36	5	2794	G	C5-C6-O6	-6.27	124.84	128.60
36	1	942	U	O5'-P-OP2	-6.27	100.06	105.70
36	1	3259	U	C5-C6-N1	6.27	125.84	122.70
36	1	1098	A	N7-C8-N9	6.27	116.93	113.80
36	5	1064	A	O4'-C1'-N9	-6.27	103.19	108.20
36	5	1642	A	N1-C6-N6	6.27	122.36	118.60
36	5	2531	C	O4'-C1'-N1	6.27	113.22	108.20
36	5	208	C	N3-C2-O2	-6.27	117.51	121.90
36	5	3050	U	N3-C2-O2	-6.27	117.81	122.20
1	2	61	A	C8-N9-C4	-6.27	103.29	105.80
36	1	1891	A	N3-C4-N9	-6.27	122.39	127.40
36	1	894	G	C5-C6-O6	-6.26	124.84	128.60
36	5	365	A	N1-C6-N6	6.26	122.36	118.60
37	7	75	G	N1-C6-O6	6.26	123.66	119.90
36	1	2376	G	C5-C6-N1	6.26	114.63	111.50
1	6	1048	G	C8-N9-C4	6.26	108.90	106.40
36	5	641	C	N1-C2-N3	6.26	123.58	119.20
36	5	1083	G	O5'-P-OP1	-6.26	100.06	105.70
36	5	2531	C	N1-C2-O2	6.26	122.66	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1835	A	C5-C6-N1	-6.26	114.57	117.70
36	5	2725	U	C5-C4-O4	-6.26	122.14	125.90
36	5	2894	C	N3-C4-C5	6.26	124.40	121.90
36	1	3351	U	C5-C6-N1	6.26	125.83	122.70
38	4	13	A	N7-C8-N9	6.26	116.93	113.80
36	5	649	A	C6-C5-N7	-6.26	127.92	132.30
36	1	329	U	C2-N3-C4	-6.26	123.25	127.00
1	6	805	U	C6-N1-C2	-6.26	117.25	121.00
36	5	92	G	N3-C2-N2	6.26	124.28	119.90
36	5	627	U	C5-C6-N1	6.26	125.83	122.70
36	5	2699	G	C8-N9-C4	6.26	108.90	106.40
36	5	3374	U	C6-N1-C2	6.26	124.75	121.00
36	1	399	A	O5'-P-OP1	-6.25	100.07	105.70
1	2	1514	U	O5'-P-OP1	-6.25	100.07	105.70
36	5	955	U	C2-N3-C4	-6.25	123.25	127.00
36	5	1130	A	C5-C6-N1	6.25	120.83	117.70
36	5	2625	C	OP1-P-O3'	6.25	118.96	105.20
36	1	102	C	N1-C2-O2	-6.25	115.15	118.90
36	1	803	C	O5'-P-OP1	6.25	118.20	110.70
36	1	983	A	N1-C6-N6	6.25	122.35	118.60
1	6	144	U	N1-C2-N3	6.25	118.65	114.90
36	5	3034	C	N1-C2-O2	-6.25	115.15	118.90
36	1	334	A	C6-N1-C2	-6.25	114.85	118.60
36	1	1434	G	C8-N9-C4	-6.25	103.90	106.40
1	6	536	C	C6-N1-C2	-6.25	117.80	120.30
36	5	1169	A	C5-C6-N1	-6.25	114.58	117.70
36	5	1348	U	O4'-C1'-N1	6.25	113.20	108.20
36	1	59	G	N1-C6-O6	6.25	123.65	119.90
36	1	766	U	O5'-P-OP1	-6.25	100.08	105.70
36	1	3121	U	OP1-P-O3'	6.25	118.95	105.20
38	4	56	G	N1-C2-N2	-6.25	110.58	116.20
1	6	1058	U	OP1-P-O3'	6.25	118.95	105.20
1	2	352	A	O5'-P-OP1	-6.25	100.08	105.70
36	1	62	A	C2-N3-C4	6.25	113.72	110.60
36	1	2824	G	C5-C6-N1	6.25	114.62	111.50
36	5	366	A	N1-C6-N6	6.25	122.35	118.60
36	5	931	C	C2-N3-C4	-6.25	116.78	119.90
36	5	1604	G	C8-N9-C1'	-6.25	118.88	127.00
36	5	2550	U	N3-C2-O2	-6.25	117.83	122.20
36	5	2860	U	N3-C2-O2	6.25	126.57	122.20
38	4	113	U	C5-C4-O4	6.25	129.65	125.90
36	1	646	A	C8-N9-C4	-6.24	103.30	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	908	G	C8-N9-C1'	-6.24	118.88	127.00
36	1	1307	G	C8-N9-C1'	6.24	135.12	127.00
36	5	946	U	O5'-P-OP2	-6.24	100.08	105.70
36	5	2211	U	N1-C2-N3	6.24	118.65	114.90
36	1	1004	U	C5-C6-N1	6.24	125.82	122.70
37	7	89	G	C8-N9-C4	6.24	108.90	106.40
1	2	1137	A	C8-N9-C4	6.24	108.30	105.80
36	1	2243	A	C8-N9-C4	6.24	108.30	105.80
38	4	12	A	N1-C2-N3	-6.24	126.18	129.30
38	4	67	U	N3-C2-O2	-6.24	117.83	122.20
36	5	652	G	O5'-P-OP2	-6.24	100.08	105.70
36	5	1519	G	C5-C6-O6	-6.24	124.86	128.60
36	5	3120	C	C6-N1-C2	-6.24	117.80	120.30
36	1	2860	U	C5-C4-O4	-6.24	122.16	125.90
37	3	73	C	N3-C2-O2	-6.24	117.53	121.90
36	5	3128	G	C2-N3-C4	6.24	115.02	111.90
36	1	2215	A	C8-N9-C4	6.24	108.30	105.80
20	C8	3	LEU	CA-CB-CG	6.24	129.64	115.30
36	1	1294	A	N1-C6-N6	-6.24	114.86	118.60
36	1	2302	G	N1-C2-N2	-6.24	110.59	116.20
36	1	2324	A	C8-N9-C4	-6.24	103.31	105.80
4	s2	73	LEU	CA-CB-CG	6.24	129.64	115.30
36	5	1468	A	C8-N9-C4	6.24	108.29	105.80
1	2	1101	G	C5-C6-O6	-6.23	124.86	128.60
36	1	2942	C	C2-N1-C1'	-6.23	111.94	118.80
1	6	1657	U	N1-C2-N3	-6.23	111.16	114.90
36	5	596	C	N3-C4-C5	-6.23	119.41	121.90
37	7	121	U	C6-N1-C1'	-6.23	112.47	121.20
36	1	86	G	O5'-P-OP1	6.23	118.18	110.70
36	1	283	G	C4-C5-N7	6.23	113.29	110.80
36	1	2817	A	OP2-P-O3'	6.23	118.91	105.20
36	1	3228	C	OP1-P-OP2	-6.23	110.25	119.60
36	5	641	C	N3-C2-O2	6.23	126.26	121.90
36	5	1461	A	C8-N9-C4	6.23	108.29	105.80
36	5	2991	A	C6-N1-C2	-6.23	114.86	118.60
36	1	959	C	C5-C4-N4	-6.23	115.84	120.20
36	1	1300	G	C5-C6-N1	6.23	114.61	111.50
36	1	1359	C	C6-N1-C2	6.23	122.79	120.30
36	1	2857	C	N3-C4-C5	6.23	124.39	121.90
36	5	1367	G	C8-N9-C1'	-6.23	118.91	127.00
36	5	2996	U	O5'-P-OP2	-6.23	100.09	105.70
47	m0	128	ARG	NE-CZ-NH1	6.23	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1308	A	C8-N9-C4	-6.23	103.31	105.80
36	5	2826	U	N3-C4-O4	-6.23	115.04	119.40
1	2	1458	G	C4-N9-C1'	6.22	134.59	126.50
36	1	1792	C	N3-C4-C5	-6.22	119.41	121.90
1	6	31	C	C5-C4-N4	6.22	124.56	120.20
1	6	1120	U	N3-C4-O4	-6.22	115.04	119.40
36	5	1119	C	C2-N3-C4	-6.22	116.79	119.90
36	5	2802	A	C8-N9-C4	-6.22	103.31	105.80
36	1	1911	A	C6-C5-N7	-6.22	127.94	132.30
36	1	2648	G	C4-C5-N7	6.22	113.29	110.80
1	6	453	U	N1-C2-O2	6.22	127.16	122.80
36	5	47	C	C5-C6-N1	-6.22	117.89	121.00
36	5	201	A	OP1-P-OP2	-6.22	110.27	119.60
36	5	391	A	C8-N9-C4	6.22	108.29	105.80
36	5	1842	A	C8-N9-C4	6.22	108.29	105.80
36	5	2155	G	C8-N9-C4	6.22	108.89	106.40
36	5	3098	G	N1-C6-O6	-6.22	116.17	119.90
36	1	201	A	C5-C6-N1	-6.22	114.59	117.70
36	1	628	A	N1-C6-N6	6.22	122.33	118.60
36	1	1133	A	C5-C6-N1	6.22	120.81	117.70
36	1	2150	G	C5-C6-O6	6.22	132.33	128.60
37	3	94	C	N1-C2-O2	-6.22	115.17	118.90
37	7	35	C	C4-C5-C6	6.22	120.51	117.40
70	O4	8	ARG	NE-CZ-NH1	6.22	123.41	120.30
36	1	2954	U	C6-N1-C2	6.22	124.73	121.00
36	1	3178	A	C8-N9-C4	6.22	108.29	105.80
36	1	3309	G	C6-C5-N7	-6.22	126.67	130.40
1	6	385	A	N1-C6-N6	-6.22	114.87	118.60
36	5	282	G	N1-C6-O6	-6.22	116.17	119.90
38	8	82	U	O5'-P-OP1	-6.22	100.11	105.70
36	1	932	U	N1-C2-O2	-6.21	118.45	122.80
36	5	2335	G	N9-C4-C5	6.21	107.89	105.40
36	5	2867	C	C5-C4-N4	6.21	124.55	120.20
36	5	2927	C	C5-C4-N4	6.21	124.55	120.20
36	5	3027	A	C8-N9-C4	6.21	108.29	105.80
1	2	145	A	C8-N9-C4	-6.21	103.31	105.80
36	5	111	C	C5-C6-N1	-6.21	117.89	121.00
36	1	1843	C	O5'-P-OP2	-6.21	100.11	105.70
36	5	295	A	C2-N3-C4	-6.21	107.49	110.60
36	5	514	G	C5-C6-O6	-6.21	124.87	128.60
36	5	3045	G	O5'-P-OP2	-6.21	100.11	105.70
1	6	54	C	N3-C4-C5	6.21	124.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1849	C	C5-C4-N4	-6.21	115.85	120.20
36	1	2928	C	C6-N1-C2	-6.21	117.82	120.30
1	6	338	C	O5'-P-OP2	-6.21	100.11	105.70
36	5	341	G	C4-C5-N7	6.21	113.28	110.80
36	5	3095	U	N3-C2-O2	-6.21	117.85	122.20
36	1	834	U	C5-C6-N1	-6.21	119.60	122.70
36	1	2406	C	N1-C2-O2	-6.21	115.18	118.90
36	5	939	U	N1-C2-O2	-6.21	118.46	122.80
36	5	1487	G	C5-C6-O6	6.21	132.32	128.60
36	5	3217	C	C6-N1-C1'	6.21	128.25	120.80
1	2	1273	G	O4'-C1'-N9	6.21	113.16	108.20
36	1	690	A	C2-N3-C4	6.21	113.70	110.60
36	5	1081	U	N3-C4-C5	6.21	118.32	114.60
36	5	1899	G	N9-C4-C5	6.21	107.88	105.40
37	7	72	A	OP2-P-O3'	6.21	118.85	105.20
36	1	944	C	C5-C6-N1	6.20	124.10	121.00
36	1	2396	G	C5-N7-C8	6.20	107.40	104.30
36	1	2762	A	N7-C8-N9	-6.20	110.70	113.80
36	5	788	C	OP2-P-O3'	6.20	118.85	105.20
36	5	2830	G	N1-C2-N3	6.20	127.62	123.90
36	1	1103	A	P-O3'-C3'	6.20	127.14	119.70
36	1	657	A	N1-C6-N6	-6.20	114.88	118.60
36	1	3293	U	N3-C2-O2	6.20	126.54	122.20
37	7	84	A	C8-N9-C4	-6.20	103.32	105.80
36	1	1198	C	N1-C2-O2	-6.20	115.18	118.90
36	1	1382	G	OP1-P-OP2	-6.20	110.30	119.60
36	1	1389	G	N3-C4-N9	6.20	129.72	126.00
36	1	2139	A	N9-C4-C5	6.20	108.28	105.80
36	1	2975	U	N1-C2-O2	6.20	127.14	122.80
38	4	46	G	N3-C4-N9	6.20	129.72	126.00
36	5	2284	C	C2-N1-C1'	6.20	125.62	118.80
36	5	3160	U	C5-C6-N1	6.20	125.80	122.70
36	1	1153	A	N1-C6-N6	6.20	122.32	118.60
36	1	1520	G	N7-C8-N9	-6.20	110.00	113.10
36	1	2693	C	C6-N1-C2	6.20	122.78	120.30
36	5	952	A	C5-C6-N6	-6.20	118.74	123.70
36	1	368	G	N3-C2-N2	6.20	124.24	119.90
36	1	2622	C	N1-C2-O2	-6.20	115.18	118.90
36	1	2706	G	N3-C4-N9	6.20	129.72	126.00
36	1	2993	G	N3-C4-N9	6.20	129.72	126.00
1	2	1202	A	C8-N9-C4	-6.19	103.32	105.80
36	1	411	U	O5'-P-OP2	-6.19	100.13	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2984	C	N1-C2-N3	6.19	123.54	119.20
36	1	2165	G	C8-N9-C4	-6.19	103.92	106.40
1	6	858	G	C4-N9-C1'	6.19	134.55	126.50
36	5	3039	C	C5-C4-N4	6.19	124.53	120.20
36	5	1838	G	O5'-P-OP2	-6.19	100.13	105.70
36	5	2788	C	N3-C4-C5	-6.19	119.42	121.90
36	1	102	C	N3-C4-N4	6.19	122.33	118.00
38	8	26	U	N3-C2-O2	-6.19	117.87	122.20
36	5	2816	G	C6-C5-N7	6.19	134.11	130.40
36	1	957	C	N3-C2-O2	6.18	126.23	121.90
36	1	2383	C	C2-N3-C4	-6.18	116.81	119.90
37	7	79	A	N1-C6-N6	6.18	122.31	118.60
36	1	608	A	C5-C6-N6	-6.18	118.75	123.70
36	1	651	G	N1-C2-N2	-6.18	110.64	116.20
36	1	1307	G	OP1-P-O3'	6.18	118.80	105.20
1	6	987	G	C5-C6-O6	-6.18	124.89	128.60
36	5	305	U	O4'-C1'-N1	6.18	113.15	108.20
36	5	2812	C	C4-C5-C6	6.18	120.49	117.40
36	5	2968	G	C4-C5-N7	-6.18	108.33	110.80
36	1	335	G	C8-N9-C4	-6.18	103.93	106.40
36	1	810	A	OP1-P-OP2	-6.18	110.33	119.60
36	1	2191	U	O5'-P-OP2	-6.18	100.14	105.70
1	6	1145	U	N3-C4-O4	6.18	123.73	119.40
36	5	3007	U	N3-C2-O2	-6.18	117.87	122.20
36	1	2773	C	OP1-P-OP2	6.18	128.87	119.60
36	5	34	A	OP2-P-O3'	6.18	118.79	105.20
36	5	2626	A	OP1-P-OP2	-6.18	110.33	119.60
36	1	2139	A	C4-C5-N7	-6.18	107.61	110.70
38	4	27	U	OP1-P-OP2	-6.18	110.34	119.60
1	6	52	U	N1-C2-N3	6.18	118.61	114.90
1	6	1031	U	C5-C4-O4	-6.18	122.19	125.90
36	5	686	G	C8-N9-C4	6.18	108.87	106.40
36	1	1822	C	C6-N1-C2	-6.17	117.83	120.30
36	1	2899	C	OP2-P-O3'	6.17	118.78	105.20
1	6	65	A	N1-C6-N6	6.17	122.31	118.60
1	6	387	A	N9-C4-C5	6.17	108.27	105.80
1	6	542	A	P-O3'-C3'	6.17	127.11	119.70
36	5	803	C	C6-N1-C2	-6.17	117.83	120.30
36	5	1881	A	O5'-P-OP2	-6.17	100.14	105.70
36	5	1912	U	N1-C2-N3	-6.17	111.19	114.90
36	1	51	A	C5-N7-C8	-6.17	100.81	103.90
1	6	1605	G	N1-C6-O6	-6.17	116.20	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	535	G	C8-N9-C4	6.17	108.87	106.40
36	5	776	U	N3-C4-O4	-6.17	115.08	119.40
36	5	2719	U	C6-N1-C1'	6.17	129.84	121.20
36	1	1179	A	OP2-P-O3'	6.17	118.78	105.20
36	1	3209	A	C5-N7-C8	-6.17	100.81	103.90
1	6	1750	A	N1-C6-N6	6.17	122.30	118.60
36	5	3188	G	C4-C5-N7	-6.17	108.33	110.80
36	5	1373	A	C6-C5-N7	-6.17	127.98	132.30
36	5	1905	G	C2-N3-C4	6.17	114.98	111.90
1	2	1430	U	O5'-P-OP2	-6.17	100.15	105.70
36	1	794	U	O5'-P-OP2	-6.17	100.15	105.70
36	5	339	C	N3-C4-N4	-6.17	113.68	118.00
36	5	875	G	C5-C6-N1	6.17	114.58	111.50
37	7	69	C	C6-N1-C2	6.17	122.77	120.30
36	1	404	G	N7-C8-N9	-6.17	110.02	113.10
36	1	3019	U	C6-N1-C2	-6.17	117.30	121.00
36	5	2388	U	N1-C2-O2	-6.17	118.48	122.80
36	5	3175	U	N3-C2-O2	-6.17	117.88	122.20
36	1	1130	A	N1-C2-N3	-6.17	126.22	129.30
36	1	1931	U	N3-C4-O4	-6.17	115.08	119.40
1	2	901	G	C4-N9-C1'	6.16	134.51	126.50
1	2	1780	G	C4-C5-N7	6.16	113.27	110.80
36	1	2616	C	N3-C2-O2	-6.16	117.58	121.90
36	1	2882	U	O5'-P-OP2	6.16	118.10	110.70
1	6	977	A	N1-C6-N6	6.16	122.30	118.60
1	2	625	C	O5'-P-OP2	-6.16	100.16	105.70
36	1	2363	A	N9-C4-C5	6.16	108.26	105.80
1	6	44	U	N3-C2-O2	6.16	126.51	122.20
1	6	1628	U	N3-C2-O2	-6.16	117.89	122.20
36	5	987	U	N1-C2-N3	6.16	118.60	114.90
36	5	2883	U	O5'-P-OP1	6.16	118.09	110.70
36	5	3335	A	C6-C5-N7	-6.16	127.99	132.30
37	7	32	U	C2-N3-C4	-6.16	123.30	127.00
1	2	1082	C	C6-N1-C2	-6.16	117.84	120.30
36	5	718	G	O4'-C1'-N9	6.16	113.13	108.20
36	5	2848	G	N3-C4-C5	-6.16	125.52	128.60
37	7	95	A	N1-C6-N6	-6.16	114.90	118.60
1	2	89	G	C8-N9-C4	6.16	108.86	106.40
1	2	1270	G	N1-C6-O6	-6.16	116.21	119.90
36	1	3326	G	N7-C8-N9	-6.16	110.02	113.10
36	5	421	G	N1-C6-O6	6.16	123.59	119.90
36	5	882	A	N1-C2-N3	6.16	132.38	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	982	C	OP2-P-O3'	6.16	118.74	105.20
36	5	1875	G	O5'-P-OP2	-6.16	100.16	105.70
36	1	37	U	O5'-P-OP1	6.15	118.08	110.70
36	1	2942	C	C6-N1-C2	6.15	122.76	120.30
36	1	3057	U	N1-C2-N3	6.15	118.59	114.90
36	1	797	U	OP2-P-O3'	6.15	118.73	105.20
36	1	1878	G	O4'-C1'-N9	-6.15	103.28	108.20
38	4	5	U	C5-C4-O4	-6.15	122.21	125.90
36	5	1723	A	C5-C6-N1	6.15	120.78	117.70
36	1	88	A	N1-C6-N6	6.15	122.29	118.60
1	6	647	G	N3-C2-N2	-6.15	115.59	119.90
1	2	1241	G	N7-C8-N9	6.15	116.17	113.10
36	1	999	G	C5-C6-O6	-6.15	124.91	128.60
36	5	21	G	C5-C6-O6	-6.15	124.91	128.60
36	5	1195	A	C8-N9-C4	-6.15	103.34	105.80
36	1	696	C	C4-C5-C6	-6.15	114.33	117.40
36	1	1314	C	N1-C2-O2	-6.15	115.21	118.90
38	4	13	A	C8-N9-C4	-6.15	103.34	105.80
36	5	804	C	N3-C2-O2	6.15	126.20	121.90
36	5	3142	A	C8-N9-C4	6.15	108.26	105.80
36	1	356	C	N3-C4-C5	6.15	124.36	121.90
1	6	1537	C	C6-N1-C1'	6.15	128.18	120.80
36	1	1611	G	C2-N3-C4	-6.14	108.83	111.90
36	1	2306	C	C6-N1-C2	-6.14	117.84	120.30
37	3	39	C	N3-C4-N4	-6.14	113.70	118.00
1	6	1035	G	C8-N9-C4	6.14	108.86	106.40
36	5	2802	A	N1-C6-N6	-6.14	114.91	118.60
36	1	988	U	C5-C6-N1	-6.14	119.63	122.70
36	1	2400	G	N1-C2-N2	6.14	121.73	116.20
36	5	969	C	C6-N1-C2	6.14	122.76	120.30
36	5	2645	G	C5-C6-N1	6.14	114.57	111.50
36	1	2977	G	C2-N3-C4	6.14	114.97	111.90
36	5	1164	G	C5-C6-N1	-6.14	108.43	111.50
36	1	155	G	N3-C4-C5	-6.14	125.53	128.60
38	4	29	U	N3-C4-O4	6.14	123.70	119.40
1	2	1744	A	O5'-P-OP1	-6.14	100.18	105.70
36	1	907	G	O4'-C1'-N9	6.14	113.11	108.20
36	1	681	U	N1-C2-O2	-6.14	118.50	122.80
36	1	1133	A	C8-N9-C4	6.14	108.25	105.80
36	5	1127	G	N9-C4-C5	-6.14	102.95	105.40
36	5	1340	G	C5-N7-C8	6.14	107.37	104.30
36	1	639	G	N9-C1'-C2'	-6.13	105.25	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1313	G	C4-C5-N7	6.13	113.25	110.80
36	1	2658	G	N7-C8-N9	-6.13	110.03	113.10
36	5	388	G	C5-C6-O6	-6.13	124.92	128.60
36	5	611	A	N7-C8-N9	-6.13	110.73	113.80
36	5	942	U	OP1-P-OP2	-6.13	110.40	119.60
36	5	2531	C	C6-N1-C1'	-6.13	113.44	120.80
36	1	938	C	N3-C4-C5	6.13	124.35	121.90
71	O5	69	LEU	CA-CB-CG	6.13	129.40	115.30
1	6	427	C	C6-N1-C2	-6.13	117.85	120.30
1	6	558	U	P-O3'-C3'	6.13	127.06	119.70
36	5	213	A	O5'-P-OP1	6.13	118.06	110.70
36	5	329	U	C2-N3-C4	-6.13	123.32	127.00
36	5	927	C	N3-C2-O2	6.13	126.19	121.90
1	2	1652	C	C6-N1-C2	-6.13	117.85	120.30
37	3	103	A	N1-C6-N6	6.13	122.28	118.60
1	2	1012	U	C2-N3-C4	6.13	130.68	127.00
1	2	1778	G	O5'-P-OP1	-6.13	100.19	105.70
36	5	925	A	C8-N9-C4	6.13	108.25	105.80
36	5	1681	U	N1-C2-O2	-6.13	118.51	122.80
36	5	1750	A	N1-C6-N6	6.13	122.28	118.60
36	1	770	G	C5-C6-O6	-6.13	124.92	128.60
36	1	2614	G	OP1-P-OP2	6.13	128.79	119.60
1	6	56	U	C2-N3-C4	-6.13	123.32	127.00
1	6	1036	A	N1-C6-N6	-6.13	114.92	118.60
36	5	2813	A	N7-C8-N9	6.13	116.86	113.80
36	5	3076	C	N3-C2-O2	-6.13	117.61	121.90
36	1	68	C	OP2-P-O3'	6.12	118.67	105.20
36	1	631	U	OP2-P-O3'	6.12	118.67	105.20
36	5	1462	A	C6-C5-N7	-6.12	128.01	132.30
36	5	2976	A	OP2-P-O3'	6.12	118.67	105.20
37	7	80	G	N3-C4-N9	6.12	129.67	126.00
36	1	867	G	O5'-P-OP1	6.12	118.05	110.70
36	1	1160	C	C2-N3-C4	6.12	122.96	119.90
36	1	1848	G	C5-C6-O6	-6.12	124.93	128.60
36	5	1059	G	C6-N1-C2	-6.12	121.43	125.10
36	5	1178	G	N7-C8-N9	6.12	116.16	113.10
36	5	1935	G	N9-C4-C5	-6.12	102.95	105.40
36	5	2930	A	N9-C4-C5	6.12	108.25	105.80
36	1	2956	A	OP1-P-OP2	-6.12	110.42	119.60
36	5	1868	G	N3-C4-N9	6.12	129.67	126.00
1	2	314	C	O5'-P-OP1	-6.12	100.19	105.70
38	4	21	C	C6-N1-C2	6.12	122.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1737	G	C4-C5-N7	6.12	113.25	110.80
36	5	704	U	C2-N1-C1'	-6.12	110.36	117.70
37	7	28	C	N1-C2-O2	-6.12	115.23	118.90
36	1	1008	U	N1-C2-O2	-6.12	118.52	122.80
1	6	1297	G	O5'-P-OP2	-6.12	100.19	105.70
36	1	2627	C	N3-C4-C5	6.12	124.35	121.90
36	5	2246	G	O5'-P-OP2	6.12	118.04	110.70
36	5	628	A	C8-N9-C4	6.11	108.25	105.80
36	5	780	A	N9-C4-C5	-6.11	103.36	105.80
36	5	1193	A	C4-C5-C6	6.11	120.06	117.00
36	5	3013	U	C2-N1-C1'	6.11	125.04	117.70
36	5	3325	G	C5-C6-O6	6.11	132.27	128.60
1	2	1145	U	N3-C2-O2	6.11	126.48	122.20
36	1	718	G	C5-N7-C8	-6.11	101.24	104.30
36	5	815	G	N3-C4-C5	-6.11	125.54	128.60
36	5	2622	C	C4-C5-C6	6.11	120.46	117.40
36	5	2830	G	C5-N7-C8	6.11	107.36	104.30
1	2	959	U	N3-C2-O2	-6.11	117.92	122.20
36	1	1336	U	C5-C6-N1	-6.11	119.64	122.70
36	1	1881	A	C8-N9-C4	6.11	108.24	105.80
36	1	2984	C	C5-C6-N1	-6.11	117.94	121.00
1	6	1751	C	C6-N1-C2	6.11	122.74	120.30
36	5	2825	C	C6-N1-C2	6.11	122.74	120.30
36	5	3196	U	O5'-P-OP1	-6.11	100.20	105.70
36	1	3103	A	N1-C2-N3	6.11	132.35	129.30
36	5	960	U	N3-C2-O2	-6.11	117.92	122.20
1	6	1399	C	C5-C6-N1	6.11	124.05	121.00
1	6	1744	A	N1-C6-N6	6.11	122.26	118.60
36	5	3244	A	O5'-P-OP1	-6.10	100.21	105.70
1	2	933	A	C8-N9-C4	-6.10	103.36	105.80
36	5	41	G	OP2-P-O3'	6.10	118.62	105.20
36	5	57	A	N1-C6-N6	6.10	122.26	118.60
36	1	1049	C	N1-C2-O2	6.10	122.56	118.90
1	6	1698	G	P-O3'-C3'	6.10	127.02	119.70
36	1	203	G	OP2-P-O3'	6.10	118.62	105.20
36	1	1855	U	N3-C2-O2	-6.10	117.93	122.20
36	1	2139	A	C5-C6-N6	6.10	128.58	123.70
1	6	794	U	N3-C2-O2	-6.10	117.93	122.20
36	5	267	G	O4'-C1'-N9	-6.10	103.32	108.20
36	5	1880	U	C4-C5-C6	-6.10	116.04	119.70
36	5	3047	U	C4-C5-C6	6.10	123.36	119.70
36	5	3276	G	O5'-P-OP1	-6.10	100.21	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	361	A	C6-N1-C2	-6.10	114.94	118.60
36	1	954	U	N1-C2-O2	-6.10	118.53	122.80
36	1	1630	U	O5'-P-OP2	-6.10	100.21	105.70
36	1	2725	U	C5-C6-N1	-6.10	119.65	122.70
1	6	380	U	N1-C2-O2	6.10	127.07	122.80
38	4	81	U	N1-C2-O2	6.10	127.07	122.80
1	2	610	G	C4-N9-C1'	6.09	134.42	126.50
36	1	636	C	C2-N3-C4	-6.09	116.85	119.90
36	1	1199	C	C5-C6-N1	-6.09	117.95	121.00
36	1	1445	U	N3-C2-O2	6.09	126.47	122.20
36	1	2944	U	OP1-P-O3'	6.09	118.61	105.20
1	6	90	C	N3-C4-C5	6.09	124.34	121.90
1	6	1578	U	O5'-P-OP1	-6.09	100.22	105.70
36	5	1323	G	N1-C6-O6	-6.09	116.24	119.90
36	5	1908	A	C8-N9-C4	-6.09	103.36	105.80
36	5	2297	U	C6-N1-C1'	6.09	129.73	121.20
24	D2	104	LEU	CA-CB-CG	6.09	129.31	115.30
36	1	1173	U	C5-C6-N1	-6.09	119.66	122.70
36	1	644	G	O5'-P-OP1	-6.09	100.22	105.70
36	1	1157	G	C8-N9-C4	-6.09	103.97	106.40
36	1	2392	C	N1-C2-O2	-6.09	115.25	118.90
36	1	2525	G	C4-C5-N7	6.09	113.24	110.80
36	1	2572	C	N1-C2-O2	6.09	122.55	118.90
36	1	2830	G	C4-C5-N7	-6.09	108.36	110.80
38	4	151	C	N3-C4-C5	-6.09	119.46	121.90
79	Q3	17	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	6	416	A	N1-C6-N6	6.09	122.25	118.60
36	5	832	G	N3-C4-C5	-6.09	125.56	128.60
36	1	1472	U	C5-C6-N1	-6.09	119.66	122.70
1	6	1164	G	N1-C6-O6	6.09	123.55	119.90
1	6	1796	C	C4-C5-C6	6.09	120.44	117.40
36	5	1408	G	OP2-P-O3'	6.09	118.59	105.20
37	7	95	A	C5-C6-N6	6.09	128.57	123.70
36	1	2374	C	C4-C5-C6	6.09	120.44	117.40
36	1	2378	C	N3-C4-N4	6.09	122.26	118.00
36	5	2932	U	C2-N3-C4	-6.09	123.35	127.00
36	1	3140	G	N9-C4-C5	-6.08	102.97	105.40
36	5	2830	G	N9-C4-C5	6.08	107.83	105.40
36	1	1340	G	N3-C2-N2	6.08	124.16	119.90
36	1	2522	G	C4-N9-C1'	6.08	134.41	126.50
1	6	1747	G	N7-C8-N9	-6.08	110.06	113.10
36	5	1409	G	N3-C4-C5	-6.08	125.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3120	C	C2-N3-C4	6.08	122.94	119.90
43	16	173	MET	CB-CG-SD	-6.08	94.15	112.40
36	1	1171	G	O5'-P-OP1	-6.08	100.23	105.70
36	5	229	G	N1-C6-O6	6.08	123.55	119.90
36	5	1300	G	N1-C6-O6	6.08	123.55	119.90
36	1	685	G	C5-C6-O6	-6.08	124.95	128.60
36	1	2956	A	N7-C8-N9	6.08	116.84	113.80
36	1	55	G	N3-C2-N2	6.08	124.15	119.90
36	1	189	G	N3-C4-C5	-6.08	125.56	128.60
36	1	2723	U	C5-C6-N1	-6.08	119.66	122.70
36	1	3009	G	C2-N3-C4	6.08	114.94	111.90
36	5	952	A	O5'-P-OP2	-6.08	100.23	105.70
36	5	1127	G	C8-N9-C4	6.08	108.83	106.40
38	4	32	C	C6-N1-C1'	6.08	128.09	120.80
36	5	890	C	C2-N3-C4	-6.08	116.86	119.90
36	5	1113	G	N1-C2-N3	6.08	127.55	123.90
38	8	39	G	N3-C4-C5	-6.08	125.56	128.60
1	2	1560	U	C5-C4-O4	6.08	129.55	125.90
36	1	123	A	N7-C8-N9	6.08	116.84	113.80
36	1	2648	G	N3-C2-N2	6.08	124.15	119.90
36	5	1448	U	C5-C6-N1	-6.08	119.66	122.70
1	2	756	A	N9-C4-C5	6.07	108.23	105.80
36	1	427	C	N1-C2-N3	6.07	123.45	119.20
36	1	972	A	C8-N9-C4	6.07	108.23	105.80
36	5	984	G	N3-C4-C5	-6.07	125.56	128.60
36	5	1430	U	C5-C6-N1	-6.07	119.66	122.70
36	5	2616	C	OP2-P-O3'	6.07	118.56	105.20
36	1	94	G	C5-C6-O6	-6.07	124.96	128.60
36	1	426	G	N3-C4-N9	6.07	129.64	126.00
36	5	283	G	C5-C6-N1	6.07	114.54	111.50
36	1	608	A	N9-C4-C5	-6.07	103.37	105.80
36	1	1081	U	C5-C4-O4	-6.07	122.26	125.90
1	6	327	U	C5-C4-O4	6.07	129.54	125.90
1	6	616	G	C5-C6-O6	6.07	132.24	128.60
36	5	760	G	O4'-C1'-N9	6.07	113.06	108.20
36	5	2391	G	OP1-P-OP2	-6.07	110.49	119.60
36	5	2611	U	C4-C5-C6	6.07	123.34	119.70
36	1	1404	G	C8-N9-C4	6.07	108.83	106.40
36	1	1445	U	C6-N1-C2	6.07	124.64	121.00
36	1	2362	C	C2-N1-C1'	6.07	125.48	118.80
1	6	1124	A	O5'-P-OP2	6.07	117.98	110.70
36	5	2620	G	N3-C2-N2	-6.07	115.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	920	A	C8-N9-C4	6.07	108.23	105.80
36	1	2619	G	C5-N7-C8	6.07	107.33	104.30
36	1	656	A	C4-C5-C6	6.07	120.03	117.00
1	6	687	G	N3-C2-N2	-6.07	115.65	119.90
36	5	1458	U	O5'-P-OP1	-6.07	100.24	105.70
36	5	2323	G	OP1-P-OP2	-6.07	110.50	119.60
1	2	1568	C	C6-N1-C2	-6.06	117.87	120.30
36	1	57	A	C8-N9-C4	6.06	108.23	105.80
1	6	173	A	C2-N3-C4	-6.06	107.57	110.60
1	2	192	U	O4'-C1'-N1	6.06	113.05	108.20
36	1	336	A	OP2-P-O3'	6.06	118.54	105.20
36	1	380	U	C5-C6-N1	6.06	125.73	122.70
36	1	619	A	N1-C6-N6	6.06	122.24	118.60
36	1	2618	G	N3-C4-C5	-6.06	125.57	128.60
38	4	79	A	N3-C4-C5	-6.06	122.56	126.80
38	8	47	C	C4-C5-C6	6.06	120.43	117.40
36	5	341	G	N1-C6-O6	6.06	123.54	119.90
36	5	1433	A	N1-C6-N6	6.06	122.24	118.60
36	5	1848	G	C5-C6-N1	6.06	114.53	111.50
36	1	969	C	C5-C4-N4	-6.06	115.96	120.20
36	1	2891	U	C5-C6-N1	-6.06	119.67	122.70
36	5	2847	A	O5'-P-OP1	-6.06	100.25	105.70
36	5	2857	C	N3-C4-C5	6.06	124.32	121.90
36	1	1307	G	C2'-C3'-O3'	6.06	123.39	113.70
36	1	2177	G	N3-C4-C5	-6.06	125.57	128.60
36	5	210	U	N3-C4-O4	-6.06	115.16	119.40
36	5	2399	A	OP1-P-OP2	-6.06	110.52	119.60
38	8	25	G	N3-C4-N9	6.05	129.63	126.00
1	2	448	C	N3-C4-C5	-6.05	119.48	121.90
36	1	2180	G	N1-C2-N3	6.05	127.53	123.90
36	1	3244	A	O4'-C1'-N9	-6.05	103.36	108.20
36	5	1879	A	C8-N9-C4	-6.05	103.38	105.80
36	1	361	A	N9-C4-C5	6.05	108.22	105.80
1	6	19	A	O5'-P-OP1	-6.05	100.25	105.70
1	6	57	G	N3-C4-C5	-6.05	125.57	128.60
38	8	103	G	N3-C4-C5	-6.05	125.57	128.60
36	1	999	G	OP2-P-O3'	6.05	118.51	105.20
36	1	2427	U	N3-C2-O2	-6.05	117.97	122.20
36	1	2969	A	O5'-P-OP2	-6.05	100.25	105.70
1	6	1781	A	C4-C5-C6	6.05	120.02	117.00
36	5	338	A	N9-C4-C5	-6.05	103.38	105.80
36	5	389	A	N1-C6-N6	-6.05	114.97	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2524	A	C8-N9-C4	-6.05	103.38	105.80
36	1	47	C	OP1-P-OP2	-6.05	110.53	119.60
36	1	2705	A	C8-N9-C4	6.05	108.22	105.80
1	6	305	C	N1-C2-O2	-6.05	115.27	118.90
36	5	1495	U	C2-N1-C1'	6.05	124.96	117.70
36	5	2524	A	N7-C8-N9	6.05	116.82	113.80
36	5	2873	U	C4-C5-C6	6.05	123.33	119.70
36	1	1108	U	OP1-P-OP2	6.05	128.67	119.60
36	1	2798	C	N3-C4-C5	-6.05	119.48	121.90
36	1	2808	A	N9-C4-C5	-6.05	103.38	105.80
38	4	40	A	N9-C4-C5	-6.05	103.38	105.80
62	N6	75	ARG	NE-CZ-NH2	6.05	123.32	120.30
36	5	953	G	C5-C6-O6	-6.05	124.97	128.60
36	5	1427	U	N3-C4-C5	6.05	118.23	114.60
36	1	728	G	OP2-P-O3'	6.04	118.50	105.20
36	1	3062	G	C5-C6-O6	-6.04	124.97	128.60
36	5	1754	G	N3-C4-C5	-6.04	125.58	128.60
36	5	2798	C	C5-C4-N4	6.04	124.43	120.20
36	5	3315	G	N9-C4-C5	6.04	107.82	105.40
1	2	1207	C	C6-N1-C2	6.04	122.72	120.30
36	1	1584	U	C5-C4-O4	6.04	129.53	125.90
1	6	459	G	N1-C6-O6	6.04	123.53	119.90
1	2	551	G	C5-N7-C8	-6.04	101.28	104.30
36	1	53	G	N3-C4-N9	6.04	129.62	126.00
36	1	3151	U	O5'-P-OP2	-6.04	100.26	105.70
36	1	196	G	C4-C5-N7	6.04	113.22	110.80
36	1	1180	A	C5-N7-C8	6.04	106.92	103.90
36	1	1374	G	C5-C6-O6	6.04	132.22	128.60
36	5	2634	U	C5-C4-O4	-6.04	122.28	125.90
36	1	1127	G	N1-C6-O6	6.04	123.52	119.90
36	1	2142	A	C4-C5-N7	-6.04	107.68	110.70
36	1	2943	G	O5'-P-OP1	6.04	117.95	110.70
38	4	81	U	C2-N1-C1'	6.04	124.95	117.70
36	5	334	A	C8-N9-C4	6.04	108.22	105.80
36	5	2709	C	N3-C4-C5	6.04	124.31	121.90
36	1	1139	G	OP2-P-O3'	6.04	118.48	105.20
36	1	1450	G	C8-N9-C4	6.04	108.81	106.40
36	1	1713	G	N9-C4-C5	-6.04	102.99	105.40
67	O1	62	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	6	451	A	N1-C6-N6	6.04	122.22	118.60
1	6	1139	A	N1-C6-N6	-6.04	114.98	118.60
36	5	81	C	N3-C4-N4	-6.04	113.78	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2816	G	C4-N9-C1'	-6.04	118.66	126.50
36	5	3039	C	N3-C2-O2	-6.04	117.67	121.90
38	8	83	C	N3-C4-N4	6.04	122.23	118.00
36	1	698	U	N1-C2-O2	-6.03	118.58	122.80
36	1	1008	U	C2-N1-C1'	-6.03	110.46	117.70
36	1	1307	G	C4-C5-N7	-6.03	108.39	110.80
36	1	2160	G	C5-C6-O6	6.03	132.22	128.60
36	5	993	G	OP1-P-OP2	6.03	128.65	119.60
36	5	1116	G	C4-C5-N7	-6.03	108.39	110.80
36	5	3374	U	C5-C6-N1	-6.03	119.68	122.70
1	2	192	U	N1-C2-O2	6.03	127.02	122.80
36	1	962	A	C6-N1-C2	-6.03	114.98	118.60
1	6	1	U	C2-N1-C1'	6.03	124.94	117.70
1	2	158	U	C6-N1-C2	-6.03	117.38	121.00
36	1	1931	U	N3-C4-C5	6.03	118.22	114.60
1	6	418	G	C4-C5-N7	6.03	113.21	110.80
36	5	651	G	C2-N3-C4	6.03	114.92	111.90
36	5	756	U	O5'-P-OP2	-6.03	100.27	105.70
36	5	973	A	N1-C6-N6	6.03	122.22	118.60
36	5	2326	A	C8-N9-C4	6.03	108.21	105.80
36	5	2960	C	OP2-P-O3'	6.03	118.47	105.20
36	1	893	C	C6-N1-C2	-6.03	117.89	120.30
36	1	2209	U	C6-N1-C2	-6.03	117.38	121.00
38	4	8	C	N1-C2-O2	-6.03	115.28	118.90
1	6	1	U	O4'-C1'-N1	6.03	113.02	108.20
1	6	624	G	N1-C2-N3	-6.03	120.28	123.90
36	5	387	A	O5'-P-OP2	-6.03	100.27	105.70
36	1	2314	U	N3-C4-O4	6.03	123.62	119.40
36	1	2698	G	N9-C4-C5	6.03	107.81	105.40
36	1	2763	U	N3-C4-O4	6.03	123.62	119.40
36	5	1000	C	O4'-C1'-N1	6.03	113.02	108.20
36	5	2363	A	N1-C6-N6	-6.03	114.98	118.60
1	2	1426	C	N3-C4-C5	6.03	124.31	121.90
36	1	2748	A	C2-N3-C4	-6.03	107.59	110.60
36	5	2361	A	C5-C6-N6	-6.03	118.88	123.70
36	5	2376	G	OP1-P-OP2	6.02	128.64	119.60
36	1	576	C	N3-C4-C5	6.02	124.31	121.90
36	1	1325	U	C5-C4-O4	6.02	129.51	125.90
36	1	2354	C	C4-C5-C6	6.02	120.41	117.40
36	5	1116	G	N3-C4-C5	-6.02	125.59	128.60
37	7	44	C	N1-C2-O2	-6.02	115.29	118.90
36	5	1393	A	C4-C5-N7	6.02	113.71	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2879	C	N3-C4-C5	6.02	124.31	121.90
36	5	43	A	O4'-C1'-N9	6.02	113.02	108.20
36	5	807	A	O4'-C1'-N9	6.02	113.02	108.20
36	5	2176	U	C2-N1-C1'	6.02	124.92	117.70
36	1	1084	A	C8-N9-C4	-6.02	103.39	105.80
1	6	46	A	O5'-P-OP1	-6.02	100.28	105.70
36	5	936	A	P-O3'-C3'	6.02	126.92	119.70
36	5	3228	C	N1-C2-O2	6.02	122.51	118.90
1	2	595	G	O5'-P-OP2	-6.01	100.29	105.70
36	1	636	C	N3-C4-C5	6.01	124.31	121.90
36	1	1081	U	C2-N1-C1'	6.01	124.92	117.70
1	6	646	C	C5-C6-N1	6.01	124.01	121.00
36	1	380	U	C6-N1-C2	-6.01	117.39	121.00
36	1	2424	A	N9-C4-C5	-6.01	103.39	105.80
36	5	1496	C	OP1-P-OP2	-6.01	110.58	119.60
1	2	557	G	N3-C4-N9	6.01	129.61	126.00
36	1	2298	U	C2-N3-C4	-6.01	123.39	127.00
1	6	1537	C	N1-C2-O2	-6.01	115.30	118.90
70	o4	58	ARG	NE-CZ-NH1	6.01	123.31	120.30
36	1	1792	C	N1-C2-O2	-6.01	115.30	118.90
36	1	3228	C	O5'-P-OP1	6.01	117.91	110.70
36	1	53	G	O5'-P-OP2	-6.01	100.29	105.70
36	1	2970	C	C6-N1-C2	6.01	122.70	120.30
1	6	458	G	C5-C6-O6	-6.01	125.00	128.60
36	5	421	G	O5'-P-OP2	-6.01	100.29	105.70
36	5	717	C	OP2-P-O3'	6.01	118.42	105.20
36	5	1008	U	C2-N1-C1'	-6.01	110.49	117.70
36	1	2550	U	N1-C2-O2	6.00	127.00	122.80
36	5	2347	U	C5-C4-O4	-6.00	122.30	125.90
1	2	1629	G	C8-N9-C4	-6.00	104.00	106.40
36	1	1353	U	N3-C2-O2	-6.00	118.00	122.20
36	1	2726	C	C5-C6-N1	-6.00	118.00	121.00
1	6	616	G	O5'-P-OP1	-6.00	100.30	105.70
1	6	362	G	N3-C4-N9	6.00	129.60	126.00
36	5	805	G	OP2-P-O3'	6.00	118.40	105.20
36	5	1127	G	C5-C6-O6	-6.00	125.00	128.60
36	5	2735	U	C2-N3-C4	6.00	130.60	127.00
36	1	2611	U	C2-N3-C4	-6.00	123.40	127.00
36	1	3111	U	N1-C2-O2	6.00	127.00	122.80
36	5	1012	G	C8-N9-C1'	6.00	134.80	127.00
36	5	3195	U	N3-C2-O2	-6.00	118.00	122.20
36	1	282	G	C2'-C3'-O3'	6.00	123.30	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	63	A	OP1-P-OP2	-6.00	110.60	119.60
36	1	78	U	C4-C5-C6	6.00	123.30	119.70
36	1	667	C	N3-C4-N4	-6.00	113.80	118.00
36	1	2370	G	OP2-P-O3'	6.00	118.39	105.20
1	6	136	C	C2-N1-C1'	6.00	125.40	118.80
36	5	2109	U	N1-C2-N3	6.00	118.50	114.90
36	5	2399	A	N1-C2-N3	6.00	132.30	129.30
36	1	1103	A	O5'-P-OP2	6.00	117.89	110.70
36	1	1434	G	N9-C4-C5	6.00	107.80	105.40
36	1	2176	U	C5-C4-O4	6.00	129.50	125.90
36	1	2996	U	C5-C6-N1	6.00	125.70	122.70
1	6	339	C	N1-C2-O2	-6.00	115.30	118.90
36	5	2618	G	N1-C6-O6	-6.00	116.30	119.90
1	2	61	A	C5-N7-C8	-5.99	100.90	103.90
36	1	709	A	C5-N7-C8	5.99	106.90	103.90
38	4	79	A	P-O3'-C3'	5.99	126.89	119.70
36	5	1448	U	C2-N3-C4	-5.99	123.40	127.00
36	5	2763	U	N3-C2-O2	5.99	126.39	122.20
54	m8	92	ARG	NE-CZ-NH2	-5.99	117.30	120.30
6	S4	3	ARG	NE-CZ-NH1	-5.99	117.31	120.30
36	1	613	G	N9-C4-C5	-5.99	103.00	105.40
36	1	632	G	OP2-P-O3'	5.99	118.38	105.20
36	1	1126	G	N1-C6-O6	5.99	123.49	119.90
36	1	424	G	C5-N7-C8	5.99	107.30	104.30
36	1	946	U	N1-C2-N3	5.99	118.49	114.90
36	1	1210	U	C5-C6-N1	-5.99	119.71	122.70
36	1	1498	A	C6-N1-C2	-5.99	115.01	118.60
36	5	2138	A	C5-C6-N1	-5.99	114.70	117.70
36	5	2947	G	C2-N3-C4	5.99	114.89	111.90
36	1	3210	A	O5'-P-OP2	-5.99	100.31	105.70
36	5	928	C	O5'-P-OP1	5.99	117.89	110.70
36	5	3058	U	O4'-C1'-N1	5.99	112.99	108.20
36	1	1496	C	C2-N1-C1'	5.99	125.38	118.80
36	1	2728	G	O4'-C1'-N9	5.99	112.99	108.20
38	4	16	G	C8-N9-C4	5.99	108.79	106.40
36	5	2820	A	OP2-P-O3'	-5.99	92.03	105.20
36	5	2849	C	C5-C6-N1	5.99	123.99	121.00
1	2	1518	C	O5'-P-OP1	-5.98	100.31	105.70
36	1	2411	U	C2-N1-C1'	-5.98	110.52	117.70
36	5	1436	U	C5-C4-O4	-5.98	122.31	125.90
38	4	94	C	C6-N1-C2	5.98	122.69	120.30
36	1	319	A	O5'-P-OP1	-5.98	100.32	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	783	A	C2-N3-C4	-5.98	107.61	110.60
36	5	993	G	O4'-C1'-N9	5.98	112.98	108.20
36	5	2366	C	N3-C4-N4	5.98	122.19	118.00
36	5	2891	U	N1-C2-N3	5.98	118.49	114.90
36	1	1178	G	N3-C4-C5	-5.98	125.61	128.60
36	1	1793	C	N3-C4-C5	5.98	124.29	121.90
36	5	822	G	O5'-P-OP2	5.98	117.87	110.70
36	5	2379	U	C6-N1-C2	5.98	124.59	121.00
36	5	3130	A	C8-N9-C4	5.98	108.19	105.80
37	7	110	G	O4'-C1'-N9	5.98	112.98	108.20
36	1	1316	C	C2-N3-C4	-5.98	116.91	119.90
36	5	205	C	N3-C4-C5	5.98	124.29	121.90
38	4	32	C	C2-N1-C1'	-5.97	112.23	118.80
36	5	1192	C	N3-C4-C5	5.97	124.29	121.90
36	5	3347	A	C8-N9-C4	5.97	108.19	105.80
36	1	3055	U	N3-C4-O4	5.97	123.58	119.40
36	5	1314	C	N3-C2-O2	-5.97	117.72	121.90
1	2	551	G	C4-C5-N7	5.97	113.19	110.80
36	1	341	G	C5-C6-N1	5.97	114.48	111.50
36	1	2828	G	O5'-P-OP2	5.97	117.86	110.70
36	5	1193	A	N7-C8-N9	5.97	116.78	113.80
36	1	44	U	C2-N1-C1'	-5.97	110.54	117.70
36	1	709	A	O5'-P-OP2	5.97	117.86	110.70
36	1	371	G	N9-C4-C5	-5.97	103.01	105.40
36	1	1594	A	N9-C4-C5	5.97	108.19	105.80
36	5	204	A	C4-C5-N7	-5.97	107.72	110.70
36	5	2234	G	C6-N1-C2	-5.97	121.52	125.10
36	5	2705	A	N9-C4-C5	-5.97	103.41	105.80
36	5	2922	G	N1-C6-O6	-5.97	116.32	119.90
36	5	2955	U	N1-C2-N3	5.97	118.48	114.90
38	8	81	U	N3-C2-O2	-5.97	118.02	122.20
36	1	102	C	C5-C4-N4	-5.96	116.02	120.20
36	1	214	G	C8-N9-C4	5.96	108.79	106.40
36	1	1879	A	C8-N9-C4	-5.96	103.41	105.80
36	1	2731	U	N1-C2-O2	-5.96	118.62	122.80
1	6	901	G	C5-N7-C8	-5.96	101.32	104.30
36	5	937	G	C5-N7-C8	5.96	107.28	104.30
36	5	1047	A	C6-C5-N7	-5.96	128.12	132.30
36	5	2244	A	O5'-P-OP1	5.96	117.86	110.70
36	5	3304	U	N1-C2-O2	-5.96	118.62	122.80
36	1	924	G	C4-C5-N7	5.96	113.19	110.80
36	1	1586	G	O5'-P-OP2	-5.96	100.33	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	804	A	N1-C6-N6	5.96	122.18	118.60
36	5	1847	A	N3-C4-C5	5.96	130.97	126.80
36	5	1870	C	N3-C4-C5	5.96	124.28	121.90
36	5	2400	G	N1-C2-N3	5.96	127.48	123.90
36	5	2614	G	C5-N7-C8	5.96	107.28	104.30
36	5	2928	C	C6-N1-C2	-5.96	117.92	120.30
36	1	2376	G	N3-C4-C5	-5.96	125.62	128.60
36	5	966	U	O5'-P-OP2	-5.96	100.33	105.70
36	5	1838	G	N1-C2-N2	5.96	121.56	116.20
36	5	2290	C	N3-C4-C5	5.96	124.28	121.90
36	5	2692	A	N9-C4-C5	5.96	108.19	105.80
36	5	3060	C	C5-C4-N4	-5.96	116.03	120.20
36	1	2149	A	C5-C6-N1	-5.96	114.72	117.70
1	6	1613	U	N3-C2-O2	-5.96	118.03	122.20
36	5	1592	G	C8-N9-C4	-5.96	104.02	106.40
36	1	652	G	N3-C2-N2	5.96	124.07	119.90
36	1	1440	G	C6-N1-C2	5.96	128.68	125.10
36	5	277	G	O5'-P-OP1	-5.96	100.34	105.70
36	5	2373	A	C5-C6-N6	-5.96	118.93	123.70
36	5	3028	G	N3-C4-N9	5.96	129.57	126.00
37	7	94	C	O5'-P-OP2	5.96	117.85	110.70
37	7	100	C	C5-C6-N1	-5.96	118.02	121.00
36	1	1340	G	N9-C4-C5	-5.96	103.02	105.40
36	5	1884	A	OP2-P-O3'	5.96	118.30	105.20
36	5	2725	U	OP2-P-O3'	5.96	118.31	105.20
36	5	2816	G	C2-N3-C4	5.96	114.88	111.90
36	5	3285	C	C2-N1-C1'	5.96	125.35	118.80
1	2	577	G	N3-C4-C5	5.96	131.58	128.60
1	2	1291	G	N3-C4-C5	5.96	131.58	128.60
36	1	1177	G	N1-C2-N2	5.96	121.56	116.20
1	6	1614	A	N1-C6-N6	5.96	122.17	118.60
36	5	3228	C	C2-N1-C1'	5.96	125.35	118.80
1	2	1340	U	C5-C4-O4	5.95	129.47	125.90
36	1	960	U	OP2-P-O3'	5.95	118.30	105.20
36	5	192	C	OP1-P-O3'	5.95	118.30	105.20
36	5	372	A	C4-C5-N7	5.95	113.68	110.70
36	5	2818	U	C4-C5-C6	-5.95	116.13	119.70
36	1	1835	A	C2-N3-C4	-5.95	107.62	110.60
36	1	3040	A	OP2-P-O3'	5.95	118.29	105.20
36	5	1312	C	C5-C4-N4	5.95	124.37	120.20
36	5	2335	G	C5-C6-O6	5.95	132.17	128.60
36	1	637	C	C2-N1-C1'	-5.95	112.25	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2218	G	N1-C6-O6	-5.95	116.33	119.90
36	1	2359	C	N1-C2-O2	-5.95	115.33	118.90
36	5	1556	C	N1-C2-O2	5.95	122.47	118.90
36	5	1870	C	C5-C6-N1	-5.95	118.03	121.00
36	5	1917	C	C4-C5-C6	5.95	120.38	117.40
36	5	2944	U	N3-C2-O2	-5.95	118.03	122.20
37	7	10	C	N3-C4-C5	5.95	124.28	121.90
36	1	504	A	O5'-P-OP2	-5.95	100.35	105.70
36	1	786	A	C5-C6-N6	5.95	128.46	123.70
36	1	2178	A	N1-C6-N6	-5.95	115.03	118.60
36	1	2799	A	C8-N9-C4	5.95	108.18	105.80
36	1	2818	U	O5'-P-OP2	-5.95	100.35	105.70
38	4	5	U	N3-C4-C5	5.95	118.17	114.60
11	s9	99	LEU	CA-CB-CG	5.95	128.98	115.30
36	5	1371	G	C5-N7-C8	5.95	107.27	104.30
38	8	139	U	C5-C4-O4	5.95	129.47	125.90
36	1	71	A	N1-C2-N3	5.95	132.27	129.30
36	5	13	A	N1-C6-N6	-5.95	115.03	118.60
36	5	72	C	N3-C4-C5	5.95	124.28	121.90
36	1	280	U	C5-C4-O4	-5.95	122.33	125.90
36	1	776	U	N3-C2-O2	-5.95	118.04	122.20
36	1	932	U	OP1-P-O3'	5.95	118.28	105.20
36	1	2660	G	C5-C6-N1	5.95	114.47	111.50
1	6	678	A	P-O3'-C3'	5.95	126.83	119.70
36	5	831	G	C2-N3-C4	5.95	114.87	111.90
36	5	1161	G	N7-C8-N9	-5.95	110.13	113.10
36	5	2402	A	N1-C6-N6	-5.95	115.03	118.60
36	5	2422	C	N3-C4-N4	-5.95	113.84	118.00
36	5	3074	G	N3-C2-N2	5.95	124.06	119.90
37	7	73	C	OP1-P-OP2	-5.95	110.68	119.60
36	1	1867	A	C8-N9-C4	5.94	108.18	105.80
36	5	705	A	O5'-P-OP2	-5.94	100.35	105.70
1	2	734	A	OP1-P-O3'	5.94	118.27	105.20
36	1	2423	U	N1-C2-O2	-5.94	118.64	122.80
36	5	1298	C	N1-C2-O2	-5.94	115.33	118.90
36	5	1561	G	O4'-C1'-N9	5.94	112.95	108.20
36	5	2392	C	C5-C6-N1	-5.94	118.03	121.00
36	1	196	G	C5-C6-O6	-5.94	125.04	128.60
1	6	815	G	C8-N9-C4	-5.94	104.02	106.40
36	5	816	A	O5'-P-OP2	-5.94	100.35	105.70
36	5	841	A	C5-C6-N1	5.94	120.67	117.70
36	1	2340	U	C5-C6-N1	5.94	125.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2121	G	O5'-P-OP1	5.94	117.83	110.70
36	5	3309	G	N3-C4-N9	5.94	129.56	126.00
36	1	760	G	O4'-C1'-N9	5.94	112.95	108.20
36	1	765	C	N1-C2-O2	5.94	122.46	118.90
36	1	1296	C	C4-C5-C6	5.94	120.37	117.40
36	1	1448	U	C2-N3-C4	-5.94	123.44	127.00
1	6	272	U	P-O3'-C3'	5.94	126.83	119.70
36	5	393	U	C6-N1-C2	-5.94	117.44	121.00
36	5	3195	U	N1-C2-O2	5.94	126.95	122.80
37	7	43	U	N1-C2-N3	5.94	118.46	114.90
37	3	11	A	C8-N9-C4	5.93	108.17	105.80
1	6	385	A	C5-C6-N6	5.93	128.45	123.70
36	5	869	G	C5-C6-N1	5.93	114.47	111.50
36	5	908	G	C4-N9-C1'	5.93	134.22	126.50
36	1	112	U	N3-C4-O4	5.93	123.55	119.40
36	1	1048	A	C5-N7-C8	5.93	106.87	103.90
36	1	2247	G	N9-C4-C5	-5.93	103.03	105.40
36	1	2623	G	OP1-P-OP2	-5.93	110.70	119.60
36	5	2339	C	C6-N1-C2	-5.93	117.93	120.30
36	5	2614	G	O5'-P-OP2	-5.93	100.36	105.70
36	5	2859	U	C5-C6-N1	5.93	125.67	122.70
36	1	3247	G	C6-C5-N7	-5.93	126.84	130.40
36	1	1599	G	N1-C6-O6	-5.93	116.34	119.90
36	1	2899	C	C4-C5-C6	5.93	120.36	117.40
78	Q2	35	LEU	CA-CB-CG	5.93	128.94	115.30
12	c0	83	PRO	N-CA-CB	5.93	110.42	103.30
36	5	1480	G	O4'-C1'-N9	5.93	112.94	108.20
36	1	1868	G	N3-C4-N9	5.93	129.56	126.00
36	5	3123	A	N7-C8-N9	-5.93	110.84	113.80
24	D2	93	LEU	CA-CB-CG	5.93	128.93	115.30
36	1	961	C	C6-N1-C2	5.93	122.67	120.30
36	1	2732	G	C4-C5-N7	5.93	113.17	110.80
37	7	50	U	C6-N1-C2	-5.93	117.44	121.00
18	C6	40	GLU	C-N-CD	-5.92	107.56	120.60
36	1	110	G	C2-N3-C4	-5.92	108.94	111.90
1	6	337	G	O4'-C1'-N9	-5.92	103.46	108.20
1	6	1656	U	O5'-P-OP1	5.92	117.81	110.70
36	5	2961	G	C8-N9-C4	-5.92	104.03	106.40
36	5	3018	C	O5'-P-OP2	-5.92	100.37	105.70
37	7	32	U	C5-C6-N1	-5.92	119.74	122.70
1	2	1556	A	OP1-P-O3'	5.92	118.23	105.20
36	1	57	A	C2-N3-C4	-5.92	107.64	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2434	U	C5-C4-O4	5.92	129.45	125.90
36	1	2777	G	N9-C4-C5	5.92	107.77	105.40
36	5	22	G	C8-N9-C4	5.92	108.77	106.40
36	5	960	U	N1-C1'-C2'	5.92	121.70	114.00
36	1	1367	G	N3-C4-N9	5.92	129.55	126.00
36	1	2389	C	C6-N1-C2	5.92	122.67	120.30
36	5	415	G	N1-C6-O6	-5.92	116.35	119.90
36	5	972	A	OP2-P-O3'	5.92	118.23	105.20
36	5	297	G	O4'-C1'-N9	5.92	112.94	108.20
52	m6	16	VAL	CG1-CB-CG2	-5.92	101.43	110.90
36	1	1443	G	C5-N7-C8	-5.92	101.34	104.30
36	1	3123	A	C2-N3-C4	-5.92	107.64	110.60
36	1	3344	A	C2-N3-C4	-5.92	107.64	110.60
52	M6	84	LEU	CB-CG-CD2	-5.92	100.94	111.00
36	5	1445	U	N1-C2-N3	5.92	118.45	114.90
36	5	3280	U	OP1-P-OP2	-5.92	110.72	119.60
36	1	81	C	C2-N3-C4	-5.92	116.94	119.90
36	1	983	A	C5-C6-N6	-5.92	118.97	123.70
36	1	1372	C	C6-N1-C2	5.92	122.67	120.30
1	6	1746	A	C8-N9-C4	-5.92	103.43	105.80
36	5	1209	G	N1-C6-O6	-5.92	116.35	119.90
36	5	3228	C	N3-C2-O2	-5.92	117.76	121.90
36	1	2942	C	O5'-P-OP1	5.92	117.80	110.70
1	2	1198	G	N7-C8-N9	5.91	116.06	113.10
36	1	3178	A	N1-C6-N6	5.91	122.15	118.60
36	5	304	G	C2-N3-C4	5.91	114.86	111.90
36	5	337	G	C8-N9-C4	-5.91	104.03	106.40
1	2	314	C	C6-N1-C2	-5.91	117.94	120.30
36	1	890	C	C6-N1-C2	-5.91	117.94	120.30
36	1	1313	G	N1-C6-O6	5.91	123.45	119.90
36	1	1320	C	N1-C2-O2	-5.91	115.35	118.90
36	5	935	U	C2-N3-C4	-5.91	123.45	127.00
36	1	967	A	N1-C2-N3	5.91	132.25	129.30
36	1	2735	U	N3-C4-O4	-5.91	115.26	119.40
36	1	2834	G	C5-C6-O6	-5.91	125.05	128.60
1	6	435	C	N1-C2-O2	5.91	122.45	118.90
36	5	215	G	C8-N9-C4	-5.91	104.04	106.40
36	5	1164	G	C4-C5-N7	-5.91	108.44	110.80
36	5	1365	G	N3-C4-N9	5.91	129.55	126.00
36	5	2253	G	O5'-P-OP2	-5.91	100.38	105.70
1	2	1611	A	C8-N9-C4	-5.91	103.44	105.80
36	1	1155	C	N3-C4-N4	-5.91	113.86	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3362	A	C4-N9-C1'	5.91	136.94	126.30
37	3	104	A	C8-N9-C4	5.91	108.16	105.80
36	5	946	U	C5-C6-N1	-5.91	119.75	122.70
36	5	2369	G	C8-N9-C4	5.91	108.76	106.40
36	1	3045	G	N3-C4-C5	-5.91	125.65	128.60
15	c3	114	ARG	NE-CZ-NH1	5.91	123.25	120.30
36	5	1307	G	N1-C2-N3	-5.91	120.36	123.90
36	1	2152	A	C5-N7-C8	5.91	106.85	103.90
1	6	1027	A	C5-N7-C8	-5.91	100.95	103.90
1	6	1100	G	C6-N1-C2	-5.91	121.56	125.10
36	5	2861	U	C4-C5-C6	5.91	123.24	119.70
36	1	948	C	C6-N1-C2	5.90	122.66	120.30
36	1	2626	A	N1-C2-N3	5.90	132.25	129.30
12	c0	88	PRO	N-CA-CB	5.90	110.38	103.30
36	5	1124	U	C4-C5-C6	-5.90	116.16	119.70
36	5	3181	C	N3-C4-C5	-5.90	119.54	121.90
5	S3	143	ARG	NE-CZ-NH2	5.90	123.25	120.30
36	1	188	U	N1-C2-O2	-5.90	118.67	122.80
36	1	366	A	C2-N3-C4	5.90	113.55	110.60
36	1	2177	G	N9-C4-C5	-5.90	103.04	105.40
1	6	1703	C	C5-C6-N1	5.90	123.95	121.00
36	5	785	G	C2-N3-C4	5.90	114.85	111.90
36	5	2420	C	N3-C2-O2	5.90	126.03	121.90
36	1	701	G	OP2-P-O3'	5.90	118.18	105.20
36	1	859	G	N3-C4-C5	-5.90	125.65	128.60
36	5	427	C	N3-C4-N4	-5.90	113.87	118.00
65	n9	23	LYS	C-N-CD	5.90	140.79	128.40
36	1	956	U	O5'-P-OP1	-5.90	100.39	105.70
36	1	3107	U	O5'-P-OP2	-5.90	100.39	105.70
1	6	403	G	C8-N9-C4	5.90	108.76	106.40
36	5	980	A	C8-N9-C4	5.90	108.16	105.80
36	5	2968	G	N1-C6-O6	-5.90	116.36	119.90
1	2	1118	G	N3-C2-N2	-5.90	115.77	119.90
1	6	272	U	N3-C2-O2	-5.90	118.07	122.20
36	1	2417	U	N1-C2-N3	5.89	118.44	114.90
36	1	2694	A	O5'-P-OP2	-5.89	100.39	105.70
36	1	2725	U	C6-N1-C2	5.89	124.54	121.00
38	4	72	A	O5'-P-OP1	-5.89	100.40	105.70
1	6	31	C	N1-C2-O2	-5.89	115.36	118.90
1	6	163	G	C8-N9-C1'	5.89	134.66	127.00
36	5	916	G	N3-C2-N2	-5.89	115.77	119.90
36	1	941	G	N1-C6-O6	-5.89	116.36	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1365	G	N7-C8-N9	5.89	116.05	113.10
36	5	2112	U	C5-C6-N1	5.89	125.65	122.70
36	5	2823	G	C5-C6-O6	5.89	132.13	128.60
1	2	343	C	N1-C2-O2	5.89	122.43	118.90
36	1	2145	A	C8-N9-C4	-5.89	103.44	105.80
36	1	2960	C	N3-C4-C5	5.89	124.26	121.90
36	5	1367	G	C4-N9-C1'	5.89	134.16	126.50
36	5	3048	A	C2-N3-C4	5.89	113.55	110.60
36	5	3140	G	N1-C6-O6	5.89	123.43	119.90
1	2	1141	G	N1-C6-O6	-5.89	116.37	119.90
36	1	225	C	N3-C4-N4	5.89	122.12	118.00
36	1	1923	C	C6-N1-C2	5.89	122.66	120.30
36	1	2163	C	C2-N3-C4	-5.89	116.95	119.90
37	3	88	G	N3-C4-N9	5.89	129.53	126.00
1	6	1137	A	O5'-P-OP2	5.89	117.76	110.70
36	5	2327	U	C6-N1-C2	5.89	124.53	121.00
36	5	3330	A	N1-C6-N6	-5.89	115.07	118.60
36	1	960	U	C4-C5-C6	-5.88	116.17	119.70
36	1	2937	G	C8-N9-C4	5.88	108.75	106.40
36	1	3277	U	C6-N1-C2	-5.88	117.47	121.00
36	5	1373	A	N9-C4-C5	-5.88	103.45	105.80
36	5	2660	G	N3-C4-N9	5.88	129.53	126.00
36	5	3194	C	C2-N1-C1'	-5.88	112.33	118.80
38	8	37	A	N1-C6-N6	-5.88	115.07	118.60
36	1	267	G	C6-C5-N7	-5.88	126.87	130.40
36	1	3086	A	OP2-P-O3'	5.88	118.14	105.20
36	5	971	G	N3-C2-N2	-5.88	115.78	119.90
36	1	55	G	C5-N7-C8	5.88	107.24	104.30
36	1	400	G	N1-C6-O6	5.88	123.43	119.90
36	1	575	G	C6-C5-N7	5.88	133.93	130.40
36	1	1165	A	O5'-P-OP2	-5.88	100.41	105.70
36	1	2287	C	C6-N1-C2	-5.88	117.95	120.30
36	1	2920	U	N3-C4-C5	5.88	118.13	114.60
1	6	945	U	O5'-P-OP1	-5.88	100.41	105.70
36	5	571	U	N3-C2-O2	-5.88	118.08	122.20
36	5	1179	A	O5'-P-OP1	-5.88	100.41	105.70
36	5	1360	C	N1-C2-O2	-5.88	115.37	118.90
36	5	1880	U	N3-C4-O4	-5.88	115.28	119.40
36	5	1908	A	N9-C4-C5	5.88	108.15	105.80
36	5	2649	A	N9-C4-C5	-5.88	103.45	105.80
36	1	674	G	C4-C5-N7	-5.88	108.45	110.80
36	1	2818	U	C5-C4-O4	-5.88	122.37	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3050	U	N1-C2-O2	5.88	126.92	122.80
1	6	52	U	N3-C2-O2	-5.88	118.08	122.20
36	1	344	A	N1-C2-N3	-5.88	126.36	129.30
36	1	3172	A	C8-N9-C4	5.88	108.15	105.80
1	6	871	G	C6-C5-N7	-5.88	126.87	130.40
36	5	2875	U	N1-C2-O2	-5.88	118.69	122.80
1	6	417	A	P-O3'-C3'	5.88	126.75	119.70
36	1	22	G	N3-C4-C5	-5.88	125.66	128.60
36	5	871	U	N1-C2-N3	5.88	118.42	114.90
36	5	645	A	C8-N9-C4	-5.87	103.45	105.80
36	5	1935	G	C8-N9-C4	5.87	108.75	106.40
36	5	2404	A	N1-C6-N6	5.87	122.12	118.60
36	5	2824	G	N1-C2-N3	5.87	127.42	123.90
36	1	212	G	N3-C4-N9	5.87	129.52	126.00
36	1	938	C	N3-C2-O2	5.87	126.01	121.90
36	1	1847	A	C5-C6-N1	5.87	120.64	117.70
1	6	1188	G	N1-C6-O6	5.87	123.42	119.90
37	3	83	U	C2-N3-C4	-5.87	123.48	127.00
1	2	1363	U	C2-N1-C1'	5.87	124.74	117.70
36	1	1114	U	C6-N1-C2	5.87	124.52	121.00
36	1	2815	G	N9-C4-C5	-5.87	103.05	105.40
36	1	3120	C	N1-C2-O2	-5.87	115.38	118.90
36	1	3141	A	OP2-P-O3'	5.87	118.11	105.20
1	6	870	C	O5'-P-OP1	-5.87	100.42	105.70
36	5	285	A	C4-C5-N7	-5.87	107.77	110.70
36	5	2651	G	C6-C5-N7	5.87	133.92	130.40
36	5	3050	U	N1-C2-O2	5.87	126.91	122.80
1	2	427	C	C2-N1-C1'	5.87	125.25	118.80
1	2	580	A	C8-N9-C4	-5.87	103.45	105.80
1	2	396	G	C5-C6-O6	-5.87	125.08	128.60
1	2	1196	A	P-O3'-C3'	5.87	126.74	119.70
36	1	918	C	N1-C2-N3	5.87	123.31	119.20
36	1	1858	A	C8-N9-C1'	-5.87	117.14	127.70
1	6	609	U	N3-C2-O2	-5.87	118.09	122.20
1	6	616	G	N3-C4-N9	-5.87	122.48	126.00
36	5	1432	C	N1-C2-O2	-5.87	115.38	118.90
36	5	2617	U	N3-C2-O2	5.87	126.31	122.20
37	7	48	U	O5'-P-OP1	5.87	117.74	110.70
36	1	1051	U	N1-C2-O2	-5.86	118.69	122.80
36	1	1366	A	N7-C8-N9	5.86	116.73	113.80
36	1	1389	G	C6-C5-N7	-5.86	126.88	130.40
36	1	2128	C	O5'-P-OP2	-5.86	100.42	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2283	G	C5-C6-O6	-5.86	125.08	128.60
36	1	2383	C	C4-C5-C6	5.86	120.33	117.40
1	6	65	A	N3-C4-C5	5.86	130.91	126.80
1	6	941	A	N9-C4-C5	5.86	108.14	105.80
1	6	1110	G	C8-N9-C4	-5.86	104.06	106.40
36	5	197	G	C6-C5-N7	-5.86	126.88	130.40
36	5	348	A	C8-N9-C4	5.86	108.15	105.80
36	5	499	G	O5'-P-OP1	-5.86	100.42	105.70
36	5	2611	U	O5'-P-OP2	-5.86	100.42	105.70
36	5	2693	C	C6-N1-C2	5.86	122.64	120.30
36	1	331	G	N1-C2-N2	5.86	121.48	116.20
36	5	1854	C	C2-N3-C4	5.86	122.83	119.90
36	5	3053	G	OP2-P-O3'	5.86	118.10	105.20
36	5	3125	U	O5'-P-OP1	-5.86	100.42	105.70
36	1	369	A	N9-C4-C5	5.86	108.14	105.80
36	1	3269	U	N1-C2-N3	5.86	118.42	114.90
38	4	85	G	C8-N9-C4	-5.86	104.06	106.40
39	L2	123	ARG	NE-CZ-NH1	-5.86	117.37	120.30
36	5	1464	G	C8-N9-C4	5.86	108.74	106.40
36	5	2871	G	N1-C6-O6	-5.86	116.38	119.90
1	2	704	C	O4'-C1'-N1	5.86	112.89	108.20
1	2	1798	U	C5-C6-N1	5.86	125.63	122.70
36	1	1193	A	C5-C6-N6	-5.86	119.01	123.70
36	1	3017	A	O5'-P-OP2	-5.86	100.43	105.70
36	5	1012	G	N3-C4-C5	5.86	131.53	128.60
36	1	1120	A	C5-C6-N1	5.86	120.63	117.70
1	6	610	G	C4-N9-C1'	5.86	134.11	126.50
1	6	1133	A	O5'-P-OP2	5.86	117.73	110.70
36	5	1680	G	C5-C6-O6	5.86	132.11	128.60
36	1	930	U	C5-C6-N1	-5.85	119.77	122.70
36	1	962	A	N1-C2-N3	5.85	132.23	129.30
36	1	2423	U	N3-C4-O4	5.85	123.50	119.40
36	1	3011	A	C8-N9-C4	5.85	108.14	105.80
38	4	103	G	C8-N9-C4	-5.85	104.06	106.40
1	6	638	U	N3-C2-O2	-5.85	118.10	122.20
1	6	904	G	N3-C4-C5	-5.85	125.67	128.60
11	s9	109	LEU	CA-CB-CG	5.85	128.76	115.30
36	5	933	A	N3-C4-C5	-5.85	122.70	126.80
36	5	2643	A	O5'-P-OP2	-5.85	100.43	105.70
36	5	2796	G	O5'-P-OP1	5.85	117.72	110.70
36	5	3031	G	C8-N9-C4	5.85	108.74	106.40
1	2	394	C	N1-C2-O2	5.85	122.41	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2278	C	C5-C6-N1	5.85	123.92	121.00
1	2	720	G	OP1-P-O3'	5.85	118.07	105.20
36	1	646	A	N7-C8-N9	5.85	116.72	113.80
36	1	921	A	O4'-C1'-N9	-5.85	103.52	108.20
36	1	997	A	C8-N9-C4	-5.85	103.46	105.80
36	1	3178	A	N9-C4-C5	-5.85	103.46	105.80
36	5	2725	U	O5'-P-OP1	-5.85	100.44	105.70
36	5	3343	G	N3-C4-N9	5.85	129.51	126.00
36	1	72	C	N1-C2-O2	-5.85	115.39	118.90
36	1	2762	A	N1-C6-N6	-5.85	115.09	118.60
36	5	112	U	O4'-C1'-N1	5.85	112.88	108.20
36	5	506	U	C4-C5-C6	5.85	123.21	119.70
36	1	1003	A	C4-C5-C6	5.85	119.92	117.00
36	1	2722	U	N3-C2-O2	-5.85	118.11	122.20
36	1	2904	U	O5'-P-OP2	-5.85	100.44	105.70
36	5	1307	G	N1-C6-O6	-5.85	116.39	119.90
36	5	2807	U	OP1-P-O3'	5.85	118.06	105.20
1	6	542	A	OP1-P-O3'	5.84	118.06	105.20
1	6	1568	C	P-O3'-C3'	5.84	126.71	119.70
36	5	590	G	O5'-P-OP1	-5.84	100.44	105.70
36	5	1133	A	N1-C6-N6	-5.84	115.09	118.60
36	5	1912	U	N3-C2-O2	5.84	126.29	122.20
36	5	2386	A	C4-C5-C6	5.84	119.92	117.00
36	5	3022	G	N1-C6-O6	-5.84	116.39	119.90
36	1	2836	C	N1-C2-N3	5.84	123.29	119.20
1	2	1761	U	N1-C2-N3	5.84	118.41	114.90
36	1	1000	C	O4'-C1'-N1	5.84	112.87	108.20
36	1	1060	U	C5-C6-N1	-5.84	119.78	122.70
36	1	2295	A	C6-C5-N7	-5.84	128.21	132.30
36	1	2930	A	C2-N3-C4	5.84	113.52	110.60
36	1	2949	U	OP2-P-O3'	5.84	118.05	105.20
36	1	2950	G	C5-C6-N1	5.84	114.42	111.50
38	4	40	A	C6-C5-N7	-5.84	128.21	132.30
38	4	113	U	N1-C2-N3	5.84	118.41	114.90
52	M6	94	ARG	NE-CZ-NH2	5.84	123.22	120.30
36	5	2594	C	C5-C4-N4	-5.84	116.11	120.20
36	5	2611	U	C2-N3-C4	-5.84	123.50	127.00
36	5	1149	G	C4-C5-C6	5.84	122.30	118.80
36	5	2860	U	N1-C2-N3	-5.84	111.40	114.90
36	1	500	C	N3-C4-C5	-5.84	119.56	121.90
36	1	686	G	OP2-P-O3'	5.84	118.04	105.20
36	1	932	U	C2-N3-C4	-5.84	123.50	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	815	G	C4-N9-C1'	5.84	134.09	126.50
36	1	1000	C	O5'-P-OP2	-5.84	100.45	105.70
36	1	1155	C	OP1-P-O3'	5.84	118.04	105.20
36	1	2920	U	OP2-P-O3'	5.84	118.04	105.20
36	5	269	G	C8-N9-C4	5.84	108.73	106.40
36	5	812	G	N1-C6-O6	-5.84	116.40	119.90
36	5	1306	G	OP1-P-O3'	5.84	118.04	105.20
36	5	2418	G	O4'-C1'-N9	5.84	112.87	108.20
1	2	1611	A	N1-C2-N3	5.83	132.22	129.30
37	3	44	C	N3-C2-O2	-5.83	117.81	121.90
1	6	1630	U	C5-C6-N1	-5.83	119.78	122.70
1	6	1657	U	OP1-P-OP2	5.83	128.35	119.60
36	5	75	G	N9-C4-C5	-5.83	103.07	105.40
36	5	875	G	C6-N1-C2	-5.83	121.60	125.10
36	1	281	G	C6-N1-C2	-5.83	121.60	125.10
36	1	659	G	N3-C4-N9	5.83	129.50	126.00
36	1	2783	U	C4-C5-C6	5.83	123.20	119.70
36	5	2850	G	OP1-P-OP2	5.83	128.35	119.60
36	1	859	G	C4-C5-C6	5.83	122.30	118.80
36	1	3212	C	C6-N1-C2	5.83	122.63	120.30
36	5	1307	G	N3-C2-N2	5.83	123.98	119.90
36	5	2281	A	N7-C8-N9	-5.83	110.88	113.80
36	5	2350	C	OP1-P-OP2	-5.83	110.85	119.60
36	5	2887	A	OP2-P-O3'	5.83	118.03	105.20
36	5	3161	C	N3-C4-N4	5.83	122.08	118.00
36	1	2124	G	N1-C6-O6	5.83	123.40	119.90
36	1	2374	C	C6-N1-C2	-5.83	117.97	120.30
36	1	2653	C	N1-C2-N3	5.83	123.28	119.20
1	6	1001	A	N1-C6-N6	5.83	122.10	118.60
36	5	1155	C	OP1-P-O3'	5.83	118.02	105.20
36	5	1312	C	C6-N1-C2	-5.83	117.97	120.30
41	14	230	VAL	CB-CA-C	-5.83	100.33	111.40
1	2	577	G	C5-N7-C8	-5.83	101.39	104.30
1	6	194	U	C2-N1-C1'	5.83	124.69	117.70
1	6	1499	G	C5-C6-O6	5.83	132.09	128.60
36	5	374	A	P-O3'-C3'	5.83	126.69	119.70
36	5	1002	A	O5'-P-OP1	5.83	117.69	110.70
1	2	53	G	C5-C6-O6	5.82	132.09	128.60
1	2	553	G	N3-C2-N2	-5.82	115.82	119.90
36	1	404	G	C8-N9-C4	5.82	108.73	106.40
36	1	404	G	C5-N7-C8	5.82	107.21	104.30
36	1	419	G	N3-C2-N2	5.82	123.98	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	584	G	N1-C6-O6	-5.82	116.41	119.90
36	1	906	A	C5-C6-N1	5.82	120.61	117.70
36	5	952	A	N1-C6-N6	5.82	122.09	118.60
36	1	1420	C	N3-C2-O2	-5.82	117.83	121.90
36	5	216	G	N9-C4-C5	-5.82	103.07	105.40
36	5	531	G	O5'-P-OP1	-5.82	100.46	105.70
1	6	390	G	N1-C6-O6	5.82	123.39	119.90
36	5	2887	A	C4-C5-C6	5.82	119.91	117.00
36	1	3380	U	O5'-P-OP2	-5.82	100.46	105.70
36	5	2377	G	C5-C6-O6	5.82	132.09	128.60
36	1	284	A	N7-C8-N9	5.82	116.71	113.80
36	1	604	G	C8-N9-C4	-5.82	104.07	106.40
36	1	2414	G	N1-C2-N3	5.82	127.39	123.90
37	3	96	U	C2-N3-C4	-5.82	123.51	127.00
36	5	412	G	OP1-P-OP2	-5.82	110.87	119.60
36	5	571	U	N3-C4-O4	-5.82	115.33	119.40
36	5	2860	U	N3-C4-C5	5.82	118.09	114.60
36	5	3179	U	N3-C2-O2	-5.82	118.13	122.20
1	2	1654	G	C5-C6-N1	5.82	114.41	111.50
36	1	633	C	C5-C6-N1	-5.82	118.09	121.00
36	1	1926	C	C5-C4-N4	-5.82	116.13	120.20
1	6	406	U	N1-C2-O2	5.82	126.87	122.80
36	5	715	A	C8-N9-C4	-5.82	103.47	105.80
36	5	2937	G	O5'-P-OP2	5.82	117.68	110.70
36	5	3097	C	N1-C2-O2	-5.82	115.41	118.90
36	5	2351	U	OP1-P-OP2	-5.81	110.88	119.60
36	1	320	G	C5-C6-O6	-5.81	125.11	128.60
36	1	1008	U	N3-C2-O2	5.81	126.27	122.20
36	1	1154	A	N3-C4-C5	-5.81	122.73	126.80
36	1	1394	A	N3-C4-C5	5.81	130.87	126.80
36	1	2653	C	N3-C2-O2	-5.81	117.83	121.90
36	5	106	A	C8-N9-C4	5.81	108.12	105.80
36	5	649	A	C5-N7-C8	-5.81	100.99	103.90
36	1	3166	C	C6-N1-C2	-5.81	117.97	120.30
36	1	1516	C	N1-C2-O2	-5.81	115.41	118.90
36	1	2388	U	N1-C2-O2	-5.81	118.73	122.80
36	1	2892	A	N1-C6-N6	-5.81	115.11	118.60
1	6	412	A	C2-N3-C4	5.81	113.50	110.60
36	5	334	A	C5-N7-C8	5.81	106.81	103.90
36	5	1432	C	N3-C4-C5	5.81	124.22	121.90
36	5	2297	U	N1-C2-O2	-5.81	118.73	122.80
36	5	2383	C	C5-C4-N4	-5.81	116.13	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2836	C	O4'-C1'-N1	5.81	112.85	108.20
37	7	75	G	N3-C2-N2	-5.81	115.83	119.90
1	2	1596	C	C2-N1-C1'	5.81	125.19	118.80
36	1	545	U	C2-N1-C1'	5.81	124.67	117.70
36	1	1103	A	C8-N9-C4	5.81	108.12	105.80
36	1	1307	G	C4-N9-C1'	-5.81	118.95	126.50
36	5	1083	G	OP1-P-OP2	5.81	128.31	119.60
36	5	1917	C	N1-C2-O2	-5.81	115.42	118.90
36	5	2357	A	N9-C4-C5	-5.81	103.48	105.80
36	5	2831	G	N3-C4-C5	-5.81	125.70	128.60
36	5	2948	C	C6-N1-C2	5.81	122.62	120.30
36	1	66	A	O5'-P-OP2	5.81	117.67	110.70
36	5	309	U	N3-C2-O2	5.81	126.26	122.20
36	1	2620	G	C4-N9-C1'	-5.80	118.95	126.50
36	5	825	U	N1-C2-O2	5.80	126.86	122.80
36	5	1365	G	N1-C2-N2	-5.80	110.98	116.20
36	5	2113	A	O4'-C1'-N9	-5.80	103.56	108.20
36	1	1530	U	N3-C2-O2	5.80	126.26	122.20
36	1	2152	A	C4-C5-N7	-5.80	107.80	110.70
1	6	609	U	N3-C4-O4	-5.80	115.34	119.40
36	5	1441	G	C5-C6-O6	-5.80	125.12	128.60
36	5	2249	G	C2-N3-C4	5.80	114.80	111.90
36	5	2850	G	O5'-P-OP2	-5.80	100.48	105.70
36	1	2619	G	OP1-P-OP2	5.80	128.30	119.60
36	5	1156	C	C6-N1-C2	-5.80	117.98	120.30
36	5	2136	C	OP2-P-O3'	5.80	117.96	105.20
1	2	1462	G	N1-C6-O6	5.80	123.38	119.90
36	1	2722	U	N1-C2-O2	5.80	126.86	122.80
36	1	3174	A	N7-C8-N9	5.80	116.70	113.80
1	6	378	A	N1-C6-N6	5.80	122.08	118.60
36	5	2117	A	N1-C6-N6	-5.80	115.12	118.60
36	5	2914	G	C2-N3-C4	5.80	114.80	111.90
36	1	1197	A	C5-C6-N6	-5.80	119.06	123.70
38	4	38	U	N1-C2-N3	5.80	118.38	114.90
1	6	613	G	N3-C4-N9	5.80	129.48	126.00
1	2	380	U	N3-C2-O2	-5.80	118.14	122.20
36	1	201	A	C2-N3-C4	-5.80	107.70	110.60
36	1	2396	G	C8-N9-C4	5.80	108.72	106.40
36	1	3362	A	C4-C5-C6	5.80	119.90	117.00
38	4	51	G	C4-C5-N7	5.80	113.12	110.80
36	5	1548	C	N3-C2-O2	5.80	125.96	121.90
36	5	2182	A	N1-C2-N3	5.80	132.20	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3244	A	O4'-C1'-N9	-5.80	103.56	108.20
1	6	449	C	N3-C4-N4	-5.79	113.94	118.00
36	5	304	G	N3-C2-N2	-5.79	115.84	119.90
1	2	1093	A	N1-C6-N6	5.79	122.08	118.60
36	1	1593	A	C8-N9-C4	5.79	108.12	105.80
38	4	116	G	C8-N9-C4	5.79	108.72	106.40
36	5	3388	C	N3-C4-N4	-5.79	113.94	118.00
1	6	1700	C	C6-N1-C1'	-5.79	113.85	120.80
36	5	503	C	C5-C4-N4	-5.79	116.14	120.20
36	5	715	A	O4'-C1'-N9	5.79	112.83	108.20
36	5	861	C	C2-N3-C4	-5.79	117.00	119.90
36	5	1842	A	N1-C6-N6	5.79	122.07	118.60
36	1	922	U	N3-C2-O2	-5.79	118.15	122.20
36	5	2402	A	N9-C4-C5	5.79	108.12	105.80
36	5	2818	U	C5'-C4'-O4'	-5.79	102.15	109.10
36	1	652	G	C4-C5-N7	5.79	113.12	110.80
36	5	2191	U	N1-C2-O2	5.79	126.85	122.80
36	5	3058	U	C6-N1-C1'	-5.79	113.09	121.20
36	1	1920	U	N3-C2-O2	-5.79	118.15	122.20
36	1	2857	C	C6-N1-C2	5.79	122.61	120.30
1	6	1537	C	C4-C5-C6	5.79	120.29	117.40
36	5	579	G	OP2-P-O3'	5.79	117.93	105.20
36	1	329	U	C5-C6-N1	-5.79	119.81	122.70
36	1	971	G	O5'-P-OP2	-5.79	100.49	105.70
36	1	1541	G	N1-C6-O6	5.79	123.37	119.90
36	1	1793	C	C2-N3-C4	-5.79	117.01	119.90
36	1	2303	A	N1-C6-N6	-5.79	115.13	118.60
36	1	2637	A	O5'-P-OP1	-5.79	100.49	105.70
36	1	3135	U	OP1-P-OP2	5.79	128.28	119.60
1	6	402	C	O5'-P-OP1	5.79	117.64	110.70
36	5	3042	U	N3-C4-O4	-5.79	115.35	119.40
36	5	3303	G	O5'-P-OP2	-5.79	100.49	105.70
1	2	1761	U	C6-N1-C2	-5.78	117.53	121.00
36	1	655	C	N3-C2-O2	-5.78	117.85	121.90
36	1	2302	G	N3-C2-N2	5.78	123.95	119.90
36	1	2354	C	N3-C2-O2	-5.78	117.85	121.90
36	1	2906	C	N3-C2-O2	-5.78	117.85	121.90
36	1	2983	C	O4'-C1'-N1	5.78	112.83	108.20
1	6	1703	C	C2-N1-C1'	5.78	125.16	118.80
38	8	69	U	O5'-P-OP2	-5.78	100.49	105.70
36	1	331	G	N3-C2-N2	-5.78	115.85	119.90
36	5	197	G	O5'-P-OP2	-5.78	100.50	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1150	A	O5'-P-OP2	-5.78	100.50	105.70
36	5	1152	G	N9-C4-C5	5.78	107.71	105.40
1	6	4	C	O5'-P-OP1	-5.78	100.50	105.70
1	6	795	U	C2-N1-C1'	5.78	124.64	117.70
36	5	1164	G	C5-N7-C8	5.78	107.19	104.30
36	5	2615	G	N9-C4-C5	-5.78	103.09	105.40
1	2	769	A	N1-C6-N6	-5.78	115.13	118.60
36	1	340	C	C5-C6-N1	-5.78	118.11	121.00
36	1	1472	U	C6-N1-C2	5.78	124.47	121.00
36	5	406	G	C5-C6-N1	5.78	114.39	111.50
36	5	2732	G	C4-C5-C6	5.78	122.27	118.80
1	2	1051	G	O4'-C1'-N9	5.78	112.82	108.20
36	1	63	A	N7-C8-N9	5.78	116.69	113.80
36	1	2585	G	C2-N3-C4	5.78	114.79	111.90
1	6	1765	A	O4'-C1'-N9	5.78	112.82	108.20
36	5	878	G	OP1-P-O3'	5.78	117.91	105.20
36	5	1847	A	C4-C5-C6	-5.78	114.11	117.00
38	8	8	C	C6-N1-C2	-5.78	117.99	120.30
36	1	171	G	N3-C4-C5	5.78	131.49	128.60
36	1	2371	G	N1-C6-O6	5.78	123.36	119.90
36	1	3181	C	C4-C5-C6	5.78	120.29	117.40
36	5	504	A	C8-N9-C4	5.78	108.11	105.80
36	5	1045	C	OP2-P-O3'	5.78	117.91	105.20
36	5	1891	A	O5'-P-OP2	-5.78	100.50	105.70
36	5	2418	G	OP1-P-O3'	5.78	117.90	105.20
36	5	3362	A	N7-C8-N9	5.78	116.69	113.80
1	2	408	C	O5'-P-OP2	-5.77	100.50	105.70
1	2	1274	C	C5-C4-N4	5.77	124.24	120.20
36	1	1148	G	N3-C2-N2	5.77	123.94	119.90
36	5	407	A	N3-C4-N9	5.77	132.02	127.40
36	5	617	G	C5-C6-O6	-5.77	125.14	128.60
36	5	1907	C	N3-C2-O2	5.77	125.94	121.90
36	5	2284	C	C6-N1-C1'	-5.77	113.87	120.80
36	5	2430	A	C2-N3-C4	-5.77	107.71	110.60
36	5	2867	C	N1-C2-O2	5.77	122.36	118.90
37	7	91	G	N3-C2-N2	-5.77	115.86	119.90
36	5	339	C	C5-C4-N4	5.77	124.24	120.20
36	1	3256	G	N3-C4-C5	5.77	131.48	128.60
36	5	1175	C	C4-C5-C6	-5.77	114.52	117.40
36	5	1582	C	C6-N1-C2	-5.77	117.99	120.30
38	8	36	G	C5-C6-O6	5.77	132.06	128.60
36	5	1390	A	N9-C4-C5	5.77	108.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1770	G	C4-N9-C1'	5.77	134.00	126.50
36	5	2704	A	OP2-P-O3'	5.77	117.89	105.20
36	5	1722	U	C5-C6-N1	-5.77	119.82	122.70
36	5	2987	A	C5-N7-C8	5.77	106.78	103.90
36	5	3374	U	N3-C4-O4	-5.77	115.36	119.40
38	8	63	G	C6-C5-N7	5.77	133.86	130.40
36	1	1480	G	OP2-P-O3'	5.76	117.88	105.20
36	1	2121	G	C5-N7-C8	5.76	107.18	104.30
36	1	2135	U	C4-C5-C6	-5.76	116.24	119.70
36	1	2150	G	C4-C5-N7	-5.76	108.49	110.80
1	6	371	G	C5-C6-O6	-5.76	125.14	128.60
1	6	619	A	OP2-P-O3'	5.76	117.88	105.20
1	6	1004	U	N1-C2-O2	-5.76	118.77	122.80
36	5	880	G	C4-N9-C1'	-5.76	119.01	126.50
36	5	2197	C	C6-N1-C1'	5.76	127.72	120.80
36	5	2639	G	C4-C5-C6	5.76	122.26	118.80
36	5	2772	C	O5'-P-OP1	-5.76	100.51	105.70
51	m5	153	ASP	CB-CG-OD2	-5.76	113.11	118.30
36	1	1116	G	C8-N9-C4	-5.76	104.09	106.40
1	6	1607	G	C5-N7-C8	5.76	107.18	104.30
1	2	1669	U	C5-C6-N1	5.76	125.58	122.70
36	1	351	A	N1-C2-N3	5.76	132.18	129.30
36	1	730	C	N3-C4-C5	5.76	124.20	121.90
36	1	1062	A	C5-N7-C8	-5.76	101.02	103.90
36	1	1194	G	C4-C5-N7	-5.76	108.50	110.80
36	5	40	A	C8-N9-C4	-5.76	103.50	105.80
36	5	938	C	N1-C2-O2	-5.76	115.44	118.90
36	5	1117	G	C6-C5-N7	5.76	133.86	130.40
36	5	1466	G	OP2-P-O3'	5.76	117.87	105.20
36	5	2788	C	C5-C4-N4	5.76	124.23	120.20
1	2	742	U	C5-C6-N1	5.76	125.58	122.70
36	1	57	A	OP2-P-O3'	5.76	117.87	105.20
36	1	1541	G	N9-C4-C5	-5.76	103.10	105.40
36	1	2920	U	N3-C4-O4	-5.76	115.37	119.40
38	4	49	G	C5-C6-O6	-5.76	125.14	128.60
1	6	73	U	N3-C2-O2	5.76	126.23	122.20
36	5	861	C	C4-C5-C6	5.76	120.28	117.40
36	5	1884	A	C6-C5-N7	-5.76	128.27	132.30
36	5	3217	C	N3-C4-N4	-5.76	113.97	118.00
36	1	59	G	C6-C5-N7	-5.76	126.94	130.40
1	6	639	U	C2-N1-C1'	5.76	124.61	117.70
1	6	687	G	N9-C4-C5	5.76	107.70	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1059	G	C5-C6-N1	5.76	114.38	111.50
36	5	2609	A	N1-C6-N6	-5.76	115.14	118.60
36	1	956	U	N3-C2-O2	-5.76	118.17	122.20
36	1	1492	G	C4-C5-C6	5.76	122.25	118.80
62	N6	13	ARG	NE-CZ-NH2	-5.76	117.42	120.30
36	5	404	G	C4-C5-C6	5.76	122.25	118.80
36	5	681	U	N3-C4-O4	5.76	123.43	119.40
36	5	2384	A	OP2-P-O3'	5.76	117.87	105.20
36	5	3285	C	N1-C2-O2	5.76	122.35	118.90
38	8	113	U	N1-C2-O2	5.76	126.83	122.80
36	1	291	C	OP2-P-O3'	5.75	117.86	105.20
36	1	1496	C	C6-N1-C2	-5.75	118.00	120.30
36	5	1600	U	OP1-P-OP2	-5.75	110.97	119.60
36	1	1365	G	N1-C2-N2	-5.75	111.02	116.20
36	1	1389	G	C5-N7-C8	-5.75	101.42	104.30
36	1	1392	G	C2-N3-C4	5.75	114.78	111.90
36	1	2762	A	C5-C6-N6	5.75	128.30	123.70
36	1	3135	U	O5'-P-OP1	-5.75	100.52	105.70
1	6	1602	C	N1-C2-O2	5.75	122.35	118.90
36	5	157	A	O5'-P-OP2	-5.75	100.52	105.70
36	5	1113	G	N3-C2-N2	-5.75	115.87	119.90
36	5	1492	G	C2-N3-C4	5.75	114.78	111.90
36	5	2861	U	O5'-P-OP1	5.75	117.60	110.70
36	1	1458	U	C5-C6-N1	-5.75	119.82	122.70
36	5	640	U	N1-C2-N3	5.75	118.35	114.90
36	5	2371	G	C8-N9-C4	5.75	108.70	106.40
36	1	2141	U	N3-C4-O4	-5.75	115.38	119.40
36	1	3275	U	C6-N1-C2	-5.75	117.55	121.00
76	Q0	103	LEU	CA-CB-CG	-5.75	102.08	115.30
36	5	1139	G	N3-C2-N2	-5.75	115.88	119.90
36	1	2787	G	C8-N9-C4	-5.75	104.10	106.40
1	6	536	C	C5-C6-N1	5.75	123.87	121.00
36	5	425	G	C8-N9-C4	5.75	108.70	106.40
36	5	806	A	N9-C4-C5	-5.75	103.50	105.80
36	5	875	G	O5'-P-OP1	5.75	117.60	110.70
36	5	2271	A	C5-C6-N1	5.75	120.57	117.70
36	5	2689	A	C6-N1-C2	-5.75	115.15	118.60
36	5	3001	C	N1-C2-O2	-5.75	115.45	118.90
37	7	92	A	N3-C4-N9	5.75	132.00	127.40
36	1	755	A	N1-C6-N6	-5.75	115.15	118.60
36	1	2434	U	N3-C4-O4	-5.75	115.38	119.40
36	1	3157	U	C5-C4-O4	-5.75	122.45	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	630	A	C8-N9-C4	5.75	108.10	105.80
36	5	994	G	C5-C6-N1	5.75	114.37	111.50
36	5	1882	G	O5'-P-OP2	5.75	117.60	110.70
36	5	2250	G	N1-C6-O6	-5.75	116.45	119.90
1	2	581	U	C5-C6-N1	5.75	125.57	122.70
36	1	2648	G	C4-C5-C6	-5.75	115.35	118.80
1	2	577	G	C4-C5-N7	5.74	113.10	110.80
36	1	227	G	N1-C6-O6	5.74	123.35	119.90
36	1	635	G	N3-C2-N2	5.74	123.92	119.90
36	1	1374	G	N1-C6-O6	-5.74	116.45	119.90
36	1	2611	U	N3-C4-O4	-5.74	115.38	119.40
38	4	102	U	C4-C5-C6	5.74	123.15	119.70
1	6	390	G	C5-C6-O6	-5.74	125.15	128.60
36	5	840	C	N1-C2-N3	5.74	123.22	119.20
36	5	3042	U	N3-C4-C5	5.74	118.05	114.60
36	5	3180	A	C5-C6-N6	-5.74	119.11	123.70
36	1	515	C	C2-N3-C4	5.74	122.77	119.90
36	1	1204	A	N1-C6-N6	5.74	122.05	118.60
36	5	815	G	C8-N9-C1'	-5.74	119.53	127.00
36	1	2790	A	O5'-P-OP2	-5.74	100.53	105.70
36	1	3269	U	N3-C2-O2	-5.74	118.18	122.20
1	6	1666	U	N1-C2-O2	-5.74	118.78	122.80
36	5	1420	C	C5-C6-N1	-5.74	118.13	121.00
36	1	743	C	N1-C2-O2	-5.74	115.46	118.90
1	6	792	U	C5-C6-N1	5.74	125.57	122.70
36	5	2334	U	N3-C2-O2	-5.74	118.18	122.20
36	1	1064	A	O4'-C1'-N9	-5.74	103.61	108.20
36	1	1389	G	C5-C6-N1	5.74	114.37	111.50
1	2	1006	C	N1-C2-O2	-5.74	115.46	118.90
36	1	43	A	N3-C4-C5	5.74	130.81	126.80
36	1	2522	G	N3-C4-N9	5.74	129.44	126.00
36	1	2831	G	N1-C6-O6	5.74	123.34	119.90
38	4	58	G	N3-C4-C5	-5.74	125.73	128.60
41	L4	139	GLY	N-CA-C	-5.74	98.76	113.10
36	5	189	G	C5-C6-O6	5.74	132.04	128.60
36	1	639	G	N9-C4-C5	-5.73	103.11	105.40
36	1	3101	G	C8-N9-C4	5.73	108.69	106.40
36	5	907	G	N3-C2-N2	5.73	123.91	119.90
36	5	3044	G	C6-N1-C2	-5.73	121.66	125.10
36	1	2924	U	C5-C6-N1	-5.73	119.83	122.70
1	6	43	A	OP2-P-O3'	5.73	117.81	105.20
36	5	1937	U	C2-N3-C4	-5.73	123.56	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	793	C	N1-C2-O2	-5.73	115.46	118.90
36	1	1145	G	N9-C4-C5	-5.73	103.11	105.40
36	1	1716	U	P-O3'-C3'	5.73	126.58	119.70
1	6	815	G	C5-C6-O6	-5.73	125.16	128.60
1	6	1641	C	C6-N1-C2	5.73	122.59	120.30
36	5	1114	U	O5'-P-OP2	-5.73	100.54	105.70
36	5	2879	C	C6-N1-C2	5.73	122.59	120.30
36	5	3053	G	N1-C2-N3	-5.73	120.46	123.90
38	8	12	A	C4-C5-C6	-5.73	114.14	117.00
36	1	809	G	N1-C6-O6	5.73	123.34	119.90
36	1	971	G	C5-C6-N1	5.73	114.36	111.50
36	1	1119	C	C5-C4-N4	5.73	124.21	120.20
36	1	1841	A	N3-C4-N9	5.73	131.98	127.40
36	1	2622	C	C5-C6-N1	5.73	123.86	121.00
1	6	1789	G	N1-C6-O6	5.73	123.34	119.90
36	5	76	G	N3-C4-C5	5.73	131.47	128.60
1	2	16	G	N3-C2-N2	5.73	123.91	119.90
36	1	18	G	C4-C5-N7	5.73	113.09	110.80
36	1	1303	A	N7-C8-N9	-5.73	110.94	113.80
36	1	1594	A	N1-C6-N6	-5.73	115.16	118.60
38	4	46	G	C4-N9-C1'	5.73	133.94	126.50
1	6	272	U	C2-N1-C1'	5.73	124.57	117.70
36	5	25	U	N1-C2-O2	-5.73	118.79	122.80
36	5	2293	C	N3-C4-N4	5.73	122.01	118.00
36	5	2623	G	N9-C4-C5	-5.73	103.11	105.40
36	5	2730	G	C5-C6-O6	-5.73	125.16	128.60
36	1	99	A	O4'-C1'-N9	5.73	112.78	108.20
36	1	1929	G	N9-C4-C5	-5.73	103.11	105.40
36	5	1054	A	N1-C2-N3	-5.73	126.44	129.30
1	2	348	U	OP2-P-O3'	5.72	117.79	105.20
1	2	1595	U	C4-C5-C6	5.72	123.14	119.70
36	1	229	G	C5-C6-O6	-5.72	125.17	128.60
36	1	3217	C	C6-N1-C1'	-5.72	113.93	120.80
36	5	926	A	N1-C2-N3	5.72	132.16	129.30
36	5	1051	U	C2-N3-C4	-5.72	123.56	127.00
36	5	2109	U	C5-C4-O4	5.72	129.33	125.90
36	5	2959	C	N3-C4-C5	-5.72	119.61	121.90
36	5	3089	C	O5'-P-OP2	-5.72	100.55	105.70
1	2	720	G	P-O3'-C3'	5.72	126.57	119.70
1	2	992	A	N3-C4-C5	5.72	130.81	126.80
1	2	1385	G	N3-C4-N9	5.72	129.43	126.00
36	1	53	G	C8-N9-C1'	-5.72	119.56	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	786	A	C4-C5-N7	-5.72	107.84	110.70
1	6	1025	A	N1-C6-N6	5.72	122.03	118.60
36	5	664	U	N3-C2-O2	-5.72	118.19	122.20
36	5	1048	A	C8-N9-C4	5.72	108.09	105.80
36	5	1520	G	C5-C6-N1	5.72	114.36	111.50
36	1	953	G	P-O3'-C3'	5.72	126.56	119.70
36	5	1081	U	C5-C4-O4	-5.72	122.47	125.90
36	5	1445	U	N3-C4-C5	5.72	118.03	114.60
36	1	1421	G	N7-C8-N9	-5.72	110.24	113.10
36	1	2800	G	C5-N7-C8	5.72	107.16	104.30
36	1	3041	U	C6-N1-C2	-5.72	117.57	121.00
1	6	352	A	OP2-P-O3'	5.72	117.78	105.20
1	6	416	A	C5-C6-N1	-5.72	114.84	117.70
1	6	1596	C	C6-N1-C2	-5.72	118.01	120.30
36	5	2396	G	N9-C4-C5	5.72	107.69	105.40
36	5	3028	G	N9-C4-C5	-5.72	103.11	105.40
36	5	3104	U	N3-C4-C5	5.72	118.03	114.60
1	2	1634	C	C2-N1-C1'	-5.72	112.51	118.80
36	1	718	G	C2-N3-C4	-5.72	109.04	111.90
36	1	846	A	C2-N3-C4	-5.72	107.74	110.60
36	1	908	G	N3-C2-N2	-5.72	115.90	119.90
36	5	1910	A	OP2-P-O3'	5.72	117.78	105.20
36	5	2758	A	N9-C4-C5	5.72	108.09	105.80
36	5	2772	C	N3-C2-O2	5.72	125.90	121.90
36	1	653	A	C5-C6-N6	-5.72	119.13	123.70
36	1	1606	U	N3-C2-O2	5.72	126.20	122.20
36	1	1893	A	N1-C2-N3	5.72	132.16	129.30
36	1	2996	U	N1-C1'-C2'	5.72	121.43	114.00
36	1	3174	A	N1-C6-N6	5.72	122.03	118.60
36	5	3257	C	O5'-P-OP1	-5.72	100.55	105.70
1	2	1478	G	C8-N9-C4	-5.71	104.11	106.40
36	1	1834	U	N3-C4-C5	-5.71	111.17	114.60
36	5	427	C	C5-C6-N1	-5.71	118.14	121.00
36	5	1487	G	C4-C5-N7	-5.71	108.51	110.80
36	1	22	G	N1-C2-N3	5.71	127.33	123.90
36	1	1547	G	N1-C2-N3	-5.71	120.47	123.90
1	2	736	C	C2-N1-C1'	5.71	125.08	118.80
1	2	994	G	C5-C6-O6	5.71	132.03	128.60
36	1	340	C	C4-C5-C6	5.71	120.26	117.40
36	1	2632	G	OP1-P-O3'	5.71	117.77	105.20
38	4	83	C	O5'-P-OP1	-5.71	100.56	105.70
44	L7	177	GLY	N-CA-C	-5.71	98.82	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	980	G	C6-C5-N7	5.71	133.83	130.40
36	5	610	G	N9-C4-C5	5.71	107.69	105.40
36	5	691	A	N9-C4-C5	5.71	108.08	105.80
36	5	715	A	C4-C5-N7	-5.71	107.84	110.70
36	5	1355	A	OP2-P-O3'	5.71	117.77	105.20
36	5	2137	U	C2-N3-C4	-5.71	123.57	127.00
36	5	1481	A	C5-N7-C8	-5.71	101.05	103.90
1	2	1455	G	N3-C2-N2	-5.71	115.90	119.90
1	2	1773	C	C5-C6-N1	5.71	123.86	121.00
36	1	1169	A	C8-N9-C4	5.71	108.08	105.80
36	1	1394	A	OP1-P-O3'	-5.71	92.64	105.20
38	4	46	G	N3-C4-C5	-5.71	125.75	128.60
36	5	2169	G	C4-C5-N7	-5.71	108.52	110.80
38	8	4	C	C5-C6-N1	-5.71	118.15	121.00
38	8	126	A	OP1-P-O3'	5.71	117.76	105.20
1	2	619	A	OP2-P-O3'	5.71	117.75	105.20
1	2	756	A	C8-N9-C4	-5.71	103.52	105.80
36	1	365	A	N1-C6-N6	5.71	122.02	118.60
36	5	1420	C	C2-N1-C1'	-5.71	112.52	118.80
36	5	2386	A	C8-N9-C4	-5.71	103.52	105.80
36	5	2399	A	N1-C6-N6	5.71	122.02	118.60
36	5	2685	C	N3-C2-O2	-5.71	117.91	121.90
36	5	3044	G	N1-C2-N3	5.71	127.32	123.90
1	6	1184	A	C8-N9-C4	-5.71	103.52	105.80
1	2	142	G	N3-C4-N9	-5.70	122.58	126.00
1	2	1654	G	C5-C6-O6	-5.70	125.18	128.60
36	1	517	G	C5-C6-O6	-5.70	125.18	128.60
36	1	3308	C	N1-C2-O2	-5.70	115.48	118.90
56	N0	40	ARG	NE-CZ-NH1	-5.70	117.45	120.30
36	5	51	A	OP1-P-OP2	-5.70	111.04	119.60
36	5	694	C	N3-C2-O2	-5.70	117.91	121.90
36	5	826	G	N1-C2-N2	5.70	121.33	116.20
36	5	961	C	N3-C4-N4	5.70	121.99	118.00
36	5	1300	G	C6-C5-N7	-5.70	126.98	130.40
36	5	1944	U	C6-N1-C2	-5.70	117.58	121.00
37	7	92	A	C8-N9-C1'	-5.70	117.43	127.70
38	8	38	U	C5-C6-N1	-5.70	119.85	122.70
36	1	859	G	C4-N9-C1'	5.70	133.91	126.50
37	7	99	G	OP2-P-O3'	5.70	117.75	105.20
36	1	384	A	C8-N9-C4	5.70	108.08	105.80
36	1	2836	C	C5-C6-N1	-5.70	118.15	121.00
36	5	410	U	OP2-P-O3'	5.70	117.74	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	934	C	C6-N1-C1'	-5.70	113.96	120.80
36	1	2181	C	C5-C6-N1	-5.70	118.15	121.00
36	1	2812	C	N3-C4-C5	-5.70	119.62	121.90
65	N9	18	ARG	NE-CZ-NH2	-5.70	117.45	120.30
21	c9	57	ARG	NE-CZ-NH2	-5.70	117.45	120.30
36	5	3054	U	N3-C4-O4	5.70	123.39	119.40
49	m3	21	ARG	NE-CZ-NH1	-5.70	117.45	120.30
36	1	640	U	O5'-P-OP2	5.70	117.54	110.70
36	1	968	G	C4-C5-N7	5.70	113.08	110.80
36	1	1203	A	OP2-P-O3'	5.70	117.73	105.20
36	5	339	C	OP1-P-OP2	-5.70	111.06	119.60
36	5	2897	A	C5-C6-N1	5.70	120.55	117.70
1	2	1042	G	C4-C5-N7	-5.70	108.52	110.80
36	1	3052	G	C5-C6-N1	-5.70	108.65	111.50
1	6	965	U	C6-N1-C1'	-5.70	113.22	121.20
36	5	667	C	N3-C4-N4	-5.70	114.01	118.00
36	5	1426	C	C2-N3-C4	-5.70	117.05	119.90
36	5	1520	G	N3-C2-N2	-5.70	115.91	119.90
1	2	941	A	N1-C6-N6	-5.69	115.18	118.60
36	1	2643	A	C8-N9-C4	5.69	108.08	105.80
36	1	64	G	N3-C4-N9	-5.69	122.58	126.00
36	1	1147	G	N1-C6-O6	-5.69	116.48	119.90
36	1	1375	G	C4-C5-N7	5.69	113.08	110.80
1	6	1681	A	C2-N3-C4	-5.69	107.75	110.60
36	5	1049	C	C5-C6-N1	5.69	123.85	121.00
36	5	2606	G	N7-C8-N9	5.69	115.95	113.10
36	1	384	A	N1-C6-N6	5.69	122.01	118.60
36	1	2294	U	N1-C2-O2	-5.69	118.82	122.80
36	5	1301	A	N9-C4-C5	-5.69	103.52	105.80
36	5	2992	U	N1-C2-O2	5.69	126.78	122.80
44	17	229	PHE	CB-CG-CD2	-5.69	116.82	120.80
36	1	1227	C	C6-N1-C2	-5.69	118.02	120.30
36	1	1611	G	C5-C6-N1	-5.69	108.66	111.50
1	2	1202	A	N7-C8-N9	5.69	116.64	113.80
36	1	1851	G	O5'-P-OP2	-5.69	100.58	105.70
36	1	2130	G	N3-C4-C5	-5.69	125.76	128.60
36	5	52	A	C2-N3-C4	-5.69	107.76	110.60
36	5	695	C	O5'-P-OP2	5.69	117.53	110.70
36	5	796	U	N3-C2-O2	-5.69	118.22	122.20
36	5	868	C	C5-C6-N1	-5.69	118.16	121.00
36	5	2620	G	C5-C6-O6	-5.69	125.19	128.60
36	5	2806	U	C2-N3-C4	-5.69	123.59	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1429	G	C5-N7-C8	5.69	107.14	104.30
36	1	3192	U	N1-C2-O2	-5.69	118.82	122.80
1	6	1600	A	N1-C2-N3	5.69	132.14	129.30
36	5	2726	C	C4-C5-C6	5.69	120.24	117.40
36	5	2930	A	O4'-C1'-N9	5.69	112.75	108.20
36	5	3132	C	O5'-P-OP1	5.69	117.52	110.70
36	1	609	G	N3-C4-N9	5.68	129.41	126.00
36	1	685	G	N1-C6-O6	5.68	123.31	119.90
36	1	1926	C	N1-C2-O2	-5.68	115.49	118.90
36	1	2145	A	N7-C8-N9	5.68	116.64	113.80
1	6	1796	C	N3-C4-N4	-5.68	114.02	118.00
36	5	103	G	N1-C6-O6	-5.68	116.49	119.90
36	5	1665	C	N1-C2-O2	5.68	122.31	118.90
36	5	3058	U	N3-C2-O2	-5.68	118.22	122.20
36	1	981	U	C6-N1-C2	-5.68	117.59	121.00
36	1	2836	C	N3-C2-O2	-5.68	117.92	121.90
1	6	31	C	C6-N1-C1'	5.68	127.62	120.80
36	5	630	A	N9-C4-C5	-5.68	103.53	105.80
1	2	1180	C	N3-C2-O2	-5.68	117.92	121.90
1	6	337	G	N9-C4-C5	-5.68	103.13	105.40
1	6	1032	G	C8-N9-C4	5.68	108.67	106.40
1	2	65	A	C2-N3-C4	-5.68	107.76	110.60
36	1	2131	A	OP1-P-OP2	-5.68	111.08	119.60
36	1	2878	G	C5-C6-N1	5.68	114.34	111.50
1	6	144	U	C6-N1-C2	-5.68	117.59	121.00
36	5	641	C	C6-N1-C2	-5.68	118.03	120.30
36	5	805	G	N7-C8-N9	-5.68	110.26	113.10
36	5	1054	A	O4'-C1'-N9	-5.68	103.66	108.20
36	5	2971	A	C8-N9-C4	5.68	108.07	105.80
36	5	3371	G	N3-C4-C5	5.68	131.44	128.60
36	1	85	A	C4-C5-N7	5.68	113.54	110.70
36	1	808	A	N7-C8-N9	-5.68	110.96	113.80
51	M5	203	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	6	60	U	C2-N1-C1'	5.68	124.51	117.70
36	5	1315	U	N3-C4-O4	5.68	123.38	119.40
36	5	2150	G	C2-N3-C4	5.68	114.74	111.90
1	2	102	U	N1-C2-O2	-5.68	118.83	122.80
36	1	3142	A	C6-N1-C2	-5.68	115.19	118.60
36	5	908	G	C8-N9-C1'	-5.68	119.62	127.00
36	5	1364	C	OP2-P-O3'	5.68	117.69	105.20
36	5	3142	A	N9-C4-C5	-5.68	103.53	105.80
36	1	1841	A	N3-C4-C5	-5.67	122.83	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2379	U	O5'-P-OP1	5.67	117.51	110.70
36	5	2146	C	C5-C6-N1	-5.67	118.16	121.00
36	5	2276	G	C5-C6-O6	-5.67	125.19	128.60
36	5	3275	U	O5'-P-OP1	5.67	117.51	110.70
37	7	83	U	OP1-P-OP2	-5.67	111.09	119.60
37	3	105	C	OP2-P-O3'	5.67	117.68	105.20
1	6	566	C	N3-C4-C5	-5.67	119.63	121.90
36	1	400	G	C5-C6-O6	-5.67	125.20	128.60
37	3	86	U	N3-C4-C5	5.67	118.00	114.60
36	5	1107	C	OP2-P-O3'	5.67	117.68	105.20
36	5	2770	G	C2-N3-C4	5.67	114.74	111.90
36	5	3278	C	C6-N1-C2	5.67	122.57	120.30
36	1	589	A	C8-N9-C4	5.67	108.07	105.80
1	6	1285	U	C6-N1-C2	-5.67	117.60	121.00
36	5	832	G	C4-C5-C6	5.67	122.20	118.80
36	1	106	A	C8-N9-C4	5.67	108.07	105.80
36	1	123	A	C8-N9-C4	-5.67	103.53	105.80
36	1	887	G	C5-N7-C8	5.67	107.13	104.30
36	1	2611	U	C5-C6-N1	-5.67	119.87	122.70
36	5	1148	G	C8-N9-C4	5.67	108.67	106.40
36	1	304	G	N1-C6-O6	-5.67	116.50	119.90
36	1	867	G	C4-C5-N7	-5.67	108.53	110.80
36	1	2281	A	N3-C4-C5	5.67	130.77	126.80
36	1	2309	A	OP1-P-OP2	5.67	128.10	119.60
36	1	2362	C	C2-N3-C4	5.67	122.73	119.90
1	6	913	G	O5'-P-OP1	-5.67	100.60	105.70
1	6	1058	U	P-O3'-C3'	5.67	126.50	119.70
1	6	1503	A	O4'-C1'-N9	5.67	112.73	108.20
36	5	776	U	N3-C2-O2	-5.67	118.23	122.20
36	5	1152	G	N1-C2-N3	5.67	127.30	123.90
36	5	2156	C	N1-C2-O2	-5.67	115.50	118.90
1	6	1145	U	C4-C5-C6	5.67	123.10	119.70
36	5	945	C	C6-N1-C2	5.67	122.57	120.30
36	5	2938	G	C2-N3-C4	5.67	114.73	111.90
54	m8	178	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	2	527	A	N7-C8-N9	5.66	116.63	113.80
36	1	272	G	C5-C6-O6	-5.66	125.20	128.60
36	1	833	G	N1-C2-N2	-5.66	111.10	116.20
36	1	2649	A	N1-C6-N6	5.66	122.00	118.60
36	5	2148	U	C2-N3-C4	-5.66	123.60	127.00
36	5	2191	U	N3-C4-C5	5.66	118.00	114.60
1	2	696	C	C6-N1-C2	-5.66	118.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2146	C	OP1-P-O3'	5.66	117.66	105.20
36	5	415	G	N3-C2-N2	5.66	123.86	119.90
36	5	3028	G	N1-C2-N2	-5.66	111.10	116.20
37	7	40	C	C5-C4-N4	-5.66	116.24	120.20
36	1	2645	G	N3-C2-N2	-5.66	115.94	119.90
41	L4	188	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	6	174	U	O5'-P-OP1	-5.66	100.61	105.70
1	6	558	U	C2-N1-C1'	5.66	124.49	117.70
36	1	98	G	OP2-P-O3'	5.66	117.65	105.20
36	1	651	G	C4-C5-C6	5.66	122.19	118.80
36	1	2206	G	C5-C6-O6	-5.66	125.20	128.60
38	4	61	A	N1-C6-N6	5.66	122.00	118.60
36	5	41	G	C4-C5-N7	5.66	113.06	110.80
36	5	1403	C	C5-C6-N1	-5.66	118.17	121.00
36	5	3326	G	C4-C5-N7	5.66	113.06	110.80
1	2	158	U	P-O3'-C3'	5.66	126.49	119.70
36	1	922	U	C4-C5-C6	-5.66	116.31	119.70
36	5	404	G	C4-C5-N7	-5.66	108.54	110.80
36	5	653	A	C6-C5-N7	-5.66	128.34	132.30
36	1	1435	A	O5'-P-OP2	5.66	117.49	110.70
36	1	1472	U	C2-N3-C4	-5.66	123.61	127.00
36	1	1661	G	N3-C2-N2	5.66	123.86	119.90
36	1	2362	C	OP1-P-OP2	5.66	128.08	119.60
36	1	2670	G	N3-C2-N2	-5.66	115.94	119.90
1	6	449	C	C5-C4-N4	5.66	124.16	120.20
36	5	911	C	C2-N3-C4	-5.66	117.07	119.90
38	8	11	C	C2-N3-C4	5.66	122.73	119.90
1	2	48	G	C5-C6-O6	5.65	131.99	128.60
36	1	1194	G	C5-C6-O6	5.65	131.99	128.60
36	1	2402	A	C2-N3-C4	5.65	113.43	110.60
36	5	2948	C	OP1-P-OP2	-5.65	111.12	119.60
1	2	36	C	C6-N1-C2	5.65	122.56	120.30
36	1	1051	U	OP1-P-O3'	5.65	117.64	105.20
36	1	1164	G	C5-C6-O6	5.65	131.99	128.60
36	1	2180	G	C4-C5-C6	5.65	122.19	118.80
36	5	285	A	N9-C4-C5	5.65	108.06	105.80
36	5	1123	U	C5-C6-N1	-5.65	119.87	122.70
36	5	1206	G	C4-C5-N7	-5.65	108.54	110.80
36	5	1338	C	OP1-P-O3'	5.65	117.64	105.20
1	2	1082	C	P-O3'-C3'	5.65	126.48	119.70
11	S9	60	LEU	CA-CB-CG	5.65	128.30	115.30
36	1	940	G	C4-C5-N7	-5.65	108.54	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1522	U	C5-C4-O4	-5.65	122.51	125.90
36	1	2812	C	C6-N1-C2	5.65	122.56	120.30
36	5	113	C	C6-N1-C2	5.65	122.56	120.30
36	5	3206	C	OP1-P-OP2	5.65	128.07	119.60
38	8	57	C	N3-C4-C5	5.65	124.16	121.90
1	2	1482	C	C6-N1-C2	5.65	122.56	120.30
36	1	1581	C	N3-C2-O2	-5.65	117.95	121.90
36	1	2249	G	C5-C6-N1	5.65	114.33	111.50
37	3	5	G	N3-C4-N9	-5.65	122.61	126.00
1	6	554	C	N3-C2-O2	-5.65	117.95	121.90
36	5	226	C	C6-N1-C2	-5.65	118.04	120.30
36	5	313	A	C8-N9-C4	-5.65	103.54	105.80
37	7	37	G	C6-C5-N7	-5.65	127.01	130.40
36	1	1340	G	N3-C4-N9	5.65	129.39	126.00
36	1	2135	U	N3-C4-C5	5.65	117.99	114.60
36	1	2363	A	C4-C5-N7	-5.65	107.88	110.70
1	6	1	U	N1-C2-O2	5.65	126.75	122.80
1	6	416	A	C2-N3-C4	-5.65	107.78	110.60
36	5	3328	G	N3-C4-C5	-5.65	125.78	128.60
1	2	967	A	C8-N9-C4	5.64	108.06	105.80
36	1	196	G	N9-C4-C5	-5.64	103.14	105.40
36	1	371	G	N3-C2-N2	5.64	123.85	119.90
36	1	1394	A	N3-C4-N9	-5.64	122.88	127.40
36	1	2121	G	C4-C5-N7	-5.64	108.54	110.80
36	1	2417	U	N1-C2-O2	-5.64	118.85	122.80
36	1	2810	C	C5-C6-N1	-5.64	118.18	121.00
36	1	2915	U	C2-N3-C4	-5.64	123.61	127.00
1	6	308	C	C6-N1-C1'	5.64	127.57	120.80
36	5	2356	A	C5-C6-N1	-5.64	114.88	117.70
36	5	2641	U	OP1-P-O3'	5.64	117.62	105.20
36	5	3003	G	C5-C6-N1	5.64	114.32	111.50
1	2	1652	C	C5-C6-N1	5.64	123.82	121.00
36	1	1122	U	C2-N3-C4	-5.64	123.61	127.00
36	1	2952	G	N1-C6-O6	5.64	123.29	119.90
36	1	2985	C	N1-C2-O2	5.64	122.28	118.90
36	1	3111	U	N3-C2-O2	-5.64	118.25	122.20
36	5	422	A	N1-C6-N6	-5.64	115.22	118.60
36	5	2134	G	N9-C4-C5	-5.64	103.14	105.40
36	5	2816	G	N7-C8-N9	-5.64	110.28	113.10
36	5	3190	C	C6-N1-C2	-5.64	118.04	120.30
36	5	3275	U	P-O3'-C3'	5.64	126.47	119.70
1	2	734	A	P-O3'-C3'	5.64	126.47	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	325	A	C6-N1-C2	-5.64	115.22	118.60
36	1	856	G	C5-C6-O6	-5.64	125.22	128.60
1	6	1027	A	P-O3'-C3'	5.64	126.47	119.70
36	5	1847	A	C5-N7-C8	-5.64	101.08	103.90
1	2	765	G	C5-C6-O6	-5.64	125.22	128.60
36	1	1801	U	C4-C5-C6	5.64	123.08	119.70
36	1	2168	A	C5-C6-N1	5.64	120.52	117.70
36	1	2954	U	OP1-P-OP2	-5.64	111.14	119.60
37	3	44	C	C6-N1-C2	-5.64	118.04	120.30
1	6	524	U	N3-C2-O2	-5.64	118.25	122.20
36	5	611	A	C8-N9-C4	5.64	108.06	105.80
36	5	2693	C	C5-C6-N1	-5.64	118.18	121.00
36	1	785	G	N3-C4-C5	-5.64	125.78	128.60
36	1	1807	G	C8-N9-C4	-5.64	104.14	106.40
36	5	1660	C	N1-C2-O2	-5.64	115.52	118.90
36	5	2936	A	O5'-P-OP1	-5.64	100.63	105.70
36	1	895	A	O5'-P-OP1	-5.64	100.63	105.70
36	1	1269	U	N1-C2-O2	5.64	126.75	122.80
36	1	2608	G	N1-C6-O6	5.64	123.28	119.90
1	6	1747	G	C5-C6-N1	5.64	114.32	111.50
36	5	1154	A	C2-N3-C4	5.64	113.42	110.60
36	5	1496	C	N3-C2-O2	-5.64	117.95	121.90
37	3	49	G	N3-C2-N2	5.63	123.84	119.90
36	5	645	A	N3-C4-C5	-5.63	122.86	126.80
36	5	1657	C	C2-N1-C1'	5.63	125.00	118.80
36	5	2833	A	C5-C6-N6	-5.63	119.19	123.70
36	5	3196	U	C2-N1-C1'	-5.63	110.94	117.70
1	2	1289	U	C5-C6-N1	-5.63	119.88	122.70
36	1	2286	U	C5-C4-O4	5.63	129.28	125.90
36	5	544	C	C2-N1-C1'	5.63	125.00	118.80
36	5	2385	G	C5-C6-O6	-5.63	125.22	128.60
36	5	2631	U	N1-C2-N3	5.63	118.28	114.90
37	7	37	G	N1-C6-O6	5.63	123.28	119.90
36	1	2608	G	N3-C4-C5	5.63	131.42	128.60
36	5	2307	G	C5-C6-O6	5.63	131.98	128.60
36	5	2694	A	N9-C4-C5	5.63	108.05	105.80
36	5	3373	U	C2-N3-C4	-5.63	123.62	127.00
1	2	1100	G	N3-C4-N9	5.63	129.38	126.00
36	1	1145	G	N3-C4-C5	5.63	131.41	128.60
36	1	1367	G	C8-N9-C4	5.63	108.65	106.40
36	1	1815	U	P-O3'-C3'	5.63	126.46	119.70
36	1	2377	G	C5-C6-O6	5.63	131.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	62	C	C6-N1-C2	5.63	122.55	120.30
1	2	18	C	C6-N1-C2	-5.63	118.05	120.30
1	2	994	G	C5-C6-N1	-5.63	108.69	111.50
36	1	906	A	C5-C6-N6	-5.63	119.20	123.70
36	1	1555	U	C6-N1-C2	5.63	124.38	121.00
36	1	2811	A	C6-N1-C2	-5.63	115.22	118.60
1	6	864	U	C2-N1-C1'	5.63	124.45	117.70
36	5	1122	U	C4-C5-C6	5.63	123.08	119.70
36	5	1208	U	O5'-P-OP2	-5.63	100.64	105.70
36	5	1476	G	O5'-P-OP2	-5.63	100.64	105.70
36	5	2201	G	N3-C4-C5	-5.63	125.79	128.60
36	5	2899	C	C2-N3-C4	-5.63	117.09	119.90
1	2	1600	A	C5-N7-C8	-5.62	101.09	103.90
36	1	1325	U	OP1-P-OP2	5.62	128.04	119.60
38	4	25	G	C5-N7-C8	5.62	107.11	104.30
1	6	92	A	C8-N9-C4	5.62	108.05	105.80
1	6	355	G	N3-C2-N2	-5.62	115.96	119.90
36	1	1200	A	O4'-C1'-N9	5.62	112.70	108.20
36	1	1738	C	N3-C4-C5	5.62	124.15	121.90
38	4	60	U	C2-N3-C4	-5.62	123.62	127.00
1	6	1514	U	N3-C4-O4	-5.62	115.46	119.40
36	5	41	G	C5-N7-C8	-5.62	101.49	104.30
36	5	918	C	N1-C2-O2	5.62	122.27	118.90
36	5	1484	U	C5-C6-N1	-5.62	119.89	122.70
36	5	2293	C	C2-N1-C1'	5.62	124.98	118.80
1	2	553	G	C8-N9-C4	-5.62	104.15	106.40
1	2	1267	G	N3-C4-C5	-5.62	125.79	128.60
1	2	1600	A	N3-C4-C5	5.62	130.73	126.80
36	1	320	G	O5'-P-OP2	-5.62	100.64	105.70
36	1	3043	C	N3-C4-C5	5.62	124.15	121.90
38	4	113	U	N3-C2-O2	-5.62	118.27	122.20
1	6	815	G	C5-N7-C8	-5.62	101.49	104.30
36	5	2279	A	OP1-P-OP2	-5.62	111.17	119.60
36	5	2871	G	N3-C4-C5	-5.62	125.79	128.60
1	2	1455	G	C5-C6-N1	-5.62	108.69	111.50
48	m1	61	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	2	158	U	C5-C6-N1	5.62	125.51	122.70
36	1	1124	U	C5-C6-N1	5.62	125.51	122.70
36	1	3207	U	N3-C4-O4	-5.62	115.47	119.40
37	3	82	G	N1-C2-N2	-5.62	111.14	116.20
1	6	631	G	C8-N9-C4	-5.62	104.15	106.40
36	5	225	C	N3-C4-N4	5.62	121.93	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2708	C	N3-C4-C5	5.62	124.15	121.90
38	8	17	A	N1-C6-N6	5.62	121.97	118.60
38	8	116	G	C4-C5-N7	5.62	113.05	110.80
1	2	393	C	N3-C4-C5	5.62	124.15	121.90
1	2	1654	G	N3-C4-N9	5.62	129.37	126.00
36	1	2351	U	O5'-P-OP2	5.62	117.44	110.70
36	1	2621	G	O5'-P-OP2	-5.62	100.64	105.70
36	5	1296	C	N3-C4-C5	-5.62	119.65	121.90
1	2	687	G	N3-C2-N2	-5.62	115.97	119.90
36	1	1145	G	N1-C6-O6	5.62	123.27	119.90
38	4	14	C	N3-C4-C5	5.62	124.15	121.90
1	6	431	C	C5-C4-N4	5.62	124.13	120.20
36	5	197	G	C8-N9-C1'	-5.62	119.70	127.00
36	5	631	U	OP1-P-OP2	5.62	128.02	119.60
1	2	1426	C	C6-N1-C2	5.61	122.55	120.30
36	1	267	G	O4'-C1'-N9	-5.61	103.71	108.20
36	1	1713	G	N3-C4-C5	5.61	131.41	128.60
37	3	73	C	C6-N1-C2	-5.61	118.06	120.30
1	6	426	G	C8-N9-C4	-5.61	104.16	106.40
36	5	500	C	OP1-P-O3'	5.61	117.55	105.20
36	1	1125	U	O5'-P-OP1	-5.61	100.65	105.70
36	1	1145	G	N1-C2-N2	5.61	121.25	116.20
20	c8	15	LEU	CA-CB-CG	5.61	128.21	115.30
49	m3	67	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	2	1673	G	C6-C5-N7	-5.61	127.03	130.40
36	1	1124	U	N1-C2-O2	5.61	126.73	122.80
36	1	1319	G	C5-C6-O6	5.61	131.97	128.60
36	5	41	G	N9-C4-C5	-5.61	103.16	105.40
36	5	201	A	O5'-P-OP1	5.61	117.43	110.70
36	5	622	A	C5-C6-N6	-5.61	119.21	123.70
36	1	1133	A	N1-C6-N6	5.61	121.97	118.60
36	1	2392	C	N1-C2-N3	5.61	123.13	119.20
36	1	3142	A	N1-C2-N3	5.61	132.10	129.30
1	6	1560	U	N3-C4-O4	-5.61	115.47	119.40
36	5	1885	U	N1-C2-N3	5.61	118.27	114.90
36	5	2572	C	C6-N1-C1'	-5.61	114.07	120.80
40	l3	347	SER	N-CA-C	5.61	126.14	111.00
36	1	270	U	N3-C2-O2	-5.61	118.27	122.20
36	1	331	G	C2-N3-C4	5.61	114.70	111.90
36	1	754	G	OP2-P-O3'	5.61	117.53	105.20
36	5	1750	A	C5-C6-N6	-5.61	119.21	123.70
36	5	2263	C	N1-C2-O2	5.61	122.27	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1783	C	O5'-P-OP2	-5.61	100.65	105.70
36	1	347	G	C8-N9-C1'	-5.61	119.71	127.00
36	1	1349	G	N3-C4-N9	5.61	129.36	126.00
1	6	542	A	N7-C8-N9	5.61	116.60	113.80
1	6	754	A	N1-C6-N6	5.61	121.96	118.60
36	5	587	U	N3-C2-O2	5.61	126.12	122.20
36	5	1891	A	C6-N1-C2	-5.61	115.24	118.60
36	1	1165	A	C8-N9-C4	5.60	108.04	105.80
36	1	2152	A	C2-N3-C4	5.60	113.40	110.60
36	5	959	C	P-O3'-C3'	5.60	126.42	119.70
36	5	2641	U	C4-C5-C6	5.60	123.06	119.70
36	5	3383	G	N3-C4-C5	-5.60	125.80	128.60
1	2	344	A	N1-C6-N6	-5.60	115.24	118.60
36	1	1134	G	N1-C6-O6	5.60	123.26	119.90
36	1	1906	G	N1-C6-O6	5.60	123.26	119.90
36	1	3261	C	N1-C2-O2	-5.60	115.54	118.90
36	5	1926	C	C2-N3-C4	-5.60	117.10	119.90
1	2	404	G	O5'-P-OP1	-5.60	100.66	105.70
36	5	2824	G	OP1-P-OP2	5.60	128.00	119.60
1	2	1180	C	C2-N1-C1'	5.60	124.96	118.80
1	2	1491	U	O5'-P-OP1	-5.60	100.66	105.70
36	1	2800	G	N7-C8-N9	-5.60	110.30	113.10
38	4	55	U	C2-N3-C4	-5.60	123.64	127.00
1	6	1028	C	O5'-P-OP1	-5.60	100.66	105.70
20	c8	116	LEU	CA-CB-CG	5.60	128.18	115.30
36	5	786	A	C8-N9-C4	-5.60	103.56	105.80
1	2	325	G	N3-C4-C5	5.60	131.40	128.60
36	1	2688	U	N1-C2-O2	5.60	126.72	122.80
38	4	79	A	C4-C5-C6	5.60	119.80	117.00
1	6	331	A	N3-C4-C5	5.60	130.72	126.80
36	5	1082	U	N3-C4-O4	5.60	123.32	119.40
36	5	2414	G	C5-C6-N1	-5.60	108.70	111.50
36	5	2872	A	C8-N9-C1'	5.60	137.78	127.70
1	2	527	A	C8-N9-C4	-5.60	103.56	105.80
36	1	2130	G	N3-C2-N2	5.60	123.82	119.90
43	L6	64	LEU	CA-CB-CG	5.60	128.17	115.30
36	5	1747	G	C4-C5-N7	-5.60	108.56	110.80
36	5	3098	G	C2-N3-C4	5.60	114.70	111.90
36	1	2877	G	N9-C4-C5	5.59	107.64	105.40
36	1	2930	A	O4'-C1'-N9	5.59	112.68	108.20
71	O5	63	ARG	NE-CZ-NH1	-5.59	117.50	120.30
36	5	2673	A	C8-N9-C4	5.59	108.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2985	C	C2-N3-C4	5.59	122.70	119.90
36	1	1396	C	N1-C2-N3	-5.59	115.28	119.20
36	1	2918	G	OP1-P-OP2	5.59	127.99	119.60
36	1	3344	A	C4-C5-N7	5.59	113.50	110.70
1	6	1162	C	N3-C4-C5	-5.59	119.66	121.90
36	5	356	C	O5'-P-OP2	-5.59	100.67	105.70
36	5	2758	A	N3-C4-C5	-5.59	122.89	126.80
36	5	2878	G	C5-C6-N1	5.59	114.30	111.50
36	5	2940	A	C6-N1-C2	-5.59	115.25	118.60
36	5	3174	A	C8-N9-C4	-5.59	103.56	105.80
36	1	2952	G	C5-C6-O6	-5.59	125.25	128.60
2	s0	62	ARG	NE-CZ-NH1	5.59	123.09	120.30
36	5	644	G	N1-C6-O6	-5.59	116.55	119.90
36	5	2339	C	OP1-P-O3'	5.59	117.50	105.20
36	5	2703	A	C8-N9-C4	-5.59	103.56	105.80
57	n1	8	ARG	NE-CZ-NH2	-5.59	117.51	120.30
36	1	698	U	N3-C2-O2	5.59	126.11	122.20
36	1	3361	G	N3-C4-C5	-5.59	125.81	128.60
37	3	89	G	N3-C4-N9	5.59	129.35	126.00
36	5	924	G	N3-C2-N2	-5.59	115.99	119.90
36	5	1053	A	C5-C6-N1	5.59	120.49	117.70
36	5	1769	G	N1-C6-O6	5.59	123.25	119.90
36	5	2141	U	N3-C2-O2	-5.59	118.29	122.20
36	5	2763	U	C2-N3-C4	-5.59	123.65	127.00
1	2	54	C	N3-C4-C5	5.59	124.14	121.90
1	6	1736	G	N3-C2-N2	-5.59	115.99	119.90
25	d3	104	LEU	CA-CB-CG	5.59	128.15	115.30
38	8	25	G	N1-C6-O6	-5.59	116.55	119.90
36	1	1531	C	C6-N1-C2	-5.58	118.07	120.30
36	1	2912	G	C5-C6-N1	5.58	114.29	111.50
1	6	1285	U	C5-C4-O4	5.58	129.25	125.90
36	1	320	G	N1-C6-O6	5.58	123.25	119.90
36	1	658	G	C8-N9-C4	5.58	108.63	106.40
36	1	896	A	N7-C8-N9	5.58	116.59	113.80
36	1	1398	U	N3-C4-C5	5.58	117.95	114.60
36	1	2816	G	N1-C6-O6	5.58	123.25	119.90
36	1	3000	A	C2-N3-C4	-5.58	107.81	110.60
36	5	1906	G	N9-C4-C5	-5.58	103.17	105.40
36	5	3000	A	C5-C6-N6	-5.58	119.23	123.70
36	5	3101	G	C5-C6-O6	5.58	131.95	128.60
1	2	1654	G	N3-C4-C5	-5.58	125.81	128.60
36	1	2295	A	N1-C6-N6	5.58	121.95	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3278	C	C6-N1-C2	-5.58	118.07	120.30
37	7	6	C	C2-N3-C4	-5.58	117.11	119.90
36	1	1294	A	O4'-C1'-N9	5.58	112.66	108.20
36	1	2116	G	C5-N7-C8	5.58	107.09	104.30
1	2	458	G	C5-C6-N1	-5.58	108.71	111.50
1	2	1589	C	O5'-P-OP2	-5.58	100.68	105.70
36	1	2275	A	O5'-P-OP1	-5.58	100.68	105.70
1	6	21	U	C5-C4-O4	-5.58	122.55	125.90
36	5	128	G	N3-C4-N9	5.58	129.35	126.00
36	5	950	G	C5-C6-O6	5.58	131.95	128.60
36	5	2891	U	C5-C6-N1	-5.58	119.91	122.70
37	7	50	U	C5-C6-N1	5.58	125.49	122.70
1	2	1639	C	N3-C4-N4	5.58	121.90	118.00
36	1	1881	A	OP1-P-OP2	5.58	127.97	119.60
36	1	2658	G	C5-N7-C8	5.58	107.09	104.30
36	1	1659	U	N1-C2-N3	5.58	118.25	114.90
36	1	2298	U	C4-C5-C6	5.58	123.05	119.70
36	1	2760	C	N3-C4-C5	-5.58	119.67	121.90
38	4	35	C	C4-C5-C6	5.58	120.19	117.40
38	4	48	A	N1-C6-N6	5.58	121.94	118.60
36	5	1407	A	O5'-P-OP1	5.58	117.39	110.70
36	5	1420	C	OP2-P-O3'	5.58	117.47	105.20
36	5	2161	G	N3-C2-N2	-5.58	116.00	119.90
36	5	3078	U	C3'-C2'-C1'	5.58	105.96	101.50
36	1	1199	C	C4-C5-C6	5.57	120.19	117.40
36	1	2150	G	N3-C4-C5	-5.57	125.81	128.60
36	1	2627	C	C2-N1-C1'	-5.57	112.67	118.80
36	1	2728	G	C5-C6-N1	5.57	114.29	111.50
38	4	58	G	N3-C4-N9	5.57	129.34	126.00
1	6	767	U	N3-C2-O2	-5.57	118.30	122.20
36	5	410	U	C5-C6-N1	5.57	125.49	122.70
36	5	425	G	C5-C6-O6	-5.57	125.25	128.60
36	5	1110	U	C5-C6-N1	5.57	125.49	122.70
36	5	2136	C	C5-C4-N4	-5.57	116.30	120.20
36	1	272	G	C6-C5-N7	-5.57	127.06	130.40
36	1	809	G	C8-N9-C4	5.57	108.63	106.40
36	1	2129	U	C6-N1-C2	-5.57	117.66	121.00
37	7	8	G	N3-C4-C5	-5.57	125.81	128.60
36	1	1700	G	N3-C4-N9	5.57	129.34	126.00
36	1	1733	G	N3-C4-N9	5.57	129.34	126.00
38	4	140	G	C8-N9-C4	-5.57	104.17	106.40
36	5	326	U	OP2-P-O3'	5.57	117.46	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	596	C	C2-N3-C4	5.57	122.69	119.90
36	5	1381	A	O5'-P-OP1	-5.57	100.69	105.70
36	5	1391	C	N1-C2-O2	-5.57	115.56	118.90
36	5	2116	G	N1-C6-O6	5.57	123.24	119.90
38	8	8	C	O5'-P-OP1	5.57	117.38	110.70
38	8	115	C	N3-C2-O2	5.57	125.80	121.90
36	1	143	G	C5-C6-N1	5.57	114.28	111.50
36	5	785	G	C5-C6-N1	5.57	114.28	111.50
36	5	1333	C	C2-N3-C4	5.57	122.68	119.90
36	5	2365	C	OP1-P-OP2	5.57	127.95	119.60
36	1	104	G	C5-N7-C8	-5.57	101.52	104.30
36	1	2181	C	N3-C4-C5	5.57	124.13	121.90
36	1	3368	U	N1-C2-O2	-5.57	118.90	122.80
36	5	646	A	C2-N3-C4	-5.57	107.82	110.60
36	5	1450	G	OP2-P-O3'	5.57	117.45	105.20
36	5	2871	G	C5-C6-N1	5.57	114.28	111.50
36	1	102	C	N3-C2-O2	5.57	125.80	121.90
36	1	200	C	N3-C4-N4	5.57	121.90	118.00
36	1	361	A	C5-C6-N1	5.57	120.48	117.70
36	1	1489	A	N1-C6-N6	5.57	121.94	118.60
36	1	2572	C	N3-C2-O2	-5.57	118.00	121.90
1	6	163	G	N9-C4-C5	5.57	107.63	105.40
1	6	960	U	N3-C2-O2	-5.57	118.30	122.20
36	5	283	G	C2-N3-C4	5.57	114.68	111.90
36	5	1852	G	N7-C8-N9	5.57	115.88	113.10
36	5	2886	U	C5-C4-O4	5.57	129.24	125.90
36	5	2889	C	N3-C4-C5	5.57	124.13	121.90
47	m0	88	ARG	NE-CZ-NH1	-5.57	117.52	120.30
36	1	584	G	N9-C4-C5	5.56	107.63	105.40
36	1	1368	U	C2-N3-C4	-5.56	123.66	127.00
36	1	1425	U	N3-C2-O2	-5.56	118.31	122.20
36	5	1297	C	C6-N1-C2	-5.56	118.08	120.30
36	5	2249	G	N1-C6-O6	-5.56	116.56	119.90
36	5	2385	G	C8-N9-C4	5.56	108.62	106.40
36	1	796	U	OP2-P-O3'	5.56	117.44	105.20
36	1	1122	U	C5-C6-N1	-5.56	119.92	122.70
36	1	3137	C	N1-C2-O2	-5.56	115.56	118.90
36	5	358	G	C6-N1-C2	5.56	128.44	125.10
36	5	571	U	N1-C2-N3	5.56	118.24	114.90
36	5	2378	C	N3-C4-C5	5.56	124.12	121.90
36	5	2873	U	C5-C6-N1	-5.56	119.92	122.70
36	1	112	U	C5-C4-O4	-5.56	122.56	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1505	C	C6-N1-C2	5.56	122.52	120.30
1	6	1048	G	N1-C6-O6	5.56	123.24	119.90
36	5	948	C	N3-C4-N4	5.56	121.89	118.00
36	5	1314	C	N1-C2-O2	5.56	122.24	118.90
36	1	2431	C	C2-N3-C4	-5.56	117.12	119.90
36	1	3175	U	N1-C2-N3	5.56	118.24	114.90
1	6	402	C	O4'-C1'-N1	5.56	112.65	108.20
1	6	1696	G	P-O3'-C3'	5.56	126.37	119.70
36	5	1433	A	OP2-P-O3'	5.56	117.43	105.20
36	5	3078	U	N1-C1'-C2'	-5.56	105.88	112.00
38	8	11	C	N1-C2-O2	5.56	122.23	118.90
52	m6	69	GLY	N-CA-C	-5.56	99.20	113.10
36	1	428	A	OP2-P-O3'	5.56	117.42	105.20
36	1	580	C	N1-C2-O2	-5.56	115.56	118.90
1	6	172	C	C6-N1-C2	-5.56	118.08	120.30
36	5	935	U	C5-C4-O4	-5.56	122.56	125.90
36	5	2425	G	N3-C4-C5	5.56	131.38	128.60
36	5	2978	U	N3-C2-O2	-5.56	118.31	122.20
36	5	3260	G	N1-C2-N2	-5.56	111.20	116.20
1	2	1595	U	N3-C4-C5	-5.56	111.27	114.60
36	5	658	G	N1-C6-O6	5.56	123.23	119.90
1	2	440	U	C2-N1-C1'	-5.55	111.03	117.70
36	1	1520	G	C8-N9-C4	5.55	108.62	106.40
36	1	1586	G	N3-C4-C5	-5.55	125.82	128.60
36	1	2899	C	C2-N1-C1'	5.55	124.91	118.80
36	1	3063	C	N3-C4-C5	5.55	124.12	121.90
1	6	308	C	C5-C4-N4	5.55	124.09	120.20
36	5	1208	U	N3-C4-O4	-5.55	115.51	119.40
36	5	2142	A	N1-C6-N6	-5.55	115.27	118.60
36	5	2314	U	N3-C4-O4	5.55	123.29	119.40
36	5	2373	A	C5-C6-N1	5.55	120.48	117.70
36	1	1430	U	C5-C4-O4	-5.55	122.57	125.90
1	2	863	A	C5-C6-N6	-5.55	119.26	123.70
36	1	934	G	C8-N9-C1'	-5.55	119.78	127.00
36	1	1830	G	C5-C6-O6	-5.55	125.27	128.60
36	1	3341	U	O4'-C1'-N1	5.55	112.64	108.20
1	6	1674	C	N1-C2-O2	-5.55	115.57	118.90
36	5	782	U	N3-C2-O2	-5.55	118.31	122.20
36	5	2141	U	C5-C4-O4	5.55	129.23	125.90
36	5	2826	U	C5-C4-O4	5.55	129.23	125.90
36	5	3093	C	O4'-C1'-N1	-5.55	103.76	108.20
1	2	327	U	C5-C4-O4	-5.55	122.57	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	496	C	C6-N1-C2	-5.55	118.08	120.30
36	1	2549	G	N1-C6-O6	-5.55	116.57	119.90
36	1	2986	U	N1-C2-N3	5.55	118.23	114.90
38	4	34	U	C6-N1-C2	5.55	124.33	121.00
1	6	1140	G	C5-C6-N1	5.55	114.28	111.50
36	5	1181	U	C5-C6-N1	-5.55	119.92	122.70
36	5	2388	U	OP2-P-O3'	5.55	117.41	105.20
1	2	1502	G	N3-C4-N9	5.55	129.33	126.00
36	1	2343	C	N3-C4-N4	-5.55	114.12	118.00
36	1	439	C	C6-N1-C1'	-5.55	114.14	120.80
36	1	718	G	C8-N9-C1'	5.55	134.21	127.00
36	1	1793	C	C6-N1-C2	5.55	122.52	120.30
36	1	2732	G	N1-C2-N2	-5.55	111.21	116.20
36	1	3259	U	O4'-C1'-N1	-5.55	103.76	108.20
36	1	3308	C	N3-C4-C5	-5.55	119.68	121.90
36	5	421	G	N1-C2-N3	5.55	127.23	123.90
36	5	1065	A	N1-C6-N6	-5.55	115.27	118.60
37	7	99	G	OP1-P-O3'	-5.55	93.00	105.20
36	5	2376	G	N3-C4-C5	-5.54	125.83	128.60
36	5	2817	A	O5'-P-OP1	5.54	117.35	110.70
36	5	3028	G	C6-C5-N7	-5.54	127.07	130.40
37	7	1	G	N3-C4-N9	5.54	129.33	126.00
1	2	248	U	N3-C2-O2	5.54	126.08	122.20
36	1	994	G	N1-C6-O6	-5.54	116.57	119.90
36	1	2195	C	C6-N1-C2	-5.54	118.08	120.30
36	1	3186	A	C8-N9-C4	-5.54	103.58	105.80
1	6	16	G	N9-C4-C5	5.54	107.62	105.40
36	5	749	C	N1-C2-O2	-5.54	115.57	118.90
36	5	1911	A	O5'-P-OP2	-5.54	100.71	105.70
36	5	2983	C	N3-C4-C5	-5.54	119.68	121.90
36	5	3266	G	C5-C6-O6	5.54	131.93	128.60
24	D2	65	LEU	CA-CB-CG	5.54	128.04	115.30
36	1	776	U	N3-C4-O4	-5.54	115.52	119.40
36	1	1952	G	N3-C4-C5	-5.54	125.83	128.60
38	4	102	U	C6-N1-C2	-5.54	117.67	121.00
54	M8	138	LEU	CA-CB-CG	5.54	128.05	115.30
36	5	1047	A	O5'-P-OP1	-5.54	100.71	105.70
36	5	1120	A	OP1-P-O3'	-5.54	93.01	105.20
36	5	2710	C	N3-C4-C5	-5.54	119.68	121.90
36	5	2728	G	C8-N9-C4	-5.54	104.18	106.40
36	5	2736	A	N1-C6-N6	-5.54	115.28	118.60
36	1	1187	C	O5'-P-OP1	-5.54	100.71	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	412	G	C2-N3-C4	5.54	114.67	111.90
36	5	1376	C	C5-C4-N4	5.54	124.08	120.20
36	5	2947	G	N1-C2-N2	5.54	121.19	116.20
15	C3	22	ALA	C-N-CA	5.54	145.26	122.00
36	1	1116	G	OP2-P-O3'	5.54	117.39	105.20
36	1	3125	U	C6-N1-C2	5.54	124.32	121.00
36	5	645	A	N9-C4-C5	5.54	108.02	105.80
36	5	3120	C	C5-C6-N1	5.54	123.77	121.00
39	12	216	HIS	N-CA-C	-5.54	96.04	111.00
36	1	652	G	N3-C4-N9	5.54	129.32	126.00
36	1	2878	G	N9-C4-C5	-5.54	103.19	105.40
36	1	2912	G	N3-C4-C5	-5.54	125.83	128.60
36	5	1902	G	C5-C6-N1	5.54	114.27	111.50
36	1	435	C	N3-C2-O2	5.54	125.78	121.90
36	1	1362	G	OP2-P-O3'	5.54	117.38	105.20
36	1	2349	U	N3-C4-C5	5.54	117.92	114.60
36	1	3228	C	C2-N1-C1'	5.54	124.89	118.80
36	1	3353	G	P-O3'-C3'	5.54	126.34	119.70
37	3	119	U	N3-C2-O2	-5.54	118.33	122.20
36	5	835	G	C6-N1-C2	-5.54	121.78	125.10
36	5	2796	G	O5'-P-OP2	-5.54	100.72	105.70
1	2	1600	A	C4-C5-N7	5.53	113.47	110.70
36	1	812	G	N9-C4-C5	5.53	107.61	105.40
36	1	1724	U	O4'-C1'-N1	5.53	112.63	108.20
36	1	3086	A	O5'-P-OP2	-5.53	100.72	105.70
1	6	387	A	N1-C6-N6	-5.53	115.28	118.60
1	6	1739	C	N1-C2-O2	-5.53	115.58	118.90
36	5	396	A	N1-C6-N6	-5.53	115.28	118.60
36	5	672	A	C8-N9-C4	-5.53	103.59	105.80
36	5	1909	A	C8-N9-C4	5.53	108.01	105.80
36	5	2306	C	O4'-C1'-N1	-5.53	103.77	108.20
36	5	2869	U	C5-C6-N1	-5.53	119.93	122.70
36	5	3243	A	O4'-C1'-N9	-5.53	103.77	108.20
36	1	903	U	C5-C6-N1	-5.53	119.93	122.70
37	3	61	G	N3-C4-N9	-5.53	122.68	126.00
37	7	85	G	OP2-P-O3'	5.53	117.37	105.20
36	1	804	C	C5-C4-N4	-5.53	116.33	120.20
36	1	1901	A	N1-C6-N6	-5.53	115.28	118.60
37	3	89	G	N3-C4-C5	-5.53	125.83	128.60
36	5	645	A	OP1-P-OP2	-5.53	111.30	119.60
36	5	1556	C	C2-N1-C1'	5.53	124.89	118.80
36	5	2150	G	C8-N9-C4	-5.53	104.19	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2732	G	C4-N9-C1'	5.53	133.69	126.50
1	2	696	C	N1-C2-O2	5.53	122.22	118.90
36	1	69	C	N3-C2-O2	5.53	125.77	121.90
36	1	1203	A	N9-C4-C5	5.53	108.01	105.80
36	1	3000	A	N3-C4-C5	5.53	130.67	126.80
36	1	1165	A	C5-C6-N1	-5.53	114.94	117.70
38	4	8	C	N3-C2-O2	5.53	125.77	121.90
1	6	50	C	C5-C4-N4	-5.53	116.33	120.20
36	5	907	G	N1-C2-N2	-5.53	111.22	116.20
36	5	939	U	N1-C2-N3	5.53	118.22	114.90
36	5	1336	U	C5-C4-O4	-5.53	122.58	125.90
36	5	1864	A	N1-C6-N6	5.53	121.92	118.60
36	5	1885	U	C6-N1-C1'	5.53	128.94	121.20
36	1	84	U	N3-C4-O4	5.53	123.27	119.40
41	L4	95	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	6	137	U	C2-N1-C1'	5.53	124.33	117.70
1	6	1744	A	C8-N9-C4	5.53	108.01	105.80
36	5	1117	G	C4-C5-C6	-5.53	115.48	118.80
36	1	935	U	N3-C2-O2	-5.52	118.33	122.20
36	1	1419	A	C5'-C4'-O4'	5.52	115.73	109.10
36	1	2742	C	C6-N1-C2	-5.52	118.09	120.30
38	4	37	A	C8-N9-C4	-5.52	103.59	105.80
36	5	338	A	C6-C5-N7	-5.52	128.43	132.30
1	2	110	U	N3-C2-O2	-5.52	118.33	122.20
1	2	1164	G	N9-C4-C5	-5.52	103.19	105.40
36	1	366	A	N3-C4-N9	5.52	131.82	127.40
36	1	716	A	O4'-C1'-N9	-5.52	103.78	108.20
36	1	1917	C	N1-C2-O2	5.52	122.21	118.90
38	4	58	G	O5'-P-OP2	-5.52	100.73	105.70
1	6	978	A	N7-C8-N9	5.52	116.56	113.80
1	6	1313	A	C8-N9-C4	-5.52	103.59	105.80
36	5	1108	U	OP1-P-OP2	5.52	127.88	119.60
36	5	2144	A	OP1-P-O3'	5.52	117.35	105.20
36	1	983	A	N9-C4-C5	-5.52	103.59	105.80
36	5	2376	G	C8-N9-C4	-5.52	104.19	106.40
36	5	668	G	N1-C2-N2	-5.52	111.23	116.20
36	5	796	U	C2-N3-C4	-5.52	123.69	127.00
1	2	901	G	O4'-C1'-N9	5.52	112.61	108.20
36	1	357	A	O5'-P-OP2	-5.52	100.73	105.70
36	1	2265	C	N3-C2-O2	-5.52	118.04	121.90
36	1	2268	U	C5-C4-O4	-5.52	122.59	125.90
1	6	1027	A	C2-N3-C4	-5.52	107.84	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	229	G	C5-C6-O6	-5.52	125.29	128.60
36	5	1453	A	O5'-P-OP1	-5.52	100.73	105.70
36	5	3043	C	N3-C4-C5	5.52	124.11	121.90
38	8	82	U	N1-C2-N3	5.52	118.21	114.90
38	8	113	U	OP2-P-O3'	5.52	117.34	105.20
36	1	366	A	N3-C4-C5	-5.52	122.94	126.80
36	1	1203	A	C8-N9-C4	-5.52	103.59	105.80
36	1	2187	G	C6-C5-N7	-5.52	127.09	130.40
36	1	2604	U	OP1-P-O3'	5.52	117.34	105.20
1	2	621	A	O4'-C1'-N9	-5.51	103.79	108.20
1	2	1022	C	C2-N3-C4	-5.51	117.14	119.90
36	1	97	U	C2-N3-C4	-5.51	123.69	127.00
36	1	907	G	C5-C6-O6	-5.51	125.29	128.60
36	1	1139	G	C5-C6-N1	-5.51	108.74	111.50
36	1	1844	C	OP1-P-O3'	5.51	117.33	105.20
36	1	2412	G	C8-N9-C4	-5.51	104.19	106.40
36	1	3262	U	C5-C4-O4	5.51	129.21	125.90
1	6	1100	G	N3-C4-C5	-5.51	125.84	128.60
1	6	1773	C	N3-C2-O2	5.51	125.76	121.90
36	5	1861	G	C8-N9-C4	-5.51	104.19	106.40
36	5	2724	U	C6-N1-C2	-5.51	117.69	121.00
36	5	2956	A	C8-N9-C4	-5.51	103.59	105.80
36	5	3206	C	N3-C2-O2	-5.51	118.04	121.90
1	2	275	C	C5-C6-N1	5.51	123.76	121.00
36	1	225	C	C4-C5-C6	5.51	120.16	117.40
36	1	718	G	C4-C5-N7	5.51	113.00	110.80
36	1	2937	G	N7-C8-N9	-5.51	110.34	113.10
36	1	3207	U	C5-C6-N1	-5.51	119.94	122.70
36	5	805	G	N9-C1'-C2'	-5.51	105.94	112.00
25	D3	111	GLY	N-CA-C	-5.51	99.32	113.10
36	1	423	A	OP2-P-O3'	5.51	117.33	105.20
36	1	1356	U	N3-C4-O4	5.51	123.26	119.40
36	1	1373	A	OP2-P-O3'	5.51	117.32	105.20
36	1	2644	C	O4'-C1'-N1	-5.51	103.79	108.20
1	6	1729	C	C5-C6-N1	-5.51	118.25	121.00
36	5	892	U	C2-N1-C1'	-5.51	111.08	117.70
36	5	1144	U	N1-C2-O2	-5.51	118.94	122.80
1	2	360	A	C8-N9-C4	5.51	108.00	105.80
36	1	73	C	N3-C4-N4	5.51	121.86	118.00
36	1	111	C	C5-C6-N1	-5.51	118.25	121.00
36	1	1670	C	C2-N3-C4	-5.51	117.14	119.90
36	1	2247	G	C5-C6-O6	-5.51	125.30	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2688	U	C6-N1-C1'	-5.51	113.48	121.20
36	1	3222	U	N3-C4-O4	5.51	123.26	119.40
37	3	1	G	C4-N9-C1'	5.51	133.66	126.50
1	6	359	A	C6-N1-C2	5.51	121.91	118.60
1	6	449	C	N3-C2-O2	-5.51	118.04	121.90
36	5	679	U	N3-C4-O4	-5.51	115.54	119.40
36	5	1110	U	N3-C2-O2	-5.51	118.34	122.20
36	5	2121	G	C4-C5-N7	5.51	113.00	110.80
36	5	2819	A	O5'-P-OP2	-5.51	100.74	105.70
36	5	2833	A	C5-C6-N1	5.51	120.45	117.70
36	5	3091	A	C8-N9-C4	-5.51	103.60	105.80
36	5	3362	A	C8-N9-C4	-5.51	103.60	105.80
37	7	48	U	C5-C4-O4	-5.51	122.59	125.90
1	2	631	G	N3-C4-C5	5.51	131.35	128.60
36	1	863	C	OP2-P-O3'	5.51	117.32	105.20
36	1	922	U	N3-C4-O4	-5.51	115.54	119.40
36	1	636	C	OP1-P-OP2	5.51	127.86	119.60
36	1	640	U	OP1-P-O3'	-5.51	93.09	105.20
36	1	836	A	N1-C2-N3	5.51	132.05	129.30
36	1	1846	C	N3-C4-C5	-5.51	119.70	121.90
36	1	2405	C	C6-N1-C2	-5.51	118.10	120.30
36	1	2552	C	N3-C4-N4	-5.51	114.14	118.00
36	1	2873	U	N1-C2-N3	5.51	118.20	114.90
36	1	3078	U	C5-C6-N1	5.51	125.45	122.70
36	5	21	G	C5-C6-N1	5.51	114.25	111.50
36	5	2758	A	C5-N7-C8	5.51	106.65	103.90
36	5	2991	A	N9-C4-C5	5.51	108.00	105.80
56	n0	113	ARG	NE-CZ-NH1	-5.51	117.55	120.30
36	1	1296	C	N1-C2-N3	5.50	123.05	119.20
1	6	14	C	C6-N1-C2	-5.50	118.10	120.30
36	5	958	C	O5'-P-OP1	-5.50	100.75	105.70
1	2	158	U	N1-C2-O2	5.50	126.65	122.80
1	2	1118	G	C5-C6-O6	-5.50	125.30	128.60
1	2	1780	G	N1-C6-O6	5.50	123.20	119.90
36	1	427	C	C6-N1-C2	-5.50	118.10	120.30
36	1	978	G	P-O3'-C3'	-5.50	113.09	119.70
38	4	8	C	N3-C4-N4	5.50	121.85	118.00
36	5	428	A	OP2-P-O3'	5.50	117.31	105.20
36	5	818	C	N1-C2-O2	-5.50	115.60	118.90
36	5	1376	C	N3-C4-N4	-5.50	114.15	118.00
36	5	1641	U	C5-C4-O4	-5.50	122.60	125.90
36	5	2997	G	C4-C5-N7	5.50	113.00	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	647	G	N9-C4-C5	5.50	107.60	105.40
1	2	1189	A	C8-N9-C4	5.50	108.00	105.80
36	1	98	G	C2-N3-C4	-5.50	109.15	111.90
36	1	337	G	C8-N9-C4	5.50	108.60	106.40
36	1	717	C	OP2-P-O3'	5.50	117.31	105.20
36	1	1116	G	O5'-P-OP1	-5.50	100.75	105.70
36	1	1169	A	N7-C8-N9	-5.50	111.05	113.80
36	1	1293	U	N1-C2-O2	-5.50	118.95	122.80
36	5	896	A	C2-N3-C4	5.50	113.35	110.60
36	5	2991	A	C5-C6-N1	5.50	120.45	117.70
36	1	1903	U	N3-C4-O4	5.50	123.25	119.40
36	1	2706	G	C5-C6-O6	-5.50	125.30	128.60
38	4	13	A	C6-C5-N7	-5.50	128.45	132.30
1	6	1757	G	N1-C6-O6	-5.50	116.60	119.90
36	5	1662	G	C5-C6-N1	-5.50	108.75	111.50
36	5	1712	G	C8-N9-C4	-5.50	104.20	106.40
36	5	2169	G	N9-C4-C5	5.50	107.60	105.40
36	5	2877	G	N1-C2-N3	5.50	127.20	123.90
36	5	2890	A	C5-C6-N1	-5.50	114.95	117.70
1	2	631	G	N3-C4-N9	-5.50	122.70	126.00
36	1	2295	A	N7-C8-N9	5.50	116.55	113.80
37	3	39	C	N3-C4-C5	5.50	124.10	121.90
38	4	98	U	C5-C4-O4	-5.50	122.60	125.90
1	6	100	A	C5-C6-N1	-5.50	114.95	117.70
1	6	558	U	N3-C2-O2	-5.50	118.35	122.20
36	5	1445	U	C5-C6-N1	-5.50	119.95	122.70
36	5	3183	A	C6-C5-N7	-5.50	128.45	132.30
36	1	382	U	N1-C2-O2	-5.50	118.95	122.80
36	1	661	G	N3-C4-N9	5.50	129.30	126.00
36	1	816	A	C6-N1-C2	5.50	121.90	118.60
36	1	1592	G	N1-C2-N2	-5.50	111.25	116.20
1	6	393	C	C5-C6-N1	5.50	123.75	121.00
36	5	333	G	N1-C2-N3	5.50	127.20	123.90
36	5	636	C	C2-N3-C4	-5.50	117.15	119.90
36	5	1046	A	OP2-P-O3'	5.50	117.29	105.20
36	5	1367	G	C5-C6-N1	-5.50	108.75	111.50
36	5	1712	G	N3-C4-C5	-5.50	125.85	128.60
36	5	2149	A	O5'-P-OP2	-5.50	100.75	105.70
36	5	2980	U	N3-C4-O4	-5.50	115.55	119.40
37	7	74	C	C5-C4-N4	-5.50	116.35	120.20
36	1	2541	U	P-O3'-C3'	5.50	126.29	119.70
36	1	2646	C	C6-N1-C2	5.50	122.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1726	G	OP2-P-O3'	5.50	117.29	105.20
36	1	1654	A	N7-C8-N9	-5.49	111.05	113.80
36	1	2597	U	OP2-P-O3'	5.49	117.28	105.20
1	6	565	C	C5-C6-N1	-5.49	118.25	121.00
36	5	1170	A	C6-C5-N7	-5.49	128.46	132.30
36	5	1387	G	OP1-P-OP2	5.49	127.84	119.60
36	5	2129	U	C5-C6-N1	5.49	125.45	122.70
36	5	2836	C	OP1-P-OP2	5.49	127.84	119.60
1	2	619	A	N1-C6-N6	-5.49	115.31	118.60
36	1	1304	A	C8-N9-C4	5.49	108.00	105.80
36	1	1403	C	C5-C6-N1	-5.49	118.25	121.00
36	5	1430	U	N1-C2-N3	-5.49	111.61	114.90
36	5	1841	A	O4'-C1'-N9	5.49	112.59	108.20
36	5	2925	C	O5'-P-OP2	5.49	117.29	110.70
64	n8	46	ASP	CB-CG-OD1	5.49	123.24	118.30
36	1	296	A	C8-N9-C4	-5.49	103.61	105.80
36	1	325	A	OP1-P-OP2	-5.49	111.37	119.60
36	1	829	U	N3-C2-O2	-5.49	118.36	122.20
36	1	2615	G	C4-C5-N7	5.49	113.00	110.80
36	1	2942	C	C4-C5-C6	-5.49	114.66	117.40
36	1	3076	C	N1-C2-O2	-5.49	115.61	118.90
38	4	26	U	N3-C4-O4	-5.49	115.56	119.40
1	6	1786	G	C8-N9-C4	5.49	108.60	106.40
36	5	878	G	N7-C8-N9	5.49	115.84	113.10
36	5	1392	G	N3-C4-N9	5.49	129.29	126.00
36	1	109	A	OP1-P-O3'	5.49	117.27	105.20
36	5	1509	A	N9-C4-C5	-5.49	103.61	105.80
36	5	3330	A	C8-N9-C4	5.49	108.00	105.80
36	1	628	A	OP2-P-O3'	5.49	117.27	105.20
36	1	902	G	N1-C6-O6	5.49	123.19	119.90
36	1	3002	C	N3-C4-C5	5.49	124.09	121.90
36	1	3062	G	C4-C5-N7	5.49	112.99	110.80
36	5	350	C	N1-C2-N3	5.49	123.04	119.20
36	5	1149	G	C6-N1-C2	-5.49	121.81	125.10
36	5	1300	G	N3-C4-N9	5.49	129.29	126.00
36	5	1321	G	O5'-P-OP2	-5.49	100.76	105.70
36	5	1604	G	C4-N9-C1'	5.49	133.63	126.50
36	5	3217	C	C5-C6-N1	-5.49	118.26	121.00
36	1	2177	G	C6-C5-N7	-5.48	127.11	130.40
36	1	2376	G	N7-C8-N9	5.48	115.84	113.10
36	1	2821	C	C2-N3-C4	-5.48	117.16	119.90
36	5	2721	A	O5'-P-OP2	5.48	117.28	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	m0	153	ARG	NE-CZ-NH1	5.48	123.04	120.30
36	1	2625	C	C5-C6-N1	-5.48	118.26	121.00
36	5	636	C	C5-C6-N1	-5.48	118.26	121.00
36	1	51	A	C4-C5-N7	5.48	113.44	110.70
36	1	1332	A	N7-C8-N9	5.48	116.54	113.80
1	6	988	A	N1-C6-N6	-5.48	115.31	118.60
36	5	1466	G	OP1-P-OP2	-5.48	111.38	119.60
36	5	2857	C	C6-N1-C1'	-5.48	114.22	120.80
36	1	933	A	C4-C5-C6	5.48	119.74	117.00
36	1	1048	A	N1-C6-N6	-5.48	115.31	118.60
36	1	1377	G	N3-C2-N2	5.48	123.73	119.90
1	2	1180	C	N1-C2-O2	5.48	122.19	118.90
36	1	1421	G	N3-C2-N2	5.48	123.73	119.90
36	1	2356	A	N9-C4-C5	-5.48	103.61	105.80
36	1	2761	G	N7-C8-N9	-5.48	110.36	113.10
36	1	3344	A	N1-C2-N3	5.48	132.04	129.30
38	4	144	G	N9-C4-C5	5.48	107.59	105.40
36	5	918	C	C5-C6-N1	5.48	123.74	121.00
36	1	1434	G	N3-C2-N2	-5.48	116.07	119.90
36	5	2185	G	C5-C6-N1	-5.48	108.76	111.50
36	5	2584	G	OP2-P-O3'	5.48	117.25	105.20
36	5	2928	C	N3-C2-O2	-5.48	118.07	121.90
36	1	1405	U	C6-N1-C2	5.47	124.28	121.00
36	1	2391	G	C8-N9-C4	-5.47	104.21	106.40
36	1	2873	U	O5'-P-OP2	-5.47	100.77	105.70
1	6	922	G	OP1-P-OP2	5.47	127.81	119.60
37	7	37	G	N9-C4-C5	-5.47	103.21	105.40
40	l3	4	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	2	572	C	O5'-P-OP1	-5.47	100.77	105.70
36	1	304	G	C6-C5-N7	5.47	133.68	130.40
36	1	1227	C	C2-N1-C1'	5.47	124.82	118.80
1	6	1285	U	N3-C2-O2	-5.47	118.37	122.20
36	5	2748	A	C8-N9-C4	5.47	107.99	105.80
36	5	3148	U	N1-C2-O2	-5.47	118.97	122.80
36	1	113	C	N3-C4-C5	-5.47	119.71	121.90
36	1	661	G	C5-C6-N1	5.47	114.23	111.50
36	1	884	A	OP1-P-OP2	5.47	127.81	119.60
36	1	1294	A	C2-N3-C4	5.47	113.34	110.60
36	1	3214	U	OP2-P-O3'	5.47	117.24	105.20
1	6	991	G	C5-C6-O6	-5.47	125.32	128.60
36	5	2961	G	N9-C4-C5	5.47	107.59	105.40
36	5	3088	G	O5'-P-OP1	-5.47	100.78	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1762	A	C2-N3-C4	-5.47	107.86	110.60
36	1	182	U	C2-N1-C1'	-5.47	111.14	117.70
1	6	454	U	C6-N1-C2	5.47	124.28	121.00
36	5	304	G	N9-C4-C5	5.47	107.59	105.40
36	5	815	G	C6-N1-C2	-5.47	121.82	125.10
36	5	908	G	C6-C5-N7	-5.47	127.12	130.40
36	5	1379	G	N3-C2-N2	5.47	123.73	119.90
36	5	2794	G	N3-C4-N9	5.47	129.28	126.00
36	5	2883	U	C2-N3-C4	5.47	130.28	127.00
36	1	345	G	C6-N1-C2	-5.47	121.82	125.10
36	1	2282	U	C2-N3-C4	-5.47	123.72	127.00
36	1	2874	G	N3-C2-N2	-5.47	116.07	119.90
38	8	83	C	N3-C4-C5	-5.47	119.71	121.90
36	1	678	G	N3-C4-C5	-5.47	125.87	128.60
36	5	644	G	C5-C6-N1	-5.47	108.77	111.50
36	5	884	A	C8-N9-C4	5.47	107.99	105.80
36	5	1680	G	N9-C4-C5	5.47	107.59	105.40
36	5	3084	C	C6-N1-C2	5.47	122.49	120.30
60	n4	25	ASP	CB-CG-OD2	-5.47	113.38	118.30
36	1	2824	G	N1-C6-O6	-5.46	116.62	119.90
36	1	3205	G	C8-N9-C4	5.46	108.59	106.40
36	5	146	U	C5-C6-N1	-5.46	119.97	122.70
36	5	1201	C	C6-N1-C1'	5.46	127.36	120.80
36	5	1659	U	OP2-P-O3'	5.46	117.22	105.20
36	5	2693	C	C2-N3-C4	-5.46	117.17	119.90
36	1	1792	C	C4-C5-C6	5.46	120.13	117.40
36	1	3052	G	C2-N3-C4	-5.46	109.17	111.90
37	3	88	G	N3-C4-C5	-5.46	125.87	128.60
1	6	538	A	N9-C4-C5	5.46	107.98	105.80
1	6	1031	U	N3-C2-O2	5.46	126.02	122.20
36	5	1014	U	C2-N1-C1'	5.46	124.26	117.70
36	5	2975	U	N1-C2-O2	5.46	126.62	122.80
1	2	553	G	C2-N3-C4	-5.46	109.17	111.90
36	1	1373	A	O5'-P-OP2	-5.46	100.78	105.70
36	1	2571	U	N1-C2-O2	5.46	126.62	122.80
1	6	1796	C	N3-C2-O2	-5.46	118.08	121.90
36	5	651	G	C8-N9-C4	-5.46	104.22	106.40
36	5	1840	U	N3-C2-O2	-5.46	118.38	122.20
36	5	2608	G	C8-N9-C4	5.46	108.58	106.40
36	5	2622	C	OP1-P-O3'	5.46	117.22	105.20
36	1	801	A	C5-C6-N6	-5.46	119.33	123.70
36	1	1309	U	N1-C2-N3	5.46	118.18	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1321	G	O5'-P-OP1	-5.46	100.79	105.70
36	5	392	G	C5-C6-O6	-5.46	125.32	128.60
36	5	876	A	C5-C6-N1	5.46	120.43	117.70
36	5	2426	U	N3-C4-O4	-5.46	115.58	119.40
56	n0	115	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	2	968	U	C5-C6-N1	-5.46	119.97	122.70
1	2	1201	G	N3-C4-N9	-5.46	122.72	126.00
36	1	908	G	C6-C5-N7	-5.46	127.12	130.40
36	1	969	C	C5-C6-N1	-5.46	118.27	121.00
36	1	2709	C	N3-C2-O2	-5.46	118.08	121.90
36	1	2818	U	C5'-C4'-O4'	-5.46	102.55	109.10
36	1	2975	U	C2-N1-C1'	5.46	124.25	117.70
1	6	542	A	C5-N7-C8	-5.46	101.17	103.90
36	5	2393	G	C5-C6-O6	-5.46	125.33	128.60
36	5	2692	A	C5-C6-N6	5.46	128.07	123.70
1	2	347	G	N3-C4-C5	-5.46	125.87	128.60
36	1	422	A	N9-C4-C5	5.46	107.98	105.80
36	1	619	A	N9-C4-C5	-5.46	103.62	105.80
36	1	2322	C	N3-C2-O2	5.46	125.72	121.90
36	1	2660	G	C5-C6-O6	-5.46	125.33	128.60
16	c4	127	ARG	NE-CZ-NH1	5.46	123.03	120.30
36	5	201	A	N7-C8-N9	5.46	116.53	113.80
36	5	1144	U	C2-N1-C1'	-5.46	111.15	117.70
36	1	1654	A	C5-N7-C8	5.46	106.63	103.90
36	5	934	G	C2-N3-C4	5.46	114.63	111.90
36	5	1386	A	C2-N3-C4	-5.46	107.87	110.60
1	2	42	G	N1-C6-O6	-5.45	116.63	119.90
1	2	402	C	C6-N1-C2	5.45	122.48	120.30
1	2	1200	G	N7-C8-N9	5.45	115.83	113.10
1	2	1273	G	O5'-P-OP1	-5.45	100.79	105.70
1	6	543	C	C2-N1-C1'	5.45	124.80	118.80
36	5	1847	A	C4-C5-N7	5.45	113.43	110.70
36	1	909	G	O5'-P-OP2	5.45	117.24	110.70
36	1	3140	G	C4-C5-N7	5.45	112.98	110.80
1	6	83	G	N7-C8-N9	5.45	115.83	113.10
1	6	1680	G	C5-C6-O6	-5.45	125.33	128.60
36	5	805	G	OP1-P-OP2	-5.45	111.42	119.60
36	5	2733	A	O5'-P-OP1	5.45	117.24	110.70
37	7	101	G	C6-C5-N7	-5.45	127.13	130.40
36	1	374	A	P-O3'-C3'	5.45	126.24	119.70
1	6	871	G	C4-C5-N7	5.45	112.98	110.80
36	5	437	G	C5-N7-C8	-5.45	101.58	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2838	A	O5'-P-OP1	5.45	117.24	110.70
36	5	3093	C	C2-N3-C4	-5.45	117.17	119.90
37	7	121	U	N1-C2-O2	5.45	126.61	122.80
36	1	62	A	N3-C4-C5	-5.45	122.99	126.80
36	1	711	A	C4-C5-N7	-5.45	107.98	110.70
36	1	1129	A	C5-C6-N1	5.45	120.42	117.70
36	1	2812	C	N1-C2-O2	5.45	122.17	118.90
36	1	3029	A	C8-N9-C4	-5.45	103.62	105.80
36	1	3275	U	C5-C6-N1	5.45	125.42	122.70
40	L3	238	LEU	CA-CB-CG	5.45	127.83	115.30
1	6	572	C	N3-C4-N4	5.45	121.81	118.00
36	5	282	G	C5-C6-O6	5.45	131.87	128.60
36	5	644	G	C8-N9-C4	-5.45	104.22	106.40
37	7	97	A	N1-C6-N6	-5.45	115.33	118.60
65	n9	39	PHE	N-CA-CB	5.45	120.41	110.60
36	1	3122	A	C8-N9-C4	-5.45	103.62	105.80
36	5	900	G	C4-C5-N7	-5.45	108.62	110.80
36	1	1509	A	N1-C6-N6	5.45	121.87	118.60
36	1	1891	A	C4-N9-C1'	-5.45	116.50	126.30
37	3	53	U	N1-C2-O2	-5.45	118.99	122.80
36	5	681	U	C5-C4-O4	-5.45	122.63	125.90
37	7	48	U	O5'-P-OP2	-5.45	100.80	105.70
1	2	728	U	C2-N1-C1'	5.44	124.23	117.70
1	2	351	C	C2-N3-C4	-5.44	117.18	119.90
36	5	1098	A	N7-C8-N9	5.44	116.52	113.80
36	1	637	C	N3-C2-O2	-5.44	118.09	121.90
36	1	1117	G	C8-N9-C4	5.44	108.58	106.40
36	1	2373	A	C4-C5-C6	5.44	119.72	117.00
36	1	2731	U	N3-C2-O2	5.44	126.01	122.20
36	1	2993	G	N3-C4-C5	-5.44	125.88	128.60
36	1	3305	A	N1-C6-N6	-5.44	115.34	118.60
36	5	1370	G	C5-C6-O6	5.44	131.86	128.60
36	5	2349	U	N3-C2-O2	-5.44	118.39	122.20
36	5	2634	U	N3-C4-C5	5.44	117.86	114.60
36	5	3303	G	N1-C6-O6	-5.44	116.64	119.90
1	2	1057	U	C5-C6-N1	5.44	125.42	122.70
36	1	387	A	C8-N9-C4	-5.44	103.62	105.80
36	1	1513	G	C5-C6-N1	5.44	114.22	111.50
36	5	103	G	C5-C6-O6	5.44	131.86	128.60
36	1	1939	G	N3-C2-N2	-5.44	116.09	119.90
1	6	1751	C	N1-C2-O2	5.44	122.16	118.90
36	5	339	C	C2-N1-C1'	-5.44	112.82	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1017	C	C2-N3-C4	5.44	122.62	119.90
36	5	2376	G	N9-C4-C5	5.44	107.58	105.40
36	1	351	A	C5-N7-C8	5.44	106.62	103.90
1	6	427	C	N1-C2-O2	-5.44	115.64	118.90
36	1	54	C	C2-N1-C1'	-5.43	112.82	118.80
36	1	77	A	C2-N3-C4	5.43	113.32	110.60
36	1	545	U	N1-C2-O2	5.43	126.60	122.80
36	1	924	G	C5-N7-C8	-5.43	101.58	104.30
36	1	2915	U	N1-C2-O2	-5.43	119.00	122.80
1	6	399	A	C8-N9-C4	5.43	107.97	105.80
1	6	510	G	C6-C5-N7	-5.43	127.14	130.40
36	5	2610	G	C5-C6-N1	-5.43	108.78	111.50
36	5	2942	C	C2-N3-C4	-5.43	117.18	119.90
1	2	140	A	N1-C6-N6	5.43	121.86	118.60
1	2	1611	A	C2-N3-C4	-5.43	107.88	110.60
18	C6	53	LEU	CA-CB-CG	-5.43	102.80	115.30
36	1	1107	C	C6-N1-C2	5.43	122.47	120.30
1	6	327	U	N1-C2-N3	5.43	118.16	114.90
1	6	334	G	C5-C6-O6	5.43	131.86	128.60
36	5	43	A	C2-N3-C4	-5.43	107.88	110.60
36	1	1141	C	N3-C4-N4	5.43	121.80	118.00
36	1	1370	G	N9-C4-C5	-5.43	103.23	105.40
36	1	1444	G	C4-C5-N7	5.43	112.97	110.80
36	1	2417	U	C5-C6-N1	-5.43	119.98	122.70
38	4	39	G	N3-C2-N2	5.43	123.70	119.90
36	5	38	U	C6-N1-C2	5.43	124.26	121.00
36	5	1192	C	O5'-P-OP2	5.43	117.22	110.70
36	5	1451	C	N1-C2-O2	5.43	122.16	118.90
36	5	2413	A	N7-C8-N9	-5.43	111.08	113.80
36	1	1541	G	C4-C5-N7	5.43	112.97	110.80
36	1	2649	A	C5-C6-N1	5.43	120.41	117.70
36	5	56	G	O5'-P-OP1	5.43	117.21	110.70
36	5	1493	G	C4-C5-N7	5.43	112.97	110.80
36	1	647	A	C8-N9-C4	5.43	107.97	105.80
36	1	760	G	N3-C4-N9	5.43	129.26	126.00
36	1	2861	U	N3-C2-O2	-5.43	118.40	122.20
36	5	2985	C	N3-C4-C5	-5.43	119.73	121.90
36	1	585	A	C8-N9-C4	5.43	107.97	105.80
36	1	2116	G	N7-C8-N9	-5.43	110.39	113.10
36	5	1048	A	N1-C2-N3	-5.43	126.59	129.30
36	5	1820	U	O4'-C1'-N1	5.43	112.54	108.20
36	5	2298	U	OP1-P-OP2	5.43	127.74	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1762	A	O5'-P-OP2	5.42	117.21	110.70
36	1	49	A	C5-C6-N1	-5.42	114.99	117.70
36	1	52	A	C6-N1-C2	5.42	121.86	118.60
36	1	54	C	N3-C4-C5	5.42	124.07	121.90
36	1	662	U	N1-C2-O2	5.42	126.60	122.80
36	1	788	C	C2-N1-C1'	-5.42	112.83	118.80
36	1	1006	A	OP1-P-OP2	5.42	127.74	119.60
36	5	503	C	N3-C4-N4	5.42	121.80	118.00
36	5	2260	U	O5'-P-OP1	-5.42	100.82	105.70
36	5	2898	G	C4-N9-C1'	-5.42	119.45	126.50
36	1	1507	G	C4-C5-C6	5.42	122.05	118.80
36	1	1660	C	N1-C2-N3	5.42	123.00	119.20
36	5	974	G	C8-N9-C4	-5.42	104.23	106.40
37	7	74	C	N3-C2-O2	5.42	125.70	121.90
1	2	1446	A	C8-N9-C4	-5.42	103.63	105.80
9	S7	118	LEU	CA-CB-CG	5.42	127.77	115.30
36	1	421	G	O5'-P-OP1	-5.42	100.82	105.70
36	1	943	U	C2-N3-C4	-5.42	123.75	127.00
36	1	1185	C	C2-N3-C4	-5.42	117.19	119.90
36	1	2829	U	OP2-P-O3'	5.42	117.13	105.20
1	6	1697	G	N3-C4-C5	-5.42	125.89	128.60
36	5	369	A	C5-N7-C8	-5.42	101.19	103.90
36	5	779	G	C5-C6-O6	-5.42	125.35	128.60
36	5	1128	U	C4-C5-C6	5.42	122.95	119.70
36	5	1456	A	C8-N9-C4	5.42	107.97	105.80
36	5	2137	U	N3-C4-C5	5.42	117.85	114.60
36	5	2409	G	N3-C4-N9	-5.42	122.75	126.00
36	5	3115	C	N3-C2-O2	5.42	125.69	121.90
36	5	3214	U	N1-C2-O2	5.42	126.59	122.80
1	2	1241	G	C4-N9-C1'	5.42	133.55	126.50
1	2	1653	C	C6-N1-C2	-5.42	118.13	120.30
36	1	690	A	N9-C4-C5	5.42	107.97	105.80
1	6	1653	C	N1-C2-N3	5.42	122.99	119.20
36	5	562	C	C5-C4-N4	-5.42	116.41	120.20
36	5	1056	U	C5-C6-N1	5.42	125.41	122.70
36	5	1157	G	C6-C5-N7	5.42	133.65	130.40
36	5	3127	A	C8-N9-C4	-5.42	103.63	105.80
36	1	688	G	C4-C5-N7	-5.42	108.63	110.80
36	1	2171	G	N3-C4-C5	-5.42	125.89	128.60
36	1	3192	U	N3-C2-O2	5.42	125.99	122.20
36	5	1409	G	C5-C6-N1	5.42	114.21	111.50
36	5	2352	A	OP2-P-O3'	5.42	117.12	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	648	C	C6-N1-C1'	-5.42	114.30	120.80
36	1	908	G	C4-N9-C1'	5.42	133.54	126.50
36	1	1915	A	C5-C6-N1	5.42	120.41	117.70
36	1	2249	G	C3'-C2'-C1'	-5.42	97.17	101.50
36	1	2550	U	N3-C4-O4	-5.42	115.61	119.40
36	1	2800	G	N1-C2-N3	5.42	127.15	123.90
36	1	2954	U	C5-C6-N1	-5.42	119.99	122.70
36	5	1475	A	C4-C5-C6	5.42	119.71	117.00
36	5	1844	C	N1-C2-N3	5.42	122.99	119.20
36	5	2134	G	N3-C2-N2	5.42	123.69	119.90
36	5	2186	U	N1-C2-O2	5.42	126.59	122.80
38	8	63	G	C4-C5-N7	-5.42	108.63	110.80
1	2	549	G	N1-C6-O6	-5.42	116.65	119.90
36	1	2404	A	C4-C5-C6	-5.42	114.29	117.00
36	5	1122	U	C2-N3-C4	-5.42	123.75	127.00
36	5	1922	A	OP1-P-OP2	-5.42	111.48	119.60
36	1	78	U	C5-C4-O4	-5.41	122.65	125.90
36	1	1832	C	N1-C2-O2	5.41	122.15	118.90
36	1	2149	A	C6-N1-C2	5.41	121.85	118.60
36	1	2877	G	C4-C5-N7	-5.41	108.64	110.80
36	1	3036	G	N3-C4-C5	-5.41	125.89	128.60
36	1	3368	U	C6-N1-C1'	5.41	128.78	121.20
38	4	23	U	C5-C6-N1	-5.41	119.99	122.70
1	6	1347	U	N1-C2-N3	5.41	118.15	114.90
36	5	328	U	N1-C2-N3	5.41	118.15	114.90
36	5	2169	G	C6-C5-N7	5.41	133.65	130.40
36	5	2281	A	N9-C4-C5	-5.41	103.64	105.80
36	5	2744	U	N1-C2-O2	5.41	126.59	122.80
36	5	3317	U	C5-C4-O4	5.41	129.15	125.90
37	7	52	G	C8-N9-C4	5.41	108.56	106.40
36	1	651	G	N3-C2-N2	5.41	123.69	119.90
36	1	2291	A	OP1-P-O3'	5.41	117.11	105.20
36	1	3361	G	N3-C4-N9	5.41	129.25	126.00
1	6	1000	C	N3-C2-O2	-5.41	118.11	121.90
36	5	372	A	C6-C5-N7	-5.41	128.51	132.30
36	5	2887	A	OP1-P-OP2	5.41	127.72	119.60
36	5	3332	U	N3-C4-O4	-5.41	115.61	119.40
36	1	1421	G	N9-C4-C5	-5.41	103.24	105.40
36	1	1700	G	C6-C5-N7	-5.41	127.15	130.40
36	1	2877	G	N3-C4-C5	-5.41	125.89	128.60
38	4	115	C	O5'-P-OP2	-5.41	100.83	105.70
1	6	1765	A	N1-C6-N6	-5.41	115.35	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	869	G	N1-C6-O6	-5.41	116.65	119.90
36	5	942	U	O5'-P-OP1	5.41	117.19	110.70
36	5	1661	G	N3-C4-C5	-5.41	125.89	128.60
36	5	2833	A	C8-N9-C4	5.41	107.96	105.80
36	5	3267	A	C8-N9-C4	5.41	107.96	105.80
36	1	155	G	O5'-P-OP2	-5.41	100.83	105.70
36	1	213	A	C6-N1-C2	5.41	121.84	118.60
36	1	2197	C	N1-C2-O2	5.41	122.15	118.90
36	5	506	U	OP2-P-O3'	5.41	117.10	105.20
36	5	667	C	C6-N1-C2	5.41	122.46	120.30
36	5	969	C	C2-N1-C1'	-5.41	112.85	118.80
36	1	602	A	N1-C6-N6	-5.41	115.36	118.60
36	1	2772	C	P-O3'-C3'	5.41	126.19	119.70
38	4	100	U	C2-N1-C1'	5.41	124.19	117.70
36	5	2210	G	C6-C5-N7	-5.41	127.16	130.40
36	5	2550	U	N3-C4-O4	-5.41	115.61	119.40
1	6	1560	U	C5-C4-O4	5.41	129.14	125.90
36	5	328	U	N3-C4-O4	-5.41	115.62	119.40
36	5	2136	C	C4-C5-C6	5.41	120.10	117.40
36	5	2855	U	N3-C4-O4	-5.41	115.62	119.40
36	5	2974	U	N3-C4-O4	5.41	123.18	119.40
36	5	3242	G	C8-N9-C4	-5.41	104.24	106.40
36	1	1065	A	O5'-P-OP1	-5.40	100.84	105.70
36	1	1332	A	C8-N9-C4	-5.40	103.64	105.80
37	3	88	G	C4-C5-N7	-5.40	108.64	110.80
38	4	6	U	C5-C4-O4	-5.40	122.66	125.90
36	5	1411	C	N3-C4-C5	5.40	124.06	121.90
1	2	1092	A	N9-C4-C5	-5.40	103.64	105.80
36	1	806	A	OP1-P-OP2	5.40	127.70	119.60
36	1	2388	U	OP2-P-O3'	5.40	117.09	105.20
36	1	2399	A	OP1-P-OP2	-5.40	111.50	119.60
36	1	2894	C	C6-N1-C2	-5.40	118.14	120.30
36	1	3001	C	O5'-P-OP1	5.40	117.18	110.70
1	6	365	G	N3-C4-C5	-5.40	125.90	128.60
1	6	1619	C	C6-N1-C2	-5.40	118.14	120.30
1	6	1658	G	C6-C5-N7	5.40	133.64	130.40
36	5	887	G	C5-C6-O6	5.40	131.84	128.60
36	5	2358	A	N1-C6-N6	5.40	121.84	118.60
3	S1	96	LEU	CA-CB-CG	5.40	127.72	115.30
36	1	171	G	N3-C4-N9	-5.40	122.76	126.00
36	1	716	A	N3-C4-C5	5.40	130.58	126.80
36	1	893	C	C5-C6-N1	5.40	123.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	927	C	N3-C4-C5	5.40	124.06	121.90
36	1	938	C	C5-C6-N1	5.40	123.70	121.00
36	1	966	U	N3-C2-O2	-5.40	118.42	122.20
36	1	1529	A	C2-N3-C4	-5.40	107.90	110.60
36	1	2793	G	C8-N9-C1'	-5.40	119.98	127.00
38	4	35	C	C2-N3-C4	-5.40	117.20	119.90
1	6	883	C	O5'-P-OP1	-5.40	100.84	105.70
36	5	101	G	O4'-C1'-N9	5.40	112.52	108.20
36	5	287	G	N1-C6-O6	-5.40	116.66	119.90
36	5	395	A	C5-C6-N6	-5.40	119.38	123.70
36	5	2637	A	N1-C6-N6	5.40	121.84	118.60
36	5	2871	G	O5'-P-OP1	5.40	117.18	110.70
73	o7	65	ARG	NE-CZ-NH1	5.40	123.00	120.30
36	1	592	A	N1-C2-N3	5.40	132.00	129.30
37	3	85	G	OP2-P-O3'	5.40	117.08	105.20
36	5	2808	A	N9-C4-C5	-5.40	103.64	105.80
1	2	347	G	C8-N9-C4	-5.40	104.24	106.40
1	2	557	G	N3-C4-C5	-5.40	125.90	128.60
36	1	1937	U	N3-C4-C5	5.40	117.84	114.60
1	6	858	G	C4-C5-N7	5.40	112.96	110.80
36	5	78	U	C5-C4-O4	-5.40	122.66	125.90
36	5	1320	C	C2-N3-C4	5.40	122.60	119.90
36	5	2401	A	N3-C4-N9	-5.40	123.08	127.40
36	5	2866	U	C6-N1-C2	-5.40	117.76	121.00
36	1	1849	C	N1-C2-O2	-5.40	115.66	118.90
36	1	2802	A	C5-N7-C8	-5.40	101.20	103.90
1	6	557	G	N3-C4-C5	-5.40	125.90	128.60
1	6	639	U	N3-C2-O2	-5.40	118.42	122.20
36	1	327	A	C4-C5-C6	-5.39	114.30	117.00
36	1	2657	A	N9-C4-C5	5.39	107.96	105.80
36	1	3207	U	N1-C2-O2	-5.39	119.02	122.80
54	M8	99	THR	N-CA-C	5.39	125.56	111.00
1	6	448	C	N3-C4-C5	-5.39	119.74	121.90
1	6	1642	G	N1-C6-O6	5.39	123.14	119.90
36	5	337	G	N3-C4-C5	-5.39	125.90	128.60
36	5	721	G	O5'-P-OP1	-5.39	100.84	105.70
36	5	2988	C	C2-N3-C4	-5.39	117.20	119.90
1	2	852	C	N1-C2-O2	5.39	122.14	118.90
1	2	1206	U	N3-C4-O4	5.39	123.17	119.40
36	1	112	U	C5-C6-N1	5.39	125.40	122.70
36	1	227	G	C5-C6-O6	-5.39	125.36	128.60
36	1	1062	A	C4-C5-N7	5.39	113.40	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1508	C	N3-C4-N4	-5.39	114.23	118.00
1	6	1210	C	C6-N1-C2	-5.39	118.14	120.30
36	5	1170	A	C4-C5-C6	5.39	119.70	117.00
36	5	2223	A	C8-N9-C4	-5.39	103.64	105.80
36	5	2360	C	OP1-P-OP2	-5.39	111.51	119.60
37	7	44	C	C2-N1-C1'	-5.39	112.87	118.80
1	2	61	A	O4'-C1'-N9	5.39	112.51	108.20
36	1	1881	A	N7-C8-N9	-5.39	111.11	113.80
1	6	595	G	C5-C6-O6	5.39	131.84	128.60
36	5	2145	A	C6-N1-C2	-5.39	115.36	118.60
36	1	574	U	C5-C6-N1	-5.39	120.00	122.70
36	1	950	G	C4-C5-N7	5.39	112.96	110.80
36	1	2924	U	C6-N1-C2	5.39	124.23	121.00
1	6	362	G	C4-N9-C1'	5.39	133.50	126.50
36	5	1402	C	C2-N3-C4	-5.39	117.20	119.90
36	5	2622	C	C5-C6-N1	-5.39	118.31	121.00
36	5	2705	A	C8-N9-C4	5.39	107.95	105.80
36	5	2866	U	N3-C4-O4	5.39	123.17	119.40
37	7	6	C	C5-C6-N1	-5.39	118.31	121.00
36	1	2372	A	N3-C4-C5	-5.39	123.03	126.80
1	6	142	G	C6-C5-N7	-5.39	127.17	130.40
36	1	29	C	N3-C4-C5	5.39	124.05	121.90
36	1	346	C	O5'-P-OP2	-5.39	100.85	105.70
36	1	909	G	N7-C8-N9	-5.39	110.41	113.10
36	1	1178	G	N3-C4-N9	5.39	129.23	126.00
36	1	3179	U	O5'-P-OP2	5.39	117.17	110.70
37	3	21	G	N7-C8-N9	-5.39	110.41	113.10
38	4	47	C	N1-C2-O2	5.39	122.13	118.90
1	6	793	A	O4'-C1'-N9	5.39	112.51	108.20
1	6	1117	U	N3-C4-C5	-5.39	111.37	114.60
36	5	1192	C	C2-N3-C4	-5.39	117.21	119.90
36	5	1192	C	N3-C2-O2	-5.39	118.13	121.90
36	1	213	A	N1-C2-N3	-5.38	126.61	129.30
36	1	878	G	C5-C6-O6	5.38	131.83	128.60
36	1	1056	U	C5-C6-N1	5.38	125.39	122.70
36	1	2572	C	C6-N1-C2	-5.38	118.15	120.30
37	3	60	G	N1-C6-O6	5.38	123.13	119.90
37	3	61	G	N3-C4-C5	5.38	131.29	128.60
36	5	277	G	OP2-P-O3'	5.38	117.05	105.20
36	5	701	G	C4-C5-N7	-5.38	108.65	110.80
36	5	2922	G	C8-N9-C4	5.38	108.55	106.40
36	5	2971	A	N1-C2-N3	-5.38	126.61	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2971	A	N9-C4-C5	-5.38	103.65	105.80
36	5	2986	U	C2-N1-C1'	5.38	124.16	117.70
36	5	3278	C	P-O3'-C3'	5.38	126.16	119.70
36	5	3315	G	N1-C6-O6	-5.38	116.67	119.90
1	2	28	A	C8-N9-C4	5.38	107.95	105.80
36	5	667	C	N3-C4-C5	5.38	124.05	121.90
36	5	873	C	C4-C5-C6	5.38	120.09	117.40
36	1	1154	A	N9-C4-C5	5.38	107.95	105.80
36	1	2127	U	C6-N1-C2	-5.38	117.77	121.00
36	1	2210	G	C4-N9-C1'	-5.38	119.50	126.50
36	1	3181	C	N1-C2-O2	5.38	122.13	118.90
1	6	196	G	O4'-C1'-N9	5.38	112.50	108.20
36	5	335	G	C2-N3-C4	5.38	114.59	111.90
36	5	1452	A	C5-C6-N1	5.38	120.39	117.70
41	14	313	LEU	CA-CB-CG	5.38	127.68	115.30
36	5	2636	A	N1-C6-N6	-5.38	115.37	118.60
36	5	3146	G	N3-C2-N2	5.38	123.67	119.90
36	1	20	A	N1-C2-N3	5.38	131.99	129.30
36	1	25	U	N3-C2-O2	5.38	125.97	122.20
36	1	939	U	O5'-P-OP2	-5.38	100.86	105.70
36	1	974	G	C8-N9-C1'	-5.38	120.01	127.00
36	1	3044	G	N1-C2-N2	-5.38	111.36	116.20
38	4	111	A	C6-C5-N7	-5.38	128.53	132.30
1	6	1423	U	C5-C6-N1	-5.38	120.01	122.70
36	5	43	A	O5'-P-OP1	-5.38	100.86	105.70
36	5	1840	U	OP1-P-OP2	5.38	127.67	119.60
36	5	2818	U	C5-C4-O4	-5.38	122.67	125.90
36	5	3306	U	O5'-P-OP2	-5.38	100.86	105.70
1	2	399	A	C8-N9-C4	5.38	107.95	105.80
36	1	66	A	C8-N9-C4	5.38	107.95	105.80
36	1	1365	G	N1-C6-O6	-5.38	116.67	119.90
36	1	2143	A	N7-C8-N9	5.38	116.49	113.80
1	6	16	G	N1-C6-O6	-5.38	116.67	119.90
1	6	339	C	C6-N1-C2	-5.38	118.15	120.30
36	5	1075	A	N7-C8-N9	-5.38	111.11	113.80
36	5	1833	G	C5-C6-O6	5.38	131.82	128.60
36	5	2343	C	C5-C6-N1	-5.38	118.31	121.00
36	5	2987	A	C4-C5-N7	-5.38	108.01	110.70
1	6	1050	G	C8-N9-C4	-5.38	104.25	106.40
36	5	399	A	O5'-P-OP1	-5.38	100.86	105.70
36	1	368	G	N9-C4-C5	-5.37	103.25	105.40
36	1	950	G	N9-C4-C5	-5.37	103.25	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1753	A	N9-C4-C5	5.37	107.95	105.80
36	5	973	A	C5-C6-N6	-5.37	119.40	123.70
36	5	1127	G	C5-C6-N1	5.37	114.19	111.50
36	5	1348	U	N3-C4-C5	-5.37	111.38	114.60
36	1	416	A	N1-C6-N6	-5.37	115.38	118.60
36	1	2245	C	C6-N1-C2	-5.37	118.15	120.30
1	6	858	G	O4'-C1'-N9	5.37	112.50	108.20
36	5	606	C	C5-C6-N1	-5.37	118.31	121.00
36	5	1452	A	C4-C5-C6	-5.37	114.31	117.00
36	5	2192	C	N1-C2-O2	5.37	122.12	118.90
36	1	613	G	C6-N1-C2	5.37	128.32	125.10
36	5	25	U	N1-C2-N3	5.37	118.12	114.90
36	5	2390	A	OP2-P-O3'	5.37	117.01	105.20
36	5	3332	U	C5-C4-O4	5.37	129.12	125.90
1	2	440	U	C5-C4-O4	5.37	129.12	125.90
36	1	1144	U	C5-C6-N1	-5.37	120.02	122.70
36	1	1269	U	N3-C2-O2	-5.37	118.44	122.20
36	1	1381	A	N1-C6-N6	5.37	121.82	118.60
36	1	1427	U	C6-N1-C2	5.37	124.22	121.00
36	1	1531	C	N3-C4-N4	-5.37	114.24	118.00
36	1	3108	G	C5-N7-C8	5.37	106.98	104.30
36	5	210	U	C5-C4-O4	5.37	129.12	125.90
36	5	861	C	C5-C6-N1	-5.37	118.32	121.00
36	5	1519	G	N1-C6-O6	5.37	123.12	119.90
36	5	2351	U	O5'-P-OP2	5.37	117.14	110.70
36	5	2513	U	P-O3'-C3'	5.37	126.14	119.70
36	1	1807	G	C6-C5-N7	-5.37	127.18	130.40
36	1	2795	U	O5'-P-OP1	-5.37	100.87	105.70
36	1	2856	G	C4-C5-N7	-5.37	108.65	110.80
36	5	3309	G	C8-N9-C1'	-5.37	120.02	127.00
39	12	55	GLY	N-CA-C	-5.37	99.68	113.10
1	2	1180	C	C6-N1-C2	-5.37	118.15	120.30
36	1	958	C	N1-C2-N3	5.37	122.95	119.20
36	1	1116	G	C2-N3-C4	5.37	114.58	111.90
36	1	1445	U	N3-C4-C5	5.37	117.82	114.60
36	1	2380	U	N3-C4-O4	-5.37	115.64	119.40
36	1	2643	A	C2-N3-C4	-5.37	107.92	110.60
1	6	418	G	N9-C4-C5	-5.37	103.25	105.40
36	5	1613	A	C8-N9-C4	5.37	107.95	105.80
36	5	2763	U	N3-C4-O4	5.37	123.16	119.40
36	1	64	G	N9-C4-C5	5.36	107.55	105.40
36	1	1164	G	C5-C6-N1	-5.36	108.82	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1367	G	N1-C6-O6	5.36	123.12	119.90
36	1	2171	G	C2-N3-C4	5.36	114.58	111.90
47	M0	24	ARG	CD-NE-CZ	5.36	131.11	123.60
36	5	285	A	N1-C2-N3	5.36	131.98	129.30
36	5	607	A	N1-C6-N6	-5.36	115.38	118.60
36	5	1879	A	P-O3'-C3'	5.36	126.14	119.70
36	5	2651	G	C5-C6-O6	5.36	131.82	128.60
38	8	2	A	OP2-P-O3'	5.36	117.00	105.20
36	1	1103	A	OP1-P-O3'	5.36	116.99	105.20
36	1	1156	C	N1-C2-O2	5.36	122.12	118.90
36	1	1837	U	N1-C2-O2	-5.36	119.05	122.80
1	6	65	A	C4-C5-N7	5.36	113.38	110.70
1	6	572	C	C5-C6-N1	5.36	123.68	121.00
1	6	1266	U	C5-C6-N1	5.36	125.38	122.70
36	5	875	G	C8-N9-C4	-5.36	104.26	106.40
36	5	933	A	OP1-P-O3'	5.36	116.99	105.20
36	5	1306	G	N9-C4-C5	-5.36	103.26	105.40
36	5	1506	A	C8-N9-C4	-5.36	103.66	105.80
36	5	1528	G	C4-N9-C1'	5.36	133.47	126.50
38	8	95	G	N3-C4-N9	-5.36	122.78	126.00
36	1	30	G	N1-C6-O6	-5.36	116.68	119.90
36	1	325	A	C5-N7-C8	5.36	106.58	103.90
36	1	782	U	N1-C2-O2	5.36	126.55	122.80
36	1	2242	A	N1-C2-N3	5.36	131.98	129.30
1	6	1111	G	N3-C4-C5	-5.36	125.92	128.60
36	5	988	U	N3-C4-O4	-5.36	115.65	119.40
36	5	1130	A	N3-C4-N9	5.36	131.69	127.40
36	5	2112	U	P-O3'-C3'	5.36	126.13	119.70
36	5	2401	A	O4'-C1'-N9	5.36	112.49	108.20
36	5	2945	G	C4-C5-N7	5.36	112.94	110.80
36	1	1116	G	N9-C4-C5	5.36	107.54	105.40
36	1	1387	G	N1-C6-O6	-5.36	116.69	119.90
36	1	2631	U	N3-C4-O4	-5.36	115.65	119.40
36	1	2761	G	C8-N9-C4	5.36	108.54	106.40
1	6	934	C	C2-N1-C1'	5.36	124.69	118.80
36	5	1096	U	C5-C4-O4	-5.36	122.69	125.90
36	5	2661	G	N3-C4-C5	-5.36	125.92	128.60
36	1	1547	G	C5-N7-C8	5.36	106.98	104.30
36	1	2286	U	N3-C4-O4	-5.36	115.65	119.40
36	1	2422	C	N3-C4-N4	-5.36	114.25	118.00
1	6	628	G	N1-C2-N2	-5.36	111.38	116.20
36	1	1145	G	C4-C5-N7	5.35	112.94	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2859	U	N3-C4-C5	-5.35	111.39	114.60
1	6	908	U	N3-C4-O4	-5.35	115.65	119.40
36	5	1381	A	C8-N9-C4	5.35	107.94	105.80
36	5	2704	A	C5-C6-N6	-5.35	119.42	123.70
1	2	144	U	C4-C5-C6	5.35	122.91	119.70
36	1	665	A	C5-C6-N6	5.35	127.98	123.70
36	1	728	G	C5-C6-O6	5.35	131.81	128.60
36	1	1305	U	N1-C2-N3	-5.35	111.69	114.90
36	1	1939	G	N1-C2-N2	5.35	121.02	116.20
36	1	2371	G	N9-C4-C5	-5.35	103.26	105.40
36	1	3174	A	C2-N3-C4	-5.35	107.92	110.60
1	6	1549	C	N3-C4-C5	-5.35	119.76	121.90
36	5	300	G	C5-C6-O6	5.35	131.81	128.60
36	1	2881	C	C6-N1-C2	5.35	122.44	120.30
36	5	686	G	OP1-P-OP2	-5.35	111.57	119.60
36	1	283	G	C5-C6-O6	-5.35	125.39	128.60
36	1	942	U	N1-C2-N3	5.35	118.11	114.90
36	1	1047	A	O5'-P-OP1	-5.35	100.89	105.70
36	1	2120	A	C4-C5-C6	5.35	119.67	117.00
36	1	3300	U	C5-C4-O4	5.35	129.11	125.90
1	6	1000	C	C6-N1-C1'	-5.35	114.38	120.80
36	5	661	G	OP1-P-O3'	5.35	116.97	105.20
36	5	918	C	C2-N3-C4	5.35	122.58	119.90
36	5	1512	U	OP2-P-O3'	5.35	116.97	105.20
36	5	1880	U	N1-C2-O2	5.35	126.55	122.80
36	5	2351	U	N3-C2-O2	-5.35	118.45	122.20
1	2	307	G	C8-N9-C4	5.35	108.54	106.40
1	2	549	G	C5-C6-O6	5.35	131.81	128.60
36	1	2624	G	C5-C6-O6	-5.35	125.39	128.60
36	1	3293	U	C6-N1-C2	5.35	124.21	121.00
1	6	421	A	N9-C4-C5	-5.35	103.66	105.80
1	6	901	G	O4'-C1'-N9	5.35	112.48	108.20
36	5	395	A	N3-C4-N9	5.35	131.68	127.40
36	5	1205	A	OP1-P-OP2	5.35	127.62	119.60
36	5	1367	G	N1-C6-O6	5.35	123.11	119.90
36	5	2336	U	C4-C5-C6	-5.35	116.49	119.70
36	5	2843	U	C5-C4-O4	5.35	129.11	125.90
37	7	95	A	N9-C4-C5	5.35	107.94	105.80
37	7	120	C	N3-C4-C5	5.35	124.04	121.90
38	4	36	G	C5-C6-O6	-5.35	125.39	128.60
36	5	95	A	C5-N7-C8	5.35	106.57	103.90
36	5	225	C	C5-C4-N4	-5.35	116.46	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	845	G	OP2-P-O3'	5.35	116.96	105.20
36	1	817	A	C4-C5-C6	5.34	119.67	117.00
36	5	1369	A	N1-C6-N6	5.34	121.81	118.60
70	O4	60	ARG	NE-CZ-NH1	5.34	122.97	120.30
36	5	633	C	C4-C5-C6	5.34	120.07	117.40
1	2	192	U	N3-C2-O2	-5.34	118.46	122.20
36	1	1075	A	C8-N9-C4	5.34	107.94	105.80
36	1	1344	G	N9-C4-C5	-5.34	103.26	105.40
36	1	2140	U	O5'-P-OP1	5.34	117.11	110.70
36	1	2968	G	N3-C2-N2	5.34	123.64	119.90
1	6	1796	C	C5-C4-N4	5.34	123.94	120.20
36	5	715	A	N3-C4-C5	-5.34	123.06	126.80
36	5	969	C	C5-C4-N4	5.34	123.94	120.20
36	5	2136	C	C2-N1-C1'	5.34	124.67	118.80
1	2	1780	G	C5-N7-C8	-5.34	101.63	104.30
36	1	42	C	O5'-P-OP2	5.34	117.11	110.70
36	1	648	C	OP1-P-OP2	5.34	127.61	119.60
1	6	1614	A	C2-N3-C4	-5.34	107.93	110.60
36	5	608	A	N3-C4-N9	5.34	131.67	127.40
36	5	2870	C	N3-C4-C5	5.34	124.04	121.90
36	1	283	G	N3-C2-N2	-5.34	116.16	119.90
36	1	1334	U	C6-N1-C2	-5.34	117.80	121.00
36	1	2650	U	C2-N3-C4	-5.34	123.80	127.00
37	3	54	U	C5-C4-O4	-5.34	122.70	125.90
56	N0	155	ARG	NE-CZ-NH1	-5.34	117.63	120.30
36	5	1050	U	C5-C4-O4	5.34	129.10	125.90
36	5	2623	G	OP1-P-OP2	-5.34	111.59	119.60
36	5	2945	G	C6-C5-N7	-5.34	127.20	130.40
40	l3	4	ARG	CG-CD-NE	5.34	123.01	111.80
1	2	1572	G	C4-C5-N7	5.34	112.93	110.80
36	1	1164	G	C4-N9-C1'	5.34	133.44	126.50
36	1	1503	A	N3-C4-C5	5.34	130.53	126.80
36	1	1837	U	OP2-P-O3'	5.34	116.94	105.20
1	6	1641	C	N3-C2-O2	5.34	125.64	121.90
36	5	114	A	N1-C6-N6	5.34	121.80	118.60
36	5	915	A	OP1-P-O3'	5.34	116.94	105.20
36	5	3211	C	C6-N1-C2	5.34	122.43	120.30
36	1	2824	G	C8-N9-C4	5.33	108.53	106.40
1	6	35	U	N3-C2-O2	-5.33	118.47	122.20
36	5	589	A	O4'-C1'-N9	-5.33	103.93	108.20
36	5	2817	A	N3-C4-C5	-5.33	123.06	126.80
59	n3	87	ARG	NE-CZ-NH1	5.33	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	227	G	N3-C2-N2	-5.33	116.17	119.90
36	1	2343	C	O5'-P-OP2	-5.33	100.90	105.70
68	O2	47	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	6	52	U	C6-N1-C2	-5.33	117.80	121.00
36	5	966	U	C2-N1-C1'	5.33	124.10	117.70
36	5	1437	C	C6-N1-C2	-5.33	118.17	120.30
36	5	1898	G	O4'-C1'-N9	5.33	112.47	108.20
36	5	2138	A	C4-C5-C6	5.33	119.67	117.00
36	1	62	A	N3-C4-N9	5.33	131.66	127.40
36	1	282	G	P-O3'-C3'	5.33	126.10	119.70
36	1	1832	C	N3-C2-O2	-5.33	118.17	121.90
44	L7	179	LEU	CA-CB-CG	5.33	127.56	115.30
36	5	2345	A	C5-C6-N6	-5.33	119.43	123.70
36	1	105	C	C5-C4-N4	-5.33	116.47	120.20
36	1	2331	C	N1-C2-O2	-5.33	115.70	118.90
36	5	2156	C	C2-N1-C1'	-5.33	112.94	118.80
36	5	2948	C	N3-C4-N4	-5.33	114.27	118.00
1	2	1522	U	N1-C2-O2	-5.33	119.07	122.80
36	1	2298	U	O4'-C1'-N1	5.33	112.46	108.20
36	1	2916	U	OP1-P-O3'	5.33	116.92	105.20
36	5	41	G	C5-C6-O6	-5.33	125.40	128.60
36	5	1556	C	C5-C6-N1	5.33	123.66	121.00
36	5	2246	G	C4-C5-N7	-5.33	108.67	110.80
36	5	2420	C	N1-C2-O2	-5.33	115.70	118.90
36	5	2978	U	O4'-C1'-N1	5.33	112.46	108.20
1	2	359	A	N9-C4-C5	-5.33	103.67	105.80
36	1	142	C	N3-C4-C5	-5.33	119.77	121.90
36	1	402	A	O5'-P-OP1	-5.33	100.91	105.70
36	1	2952	G	C6-C5-N7	-5.33	127.20	130.40
1	6	1596	C	C2-N1-C1'	5.33	124.66	118.80
36	5	1122	U	N3-C2-O2	-5.33	118.47	122.20
1	2	1030	A	C8-N9-C4	5.33	107.93	105.80
36	1	69	C	N1-C2-O2	-5.33	115.70	118.90
36	1	647	A	N7-C8-N9	-5.33	111.14	113.80
36	1	1048	A	C5-C6-N1	5.33	120.36	117.70
36	1	2815	G	N3-C2-N2	5.33	123.63	119.90
36	5	934	G	C8-N9-C1'	-5.33	120.08	127.00
38	8	82	U	C5-C4-O4	5.33	129.10	125.90
36	1	25	U	N1-C2-N3	5.32	118.09	114.90
36	1	695	C	C5-C6-N1	-5.32	118.34	121.00
36	1	776	U	C2-N3-C4	-5.32	123.81	127.00
36	1	2537	U	P-O3'-C3'	5.32	126.09	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	945	U	N3-C2-O2	-5.32	118.47	122.20
1	6	1788	G	N1-C2-N3	5.32	127.09	123.90
36	5	575	G	N1-C6-O6	-5.32	116.71	119.90
36	5	776	U	C5-C4-O4	5.32	129.09	125.90
36	5	3043	C	C6-N1-C2	5.32	122.43	120.30
50	m4	109	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	2	1486	G	C4-C5-N7	5.32	112.93	110.80
36	1	1328	C	C2-N3-C4	-5.32	117.24	119.90
36	1	2649	A	N3-C4-N9	5.32	131.66	127.40
36	1	2661	G	C6-C5-N7	-5.32	127.21	130.40
36	1	2874	G	N1-C2-N3	5.32	127.09	123.90
38	4	39	G	O5'-P-OP2	-5.32	100.91	105.70
36	5	270	U	C6-N1-C1'	-5.32	113.75	121.20
36	5	815	G	C4-N9-C1'	5.32	133.42	126.50
36	1	2409	G	N3-C2-N2	5.32	123.62	119.90
36	1	3071	U	N1-C2-O2	-5.32	119.08	122.80
36	5	1906	G	N1-C2-N3	5.32	127.09	123.90
36	5	2627	C	N3-C4-N4	-5.32	114.28	118.00
36	5	3050	U	N3-C4-O4	-5.32	115.68	119.40
36	5	3103	A	C5-C6-N6	-5.32	119.44	123.70
36	1	1216	C	O5'-P-OP2	-5.32	100.91	105.70
36	1	1371	G	OP2-P-O3'	5.32	116.90	105.20
36	1	1407	A	C8-N9-C4	5.32	107.93	105.80
36	1	2380	U	N1-C2-N3	5.32	118.09	114.90
36	5	606	C	C2-N3-C4	-5.32	117.24	119.90
36	5	946	U	N3-C4-C5	5.32	117.79	114.60
36	1	105	C	C2-N3-C4	-5.32	117.24	119.90
36	5	728	G	C5-C6-O6	5.32	131.79	128.60
36	5	1403	C	N3-C4-C5	5.32	124.03	121.90
36	5	1514	G	N9-C4-C5	-5.32	103.27	105.40
36	5	2425	G	C5-N7-C8	-5.32	101.64	104.30
36	5	2813	A	N9-C4-C5	5.32	107.93	105.80
36	5	3243	A	C6-N1-C2	-5.32	115.41	118.60
1	2	1747	G	N1-C6-O6	5.32	123.09	119.90
36	1	1819	U	C5-C6-N1	5.32	125.36	122.70
36	1	2553	U	C5-C6-N1	-5.32	120.04	122.70
36	1	2623	G	C4-C5-N7	5.32	112.93	110.80
1	6	10	G	C5-C6-O6	5.32	131.79	128.60
1	6	1117	U	N3-C4-O4	5.32	123.12	119.40
36	5	339	C	N1-C2-N3	5.32	122.92	119.20
36	5	432	G	C2-N3-C4	-5.32	109.24	111.90
36	5	2834	G	OP1-P-OP2	5.32	127.57	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2297	U	P-O3'-C3'	5.31	126.08	119.70
1	6	858	G	N7-C8-N9	5.31	115.76	113.10
36	5	907	G	N3-C4-N9	5.31	129.19	126.00
1	2	1175	U	OP1-P-O3'	5.31	116.89	105.20
1	2	1277	G	N3-C4-N9	-5.31	122.81	126.00
36	1	338	A	O5'-P-OP1	-5.31	100.92	105.70
36	1	2180	G	C5-C6-N1	-5.31	108.84	111.50
36	1	2549	G	N3-C4-C5	-5.31	125.94	128.60
1	6	299	A	O5'-P-OP2	-5.31	100.92	105.70
36	5	669	U	N1-C2-O2	-5.31	119.08	122.80
36	5	1122	U	C5-C6-N1	-5.31	120.04	122.70
36	5	2392	C	C2-N1-C1'	-5.31	112.95	118.80
36	5	3050	U	O5'-P-OP2	5.31	117.08	110.70
36	1	3123	A	N7-C8-N9	5.31	116.45	113.80
36	1	3201	C	C6-N1-C2	-5.31	118.18	120.30
36	5	2366	C	C2-N1-C1'	5.31	124.64	118.80
36	5	2593	A	P-O3'-C3'	5.31	126.07	119.70
36	5	3054	U	N3-C2-O2	5.31	125.92	122.20
36	1	1544	G	O5'-P-OP2	-5.31	100.92	105.70
36	1	2194	G	C4-C5-C6	5.31	121.99	118.80
36	1	2656	A	N3-C4-C5	-5.31	123.08	126.80
1	6	1032	G	N3-C4-C5	5.31	131.25	128.60
36	5	192	C	C2-N1-C1'	5.31	124.64	118.80
36	5	1314	C	C2-N1-C1'	5.31	124.64	118.80
36	5	2849	C	O5'-P-OP1	-5.31	100.92	105.70
1	2	1456	C	C4-C5-C6	5.31	120.05	117.40
36	1	86	G	C5-C6-O6	5.31	131.78	128.60
36	1	363	G	OP1-P-O3'	5.31	116.88	105.20
36	1	594	U	C5-C6-N1	-5.31	120.05	122.70
36	1	805	G	C5-N7-C8	5.31	106.95	104.30
36	1	2402	A	P-O3'-C3'	5.31	126.07	119.70
1	6	1680	G	C4-C5-N7	5.31	112.92	110.80
36	5	897	U	N1-C2-N3	5.31	118.08	114.90
36	5	1846	C	C2-N3-C4	-5.31	117.25	119.90
36	5	2364	G	O4'-C1'-N9	5.31	112.44	108.20
36	5	2641	U	N1-C2-N3	5.31	118.08	114.90
36	5	2705	A	O5'-P-OP1	-5.31	100.92	105.70
36	5	3067	C	C6-N1-C2	5.31	122.42	120.30
1	2	1101	G	C5-C6-N1	5.31	114.15	111.50
36	1	176	G	N3-C4-N9	5.31	129.18	126.00
36	1	638	C	OP2-P-O3'	5.31	116.87	105.20
36	1	985	U	C4-C5-C6	-5.31	116.52	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2912	G	C2-N3-C4	5.31	114.55	111.90
36	1	2968	G	C2-N3-C4	-5.31	109.25	111.90
1	6	345	U	C5-C6-N1	-5.31	120.05	122.70
36	5	2405	C	N1-C2-N3	5.31	122.92	119.20
38	8	14	C	O5'-P-OP2	-5.31	100.92	105.70
52	m6	66	LYS	CD-CE-NZ	5.31	123.90	111.70
36	1	1101	G	C4-C5-N7	-5.30	108.68	110.80
36	1	2161	G	N3-C4-C5	-5.30	125.95	128.60
36	1	2865	U	C5-C4-O4	-5.30	122.72	125.90
36	1	2944	U	OP2-P-O3'	5.30	116.87	105.20
38	4	45	C	O5'-P-OP2	-5.30	100.93	105.70
1	6	16	G	C5-C6-O6	5.30	131.78	128.60
1	6	355	G	C4-C5-N7	-5.30	108.68	110.80
36	5	143	G	C8-N9-C4	5.30	108.52	106.40
36	5	729	C	N3-C4-C5	5.30	124.02	121.90
36	5	2892	A	O5'-P-OP2	-5.30	100.93	105.70
36	1	208	C	N1-C2-N3	5.30	122.91	119.20
36	1	2144	A	C5-C6-N6	-5.30	119.46	123.70
36	1	2418	G	C8-N9-C4	-5.30	104.28	106.40
36	5	2148	U	N1-C2-O2	-5.30	119.09	122.80
36	1	936	A	P-O3'-C3'	5.30	126.06	119.70
36	1	1125	U	OP2-P-O3'	5.30	116.86	105.20
36	1	1878	G	O5'-P-OP1	-5.30	100.93	105.70
36	1	3112	G	N1-C2-N3	-5.30	120.72	123.90
36	5	2243	A	C8-N9-C4	5.30	107.92	105.80
36	5	2318	U	N1-C2-O2	5.30	126.51	122.80
36	5	3104	U	C5-C4-O4	-5.30	122.72	125.90
36	1	132	C	C2-N1-C1'	-5.30	112.97	118.80
36	5	315	C	N3-C4-C5	5.30	124.02	121.90
36	5	980	A	C6-C5-N7	5.30	136.01	132.30
36	5	2415	C	N3-C4-C5	5.30	124.02	121.90
38	8	81	U	N1-C2-O2	5.30	126.51	122.80
36	1	354	U	OP1-P-OP2	5.30	127.55	119.60
36	1	1380	G	O5'-P-OP1	5.30	117.06	110.70
36	1	2356	A	C4-C5-N7	5.30	113.35	110.70
37	3	90	U	C2-N1-C1'	-5.30	111.34	117.70
1	6	574	G	C5-N7-C8	5.30	106.95	104.30
1	6	1615	C	N1-C1'-C2'	-5.30	106.17	112.00
36	5	1179	A	N1-C2-N3	5.30	131.95	129.30
36	5	2225	U	O5'-P-OP1	-5.30	100.93	105.70
36	1	2615	G	C5-C6-N1	5.30	114.15	111.50
36	1	3041	U	N1-C2-O2	-5.30	119.09	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	81	U	C6-N1-C2	-5.30	117.82	121.00
44	L7	239	LEU	CA-CB-CG	5.30	127.48	115.30
36	5	2662	G	OP2-P-O3'	5.30	116.85	105.20
1	2	158	U	C2-N1-C1'	5.29	124.06	117.70
36	1	99	A	C5-C6-N1	5.29	120.35	117.70
36	1	1431	G	N3-C4-C5	-5.29	125.95	128.60
36	1	1507	G	C6-N1-C2	-5.29	121.92	125.10
38	4	78	G	N3-C2-N2	5.29	123.61	119.90
36	5	2372	A	N1-C2-N3	5.29	131.95	129.30
36	5	2802	A	C2-N3-C4	5.29	113.25	110.60
1	2	1370	U	P-O3'-C3'	5.29	126.05	119.70
36	1	788	C	N3-C4-N4	-5.29	114.30	118.00
1	6	1440	C	C5-C6-N1	5.29	123.65	121.00
36	5	957	C	N3-C2-O2	-5.29	118.19	121.90
36	5	1164	G	C5-C6-O6	5.29	131.78	128.60
36	5	3184	A	C8-N9-C4	5.29	107.92	105.80
1	2	765	G	C5-C6-N1	5.29	114.15	111.50
36	1	633	C	C6-N1-C2	5.29	122.42	120.30
1	6	1039	A	O4'-C1'-N9	5.29	112.43	108.20
36	5	414	U	C6-N1-C2	5.29	124.17	121.00
36	5	832	G	N3-C4-N9	5.29	129.18	126.00
36	5	1610	G	O5'-P-OP1	5.29	117.05	110.70
36	5	2704	A	C5'-C4'-O4'	-5.29	102.75	109.10
36	5	3042	U	C2-N3-C4	-5.29	123.83	127.00
38	8	4	C	C4-C5-C6	5.29	120.05	117.40
36	1	2708	C	N3-C4-C5	5.29	124.02	121.90
1	6	1125	A	C2-N3-C4	-5.29	107.95	110.60
36	5	3090	U	N3-C4-C5	5.29	117.77	114.60
36	5	3123	A	C5-N7-C8	5.29	106.55	103.90
36	1	1433	A	N1-C6-N6	5.29	121.77	118.60
36	1	3280	U	O4'-C1'-N1	5.29	112.43	108.20
36	5	1657	C	C6-N1-C1'	-5.29	114.45	120.80
36	5	2211	U	C5-C6-N1	-5.29	120.06	122.70
36	5	2271	A	N1-C6-N6	-5.29	115.43	118.60
36	5	2754	G	C5-C6-O6	5.29	131.77	128.60
36	5	2927	C	N3-C4-C5	-5.29	119.78	121.90
36	1	878	G	N9-C4-C5	5.29	107.52	105.40
36	1	1855	U	N1-C2-N3	5.29	118.07	114.90
36	5	534	U	N3-C2-O2	-5.29	118.50	122.20
1	6	1658	G	N7-C8-N9	-5.29	110.46	113.10
36	5	655	C	C6-N1-C2	-5.29	118.19	120.30
36	5	809	G	C5-C6-N1	5.29	114.14	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	893	C	N3-C4-C5	-5.29	119.79	121.90
36	5	1001	G	OP1-P-OP2	5.29	127.53	119.60
36	5	1201	C	C2-N1-C1'	-5.29	112.99	118.80
36	5	2980	U	N1-C2-O2	5.29	126.50	122.80
36	5	3148	U	C5-C4-O4	-5.29	122.73	125.90
36	5	3242	G	C5-C6-O6	5.29	131.77	128.60
1	2	992	A	C5-N7-C8	-5.28	101.26	103.90
36	1	22	G	C5-C6-N1	5.28	114.14	111.50
36	1	375	A	C2-N3-C4	5.28	113.24	110.60
36	1	823	C	C6-N1-C2	-5.28	118.19	120.30
36	1	1646	G	O4'-C1'-N9	5.28	112.43	108.20
36	1	2815	G	N1-C2-N2	-5.28	111.45	116.20
36	5	40	A	N7-C8-N9	5.28	116.44	113.80
36	5	2705	A	C5-C6-N6	-5.28	119.47	123.70
36	5	3003	G	C5-N7-C8	-5.28	101.66	104.30
36	5	3107	U	OP2-P-O3'	5.28	116.82	105.20
37	7	37	G	N3-C4-N9	5.28	129.17	126.00
36	1	1838	G	OP1-P-O3'	5.28	116.82	105.20
36	5	200	C	C2-N3-C4	5.28	122.54	119.90
36	5	1186	G	N7-C8-N9	5.28	115.74	113.10
36	5	1855	U	O5'-P-OP2	-5.28	100.95	105.70
36	5	2631	U	C2-N3-C4	-5.28	123.83	127.00
36	5	3277	U	O5'-P-OP1	-5.28	100.95	105.70
1	2	1595	U	N3-C4-O4	5.28	123.10	119.40
36	1	919	U	N3-C4-C5	5.28	117.77	114.60
36	1	1940	G	N3-C4-N9	5.28	129.17	126.00
36	1	2163	C	N1-C2-N3	5.28	122.90	119.20
36	1	2865	U	O5'-P-OP2	-5.28	100.95	105.70
36	1	2878	G	C5-C6-O6	-5.28	125.43	128.60
36	5	636	C	C4-C5-C6	5.28	120.04	117.40
36	5	1017	C	C5-C6-N1	5.28	123.64	121.00
36	5	1442	U	O5'-P-OP1	-5.28	100.95	105.70
36	5	2605	G	C5-C6-O6	-5.28	125.43	128.60
36	5	3392	U	C2-N1-C1'	-5.28	111.36	117.70
36	1	1841	A	C4-C5-C6	5.28	119.64	117.00
36	5	659	G	P-O3'-C3'	5.28	126.03	119.70
36	5	1730	G	N3-C4-N9	5.28	129.17	126.00
36	5	2599	U	N1-C2-O2	-5.28	119.11	122.80
1	2	1280	C	O5'-P-OP1	-5.28	100.95	105.70
36	1	75	G	O5'-P-OP2	-5.28	100.95	105.70
36	1	927	C	C6-N1-C2	5.28	122.41	120.30
36	1	1884	A	OP2-P-O3'	5.28	116.81	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2865	U	OP2-P-O3'	5.28	116.81	105.20
1	6	467	G	N3-C4-N9	5.28	129.17	126.00
36	5	818	C	N1-C2-N3	5.28	122.89	119.20
36	5	1547	G	O5'-P-OP1	-5.28	100.95	105.70
36	5	2201	G	N3-C2-N2	5.28	123.59	119.90
36	5	2211	U	N3-C4-C5	-5.28	111.43	114.60
36	5	3195	U	P-O3'-C3'	5.28	126.03	119.70
1	2	1446	A	N1-C6-N6	-5.28	115.44	118.60
36	1	509	U	C2-N3-C4	-5.28	123.83	127.00
36	1	2821	C	C4-C5-C6	5.28	120.04	117.40
36	5	1388	U	O5'-P-OP2	-5.28	100.95	105.70
36	5	2334	U	N1-C2-N3	5.28	118.07	114.90
36	5	3142	A	C5-C6-N6	-5.28	119.48	123.70
36	1	1604	G	C4-N9-C1'	5.27	133.36	126.50
1	6	1027	A	OP1-P-O3'	5.27	116.80	105.20
36	5	128	G	C5-C6-O6	-5.27	125.44	128.60
36	5	644	G	N3-C4-C5	-5.27	125.96	128.60
36	5	2347	U	C4-C5-C6	-5.27	116.53	119.70
36	1	439	C	C2-N3-C4	5.27	122.54	119.90
36	1	2955	U	OP1-P-O3'	5.27	116.80	105.20
37	3	96	U	C5-C6-N1	-5.27	120.06	122.70
36	5	2623	G	O5'-P-OP2	5.27	117.03	110.70
37	7	77	G	N3-C4-C5	-5.27	125.96	128.60
1	2	587	C	N3-C4-C5	-5.27	119.79	121.90
36	1	1594	A	C8-N9-C4	-5.27	103.69	105.80
36	1	2242	A	OP2-P-O3'	5.27	116.80	105.20
37	3	73	C	C5-C6-N1	5.27	123.64	121.00
36	5	2878	G	OP1-P-O3'	5.27	116.80	105.20
37	7	8	G	N3-C4-N9	5.27	129.16	126.00
36	1	309	U	OP1-P-OP2	-5.27	111.70	119.60
36	1	946	U	N3-C2-O2	-5.27	118.51	122.20
41	L4	182	LEU	CA-CB-CG	5.27	127.42	115.30
1	6	308	C	C5-C6-N1	-5.27	118.36	121.00
36	5	1450	G	N1-C2-N2	5.27	120.94	116.20
36	5	2412	G	N3-C4-C5	-5.27	125.97	128.60
36	5	2727	A	C2-N3-C4	5.27	113.23	110.60
43	l6	18	LEU	CA-CB-CG	-5.27	103.18	115.30
1	2	545	A	OP1-P-O3'	5.27	116.79	105.20
36	1	2719	U	C2-N3-C4	-5.27	123.84	127.00
36	1	2894	C	OP2-P-O3'	5.27	116.79	105.20
36	1	2941	A	C4-C5-N7	5.27	113.33	110.70
36	1	3123	A	C5-N7-C8	-5.27	101.27	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	625	C	N3-C4-N4	5.27	121.69	118.00
1	6	1526	A	C5-C6-N6	5.27	127.91	123.70
36	5	1725	C	O4'-C1'-N1	5.27	112.41	108.20
36	5	2550	U	C6-N1-C2	-5.27	117.84	121.00
36	5	3041	U	C4-C5-C6	-5.27	116.54	119.70
36	5	3258	U	OP2-P-O3'	5.27	116.79	105.20
36	1	637	C	C6-N1-C1'	5.27	127.12	120.80
1	6	2	A	C8-N9-C4	5.27	107.91	105.80
1	6	187	G	P-O3'-C3'	5.27	126.02	119.70
36	1	101	G	O4'-C1'-N9	5.26	112.41	108.20
36	1	304	G	C5-C6-N1	5.26	114.13	111.50
1	6	142	G	C8-N9-C1'	-5.26	120.16	127.00
1	6	1614	A	O4'-C1'-N9	5.26	112.41	108.20
1	6	1766	A	C5-C6-N1	-5.26	115.07	117.70
36	5	210	U	C5'-C4'-O4'	-5.26	102.78	109.10
36	5	1832	C	C5-C6-N1	-5.26	118.37	121.00
36	5	2210	G	C4-N9-C1'	5.26	133.34	126.50
36	5	3115	C	C6-N1-C1'	5.26	127.12	120.80
40	13	26	ARG	NE-CZ-NH1	-5.26	117.67	120.30
36	1	27	C	N1-C2-N3	5.26	122.88	119.20
36	1	1097	G	N1-C6-O6	5.26	123.06	119.90
36	1	2370	G	C5-C6-O6	-5.26	125.44	128.60
1	6	1789	G	C5-C6-O6	-5.26	125.44	128.60
36	5	3028	G	C4-C5-N7	5.26	112.91	110.80
36	1	629	U	N3-C2-O2	-5.26	118.52	122.20
36	1	2623	G	C6-C5-N7	-5.26	127.24	130.40
36	5	63	A	N9-C4-C5	-5.26	103.70	105.80
36	5	990	U	C2-N3-C4	5.26	130.16	127.00
36	5	2753	G	C8-N9-C4	-5.26	104.30	106.40
36	5	3368	U	N1-C2-O2	-5.26	119.12	122.80
37	7	53	U	O5'-P-OP2	-5.26	100.97	105.70
37	7	112	G	C8-N9-C4	-5.26	104.30	106.40
36	1	497	C	OP2-P-O3'	5.26	116.77	105.20
36	1	1433	A	OP1-P-O3'	5.26	116.77	105.20
36	1	2688	U	C5-C4-O4	-5.26	122.74	125.90
1	6	1667	A	OP1-P-OP2	-5.26	111.71	119.60
36	5	2133	U	C6-N1-C2	5.26	124.16	121.00
36	5	3189	G	C5-C6-N1	5.26	114.13	111.50
1	2	624	G	N1-C6-O6	-5.26	116.75	119.90
1	2	959	U	C6-N1-C1'	-5.26	113.84	121.20
36	1	26	A	O5'-P-OP1	-5.26	100.97	105.70
36	1	2631	U	C5-C6-N1	-5.26	120.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2899	C	C5-C6-N1	-5.26	118.37	121.00
1	2	453	U	C6-N1-C1'	-5.26	113.84	121.20
31	D9	36	LEU	CA-CB-CG	5.26	127.39	115.30
36	1	375	A	N1-C2-N3	-5.26	126.67	129.30
36	1	1440	G	N3-C2-N2	5.26	123.58	119.90
36	1	2915	U	N1-C2-N3	5.26	118.05	114.90
36	1	3157	U	C6-N1-C1'	-5.26	113.84	121.20
38	4	101	U	N1-C2-O2	5.26	126.48	122.80
1	6	174	U	C5-C4-O4	-5.26	122.75	125.90
36	5	887	G	C6-N1-C2	5.26	128.25	125.10
36	5	900	G	C2-N3-C4	5.26	114.53	111.90
36	5	2137	U	OP1-P-OP2	-5.26	111.71	119.60
36	5	3330	A	C4-C5-N7	-5.26	108.07	110.70
36	1	1935	G	N3-C2-N2	5.25	123.58	119.90
1	2	1081	A	P-O3'-C3'	5.25	126.00	119.70
1	2	1374	C	C6-N1-C2	-5.25	118.20	120.30
3	S1	181	LEU	CA-CB-CG	5.25	127.38	115.30
36	1	2877	G	N1-C2-N3	5.25	127.05	123.90
36	1	3246	G	O4'-C1'-N9	5.25	112.40	108.20
36	5	96	G	C4-N9-C1'	-5.25	119.67	126.50
36	5	889	U	C5-C4-O4	-5.25	122.75	125.90
36	5	1137	C	N3-C4-C5	-5.25	119.80	121.90
36	5	3260	G	N1-C6-O6	-5.25	116.75	119.90
36	1	141	C	C5-C6-N1	5.25	123.63	121.00
36	1	1779	C	N1-C2-O2	-5.25	115.75	118.90
36	1	2296	A	OP2-P-O3'	5.25	116.75	105.20
36	1	2867	C	C6-N1-C2	5.25	122.40	120.30
73	O7	67	LEU	CA-CB-CG	5.25	127.38	115.30
36	5	955	U	N1-C2-N3	5.25	118.05	114.90
36	5	1592	G	OP2-P-O3'	5.25	116.75	105.20
1	2	418	G	O5'-P-OP2	5.25	117.00	110.70
36	1	862	U	C5-C4-O4	-5.25	122.75	125.90
36	1	1100	U	C2-N3-C4	-5.25	123.85	127.00
36	1	3264	G	C2-N3-C4	-5.25	109.28	111.90
1	6	1081	A	C5-C6-N6	-5.25	119.50	123.70
36	5	2832	C	C5-C6-N1	-5.25	118.38	121.00
36	1	1949	G	O5'-P-OP1	-5.25	100.98	105.70
36	1	3044	G	N1-C6-O6	-5.25	116.75	119.90
1	6	977	A	C8-N9-C4	5.25	107.90	105.80
36	5	44	U	C5-C6-N1	-5.25	120.08	122.70
36	5	528	U	N3-C2-O2	-5.25	118.53	122.20
36	5	2190	U	N1-C2-N3	5.25	118.05	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	m1	112	LEU	CA-CB-CG	5.25	127.37	115.30
54	m8	22	ASP	CB-CG-OD1	-5.25	113.58	118.30
36	1	150	A	C8-N9-C4	-5.25	103.70	105.80
36	1	652	G	O5'-P-OP2	-5.25	100.98	105.70
36	1	947	G	N3-C4-N9	5.25	129.15	126.00
36	1	3133	C	N3-C2-O2	-5.25	118.23	121.90
1	6	26	A	O5'-P-OP1	-5.25	100.98	105.70
36	5	571	U	C5-C4-O4	5.25	129.05	125.90
36	5	1048	A	N7-C8-N9	-5.25	111.18	113.80
36	5	1121	U	N3-C2-O2	5.25	125.87	122.20
36	5	1302	A	C8-N9-C4	-5.25	103.70	105.80
36	5	1528	G	N3-C4-C5	-5.25	125.98	128.60
36	5	2845	A	N9-C4-C5	-5.25	103.70	105.80
37	7	33	U	O5'-P-OP1	-5.25	100.98	105.70
36	1	826	G	C5-C6-N1	5.25	114.12	111.50
36	5	1141	C	O5'-P-OP1	-5.25	100.98	105.70
1	2	1458	G	C8-N9-C1'	-5.24	120.18	127.00
36	1	659	G	P-O3'-C3'	5.24	125.99	119.70
36	1	1671	C	C6-N1-C2	-5.24	118.20	120.30
36	1	2410	U	N1-C2-N3	5.24	118.05	114.90
36	1	2960	C	C2-N3-C4	-5.24	117.28	119.90
36	1	3140	G	C6-C5-N7	-5.24	127.25	130.40
37	3	39	C	C6-N1-C2	5.24	122.40	120.30
36	5	665	A	N1-C6-N6	5.24	121.75	118.60
36	5	1868	G	C5-C6-O6	-5.24	125.45	128.60
36	5	2617	U	N1-C2-O2	-5.24	119.13	122.80
36	5	3183	A	C4-C5-N7	5.24	113.32	110.70
36	1	1318	A	C5-N7-C8	-5.24	101.28	103.90
36	1	3120	C	N3-C2-O2	5.24	125.57	121.90
1	6	1456	C	N3-C2-O2	-5.24	118.23	121.90
36	5	382	U	N1-C2-N3	5.24	118.05	114.90
36	5	3038	U	N3-C4-C5	-5.24	111.45	114.60
36	1	2823	G	N3-C4-C5	-5.24	125.98	128.60
1	6	536	C	C2-N1-C1'	5.24	124.56	118.80
1	6	1526	A	N1-C6-N6	-5.24	115.45	118.60
1	6	1768	G	N1-C6-O6	-5.24	116.75	119.90
36	5	388	G	C6-C5-N7	-5.24	127.25	130.40
36	5	648	C	C2-N1-C1'	5.24	124.56	118.80
36	5	746	A	N9-C4-C5	5.24	107.90	105.80
36	5	796	U	C4-C5-C6	5.24	122.84	119.70
36	1	743	C	N3-C4-C5	5.24	124.00	121.90
36	1	1518	U	N1-C2-N3	5.24	118.04	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2661	G	O5'-P-OP1	-5.24	100.99	105.70
1	6	754	A	C5-C6-N6	-5.24	119.51	123.70
1	6	1135	U	C2-N3-C4	-5.24	123.86	127.00
31	d9	36	LEU	CA-CB-CG	5.24	127.35	115.30
36	5	103	G	N1-C2-N3	5.24	127.04	123.90
36	5	2132	C	C6-N1-C2	-5.24	118.20	120.30
36	5	2372	A	N1-C6-N6	-5.24	115.46	118.60
36	5	2601	A	C6-C5-N7	5.24	135.97	132.30
36	1	757	C	O5'-P-OP2	-5.24	100.99	105.70
36	5	189	G	N1-C2-N2	-5.24	111.49	116.20
36	5	1296	C	C4-C5-C6	5.24	120.02	117.40
36	5	3354	U	C6-N1-C2	-5.24	117.86	121.00
36	1	1838	G	N1-C6-O6	5.24	123.04	119.90
36	1	1899	G	N1-C6-O6	-5.24	116.76	119.90
36	1	3270	U	N1-C2-O2	-5.24	119.14	122.80
1	6	106	U	OP2-P-O3'	5.24	116.72	105.20
36	5	636	C	N3-C4-N4	5.24	121.67	118.00
36	5	804	C	N3-C4-N4	5.24	121.66	118.00
36	5	1355	A	P-O3'-C3'	5.24	125.98	119.70
36	5	3264	G	C6-N1-C2	5.24	128.24	125.10
36	5	3316	A	N1-C6-N6	5.24	121.74	118.60
36	5	3343	G	N3-C2-N2	5.24	123.56	119.90
36	1	2647	A	C6-N1-C2	-5.23	115.46	118.60
1	6	136	C	N1-C2-O2	5.23	122.04	118.90
36	5	85	A	N1-C6-N6	5.23	121.74	118.60
1	2	192	U	C5-C6-N1	5.23	125.32	122.70
6	S4	38	LEU	CA-CB-CG	5.23	127.33	115.30
36	1	684	G	N9-C4-C5	-5.23	103.31	105.40
36	1	940	G	N3-C2-N2	-5.23	116.24	119.90
36	1	1126	G	C6-C5-N7	-5.23	127.26	130.40
36	1	1918	C	C6-N1-C2	-5.23	118.21	120.30
77	Q1	17	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	6	16	G	C8-N9-C4	-5.23	104.31	106.40
36	5	41	G	N3-C4-C5	5.23	131.22	128.60
36	5	365	A	N9-C4-C5	-5.23	103.71	105.80
36	5	747	A	O5'-P-OP2	-5.23	100.99	105.70
36	5	1450	G	N3-C2-N2	-5.23	116.24	119.90
36	5	3034	C	N3-C2-O2	5.23	125.56	121.90
36	1	410	U	OP2-P-O3'	5.23	116.71	105.20
36	1	656	A	O5'-P-OP1	-5.23	100.99	105.70
37	3	21	G	N9-C4-C5	-5.23	103.31	105.40
73	O7	24	ARG	NE-CZ-NH1	-5.23	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	887	G	C5-C6-N1	-5.23	108.88	111.50
36	5	1330	A	OP2-P-O3'	5.23	116.71	105.20
36	5	2994	A	C6-N1-C2	-5.23	115.46	118.60
36	1	41	G	N1-C6-O6	-5.23	116.76	119.90
36	5	1365	G	C6-C5-N7	-5.23	127.26	130.40
1	2	1454	G	N3-C4-C5	-5.23	125.99	128.60
36	1	2860	U	N3-C2-O2	5.23	125.86	122.20
36	1	3143	C	OP1-P-O3'	5.23	116.70	105.20
37	3	104	A	N7-C8-N9	-5.23	111.19	113.80
36	5	828	A	N1-C6-N6	-5.23	115.46	118.60
36	5	1865	A	OP1-P-OP2	-5.23	111.76	119.60
36	5	2249	G	C3'-C2'-C1'	-5.23	97.32	101.50
36	5	2797	C	N3-C4-C5	-5.23	119.81	121.90
36	5	3343	G	N9-C4-C5	-5.23	103.31	105.40
37	7	8	G	C6-C5-N7	-5.23	127.26	130.40
38	8	21	C	OP2-P-O3'	5.23	116.70	105.20
1	2	728	U	N1-C2-O2	5.23	126.46	122.80
36	1	419	G	OP2-P-O3'	5.23	116.70	105.20
36	1	2634	U	N3-C2-O2	-5.23	118.54	122.20
37	3	71	G	C5-C6-O6	5.23	131.74	128.60
44	L7	215	GLY	N-CA-C	-5.23	100.04	113.10
36	5	1842	A	C8-N9-C1'	-5.23	118.29	127.70
1	2	328	A	OP1-P-OP2	5.22	127.44	119.60
36	1	719	U	N3-C2-O2	5.22	125.86	122.20
36	1	780	A	N1-C6-N6	-5.22	115.47	118.60
36	1	1340	G	C8-N9-C4	5.22	108.49	106.40
36	1	1605	A	O4'-C1'-N9	5.22	112.38	108.20
36	1	2706	G	N1-C6-O6	5.22	123.03	119.90
52	M6	52	LEU	CB-CG-CD1	-5.22	102.12	111.00
36	5	643	U	C5-C6-N1	-5.22	120.09	122.70
36	5	929	A	C5-C6-N6	5.22	127.88	123.70
36	5	2698	G	N1-C6-O6	-5.22	116.77	119.90
36	5	2763	U	OP1-P-O3'	5.22	116.70	105.20
36	5	2915	U	OP1-P-OP2	-5.22	111.76	119.60
36	5	3275	U	OP1-P-OP2	-5.22	111.76	119.60
1	2	402	C	P-O3'-C3'	5.22	125.97	119.70
1	2	975	C	O5'-P-OP1	-5.22	101.00	105.70
36	1	212	G	C8-N9-C1'	-5.22	120.21	127.00
36	1	226	C	N3-C4-N4	5.22	121.66	118.00
36	1	1049	C	N3-C2-O2	-5.22	118.24	121.90
36	5	1002	A	OP2-P-O3'	5.22	116.69	105.20
36	5	1844	C	N3-C2-O2	-5.22	118.24	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2848	G	C6-C5-N7	-5.22	127.27	130.40
36	5	3313	U	O5'-P-OP2	-5.22	101.00	105.70
37	7	102	A	C5-C6-N1	-5.22	115.09	117.70
1	2	944	A	C8-N9-C4	5.22	107.89	105.80
36	1	1452	A	N3-C4-C5	5.22	130.45	126.80
36	5	966	U	N1-C2-O2	5.22	126.45	122.80
36	1	337	G	O5'-P-OP2	-5.22	101.00	105.70
36	1	500	C	C6-N1-C2	-5.22	118.21	120.30
37	3	5	G	N3-C4-C5	5.22	131.21	128.60
1	6	406	U	N3-C2-O2	-5.22	118.55	122.20
1	6	629	U	O5'-P-OP2	-5.22	101.00	105.70
1	6	1180	C	C6-N1-C2	-5.22	118.21	120.30
36	5	40	A	N1-C2-N3	5.22	131.91	129.30
36	5	75	G	N3-C4-N9	5.22	129.13	126.00
36	5	1198	C	N1-C2-N3	5.22	122.85	119.20
36	5	1725	C	C2-N3-C4	-5.22	117.29	119.90
36	5	2172	A	O5'-P-OP2	-5.22	101.00	105.70
36	5	2290	C	C5-C4-N4	-5.22	116.55	120.20
36	5	3328	G	C5-C6-N1	5.22	114.11	111.50
1	2	445	A	N1-C2-N3	-5.22	126.69	129.30
17	C5	42	ARG	NE-CZ-NH2	-5.22	117.69	120.30
36	5	1517	G	C8-N9-C4	-5.22	104.31	106.40
36	5	1873	U	N1-C2-O2	-5.22	119.15	122.80
1	2	297	U	C6-N1-C2	-5.22	117.87	121.00
36	1	804	C	N1-C2-O2	-5.22	115.77	118.90
1	6	1700	C	N3-C2-O2	-5.22	118.25	121.90
36	5	1174	G	C4-N9-C1'	5.22	133.28	126.50
36	5	2728	G	O4'-C1'-N9	5.22	112.37	108.20
37	7	69	C	N3-C4-C5	5.22	123.99	121.90
36	1	32	U	N1-C2-N3	5.21	118.03	114.90
36	1	658	G	C5-C6-O6	-5.21	125.47	128.60
36	1	1480	G	O4'-C1'-N9	5.21	112.37	108.20
36	1	1522	U	C2-N3-C4	-5.21	123.87	127.00
36	1	2353	G	C4-C5-N7	-5.21	108.71	110.80
36	1	2395	G	N3-C4-N9	5.21	129.13	126.00
36	1	2618	G	C5-C6-O6	5.21	131.73	128.60
36	1	2861	U	N3-C4-O4	-5.21	115.75	119.40
36	5	1126	G	C8-N9-C4	-5.21	104.31	106.40
36	5	1126	G	C5-C6-O6	5.21	131.73	128.60
36	5	1501	U	C5-C6-N1	5.21	125.31	122.70
36	5	1522	U	C5-C4-O4	-5.21	122.77	125.90
36	5	1874	A	C2-N3-C4	-5.21	107.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2159	U	C2-N3-C4	-5.21	123.87	127.00
36	5	2673	A	N7-C8-N9	-5.21	111.19	113.80
1	2	1733	C	C5-C4-N4	-5.21	116.55	120.20
36	1	424	G	N1-C6-O6	-5.21	116.77	119.90
1	6	1615	C	N3-C2-O2	5.21	125.55	121.90
1	6	1770	U	N1-C2-O2	5.21	126.45	122.80
36	5	1371	G	C6-N1-C2	-5.21	121.97	125.10
36	5	2703	A	C4-C5-C6	5.21	119.61	117.00
1	2	1448	G	O5'-P-OP1	-5.21	101.01	105.70
36	1	1739	U	C2-N1-C1'	-5.21	111.45	117.70
36	1	2985	C	OP2-P-O3'	5.21	116.66	105.20
38	4	82	U	C5-C6-N1	5.21	125.31	122.70
51	M5	153	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	6	510	G	N3-C4-N9	5.21	129.13	126.00
1	6	514	G	N3-C2-N2	5.21	123.55	119.90
36	5	352	A	C4-C5-C6	-5.21	114.39	117.00
36	5	437	G	N3-C4-N9	-5.21	122.87	126.00
36	5	947	G	C5-C6-N1	5.21	114.11	111.50
36	5	2234	G	N9-C4-C5	-5.21	103.31	105.40
36	5	2271	A	C2-N3-C4	5.21	113.21	110.60
36	5	3276	G	OP1-P-O3'	5.21	116.67	105.20
36	1	817	A	N3-C4-C5	-5.21	123.15	126.80
38	4	111	A	C4-C5-N7	5.21	113.31	110.70
36	5	225	C	O5'-P-OP1	-5.21	101.01	105.70
36	5	2165	G	C5-C6-O6	-5.21	125.47	128.60
40	l3	232	ARG	NE-CZ-NH2	-5.21	117.69	120.30
36	1	979	U	C5-C4-O4	5.21	129.03	125.90
36	1	1474	A	N1-C2-N3	5.21	131.90	129.30
36	1	1837	U	C6-N1-C2	5.21	124.12	121.00
36	1	2541	U	C2-N1-C1'	5.21	123.95	117.70
36	1	2941	A	O4'-C1'-N9	-5.21	104.03	108.20
38	4	84	C	C5-C6-N1	-5.21	118.40	121.00
1	6	47	A	N1-C2-N3	-5.21	126.70	129.30
36	5	579	G	C4-N9-C1'	-5.21	119.73	126.50
36	5	2819	A	OP2-P-O3'	5.21	116.66	105.20
1	2	1339	C	C2-N1-C1'	5.21	124.53	118.80
36	1	1441	G	O5'-P-OP2	-5.21	101.01	105.70
36	1	2643	A	N1-C6-N6	5.21	121.72	118.60
36	1	3182	G	N7-C8-N9	-5.21	110.50	113.10
1	6	889	U	N3-C2-O2	5.21	125.84	122.20
36	5	2743	A	C8-N9-C4	5.21	107.88	105.80
36	1	829	U	C2-N3-C4	-5.21	123.88	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	920	A	N1-C2-N3	5.21	131.90	129.30
36	5	590	G	C4-C5-N7	5.21	112.88	110.80
36	5	1199	C	C4-C5-C6	5.21	120.00	117.40
36	5	2603	G	C5-C6-O6	5.21	131.72	128.60
36	5	2774	C	C4-C5-C6	5.21	120.00	117.40
36	1	585	A	N7-C8-N9	-5.20	111.20	113.80
36	1	878	G	N1-C2-N3	5.20	127.02	123.90
36	1	1081	U	N3-C4-O4	5.20	123.04	119.40
36	1	2909	U	OP2-P-O3'	5.20	116.65	105.20
36	1	3049	A	C8-N9-C4	5.20	107.88	105.80
36	1	3175	U	C5-C6-N1	-5.20	120.10	122.70
36	5	658	G	OP1-P-O3'	5.20	116.65	105.20
36	5	1551	C	C6-N1-C2	-5.20	118.22	120.30
36	5	1896	A	N1-C2-N3	5.20	131.90	129.30
36	1	111	C	N3-C2-O2	5.20	125.54	121.90
38	4	57	C	N3-C4-N4	-5.20	114.36	118.00
1	6	957	G	N3-C2-N2	-5.20	116.26	119.90
36	5	2843	U	C2-N1-C1'	5.20	123.94	117.70
36	5	3287	U	N1-C2-O2	5.20	126.44	122.80
37	7	43	U	C2-N3-C4	-5.20	123.88	127.00
1	2	150	U	N1-C2-O2	5.20	126.44	122.80
1	2	1280	C	C6-N1-C2	-5.20	118.22	120.30
36	1	939	U	C5-C4-O4	-5.20	122.78	125.90
36	1	1653	G	C2-N3-C4	5.20	114.50	111.90
36	1	2878	G	C4-C5-N7	5.20	112.88	110.80
36	1	2884	C	C4-C5-C6	-5.20	114.80	117.40
1	6	103	A	O4'-C1'-N9	5.20	112.36	108.20
1	6	815	G	N1-C6-O6	5.20	123.02	119.90
1	6	1657	U	C5-C4-O4	-5.20	122.78	125.90
36	5	590	G	N1-C6-O6	5.20	123.02	119.90
36	5	643	U	C2-N3-C4	-5.20	123.88	127.00
37	7	40	C	N3-C2-O2	5.20	125.54	121.90
1	2	1389	C	N3-C2-O2	-5.20	118.26	121.90
36	1	876	A	N9-C4-C5	-5.20	103.72	105.80
36	1	1331	U	N1-C1'-C2'	5.20	120.76	114.00
36	1	1379	G	N1-C2-N3	5.20	127.02	123.90
36	1	2710	C	N3-C2-O2	5.20	125.54	121.90
36	1	2841	G	OP1-P-O3'	5.20	116.64	105.20
1	6	454	U	N3-C2-O2	5.20	125.84	122.20
1	6	1149	G	C8-N9-C4	-5.20	104.32	106.40
36	5	391	A	C5-N7-C8	5.20	106.50	103.90
36	1	280	U	C2-N3-C4	-5.20	123.88	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2366	C	C6-N1-C2	-5.20	118.22	120.30
1	6	280	U	N1-C2-O2	5.20	126.44	122.80
1	6	1410	A	N1-C6-N6	5.20	121.72	118.60
36	5	1368	U	N3-C4-O4	5.20	123.04	119.40
36	5	1446	A	OP1-P-O3'	5.20	116.63	105.20
1	2	1463	C	C6-N1-C2	5.20	122.38	120.30
36	1	1548	C	N1-C2-O2	-5.20	115.78	118.90
36	1	2304	C	C4-C5-C6	5.20	120.00	117.40
36	1	2410	U	N3-C2-O2	5.20	125.84	122.20
36	1	2714	G	C8-N9-C1'	5.20	133.75	127.00
36	1	2936	A	C5-C6-N6	5.20	127.86	123.70
51	M5	201	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	6	1750	A	N9-C4-C5	-5.20	103.72	105.80
36	5	31	C	OP1-P-OP2	-5.20	111.81	119.60
36	5	718	G	C4-N9-C1'	5.20	133.25	126.50
37	7	103	A	C2-N3-C4	5.20	113.20	110.60
36	1	111	C	N3-C4-C5	5.19	123.98	121.90
1	6	1751	C	C5-C6-N1	-5.19	118.40	121.00
36	5	2164	A	C4-C5-C6	5.19	119.60	117.00
1	2	1654	G	C6-N1-C2	-5.19	121.98	125.10
36	1	2714	G	O5'-P-OP2	5.19	116.93	110.70
36	1	2975	U	N3-C2-O2	-5.19	118.56	122.20
1	6	26	A	C8-N9-C4	-5.19	103.72	105.80
1	6	778	G	C8-N9-C4	5.19	108.48	106.40
1	6	1127	G	C4-C5-N7	-5.19	108.72	110.80
36	5	1193	A	N9-C4-C5	5.19	107.88	105.80
36	5	1440	G	N9-C4-C5	5.19	107.48	105.40
36	5	1665	C	N3-C2-O2	-5.19	118.27	121.90
36	5	2692	A	C8-N9-C4	-5.19	103.72	105.80
36	1	376	G	O5'-P-OP1	-5.19	101.03	105.70
36	1	497	C	OP1-P-OP2	-5.19	111.81	119.60
36	1	1069	C	C5-C6-N1	5.19	123.59	121.00
36	1	2318	U	C2-N3-C4	-5.19	123.89	127.00
1	2	1200	G	C5-C6-N1	-5.19	108.91	111.50
36	1	2651	G	N3-C2-N2	-5.19	116.27	119.90
36	5	2268	U	C5-C6-N1	5.19	125.29	122.70
36	5	2797	C	C5-C6-N1	5.19	123.59	121.00
36	5	3078	U	N3-C2-O2	-5.19	118.57	122.20
36	1	1478	C	N1-C2-O2	-5.19	115.79	118.90
36	5	804	C	OP1-P-OP2	-5.19	111.82	119.60
36	5	2235	C	C6-N1-C2	5.19	122.38	120.30
1	2	303	U	N1-C2-O2	5.19	126.43	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	828	A	OP1-P-O3'	5.19	116.61	105.20
1	2	1611	A	C5-N7-C8	-5.18	101.31	103.90
36	1	325	A	O5'-P-OP2	5.18	116.92	110.70
36	1	2163	C	C4-C5-C6	5.18	119.99	117.40
36	5	621	A	N1-C6-N6	-5.18	115.49	118.60
36	5	1348	U	N3-C4-O4	5.18	123.03	119.40
36	1	386	A	O4'-C1'-N9	-5.18	104.05	108.20
36	1	2773	C	N3-C4-C5	5.18	123.97	121.90
38	4	56	G	N3-C2-N2	5.18	123.53	119.90
36	5	3126	C	N3-C4-C5	5.18	123.97	121.90
38	8	37	A	C8-N9-C4	-5.18	103.73	105.80
36	1	1555	U	C2-N1-C1'	-5.18	111.48	117.70
36	1	2620	G	N9-C4-C5	-5.18	103.33	105.40
36	1	2636	A	N7-C8-N9	5.18	116.39	113.80
36	5	1101	G	N1-C6-O6	-5.18	116.79	119.90
36	5	2830	G	N7-C8-N9	-5.18	110.51	113.10
36	1	304	G	N3-C4-C5	-5.18	126.01	128.60
36	1	1113	G	C8-N9-C4	-5.18	104.33	106.40
36	1	1854	C	O5'-P-OP2	-5.18	101.04	105.70
36	1	1921	A	C8-N9-C4	-5.18	103.73	105.80
1	6	53	G	N3-C4-C5	-5.18	126.01	128.60
1	6	1112	G	N3-C4-N9	5.18	129.11	126.00
36	5	299	G	N1-C6-O6	-5.18	116.79	119.90
36	5	627	U	C4-C5-C6	-5.18	116.59	119.70
36	5	636	C	C6-N1-C1'	-5.18	114.58	120.80
36	5	1330	A	OP1-P-OP2	5.18	127.37	119.60
36	5	1880	U	C6-N1-C2	5.18	124.11	121.00
36	5	3189	G	C6-N1-C2	-5.18	121.99	125.10
36	5	3194	C	N1-C2-O2	-5.18	115.79	118.90
36	5	2308	C	N3-C2-O2	5.18	125.53	121.90
36	5	2383	C	N3-C4-C5	-5.18	119.83	121.90
36	1	1320	C	C6-N1-C2	-5.18	118.23	120.30
36	1	2331	C	C4-C5-C6	5.18	119.99	117.40
36	1	2366	C	C5-C6-N1	5.18	123.59	121.00
1	6	1697	G	N3-C4-N9	5.18	129.11	126.00
4	s2	148	LEU	CA-CB-CG	5.18	127.20	115.30
36	5	579	G	C5-C6-N1	5.18	114.09	111.50
1	2	864	U	N3-C2-O2	-5.17	118.58	122.20
36	1	499	G	OP1-P-O3'	5.17	116.58	105.20
36	1	1304	A	OP1-P-OP2	5.17	127.36	119.60
36	1	2799	A	C5-N7-C8	5.17	106.49	103.90
36	1	3090	U	N3-C2-O2	5.17	125.82	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	4	C	C5-C6-N1	5.17	123.59	121.00
1	6	541	A	P-O3'-C3'	-5.17	113.49	119.70
1	6	613	G	N9-C4-C5	-5.17	103.33	105.40
36	5	283	G	N3-C2-N2	-5.17	116.28	119.90
36	5	852	U	OP2-P-O3'	5.17	116.58	105.20
36	5	1208	U	N1-C2-N3	5.17	118.00	114.90
36	5	1386	A	C5-C6-N1	-5.17	115.11	117.70
36	5	2736	A	N1-C2-N3	5.17	131.89	129.30
36	5	2748	A	C4-C5-C6	-5.17	114.41	117.00
36	1	974	G	C5-N7-C8	5.17	106.89	104.30
38	8	10	A	C8-N9-C4	-5.17	103.73	105.80
36	1	157	A	N1-C6-N6	5.17	121.70	118.60
36	1	718	G	C4-N9-C1'	-5.17	119.78	126.50
36	1	832	G	N7-C8-N9	-5.17	110.51	113.10
44	L7	160	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	6	137	U	C5-C6-N1	5.17	125.29	122.70
36	5	384	A	C8-N9-C4	5.17	107.87	105.80
36	5	408	A	C5-C6-N1	5.17	120.29	117.70
36	5	961	C	OP2-P-O3'	5.17	116.58	105.20
36	5	1133	A	N3-C4-C5	-5.17	123.18	126.80
36	5	3195	U	OP1-P-O3'	5.17	116.58	105.20
36	5	581	U	C5-C6-N1	5.17	125.28	122.70
36	5	1865	A	N3-C4-C5	5.17	130.42	126.80
36	5	2632	G	C5-N7-C8	5.17	106.89	104.30
38	8	42	G	O5'-P-OP1	5.17	116.90	110.70
1	2	247	A	N1-C6-N6	5.17	121.70	118.60
36	1	954	U	N3-C2-O2	5.17	125.82	122.20
36	5	340	C	C4-C5-C6	5.17	119.98	117.40
36	5	1190	A	N9-C4-C5	5.17	107.87	105.80
36	5	1842	A	O4'-C1'-N9	-5.17	104.06	108.20
36	5	2837	A	C4-C5-C6	5.17	119.58	117.00
36	5	2886	U	N3-C4-O4	-5.17	115.78	119.40
36	1	1101	G	C6-C5-N7	5.17	133.50	130.40
36	1	1129	A	C4-C5-N7	5.17	113.28	110.70
36	1	2331	C	C5-C6-N1	-5.17	118.42	121.00
41	L4	339	LEU	CA-CB-CG	5.17	127.18	115.30
1	6	594	A	OP1-P-O3'	5.17	116.56	105.20
36	5	371	G	N1-C6-O6	-5.17	116.80	119.90
36	5	1111	U	C4-C5-C6	-5.17	116.60	119.70
36	5	1115	G	C4-N9-C1'	5.17	133.22	126.50
36	5	2830	G	C6-N1-C2	-5.17	122.00	125.10
36	1	721	G	C6-C5-N7	-5.17	127.30	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	944	C	C2-N3-C4	5.17	122.48	119.90
36	1	1344	G	C6-C5-N7	-5.17	127.30	130.40
36	1	1882	G	N3-C2-N2	-5.17	116.28	119.90
36	5	1426	C	C6-N1-C2	5.17	122.37	120.30
36	5	1680	G	C4-C5-N7	-5.17	108.73	110.80
36	5	2949	U	N3-C2-O2	-5.17	118.58	122.20
38	8	113	U	C5-C6-N1	5.17	125.28	122.70
36	1	670	C	OP1-P-O3'	5.16	116.56	105.20
36	1	701	G	C2-N3-C4	-5.16	109.32	111.90
36	1	1323	G	OP2-P-O3'	5.16	116.56	105.20
36	1	1378	U	OP1-P-O3'	5.16	116.56	105.20
36	1	2772	C	C3'-C2'-C1'	-5.16	97.37	101.50
36	1	2802	A	N1-C6-N6	-5.16	115.50	118.60
60	N4	80	ARG	C-N-CA	5.16	143.68	122.00
36	5	318	A	N1-C6-N6	5.16	121.70	118.60
36	5	1174	G	C8-N9-C1'	-5.16	120.29	127.00
36	5	1329	U	N1-C2-N3	5.16	118.00	114.90
36	5	1927	G	N3-C2-N2	-5.16	116.29	119.90
36	5	2860	U	OP1-P-OP2	5.16	127.34	119.60
36	5	3046	A	C4-C5-N7	-5.16	108.12	110.70
36	1	1203	A	O5'-P-OP1	-5.16	101.05	105.70
36	1	1501	U	OP2-P-O3'	5.16	116.56	105.20
36	1	1940	G	N1-C2-N2	-5.16	111.55	116.20
36	1	2917	G	C2-N3-C4	5.16	114.48	111.90
36	1	3133	C	N1-C2-O2	5.16	122.00	118.90
16	c4	124	ASP	CB-CG-OD1	-5.16	113.65	118.30
36	5	2585	G	C2-N3-C4	5.16	114.48	111.90
36	5	3110	C	N3-C4-N4	-5.16	114.39	118.00
36	5	3144	G	N1-C6-O6	-5.16	116.80	119.90
1	2	325	G	N1-C6-O6	5.16	123.00	119.90
1	6	711	U	C2-N1-C1'	5.16	123.89	117.70
36	5	912	G	O5'-P-OP2	-5.16	101.06	105.70
36	5	2709	C	O5'-P-OP2	-5.16	101.06	105.70
36	1	230	U	N1-C2-N3	5.16	118.00	114.90
36	1	315	C	OP1-P-OP2	5.16	127.34	119.60
36	1	1180	A	N7-C8-N9	-5.16	111.22	113.80
36	1	1661	G	N3-C4-N9	5.16	129.09	126.00
36	1	2351	U	C5-C6-N1	5.16	125.28	122.70
36	1	2384	A	C5-C6-N6	-5.16	119.57	123.70
36	1	2623	G	C8-N9-C4	5.16	108.46	106.40
36	1	2834	G	C6-C5-N7	-5.16	127.31	130.40
36	1	2878	G	O5'-P-OP1	5.16	116.89	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	3	44	C	C5-C6-N1	5.16	123.58	121.00
1	6	142	G	N9-C4-C5	-5.16	103.34	105.40
1	6	542	A	O4'-C1'-N9	5.16	112.33	108.20
1	6	1119	G	C8-N9-C4	-5.16	104.34	106.40
1	6	1641	C	N1-C2-O2	-5.16	115.81	118.90
36	5	954	U	C6-N1-C2	-5.16	117.91	121.00
36	5	3245	A	C5-C6-N6	-5.16	119.57	123.70
35	SM	134	ASP	CB-CG-OD2	5.16	122.94	118.30
36	1	1899	G	C2-N3-C4	5.16	114.48	111.90
36	5	2248	C	C5-C6-N1	-5.16	118.42	121.00
36	5	2367	A	C8-N9-C4	-5.16	103.74	105.80
36	1	55	G	N1-C6-O6	-5.16	116.81	119.90
36	1	314	U	O5'-P-OP1	-5.16	101.06	105.70
36	1	638	C	N1-C2-O2	5.16	121.99	118.90
36	1	1329	U	C3'-C2'-C1'	5.16	105.62	101.50
36	1	2704	A	OP2-P-O3'	5.16	116.54	105.20
1	2	378	A	OP2-P-O3'	5.15	116.54	105.20
1	2	1600	A	N1-C6-N6	5.15	121.69	118.60
36	1	2180	G	C6-C5-N7	-5.15	127.31	130.40
36	1	2936	A	O5'-P-OP2	5.15	116.88	110.70
1	6	142	G	N3-C4-N9	5.15	129.09	126.00
36	5	38	U	O5'-P-OP2	-5.15	101.06	105.70
36	5	639	G	N3-C2-N2	-5.15	116.29	119.90
36	5	2836	C	C4-C5-C6	5.15	119.98	117.40
38	8	3	A	C5-C6-N1	5.15	120.28	117.70
1	2	315	A	N1-C6-N6	5.15	121.69	118.60
1	2	863	A	N9-C4-C5	-5.15	103.74	105.80
36	1	116	A	O4'-C1'-N9	5.15	112.32	108.20
36	1	2423	U	N3-C2-O2	5.15	125.81	122.20
36	1	3154	C	N1-C2-O2	5.15	121.99	118.90
1	6	114	C	C2-N1-C1'	5.15	124.47	118.80
36	5	746	A	OP2-P-O3'	5.15	116.53	105.20
36	5	1362	G	OP2-P-O3'	5.15	116.54	105.20
36	5	2133	U	C2-N3-C4	-5.15	123.91	127.00
36	5	2415	C	N3-C4-N4	-5.15	114.39	118.00
36	1	1117	G	C5-C6-O6	-5.15	125.51	128.60
36	1	3213	A	C4-C5-C6	5.15	119.58	117.00
1	6	1663	G	N7-C8-N9	5.15	115.67	113.10
36	5	353	G	C8-N9-C1'	5.15	133.69	127.00
36	5	832	G	C4-N9-C1'	5.15	133.19	126.50
36	5	1405	U	C2-N3-C4	-5.15	123.91	127.00
36	5	1416	C	C2-N1-C1'	5.15	124.47	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2946	A	C5-C6-N6	5.15	127.82	123.70
1	2	551	G	N1-C2-N3	-5.15	120.81	123.90
36	1	953	G	O4'-C1'-N9	5.15	112.32	108.20
36	1	2144	A	OP1-P-O3'	5.15	116.53	105.20
36	1	2524	A	O4'-C1'-N9	5.15	112.32	108.20
1	6	11	A	C5-N7-C8	5.15	106.47	103.90
1	6	457	G	C2-N3-C4	-5.15	109.33	111.90
36	5	939	U	C2-N3-C4	-5.15	123.91	127.00
36	5	1412	G	N9-C4-C5	5.15	107.46	105.40
36	5	2815	G	C5-C6-N1	5.15	114.07	111.50
36	5	2875	U	N3-C2-O2	5.15	125.80	122.20
36	5	3309	G	C8-N9-C4	-5.15	104.34	106.40
36	1	816	A	N1-C2-N3	-5.15	126.73	129.30
36	1	872	U	C4-C5-C6	5.15	122.79	119.70
36	1	1444	G	C5-C6-O6	-5.15	125.51	128.60
36	1	1858	A	O4'-C1'-N9	5.15	112.32	108.20
36	1	2138	A	C8-N9-C4	-5.15	103.74	105.80
36	1	2645	G	C6-N1-C2	-5.15	122.01	125.10
36	1	3277	U	C2-N1-C1'	5.15	123.88	117.70
36	5	2190	U	C6-N1-C2	-5.15	117.91	121.00
36	5	2367	A	C4-C5-C6	5.15	119.57	117.00
36	5	2882	U	C5-C4-O4	-5.15	122.81	125.90
1	2	1747	G	C8-N9-C4	5.15	108.46	106.40
36	1	78	U	N3-C2-O2	5.15	125.80	122.20
36	1	2719	U	C6-N1-C2	-5.15	117.91	121.00
36	1	3005	A	C4-C5-C6	-5.15	114.43	117.00
1	6	1723	U	N3-C2-O2	-5.15	118.60	122.20
36	5	1506	A	N7-C8-N9	5.15	116.37	113.80
36	5	3054	U	N3-C4-C5	-5.15	111.51	114.60
36	1	517	G	N1-C6-O6	5.14	122.99	119.90
36	1	690	A	OP1-P-O3'	5.14	116.52	105.20
36	1	877	C	C5-C4-N4	-5.14	116.60	120.20
36	1	1183	C	N1-C2-O2	-5.14	115.81	118.90
36	1	1642	A	O5'-P-OP1	-5.14	101.07	105.70
36	1	1841	A	O5'-P-OP1	5.14	116.87	110.70
36	1	3057	U	C2-N3-C4	-5.14	123.91	127.00
1	6	957	G	C5-C6-N1	-5.14	108.93	111.50
36	5	215	G	N3-C4-C5	-5.14	126.03	128.60
36	5	1191	U	C5-C6-N1	-5.14	120.13	122.70
36	5	2654	C	OP2-P-O3'	5.14	116.52	105.20
36	5	2873	U	N3-C4-O4	5.14	123.00	119.40
62	n6	76	LEU	CA-CB-CG	5.14	127.13	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	124	A	C8-N9-C4	-5.14	103.74	105.80
36	1	2653	C	N3-C4-N4	-5.14	114.40	118.00
38	4	120	C	N3-C2-O2	5.14	125.50	121.90
1	6	321	C	N1-C2-O2	5.14	121.99	118.90
36	1	820	A	C5-N7-C8	-5.14	101.33	103.90
36	1	1329	U	C5-C4-O4	-5.14	122.81	125.90
36	1	2403	G	O4'-C1'-N9	5.14	112.31	108.20
38	8	54	A	C4-C5-N7	5.14	113.27	110.70
1	2	1573	A	P-O3'-C3'	5.14	125.87	119.70
36	1	123	A	C5-N7-C8	-5.14	101.33	103.90
36	1	673	U	N3-C4-C5	5.14	117.68	114.60
36	1	905	U	C4-C5-C6	5.14	122.78	119.70
36	1	2917	G	O5'-P-OP1	-5.14	101.07	105.70
68	O2	105	ARG	NE-CZ-NH1	5.14	122.87	120.30
36	5	44	U	N3-C2-O2	5.14	125.80	122.20
36	5	313	A	C6-N1-C2	-5.14	115.52	118.60
36	5	3185	U	O5'-P-OP2	-5.14	101.08	105.70
36	1	1429	G	N3-C4-N9	5.14	129.08	126.00
36	1	2323	G	N1-C2-N2	-5.14	111.58	116.20
36	1	2695	A	C8-N9-C4	-5.14	103.75	105.80
1	6	280	U	C2-N1-C1'	5.14	123.86	117.70
36	5	37	U	OP2-P-O3'	5.14	116.50	105.20
36	5	116	A	O5'-P-OP1	-5.14	101.08	105.70
36	5	1311	G	C5-C6-N1	5.14	114.07	111.50
36	1	84	U	C5-C4-O4	-5.14	122.82	125.90
36	1	1468	A	C4-C5-C6	5.14	119.57	117.00
36	1	2125	A	N1-C2-N3	-5.14	126.73	129.30
36	1	2707	C	OP2-P-O3'	5.14	116.50	105.20
36	5	189	G	N3-C2-N2	5.14	123.50	119.90
36	5	1114	U	OP1-P-O3'	5.14	116.50	105.20
36	5	2572	C	C6-N1-C2	-5.14	118.25	120.30
36	5	2767	U	N3-C4-O4	-5.14	115.81	119.40
36	5	3154	C	C6-N1-C1'	-5.14	114.64	120.80
36	1	334	A	N1-C2-N3	5.13	131.87	129.30
36	1	340	C	N1-C2-N3	5.13	122.80	119.20
36	1	351	A	O5'-P-OP1	-5.13	101.08	105.70
36	1	1379	G	OP2-P-O3'	5.13	116.50	105.20
36	1	2819	A	C5-N7-C8	5.13	106.47	103.90
36	1	3150	A	C4-C5-C6	-5.13	114.43	117.00
1	6	538	A	C5-C6-N6	5.13	127.81	123.70
36	5	728	G	OP2-P-O3'	5.13	116.50	105.20
36	5	1419	A	N9-C1'-C2'	-5.13	106.35	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2353	G	C5-C6-O6	-5.13	125.52	128.60
36	1	918	C	C6-N1-C1'	5.13	126.96	120.80
36	5	961	C	N3-C4-C5	-5.13	119.85	121.90
36	1	719	U	O5'-P-OP1	-5.13	101.08	105.70
36	1	2144	A	N1-C6-N6	5.13	121.68	118.60
36	1	2656	A	C2-N3-C4	5.13	113.17	110.60
1	6	1742	U	OP2-P-O3'	5.13	116.49	105.20
36	5	1011	A	OP2-P-O3'	5.13	116.49	105.20
36	5	1117	G	C5-C6-N1	5.13	114.07	111.50
36	5	2661	G	N3-C2-N2	5.13	123.49	119.90
1	2	885	G	N1-C6-O6	5.13	122.98	119.90
36	1	146	U	C5-C6-N1	-5.13	120.14	122.70
36	1	3135	U	N3-C4-O4	-5.13	115.81	119.40
36	5	347	G	C5-C6-O6	5.13	131.68	128.60
36	5	1116	G	N1-C2-N3	5.13	126.98	123.90
36	5	2747	A	C8-N9-C4	-5.13	103.75	105.80
38	8	39	G	C2-N3-C4	5.13	114.47	111.90
1	2	639	U	C2-N1-C1'	5.13	123.85	117.70
36	1	1433	A	C5-C6-N1	5.13	120.26	117.70
36	1	1660	C	C4-C5-C6	5.13	119.96	117.40
36	1	2418	G	OP2-P-O3'	5.13	116.48	105.20
36	1	2714	G	C4-C5-C6	-5.13	115.72	118.80
36	1	2796	G	C4-C5-N7	5.13	112.85	110.80
36	1	2836	C	OP2-P-O3'	5.13	116.48	105.20
36	1	2940	A	N1-C2-N3	5.13	131.86	129.30
36	1	3085	G	N1-C6-O6	5.13	122.98	119.90
1	6	607	G	N3-C4-C5	-5.13	126.04	128.60
36	5	378	A	N7-C8-N9	-5.13	111.24	113.80
1	2	343	C	O4'-C1'-N1	5.13	112.30	108.20
1	2	1052	U	C2-N1-C1'	5.13	123.85	117.70
36	1	212	G	N1-C6-O6	5.13	122.98	119.90
36	1	2383	C	C6-N1-C2	5.13	122.35	120.30
38	4	46	G	C5-N7-C8	5.13	106.86	104.30
1	6	628	G	N9-C4-C5	-5.13	103.35	105.40
36	5	367	A	O5'-P-OP1	-5.13	101.09	105.70
36	5	649	A	C8-N9-C4	-5.13	103.75	105.80
36	5	715	A	C5-C6-N1	5.13	120.26	117.70
38	8	54	A	N1-C6-N6	5.13	121.68	118.60
36	1	1494	U	C2-N3-C4	-5.12	123.92	127.00
36	1	3138	U	OP2-P-O3'	5.12	116.48	105.20
1	6	402	C	N3-C4-N4	5.12	121.59	118.00
36	5	1074	U	C5-C4-O4	-5.12	122.83	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1191	U	N3-C2-O2	5.12	125.79	122.20
36	5	2712	U	N3-C2-O2	-5.12	118.61	122.20
1	2	284	G	C8-N9-C4	5.12	108.45	106.40
36	1	1336	U	N3-C2-O2	-5.12	118.61	122.20
36	5	942	U	C5-C4-O4	-5.12	122.83	125.90
36	5	1787	A	N1-C2-N3	-5.12	126.74	129.30
78	q2	77	CYS	CA-CB-SG	-5.12	104.78	114.00
36	1	634	C	C5-C6-N1	-5.12	118.44	121.00
36	1	2181	C	C6-N1-C2	5.12	122.35	120.30
36	1	2182	A	N9-C4-C5	5.12	107.85	105.80
36	1	2572	C	C2-N1-C1'	5.12	124.43	118.80
1	6	464	A	N1-C6-N6	-5.12	115.53	118.60
1	6	1162	C	C6-N1-C2	-5.12	118.25	120.30
36	5	216	G	C4-C5-N7	5.12	112.85	110.80
36	5	2660	G	C8-N9-C1'	-5.12	120.34	127.00
36	5	2937	G	C5-C6-N1	5.12	114.06	111.50
36	1	1329	U	C5'-C4'-O4'	-5.12	102.96	109.10
36	5	415	G	N3-C4-C5	-5.12	126.04	128.60
36	5	1114	U	OP1-P-OP2	5.12	127.28	119.60
36	5	1295	G	C5-C6-O6	5.12	131.67	128.60
36	5	3196	U	C5-C6-N1	-5.12	120.14	122.70
1	2	12	U	N3-C4-O4	-5.12	115.82	119.40
36	1	415	G	C8-N9-C4	-5.12	104.35	106.40
36	1	433	A	C5-C6-N1	5.12	120.26	117.70
36	1	3306	U	C5-C6-N1	-5.12	120.14	122.70
38	4	113	U	N3-C4-O4	-5.12	115.82	119.40
39	L2	156	LYS	CD-CE-NZ	-5.12	99.93	111.70
41	L4	95	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	6	457	G	N3-C4-C5	5.12	131.16	128.60
36	5	2296	A	C2-N3-C4	5.12	113.16	110.60
36	5	2698	G	C4-C5-N7	-5.12	108.75	110.80
37	7	35	C	C6-N1-C2	5.12	122.35	120.30
36	1	94	G	N1-C2-N3	-5.12	120.83	123.90
36	1	678	G	C4-N9-C1'	5.12	133.15	126.50
36	1	940	G	O5'-P-OP1	-5.12	101.09	105.70
1	6	1361	U	N1-C2-O2	5.12	126.38	122.80
36	5	1120	A	C5-C6-N1	5.12	120.26	117.70
36	5	1432	C	N1-C2-N3	5.12	122.78	119.20
36	5	2385	G	N9-C4-C5	-5.12	103.35	105.40
36	5	3060	C	C6-N1-C2	-5.12	118.25	120.30
1	2	1456	C	C5-C6-N1	-5.12	118.44	121.00
36	1	328	U	OP2-P-O3'	5.12	116.45	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	582	G	N1-C2-N2	5.12	120.80	116.20
36	1	1300	G	N3-C4-N9	5.12	129.07	126.00
36	1	2766	U	C2-N1-C1'	5.12	123.84	117.70
36	5	687	U	C6-N1-C2	5.12	124.07	121.00
38	8	25	G	N1-C2-N2	-5.12	111.60	116.20
36	1	304	G	N1-C2-N2	5.11	120.80	116.20
36	1	615	U	C5-C4-O4	5.11	128.97	125.90
36	1	1528	G	C5-C6-N1	-5.11	108.94	111.50
36	1	2857	C	C5-C4-N4	-5.11	116.62	120.20
1	6	1081	A	N1-C6-N6	5.11	121.67	118.60
36	5	300	G	N1-C6-O6	-5.11	116.83	119.90
36	5	1200	A	OP1-P-O3'	5.11	116.45	105.20
36	1	947	G	N3-C2-N2	5.11	123.48	119.90
1	6	1421	A	C8-N9-C4	5.11	107.84	105.80
36	5	201	A	O5'-P-OP2	-5.11	101.10	105.70
36	5	494	G	N1-C6-O6	-5.11	116.83	119.90
36	5	1833	G	C4-C5-N7	-5.11	108.75	110.80
36	5	2413	A	C2-N3-C4	-5.11	108.04	110.60
36	5	2963	C	C6-N1-C2	-5.11	118.25	120.30
36	1	1100	U	N1-C2-N3	5.11	117.97	114.90
36	1	1439	U	O5'-P-OP2	5.11	116.83	110.70
36	1	2247	G	C6-C5-N7	-5.11	127.33	130.40
36	1	2363	A	C6-C5-N7	5.11	135.88	132.30
1	6	119	A	N1-C2-N3	5.11	131.85	129.30
36	5	633	C	O5'-P-OP1	-5.11	101.10	105.70
38	8	116	G	N1-C6-O6	5.11	122.97	119.90
36	1	1349	G	O4'-C1'-N9	5.11	112.29	108.20
36	1	2189	U	N3-C4-O4	5.11	122.98	119.40
36	1	2852	C	O5'-P-OP1	5.11	116.83	110.70
36	1	3207	U	O4'-C1'-N1	5.11	112.29	108.20
36	5	906	A	C6-N1-C2	-5.11	115.53	118.60
36	5	2314	U	C6-N1-C2	-5.11	117.93	121.00
36	5	2977	G	C5-C6-N1	5.11	114.06	111.50
36	5	3278	C	OP2-P-O3'	5.11	116.44	105.20
1	2	1399	C	C2-N1-C1'	5.11	124.42	118.80
36	1	182	U	N3-C4-O4	-5.11	115.82	119.40
36	1	809	G	O5'-P-OP1	5.11	116.83	110.70
36	1	2644	C	C2-N1-C1'	5.11	124.42	118.80
36	1	2887	A	C5-C6-N6	-5.11	119.61	123.70
36	1	2929	C	C6-N1-C2	5.11	122.34	120.30
36	1	2934	A	C4-C5-C6	5.11	119.55	117.00
36	1	3057	U	C5-C6-N1	-5.11	120.15	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3187	A	C5-C6-N6	-5.11	119.61	123.70
1	6	964	U	N3-C2-O2	-5.11	118.62	122.20
36	5	1205	A	N1-C6-N6	-5.11	115.53	118.60
36	5	1526	U	N1-C2-O2	-5.11	119.22	122.80
36	5	2831	G	N3-C2-N2	5.11	123.48	119.90
36	5	2979	U	C2-N3-C4	5.11	130.06	127.00
36	5	3275	U	C6-N1-C1'	5.11	128.35	121.20
38	8	111	A	C5-N7-C8	-5.11	101.35	103.90
1	2	628	G	C5-C6-O6	5.11	131.66	128.60
36	1	303	G	O4'-C1'-N9	5.11	112.28	108.20
36	1	689	U	N1-C2-O2	5.11	126.37	122.80
36	1	2810	C	C4-C5-C6	5.11	119.95	117.40
36	1	3219	G	N3-C4-C5	-5.11	126.05	128.60
36	5	2399	A	C2-N3-C4	-5.11	108.05	110.60
1	2	1591	C	N3-C2-O2	-5.10	118.33	121.90
36	1	64	G	C6-C5-N7	5.10	133.46	130.40
36	1	211	A	N1-C2-N3	5.10	131.85	129.30
36	1	953	G	C4-N9-C1'	-5.10	119.86	126.50
36	5	928	C	N3-C2-O2	-5.10	118.33	121.90
36	5	1765	U	O5'-P-OP1	5.10	116.83	110.70
36	5	2875	U	C2-N1-C1'	-5.10	111.58	117.70
36	5	2941	A	N9-C1'-C2'	5.10	120.64	114.00
36	5	2968	G	C5-N7-C8	5.10	106.85	104.30
36	5	3211	C	O5'-P-OP2	5.10	116.83	110.70
37	7	1	G	C6-C5-N7	-5.10	127.34	130.40
36	1	687	U	OP2-P-O3'	5.10	116.43	105.20
36	1	1328	C	C5-C6-N1	-5.10	118.45	121.00
36	1	2418	G	N7-C8-N9	5.10	115.65	113.10
36	1	2814	G	N3-C4-C5	-5.10	126.05	128.60
52	M6	33	ILE	CG1-CB-CG2	-5.10	100.17	111.40
36	5	3335	A	N1-C6-N6	5.10	121.66	118.60
36	5	3388	C	C5-C4-N4	5.10	123.77	120.20
36	1	664	U	OP1-P-OP2	-5.10	111.95	119.60
36	1	1122	U	N3-C4-C5	5.10	117.66	114.60
36	1	3317	U	N3-C2-O2	-5.10	118.63	122.20
38	4	58	G	OP1-P-OP2	-5.10	111.95	119.60
36	5	2643	A	N1-C6-N6	5.10	121.66	118.60
36	5	2771	U	N1-C2-O2	-5.10	119.23	122.80
38	8	36	G	O5'-P-OP1	-5.10	101.11	105.70
36	1	188	U	N1-C2-N3	5.10	117.96	114.90
36	1	2993	G	C5-C6-N1	5.10	114.05	111.50
36	5	1858	A	C8-N9-C4	-5.10	103.76	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2406	C	C5-C6-N1	-5.10	118.45	121.00
36	5	2695	A	C6-N1-C2	-5.10	115.54	118.60
36	5	2891	U	C2-N3-C4	-5.10	123.94	127.00
36	5	2919	A	C5-C6-N6	5.10	127.78	123.70
36	5	3091	A	OP1-P-OP2	-5.10	111.95	119.60
1	2	3	U	C6-N1-C2	5.10	124.06	121.00
36	1	2619	G	N7-C8-N9	-5.10	110.55	113.10
44	L7	178	ILE	CB-CA-C	-5.10	101.41	111.60
36	5	7	C	C6-N1-C2	5.10	122.34	120.30
36	5	1396	C	C4-C5-C6	-5.10	114.85	117.40
36	5	1899	G	C6-N1-C2	5.10	128.16	125.10
36	1	728	G	N1-C6-O6	-5.10	116.84	119.90
36	1	1175	C	O5'-P-OP1	-5.10	101.11	105.70
36	1	2281	A	O4'-C1'-N9	5.10	112.28	108.20
38	4	64	U	OP2-P-O3'	5.10	116.41	105.20
36	5	38	U	C5-C4-O4	-5.10	122.84	125.90
36	5	234	G	C5-C6-O6	-5.10	125.54	128.60
36	5	3028	G	N3-C2-N2	5.10	123.47	119.90
36	5	3371	G	C5-C6-O6	5.10	131.66	128.60
1	2	440	U	N3-C4-O4	-5.09	115.83	119.40
1	2	755	A	P-O3'-C3'	5.09	125.81	119.70
36	1	214	G	N7-C8-N9	-5.09	110.55	113.10
36	1	1323	G	N1-C2-N2	-5.09	111.62	116.20
36	1	2619	G	C5-C6-O6	5.09	131.66	128.60
1	6	1747	G	O5'-P-OP1	5.09	116.81	110.70
36	5	52	A	C5-C6-N1	-5.09	115.15	117.70
36	5	280	U	N1-C2-N3	5.09	117.96	114.90
36	5	958	C	N3-C2-O2	-5.09	118.33	121.90
36	5	1203	A	OP1-P-OP2	5.09	127.24	119.60
36	5	3154	C	C2-N3-C4	5.09	122.45	119.90
36	1	1301	A	C8-N9-C4	-5.09	103.76	105.80
36	1	2198	A	C8-N9-C4	5.09	107.84	105.80
1	6	1027	A	N3-C4-C5	5.09	130.37	126.80
36	5	276	U	O5'-P-OP2	5.09	116.81	110.70
36	5	2626	A	N1-C2-N3	5.09	131.85	129.30
1	2	140	A	C6-C5-N7	-5.09	128.74	132.30
1	2	1746	A	N1-C2-N3	-5.09	126.75	129.30
36	1	82	C	C6-N1-C2	5.09	122.34	120.30
36	1	1206	G	O5'-P-OP1	5.09	116.81	110.70
36	1	1352	A	P-O3'-C3'	5.09	125.81	119.70
36	1	1530	U	C6-N1-C2	5.09	124.06	121.00
1	6	31	C	C2-N1-C1'	-5.09	113.20	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	76	G	C8-N9-C4	5.09	108.44	106.40
36	5	412	G	N3-C4-N9	5.09	129.06	126.00
36	5	794	U	N3-C2-O2	-5.09	118.64	122.20
36	5	1051	U	C4-C5-C6	-5.09	116.64	119.70
36	5	1589	A	C5-C6-N6	-5.09	119.63	123.70
36	5	1729	A	N1-C6-N6	5.09	121.66	118.60
36	5	1792	C	N1-C2-O2	-5.09	115.85	118.90
36	5	2119	A	C5-C6-N6	-5.09	119.63	123.70
36	5	2964	G	C4-C5-N7	-5.09	108.76	110.80
36	5	3138	U	C5-C6-N1	5.09	125.25	122.70
36	5	3339	A	N1-C6-N6	5.09	121.66	118.60
36	1	834	U	C2-N3-C4	-5.09	123.95	127.00
1	6	1503	A	C2-N3-C4	-5.09	108.06	110.60
36	5	63	A	N1-C2-N3	-5.09	126.75	129.30
36	5	285	A	N1-C6-N6	-5.09	115.55	118.60
36	5	939	U	O5'-P-OP1	5.09	116.81	110.70
36	5	1064	A	P-O3'-C3'	5.09	125.81	119.70
36	5	2821	C	OP1-P-O3'	5.09	116.40	105.20
36	5	3298	C	O5'-P-OP2	-5.09	101.12	105.70
1	2	1481	C	C6-N1-C2	-5.09	118.27	120.30
36	1	276	U	OP1-P-OP2	5.09	127.23	119.60
36	1	1389	G	OP1-P-OP2	5.09	127.23	119.60
36	1	1829	G	N3-C4-C5	-5.09	126.06	128.60
36	5	2860	U	C5-C6-N1	-5.09	120.16	122.70
36	5	2932	U	OP1-P-OP2	-5.09	111.97	119.60
37	7	83	U	C5-C4-O4	5.09	128.95	125.90
1	2	1118	G	N1-C6-O6	5.09	122.95	119.90
36	1	945	C	N3-C4-N4	-5.09	114.44	118.00
36	1	972	A	N7-C8-N9	-5.09	111.26	113.80
36	1	2522	G	C6-C5-N7	-5.09	127.35	130.40
36	1	2815	G	N7-C8-N9	-5.09	110.56	113.10
36	1	2977	G	C6-C5-N7	5.09	133.45	130.40
1	6	1729	C	C2-N3-C4	-5.09	117.36	119.90
36	5	567	G	N1-C6-O6	5.09	122.95	119.90
36	5	1123	U	C2-N3-C4	-5.09	123.95	127.00
36	5	1140	G	N3-C2-N2	5.09	123.46	119.90
36	5	1202	A	C5-C6-N6	5.09	127.77	123.70
36	5	2879	C	C5-C6-N1	-5.09	118.46	121.00
36	5	2954	U	C6-N1-C1'	-5.09	114.08	121.20
36	5	3058	U	P-O3'-C3'	5.09	125.80	119.70
36	5	3177	G	N3-C4-C5	5.09	131.14	128.60
36	5	3271	G	N3-C4-N9	5.09	129.05	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	12	U	C5-C4-O4	-5.09	122.85	125.90
1	2	353	A	C2-N3-C4	-5.08	108.06	110.60
37	3	40	C	C6-N1-C2	-5.08	118.27	120.30
1	6	337	G	N3-C2-N2	5.08	123.46	119.90
36	5	3371	G	C5-C6-N1	-5.08	108.96	111.50
36	1	2529	A	OP2-P-O3'	5.08	116.39	105.20
36	1	2728	G	C5-C6-O6	-5.08	125.55	128.60
36	1	2864	A	N1-C6-N6	-5.08	115.55	118.60
36	1	3239	G	C8-N9-C1'	5.08	133.61	127.00
36	1	3317	U	C5-C4-O4	5.08	128.95	125.90
36	5	657	A	N1-C2-N3	-5.08	126.76	129.30
36	5	1402	C	N3-C2-O2	-5.08	118.34	121.90
36	5	3003	G	N9-C4-C5	5.08	107.43	105.40
1	2	1497	U	C2-N1-C1'	5.08	123.80	117.70
1	2	1751	C	N3-C4-N4	-5.08	114.44	118.00
36	1	1829	G	C8-N9-C4	-5.08	104.37	106.40
36	1	3099	C	O4'-C1'-N1	5.08	112.27	108.20
36	1	3307	A	N1-C6-N6	-5.08	115.55	118.60
1	6	1279	C	C6-N1-C2	-5.08	118.27	120.30
36	5	895	A	C2-N3-C4	-5.08	108.06	110.60
36	5	900	G	C6-C5-N7	5.08	133.45	130.40
36	5	2719	U	C2-N1-C1'	-5.08	111.60	117.70
36	5	2974	U	N3-C4-C5	-5.08	111.55	114.60
36	5	3006	A	N1-C6-N6	5.08	121.65	118.60
43	16	46	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	2	501	U	OP1-P-O3'	5.08	116.38	105.20
1	2	1105	C	OP2-P-O3'	5.08	116.38	105.20
36	1	435	C	C2-N1-C1'	-5.08	113.21	118.80
36	1	2706	G	C8-N9-C1'	-5.08	120.40	127.00
36	5	378	A	C8-N9-C4	5.08	107.83	105.80
36	5	803	C	O5'-P-OP1	5.08	116.80	110.70
37	7	58	C	O5'-P-OP1	5.08	116.80	110.70
1	2	1100	G	C4-N9-C1'	5.08	133.10	126.50
36	1	883	A	C6-N1-C2	-5.08	115.55	118.60
36	1	2688	U	N3-C4-C5	5.08	117.65	114.60
36	1	3095	U	N3-C2-O2	-5.08	118.64	122.20
37	3	42	A	C5-C6-N1	-5.08	115.16	117.70
1	6	382	C	C2-N3-C4	-5.08	117.36	119.90
1	6	617	U	N3-C4-C5	-5.08	111.55	114.60
1	6	1291	G	C2-N3-C4	5.08	114.44	111.90
36	5	354	U	C4-C5-C6	5.08	122.75	119.70
36	5	2643	A	N9-C4-C5	-5.08	103.77	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	581	U	N1-C2-O2	-5.08	119.25	122.80
1	6	794	U	C6-N1-C1'	-5.08	114.09	121.20
36	5	194	U	N1-C2-O2	-5.08	119.25	122.80
36	5	2699	G	OP1-P-OP2	5.08	127.22	119.60
1	2	1291	G	C8-N9-C4	-5.08	104.37	106.40
36	1	824	C	C5-C6-N1	5.08	123.54	121.00
36	1	912	G	N3-C2-N2	-5.08	116.35	119.90
36	1	1911	A	C5-C6-N6	-5.08	119.64	123.70
36	1	2122	G	O5'-P-OP2	-5.08	101.13	105.70
47	M0	24	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	6	1001	A	C4-C5-N7	5.08	113.24	110.70
1	6	1526	A	N9-C4-C5	5.08	107.83	105.80
36	5	417	A	N7-C8-N9	-5.08	111.26	113.80
36	5	707	U	C4-C5-C6	5.08	122.75	119.70
36	5	2297	U	OP1-P-OP2	5.08	127.21	119.60
36	5	2414	G	N3-C2-N2	-5.08	116.35	119.90
1	2	150	U	C2-N1-C1'	5.07	123.79	117.70
36	1	626	U	N3-C4-O4	-5.07	115.85	119.40
36	1	1741	A	C6-C5-N7	-5.07	128.75	132.30
36	1	1908	A	OP2-P-O3'	5.07	116.36	105.20
36	1	2369	G	N3-C4-C5	-5.07	126.06	128.60
36	1	2823	G	N9-C4-C5	5.07	107.43	105.40
38	4	103	G	N1-C6-O6	-5.07	116.86	119.90
36	5	579	G	C4-C5-C6	-5.07	115.76	118.80
36	5	1312	C	C2-N3-C4	5.07	122.44	119.90
36	5	2204	C	C6-N1-C1'	5.07	126.89	120.80
36	5	2280	A	C2-N3-C4	-5.07	108.06	110.60
36	5	2300	G	O5'-P-OP1	-5.07	101.13	105.70
36	5	2816	G	C4-C5-C6	-5.07	115.76	118.80
36	5	3262	U	N1-C2-N3	5.07	117.94	114.90
36	1	816	A	C8-N9-C4	-5.07	103.77	105.80
36	1	1192	C	C5-C4-N4	5.07	123.75	120.20
36	5	2933	A	OP2-P-O3'	5.07	116.36	105.20
1	2	103	A	P-O3'-C3'	5.07	125.78	119.70
1	2	580	A	N9-C4-C5	5.07	107.83	105.80
36	1	564	G	N1-C6-O6	-5.07	116.86	119.90
36	1	1450	G	C6-C5-N7	5.07	133.44	130.40
36	1	1894	U	C5-C4-O4	-5.07	122.86	125.90
36	1	2711	C	N1-C2-O2	-5.07	115.86	118.90
36	5	876	A	OP2-P-O3'	5.07	116.36	105.20
36	5	1139	G	N1-C2-N3	5.07	126.94	123.90
38	4	61	A	O5'-P-OP1	-5.07	101.14	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1020	A	C8-N9-C4	-5.07	103.77	105.80
1	6	1075	C	N1-C2-O2	-5.07	115.86	118.90
36	5	928	C	C2-N3-C4	-5.07	117.36	119.90
36	5	2953	U	N1-C2-O2	-5.07	119.25	122.80
38	8	111	A	C2-N3-C4	-5.07	108.07	110.60
1	2	1446	A	N9-C4-C5	5.07	107.83	105.80
36	1	434	U	OP2-P-O3'	5.07	116.35	105.20
36	1	1086	C	C6-N1-C2	-5.07	118.27	120.30
36	1	2647	A	N3-C4-C5	-5.07	123.25	126.80
1	6	756	A	N7-C8-N9	5.07	116.33	113.80
1	6	1658	G	C8-N9-C4	5.07	108.43	106.40
36	5	1373	A	N3-C4-N9	5.07	131.46	127.40
36	5	1876	U	C5'-C4'-C3'	-5.07	107.89	116.00
36	5	2997	G	C2-N3-C4	-5.07	109.37	111.90
36	1	1176	C	C6-N1-C2	5.07	122.33	120.30
36	1	1494	U	C5-C6-N1	-5.07	120.17	122.70
36	1	1552	G	C5-C6-O6	-5.07	125.56	128.60
36	1	1869	C	N1-C2-O2	5.07	121.94	118.90
36	1	1886	A	O5'-P-OP2	-5.07	101.14	105.70
37	3	88	G	C8-N9-C1'	-5.07	120.42	127.00
36	5	320	G	C4-C5-N7	-5.07	108.77	110.80
36	5	813	G	C5-C6-N1	5.07	114.03	111.50
36	5	943	U	N1-C2-N3	5.07	117.94	114.90
36	5	1126	G	N9-C4-C5	5.07	107.43	105.40
36	5	1131	G	C5-C6-O6	5.07	131.64	128.60
36	5	1298	C	C6-N1-C2	-5.07	118.27	120.30
36	5	1494	U	C5-C6-N1	-5.07	120.17	122.70
36	5	2735	U	C5-C4-O4	5.07	128.94	125.90
36	5	3223	A	N1-C6-N6	-5.07	115.56	118.60
38	8	14	C	N3-C4-C5	-5.07	119.87	121.90
38	8	48	A	C5-C6-N1	5.07	120.23	117.70
51	M5	105	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	6	17	C	C6-N1-C2	-5.06	118.27	120.30
36	5	505	G	N9-C4-C5	5.06	107.43	105.40
36	5	841	A	O5'-P-OP2	-5.06	101.14	105.70
36	5	1192	C	C5-C6-N1	-5.06	118.47	121.00
36	5	2345	A	O5'-P-OP2	-5.06	101.14	105.70
36	5	2837	A	O4'-C1'-N9	5.06	112.25	108.20
36	1	112	U	N1-C1'-C2'	-5.06	106.43	112.00
36	1	1393	A	OP2-P-O3'	5.06	116.34	105.20
36	1	1416	C	N1-C2-O2	5.06	121.94	118.90
36	5	2187	G	N1-C6-O6	5.06	122.94	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2661	G	OP1-P-O3'	5.06	116.34	105.20
42	15	22	ARG	NE-CZ-NH1	-5.06	117.77	120.30
36	1	1301	A	C5-N7-C8	-5.06	101.37	103.90
36	1	1448	U	OP1-P-O3'	-5.06	94.07	105.20
1	6	1085	G	N1-C6-O6	-5.06	116.86	119.90
36	5	564	G	C4-C5-N7	-5.06	108.78	110.80
36	5	661	G	C5-C6-N1	5.06	114.03	111.50
1	2	581	U	C6-N1-C1'	-5.06	114.12	121.20
36	1	1117	G	C4-N9-C1'	-5.06	119.92	126.50
36	1	1150	A	O5'-P-OP2	-5.06	101.15	105.70
36	1	1782	U	C5-C4-O4	-5.06	122.86	125.90
38	4	28	C	C2-N1-C1'	5.06	124.37	118.80
41	L4	206	LEU	CA-CB-CG	5.06	126.94	115.30
36	5	1131	G	C4-C5-N7	-5.06	108.78	110.80
36	5	2550	U	C4-C5-C6	5.06	122.73	119.70
36	1	1125	U	N3-C4-C5	5.06	117.63	114.60
36	1	2123	G	N7-C8-N9	-5.06	110.57	113.10
38	4	67	U	C6-N1-C2	-5.06	117.97	121.00
36	5	24	G	N3-C4-N9	-5.06	122.97	126.00
36	5	514	G	N1-C6-O6	5.06	122.93	119.90
36	5	1198	C	N3-C2-O2	-5.06	118.36	121.90
36	5	1508	C	C6-N1-C2	5.06	122.32	120.30
36	5	2416	U	C6-N1-C2	-5.06	117.97	121.00
36	5	2625	C	C2-N3-C4	-5.06	117.37	119.90
36	5	3330	A	C5-N7-C8	5.06	106.43	103.90
47	m0	98	ARG	NE-CZ-NH2	5.06	122.83	120.30
36	1	2302	G	OP2-P-O3'	5.05	116.32	105.20
36	1	2604	U	C5-C4-O4	5.05	128.93	125.90
36	1	2700	G	C6-C5-N7	-5.05	127.37	130.40
1	6	1606	C	N1-C2-O2	5.05	121.93	118.90
36	5	421	G	C6-N1-C2	-5.05	122.07	125.10
36	5	746	A	C4-C5-N7	-5.05	108.17	110.70
36	5	972	A	C5-N7-C8	5.05	106.43	103.90
36	5	1348	U	N3-C2-O2	-5.05	118.66	122.20
36	5	1553	U	C6-N1-C2	5.05	124.03	121.00
36	5	1770	G	C8-N9-C1'	-5.05	120.43	127.00
36	5	2892	A	N1-C6-N6	-5.05	115.57	118.60
38	8	107	G	N1-C6-O6	5.05	122.93	119.90
36	1	85	A	N9-C4-C5	-5.05	103.78	105.80
36	1	281	G	O5'-P-OP1	-5.05	101.15	105.70
36	1	2279	A	N7-C8-N9	-5.05	111.27	113.80
1	2	990	C	C6-N1-C2	-5.05	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	48	A	O4'-C1'-N9	5.05	112.24	108.20
36	1	184	U	N3-C2-O2	-5.05	118.66	122.20
36	1	225	C	N3-C4-C5	-5.05	119.88	121.90
36	1	1301	A	N7-C8-N9	5.05	116.33	113.80
36	1	2355	G	N9-C4-C5	-5.05	103.38	105.40
36	1	3362	A	C5-C6-N6	-5.05	119.66	123.70
38	4	47	C	N3-C4-N4	-5.05	114.46	118.00
1	6	619	A	N1-C6-N6	-5.05	115.57	118.60
36	5	961	C	C4-C5-C6	5.05	119.93	117.40
36	5	2775	U	N3-C2-O2	-5.05	118.66	122.20
36	5	3209	A	C5-N7-C8	-5.05	101.37	103.90
1	2	240	U	P-O3'-C3'	5.05	125.76	119.70
1	2	1346	A	O4'-C1'-N9	5.05	112.24	108.20
36	1	1467	A	C6-N1-C2	-5.05	115.57	118.60
36	1	1918	C	N1-C2-N3	5.05	122.73	119.20
36	1	2339	C	N1-C2-O2	-5.05	115.87	118.90
36	1	2347	U	N3-C4-O4	-5.05	115.86	119.40
36	5	519	A	N1-C6-N6	5.05	121.63	118.60
36	5	841	A	C6-N1-C2	-5.05	115.57	118.60
36	5	1339	C	N3-C4-N4	5.05	121.53	118.00
36	5	1348	U	C4-C5-C6	5.05	122.73	119.70
36	5	1405	U	C5-C6-N1	-5.05	120.17	122.70
36	5	2668	U	C5-C6-N1	-5.05	120.18	122.70
36	5	2681	U	C5-C6-N1	-5.05	120.17	122.70
36	5	2695	A	N1-C2-N3	5.05	131.82	129.30
36	5	2873	U	C5-C4-O4	-5.05	122.87	125.90
36	1	1801	U	C5-C6-N1	-5.05	120.18	122.70
61	N5	34	LEU	CA-CB-CG	5.05	126.91	115.30
36	5	1475	A	N1-C2-N3	5.05	131.82	129.30
36	5	1847	A	N1-C2-N3	-5.05	126.78	129.30
36	5	2877	G	C5-C6-O6	5.05	131.63	128.60
1	2	1134	C	C6-N1-C2	-5.05	118.28	120.30
36	1	189	G	C5-C6-N1	5.05	114.02	111.50
36	1	1438	U	O5'-P-OP2	-5.05	101.16	105.70
36	1	1823	A	C4-C5-C6	5.05	119.52	117.00
50	M4	135	LEU	CA-CB-CG	5.05	126.91	115.30
1	6	858	G	C6-C5-N7	-5.05	127.37	130.40
36	5	370	U	C2-N1-C1'	5.05	123.76	117.70
36	5	909	G	C8-N9-C4	5.05	108.42	106.40
36	5	937	G	O4'-C1'-N9	5.05	112.24	108.20
36	5	1512	U	OP1-P-O3'	-5.05	94.10	105.20
36	5	2398	A	C6-N1-C2	-5.05	115.57	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2731	U	N1-C2-O2	-5.05	119.27	122.80
1	6	1002	G	O5'-P-OP2	5.04	116.75	110.70
36	5	872	U	N3-C2-O2	-5.04	118.67	122.20
36	5	908	G	C5-N7-C8	-5.04	101.78	104.30
36	5	2361	A	C6-N1-C2	-5.04	115.57	118.60
36	5	2816	G	O4'-C1'-N9	5.04	112.24	108.20
1	2	421	A	N9-C4-C5	-5.04	103.78	105.80
1	2	1419	G	N3-C4-C5	5.04	131.12	128.60
34	SR	161	LYS	N-CA-C	5.04	124.62	111.00
36	1	349	A	C8-N9-C4	-5.04	103.78	105.80
36	1	2397	A	C6-C5-N7	-5.04	128.77	132.30
36	1	2868	U	C2-N3-C4	-5.04	123.97	127.00
36	1	3222	U	C2-N1-C1'	5.04	123.75	117.70
38	4	12	A	C6-N1-C2	5.04	121.63	118.60
36	5	1399	A	C6-N1-C2	5.04	121.63	118.60
36	5	2386	A	C6-C5-N7	-5.04	128.77	132.30
1	2	194	U	C5-C6-N1	5.04	125.22	122.70
1	2	1620	C	C6-N1-C2	-5.04	118.28	120.30
36	1	894	G	OP1-P-O3'	5.04	116.29	105.20
36	1	2878	G	C8-N9-C4	5.04	108.42	106.40
36	5	289	A	C6-N1-C2	-5.04	115.58	118.60
36	5	1429	G	O5'-P-OP2	-5.04	101.16	105.70
36	5	2805	G	O5'-P-OP2	-5.04	101.16	105.70
1	2	704	C	C6-N1-C1'	-5.04	114.75	120.80
36	1	364	G	C5-C6-O6	-5.04	125.58	128.60
36	1	1321	G	N9-C4-C5	5.04	107.42	105.40
38	4	59	A	C5-C6-N1	5.04	120.22	117.70
1	6	100	A	OP1-P-OP2	-5.04	112.04	119.60
36	5	184	U	C5-C6-N1	-5.04	120.18	122.70
36	5	371	G	N3-C4-N9	-5.04	122.98	126.00
36	5	984	G	N3-C4-N9	5.04	129.02	126.00
36	5	1655	G	C5-C6-O6	-5.04	125.58	128.60
36	5	2777	G	C5-C6-O6	5.04	131.62	128.60
36	5	2808	A	C8-N9-C4	5.04	107.82	105.80
1	2	839	U	C6-N1-C2	-5.04	117.98	121.00
36	1	1438	U	OP1-P-O3'	5.04	116.28	105.20
36	1	2821	C	N1-C2-O2	5.04	121.92	118.90
36	1	3182	G	N3-C4-C5	5.04	131.12	128.60
1	6	365	G	N3-C4-N9	5.04	129.02	126.00
1	6	1032	G	N7-C8-N9	-5.04	110.58	113.10
36	5	415	G	N1-C2-N2	-5.04	111.67	116.20
36	5	1300	G	C6-N1-C2	-5.04	122.08	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2649	A	C4-C5-N7	5.04	113.22	110.70
37	7	117	A	OP2-P-O3'	5.04	116.28	105.20
36	1	1104	G	N1-C6-O6	-5.04	116.88	119.90
36	1	2324	A	N1-C6-N6	-5.04	115.58	118.60
36	5	1169	A	C4-C5-C6	5.04	119.52	117.00
36	5	1521	G	C5-C6-O6	5.04	131.62	128.60
36	5	2404	A	C6-C5-N7	-5.04	128.77	132.30
1	2	436	A	O5'-P-OP2	-5.04	101.17	105.70
1	2	1101	G	C4-C5-N7	5.04	112.81	110.80
36	1	657	A	C5-N7-C8	5.04	106.42	103.90
36	1	1512	U	N3-C4-O4	-5.04	115.88	119.40
36	1	1606	U	C2-N3-C4	-5.04	123.98	127.00
36	1	2820	A	C4-C5-N7	-5.04	108.18	110.70
36	1	2824	G	N7-C8-N9	-5.04	110.58	113.10
36	1	2977	G	N3-C4-C5	-5.04	126.08	128.60
41	L4	141	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	6	199	G	O4'-C1'-N9	5.04	112.23	108.20
1	6	1697	G	C2-N3-C4	5.04	114.42	111.90
3	s1	47	LEU	CA-CB-CG	5.04	126.88	115.30
36	5	634	C	OP2-P-O3'	5.04	116.28	105.20
36	5	1475	A	OP2-P-O3'	5.04	116.28	105.20
36	5	2410	U	C6-N1-C2	5.04	124.02	121.00
36	5	2754	G	N3-C4-C5	-5.04	126.08	128.60
36	1	368	G	N1-C2-N2	-5.03	111.67	116.20
36	1	394	G	O5'-P-OP2	-5.03	101.17	105.70
36	1	429	U	N3-C2-O2	-5.03	118.68	122.20
36	1	726	G	O5'-P-OP1	-5.03	101.17	105.70
36	1	1314	C	C5-C6-N1	5.03	123.52	121.00
36	1	2183	A	N1-C2-N3	5.03	131.82	129.30
1	6	1207	C	N1-C2-O2	-5.03	115.88	118.90
36	5	971	G	C8-N9-C4	5.03	108.41	106.40
36	5	1186	G	N1-C6-O6	-5.03	116.88	119.90
36	5	1836	C	C6-N1-C2	5.03	122.31	120.30
36	5	2427	U	O5'-P-OP1	-5.03	101.17	105.70
36	5	3088	G	O5'-P-OP2	5.03	116.74	110.70
1	2	397	A	O4'-C1'-N9	5.03	112.23	108.20
36	1	53	G	N7-C8-N9	-5.03	110.58	113.10
36	1	220	G	C5-C6-O6	-5.03	125.58	128.60
36	1	354	U	O5'-P-OP1	-5.03	101.17	105.70
36	1	634	C	N3-C4-N4	-5.03	114.48	118.00
36	1	1457	U	N3-C2-O2	-5.03	118.68	122.20
36	1	1517	G	OP2-P-O3'	5.03	116.27	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2424	A	C2-N3-C4	5.03	113.12	110.60
36	1	2964	G	OP1-P-O3'	5.03	116.27	105.20
36	1	3007	U	N3-C2-O2	-5.03	118.68	122.20
36	5	2792	A	C8-N9-C4	-5.03	103.79	105.80
36	5	2961	G	C5-C6-O6	5.03	131.62	128.60
36	5	3018	C	O5'-P-OP1	5.03	116.74	110.70
36	1	679	U	O5'-P-OP2	-5.03	101.17	105.70
36	1	1123	U	C4-C5-C6	5.03	122.72	119.70
36	1	1842	A	N1-C6-N6	-5.03	115.58	118.60
36	1	2194	G	C4-N9-C1'	5.03	133.04	126.50
36	1	2401	A	C6-N1-C2	5.03	121.62	118.60
1	6	31	C	N3-C4-C5	-5.03	119.89	121.90
1	6	154	G	C5-C6-N1	5.03	114.02	111.50
1	6	813	U	N3-C2-O2	-5.03	118.68	122.20
36	5	427	C	C2-N3-C4	-5.03	117.38	119.90
36	5	1507	G	OP1-P-OP2	5.03	127.15	119.60
36	5	1906	G	N1-C2-N2	-5.03	111.67	116.20
36	5	2949	U	N1-C2-O2	5.03	126.32	122.80
62	n6	28	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	2	1755	A	N9-C4-C5	-5.03	103.79	105.80
36	1	80	G	C4-C5-N7	-5.03	108.79	110.80
36	1	2180	G	N1-C2-N2	-5.03	111.67	116.20
1	6	758	U	N1-C2-N3	5.03	117.92	114.90
36	5	403	C	OP2-P-O3'	5.03	116.26	105.20
36	5	2212	C	C5-C6-N1	5.03	123.52	121.00
36	1	658	G	N9-C4-C5	-5.03	103.39	105.40
36	1	875	G	N3-C4-N9	5.03	129.02	126.00
36	1	2958	A	C6-N1-C2	-5.03	115.58	118.60
36	1	3147	G	N1-C2-N2	-5.03	111.68	116.20
37	3	103	A	C5-C6-N6	-5.03	119.68	123.70
1	6	345	U	C2-N1-C1'	-5.03	111.67	117.70
1	6	1048	G	C4-C5-N7	5.03	112.81	110.80
1	6	1361	U	C6-N1-C1'	-5.03	114.16	121.20
1	6	1614	A	C6-C5-N7	-5.03	128.78	132.30
36	5	530	G	N9-C4-C5	5.03	107.41	105.40
38	8	42	G	O5'-P-OP2	-5.03	101.18	105.70
64	n8	24	LYS	CD-CE-NZ	-5.03	100.14	111.70
1	2	337	G	N9-C4-C5	-5.03	103.39	105.40
36	1	1854	C	N1-C2-O2	-5.03	115.89	118.90
52	M6	27	LEU	CB-CG-CD1	-5.03	102.46	111.00
1	6	100	A	C8-N9-C4	-5.03	103.79	105.80
36	5	883	A	N7-C8-N9	-5.03	111.29	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3034	C	O5'-P-OP2	-5.03	101.18	105.70
36	1	417	A	C5-C6-N1	-5.02	115.19	117.70
36	1	657	A	C4-C5-N7	-5.02	108.19	110.70
36	1	696	C	O5'-P-OP1	-5.02	101.18	105.70
36	1	1492	G	C4-N9-C1'	5.02	133.03	126.50
36	1	2634	U	C4-C5-C6	5.02	122.71	119.70
36	1	2959	C	N1-C2-N3	5.02	122.72	119.20
36	5	619	A	OP1-P-O3'	5.02	116.25	105.20
36	5	1508	C	N3-C4-C5	5.02	123.91	121.90
36	5	3218	A	N3-C4-C5	5.02	130.32	126.80
36	5	3325	G	N1-C6-O6	-5.02	116.89	119.90
1	2	1100	G	N1-C6-O6	5.02	122.91	119.90
36	1	104	G	N7-C8-N9	5.02	115.61	113.10
36	1	424	G	N7-C8-N9	-5.02	110.59	113.10
1	6	886	U	C5-C6-N1	-5.02	120.19	122.70
36	5	1082	U	N1-C2-N3	5.02	117.91	114.90
36	5	2278	C	OP2-P-O3'	5.02	116.25	105.20
36	5	2936	A	N1-C6-N6	5.02	121.61	118.60
36	1	2345	A	C5-C6-N6	-5.02	119.68	123.70
36	1	2799	A	N7-C8-N9	-5.02	111.29	113.80
36	1	3123	A	N3-C4-N9	-5.02	123.38	127.40
36	5	58	G	C5-C6-O6	-5.02	125.59	128.60
36	5	411	U	C5-C6-N1	-5.02	120.19	122.70
36	5	417	A	C4-C5-N7	-5.02	108.19	110.70
36	5	2209	U	C2-N1-C1'	-5.02	111.67	117.70
1	2	1457	C	OP1-P-OP2	-5.02	112.07	119.60
36	1	652	G	C6-C5-N7	-5.02	127.39	130.40
36	1	1328	C	C4-C5-C6	5.02	119.91	117.40
36	1	1834	U	OP1-P-O3'	5.02	116.24	105.20
36	1	2182	A	C5-C6-N6	5.02	127.72	123.70
36	1	2905	U	N1-C2-O2	-5.02	119.29	122.80
1	6	1539	G	N3-C4-N9	-5.02	122.99	126.00
1	6	1744	A	N9-C4-C5	-5.02	103.79	105.80
36	5	567	G	C5-C6-O6	-5.02	125.59	128.60
36	5	1198	C	C2-N3-C4	-5.02	117.39	119.90
36	5	1532	C	N1-C2-O2	5.02	121.91	118.90
36	5	2531	C	C5-C6-N1	5.02	123.51	121.00
36	5	2662	G	N1-C6-O6	-5.02	116.89	119.90
1	2	1207	C	C5-C6-N1	-5.02	118.49	121.00
36	1	691	A	C6-N1-C2	5.02	121.61	118.60
36	1	913	A	C5-N7-C8	5.02	106.41	103.90
36	1	967	A	C2-N3-C4	-5.02	108.09	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3302	U	C5-C4-O4	5.02	128.91	125.90
37	3	31	U	N3-C4-O4	5.02	122.91	119.40
1	6	426	G	C8-N9-C1'	-5.02	120.48	127.00
1	6	630	A	C2-N3-C4	-5.02	108.09	110.60
1	6	647	G	N3-C4-C5	5.02	131.11	128.60
1	6	1135	U	N1-C2-N3	5.02	117.91	114.90
36	5	97	U	N3-C4-C5	-5.02	111.59	114.60
36	5	1149	G	O4'-C1'-N9	5.02	112.21	108.20
1	6	748	U	N3-C2-O2	-5.02	118.69	122.20
1	6	1122	G	C8-N9-C4	5.02	108.41	106.40
36	5	836	A	C5-C6-N6	-5.02	119.69	123.70
36	5	1858	A	O4'-C1'-N9	5.02	112.21	108.20
36	5	2597	U	OP1-P-OP2	-5.02	112.08	119.60
36	5	3070	A	OP1-P-OP2	-5.02	112.08	119.60
36	1	2339	C	OP1-P-O3'	5.01	116.23	105.20
38	4	47	C	C4-C5-C6	5.01	119.91	117.40
1	6	951	A	C8-N9-C4	5.01	107.81	105.80
1	6	1612	U	C2-N1-C1'	-5.01	111.68	117.70
36	5	1004	U	N1-C2-O2	5.01	126.31	122.80
36	5	1646	G	O4'-C1'-N9	5.01	112.21	108.20
36	5	3018	C	N1-C2-N3	5.01	122.71	119.20
36	1	2810	C	N1-C2-N3	5.01	122.71	119.20
36	1	2973	G	C8-N9-C4	5.01	108.41	106.40
1	6	1674	C	N3-C2-O2	5.01	125.41	121.90
1	6	1739	C	C2-N1-C1'	-5.01	113.28	118.80
36	5	200	C	C6-N1-C2	-5.01	118.30	120.30
36	5	1149	G	C4-C5-N7	-5.01	108.80	110.80
36	1	64	G	C4-C5-N7	-5.01	108.80	110.80
36	1	642	U	N1-C2-O2	5.01	126.31	122.80
36	1	1835	A	C8-N9-C4	5.01	107.80	105.80
36	1	3216	G	C4-C5-N7	-5.01	108.80	110.80
1	6	1112	G	C5-C6-N1	5.01	114.01	111.50
36	5	364	G	C6-C5-N7	-5.01	127.39	130.40
36	5	2434	U	C5-C4-O4	5.01	128.91	125.90
38	8	25	G	C5-C6-N1	5.01	114.01	111.50
38	8	95	G	C8-N9-C1'	5.01	133.51	127.00
1	2	2	A	O4'-C1'-N9	-5.01	104.19	108.20
1	2	73	U	P-O3'-C3'	5.01	125.71	119.70
36	1	1492	G	C5-C6-O6	5.01	131.61	128.60
36	1	1518	U	C2-N3-C4	-5.01	124.00	127.00
36	1	2261	G	C8-N9-C1'	-5.01	120.49	127.00
1	6	56	U	N3-C4-C5	5.01	117.61	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	240	U	P-O3'-C3'	5.01	125.71	119.70
1	6	767	U	C5-C4-O4	5.01	128.91	125.90
1	6	1031	U	C5-C6-N1	-5.01	120.19	122.70
1	6	1672	G	N1-C2-N2	-5.01	111.69	116.20
36	5	2596	U	OP2-P-O3'	5.01	116.22	105.20
36	1	1442	U	C5-C4-O4	-5.01	122.89	125.90
36	5	372	A	N3-C4-N9	5.01	131.41	127.40
36	5	2373	A	OP1-P-OP2	-5.01	112.09	119.60
1	2	1339	C	C5-C6-N1	5.01	123.50	121.00
36	1	317	A	C8-N9-C4	-5.01	103.80	105.80
36	1	425	G	OP1-P-OP2	-5.01	112.09	119.60
36	1	502	U	C4-C5-C6	5.01	122.70	119.70
36	1	1045	C	OP2-P-O3'	5.01	116.22	105.20
36	1	1157	G	N1-C2-N3	5.01	126.90	123.90
36	1	1407	A	N7-C8-N9	-5.01	111.30	113.80
36	1	1513	G	C6-N1-C2	-5.01	122.10	125.10
36	1	2873	U	C4-C5-C6	5.01	122.70	119.70
36	1	2938	G	O5'-P-OP1	-5.01	101.19	105.70
64	N8	32	ARG	NE-CZ-NH1	-5.01	117.80	120.30
36	5	1321	G	C5-C6-N1	-5.01	109.00	111.50
36	5	2183	A	OP2-P-O3'	5.01	116.21	105.20
36	5	2685	C	C2-N1-C1'	5.01	124.31	118.80
36	5	2842	U	O5'-P-OP2	5.01	116.71	110.70
36	5	3288	G	C5-C6-N1	5.01	114.00	111.50
36	1	1416	C	N3-C4-N4	-5.00	114.50	118.00
36	1	2395	G	N3-C2-N2	5.00	123.40	119.90
1	6	130	C	N1-C2-O2	5.00	121.90	118.90
36	5	1138	U	N1-C2-N3	5.00	117.90	114.90
36	5	1321	G	N1-C6-O6	5.00	122.90	119.90
36	5	2341	A	O5'-P-OP2	-5.00	101.19	105.70
39	12	70	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	2	1161	C	N1-C2-O2	-5.00	115.90	118.90
36	1	1336	U	OP2-P-O3'	5.00	116.21	105.20
36	1	2650	U	C6-N1-C2	-5.00	118.00	121.00
36	1	2712	U	N3-C4-O4	-5.00	115.90	119.40
37	3	1	G	C6-C5-N7	-5.00	127.40	130.40
36	5	21	G	N3-C4-N9	5.00	129.00	126.00
36	5	407	A	C4-N9-C1'	5.00	135.31	126.30
36	5	809	G	C5-C6-O6	-5.00	125.60	128.60
36	5	1294	A	N9-C4-C5	5.00	107.80	105.80
36	5	2687	G	N3-C4-C5	-5.00	126.10	128.60
36	5	2772	C	C6-N1-C1'	5.00	126.80	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	518	A	O4'-C1'-N9	5.00	112.20	108.20
1	2	1082	C	C5-C6-N1	5.00	123.50	121.00
36	1	271	C	N1-C2-O2	5.00	121.90	118.90
36	1	2351	U	OP2-P-O3'	5.00	116.20	105.20
36	1	2385	G	N9-C4-C5	-5.00	103.40	105.40
36	1	2634	U	N1-C2-N3	5.00	117.90	114.90
68	O2	105	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	6	425	A	OP2-P-O3'	5.00	116.20	105.20
1	6	1513	G	C8-N9-C4	-5.00	104.40	106.40
36	5	438	A	N1-C6-N6	5.00	121.60	118.60
36	5	613	G	N9-C4-C5	5.00	107.40	105.40
36	5	2934	A	N1-C6-N6	-5.00	115.60	118.60
38	8	105	A	C8-N9-C4	5.00	107.80	105.80

There are no chirality outliers.

All (65) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	124	ASP	Peptide
27	D5	94	LYS	Peptide
27	D5	96	SER	Peptide
28	D6	84	VAL	Peptide
28	D6	97	PRO	Peptide
33	E1	137	ASP	Peptide
39	L2	19	HIS	Peptide
41	L4	129	THR	Peptide
42	L5	290	ILE	Peptide
42	L5	58	LYS	Peptide
43	L6	89	THR	Peptide
44	L7	157	ASN	Peptide
48	M1	10	ARG	Peptide
49	M3	69	VAL	Peptide
51	M5	182	ASN	Peptide
52	M6	110	PRO	Peptide
53	M7	39	TRP	Peptide
56	N0	22	PRO	Peptide
57	N1	16	GLN	Peptide
63	N7	3	LYS	Peptide
64	N8	115	LYS	Peptide
65	N9	19	ASN	Peptide
67	O1	110	GLU	Peptide
67	O1	5	LYS	Peptide

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Mol	Chain	Res	Type	Group
72	O6	2	THR	Peptide
72	O6	78	GLY	Peptide
75	O9	4	GLN	Peptide
76	Q0	77	ILE	Peptide
78	Q2	29	LYS	Peptide
78	Q2	95	GLY	Peptide
3	S1	177	GLN	Peptide
6	S4	167	GLY	Peptide
7	S5	49	GLU	Peptide
9	S7	131	PHE	Peptide
9	S7	31	SER	Peptide
16	c4	124	ASP	Peptide
18	c6	40	GLU	Peptide
18	c6	41	PRO	Peptide
19	c7	87	GLU	Peptide
22	d0	70	THR	Peptide
26	d4	29	HIS	Peptide
33	e1	146	SER	Peptide
39	l2	141	PRO	Peptide
39	l2	143	GLU	Peptide
39	l2	212	GLY	Peptide
41	l4	91	GLY	Peptide
42	l5	270	LYS	Peptide
44	l7	192	GLY	Peptide
45	l8	67	ILE	Peptide
52	m6	110	PRO	Peptide
56	n0	3	HIS	Peptide
59	n3	41	GLY	Peptide
60	n4	78	ALA	Peptide
64	n8	18	GLY	Peptide
64	n8	66	ALA	Peptide
65	n9	19	ASN	Peptide
65	n9	23	LYS	Peptide
67	o1	64	VAL	Peptide
71	o5	118	ILE	Peptide
75	o9	2	ALA	Peptide
3	s1	104	ASP	Peptide
5	s3	203	PRO	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide
9	s7	130	VAL	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	S0	204/251 (81%)	145 (71%)	36 (18%)	23 (11%)	0	2
2	s0	204/251 (81%)	151 (74%)	28 (14%)	25 (12%)	0	1
3	S1	212/254 (84%)	144 (68%)	40 (19%)	28 (13%)	0	1
3	s1	214/254 (84%)	169 (79%)	31 (14%)	14 (6%)	1	7
4	S2	215/253 (85%)	180 (84%)	23 (11%)	12 (6%)	2	10
4	s2	215/253 (85%)	183 (85%)	20 (9%)	12 (6%)	2	10
5	S3	221/239 (92%)	175 (79%)	32 (14%)	14 (6%)	1	7
5	s3	221/239 (92%)	182 (82%)	22 (10%)	17 (8%)	1	5
6	S4	258/260 (99%)	202 (78%)	36 (14%)	20 (8%)	1	4
6	s4	258/260 (99%)	211 (82%)	31 (12%)	16 (6%)	1	8
7	S5	204/224 (91%)	158 (78%)	25 (12%)	21 (10%)	0	2
7	s5	204/224 (91%)	152 (74%)	37 (18%)	15 (7%)	1	5
8	S6	224/236 (95%)	187 (84%)	28 (12%)	9 (4%)	3	17
8	s6	216/236 (92%)	180 (83%)	26 (12%)	10 (5%)	2	14
9	S7	182/189 (96%)	136 (75%)	28 (15%)	18 (10%)	0	2
9	s7	184/189 (97%)	133 (72%)	37 (20%)	14 (8%)	1	5
10	S8	184/200 (92%)	160 (87%)	16 (9%)	8 (4%)	2	15
10	s8	184/200 (92%)	157 (85%)	18 (10%)	9 (5%)	2	13
11	S9	183/196 (93%)	150 (82%)	25 (14%)	8 (4%)	2	15
11	s9	183/196 (93%)	143 (78%)	28 (15%)	12 (7%)	1	6
12	C0	94/105 (90%)	69 (73%)	16 (17%)	9 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	c0	92/105 (88%)	67 (73%)	9 (10%)	16 (17%)	0	0
13	C1	153/155 (99%)	123 (80%)	19 (12%)	11 (7%)	1	5
13	c1	144/155 (93%)	121 (84%)	13 (9%)	10 (7%)	1	6
14	C2	122/142 (86%)	70 (57%)	28 (23%)	24 (20%)	0	0
14	c2	122/142 (86%)	73 (60%)	32 (26%)	17 (14%)	0	1
15	C3	148/150 (99%)	120 (81%)	22 (15%)	6 (4%)	3	16
15	c3	148/150 (99%)	117 (79%)	20 (14%)	11 (7%)	1	5
16	C4	125/136 (92%)	81 (65%)	28 (22%)	16 (13%)	0	1
16	c4	126/136 (93%)	99 (79%)	14 (11%)	13 (10%)	0	2
17	C5	122/141 (86%)	91 (75%)	18 (15%)	13 (11%)	0	2
17	c5	133/141 (94%)	95 (71%)	20 (15%)	18 (14%)	0	1
18	C6	139/142 (98%)	111 (80%)	14 (10%)	14 (10%)	0	2
18	c6	140/142 (99%)	115 (82%)	17 (12%)	8 (6%)	1	10
19	C7	116/136 (85%)	86 (74%)	18 (16%)	12 (10%)	0	2
19	c7	113/136 (83%)	86 (76%)	20 (18%)	7 (6%)	1	8
20	C8	143/145 (99%)	110 (77%)	20 (14%)	13 (9%)	1	3
20	c8	143/145 (99%)	112 (78%)	22 (15%)	9 (6%)	1	7
21	C9	141/143 (99%)	116 (82%)	17 (12%)	8 (6%)	1	10
21	c9	141/143 (99%)	120 (85%)	18 (13%)	3 (2%)	7	33
22	D0	105/120 (88%)	81 (77%)	16 (15%)	8 (8%)	1	5
22	d0	108/120 (90%)	80 (74%)	19 (18%)	9 (8%)	1	4
23	D1	85/87 (98%)	62 (73%)	15 (18%)	8 (9%)	0	3
23	d1	85/87 (98%)	68 (80%)	9 (11%)	8 (9%)	0	3
24	D2	127/129 (98%)	100 (79%)	23 (18%)	4 (3%)	4	23
24	d2	127/129 (98%)	112 (88%)	13 (10%)	2 (2%)	9	40
25	D3	142/144 (99%)	112 (79%)	17 (12%)	13 (9%)	1	3
25	d3	142/144 (99%)	121 (85%)	16 (11%)	5 (4%)	3	20
26	D4	132/134 (98%)	108 (82%)	17 (13%)	7 (5%)	2	11
26	d4	132/134 (98%)	104 (79%)	16 (12%)	12 (9%)	1	3
27	D5	68/107 (64%)	46 (68%)	13 (19%)	9 (13%)	0	1
27	d5	67/107 (63%)	52 (78%)	12 (18%)	3 (4%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	D6	95/97 (98%)	55 (58%)	24 (25%)	16 (17%)	0	0
28	d6	95/97 (98%)	73 (77%)	12 (13%)	10 (10%)	0	2
29	D7	79/81 (98%)	60 (76%)	14 (18%)	5 (6%)	1	7
29	d7	79/81 (98%)	63 (80%)	9 (11%)	7 (9%)	1	3
30	D8	61/66 (92%)	47 (77%)	12 (20%)	2 (3%)	4	21
30	d8	61/66 (92%)	44 (72%)	13 (21%)	4 (7%)	1	6
31	D9	51/55 (93%)	43 (84%)	5 (10%)	3 (6%)	1	9
31	d9	51/55 (93%)	37 (72%)	9 (18%)	5 (10%)	0	2
32	E0	58/60 (97%)	44 (76%)	11 (19%)	3 (5%)	2	12
33	E1	69/76 (91%)	30 (44%)	19 (28%)	20 (29%)	0	0
33	e1	74/76 (97%)	37 (50%)	16 (22%)	21 (28%)	0	0
34	SR	316/318 (99%)	263 (83%)	45 (14%)	8 (2%)	5	28
34	sR	316/318 (99%)	256 (81%)	48 (15%)	12 (4%)	3	18
35	SM	155/273 (57%)	103 (66%)	29 (19%)	23 (15%)	0	1
35	sM	98/273 (36%)	57 (58%)	28 (29%)	13 (13%)	0	1
39	L2	250/253 (99%)	222 (89%)	19 (8%)	9 (4%)	3	19
39	l2	250/253 (99%)	211 (84%)	29 (12%)	10 (4%)	3	17
40	L3	384/386 (100%)	339 (88%)	29 (8%)	16 (4%)	3	16
40	l3	384/386 (100%)	342 (89%)	29 (8%)	13 (3%)	3	20
41	L4	359/361 (99%)	301 (84%)	39 (11%)	19 (5%)	2	11
41	l4	359/361 (99%)	303 (84%)	36 (10%)	20 (6%)	2	10
42	L5	294/296 (99%)	235 (80%)	37 (13%)	22 (8%)	1	5
42	l5	292/296 (99%)	247 (85%)	34 (12%)	11 (4%)	3	18
43	L6	152/175 (87%)	137 (90%)	12 (8%)	3 (2%)	7	34
43	l6	153/175 (87%)	129 (84%)	20 (13%)	4 (3%)	5	27
44	L7	220/243 (90%)	192 (87%)	20 (9%)	8 (4%)	3	19
44	l7	221/243 (91%)	201 (91%)	14 (6%)	6 (3%)	5	26
45	L8	231/255 (91%)	188 (81%)	36 (16%)	7 (3%)	4	24
45	l8	229/255 (90%)	180 (79%)	33 (14%)	16 (7%)	1	6
46	L9	189/191 (99%)	164 (87%)	21 (11%)	4 (2%)	7	33
46	l9	189/191 (99%)	169 (89%)	16 (8%)	4 (2%)	7	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	M0	207/220 (94%)	174 (84%)	25 (12%)	8 (4%)	3	17
47	m0	209/220 (95%)	167 (80%)	26 (12%)	16 (8%)	1	5
48	M1	167/173 (96%)	130 (78%)	21 (13%)	16 (10%)	0	3
48	m1	167/173 (96%)	139 (83%)	17 (10%)	11 (7%)	1	6
49	M3	191/198 (96%)	165 (86%)	17 (9%)	9 (5%)	2	14
49	m3	192/198 (97%)	152 (79%)	26 (14%)	14 (7%)	1	5
50	M4	134/137 (98%)	114 (85%)	10 (8%)	10 (8%)	1	5
50	m4	135/137 (98%)	122 (90%)	11 (8%)	2 (2%)	10	42
51	M5	201/203 (99%)	179 (89%)	17 (8%)	5 (2%)	5	28
51	m5	201/203 (99%)	180 (90%)	16 (8%)	5 (2%)	5	28
52	M6	195/198 (98%)	182 (93%)	10 (5%)	3 (2%)	10	42
52	m6	195/198 (98%)	172 (88%)	15 (8%)	8 (4%)	3	16
53	M7	181/183 (99%)	149 (82%)	21 (12%)	11 (6%)	1	8
53	m7	153/183 (84%)	133 (87%)	17 (11%)	3 (2%)	7	34
54	M8	183/185 (99%)	161 (88%)	16 (9%)	6 (3%)	4	21
54	m8	183/185 (99%)	148 (81%)	24 (13%)	11 (6%)	1	9
55	M9	186/188 (99%)	162 (87%)	21 (11%)	3 (2%)	9	40
55	m9	186/188 (99%)	156 (84%)	25 (13%)	5 (3%)	5	26
56	N0	170/172 (99%)	154 (91%)	14 (8%)	2 (1%)	13	48
56	n0	170/172 (99%)	153 (90%)	15 (9%)	2 (1%)	13	48
57	N1	157/159 (99%)	135 (86%)	13 (8%)	9 (6%)	1	10
57	n1	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	3	18
58	N2	98/120 (82%)	75 (76%)	18 (18%)	5 (5%)	2	12
58	n2	96/120 (80%)	77 (80%)	16 (17%)	3 (3%)	4	23
59	N3	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	10	42
59	n3	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
60	N4	96/155 (62%)	72 (75%)	16 (17%)	8 (8%)	1	4
60	n4	133/155 (86%)	101 (76%)	21 (16%)	11 (8%)	1	4
61	N5	119/141 (84%)	100 (84%)	17 (14%)	2 (2%)	9	39
61	n5	118/141 (84%)	103 (87%)	7 (6%)	8 (7%)	1	6
62	N6	124/126 (98%)	114 (92%)	8 (6%)	2 (2%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	n6	124/126 (98%)	109 (88%)	12 (10%)	3 (2%)	6	29
63	N7	133/135 (98%)	102 (77%)	21 (16%)	10 (8%)	1	5
63	n7	133/135 (98%)	101 (76%)	20 (15%)	12 (9%)	1	3
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	2	13
64	n8	146/148 (99%)	128 (88%)	14 (10%)	4 (3%)	5	26
65	N9	56/58 (97%)	43 (77%)	12 (21%)	1 (2%)	8	37
65	n9	56/58 (97%)	40 (71%)	9 (16%)	7 (12%)	0	1
66	O0	95/104 (91%)	88 (93%)	5 (5%)	2 (2%)	7	33
66	o0	98/104 (94%)	88 (90%)	8 (8%)	2 (2%)	7	34
67	O1	107/112 (96%)	95 (89%)	8 (8%)	4 (4%)	3	19
67	o1	107/112 (96%)	86 (80%)	14 (13%)	7 (6%)	1	7
68	O2	125/129 (97%)	113 (90%)	11 (9%)	1 (1%)	19	57
68	o2	125/129 (97%)	108 (86%)	12 (10%)	5 (4%)	3	17
69	O3	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	15	53
69	o3	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	8	36
70	O4	110/119 (92%)	100 (91%)	6 (6%)	4 (4%)	3	19
70	o4	110/119 (92%)	99 (90%)	7 (6%)	4 (4%)	3	19
71	O5	117/119 (98%)	108 (92%)	7 (6%)	2 (2%)	9	39
71	o5	117/119 (98%)	104 (89%)	7 (6%)	6 (5%)	2	12
72	O6	97/99 (98%)	79 (81%)	13 (13%)	5 (5%)	2	12
72	o6	97/99 (98%)	85 (88%)	10 (10%)	2 (2%)	7	33
73	O7	85/87 (98%)	71 (84%)	11 (13%)	3 (4%)	3	20
73	o7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	6	29
74	O8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	2	11
74	o8	75/77 (97%)	57 (76%)	15 (20%)	3 (4%)	3	17
75	O9	48/50 (96%)	42 (88%)	4 (8%)	2 (4%)	3	16
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	7	33
76	Q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	3	17
76	q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	7	34
77	Q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	15
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	Q2	103/105 (98%)	84 (82%)	12 (12%)	7 (7%)	1	6
78	q2	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
79	Q3	89/91 (98%)	74 (83%)	11 (12%)	4 (4%)	2	14
79	q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	6	31
80	e0	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	0	2
82	p0	139/311 (45%)	113 (81%)	22 (16%)	4 (3%)	4	24
All	All	22333/24141 (92%)	18316 (82%)	2723 (12%)	1294 (6%)	1	10

All (1294) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	5	ALA
2	S0	30	GLN
2	S0	39	ASN
2	S0	66	ALA
2	S0	95	ALA
2	S0	139	VAL
2	S0	158	VAL
2	S0	187	ALA
2	S0	191	ARG
3	S1	37	THR
3	S1	49	ASN
3	S1	63	GLY
3	S1	132	ASP
3	S1	148	ASN
3	S1	158	SER
3	S1	206	PRO
4	S2	107	SER
4	S2	236	PRO
5	S3	62	ASN
5	S3	93	ASP
5	S3	211	PRO
5	S3	220	PRO
6	S4	3	ARG
6	S4	96	ASN
6	S4	104	ASP
6	S4	142	HIS
6	S4	223	ASN
7	S5	35	GLN

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Mol	Chain	Res	Type
7	S5	39	GLU
7	S5	43	PHE
7	S5	63	GLN
7	S5	148	ARG
7	S5	154	ALA
9	S7	30	SER
9	S7	31	SER
9	S7	32	PRO
9	S7	64	VAL
9	S7	74	GLN
9	S7	85	PHE
9	S7	111	LYS
9	S7	112	ARG
9	S7	131	PHE
9	S7	133	THR
9	S7	134	GLU
9	S7	156	SER
10	S8	152	ILE
10	S8	153	GLU
10	S8	199	LYS
11	S9	134	ILE
12	C0	54	TYR
12	C0	88	PRO
13	C1	29	LYS
13	C1	96	LYS
13	C1	154	ALA
14	C2	55	GLY
14	C2	83	GLU
14	C2	89	ILE
14	C2	91	VAL
14	C2	93	ASP
14	C2	113	ARG
14	C2	130	THR
15	C3	22	ALA
15	C3	27	LYS
16	C4	42	VAL
16	C4	50	ALA
16	C4	92	LYS
16	C4	124	ASP
16	C4	125	SER
16	C4	126	THR
17	C5	22	LEU

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Mol	Chain	Res	Type
17	C5	51	SER
17	C5	125	PRO
18	C6	29	ILE
18	C6	39	VAL
18	C6	41	PRO
18	C6	58	ASP
18	C6	59	LYS
18	C6	113	ASP
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	96	SER
20	C8	8	GLN
20	C8	14	ILE
20	C8	61	LEU
20	C8	91	ASP
20	C8	92	ILE
20	C8	145	ARG
21	C9	31	PRO
21	C9	53	TRP
23	D1	2	GLU
23	D1	11	LEU
23	D1	82	VAL
24	D2	83	ILE
25	D3	40	SER
25	D3	41	SER
25	D3	78	LYS
25	D3	128	SER
25	D3	131	SER
25	D3	137	LYS
25	D3	144	ARG
26	D4	6	THR
26	D4	34	ASN
26	D4	36	SER
26	D4	60	PHE
27	D5	39	ALA
27	D5	43	ASP
27	D5	44	GLN
27	D5	71	ILE
27	D5	97	LYS
28	D6	45	VAL
28	D6	47	ALA

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Mol	Chain	Res	Type
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
29	D7	38	PRO
29	D7	62	ILE
31	D9	8	PHE
32	E0	47	VAL
33	E1	84	VAL
33	E1	102	VAL
33	E1	128	ALA
34	SR	51	ASP
34	SR	161	LYS
35	SM	17	VAL
35	SM	23	LYS
35	SM	52	PRO
35	SM	64	LYS
35	SM	102	THR
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
39	L2	143	GLU
39	L2	250	GLN
40	L3	4	ARG
40	L3	5	LYS
40	L3	140	ASP
40	L3	142	ALA
40	L3	348	ARG
41	L4	4	PRO
41	L4	291	ASN
41	L4	317	PRO
41	L4	318	LEU
41	L4	338	LYS
41	L4	361	HIS
42	L5	107	ARG
42	L5	108	ARG
42	L5	125	VAL
42	L5	215	ASP
42	L5	233	ALA
42	L5	234	ASP
42	L5	258	LYS
43	L6	98	VAL
44	L7	24	GLU

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Mol	Chain	Res	Type
44	L7	26	VAL
44	L7	216	VAL
45	L8	25	PRO
47	M0	142	ASP
48	M1	9	MET
48	M1	12	LEU
48	M1	94	ARG
48	M1	114	ILE
48	M1	165	GLN
49	M3	47	ALA
49	M3	129	ASN
50	M4	8	LYS
50	M4	9	ALA
50	M4	135	LEU
51	M5	74	PRO
52	M6	111	PRO
53	M7	157	VAL
54	M8	99	THR
56	N0	2	ALA
57	N1	122	GLN
57	N1	126	VAL
60	N4	64	THR
60	N4	81	PRO
60	N4	97	LYS
61	N5	105	VAL
62	N6	52	ARG
62	N6	84	LYS
63	N7	5	LEU
63	N7	30	ASP
63	N7	35	SER
63	N7	128	GLN
64	N8	76	ASP
64	N8	78	LEU
64	N8	96	LYS
67	O1	6	ASP
68	O2	127	ALA
70	O4	74	ARG
71	O5	119	LYS
72	O6	3	VAL
72	O6	33	ALA
75	O9	4	GLN
76	Q0	78	ILE

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Mol	Chain	Res	Type
76	Q0	79	GLU
77	Q1	23	ARG
78	Q2	15	LYS
78	Q2	100	LYS
79	Q3	58	SER
2	s0	8	ASP
2	s0	29	VAL
2	s0	30	GLN
2	s0	66	ALA
2	s0	115	PHE
2	s0	185	ARG
2	s0	189	VAL
2	s0	206	ASP
3	s1	106	THR
3	s1	147	ALA
3	s1	206	PRO
4	s2	83	ILE
4	s2	91	ARG
4	s2	92	ALA
4	s2	238	SER
5	s3	90	ARG
5	s3	115	ILE
5	s3	195	SER
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	163	ASP
6	s4	195	ILE
6	s4	196	VAL
6	s4	214	LEU
7	s5	28	PRO
7	s5	35	GLN
7	s5	36	ALA
7	s5	39	GLU
7	s5	184	PHE
8	s6	153	VAL
8	s6	173	PRO
9	s7	30	SER
9	s7	64	VAL
9	s7	74	GLN
9	s7	155	ASP
10	s8	199	LYS

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Mol	Chain	Res	Type
11	s9	91	LYS
11	s9	147	MET
12	c0	2	LEU
12	c0	32	HIS
12	c0	83	PRO
12	c0	88	PRO
12	c0	97	PRO
13	c1	3	THR
13	c1	121	ASP
13	c1	133	LYS
13	c1	144	ALA
14	c2	22	VAL
14	c2	131	ASP
15	c3	19	SER
15	c3	66	ILE
15	c3	87	ASP
15	c3	137	PRO
15	c3	139	TRP
15	c3	140	LYS
16	c4	90	ARG
17	c5	11	VAL
17	c5	51	SER
17	c5	52	LYS
17	c5	125	PRO
17	c5	126	VAL
17	c5	127	ARG
18	c6	42	GLU
19	c7	88	VAL
19	c7	99	VAL
19	c7	116	LYS
20	c8	18	LEU
20	c8	55	HIS
21	c9	29	GLU
22	d0	49	ASN
22	d0	51	VAL
22	d0	97	VAL
22	d0	118	VAL
23	d1	66	ASP
23	d1	67	ASP
25	d3	131	SER
25	d3	138	GLU
26	d4	30	PRO

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Mol	Chain	Res	Type
26	d4	35	VAL
26	d4	52	LYS
27	d5	85	LYS
27	d5	104	ALA
28	d6	61	GLU
29	d7	3	LEU
29	d7	62	ILE
29	d7	75	GLU
30	d8	61	ARG
31	d9	6	VAL
80	e0	51	ASN
80	e0	60	PRO
33	e1	83	LYS
33	e1	84	VAL
33	e1	87	THR
33	e1	98	VAL
33	e1	103	LEU
33	e1	106	TYR
33	e1	111	GLU
33	e1	136	LYS
34	sR	160	GLU
34	sR	161	LYS
34	sR	163	ASP
34	sR	165	ASP
34	sR	318	ALA
39	l2	194	ASN
40	l3	140	ASP
40	l3	142	ALA
40	l3	235	THR
40	l3	347	SER
41	l4	15	ALA
41	l4	24	ALA
41	l4	90	PHE
41	l4	272	VAL
41	l4	305	ALA
41	l4	329	PRO
41	l4	339	LEU
41	l4	345	GLU
43	l6	98	VAL
45	l8	25	PRO
45	l8	34	PHE
45	l8	112	GLU

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Mol	Chain	Res	Type
45	l8	122	LYS
45	l8	203	VAL
45	l8	223	ALA
47	m0	25	ALA
47	m0	79	VAL
47	m0	100	ASN
47	m0	101	LYS
47	m0	170	LYS
48	m1	8	PRO
48	m1	9	MET
48	m1	10	ARG
49	m3	47	ALA
49	m3	51	LEU
49	m3	93	ILE
49	m3	101	ARG
49	m3	133	PRO
49	m3	134	GLU
49	m3	141	ALA
49	m3	162	ASN
51	m5	184	LYS
52	m6	16	VAL
52	m6	110	PRO
54	m8	74	GLU
54	m8	99	THR
55	m9	100	ARG
56	n0	2	ALA
57	n1	122	GLN
57	n1	136	ARG
58	n2	91	ASP
60	n4	25	ASP
60	n4	95	SER
61	n5	38	LEU
61	n5	101	GLU
61	n5	102	LEU
62	n6	125	LYS
63	n7	105	SER
63	n7	125	GLY
63	n7	128	GLN
63	n7	129	TRP
64	n8	48	TYR
64	n8	76	ASP
65	n9	23	LYS

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Mol	Chain	Res	Type
65	n9	39	PHE
67	o1	5	LYS
67	o1	45	GLY
67	o1	99	ALA
68	o2	5	PRO
68	o2	6	HIS
68	o2	87	MET
69	o3	88	ASN
70	o4	79	SER
74	o8	18	ALA
74	o8	19	ASP
82	p0	93	LEU
2	S0	27	ARG
2	S0	36	TYR
2	S0	94	GLY
2	S0	185	ARG
2	S0	190	ASP
2	S0	195	TRP
3	S1	23	PRO
3	S1	35	PRO
3	S1	54	LEU
3	S1	58	SER
3	S1	93	GLY
3	S1	179	SER
3	S1	213	ARG
4	S2	91	ARG
4	S2	248	SER
5	S3	64	ARG
5	S3	65	ARG
5	S3	118	ALA
5	S3	216	PRO
6	S4	11	ARG
6	S4	12	LEU
6	S4	17	HIS
6	S4	86	PHE
6	S4	195	ILE
6	S4	204	GLY
7	S5	36	ALA
7	S5	58	LEU
7	S5	101	GLY
7	S5	150	GLY
7	S5	156	ARG

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Mol	Chain	Res	Type
7	S5	206	SER
8	S6	25	ARG
8	S6	59	GLN
8	S6	70	PRO
8	S6	146	GLY
8	S6	165	GLY
9	S7	155	ASP
10	S8	22	ARG
11	S9	15	PRO
11	S9	98	ALA
12	C0	11	ILE
12	C0	35	ILE
12	C0	60	SER
13	C1	55	ASP
13	C1	95	PRO
14	C2	21	GLU
14	C2	66	VAL
14	C2	127	GLY
14	C2	131	ASP
15	C3	3	ARG
15	C3	68	GLY
16	C4	51	ASP
16	C4	123	SER
17	C5	48	GLY
17	C5	101	ALA
18	C6	76	SER
18	C6	97	VAL
19	C7	59	LYS
19	C7	124	VAL
20	C8	144	ARG
21	C9	35	ASP
22	D0	44	ASN
23	D1	7	GLN
23	D1	10	GLU
23	D1	12	TYR
25	D3	3	LYS
25	D3	37	ALA
25	D3	112	LYS
25	D3	115	GLY
25	D3	138	GLU
26	D4	5	VAL
28	D6	46	GLU

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Mol	Chain	Res	Type
28	D6	63	ALA
28	D6	82	ARG
29	D7	75	GLU
30	D8	36	THR
30	D8	61	ARG
32	E0	51	ASN
33	E1	83	LYS
33	E1	89	LYS
33	E1	94	LYS
33	E1	98	VAL
33	E1	103	LEU
33	E1	127	GLY
33	E1	138	ARG
33	E1	146	SER
34	SR	50	ASP
35	SM	86	ASN
35	SM	88	ARG
35	SM	101	ASP
35	SM	139	GLU
35	SM	154	TYR
39	L2	104	LEU
39	L2	144	ASN
40	L3	113	GLU
40	L3	155	ALA
41	L4	15	ALA
41	L4	130	ALA
41	L4	146	PRO
41	L4	232	SER
41	L4	311	HIS
42	L5	57	ASN
42	L5	58	LYS
42	L5	137	ASP
42	L5	178	ASN
42	L5	239	ILE
42	L5	253	PHE
42	L5	259	LYS
42	L5	260	PHE
42	L5	295	GLY
44	L7	158	LYS
46	L9	96	HIS
47	M0	24	ARG
47	M0	194	GLY

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Mol	Chain	Res	Type
47	M0	211	ARG
48	M1	24	GLY
48	M1	115	LYS
48	M1	167	TYR
48	M1	173	ASP
50	M4	10	SER
50	M4	136	ALA
51	M5	75	VAL
51	M5	184	LYS
53	M7	75	GLU
53	M7	100	ALA
53	M7	162	GLU
53	M7	164	LYS
54	M8	4	ASP
55	M9	53	LYS
55	M9	128	LYS
57	N1	108	ARG
57	N1	120	LYS
57	N1	124	VAL
58	N2	11	ILE
60	N4	69	LYS
63	N7	3	LYS
64	N8	66	ALA
67	O1	7	VAL
70	O4	73	SER
70	O4	77	GLY
72	O6	34	SER
72	O6	64	SER
73	O7	86	ALA
74	O8	11	PHE
74	O8	33	LYS
75	O9	3	ALA
78	Q2	94	GLY
2	s0	10	THR
2	s0	44	GLY
2	s0	68	PRO
2	s0	111	ILE
2	s0	183	ARG
2	s0	191	ARG
3	s1	39	GLU
3	s1	82	ARG
3	s1	93	GLY

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Mol	Chain	Res	Type
3	s1	94	LYS
3	s1	105	PHE
3	s1	233	GLY
4	s2	107	SER
4	s2	163	GLY
6	s4	12	LEU
6	s4	66	MET
6	s4	104	ASP
6	s4	164	LEU
6	s4	245	LYS
7	s5	37	GLN
7	s5	43	PHE
7	s5	151	GLY
7	s5	209	TYR
8	s6	25	ARG
8	s6	68	LEU
8	s6	154	ARG
9	s7	159	VAL
9	s7	185	ILE
10	s8	62	THR
10	s8	101	ILE
10	s8	122	GLY
10	s8	150	ALA
11	s9	118	LEU
11	s9	134	ILE
12	c0	31	LYS
12	c0	82	LEU
12	c0	92	ILE
13	c1	55	ASP
13	c1	128	CYS
14	c2	45	LEU
14	c2	89	ILE
14	c2	101	ALA
14	c2	115	VAL
15	c3	108	ASP
16	c4	35	GLY
16	c4	48	VAL
16	c4	50	ALA
16	c4	51	ASP
16	c4	79	VAL
16	c4	131	GLY
16	c4	132	ARG

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Mol	Chain	Res	Type
17	c5	8	LYS
17	c5	71	GLU
17	c5	132	GLY
18	c6	39	VAL
18	c6	113	ASP
19	c7	104	ASN
19	c7	105	GLN
19	c7	113	LEU
19	c7	120	SER
20	c8	9	GLY
20	c8	135	GLY
21	c9	33	TYR
22	d0	15	GLN
23	d1	44	ARG
23	d1	64	GLU
24	d2	68	ARG
26	d4	32	ARG
26	d4	53	ASP
26	d4	58	PHE
26	d4	77	ASN
26	d4	123	LYS
28	d6	34	LYS
28	d6	62	TYR
29	d7	26	GLN
29	d7	59	CYS
30	d8	32	PHE
30	d8	57	MET
31	d9	7	TRP
33	e1	79	LYS
33	e1	81	LYS
33	e1	92	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	127	GLY
33	e1	128	ALA
34	sR	4	ASN
35	sM	64	LYS
39	l2	115	ASN
39	l2	213	GLY
39	l2	215	ASN
39	l2	249	SER
40	l3	333	LYS

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Mol	Chain	Res	Type
41	l4	233	LEU
41	l4	302	ALA
41	l4	311	HIS
42	l5	119	TYR
42	l5	124	GLU
42	l5	260	PHE
42	l5	270	LYS
42	l5	279	LYS
44	l7	157	ASN
44	l7	158	LYS
45	l8	117	ALA
45	l8	121	SER
45	l8	188	THR
45	l8	196	ALA
45	l8	237	ILE
46	l9	144	ILE
46	l9	190	ASP
47	m0	3	ARG
47	m0	82	ARG
47	m0	204	GLY
47	m0	207	GLU
48	m1	15	GLU
48	m1	108	GLU
48	m1	111	ASP
49	m3	152	THR
49	m3	163	GLY
50	m4	135	LEU
50	m4	136	ALA
51	m5	183	THR
51	m5	187	ARG
52	m6	122	GLN
52	m6	176	LYS
52	m6	186	ALA
53	m7	75	GLU
57	n1	16	GLN
60	n4	63	ILE
60	n4	71	ARG
60	n4	76	VAL
60	n4	83	THR
61	n5	25	LYS
61	n5	39	LYS
61	n5	47	ALA

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Mol	Chain	Res	Type
62	n6	83	ASP
62	n6	84	LYS
63	n7	16	GLY
63	n7	56	LYS
63	n7	104	PRO
64	n8	47	LYS
65	n9	21	ILE
65	n9	25	LYS
66	o0	10	ILE
67	o1	40	ALA
68	o2	17	PHE
71	o5	40	SER
71	o5	79	ASP
71	o5	119	LYS
73	o7	85	LYS
3	S1	62	LYS
3	S1	129	THR
3	S1	207	LEU
3	S1	221	PRO
4	S2	147	ASN
4	S2	150	GLN
6	S4	26	CYS
6	S4	77	ARG
6	S4	79	ASP
6	S4	164	LEU
6	S4	222	LEU
6	S4	242	LYS
6	S4	245	LYS
7	S5	64	VAL
7	S5	100	ASN
9	S7	29	ASN
9	S7	84	LYS
9	S7	98	ILE
10	S8	105	ASP
10	S8	120	THR
10	S8	154	SER
11	S9	118	LEU
11	S9	120	LYS
12	C0	61	TRP
12	C0	86	ILE
12	C0	94	GLU
13	C1	30	ARG

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Mol	Chain	Res	Type
14	C2	22	VAL
14	C2	87	PRO
14	C2	107	ASP
14	C2	115	VAL
14	C2	117	GLY
14	C2	125	ASN
14	C2	128	ALA
15	C3	28	LEU
15	C3	31	GLU
16	C4	86	THR
16	C4	109	GLY
17	C5	17	TYR
17	C5	52	LYS
17	C5	69	GLU
18	C6	42	GLU
19	C7	3	ARG
19	C7	72	LYS
19	C7	84	TYR
19	C7	87	GLU
20	C8	7	GLU
20	C8	142	GLY
21	C9	69	LYS
22	D0	17	GLN
22	D0	21	LYS
22	D0	31	VAL
23	D1	81	ASN
24	D2	66	ASN
26	D4	53	ASP
28	D6	97	PRO
29	D7	63	LEU
31	D9	37	ASN
32	E0	33	ARG
33	E1	85	TYR
33	E1	106	TYR
33	E1	111	GLU
33	E1	145	HIS
34	SR	194	GLY
35	SM	18	VAL
35	SM	65	THR
35	SM	87	THR
35	SM	89	ARG
35	SM	173	GLU

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Mol	Chain	Res	Type
35	SM	174	LEU
39	L2	14	SER
39	L2	47	GLN
40	L3	3	HIS
40	L3	187	SER
40	L3	299	ASP
40	L3	300	ARG
40	L3	385	LYS
42	L5	7	ALA
42	L5	124	GLU
42	L5	188	GLU
42	L5	292	ALA
44	L7	159	GLN
44	L7	164	SER
45	L8	156	ASP
46	L9	2	LYS
48	M1	8	PRO
48	M1	95	ASN
48	M1	108	GLU
48	M1	166	LYS
49	M3	128	ARG
49	M3	165	SER
50	M4	6	ILE
50	M4	29	ALA
52	M6	16	VAL
53	M7	40	GLU
53	M7	160	ALA
54	M8	98	LYS
55	M9	55	VAL
57	N1	121	ALA
57	N1	159	PHE
58	N2	91	ASP
59	N3	42	SER
60	N4	86	SER
63	N7	16	GLY
63	N7	36	HIS
63	N7	102	GLU
63	N7	124	ALA
64	N8	27	LYS
73	O7	68	LYS
73	O7	85	LYS
78	Q2	35	LEU

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Mol	Chain	Res	Type
78	Q2	96	GLU
2	s0	95	ALA
2	s0	184	LEU
3	s1	22	ASP
3	s1	26	ARG
3	s1	81	PHE
4	s2	47	ALA
5	s3	45	LYS
5	s3	61	GLU
5	s3	93	ASP
6	s4	80	THR
6	s4	90	ILE
6	s4	95	THR
7	s5	33	VAL
7	s5	100	ASN
8	s6	69	LEU
8	s6	149	LYS
8	s6	152	ASP
8	s6	217	SER
9	s7	5	GLN
9	s7	131	PHE
10	s8	27	PHE
11	s9	162	SER
11	s9	164	PHE
11	s9	167	ALA
12	c0	24	LYS
12	c0	94	GLU
13	c1	95	PRO
14	c2	103	LEU
14	c2	108	ARG
14	c2	111	ASN
14	c2	130	THR
15	c3	3	ARG
16	c4	11	SER
16	c4	12	GLN
17	c5	7	ALA
17	c5	117	GLY
17	c5	135	THR
20	c8	14	ILE
20	c8	23	ASP
20	c8	61	LEU
21	c9	28	LEU

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Mol	Chain	Res	Type
22	d0	17	GLN
22	d0	52	LYS
22	d0	96	PRO
22	d0	119	ALA
23	d1	42	GLU
26	d4	3	ASP
27	d5	53	GLU
28	d6	8	ASN
28	d6	13	LYS
28	d6	82	ARG
29	d7	20	LYS
31	d9	17	GLY
80	e0	54	ARG
80	e0	61	SER
33	e1	85	TYR
34	sR	186	PHE
34	sR	206	PRO
35	sM	41	SER
35	sM	42	ALA
35	sM	46	LYS
35	sM	47	ALA
35	sM	48	ARG
35	sM	50	ASN
39	l2	56	ALA
40	l3	3	HIS
40	l3	23	ALA
41	l4	146	PRO
41	l4	338	LYS
41	l4	346	LYS
42	l5	168	ASP
42	l5	178	ASN
42	l5	215	ASP
43	l6	10	TYR
43	l6	20	LYS
43	l6	171	PRO
44	l7	129	LEU
45	l8	26	LEU
45	l8	39	ALA
45	l8	69	LEU
45	l8	133	LYS
47	m0	78	THR
47	m0	102	MET

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Mol	Chain	Res	Type
47	m0	117	GLY
47	m0	214	PRO
48	m1	7	ASN
49	m3	135	ALA
52	m6	177	LYS
53	m7	109	ALA
54	m8	21	SER
54	m8	98	LYS
54	m8	113	LYS
55	m9	35	ALA
57	n1	135	PRO
58	n2	50	LEU
60	n4	64	THR
61	n5	24	LEU
61	n5	48	SER
63	n7	103	GLN
65	n9	52	LYS
66	o0	46	ALA
67	o1	84	ASP
70	o4	51	LEU
70	o4	83	ASN
71	o5	99	GLN
72	o6	33	ALA
72	o6	64	SER
2	S0	64	ILE
2	S0	103	THR
2	S0	192	THR
2	S0	203	PHE
3	S1	36	SER
3	S1	55	LYS
3	S1	79	HIS
3	S1	82	ARG
3	S1	111	ARG
3	S1	131	ASP
4	S2	92	ALA
4	S2	145	GLY
5	S3	59	LEU
5	S3	117	ARG
5	S3	217	ILE
5	S3	218	LEU
7	S5	26	ALA
7	S5	204	GLY

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Mol	Chain	Res	Type
8	S6	20	ASP
8	S6	152	ASP
11	S9	121	SER
11	S9	147	MET
13	C1	3	THR
14	C2	25	GLU
14	C2	53	THR
14	C2	68	GLU
14	C2	90	LYS
14	C2	106	ILE
16	C4	18	ARG
17	C5	56	PHE
18	C6	14	LYS
18	C6	74	HIS
19	C7	115	LEU
21	C9	28	LEU
21	C9	39	THR
21	C9	50	ALA
23	D1	44	ARG
26	D4	83	LYS
27	D5	38	HIS
27	D5	41	ILE
27	D5	69	LEU
28	D6	14	GLY
28	D6	62	TYR
28	D6	64	LEU
28	D6	91	ASP
33	E1	87	THR
33	E1	100	LEU
33	E1	118	ARG
34	SR	237	GLN
35	SM	12	VAL
35	SM	172	VAL
40	L3	302	LYS
41	L4	272	VAL
41	L4	292	SER
41	L4	320	ASN
42	L5	6	ASP
43	L6	147	ALA
45	L8	36	ILE
45	L8	76	ALA
45	L8	114	ALA

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Mol	Chain	Res	Type
45	L8	157	VAL
46	L9	110	LYS
47	M0	187	ALA
47	M0	220	GLN
48	M1	65	ILE
48	M1	117	ASP
49	M3	76	THR
49	M3	136	GLU
50	M4	95	ALA
53	M7	163	LYS
53	M7	179	GLN
54	M8	162	ALA
54	M8	170	ARG
56	N0	167	ARG
59	N3	112	SER
60	N4	77	LYS
61	N5	25	LYS
63	N7	103	GLN
66	O0	64	LYS
67	O1	82	GLU
67	O1	83	GLU
69	O3	14	LEU
70	O4	82	ALA
71	O5	75	TYR
79	Q3	91	GLU
2	s0	4	PRO
2	s0	92	HIS
2	s0	103	THR
2	s0	158	VAL
2	s0	164	ASN
3	s1	61	LEU
4	s2	235	LEU
5	s3	144	ALA
5	s3	203	PRO
7	s5	102	ARG
9	s7	111	LYS
9	s7	112	ARG
9	s7	133	THR
9	s7	156	SER
9	s7	160	GLN
10	s8	148	ALA
11	s9	150	LEU

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Mol	Chain	Res	Type
12	c0	3	MET
12	c0	23	ALA
12	c0	30	ALA
12	c0	35	ILE
14	c2	90	LYS
14	c2	106	ILE
14	c2	119	SER
16	c4	37	GLU
17	c5	6	ASN
17	c5	13	LYS
17	c5	136	SER
18	c6	97	VAL
18	c6	142	TYR
20	c8	60	GLU
23	d1	10	GLU
23	d1	46	ILE
24	d2	18	GLU
25	d3	70	LYS
25	d3	101	GLU
26	d4	50	ALA
29	d7	61	THR
30	d8	33	LEU
31	d9	5	ASN
33	e1	148	TYR
34	sR	146	GLY
34	sR	281	TYR
34	sR	317	THR
35	sM	43	ASP
35	sM	65	THR
35	sM	171	LYS
39	l2	70	ARG
40	l3	155	ALA
40	l3	386	ASP
41	l4	174	ALA
41	l4	317	PRO
42	l5	44	TYR
42	l5	125	VAL
44	l7	191	VAL
46	l9	110	LYS
46	l9	167	VAL
48	m1	116	TYR
48	m1	117	ASP

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Mol	Chain	Res	Type
48	m1	167	TYR
49	m3	60	ALA
51	m5	76	PRO
52	m6	111	PRO
54	m8	41	ASP
54	m8	49	LEU
54	m8	77	ALA
54	m8	91	ALA
55	m9	97	ARG
55	m9	99	LEU
56	n0	51	VAL
57	n1	127	GLN
60	n4	130	SER
63	n7	55	LYS
64	n8	17	ALA
65	n9	22	LYS
67	o1	41	LYS
71	o5	14	LYS
71	o5	74	LYS
75	o9	44	TRP
76	q0	78	ILE
79	q3	51	ALA
82	p0	33	VAL
2	S0	38	PHE
2	S0	189	VAL
3	S1	209	ASN
3	S1	223	PHE
4	S2	148	LEU
4	S2	235	LEU
5	S3	81	PRO
6	S4	258	GLN
7	S5	51	VAL
7	S5	109	LYS
8	S6	69	LEU
10	S8	10	LYS
11	S9	174	ARG
12	C0	30	ALA
14	C2	119	SER
16	C4	25	ASP
16	C4	105	LEU
17	C5	29	SER
17	C5	126	VAL

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Mol	Chain	Res	Type
18	C6	45	ARG
19	C7	6	THR
20	C8	10	SER
20	C8	60	GLU
21	C9	7	ARG
24	D2	112	ASP
27	D5	88	ILE
28	D6	36	ILE
31	D9	25	SER
33	E1	86	THR
33	E1	112	GLY
34	SR	163	ASP
34	SR	255	ALA
35	SM	111	GLY
35	SM	169	ALA
39	L2	32	LEU
39	L2	142	ASP
39	L2	251	LYS
40	L3	317	ILE
40	L3	386	ASP
41	L4	16	THR
41	L4	233	LEU
43	L6	97	ASN
46	L9	120	ASP
47	M0	41	ALA
47	M0	117	GLY
48	M1	74	PRO
49	M3	153	ASP
49	M3	193	ALA
50	M4	28	SER
50	M4	71	ALA
51	M5	145	ASP
53	M7	159	LYS
54	M8	147	ARG
57	N1	18	ASP
57	N1	107	GLU
58	N2	51	GLY
60	N4	18	GLY
64	N8	47	LYS
66	O0	20	SER
72	O6	21	THR
78	Q2	17	CYS

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Mol	Chain	Res	Type
2	s0	109	ASN
3	s1	129	THR
4	s2	85	PRO
4	s2	150	GLN
4	s2	152	HIS
5	s3	43	PRO
5	s3	44	THR
5	s3	64	ARG
5	s3	178	ARG
5	s3	196	ARG
6	s4	30	ARG
7	s5	29	ILE
7	s5	42	LEU
7	s5	71	ALA
10	s8	78	ILE
10	s8	136	SER
11	s9	121	SER
11	s9	165	GLY
11	s9	183	ALA
12	c0	95	ARG
13	c1	7	VAL
13	c1	129	ARG
14	c2	58	LEU
15	c3	29	SER
16	c4	92	LYS
16	c4	114	ARG
17	c5	68	PRO
17	c5	130	ARG
18	c6	4	VAL
18	c6	106	LYS
20	c8	75	ASN
26	d4	33	ALA
28	d6	47	ALA
28	d6	58	VAL
31	d9	11	PRO
33	e1	118	ARG
33	e1	131	PHE
34	sR	239	GLU
35	sM	36	ASP
35	sM	132	ALA
39	l2	96	LEU
40	l3	187	SER

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Mol	Chain	Res	Type
40	l3	247	ARG
41	l4	4	PRO
41	l4	328	ASN
41	l4	331	ALA
44	l7	178	ILE
47	m0	219	ALA
49	m3	150	PRO
52	m6	68	ARG
54	m8	112	ALA
55	m9	137	ALA
60	n4	72	SER
60	n4	96	LEU
63	n7	102	GLU
73	o7	84	SER
82	p0	198	PRO
3	S1	48	VAL
4	S2	39	THR
4	S2	108	ASN
5	S3	212	LYS
7	S5	21	THR
13	C1	4	GLU
13	C1	113	PRO
13	C1	145	ALA
16	C4	79	VAL
16	C4	108	SER
18	C6	40	GLU
20	C8	134	ARG
25	D3	97	ASP
29	D7	51	GLN
41	L4	5	GLN
41	L4	14	GLU
42	L5	221	GLU
44	L7	178	ILE
45	L8	39	ALA
51	M5	94	TYR
58	N2	87	ASN
79	Q3	60	CYS
2	s0	157	ASP
4	s2	196	VAL
6	s4	168	LYS
6	s4	260	GLY
13	c1	96	LYS

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Mol	Chain	Res	Type
14	c2	82	PRO
17	c5	128	HIS
26	d4	36	SER
28	d6	59	TYR
33	e1	99	LYS
39	l2	80	GLU
47	m0	176	LEU
48	m1	114	ILE
54	m8	84	VAL
60	n4	26	SER
63	n7	33	SER
63	n7	34	LYS
68	o2	86	THR
74	o8	35	GLY
79	q3	35	ALA
3	S1	210	ILE
7	S5	153	GLY
7	S5	199	ILE
9	S7	132	PRO
17	C5	53	PRO
28	D6	65	PRO
34	SR	15	GLY
40	L3	141	GLY
41	L4	131	VAL
44	L7	191	VAL
49	M3	130	GLY
65	N9	21	ILE
2	s0	152	PRO
9	s7	13	PRO
14	c2	87	PRO
15	c3	22	ALA
15	c3	65	VAL
18	c6	124	PRO
25	d3	44	GLY
80	e0	47	VAL
44	l7	226	GLY
47	m0	47	PRO
49	m3	130	GLY
53	m7	67	ILE
67	o1	98	VAL
69	o3	59	VAL
8	S6	162	VAL

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Mol	Chain	Res	Type
13	C1	7	VAL
18	C6	33	GLY
22	D0	59	PRO
22	D0	108	ILE
58	N2	22	PRO
74	O8	37	PRO
5	s3	91	VAL
8	s6	165	GLY
14	c2	63	VAL
80	e0	50	VAL
40	l3	141	GLY
65	n9	37	PRO
16	C4	75	GLY
22	D0	106	ILE
22	D0	118	VAL
28	D6	59	TYR
52	M6	110	PRO
74	O8	36	LYS
78	Q2	95	GLY
2	s0	194	PRO
39	l2	238	ILE
45	l8	176	PRO
51	m5	74	PRO
70	o4	78	GLY
2	S0	117	GLU
6	S4	228	ILE
17	C5	109	PRO
20	C8	5	VAL
53	M7	84	PRO
60	N4	76	VAL
79	Q3	50	GLY
6	s4	135	GLY
11	s9	163	PRO
12	c0	96	ASN
23	d1	6	GLY
28	d6	60	PRO
35	sM	166	VAL
40	l3	40	PRO
41	l4	190	GLY
42	l5	286	VAL
82	p0	30	VAL
9	S7	13	PRO

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Mol	Chain	Res	Type
64	N8	29	PRO
33	e1	124	PRO
57	n1	126	VAL
58	n2	48	GLY
24	D2	29	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	S0	164/209 (78%)	132 (80%)	32 (20%)	1	7
2	s0	165/209 (79%)	120 (73%)	45 (27%)	0	2
3	S1	191/223 (86%)	152 (80%)	39 (20%)	1	6
3	s1	192/223 (86%)	152 (79%)	40 (21%)	1	5
4	S2	176/204 (86%)	142 (81%)	34 (19%)	1	8
4	s2	176/204 (86%)	129 (73%)	47 (27%)	0	2
5	S3	182/194 (94%)	136 (75%)	46 (25%)	0	3
5	s3	182/194 (94%)	154 (85%)	28 (15%)	2	13
6	S4	221/221 (100%)	179 (81%)	42 (19%)	1	8
6	s4	221/221 (100%)	190 (86%)	31 (14%)	3	16
7	S5	173/190 (91%)	140 (81%)	33 (19%)	1	8
7	s5	173/190 (91%)	135 (78%)	38 (22%)	1	4
8	S6	188/201 (94%)	150 (80%)	38 (20%)	1	6
8	s6	187/201 (93%)	155 (83%)	32 (17%)	2	10
9	S7	165/169 (98%)	132 (80%)	33 (20%)	1	7
9	s7	165/169 (98%)	136 (82%)	29 (18%)	2	10
10	S8	150/161 (93%)	132 (88%)	18 (12%)	5	22
10	s8	150/161 (93%)	128 (85%)	22 (15%)	3	15
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	4
11	s9	158/165 (96%)	130 (82%)	28 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	C0	77/98 (79%)	63 (82%)	14 (18%)	1	9
12	c0	73/98 (74%)	62 (85%)	11 (15%)	3	14
13	C1	129/136 (95%)	106 (82%)	23 (18%)	2	9
13	c1	129/136 (95%)	101 (78%)	28 (22%)	1	5
14	C2	88/118 (75%)	64 (73%)	24 (27%)	0	2
14	c2	88/118 (75%)	64 (73%)	24 (27%)	0	2
15	C3	127/127 (100%)	106 (84%)	21 (16%)	2	11
15	c3	127/127 (100%)	106 (84%)	21 (16%)	2	11
16	C4	81/104 (78%)	55 (68%)	26 (32%)	0	1
16	c4	97/104 (93%)	74 (76%)	23 (24%)	1	3
17	C5	101/117 (86%)	81 (80%)	20 (20%)	1	7
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	10
18	C6	117/118 (99%)	86 (74%)	31 (26%)	0	2
18	c6	118/118 (100%)	93 (79%)	25 (21%)	1	5
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	6
19	c7	92/124 (74%)	76 (83%)	16 (17%)	2	10
20	C8	128/128 (100%)	97 (76%)	31 (24%)	0	3
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	4
21	C9	115/115 (100%)	89 (77%)	26 (23%)	1	4
21	c9	115/115 (100%)	96 (84%)	19 (16%)	2	11
22	D0	100/113 (88%)	71 (71%)	29 (29%)	0	2
22	d0	103/113 (91%)	77 (75%)	26 (25%)	0	3
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	5
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	5
24	D2	110/110 (100%)	85 (77%)	25 (23%)	1	4
24	d2	110/110 (100%)	95 (86%)	15 (14%)	3	17
25	D3	119/119 (100%)	97 (82%)	22 (18%)	1	8
25	d3	119/119 (100%)	94 (79%)	25 (21%)	1	5
26	D4	112/112 (100%)	89 (80%)	23 (20%)	1	6
26	d4	112/112 (100%)	90 (80%)	22 (20%)	1	7
27	D5	61/88 (69%)	44 (72%)	17 (28%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	d5	61/88 (69%)	54 (88%)	7 (12%)	5	24
28	D6	83/83 (100%)	65 (78%)	18 (22%)	1	5
28	d6	83/83 (100%)	70 (84%)	13 (16%)	2	13
29	D7	70/70 (100%)	60 (86%)	10 (14%)	3	15
29	d7	70/70 (100%)	54 (77%)	16 (23%)	1	4
30	D8	56/59 (95%)	42 (75%)	14 (25%)	0	3
30	d8	56/59 (95%)	48 (86%)	8 (14%)	3	15
31	D9	47/48 (98%)	38 (81%)	9 (19%)	1	8
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	5
32	E0	51/51 (100%)	36 (71%)	15 (29%)	0	1
33	E1	62/66 (94%)	42 (68%)	20 (32%)	0	1
33	e1	66/66 (100%)	43 (65%)	23 (35%)	0	1
34	SR	260/261 (100%)	227 (87%)	33 (13%)	4	19
34	sR	260/261 (100%)	230 (88%)	30 (12%)	5	24
35	SM	97/228 (42%)	68 (70%)	29 (30%)	0	1
35	sM	54/228 (24%)	42 (78%)	12 (22%)	1	4
39	L2	193/195 (99%)	158 (82%)	35 (18%)	1	9
39	l2	192/195 (98%)	152 (79%)	40 (21%)	1	5
40	L3	320/322 (99%)	252 (79%)	68 (21%)	1	5
40	l3	320/322 (99%)	249 (78%)	71 (22%)	1	4
41	L4	288/288 (100%)	229 (80%)	59 (20%)	1	6
41	l4	288/288 (100%)	234 (81%)	54 (19%)	1	8
42	L5	244/244 (100%)	193 (79%)	51 (21%)	1	5
42	l5	243/244 (100%)	193 (79%)	50 (21%)	1	6
43	L6	134/152 (88%)	108 (81%)	26 (19%)	1	7
43	l6	135/152 (89%)	110 (82%)	25 (18%)	1	8
44	L7	186/204 (91%)	159 (86%)	27 (14%)	3	15
44	l7	187/204 (92%)	160 (86%)	27 (14%)	3	15
45	L8	187/207 (90%)	158 (84%)	29 (16%)	2	13
45	l8	177/207 (86%)	149 (84%)	28 (16%)	2	12
46	L9	171/171 (100%)	133 (78%)	38 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	l9	171/171 (100%)	134 (78%)	37 (22%)	1	5
47	M0	177/186 (95%)	140 (79%)	37 (21%)	1	5
47	m0	179/186 (96%)	141 (79%)	38 (21%)	1	5
48	M1	147/150 (98%)	114 (78%)	33 (22%)	1	4
48	m1	147/150 (98%)	120 (82%)	27 (18%)	1	9
49	M3	154/158 (98%)	128 (83%)	26 (17%)	2	11
49	m3	154/158 (98%)	130 (84%)	24 (16%)	2	13
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	9
50	m4	108/108 (100%)	90 (83%)	18 (17%)	2	11
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	10
51	m5	175/175 (100%)	150 (86%)	25 (14%)	3	15
52	M6	160/161 (99%)	134 (84%)	26 (16%)	2	11
52	m6	160/161 (99%)	127 (79%)	33 (21%)	1	6
53	M7	140/145 (97%)	111 (79%)	29 (21%)	1	6
53	m7	125/145 (86%)	95 (76%)	30 (24%)	0	3
54	M8	150/150 (100%)	122 (81%)	28 (19%)	1	8
54	m8	150/150 (100%)	118 (79%)	32 (21%)	1	5
55	M9	153/153 (100%)	124 (81%)	29 (19%)	1	8
55	m9	153/153 (100%)	126 (82%)	27 (18%)	2	10
56	N0	156/156 (100%)	126 (81%)	30 (19%)	1	8
56	n0	156/156 (100%)	129 (83%)	27 (17%)	2	10
57	N1	136/136 (100%)	101 (74%)	35 (26%)	0	3
57	n1	136/136 (100%)	108 (79%)	28 (21%)	1	6
58	N2	87/106 (82%)	77 (88%)	10 (12%)	5	24
58	n2	85/106 (80%)	75 (88%)	10 (12%)	5	22
59	N3	104/104 (100%)	83 (80%)	21 (20%)	1	6
59	n3	104/104 (100%)	92 (88%)	12 (12%)	5	24
60	N4	57/129 (44%)	52 (91%)	5 (9%)	10	36
60	n4	100/129 (78%)	85 (85%)	15 (15%)	3	14
61	N5	104/117 (89%)	80 (77%)	24 (23%)	1	4
61	n5	104/117 (89%)	84 (81%)	20 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	N6	109/109 (100%)	79 (72%)	30 (28%)	0	2
62	n6	109/109 (100%)	88 (81%)	21 (19%)	1	8
63	N7	115/115 (100%)	85 (74%)	30 (26%)	0	2
63	n7	115/115 (100%)	84 (73%)	31 (27%)	0	2
64	N8	118/118 (100%)	95 (80%)	23 (20%)	1	7
64	n8	118/118 (100%)	94 (80%)	24 (20%)	1	6
65	N9	46/46 (100%)	35 (76%)	11 (24%)	0	3
65	n9	46/46 (100%)	34 (74%)	12 (26%)	0	2
66	O0	81/87 (93%)	67 (83%)	14 (17%)	2	10
66	o0	84/87 (97%)	66 (79%)	18 (21%)	1	5
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	4
67	o1	94/96 (98%)	72 (77%)	22 (23%)	1	4
68	O2	109/110 (99%)	86 (79%)	23 (21%)	1	5
68	o2	109/110 (99%)	87 (80%)	22 (20%)	1	6
69	O3	90/90 (100%)	78 (87%)	12 (13%)	4	17
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2	9
70	O4	95/101 (94%)	77 (81%)	18 (19%)	1	8
70	o4	95/101 (94%)	82 (86%)	13 (14%)	3	17
71	O5	104/104 (100%)	72 (69%)	32 (31%)	0	1
71	o5	103/104 (99%)	84 (82%)	19 (18%)	1	9
72	O6	81/81 (100%)	58 (72%)	23 (28%)	0	2
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0	1
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	10
73	o7	70/70 (100%)	57 (81%)	13 (19%)	1	8
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	4
74	o8	67/68 (98%)	49 (73%)	18 (27%)	0	2
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1	7
75	o9	45/45 (100%)	33 (73%)	12 (27%)	0	2
76	Q0	47/47 (100%)	37 (79%)	10 (21%)	1	5
76	q0	47/47 (100%)	37 (79%)	10 (21%)	1	5
77	Q1	23/23 (100%)	17 (74%)	6 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	q1	23/23 (100%)	13 (56%)	10 (44%)	0	0
78	Q2	90/90 (100%)	73 (81%)	17 (19%)	1	8
78	q2	90/90 (100%)	74 (82%)	16 (18%)	2	9
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1	5
79	q3	71/71 (100%)	57 (80%)	14 (20%)	1	7
80	e0	53/53 (100%)	42 (79%)	11 (21%)	1	5
82	p0	105/253 (42%)	81 (77%)	24 (23%)	1	4
All	All	18728/20239 (92%)	14998 (80%)	3730 (20%)	1	7

All (3730) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	6	THR
2	S0	9	LEU
2	S0	10	THR
2	S0	12	GLU
2	S0	27	ARG
2	S0	30	GLN
2	S0	32	HIS
2	S0	34	GLU
2	S0	37	VAL
2	S0	43	ASP
2	S0	62	ARG
2	S0	68	PRO
2	S0	84	ARG
2	S0	86	VAL
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	108	THR
2	S0	110	TYR
2	S0	119	ARG
2	S0	123	VAL
2	S0	140	ASN
2	S0	153	SER
2	S0	157	ASP
2	S0	168	HIS
2	S0	172	LEU
2	S0	177	LEU
2	S0	185	ARG

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Mol	Chain	Res	Type
2	S0	188	LEU
2	S0	196	SER
2	S0	198	MET
2	S0	200	ASP
3	S1	21	VAL
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	37	THR
3	S1	42	ASN
3	S1	46	THR
3	S1	51	SER
3	S1	52	THR
3	S1	61	LEU
3	S1	65	VAL
3	S1	70	LEU
3	S1	78	ASP
3	S1	79	HIS
3	S1	89	ASP
3	S1	97	LEU
3	S1	103	MET
3	S1	105	PHE
3	S1	107	THR
3	S1	110	LEU
3	S1	111	ARG
3	S1	115	ARG
3	S1	117	TRP
3	S1	125	VAL
3	S1	130	SER
3	S1	135	LEU
3	S1	151	LYS
3	S1	154	SER
3	S1	170	GLU
3	S1	177	GLN
3	S1	181	LEU
3	S1	184	LEU
3	S1	193	ILE
3	S1	202	LYS
3	S1	212	VAL
3	S1	214	LYS
3	S1	218	LEU
3	S1	219	LYS

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Mol	Chain	Res	Type
3	S1	223	PHE
4	S2	53	ILE
4	S2	54	GLU
4	S2	56	ILE
4	S2	58	LEU
4	S2	72	LEU
4	S2	77	GLN
4	S2	82	ASN
4	S2	91	ARG
4	S2	94	GLN
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	106	ASP
4	S2	111	VAL
4	S2	113	LEU
4	S2	117	THR
4	S2	134	LEU
4	S2	140	ARG
4	S2	141	ARG
4	S2	146	THR
4	S2	148	LEU
4	S2	159	THR
4	S2	166	THR
4	S2	178	ILE
4	S2	195	ASP
4	S2	221	THR
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	235	LEU
4	S2	240	LEU
4	S2	242	ILE
4	S2	245	ASP
4	S2	250	GLN
5	S3	4	LEU
5	S3	5	ILE
5	S3	6	SER
5	S3	9	ARG
5	S3	10	LYS
5	S3	11	LEU
5	S3	21	LEU

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Mol	Chain	Res	Type
5	S3	26	THR
5	S3	32	GLU
5	S3	38	GLU
5	S3	39	VAL
5	S3	55	THR
5	S3	59	LEU
5	S3	62	ASN
5	S3	64	ARG
5	S3	65	ARG
5	S3	76	ARG
5	S3	84	ILE
5	S3	90	ARG
5	S3	92	GLN
5	S3	93	ASP
5	S3	97	SER
5	S3	103	GLU
5	S3	105	MET
5	S3	117	ARG
5	S3	120	TYR
5	S3	122	VAL
5	S3	124	ARG
5	S3	127	MET
5	S3	128	GLU
5	S3	142	LEU
5	S3	143	ARG
5	S3	146	ARG
5	S3	151	LYS
5	S3	158	ILE
5	S3	164	VAL
5	S3	172	THR
5	S3	175	VAL
5	S3	176	LEU
5	S3	177	MET
5	S3	178	ARG
5	S3	179	GLN
5	S3	211	PRO
5	S3	218	LEU
5	S3	221	SER
5	S3	222	VAL
6	S4	6	LYS
6	S4	7	LYS
6	S4	9	LEU

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Mol	Chain	Res	Type
6	S4	23	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	39	ARG
6	S4	42	LEU
6	S4	48	LEU
6	S4	56	LEU
6	S4	65	LEU
6	S4	67	GLN
6	S4	68	ARG
6	S4	69	HIS
6	S4	70	VAL
6	S4	72	VAL
6	S4	77	ARG
6	S4	78	THR
6	S4	81	THR
6	S4	95	THR
6	S4	96	ASN
6	S4	113	ARG
6	S4	123	LEU
6	S4	129	VAL
6	S4	131	LEU
6	S4	155	LYS
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	192	ILE
6	S4	197	HIS
6	S4	198	LYS
6	S4	206	ASP
6	S4	215	ASP
6	S4	222	LEU
6	S4	223	ASN
6	S4	228	ILE
6	S4	230	GLU
6	S4	240	LYS
6	S4	242	LYS
6	S4	258	GLN
6	S4	259	GLN
7	S5	23	VAL
7	S5	25	LEU
7	S5	38	THR

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Mol	Chain	Res	Type
7	S5	42	LEU
7	S5	43	PHE
7	S5	45	LYS
7	S5	65	ARG
7	S5	66	GLN
7	S5	79	ASN
7	S5	89	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	99	MET
7	S5	119	ASP
7	S5	122	ASN
7	S5	128	ASN
7	S5	139	ASN
7	S5	146	THR
7	S5	147	THR
7	S5	156	ARG
7	S5	157	ARG
7	S5	158	GLN
7	S5	160	VAL
7	S5	162	VAL
7	S5	163	SER
7	S5	166	ARG
7	S5	172	ILE
7	S5	186	ASN
7	S5	194	LEU
7	S5	203	LYS
7	S5	205	SER
7	S5	216	GLU
7	S5	225	ARG
8	S6	13	GLN
8	S6	20	ASP
8	S6	21	GLU
8	S6	25	ARG
8	S6	32	ILE
8	S6	45	PHE
8	S6	58	LYS
8	S6	59	GLN
8	S6	67	VAL
8	S6	68	LEU
8	S6	69	LEU
8	S6	71	THR

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Mol	Chain	Res	Type
8	S6	76	LEU
8	S6	80	ASN
8	S6	81	VAL
8	S6	89	ASP
8	S6	94	ARG
8	S6	98	ARG
8	S6	108	VAL
8	S6	109	LEU
8	S6	114	VAL
8	S6	119	GLN
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	132	ARG
8	S6	137	ARG
8	S6	154	ARG
8	S6	155	ASP
8	S6	158	ILE
8	S6	169	TYR
8	S6	174	LYS
8	S6	176	GLN
8	S6	177	ARG
8	S6	193	LEU
8	S6	201	GLN
8	S6	202	ARG
8	S6	211	LEU
9	S7	15	GLU
9	S7	16	LEU
9	S7	25	VAL
9	S7	31	SER
9	S7	38	LEU
9	S7	46	ILE
9	S7	50	ASP
9	S7	51	VAL
9	S7	67	LEU
9	S7	70	PHE
9	S7	72	LYS
9	S7	75	THR
9	S7	85	PHE
9	S7	87	ASP
9	S7	95	GLU
9	S7	97	ARG

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Mol	Chain	Res	Type
9	S7	99	LEU
9	S7	104	ARG
9	S7	105	THR
9	S7	107	ARG
9	S7	111	LYS
9	S7	112	ARG
9	S7	114	ARG
9	S7	116	ARG
9	S7	129	LEU
9	S7	130	VAL
9	S7	134	GLU
9	S7	144	VAL
9	S7	147	ASN
9	S7	158	ASP
9	S7	165	LYS
9	S7	167	GLU
9	S7	185	ILE
10	S8	7	SER
10	S8	8	ARG
10	S8	17	LYS
10	S8	21	PHE
10	S8	22	ARG
10	S8	29	LEU
10	S8	36	THR
10	S8	46	VAL
10	S8	60	ILE
10	S8	64	ASN
10	S8	73	SER
10	S8	74	LYS
10	S8	135	LYS
10	S8	141	ARG
10	S8	151	LYS
10	S8	152	ILE
10	S8	159	GLN
10	S8	197	THR
11	S9	3	ARG
11	S9	7	THR
11	S9	14	THR
11	S9	21	SER
11	S9	39	LYS
11	S9	49	LEU
11	S9	61	THR

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Mol	Chain	Res	Type
11	S9	62	ARG
11	S9	63	ASP
11	S9	65	LYS
11	S9	78	ARG
11	S9	79	ARG
11	S9	82	ARG
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	97	LEU
11	S9	101	VAL
11	S9	110	GLN
11	S9	111	THR
11	S9	112	GLN
11	S9	115	LYS
11	S9	118	LEU
11	S9	121	SER
11	S9	126	ARG
11	S9	134	ILE
11	S9	138	LYS
11	S9	149	ARG
11	S9	161	THR
11	S9	162	SER
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	180	LYS
11	S9	182	GLU
11	S9	184	SER
12	C0	1	MET
12	C0	12	HIS
12	C0	20	VAL
12	C0	27	PHE
12	C0	28	ASN
12	C0	29	GLN
12	C0	32	HIS
12	C0	50	THR
12	C0	52	LYS
12	C0	56	LYS
12	C0	60	SER
12	C0	74	GLU

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Mol	Chain	Res	Type
12	C0	81	ASN
12	C0	82	LEU
13	C1	7	VAL
13	C1	10	GLU
13	C1	21	ASN
13	C1	25	VAL
13	C1	29	LYS
13	C1	40	LEU
13	C1	44	THR
13	C1	63	LEU
13	C1	67	ARG
13	C1	69	LYS
13	C1	71	LEU
13	C1	79	LYS
13	C1	80	MET
13	C1	83	THR
13	C1	99	ARG
13	C1	105	LYS
13	C1	109	VAL
13	C1	118	GLN
13	C1	123	VAL
13	C1	127	GLN
13	C1	128	CYS
13	C1	136	ARG
13	C1	140	VAL
14	C2	28	LEU
14	C2	30	VAL
14	C2	33	ARG
14	C2	34	THR
14	C2	36	LEU
14	C2	37	VAL
14	C2	43	ARG
14	C2	50	LYS
14	C2	52	LEU
14	C2	53	THR
14	C2	54	ARG
14	C2	66	VAL
14	C2	71	ILE
14	C2	83	GLU
14	C2	86	VAL
14	C2	89	ILE
14	C2	97	LEU

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Mol	Chain	Res	Type
14	C2	103	LEU
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	138	GLU
14	C2	139	HIS
14	C2	140	PHE
15	C3	3	ARG
15	C3	6	SER
15	C3	9	LYS
15	C3	12	SER
15	C3	27	LYS
15	C3	28	LEU
15	C3	39	LYS
15	C3	43	LYS
15	C3	48	SER
15	C3	56	ASP
15	C3	64	ARG
15	C3	76	LYS
15	C3	77	SER
15	C3	83	GLU
15	C3	88	LEU
15	C3	102	LEU
15	C3	114	ARG
15	C3	115	LEU
15	C3	125	LEU
15	C3	149	LEU
15	C3	151	ASN
16	C4	14	PHE
16	C4	16	VAL
16	C4	20	TYR
16	C4	24	ASN
16	C4	29	HIS
16	C4	30	VAL
16	C4	31	THR
16	C4	39	ILE
16	C4	42	VAL
16	C4	48	VAL
16	C4	51	ASP
16	C4	55	SER
16	C4	80	HIS
16	C4	81	VAL

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Mol	Chain	Res	Type
16	C4	83	ILE
16	C4	92	LYS
16	C4	102	LEU
16	C4	107	ARG
16	C4	118	VAL
16	C4	123	SER
16	C4	124	ASP
16	C4	126	THR
16	C4	128	LYS
16	C4	129	LYS
16	C4	136	ARG
16	C4	137	LEU
17	C5	13	LYS
17	C5	14	THR
17	C5	22	LEU
17	C5	23	GLU
17	C5	26	LEU
17	C5	31	GLU
17	C5	34	VAL
17	C5	36	LEU
17	C5	44	ARG
17	C5	47	ARG
17	C5	52	LYS
17	C5	57	MET
17	C5	69	GLU
17	C5	86	VAL
17	C5	100	LYS
17	C5	106	GLU
17	C5	110	GLU
17	C5	121	ILE
17	C5	124	THR
17	C5	130	ARG
18	C6	4	VAL
18	C6	17	THR
18	C6	26	LYS
18	C6	28	LEU
18	C6	29	ILE
18	C6	39	VAL
18	C6	42	GLU
18	C6	43	ILE
18	C6	45	ARG
18	C6	50	GLU

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Mol	Chain	Res	Type
18	C6	53	LEU
18	C6	54	LEU
18	C6	58	ASP
18	C6	59	LYS
18	C6	65	ILE
18	C6	66	ARG
18	C6	69	VAL
18	C6	76	SER
18	C6	89	LEU
18	C6	94	GLN
18	C6	99	GLU
18	C6	106	LYS
18	C6	114	ARG
18	C6	116	LEU
18	C6	118	ILE
18	C6	121	SER
18	C6	123	ARG
18	C6	127	LYS
18	C6	128	LYS
18	C6	137	ARG
18	C6	143	ARG
19	C7	8	THR
19	C7	25	THR
19	C7	26	LEU
19	C7	34	LEU
19	C7	38	ILE
19	C7	40	THR
19	C7	46	LEU
19	C7	49	LYS
19	C7	54	THR
19	C7	60	ARG
19	C7	69	ILE
19	C7	72	LYS
19	C7	78	ARG
19	C7	84	TYR
19	C7	88	VAL
19	C7	105	GLN
19	C7	113	LEU
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL

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Mol	Chain	Res	Type
20	C8	6	GLN
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	20	THR
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	34	THR
20	C8	40	ARG
20	C8	41	ARG
20	C8	44	ASN
20	C8	53	ASP
20	C8	54	LEU
20	C8	60	GLU
20	C8	61	LEU
20	C8	75	ASN
20	C8	80	LYS
20	C8	92	ILE
20	C8	116	LEU
20	C8	132	ARG
20	C8	133	VAL
20	C8	136	GLN
20	C8	138	THR
20	C8	140	THR
20	C8	143	ARG
20	C8	144	ARG
20	C8	145	ARG
21	C9	6	VAL
21	C9	12	GLN
21	C9	13	ASP
21	C9	18	TYR
21	C9	22	LEU
21	C9	28	LEU
21	C9	33	TYR
21	C9	34	VAL
21	C9	35	ASP
21	C9	36	ILE
21	C9	39	THR
21	C9	57	ARG
21	C9	67	MET

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Mol	Chain	Res	Type
21	C9	70	GLN
21	C9	84	LYS
21	C9	86	ARG
21	C9	88	VAL
21	C9	94	ILE
21	C9	111	ILE
21	C9	115	GLU
21	C9	126	GLU
21	C9	130	ARG
21	C9	131	ASP
21	C9	134	ARG
21	C9	140	LEU
21	C9	144	GLU
22	D0	21	LYS
22	D0	22	ILE
22	D0	23	ARG
22	D0	25	THR
22	D0	27	THR
22	D0	31	VAL
22	D0	33	GLN
22	D0	34	LEU
22	D0	40	ASN
22	D0	43	LYS
22	D0	46	GLU
22	D0	47	GLN
22	D0	50	LEU
22	D0	53	LYS
22	D0	57	ARG
22	D0	61	LYS
22	D0	66	SER
22	D0	67	THR
22	D0	70	THR
22	D0	72	ASN
22	D0	74	GLU
22	D0	76	SER
22	D0	81	THR
22	D0	88	LYS
22	D0	89	ARG
22	D0	99	ILE
22	D0	103	ILE
22	D0	108	ILE
22	D0	117	VAL

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Mol	Chain	Res	Type
23	D1	5	LYS
23	D1	7	GLN
23	D1	8	LEU
23	D1	9	VAL
23	D1	11	LEU
23	D1	27	ASP
23	D1	32	VAL
23	D1	41	GLU
23	D1	49	GLU
23	D1	52	THR
23	D1	61	SER
23	D1	62	ARG
23	D1	68	SER
23	D1	69	LEU
23	D1	78	LEU
23	D1	80	LYS
24	D2	6	VAL
24	D2	7	LEU
24	D2	24	GLN
24	D2	25	VAL
24	D2	26	LEU
24	D2	29	PRO
24	D2	30	SER
24	D2	36	LYS
24	D2	47	ILE
24	D2	51	GLU
24	D2	53	ILE
24	D2	65	LEU
24	D2	70	ASN
24	D2	81	VAL
24	D2	87	GLU
24	D2	93	LEU
24	D2	97	ARG
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR
24	D2	114	GLU
24	D2	121	VAL
24	D2	122	SER
24	D2	125	ILE
24	D2	129	VAL
25	D3	5	LYS

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Mol	Chain	Res	Type
25	D3	7	ARG
25	D3	9	LEU
25	D3	14	LYS
25	D3	16	ARG
25	D3	19	ARG
25	D3	23	ARG
25	D3	33	LEU
25	D3	47	SER
25	D3	62	LYS
25	D3	69	ARG
25	D3	84	THR
25	D3	90	ASP
25	D3	97	ASP
25	D3	103	LEU
25	D3	107	PHE
25	D3	109	ARG
25	D3	114	LYS
25	D3	117	ILE
25	D3	128	SER
25	D3	131	SER
25	D3	140	LYS
26	D4	5	VAL
26	D4	21	LYS
26	D4	34	ASN
26	D4	36	SER
26	D4	42	GLU
26	D4	46	GLU
26	D4	51	GLU
26	D4	55	VAL
26	D4	57	VAL
26	D4	61	ARG
26	D4	62	THR
26	D4	69	SER
26	D4	74	LEU
26	D4	75	VAL
26	D4	81	GLU
26	D4	84	LYS
26	D4	88	THR
26	D4	102	LYS
26	D4	105	ARG
26	D4	112	LYS
26	D4	117	LYS

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Mol	Chain	Res	Type
26	D4	123	LYS
26	D4	124	ARG
27	D5	37	GLN
27	D5	42	LEU
27	D5	43	ASP
27	D5	48	ASP
27	D5	58	ARG
27	D5	59	TYR
27	D5	60	VAL
27	D5	63	SER
27	D5	67	ASP
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	85	LYS
27	D5	95	HIS
27	D5	96	SER
27	D5	100	ILE
27	D5	105	THR
28	D6	7	SER
28	D6	12	LYS
28	D6	15	ARG
28	D6	30	ILE
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	45	VAL
28	D6	64	LEU
28	D6	67	THR
28	D6	68	TYR
28	D6	69	ASN
28	D6	71	LEU
28	D6	83	ILE
28	D6	85	ARG
28	D6	87	ARG
28	D6	88	SER
28	D6	91	ASP
29	D7	3	LEU
29	D7	20	LYS
29	D7	33	LEU
29	D7	41	LEU
29	D7	44	THR

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Mol	Chain	Res	Type
29	D7	55	THR
29	D7	56	CYS
29	D7	60	SER
29	D7	61	THR
29	D7	62	ILE
30	D8	13	ILE
30	D8	14	LYS
30	D8	15	VAL
30	D8	19	THR
30	D8	31	GLU
30	D8	33	LEU
30	D8	38	ARG
30	D8	39	THR
30	D8	40	ILE
30	D8	48	VAL
30	D8	49	ARG
30	D8	58	GLU
30	D8	64	ARG
30	D8	65	ARG
31	D9	5	ASN
31	D9	7	TRP
31	D9	12	ARG
31	D9	18	SER
31	D9	22	ARG
31	D9	30	LEU
31	D9	32	ARG
31	D9	36	LEU
31	D9	39	CYS
32	E0	8	LEU
32	E0	16	SER
32	E0	20	LYS
32	E0	21	VAL
32	E0	22	GLU
32	E0	24	THR
32	E0	28	LYS
32	E0	31	LYS
32	E0	37	ARG
32	E0	39	LEU
32	E0	41	THR
32	E0	42	ARG
32	E0	43	ARG
32	E0	47	VAL

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Mol	Chain	Res	Type
32	E0	56	MET
33	E1	83	LYS
33	E1	84	VAL
33	E1	85	TYR
33	E1	86	THR
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
33	E1	100	LEU
33	E1	109	ASP
33	E1	113	LYS
33	E1	118	ARG
33	E1	120	GLU
33	E1	130	VAL
33	E1	137	ASP
33	E1	143	LYS
33	E1	147	VAL
33	E1	149	LYS
33	E1	150	VAL
33	E1	151	ASN
34	SR	5	GLU
34	SR	10	ARG
34	SR	25	THR
34	SR	29	GLN
34	SR	52	GLN
34	SR	59	ARG
34	SR	60	SER
34	SR	62	LYS
34	SR	76	ASP
34	SR	81	LEU
34	SR	82	SER
34	SR	87	LYS
34	SR	91	LEU
34	SR	94	VAL
34	SR	117	LYS
34	SR	136	ILE
34	SR	137	LYS
34	SR	144	LEU
34	SR	163	ASP
34	SR	166	SER
34	SR	188	ILE

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Mol	Chain	Res	Type
34	SR	191	ASP
34	SR	196	ASN
34	SR	199	ILE
34	SR	213	SER
34	SR	238	ASP
34	SR	248	ASN
34	SR	268	GLN
34	SR	277	GLU
34	SR	292	LEU
34	SR	300	THR
34	SR	308	ASN
34	SR	314	GLN
35	SM	28	SER
35	SM	33	LYS
35	SM	41	SER
35	SM	45	SER
35	SM	46	LYS
35	SM	51	ARG
35	SM	53	ARG
35	SM	61	ILE
35	SM	64	LYS
35	SM	65	THR
35	SM	68	ARG
35	SM	69	ARG
35	SM	72	ARG
35	SM	78	ASP
35	SM	84	LYS
35	SM	85	SER
35	SM	88	ARG
35	SM	89	ARG
35	SM	91	THR
35	SM	96	ARG
35	SM	100	THR
35	SM	102	THR
35	SM	105	LYS
35	SM	116	GLU
35	SM	117	LEU
35	SM	121	LYS
35	SM	131	ILE
35	SM	133	GLU
35	SM	139	GLU
39	L2	14	SER

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Mol	Chain	Res	Type
39	L2	20	THR
39	L2	32	LEU
39	L2	44	ILE
39	L2	45	VAL
39	L2	49	VAL
39	L2	52	SER
39	L2	62	VAL
39	L2	70	ARG
39	L2	71	LEU
39	L2	73	GLU
39	L2	74	GLU
39	L2	79	ASN
39	L2	96	LEU
39	L2	101	VAL
39	L2	104	LEU
39	L2	114	SER
39	L2	130	SER
39	L2	135	ILE
39	L2	158	ILE
39	L2	165	VAL
39	L2	177	LYS
39	L2	179	LEU
39	L2	180	LEU
39	L2	181	LYS
39	L2	188	LYS
39	L2	191	LEU
39	L2	202	VAL
39	L2	206	PRO
39	L2	207	VAL
39	L2	226	SER
39	L2	227	ARG
39	L2	230	VAL
39	L2	241	ARG
39	L2	247	ARG
40	L3	2	SER
40	L3	10	ARG
40	L3	17	LEU
40	L3	19	ARG
40	L3	25	ILE
40	L3	30	LYS
40	L3	34	LYS
40	L3	37	ARG

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Mol	Chain	Res	Type
40	L3	39	LYS
40	L3	47	LEU
40	L3	56	ILE
40	L3	65	SER
40	L3	79	VAL
40	L3	84	VAL
40	L3	85	VAL
40	L3	100	ARG
40	L3	103	THR
40	L3	110	LEU
40	L3	111	SER
40	L3	114	VAL
40	L3	116	ARG
40	L3	124	LYS
40	L3	134	SER
40	L3	139	GLN
40	L3	140	ASP
40	L3	146	ARG
40	L3	147	GLU
40	L3	148	LEU
40	L3	157	VAL
40	L3	160	VAL
40	L3	167	ARG
40	L3	169	THR
40	L3	173	GLN
40	L3	183	LEU
40	L3	188	ILE
40	L3	192	VAL
40	L3	201	LYS
40	L3	202	THR
40	L3	205	VAL
40	L3	210	GLU
40	L3	221	THR
40	L3	229	VAL
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	238	LEU
40	L3	242	THR
40	L3	252	ILE
40	L3	261	MET
40	L3	277	SER

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Mol	Chain	Res	Type
40	L3	284	ARG
40	L3	297	SER
40	L3	304	THR
40	L3	305	ILE
40	L3	317	ILE
40	L3	319	ASN
40	L3	320	ASP
40	L3	324	VAL
40	L3	328	ILE
40	L3	332	ARG
40	L3	337	THR
40	L3	338	LEU
40	L3	341	SER
40	L3	346	THR
40	L3	352	GLU
40	L3	355	SER
40	L3	364	LYS
40	L3	382	THR
41	L4	14	GLU
41	L4	20	LEU
41	L4	25	VAL
41	L4	40	THR
41	L4	60	THR
41	L4	71	VAL
41	L4	74	ILE
41	L4	85	SER
41	L4	93	MET
41	L4	98	ARG
41	L4	99	MET
41	L4	108	LYS
41	L4	112	LYS
41	L4	117	GLU
41	L4	133	SER
41	L4	136	LEU
41	L4	148	ILE
41	L4	150	LEU
41	L4	156	LEU
41	L4	161	LYS
41	L4	163	LYS
41	L4	176	SER
41	L4	177	ASP
41	L4	179	LEU

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Mol	Chain	Res	Type
41	L4	187	LEU
41	L4	188	ARG
41	L4	193	LYS
41	L4	198	ARG
41	L4	200	THR
41	L4	201	GLN
41	L4	203	ARG
41	L4	206	LEU
41	L4	220	ARG
41	L4	222	VAL
41	L4	230	VAL
41	L4	232	SER
41	L4	233	LEU
41	L4	246	ARG
41	L4	258	LEU
41	L4	267	VAL
41	L4	270	SER
41	L4	283	THR
41	L4	287	THR
41	L4	292	SER
41	L4	293	SER
41	L4	306	THR
41	L4	307	GLN
41	L4	311	HIS
41	L4	313	LEU
41	L4	314	LYS
41	L4	323	VAL
41	L4	332	LYS
41	L4	337	GLU
41	L4	339	LEU
41	L4	343	LYS
41	L4	346	LYS
41	L4	349	THR
41	L4	356	THR
41	L4	359	LEU
42	L5	5	LYS
42	L5	23	ARG
42	L5	35	ARG
42	L5	41	LYS
42	L5	66	SER
42	L5	67	SER
42	L5	68	THR

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Mol	Chain	Res	Type
42	L5	69	ILE
42	L5	75	LEU
42	L5	81	HIS
42	L5	89	THR
42	L5	90	HIS
42	L5	101	THR
42	L5	105	ILE
42	L5	109	THR
42	L5	112	LYS
42	L5	115	LEU
42	L5	118	THR
42	L5	122	VAL
42	L5	124	GLU
42	L5	131	LEU
42	L5	132	THR
42	L5	140	ARG
42	L5	144	VAL
42	L5	146	LEU
42	L5	148	ILE
42	L5	151	GLN
42	L5	154	THR
42	L5	155	THR
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE
42	L5	188	GLU
42	L5	193	GLU
42	L5	194	LEU
42	L5	203	HIS
42	L5	211	LEU
42	L5	216	GLU
42	L5	217	GLU
42	L5	227	LEU
42	L5	236	LEU
42	L5	242	SER
42	L5	257	GLU
42	L5	259	LYS
42	L5	261	THR
42	L5	273	ARG
42	L5	274	GLN
42	L5	275	THR
42	L5	276	LYS

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Mol	Chain	Res	Type
42	L5	279	LYS
42	L5	293	LEU
43	L6	2	SER
43	L6	5	LYS
43	L6	8	LYS
43	L6	9	TRP
43	L6	15	VAL
43	L6	21	THR
43	L6	23	LYS
43	L6	31	ARG
43	L6	35	VAL
43	L6	52	VAL
43	L6	59	GLU
43	L6	64	LEU
43	L6	70	LYS
43	L6	76	LEU
43	L6	78	ARG
43	L6	79	VAL
43	L6	89	THR
43	L6	93	VAL
43	L6	98	VAL
43	L6	129	GLU
43	L6	134	ARG
43	L6	146	ILE
43	L6	152	THR
43	L6	155	LEU
43	L6	160	SER
43	L6	162	SER
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	38	LYS
44	L7	39	GLU
44	L7	45	LEU
44	L7	52	GLN
44	L7	60	ARG
44	L7	77	VAL
44	L7	82	LYS
44	L7	83	LEU
44	L7	92	ILE
44	L7	98	LYS
44	L7	100	ARG

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Mol	Chain	Res	Type
44	L7	110	ARG
44	L7	121	LYS
44	L7	124	LEU
44	L7	143	THR
44	L7	150	LYS
44	L7	157	ASN
44	L7	158	LYS
44	L7	164	SER
44	L7	178	ILE
44	L7	179	LEU
44	L7	184	LEU
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	27	THR
45	L8	41	GLN
45	L8	63	LYS
45	L8	65	LEU
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	81	THR
45	L8	84	ARG
45	L8	92	LYS
45	L8	136	LEU
45	L8	145	ASN
45	L8	149	LYS
45	L8	150	LEU
45	L8	155	ASN
45	L8	156	ASP
45	L8	160	ILE
45	L8	169	LEU
45	L8	183	LYS
45	L8	185	ARG
45	L8	189	LEU
45	L8	197	VAL
45	L8	203	VAL
45	L8	206	GLU
45	L8	214	LEU
45	L8	241	LYS
45	L8	246	MET
45	L8	248	LYS

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Mol	Chain	Res	Type
46	L9	4	ILE
46	L9	5	GLN
46	L9	6	THR
46	L9	14	GLU
46	L9	16	VAL
46	L9	19	SER
46	L9	22	SER
46	L9	33	THR
46	L9	35	THR
46	L9	36	LYS
46	L9	39	LYS
46	L9	41	ILE
46	L9	52	LEU
46	L9	55	VAL
46	L9	62	ARG
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	80	THR
46	L9	82	VAL
46	L9	84	LYS
46	L9	103	ILE
46	L9	118	LEU
46	L9	133	THR
46	L9	135	GLU
46	L9	137	SER
46	L9	138	THR
46	L9	139	ASN
46	L9	151	VAL
46	L9	157	ASN
46	L9	161	LEU
46	L9	164	ILE
46	L9	172	ILE
46	L9	173	ARG
46	L9	188	THR
46	L9	189	GLU
46	L9	190	ASP
46	L9	191	LEU
47	M0	3	ARG
47	M0	21	ARG
47	M0	24	ARG
47	M0	30	LYS

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Mol	Chain	Res	Type
47	M0	32	ARG
47	M0	33	ILE
47	M0	34	TYR
47	M0	39	LYS
47	M0	40	LYS
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	57	LEU
47	M0	77	THR
47	M0	87	LEU
47	M0	90	ARG
47	M0	91	VAL
47	M0	99	ILE
47	M0	101	LYS
47	M0	121	LYS
47	M0	137	SER
47	M0	138	VAL
47	M0	139	ARG
47	M0	140	THR
47	M0	145	LYS
47	M0	163	GLN
47	M0	165	ILE
47	M0	166	ILE
47	M0	168	SER
47	M0	177	ASP
47	M0	184	LYS
47	M0	186	GLU
47	M0	189	GLU
47	M0	200	LEU
47	M0	203	LYS
47	M0	205	SER
47	M0	210	ILE
48	M1	7	ASN
48	M1	9	MET
48	M1	10	ARG
48	M1	12	LEU
48	M1	13	LYS
48	M1	17	LEU
48	M1	23	VAL
48	M1	25	GLU
48	M1	31	THR

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Mol	Chain	Res	Type
48	M1	38	GLU
48	M1	39	GLN
48	M1	40	LEU
48	M1	44	THR
48	M1	46	VAL
48	M1	52	TYR
48	M1	65	ILE
48	M1	70	THR
48	M1	74	PRO
48	M1	78	GLU
48	M1	80	LEU
48	M1	82	ARG
48	M1	94	ARG
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	115	LYS
48	M1	126	ASP
48	M1	130	VAL
48	M1	140	ARG
48	M1	142	LYS
48	M1	145	LYS
48	M1	166	LYS
48	M1	173	ASP
49	M3	23	LYS
49	M3	35	ARG
49	M3	41	THR
49	M3	46	ILE
49	M3	54	LEU
49	M3	55	ARG
49	M3	58	VAL
49	M3	59	ARG
49	M3	63	VAL
49	M3	67	ARG
49	M3	69	VAL
49	M3	85	LEU
49	M3	114	GLN
49	M3	115	ARG
49	M3	121	SER
49	M3	124	ILE
49	M3	131	LYS
49	M3	138	VAL

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Mol	Chain	Res	Type
49	M3	154	VAL
49	M3	164	GLU
49	M3	168	ARG
49	M3	171	ARG
49	M3	174	ARG
49	M3	190	LYS
49	M3	192	GLU
49	M3	194	GLU
50	M4	8	LYS
50	M4	15	VAL
50	M4	20	VAL
50	M4	27	GLN
50	M4	38	ILE
50	M4	53	VAL
50	M4	63	VAL
50	M4	64	VAL
50	M4	72	LEU
50	M4	92	GLU
50	M4	98	SER
50	M4	102	LYS
50	M4	105	GLN
50	M4	106	ARG
50	M4	108	ARG
50	M4	113	THR
50	M4	125	LYS
50	M4	130	THR
50	M4	135	LEU
51	M5	7	LEU
51	M5	10	LEU
51	M5	19	LEU
51	M5	22	LEU
51	M5	33	LYS
51	M5	38	ARG
51	M5	49	ARG
51	M5	50	ARG
51	M5	68	ARG
51	M5	80	THR
51	M5	84	PRO
51	M5	85	THR
51	M5	92	LEU
51	M5	96	ARG
51	M5	98	LEU

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Mol	Chain	Res	Type
51	M5	109	ARG
51	M5	113	LEU
51	M5	117	ASN
51	M5	124	ASP
51	M5	133	ILE
51	M5	138	GLN
51	M5	151	ILE
51	M5	155	VAL
51	M5	157	LYS
51	M5	170	LYS
51	M5	171	SER
51	M5	183	THR
51	M5	187	ARG
51	M5	190	THR
51	M5	201	ARG
52	M6	22	VAL
52	M6	25	LYS
52	M6	33	ILE
52	M6	59	ARG
52	M6	68	ARG
52	M6	74	ARG
52	M6	77	SER
52	M6	78	ARG
52	M6	84	LEU
52	M6	85	ARG
52	M6	88	VAL
52	M6	106	GLU
52	M6	111	PRO
52	M6	116	LYS
52	M6	117	ARG
52	M6	122	GLN
52	M6	124	LEU
52	M6	126	VAL
52	M6	128	ARG
52	M6	129	LEU
52	M6	144	SER
52	M6	152	VAL
52	M6	160	ARG
52	M6	175	THR
52	M6	184	THR
52	M6	190	VAL
53	M7	9	THR

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Mol	Chain	Res	Type
53	M7	14	SER
53	M7	24	VAL
53	M7	29	THR
53	M7	32	THR
53	M7	36	ILE
53	M7	40	GLU
53	M7	41	LEU
53	M7	46	LYS
53	M7	52	LEU
53	M7	53	ASP
53	M7	56	ARG
53	M7	70	THR
53	M7	78	VAL
53	M7	94	LEU
53	M7	107	LEU
53	M7	112	LEU
53	M7	120	ASN
53	M7	126	ARG
53	M7	127	ARG
53	M7	136	ILE
53	M7	141	SER
53	M7	142	SER
53	M7	144	SER
53	M7	157	VAL
53	M7	168	LEU
53	M7	175	ARG
53	M7	180	LYS
53	M7	181	ARG
54	M8	3	ILE
54	M8	11	LYS
54	M8	17	THR
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	34	THR
54	M8	49	LEU
54	M8	57	ILE
54	M8	63	SER
54	M8	64	VAL
54	M8	66	ARG
54	M8	73	GLN
54	M8	74	GLU

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Mol	Chain	Res	Type
54	M8	80	THR
54	M8	86	THR
54	M8	95	GLU
54	M8	100	THR
54	M8	120	GLU
54	M8	122	ILE
54	M8	127	LEU
54	M8	135	GLN
54	M8	141	ARG
54	M8	150	VAL
54	M8	168	THR
54	M8	179	ARG
54	M8	180	ARG
54	M8	181	SER
55	M9	8	LYS
55	M9	17	VAL
55	M9	29	THR
55	M9	41	ILE
55	M9	44	LEU
55	M9	52	LYS
55	M9	53	LYS
55	M9	55	VAL
55	M9	60	LYS
55	M9	74	ARG
55	M9	81	ARG
55	M9	82	LYS
55	M9	99	LEU
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	110	ARG
55	M9	114	LYS
55	M9	115	ILE
55	M9	134	HIS
55	M9	138	LEU
55	M9	144	GLN
55	M9	146	LYS
55	M9	156	ASN
55	M9	164	LEU
55	M9	172	ARG
55	M9	175	GLN
55	M9	180	LYS

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Mol	Chain	Res	Type
55	M9	182	ASP
56	N0	1	MET
56	N0	3	HIS
56	N0	8	GLN
56	N0	13	ARG
56	N0	17	GLU
56	N0	39	SER
56	N0	45	LEU
56	N0	57	GLU
56	N0	58	ILE
56	N0	61	ILE
56	N0	63	GLN
56	N0	80	ARG
56	N0	85	SER
56	N0	87	THR
56	N0	92	LYS
56	N0	97	VAL
56	N0	100	VAL
56	N0	105	THR
56	N0	115	ARG
56	N0	117	ARG
56	N0	125	LYS
56	N0	136	LYS
56	N0	137	ARG
56	N0	138	GLN
56	N0	142	GLN
56	N0	155	ARG
56	N0	157	GLN
56	N0	162	THR
56	N0	169	SER
56	N0	172	TYR
57	N1	9	SER
57	N1	16	GLN
57	N1	25	VAL
57	N1	26	HIS
57	N1	27	LEU
57	N1	32	LYS
57	N1	43	LYS
57	N1	52	MET
57	N1	55	LYS
57	N1	68	THR
57	N1	75	ILE

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Mol	Chain	Res	Type
57	N1	76	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	83	ARG
57	N1	88	ARG
57	N1	89	LEU
57	N1	96	ILE
57	N1	103	GLN
57	N1	104	GLU
57	N1	106	LEU
57	N1	118	GLU
57	N1	122	GLN
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	129	LYS
57	N1	136	ARG
57	N1	139	ARG
57	N1	140	ILE
57	N1	143	THR
57	N1	147	VAL
57	N1	149	GLN
57	N1	158	THR
57	N1	159	PHE
58	N2	10	LYS
58	N2	38	ILE
58	N2	39	ASP
58	N2	52	ASN
58	N2	61	THR
58	N2	62	VAL
58	N2	66	VAL
58	N2	88	GLN
58	N2	104	ARG
58	N2	105	LEU
59	N3	13	ILE
59	N3	32	ARG
59	N3	34	LEU
59	N3	42	SER
59	N3	45	ARG
59	N3	48	ARG
59	N3	54	LEU
59	N3	63	LYS

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Mol	Chain	Res	Type
59	N3	64	LYS
59	N3	69	LEU
59	N3	72	LYS
59	N3	73	VAL
59	N3	74	MET
59	N3	83	LYS
59	N3	91	VAL
59	N3	97	ASP
59	N3	102	ILE
59	N3	110	LYS
59	N3	115	THR
59	N3	125	LEU
59	N3	128	ARG
60	N4	5	ILE
60	N4	17	ARG
60	N4	19	THR
60	N4	39	LEU
60	N4	45	ASN
61	N5	26	VAL
61	N5	27	ARG
61	N5	34	LEU
61	N5	38	LEU
61	N5	39	LYS
61	N5	40	LEU
61	N5	45	LYS
61	N5	48	SER
61	N5	49	LYS
61	N5	59	SER
61	N5	63	ILE
61	N5	71	THR
61	N5	86	VAL
61	N5	92	LYS
61	N5	108	LEU
61	N5	109	LYS
61	N5	115	ARG
61	N5	125	ARG
61	N5	127	THR
61	N5	129	ASP
61	N5	137	ASN
61	N5	138	ARG
61	N5	139	ILE
61	N5	142	ILE

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Mol	Chain	Res	Type
62	N6	3	LYS
62	N6	5	SER
62	N6	8	VAL
62	N6	10	SER
62	N6	13	ARG
62	N6	17	LYS
62	N6	36	SER
62	N6	37	LYS
62	N6	38	GLU
62	N6	39	LEU
62	N6	45	ILE
62	N6	50	ILE
62	N6	55	GLU
62	N6	56	VAL
62	N6	57	LEU
62	N6	62	SER
62	N6	64	LYS
62	N6	70	ILE
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	83	ASP
62	N6	88	GLU
62	N6	90	VAL
62	N6	95	VAL
62	N6	105	VAL
62	N6	112	ASP
62	N6	115	ARG
62	N6	126	LEU
62	N6	127	GLU
63	N7	14	VAL
63	N7	15	ARG
63	N7	17	ARG
63	N7	24	VAL
63	N7	26	VAL
63	N7	30	ASP
63	N7	34	LYS
63	N7	46	ILE
63	N7	51	LEU
63	N7	54	THR
63	N7	56	LYS
63	N7	72	ILE

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Mol	Chain	Res	Type
63	N7	75	VAL
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	87	LEU
63	N7	89	VAL
63	N7	93	LYS
63	N7	95	VAL
63	N7	98	THR
63	N7	99	GLU
63	N7	102	GLU
63	N7	103	GLN
63	N7	107	ARG
63	N7	108	GLU
63	N7	109	GLU
63	N7	123	GLN
63	N7	134	LEU
63	N7	135	ARG
64	N8	4	ARG
64	N8	6	THR
64	N8	7	LYS
64	N8	8	THR
64	N8	10	LYS
64	N8	19	LYS
64	N8	27	LYS
64	N8	34	MET
64	N8	46	ASP
64	N8	56	VAL
64	N8	60	TYR
64	N8	76	ASP
64	N8	78	LEU
64	N8	84	GLU
64	N8	88	ASP
64	N8	91	LEU
64	N8	92	LYS
64	N8	115	LYS
64	N8	118	ILE
64	N8	120	ASN
64	N8	123	VAL
64	N8	130	VAL
64	N8	133	LEU
65	N9	17	HIS

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Mol	Chain	Res	Type
65	N9	18	ARG
65	N9	21	ILE
65	N9	22	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	33	LYS
65	N9	40	ARG
65	N9	50	THR
65	N9	58	LYS
65	N9	59	LYS
66	O0	16	LEU
66	O0	20	SER
66	O0	30	THR
66	O0	32	LYS
66	O0	40	LYS
66	O0	41	LEU
66	O0	61	MET
66	O0	66	LYS
66	O0	83	LYS
66	O0	84	LEU
66	O0	86	ARG
66	O0	87	VAL
66	O0	99	ASP
66	O0	101	LEU
67	O1	8	VAL
67	O1	11	GLU
67	O1	13	THR
67	O1	16	LEU
67	O1	18	LYS
67	O1	24	SER
67	O1	26	LYS
67	O1	31	ARG
67	O1	46	THR
67	O1	55	LEU
67	O1	64	VAL
67	O1	68	GLU
67	O1	79	ARG
67	O1	84	ASP
67	O1	86	LYS
67	O1	96	VAL
67	O1	100	SER
67	O1	104	LEU

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Mol	Chain	Res	Type
67	O1	106	THR
67	O1	107	VAL
67	O1	110	GLU
68	O2	3	SER
68	O2	4	LEU
68	O2	16	LYS
68	O2	19	ARG
68	O2	21	HIS
68	O2	33	ARG
68	O2	41	VAL
68	O2	51	SER
68	O2	52	GLN
68	O2	54	LYS
68	O2	61	LYS
68	O2	62	LYS
68	O2	72	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	76	VAL
68	O2	82	LEU
68	O2	84	THR
68	O2	87	MET
68	O2	106	VAL
68	O2	109	LEU
68	O2	111	ARG
68	O2	128	LEU
69	O3	4	SER
69	O3	15	SER
69	O3	33	GLU
69	O3	48	ARG
69	O3	59	VAL
69	O3	67	MET
69	O3	70	LYS
69	O3	80	VAL
69	O3	92	LYS
69	O3	93	THR
69	O3	98	VAL
69	O3	106	ASN
70	O4	3	GLN
70	O4	5	VAL
70	O4	8	ARG
70	O4	20	ILE

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Mol	Chain	Res	Type
70	O4	21	LYS
70	O4	24	LYS
70	O4	47	CYS
70	O4	51	LEU
70	O4	56	THR
70	O4	58	ARG
70	O4	65	VAL
70	O4	71	THR
70	O4	72	VAL
70	O4	86	LYS
70	O4	90	ILE
70	O4	103	LYS
70	O4	104	VAL
70	O4	107	GLU
71	O5	4	VAL
71	O5	5	LYS
71	O5	14	LYS
71	O5	20	GLN
71	O5	21	LEU
71	O5	27	GLU
71	O5	28	LEU
71	O5	31	LEU
71	O5	36	LEU
71	O5	40	SER
71	O5	41	LEU
71	O5	44	ILE
71	O5	46	THR
71	O5	48	ARG
71	O5	49	LYS
71	O5	50	SER
71	O5	62	GLN
71	O5	68	GLN
71	O5	71	LYS
71	O5	73	LYS
71	O5	74	LYS
71	O5	85	THR
71	O5	86	ARG
71	O5	89	ARG
71	O5	90	ARG
71	O5	99	GLN
71	O5	101	THR
71	O5	102	GLU

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Mol	Chain	Res	Type
71	O5	104	GLN
71	O5	107	LYS
71	O5	115	LYS
71	O5	119	LYS
72	O6	3	VAL
72	O6	11	LEU
72	O6	16	LYS
72	O6	18	THR
72	O6	25	LYS
72	O6	26	ILE
72	O6	34	SER
72	O6	36	ARG
72	O6	45	ARG
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	62	ARG
72	O6	68	ARG
72	O6	75	LYS
72	O6	76	ARG
72	O6	81	THR
72	O6	88	GLU
72	O6	89	GLU
72	O6	90	MET
72	O6	98	ARG
72	O6	99	ARG
72	O6	100	HIS
73	O7	5	THR
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	45	ARG
73	O7	59	THR
73	O7	65	ARG
73	O7	67	LEU
73	O7	79	GLN
73	O7	85	LYS
73	O7	87	SER
74	O8	22	THR
74	O8	24	THR
74	O8	31	LEU

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Mol	Chain	Res	Type
74	O8	32	ASN
74	O8	33	LYS
74	O8	41	THR
74	O8	46	ARG
74	O8	51	LEU
74	O8	53	THR
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	72	THR
74	O8	77	ARG
74	O8	78	LEU
75	O9	4	GLN
75	O9	5	LYS
75	O9	21	ARG
75	O9	23	LEU
75	O9	29	LEU
75	O9	34	THR
75	O9	36	ARG
75	O9	45	ARG
75	O9	51	ILE
76	Q0	77	ILE
76	Q0	78	ILE
76	Q0	83	LYS
76	Q0	85	LEU
76	Q0	91	CYS
76	Q0	108	THR
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	127	LEU
76	Q0	128	LYS
77	Q1	9	ARG
77	Q1	10	THR
77	Q1	16	LYS
77	Q1	19	LYS
77	Q1	21	ARG
77	Q1	24	SER
78	Q2	4	VAL
78	Q2	22	GLN
78	Q2	27	GLN
78	Q2	29	LYS
78	Q2	38	GLN

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Mol	Chain	Res	Type
78	Q2	47	GLN
78	Q2	55	LYS
78	Q2	60	LYS
78	Q2	75	VAL
78	Q2	76	LYS
78	Q2	78	LYS
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	88	CYS
78	Q2	93	LEU
78	Q2	100	LYS
79	Q3	6	LYS
79	Q3	7	LYS
79	Q3	11	THR
79	Q3	21	SER
79	Q3	25	GLN
79	Q3	28	LYS
79	Q3	32	GLN
79	Q3	45	LYS
79	Q3	56	THR
79	Q3	59	CYS
79	Q3	60	CYS
79	Q3	64	VAL
79	Q3	73	THR
79	Q3	78	THR
79	Q3	84	ARG
2	s0	6	THR
2	s0	9	LEU
2	s0	10	THR
2	s0	18	LEU
2	s0	24	LEU
2	s0	27	ARG
2	s0	28	ASN
2	s0	29	VAL
2	s0	32	HIS
2	s0	34	GLU
2	s0	41	ARG
2	s0	45	VAL
2	s0	48	ILE
2	s0	50	VAL
2	s0	59	LEU

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Mol	Chain	Res	Type
2	s0	62	ARG
2	s0	72	ASP
2	s0	79	ARG
2	s0	87	LEU
2	s0	88	LYS
2	s0	93	THR
2	s0	96	THR
2	s0	106	SER
2	s0	110	TYR
2	s0	111	ILE
2	s0	112	THR
2	s0	124	THR
2	s0	131	GLN
2	s0	139	VAL
2	s0	144	ILE
2	s0	146	LEU
2	s0	151	SER
2	s0	153	SER
2	s0	154	GLU
2	s0	156	VAL
2	s0	158	VAL
2	s0	164	ASN
2	s0	172	LEU
2	s0	183	ARG
2	s0	184	LEU
2	s0	185	ARG
2	s0	188	LEU
2	s0	189	VAL
2	s0	197	ILE
2	s0	198	MET
3	s1	25	THR
3	s1	37	THR
3	s1	47	LEU
3	s1	51	SER
3	s1	55	LYS
3	s1	62	LYS
3	s1	65	VAL
3	s1	68	VAL
3	s1	70	LEU
3	s1	73	LEU
3	s1	81	PHE
3	s1	82	ARG

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Mol	Chain	Res	Type
3	s1	87	ARG
3	s1	97	LEU
3	s1	106	THR
3	s1	110	LEU
3	s1	125	VAL
3	s1	126	THR
3	s1	127	VAL
3	s1	129	THR
3	s1	136	ARG
3	s1	150	VAL
3	s1	159	SER
3	s1	173	THR
3	s1	175	GLU
3	s1	180	THR
3	s1	181	LEU
3	s1	183	GLN
3	s1	185	THR
3	s1	193	ILE
3	s1	195	LYS
3	s1	212	VAL
3	s1	215	VAL
3	s1	217	LEU
3	s1	219	LYS
3	s1	223	PHE
3	s1	225	VAL
3	s1	228	LEU
3	s1	229	MET
3	s1	234	GLU
4	s2	41	LEU
4	s2	46	LYS
4	s2	51	THR
4	s2	52	THR
4	s2	53	ILE
4	s2	55	GLU
4	s2	58	LEU
4	s2	60	SER
4	s2	69	ILE
4	s2	70	ASP
4	s2	72	LEU
4	s2	73	LEU
4	s2	77	GLN
4	s2	80	VAL

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Mol	Chain	Res	Type
4	s2	81	MET
4	s2	83	ILE
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	94	GLN
4	s2	97	ARG
4	s2	111	VAL
4	s2	113	LEU
4	s2	116	LYS
4	s2	117	THR
4	s2	141	ARG
4	s2	148	LEU
4	s2	150	GLN
4	s2	159	THR
4	s2	161	LYS
4	s2	164	SER
4	s2	165	VAL
4	s2	186	LYS
4	s2	195	ASP
4	s2	198	THR
4	s2	201	ASN
4	s2	206	THR
4	s2	208	GLU
4	s2	222	TYR
4	s2	225	LEU
4	s2	226	THR
4	s2	229	LEU
4	s2	233	GLN
4	s2	238	SER
4	s2	244	SER
4	s2	245	ASP
5	s3	9	ARG
5	s3	21	LEU
5	s3	35	SER
5	s3	39	VAL
5	s3	44	THR
5	s3	46	THR
5	s3	59	LEU
5	s3	69	LEU
5	s3	70	THR

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Mol	Chain	Res	Type
5	s3	84	ILE
5	s3	90	ARG
5	s3	93	ASP
5	s3	115	ILE
5	s3	120	TYR
5	s3	125	TYR
5	s3	127	MET
5	s3	129	SER
5	s3	139	SER
5	s3	142	LEU
5	s3	158	ILE
5	s3	164	VAL
5	s3	172	THR
5	s3	176	LEU
5	s3	178	ARG
5	s3	179	GLN
5	s3	209	ILE
5	s3	210	GLU
5	s3	212	LYS
6	s4	7	LYS
6	s4	23	LEU
6	s4	29	PRO
6	s4	38	LEU
6	s4	39	ARG
6	s4	42	LEU
6	s4	48	LEU
6	s4	51	ARG
6	s4	67	GLN
6	s4	78	THR
6	s4	104	ASP
6	s4	108	ARG
6	s4	112	HIS
6	s4	116	ASP
6	s4	118	GLU
6	s4	123	LEU
6	s4	146	THR
6	s4	148	ARG
6	s4	160	VAL
6	s4	164	LEU
6	s4	170	THR
6	s4	180	LEU
6	s4	182	TYR

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Mol	Chain	Res	Type
6	s4	183	VAL
6	s4	200	ARG
6	s4	210	ILE
6	s4	214	LEU
6	s4	219	VAL
6	s4	221	ARG
6	s4	222	LEU
6	s4	246	LEU
7	s5	23	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	29	ILE
7	s5	31	GLU
7	s5	39	GLU
7	s5	41	LYS
7	s5	45	LYS
7	s5	59	VAL
7	s5	63	GLN
7	s5	68	ILE
7	s5	76	ARG
7	s5	79	ASN
7	s5	89	ILE
7	s5	90	ILE
7	s5	93	LEU
7	s5	94	THR
7	s5	99	MET
7	s5	102	ARG
7	s5	112	ARG
7	s5	119	ASP
7	s5	124	LEU
7	s5	125	THR
7	s5	126	ASP
7	s5	128	ASN
7	s5	148	ARG
7	s5	157	ARG
7	s5	160	VAL
7	s5	166	ARG
7	s5	170	GLN
7	s5	186	ASN
7	s5	190	ILE
7	s5	194	LEU
7	s5	199	ILE

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Mol	Chain	Res	Type
7	s5	203	LYS
7	s5	216	GLU
7	s5	217	LEU
7	s5	219	ARG
8	s6	18	ILE
8	s6	31	ARG
8	s6	65	GLN
8	s6	68	LEU
8	s6	73	ILE
8	s6	76	LEU
8	s6	97	VAL
8	s6	98	ARG
8	s6	108	VAL
8	s6	109	LEU
8	s6	121	LEU
8	s6	126	ASP
8	s6	127	THR
8	s6	128	THR
8	s6	143	LYS
8	s6	150	GLU
8	s6	151	ASP
8	s6	153	VAL
8	s6	157	VAL
8	s6	158	ILE
8	s6	162	VAL
8	s6	168	THR
8	s6	175	ILE
8	s6	177	ARG
8	s6	180	THR
8	s6	182	GLN
8	s6	191	ARG
8	s6	193	LEU
8	s6	201	GLN
8	s6	215	ARG
8	s6	216	LEU
8	s6	217	SER
9	s7	8	ILE
9	s7	9	LEU
9	s7	10	SER
9	s7	11	GLN
9	s7	14	THR
9	s7	28	GLU

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Mol	Chain	Res	Type
9	s7	33	GLU
9	s7	39	ARG
9	s7	42	GLN
9	s7	50	ASP
9	s7	55	LYS
9	s7	67	LEU
9	s7	75	THR
9	s7	80	GLU
9	s7	97	ARG
9	s7	103	SER
9	s7	105	THR
9	s7	106	SER
9	s7	114	ARG
9	s7	116	ARG
9	s7	118	LEU
9	s7	122	HIS
9	s7	129	LEU
9	s7	136	VAL
9	s7	159	VAL
9	s7	166	LEU
9	s7	168	SER
9	s7	184	GLU
9	s7	185	ILE
10	s8	10	LYS
10	s8	18	ARG
10	s8	22	ARG
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	46	VAL
10	s8	59	ARG
10	s8	61	GLU
10	s8	62	THR
10	s8	74	LYS
10	s8	76	THR
10	s8	94	ASN
10	s8	110	ARG
10	s8	120	THR
10	s8	135	LYS
10	s8	151	LYS
10	s8	155	SER
10	s8	158	SER

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Mol	Chain	Res	Type
10	s8	183	ILE
10	s8	184	LEU
10	s8	199	LYS
11	s9	3	ARG
11	s9	6	ARG
11	s9	7	THR
11	s9	9	SER
11	s9	16	LYS
11	s9	21	SER
11	s9	28	LEU
11	s9	49	LEU
11	s9	63	ASP
11	s9	78	ARG
11	s9	87	SER
11	s9	93	LEU
11	s9	101	VAL
11	s9	109	LEU
11	s9	126	ARG
11	s9	127	VAL
11	s9	130	THR
11	s9	133	HIS
11	s9	134	ILE
11	s9	149	ARG
11	s9	150	LEU
11	s9	151	ASP
11	s9	161	THR
11	s9	162	SER
11	s9	171	ARG
11	s9	172	VAL
11	s9	175	ARG
11	s9	182	GLU
12	c0	2	LEU
12	c0	5	LYS
12	c0	15	LEU
12	c0	20	VAL
12	c0	36	ASP
12	c0	49	LEU
12	c0	51	SER
12	c0	55	VAL
12	c0	57	THR
12	c0	70	GLU
12	c0	71	GLU

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Mol	Chain	Res	Type
13	c1	5	LEU
13	c1	10	GLU
13	c1	21	ASN
13	c1	22	ASN
13	c1	27	THR
13	c1	31	THR
13	c1	32	LYS
13	c1	33	ARG
13	c1	35	TYR
13	c1	40	LEU
13	c1	44	THR
13	c1	47	THR
13	c1	60	PHE
13	c1	64	VAL
13	c1	67	ARG
13	c1	69	LYS
13	c1	76	VAL
13	c1	77	SER
13	c1	86	ILE
13	c1	109	VAL
13	c1	112	SER
13	c1	116	ARG
13	c1	123	VAL
13	c1	129	ARG
13	c1	136	ARG
13	c1	138	ASN
13	c1	140	VAL
13	c1	143	SER
14	c2	30	VAL
14	c2	36	LEU
14	c2	37	VAL
14	c2	39	ASP
14	c2	52	LEU
14	c2	58	LEU
14	c2	59	LEU
14	c2	62	LEU
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	86	VAL
14	c2	89	ILE

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Mol	Chain	Res	Type
14	c2	91	VAL
14	c2	97	LEU
14	c2	103	LEU
14	c2	116	VAL
14	c2	125	ASN
14	c2	132	GLU
14	c2	133	LEU
14	c2	137	MET
14	c2	138	GLU
14	c2	140	PHE
15	c3	12	SER
15	c3	14	SER
15	c3	16	ILE
15	c3	20	ARG
15	c3	27	LYS
15	c3	39	LYS
15	c3	53	LEU
15	c3	64	ARG
15	c3	66	ILE
15	c3	70	LYS
15	c3	75	LEU
15	c3	80	LEU
15	c3	94	LYS
15	c3	97	SER
15	c3	103	GLU
15	c3	114	ARG
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	131	THR
15	c3	149	LEU
16	c4	13	VAL
16	c4	16	VAL
16	c4	18	ARG
16	c4	20	TYR
16	c4	26	THR
16	c4	33	LEU
16	c4	43	THR
16	c4	49	LYS
16	c4	61	MET
16	c4	65	GLN
16	c4	74	VAL

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Mol	Chain	Res	Type
16	c4	81	VAL
16	c4	102	LEU
16	c4	107	ARG
16	c4	114	ARG
16	c4	117	ASP
16	c4	118	VAL
16	c4	119	THR
16	c4	127	ARG
16	c4	133	ARG
16	c4	135	ARG
16	c4	136	ARG
16	c4	137	LEU
17	c5	10	ARG
17	c5	12	PHE
17	c5	21	ASP
17	c5	24	LYS
17	c5	27	GLU
17	c5	28	MET
17	c5	36	LEU
17	c5	44	ARG
17	c5	49	MET
17	c5	52	LYS
17	c5	69	GLU
17	c5	72	LYS
17	c5	77	ARG
17	c5	107	ILE
17	c5	110	GLU
17	c5	122	THR
17	c5	124	THR
17	c5	127	ARG
18	c6	7	VAL
18	c6	17	THR
18	c6	23	LYS
18	c6	28	LEU
18	c6	37	THR
18	c6	43	ILE
18	c6	48	VAL
18	c6	53	LEU
18	c6	54	LEU
18	c6	57	LEU
18	c6	58	ASP
18	c6	66	ARG

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Mol	Chain	Res	Type
18	c6	68	ARG
18	c6	69	VAL
18	c6	81	ILE
18	c6	82	ARG
18	c6	83	GLN
18	c6	94	GLN
18	c6	98	ASP
18	c6	107	LYS
18	c6	110	THR
18	c6	114	ARG
18	c6	115	THR
18	c6	117	LEU
18	c6	137	ARG
19	c7	3	ARG
19	c7	4	VAL
19	c7	5	ARG
19	c7	7	LYS
19	c7	8	THR
19	c7	29	GLN
19	c7	34	LEU
19	c7	40	THR
19	c7	45	ARG
19	c7	46	LEU
19	c7	62	GLN
19	c7	69	ILE
19	c7	72	LYS
19	c7	78	ARG
19	c7	110	VAL
19	c7	113	LEU
20	c8	2	SER
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	13	HIS
20	c8	14	ILE
20	c8	15	LEU
20	c8	20	THR
20	c8	25	ASN
20	c8	26	ILE
20	c8	33	THR
20	c8	40	ARG

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Mol	Chain	Res	Type
20	c8	57	ARG
20	c8	63	GLN
20	c8	66	LEU
20	c8	71	GLN
20	c8	77	THR
20	c8	88	ARG
20	c8	93	THR
20	c8	105	VAL
20	c8	107	SER
20	c8	110	ARG
20	c8	116	LEU
20	c8	117	LYS
20	c8	119	ILE
20	c8	136	GLN
20	c8	138	THR
20	c8	141	THR
20	c8	143	ARG
21	c9	20	SER
21	c9	28	LEU
21	c9	36	ILE
21	c9	37	VAL
21	c9	68	ARG
21	c9	70	GLN
21	c9	71	VAL
21	c9	75	LYS
21	c9	85	SER
21	c9	86	ARG
21	c9	88	VAL
21	c9	91	TYR
21	c9	111	ILE
21	c9	126	GLU
21	c9	132	LEU
21	c9	139	THR
21	c9	140	LEU
21	c9	141	GLU
21	c9	142	GLU
22	d0	12	GLN
22	d0	16	GLN
22	d0	22	ILE
22	d0	23	ARG
22	d0	25	THR
22	d0	27	THR

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Mol	Chain	Res	Type
22	d0	30	LYS
22	d0	34	LEU
22	d0	44	ASN
22	d0	47	GLN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	70	THR
22	d0	72	ASN
22	d0	74	GLU
22	d0	77	LYS
22	d0	89	ARG
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	104	THR
22	d0	107	THR
22	d0	108	ILE
22	d0	114	VAL
22	d0	115	GLU
23	d1	2	GLU
23	d1	5	LYS
23	d1	32	VAL
23	d1	34	ILE
23	d1	38	LYS
23	d1	49	GLU
23	d1	50	TYR
23	d1	52	THR
23	d1	61	SER
23	d1	62	ARG
23	d1	68	SER
23	d1	69	LEU
23	d1	75	ASN
23	d1	78	LEU
23	d1	80	LYS
23	d1	85	TYR
24	d2	6	VAL
24	d2	7	LEU
24	d2	15	ASN
24	d2	22	LYS
24	d2	23	ARG
24	d2	25	VAL

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Mol	Chain	Res	Type
24	d2	26	LEU
24	d2	65	LEU
24	d2	81	VAL
24	d2	85	ASP
24	d2	88	LYS
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	124	LYS
25	d3	9	LEU
25	d3	14	LYS
25	d3	17	VAL
25	d3	19	ARG
25	d3	23	ARG
25	d3	28	ASN
25	d3	36	THR
25	d3	40	SER
25	d3	46	SER
25	d3	55	GLU
25	d3	69	ARG
25	d3	72	VAL
25	d3	73	ARG
25	d3	75	GLN
25	d3	83	VAL
25	d3	84	THR
25	d3	96	VAL
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	109	ARG
25	d3	125	VAL
25	d3	133	LEU
25	d3	138	GLU
25	d3	139	LYS
26	d4	5	VAL
26	d4	10	ARG
26	d4	22	GLN
26	d4	28	LEU
26	d4	32	ARG
26	d4	36	SER
26	d4	42	GLU
26	d4	43	LYS

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Mol	Chain	Res	Type
26	d4	47	VAL
26	d4	49	LYS
26	d4	55	VAL
26	d4	62	THR
26	d4	74	LEU
26	d4	83	LYS
26	d4	88	THR
26	d4	92	VAL
26	d4	100	VAL
26	d4	104	SER
26	d4	112	LYS
26	d4	116	LYS
26	d4	128	LYS
26	d4	132	ARG
27	d5	41	ILE
27	d5	43	ASP
27	d5	46	LYS
27	d5	57	TYR
27	d5	81	ARG
27	d5	90	LYS
27	d5	93	SER
28	d6	3	LYS
28	d6	4	LYS
28	d6	10	ARG
28	d6	11	ASN
28	d6	18	VAL
28	d6	42	ARG
28	d6	44	ILE
28	d6	53	LEU
28	d6	57	SER
28	d6	61	GLU
28	d6	67	THR
28	d6	82	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	8	LEU
29	d7	14	SER
29	d7	15	GLU
29	d7	22	LYS
29	d7	34	ASP
29	d7	41	LEU
29	d7	43	ILE

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Mol	Chain	Res	Type
29	d7	52	THR
29	d7	55	THR
29	d7	59	CYS
29	d7	67	THR
29	d7	72	LYS
29	d7	77	THR
29	d7	78	SER
29	d7	81	ARG
30	d8	16	LEU
30	d8	19	THR
30	d8	22	ARG
30	d8	32	PHE
30	d8	33	LEU
30	d8	54	LEU
30	d8	64	ARG
30	d8	65	ARG
31	d9	6	VAL
31	d9	10	HIS
31	d9	12	ARG
31	d9	16	LYS
31	d9	26	SER
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	38	ILE
31	d9	54	LYS
80	e0	4	VAL
80	e0	13	LYS
80	e0	22	GLU
80	e0	29	LYS
80	e0	41	THR
80	e0	46	ASN
80	e0	48	THR
80	e0	49	LEU
80	e0	51	ASN
80	e0	55	ARG
80	e0	56	MET
33	e1	80	ARG
33	e1	84	VAL
33	e1	86	THR
33	e1	90	LYS
33	e1	92	LYS

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Mol	Chain	Res	Type
33	e1	96	LYS
33	e1	97	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	107	LYS
33	e1	109	ASP
33	e1	113	LYS
33	e1	115	THR
33	e1	117	LEU
33	e1	120	GLU
33	e1	121	CYS
33	e1	122	SER
33	e1	135	HIS
33	e1	137	ASP
33	e1	140	TYR
33	e1	144	CYS
33	e1	147	VAL
34	sR	10	ARG
34	sR	17	ASN
34	sR	21	THR
34	sR	25	THR
34	sR	29	GLN
34	sR	48	THR
34	sR	52	GLN
34	sR	59	ARG
34	sR	64	HIS
34	sR	65	SER
34	sR	66	HIS
34	sR	76	ASP
34	sR	96	THR
34	sR	98	GLU
34	sR	100	TYR
34	sR	118	LYS
34	sR	123	ILE
34	sR	130	THR
34	sR	145	LEU
34	sR	149	ASP
34	sR	152	SER
34	sR	164	ASP
34	sR	176	LYS
34	sR	178	VAL

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Mol	Chain	Res	Type
34	sR	203	THR
34	sR	210	LEU
34	sR	258	THR
34	sR	275	ARG
34	sR	282	SER
34	sR	297	ASP
35	sM	23	LYS
35	sM	27	LYS
35	sM	41	SER
35	sM	43	ASP
35	sM	45	SER
35	sM	49	LYS
35	sM	50	ASN
35	sM	61	ILE
35	sM	64	LYS
35	sM	69	ARG
35	sM	74	LYS
35	sM	77	THR
39	l2	15	ILE
39	l2	23	ARG
39	l2	30	ARG
39	l2	32	LEU
39	l2	44	ILE
39	l2	46	LYS
39	l2	48	ILE
39	l2	49	VAL
39	l2	52	SER
39	l2	61	VAL
39	l2	62	VAL
39	l2	70	ARG
39	l2	71	LEU
39	l2	74	GLU
39	l2	95	SER
39	l2	101	VAL
39	l2	111	THR
39	l2	112	ILE
39	l2	113	VAL
39	l2	119	LYS
39	l2	137	ILE
39	l2	142	ASP
39	l2	147	ARG
39	l2	149	ARG

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Mol	Chain	Res	Type
39	12	155	LYS
39	12	158	ILE
39	12	165	VAL
39	12	179	LEU
39	12	180	LEU
39	12	188	LYS
39	12	193	ARG
39	12	202	VAL
39	12	204	MET
39	12	224	THR
39	12	227	ARG
39	12	241	ARG
39	12	243	THR
39	12	246	LEU
39	12	249	SER
39	12	251	LYS
40	13	3	HIS
40	13	4	ARG
40	13	5	LYS
40	13	10	ARG
40	13	17	LEU
40	13	19	ARG
40	13	20	LYS
40	13	21	ARG
40	13	24	SER
40	13	37	ARG
40	13	39	LYS
40	13	43	LEU
40	13	47	LEU
40	13	50	LYS
40	13	56	ILE
40	13	66	LYS
40	13	70	ARG
40	13	79	VAL
40	13	81	THR
40	13	84	VAL
40	13	85	VAL
40	13	103	THR
40	13	114	VAL
40	13	132	LYS
40	13	146	ARG
40	13	148	LEU

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Mol	Chain	Res	Type
40	l3	150	ARG
40	l3	156	SER
40	l3	157	VAL
40	l3	167	ARG
40	l3	169	THR
40	l3	178	LEU
40	l3	183	LEU
40	l3	188	ILE
40	l3	192	VAL
40	l3	196	ARG
40	l3	202	THR
40	l3	205	VAL
40	l3	208	VAL
40	l3	211	GLN
40	l3	214	MET
40	l3	221	THR
40	l3	222	LYS
40	l3	229	VAL
40	l3	232	ARG
40	l3	235	THR
40	l3	238	LEU
40	l3	242	THR
40	l3	247	ARG
40	l3	248	LYS
40	l3	249	VAL
40	l3	252	ILE
40	l3	281	LYS
40	l3	284	ARG
40	l3	297	SER
40	l3	301	THR
40	l3	308	MET
40	l3	317	ILE
40	l3	318	LYS
40	l3	323	MET
40	l3	328	ILE
40	l3	332	ARG
40	l3	338	LEU
40	l3	346	THR
40	l3	347	SER
40	l3	348	ARG
40	l3	354	VAL
40	l3	355	SER

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Mol	Chain	Res	Type
40	l3	361	THR
40	l3	364	LYS
40	l3	385	LYS
41	l4	3	ARG
41	l4	14	GLU
41	l4	20	LEU
41	l4	25	VAL
41	l4	47	ARG
41	l4	53	SER
41	l4	64	SER
41	l4	93	MET
41	l4	99	MET
41	l4	112	LYS
41	l4	120	TYR
41	l4	122	THR
41	l4	144	LYS
41	l4	145	ILE
41	l4	156	LEU
41	l4	158	SER
41	l4	161	LYS
41	l4	163	LYS
41	l4	170	LYS
41	l4	172	VAL
41	l4	179	LEU
41	l4	182	LEU
41	l4	186	LYS
41	l4	187	LEU
41	l4	191	LYS
41	l4	193	LYS
41	l4	200	THR
41	l4	203	ARG
41	l4	206	LEU
41	l4	230	VAL
41	l4	246	ARG
41	l4	258	LEU
41	l4	266	THR
41	l4	267	VAL
41	l4	283	THR
41	l4	287	THR
41	l4	292	SER
41	l4	293	SER
41	l4	297	SER

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Mol	Chain	Res	Type
41	14	301	PRO
41	14	306	THR
41	14	307	GLN
41	14	313	LEU
41	14	319	LYS
41	14	327	LEU
41	14	333	VAL
41	14	337	GLU
41	14	342	LYS
41	14	343	LYS
41	14	345	GLU
41	14	347	THR
41	14	349	THR
41	14	358	THR
41	14	359	LEU
42	15	4	GLN
42	15	13	SER
42	15	34	LYS
42	15	35	ARG
42	15	41	LYS
42	15	51	LEU
42	15	61	ILE
42	15	68	THR
42	15	70	THR
42	15	75	LEU
42	15	89	THR
42	15	93	THR
42	15	109	THR
42	15	110	LEU
42	15	111	GLN
42	15	112	LYS
42	15	113	LEU
42	15	115	LEU
42	15	118	THR
42	15	124	GLU
42	15	130	GLU
42	15	132	THR
42	15	133	GLU
42	15	135	VAL
42	15	140	ARG
42	15	144	VAL
42	15	146	LEU

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Mol	Chain	Res	Type
42	15	148	ILE
42	15	152	ARG
42	15	155	THR
42	15	158	ARG
42	15	183	TRP
42	15	185	PHE
42	15	186	GLU
42	15	194	LEU
42	15	211	LEU
42	15	220	SER
42	15	227	LEU
42	15	232	ASP
42	15	236	LEU
42	15	241	THR
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS
42	15	261	THR
42	15	268	GLU
42	15	271	LYS
42	15	273	ARG
42	15	282	ARG
42	15	297	GLN
43	16	12	SER
43	16	14	ASP
43	16	15	VAL
43	16	21	THR
43	16	31	ARG
43	16	46	ARG
43	16	64	LEU
43	16	65	ILE
43	16	76	LEU
43	16	78	ARG
43	16	79	VAL
43	16	82	ARG
43	16	89	THR
43	16	93	VAL
43	16	98	VAL
43	16	99	GLU
43	16	109	GLU
43	16	129	GLU
43	16	131	LYS

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Mol	Chain	Res	Type
43	16	133	GLU
43	16	152	THR
43	16	155	LEU
43	16	162	SER
43	16	170	LYS
43	16	173	MET
44	17	22	THR
44	17	24	GLU
44	17	26	VAL
44	17	33	ARG
44	17	38	LYS
44	17	54	GLU
44	17	56	GLU
44	17	60	ARG
44	17	77	VAL
44	17	80	GLN
44	17	83	LEU
44	17	88	ARG
44	17	98	LYS
44	17	100	ARG
44	17	110	ARG
44	17	121	LYS
44	17	124	LEU
44	17	130	ILE
44	17	145	ARG
44	17	156	ILE
44	17	173	LEU
44	17	179	LEU
44	17	184	LEU
44	17	218	ARG
44	17	229	PHE
44	17	234	GLU
44	17	239	LEU
45	18	41	GLN
45	18	50	VAL
45	18	63	LYS
45	18	67	ILE
45	18	68	ARG
45	18	71	VAL
45	18	74	THR
45	18	79	GLN
45	18	89	GLU

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Mol	Chain	Res	Type
45	18	90	THR
45	18	95	ASN
45	18	111	LYS
45	18	136	LEU
45	18	146	LYS
45	18	149	LYS
45	18	160	ILE
45	18	164	VAL
45	18	169	LEU
45	18	172	LYS
45	18	183	LYS
45	18	200	LEU
45	18	214	LEU
45	18	217	THR
45	18	221	ASN
45	18	224	ASP
45	18	245	LYS
45	18	246	MET
45	18	248	LYS
46	19	5	GLN
46	19	6	THR
46	19	17	THR
46	19	18	VAL
46	19	19	SER
46	19	30	PRO
46	19	31	ARG
46	19	33	THR
46	19	36	LYS
46	19	44	THR
46	19	46	THR
46	19	52	LEU
46	19	55	VAL
46	19	68	LEU
46	19	69	ARG
46	19	70	THR
46	19	80	THR
46	19	82	VAL
46	19	92	TYR
46	19	105	GLU
46	19	106	LYS
46	19	129	ARG
46	19	132	VAL

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Mol	Chain	Res	Type
46	l9	133	THR
46	l9	134	ILE
46	l9	138	THR
46	l9	144	ILE
46	l9	151	VAL
46	l9	157	ASN
46	l9	161	LEU
46	l9	162	GLN
46	l9	168	ARG
46	l9	170	LYS
46	l9	173	ARG
46	l9	179	ILE
46	l9	184	LYS
46	l9	188	THR
47	m0	3	ARG
47	m0	19	LYS
47	m0	21	ARG
47	m0	24	ARG
47	m0	33	ILE
47	m0	36	LEU
47	m0	42	THR
47	m0	44	ASP
47	m0	48	LEU
47	m0	52	LEU
47	m0	57	LEU
47	m0	58	GLU
47	m0	59	GLN
47	m0	60	LEU
47	m0	71	CYS
47	m0	74	LYS
47	m0	77	THR
47	m0	87	LEU
47	m0	91	VAL
47	m0	99	ILE
47	m0	101	LYS
47	m0	103	LEU
47	m0	130	ASP
47	m0	140	THR
47	m0	141	LYS
47	m0	143	SER
47	m0	154	ARG
47	m0	156	ARG

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Mol	Chain	Res	Type
47	m0	167	LEU
47	m0	169	LYS
47	m0	186	GLU
47	m0	197	VAL
47	m0	200	LEU
47	m0	206	LEU
47	m0	208	ASN
47	m0	211	ARG
47	m0	212	GLU
47	m0	215	GLU
48	m1	10	ARG
48	m1	12	LEU
48	m1	13	LYS
48	m1	29	ARG
48	m1	30	LEU
48	m1	31	THR
48	m1	37	LEU
48	m1	44	THR
48	m1	47	GLN
48	m1	56	THR
48	m1	61	ARG
48	m1	71	VAL
48	m1	77	GLU
48	m1	78	GLU
48	m1	80	LEU
48	m1	82	ARG
48	m1	90	GLN
48	m1	97	SER
48	m1	106	ILE
48	m1	112	LEU
48	m1	115	LYS
48	m1	119	SER
48	m1	130	VAL
48	m1	140	ARG
48	m1	145	LYS
48	m1	153	LYS
48	m1	159	THR
49	m3	9	ILE
49	m3	13	HIS
49	m3	41	THR
49	m3	46	ILE
49	m3	53	LEU

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Mol	Chain	Res	Type
49	m3	54	LEU
49	m3	59	ARG
49	m3	62	THR
49	m3	67	ARG
49	m3	68	LYS
49	m3	69	VAL
49	m3	85	LEU
49	m3	92	THR
49	m3	100	ARG
49	m3	121	SER
49	m3	123	ILE
49	m3	124	ILE
49	m3	157	ARG
49	m3	164	GLU
49	m3	165	SER
49	m3	168	ARG
49	m3	176	GLU
49	m3	182	ILE
49	m3	184	GLU
50	m4	3	THR
50	m4	15	VAL
50	m4	20	VAL
50	m4	24	LYS
50	m4	27	GLN
50	m4	53	VAL
50	m4	58	ILE
50	m4	62	GLN
50	m4	63	VAL
50	m4	72	LEU
50	m4	80	THR
50	m4	82	SER
50	m4	105	GLN
50	m4	106	ARG
50	m4	107	GLU
50	m4	108	ARG
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	10	LEU
51	m5	15	GLN
51	m5	22	LEU
51	m5	24	ARG

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Mol	Chain	Res	Type
51	m5	49	ARG
51	m5	68	ARG
51	m5	76	PRO
51	m5	80	THR
51	m5	83	LYS
51	m5	85	THR
51	m5	92	LEU
51	m5	96	ARG
51	m5	97	SER
51	m5	98	LEU
51	m5	109	ARG
51	m5	138	GLN
51	m5	151	ILE
51	m5	153	ASP
51	m5	155	VAL
51	m5	159	ARG
51	m5	170	LYS
51	m5	171	SER
51	m5	174	ILE
51	m5	190	THR
52	m6	4	GLU
52	m6	12	LYS
52	m6	25	LYS
52	m6	34	VAL
52	m6	41	LEU
52	m6	49	ARG
52	m6	58	LEU
52	m6	60	LYS
52	m6	66	LYS
52	m6	67	THR
52	m6	74	ARG
52	m6	78	ARG
52	m6	84	LEU
52	m6	85	ARG
52	m6	89	SER
52	m6	100	GLU
52	m6	106	GLU
52	m6	108	ILE
52	m6	110	PRO
52	m6	116	LYS
52	m6	117	ARG
52	m6	124	LEU

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Mol	Chain	Res	Type
52	m6	126	VAL
52	m6	129	LEU
52	m6	134	LYS
52	m6	143	THR
52	m6	159	LYS
52	m6	166	GLU
52	m6	171	LYS
52	m6	175	THR
52	m6	177	LYS
52	m6	182	ASN
52	m6	190	VAL
53	m7	7	THR
53	m7	9	THR
53	m7	24	VAL
53	m7	25	SER
53	m7	29	THR
53	m7	31	GLU
53	m7	32	THR
53	m7	41	LEU
53	m7	43	LYS
53	m7	46	LYS
53	m7	49	GLU
53	m7	52	LEU
53	m7	56	ARG
53	m7	70	THR
53	m7	79	THR
53	m7	80	LYS
53	m7	86	LYS
53	m7	89	LYS
53	m7	112	LEU
53	m7	114	VAL
53	m7	118	GLN
53	m7	119	VAL
53	m7	124	LYS
53	m7	126	ARG
53	m7	127	ARG
53	m7	128	ARG
53	m7	144	SER
53	m7	148	LEU
53	m7	154	GLU
53	m7	155	GLU
54	m8	3	ILE

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Mol	Chain	Res	Type
54	m8	7	SER
54	m8	11	LYS
54	m8	17	THR
54	m8	22	ASP
54	m8	24	VAL
54	m8	26	LEU
54	m8	31	LYS
54	m8	32	LEU
54	m8	34	THR
54	m8	41	ASP
54	m8	49	LEU
54	m8	57	ILE
54	m8	63	SER
54	m8	64	VAL
54	m8	66	ARG
54	m8	80	THR
54	m8	81	VAL
54	m8	82	VAL
54	m8	86	THR
54	m8	93	ILE
54	m8	113	LYS
54	m8	122	ILE
54	m8	125	ASP
54	m8	135	GLN
54	m8	144	ARG
54	m8	147	ARG
54	m8	159	LYS
54	m8	161	LYS
54	m8	165	ILE
54	m8	170	ARG
54	m8	180	ARG
55	m9	7	GLN
55	m9	8	LYS
55	m9	10	LEU
55	m9	20	ARG
55	m9	29	THR
55	m9	30	SER
55	m9	31	GLU
55	m9	36	ASN
55	m9	43	LYS
55	m9	49	THR
55	m9	55	VAL

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Mol	Chain	Res	Type
55	m9	56	THR
55	m9	60	LYS
55	m9	63	THR
55	m9	70	LYS
55	m9	74	ARG
55	m9	76	SER
55	m9	88	ARG
55	m9	99	LEU
55	m9	104	ARG
55	m9	106	LEU
55	m9	126	GLU
55	m9	134	HIS
55	m9	138	LEU
55	m9	153	LYS
55	m9	164	LEU
55	m9	173	ARG
56	n0	1	MET
56	n0	8	GLN
56	n0	13	ARG
56	n0	23	LYS
56	n0	49	HIS
56	n0	53	LYS
56	n0	71	LYS
56	n0	73	LYS
56	n0	80	ARG
56	n0	87	THR
56	n0	92	LYS
56	n0	97	VAL
56	n0	100	VAL
56	n0	105	THR
56	n0	115	ARG
56	n0	117	ARG
56	n0	130	GLU
56	n0	136	LYS
56	n0	137	ARG
56	n0	148	LEU
56	n0	155	ARG
56	n0	157	GLN
56	n0	160	THR
56	n0	162	THR
56	n0	167	ARG
56	n0	169	SER

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Mol	Chain	Res	Type
56	n0	172	TYR
57	n1	9	SER
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	28	SER
57	n1	35	LYS
57	n1	47	SER
57	n1	68	THR
57	n1	71	SER
57	n1	78	LYS
57	n1	80	VAL
57	n1	83	ARG
57	n1	86	GLU
57	n1	88	ARG
57	n1	89	LEU
57	n1	96	ILE
57	n1	97	LYS
57	n1	102	ARG
57	n1	104	GLU
57	n1	106	LEU
57	n1	126	VAL
57	n1	129	LYS
57	n1	130	ARG
57	n1	135	PRO
57	n1	139	ARG
57	n1	140	ILE
57	n1	143	THR
57	n1	150	THR
58	n2	11	ILE
58	n2	13	LYS
58	n2	37	LEU
58	n2	61	THR
58	n2	63	VAL
58	n2	68	THR
58	n2	74	LYS
58	n2	90	ARG
58	n2	96	VAL
58	n2	99	LYS
59	n3	13	ILE
59	n3	17	LEU
59	n3	22	ILE

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Mol	Chain	Res	Type
59	n3	40	LYS
59	n3	42	SER
59	n3	45	ARG
59	n3	48	ARG
59	n3	69	LEU
59	n3	91	VAL
59	n3	108	GLU
59	n3	110	LYS
59	n3	115	THR
60	n4	1	MET
60	n4	2	LYS
60	n4	19	THR
60	n4	23	ARG
60	n4	26	SER
60	n4	39	LEU
60	n4	54	LEU
60	n4	57	LYS
60	n4	63	ILE
60	n4	89	LEU
60	n4	97	LYS
60	n4	105	ARG
60	n4	126	GLU
60	n4	127	LYS
60	n4	135	SER
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	38	LEU
61	n5	40	LEU
61	n5	45	LYS
61	n5	55	ASN
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	65	GLN
61	n5	69	SER
61	n5	86	VAL
61	n5	109	LYS
61	n5	115	ARG
61	n5	125	ARG
61	n5	133	LEU
61	n5	137	ASN

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Mol	Chain	Res	Type
61	n5	138	ARG
61	n5	142	ILE
62	n6	4	GLN
62	n6	9	SER
62	n6	12	ARG
62	n6	13	ARG
62	n6	37	LYS
62	n6	39	LEU
62	n6	40	ARG
62	n6	45	ILE
62	n6	50	ILE
62	n6	51	ARG
62	n6	56	VAL
62	n6	57	LEU
62	n6	62	SER
62	n6	66	GLN
62	n6	74	TYR
62	n6	76	LEU
62	n6	80	VAL
62	n6	83	ASP
62	n6	97	ILE
62	n6	120	GLN
62	n6	127	GLU
63	n7	3	LYS
63	n7	14	VAL
63	n7	17	ARG
63	n7	24	VAL
63	n7	26	VAL
63	n7	28	PRO
63	n7	31	GLU
63	n7	34	LYS
63	n7	46	ILE
63	n7	52	LYS
63	n7	54	THR
63	n7	65	ARG
63	n7	66	THR
63	n7	72	ILE
63	n7	73	LYS
63	n7	75	VAL
63	n7	81	LEU
63	n7	83	THR
63	n7	86	THR

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Mol	Chain	Res	Type
63	n7	88	ASP
63	n7	92	PHE
63	n7	93	LYS
63	n7	97	SER
63	n7	99	GLU
63	n7	103	GLN
63	n7	105	SER
63	n7	119	GLU
63	n7	121	ARG
63	n7	133	LYS
63	n7	134	LEU
63	n7	135	ARG
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	9	ARG
64	n8	16	SER
64	n8	27	LYS
64	n8	42	ARG
64	n8	43	ILE
64	n8	44	ASN
64	n8	46	ASP
64	n8	47	LYS
64	n8	60	TYR
64	n8	65	GLN
64	n8	78	LEU
64	n8	80	THR
64	n8	81	LEU
64	n8	91	LEU
64	n8	95	SER
64	n8	98	THR
64	n8	124	ILE
64	n8	128	ARG
64	n8	132	LYS
64	n8	133	LEU
64	n8	144	VAL
65	n9	3	LYS
65	n9	13	THR
65	n9	14	ARG
65	n9	22	LYS
65	n9	26	THR
65	n9	31	SER

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Mol	Chain	Res	Type
65	n9	38	LYS
65	n9	44	LYS
65	n9	50	THR
65	n9	52	LYS
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	19	LYS
66	o0	32	LYS
66	o0	33	SER
66	o0	34	LEU
66	o0	40	LYS
66	o0	41	LEU
66	o0	48	THR
66	o0	55	GLU
66	o0	61	MET
66	o0	64	LYS
66	o0	66	LYS
66	o0	68	TYR
66	o0	71	GLN
66	o0	81	VAL
66	o0	86	ARG
66	o0	93	LEU
66	o0	101	LEU
67	o1	6	ASP
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	34	LYS
67	o1	36	ILE
67	o1	44	MET
67	o1	46	THR
67	o1	61	LYS
67	o1	64	VAL
67	o1	76	SER
67	o1	82	GLU
67	o1	94	GLU
67	o1	96	VAL
67	o1	98	VAL
67	o1	100	SER
67	o1	102	LYS

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Mol	Chain	Res	Type
67	o1	105	GLN
67	o1	106	THR
67	o1	107	VAL
67	o1	110	GLU
68	o2	4	LEU
68	o2	5	PRO
68	o2	15	LYS
68	o2	16	LYS
68	o2	19	ARG
68	o2	27	ARG
68	o2	31	ASN
68	o2	33	ARG
68	o2	34	LYS
68	o2	41	VAL
68	o2	51	SER
68	o2	61	LYS
68	o2	73	THR
68	o2	75	LEU
68	o2	76	VAL
68	o2	82	LEU
68	o2	89	THR
68	o2	91	THR
68	o2	109	LEU
68	o2	125	ARG
68	o2	126	LEU
68	o2	128	LEU
69	o3	10	LYS
69	o3	20	LYS
69	o3	21	ARG
69	o3	28	SER
69	o3	31	LYS
69	o3	49	ILE
69	o3	57	LYS
69	o3	58	GLU
69	o3	60	ARG
69	o3	62	SER
69	o3	70	LYS
69	o3	74	THR
69	o3	81	VAL
69	o3	92	LYS
69	o3	98	VAL
69	o3	107	ILE

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Mol	Chain	Res	Type
70	o4	5	VAL
70	o4	20	ILE
70	o4	24	LYS
70	o4	29	ILE
70	o4	30	LEU
70	o4	33	GLN
70	o4	58	ARG
70	o4	66	SER
70	o4	79	SER
70	o4	86	LYS
70	o4	98	GLN
70	o4	103	LYS
70	o4	104	VAL
71	o5	20	GLN
71	o5	21	LEU
71	o5	30	GLU
71	o5	31	LEU
71	o5	35	LYS
71	o5	37	SER
71	o5	47	VAL
71	o5	48	ARG
71	o5	62	GLN
71	o5	69	LEU
71	o5	73	LYS
71	o5	80	LEU
71	o5	81	ARG
71	o5	85	THR
71	o5	89	ARG
71	o5	90	ARG
71	o5	100	VAL
71	o5	107	LYS
71	o5	115	LYS
72	o6	7	ILE
72	o6	9	ILE
72	o6	11	LEU
72	o6	17	VAL
72	o6	21	THR
72	o6	26	ILE
72	o6	34	SER
72	o6	36	ARG
72	o6	37	THR
72	o6	38	LYS

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Mol	Chain	Res	Type
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	59	ASP
72	o6	60	LEU
72	o6	62	ARG
72	o6	71	LYS
72	o6	76	ARG
72	o6	81	THR
72	o6	84	LYS
72	o6	88	GLU
72	o6	94	ILE
72	o6	98	ARG
72	o6	100	HIS
73	o7	3	LYS
73	o7	17	THR
73	o7	19	CYS
73	o7	33	THR
73	o7	36	SER
73	o7	44	THR
73	o7	59	THR
73	o7	64	MET
73	o7	65	ARG
73	o7	67	LEU
73	o7	72	ARG
73	o7	84	SER
73	o7	87	SER
74	o8	5	ILE
74	o8	10	GLN
74	o8	12	LEU
74	o8	16	ARG
74	o8	31	LEU
74	o8	33	LYS
74	o8	41	THR
74	o8	42	LYS
74	o8	45	VAL
74	o8	46	ARG
74	o8	50	SER
74	o8	53	THR
74	o8	64	LYS
74	o8	65	LEU

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Mol	Chain	Res	Type
74	o8	67	GLN
74	o8	69	LEU
74	o8	73	LEU
74	o8	74	LYS
75	o9	4	GLN
75	o9	15	LYS
75	o9	21	ARG
75	o9	23	LEU
75	o9	27	ILE
75	o9	28	ARG
75	o9	29	LEU
75	o9	36	ARG
75	o9	45	ARG
75	o9	47	THR
75	o9	48	LYS
75	o9	51	ILE
76	q0	79	GLU
76	q0	85	LEU
76	q0	87	SER
76	q0	88	LYS
76	q0	91	CYS
76	q0	93	LYS
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	128	LYS
77	q1	2	ARG
77	q1	6	ARG
77	q1	9	ARG
77	q1	13	LEU
77	q1	16	LYS
77	q1	18	ARG
77	q1	19	LYS
77	q1	21	ARG
77	q1	23	ARG
77	q1	24	SER
78	q2	7	THR
78	q2	8	ARG
78	q2	16	THR
78	q2	35	LEU
78	q2	45	ARG
78	q2	61	LYS

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Mol	Chain	Res	Type
78	q2	71	ARG
78	q2	76	LYS
78	q2	78	LYS
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	89	LYS
78	q2	104	LEU
78	q2	105	GLN
78	q2	106	PHE
79	q3	3	LYS
79	q3	16	VAL
79	q3	20	SER
79	q3	42	CYS
79	q3	46	THR
79	q3	48	LYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	58	SER
79	q3	62	LYS
79	q3	73	THR
79	q3	78	THR
79	q3	90	VAL
82	p0	4	ILE
82	p0	7	LYS
82	p0	10	GLU
82	p0	15	LEU
82	p0	25	LEU
82	p0	30	VAL
82	p0	39	HIS
82	p0	42	ARG
82	p0	43	LYS
82	p0	44	GLU
82	p0	52	LEU
82	p0	55	LYS
82	p0	67	LEU
82	p0	70	LEU
82	p0	72	ASP
82	p0	89	THR
82	p0	91	GLU
82	p0	93	LEU

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Mol	Chain	Res	Type
82	p0	94	THR
82	p0	97	LYS
82	p0	101	VAL
82	p0	104	ARG
82	p0	185	LEU
82	p0	192	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
2	S0	15	GLN
3	S1	79	HIS
5	S3	74	GLN
8	S6	59	GLN
10	S8	64	ASN
12	C0	12	HIS
12	C0	17	GLN
12	C0	32	HIS
17	C5	103	ASN
19	C7	105	GLN
20	C8	6	GLN
20	C8	25	ASN
21	C9	70	GLN
22	D0	47	GLN
23	D1	75	ASN
27	D5	95	HIS
34	SR	319	ASN
35	SM	94	HIS
40	L3	173	GLN
41	L4	311	HIS
43	L6	28	GLN
44	L7	244	ASN
45	L8	41	GLN
48	M1	7	ASN
54	M8	145	ASN
59	N3	98	ASN
74	O8	32	ASN
2	s0	140	ASN
7	s5	100	ASN
7	s5	186	ASN
8	s6	201	GLN
9	s7	71	HIS

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Mol	Chain	Res	Type
9	s7	122	HIS
10	s8	103	GLN
11	s9	124	HIS
11	s9	155	HIS
19	c7	31	ASN
19	c7	74	GLN
20	c8	89	GLN
20	c8	103	ASN
21	c9	64	HIS
22	d0	44	ASN
22	d0	47	GLN
24	d2	56	HIS
30	d8	27	GLN
33	e1	93	HIS
39	l2	218	HIS
40	l3	211	GLN
41	l4	18	ASN
52	m6	122	GLN
55	m9	7	GLN
55	m9	36	ASN
57	n1	98	HIS
57	n1	131	GLN
59	n3	33	ASN
64	n8	44	ASN
71	o5	108	GLN
79	q3	33	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	512 (29%)	56 (3%)
1	6	1792/1800 (99%)	463 (25%)	53 (2%)
36	1	3145/3396 (92%)	702 (22%)	92 (2%)
36	5	3145/3396 (92%)	717 (22%)	94 (2%)
37	3	120/121 (99%)	24 (20%)	2 (1%)
37	7	120/121 (99%)	23 (19%)	1 (0%)
38	4	157/158 (99%)	40 (25%)	4 (2%)
38	8	157/158 (99%)	40 (25%)	4 (2%)
All	All	10383/10950 (94%)	2521 (24%)	306 (2%)

All (2521) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	45	U
1	2	46	A
1	2	47	A
1	2	57	G
1	2	60	U
1	2	61	A
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	77	U
1	2	81	G
1	2	104	A
1	2	114	C
1	2	127	G
1	2	129	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	169	A

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Mol	Chain	Res	Type
1	2	170	U
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	212	U
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	226	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	231	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	250	C
1	2	253	A
1	2	260	U
1	2	261	U
1	2	265	A
1	2	267	U
1	2	271	A
1	2	272	U
1	2	274	G

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Mol	Chain	Res	Type
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	284	G
1	2	288	A
1	2	290	G
1	2	292	U
1	2	299	A
1	2	314	C
1	2	316	A
1	2	319	U
1	2	320	U
1	2	321	C
1	2	322	G
1	2	335	U
1	2	337	G
1	2	338	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	363	G
1	2	365	G
1	2	369	A
1	2	387	A
1	2	390	G
1	2	393	C
1	2	397	A
1	2	399	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	403	G
1	2	404	G
1	2	418	G
1	2	419	G
1	2	424	C
1	2	425	A

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Mol	Chain	Res	Type
1	2	426	G
1	2	428	A
1	2	434	G
1	2	439	U
1	2	444	C
1	2	445	A
1	2	446	A
1	2	448	C
1	2	452	A
1	2	459	G
1	2	469	C
1	2	475	A
1	2	480	G
1	2	483	A
1	2	484	C
1	2	485	A
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	511	A
1	2	512	A
1	2	513	U
1	2	515	A
1	2	516	G
1	2	519	C
1	2	520	A
1	2	527	A
1	2	536	C

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Mol	Chain	Res	Type
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	546	U
1	2	548	G
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	579	A
1	2	580	A
1	2	582	U
1	2	585	A
1	2	590	C
1	2	594	A
1	2	595	G
1	2	606	A
1	2	614	C
1	2	616	G
1	2	617	U
1	2	619	A
1	2	620	A
1	2	621	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	639	U
1	2	640	U
1	2	650	U
1	2	653	C
1	2	654	C
1	2	655	G
1	2	656	G
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	684	A

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Mol	Chain	Res	Type
1	2	685	A
1	2	686	C
1	2	692	C
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	711	U
1	2	712	G
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	743	U
1	2	745	U

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Mol	Chain	Res	Type
1	2	752	A
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	779	U
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	787	G
1	2	789	A
1	2	794	U
1	2	795	U
1	2	811	A
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G
1	2	824	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	832	U
1	2	854	U
1	2	860	U
1	2	862	A
1	2	863	A
1	2	864	U
1	2	869	A
1	2	876	G
1	2	892	A
1	2	898	A

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Mol	Chain	Res	Type
1	2	911	U
1	2	912	U
1	2	914	G
1	2	915	A
1	2	916	U
1	2	921	U
1	2	926	A
1	2	933	A
1	2	935	U
1	2	941	A
1	2	942	G
1	2	951	A
1	2	952	A
1	2	953	G
1	2	960	U
1	2	966	A
1	2	982	U
1	2	991	G
1	2	992	A
1	2	993	A
1	2	995	A
1	2	997	G
1	2	1002	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1016	C
1	2	1020	A
1	2	1021	C
1	2	1026	A
1	2	1028	C
1	2	1031	U
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1072	C
1	2	1073	G

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Mol	Chain	Res	Type
1	2	1075	C
1	2	1079	U
1	2	1082	C
1	2	1083	G
1	2	1087	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1111	G
1	2	1114	G
1	2	1134	C
1	2	1135	U
1	2	1138	A
1	2	1140	G
1	2	1141	G
1	2	1146	G
1	2	1149	G
1	2	1150	G
1	2	1151	A
1	2	1155	G
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1167	G
1	2	1176	G
1	2	1185	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1198	G
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1203	A
1	2	1206	U
1	2	1207	C
1	2	1208	A
1	2	1216	C
1	2	1217	A
1	2	1218	G

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Mol	Chain	Res	Type
1	2	1226	A
1	2	1227	A
1	2	1229	G
1	2	1234	A
1	2	1235	C
1	2	1241	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1257	U
1	2	1258	U
1	2	1273	G
1	2	1286	U
1	2	1301	U
1	2	1314	U
1	2	1315	U
1	2	1316	G
1	2	1319	A
1	2	1320	U
1	2	1321	A
1	2	1337	A
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1354	G
1	2	1361	U
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1379	C
1	2	1383	G
1	2	1386	G
1	2	1388	A
1	2	1390	U
1	2	1398	U
1	2	1399	C

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Mol	Chain	Res	Type
1	2	1400	A
1	2	1412	G
1	2	1413	U
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1433	G
1	2	1446	A
1	2	1447	C
1	2	1448	G
1	2	1454	G
1	2	1457	C
1	2	1459	C
1	2	1462	G
1	2	1466	G
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1477	G
1	2	1482	C
1	2	1486	G
1	2	1487	A
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1494	C
1	2	1500	C
1	2	1506	G
1	2	1514	U
1	2	1515	A
1	2	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1526	A
1	2	1528	U
1	2	1535	U
1	2	1536	G

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Mol	Chain	Res	Type
1	2	1537	C
1	2	1538	U
1	2	1540	G
1	2	1544	U
1	2	1548	G
1	2	1557	U
1	2	1559	A
1	2	1568	C
1	2	1569	A
1	2	1573	A
1	2	1574	G
1	2	1584	G
1	2	1590	G
1	2	1600	A
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1631	A
1	2	1635	A
1	2	1637	C
1	2	1652	C
1	2	1657	U
1	2	1658	G
1	2	1663	G
1	2	1673	G
1	2	1681	A
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1729	C
1	2	1731	A
1	2	1747	G
1	2	1756	A
1	2	1757	G
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A

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Mol	Chain	Res	Type
1	2	1783	C
1	2	1789	G
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	5	G
36	1	6	A
36	1	11	A
36	1	13	A
36	1	14	U
36	1	26	A
36	1	31	C
36	1	37	U
36	1	40	A
36	1	49	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	73	C
36	1	74	G
36	1	75	G
36	1	83	U
36	1	88	A
36	1	92	G
36	1	93	C
36	1	99	A
36	1	109	A
36	1	110	G
36	1	113	C
36	1	117	U
36	1	121	A
36	1	122	A
36	1	128	G
36	1	133	U
36	1	135	C
36	1	136	G
36	1	156	G
36	1	157	A
36	1	163	C

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Mol	Chain	Res	Type
36	1	166	C
36	1	173	G
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	199	A
36	1	210	U
36	1	219	A
36	1	224	C
36	1	238	A
36	1	240	U
36	1	241	G
36	1	243	G
36	1	244	G
36	1	245	U
36	1	249	U
36	1	250	U
36	1	252	U
36	1	269	G
36	1	283	G
36	1	284	A
36	1	286	U
36	1	295	A
36	1	298	U
36	1	305	U
36	1	315	C
36	1	323	A
36	1	329	U
36	1	339	C
36	1	343	U
36	1	349	A
36	1	350	C
36	1	357	A
36	1	375	A
36	1	376	G
36	1	397	A
36	1	398	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	420	G

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Mol	Chain	Res	Type
36	1	421	G
36	1	422	A
36	1	438	A
36	1	439	C
36	1	440	A
36	1	495	G
36	1	497	C
36	1	507	U
36	1	520	U
36	1	521	A
36	1	532	A
36	1	535	G
36	1	544	C
36	1	545	U
36	1	546	C
36	1	548	G
36	1	551	A
36	1	552	G
36	1	553	U
36	1	555	U
36	1	556	U
36	1	557	A
36	1	559	A
36	1	560	G
36	1	568	G
36	1	572	A
36	1	578	A
36	1	579	G
36	1	589	A
36	1	592	A
36	1	593	C
36	1	600	G
36	1	601	U
36	1	604	G
36	1	607	A
36	1	608	A
36	1	609	G
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A
36	1	622	A

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Mol	Chain	Res	Type
36	1	624	G
36	1	636	C
36	1	639	G
36	1	642	U
36	1	649	A
36	1	656	A
36	1	660	A
36	1	661	G
36	1	667	C
36	1	677	A
36	1	681	U
36	1	683	U
36	1	691	A
36	1	705	A
36	1	712	G
36	1	715	A
36	1	716	A
36	1	726	G
36	1	736	A
36	1	738	A
36	1	741	U
36	1	763	G
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	768	C
36	1	776	U
36	1	777	U
36	1	781	G
36	1	785	G
36	1	798	G
36	1	799	G
36	1	803	C
36	1	806	A
36	1	817	A
36	1	830	A
36	1	849	C
36	1	861	C
36	1	872	U
36	1	874	U
36	1	879	U

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Mol	Chain	Res	Type
36	1	881	C
36	1	890	C
36	1	895	A
36	1	896	A
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	923	C
36	1	924	G
36	1	925	A
36	1	937	G
36	1	938	C
36	1	943	U
36	1	944	C
36	1	958	C
36	1	959	C
36	1	960	U
36	1	962	A
36	1	979	U
36	1	981	U
36	1	982	C
36	1	993	G
36	1	994	G
36	1	996	A
36	1	997	A
36	1	1000	C
36	1	1001	G
36	1	1002	A
36	1	1010	G
36	1	1014	U
36	1	1015	U
36	1	1016	C
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1021	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1035	G

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Mol	Chain	Res	Type
36	1	1036	A
36	1	1037	C
36	1	1041	U
36	1	1047	A
36	1	1048	A
36	1	1049	C
36	1	1052	U
36	1	1057	A
36	1	1064	A
36	1	1065	A
36	1	1069	C
36	1	1071	U
36	1	1072	G
36	1	1081	U
36	1	1082	U
36	1	1087	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1116	G
36	1	1117	G
36	1	1128	U
36	1	1131	G
36	1	1144	U
36	1	1153	A
36	1	1159	A
36	1	1160	C
36	1	1178	G
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1185	C
36	1	1190	A
36	1	1191	U
36	1	1192	C
36	1	1193	A

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Mol	Chain	Res	Type
36	1	1201	C
36	1	1209	G
36	1	1213	G
36	1	1216	C
36	1	1217	A
36	1	1221	A
36	1	1222	G
36	1	1225	A
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1253	U
36	1	1258	U
36	1	1259	A
36	1	1260	A
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1267	U
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1274	A
36	1	1277	C
36	1	1278	A
36	1	1279	C
36	1	1285	G
36	1	1287	A
36	1	1292	C
36	1	1303	A
36	1	1307	G
36	1	1308	A

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Mol	Chain	Res	Type
36	1	1309	U
36	1	1313	G
36	1	1329	U
36	1	1330	A
36	1	1331	U
36	1	1333	C
36	1	1344	G
36	1	1345	G
36	1	1348	U
36	1	1349	G
36	1	1350	A
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1380	G
36	1	1386	A
36	1	1399	A
36	1	1400	G
36	1	1405	U
36	1	1418	A
36	1	1419	A
36	1	1425	U
36	1	1434	G
36	1	1437	C
36	1	1446	A
36	1	1450	G
36	1	1465	A
36	1	1481	A
36	1	1482	A
36	1	1488	G
36	1	1503	A
36	1	1508	C
36	1	1524	A
36	1	1527	C
36	1	1528	G
36	1	1533	U
36	1	1536	G
36	1	1554	U
36	1	1555	U

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Mol	Chain	Res	Type
36	1	1556	C
36	1	1558	A
36	1	1560	G
36	1	1561	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1565	G
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1572	U
36	1	1576	G
36	1	1578	C
36	1	1579	C
36	1	1580	A
36	1	1581	C
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1593	A
36	1	1607	U
36	1	1620	U
36	1	1624	G
36	1	1629	U
36	1	1641	U
36	1	1643	A
36	1	1645	U
36	1	1657	C
36	1	1664	G
36	1	1668	G
36	1	1675	G
36	1	1676	A
36	1	1683	A
36	1	1687	U
36	1	1688	U
36	1	1716	U
36	1	1717	U
36	1	1721	U

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Mol	Chain	Res	Type
36	1	1724	U
36	1	1725	C
36	1	1736	G
36	1	1747	G
36	1	1750	A
36	1	1751	G
36	1	1752	A
36	1	1760	A
36	1	1762	C
36	1	1764	U
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1770	G
36	1	1772	U
36	1	1778	G
36	1	1780	G
36	1	1795	U
36	1	1797	A
36	1	1809	A
36	1	1810	A
36	1	1814	A
36	1	1816	A
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1826	C
36	1	1835	A
36	1	1839	A
36	1	1841	A
36	1	1842	A
36	1	1845	G
36	1	1846	C
36	1	1847	A
36	1	1849	C
36	1	1855	U
36	1	1866	C
36	1	1869	C
36	1	1871	U
36	1	1879	A
36	1	1884	A
36	1	1901	A

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Mol	Chain	Res	Type
36	1	1906	G
36	1	1917	C
36	1	1937	U
36	1	1948	G
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	1954	G
36	1	2097	U
36	1	2101	C
36	1	2102	U
36	1	2106	A
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2121	G
36	1	2122	G
36	1	2131	A
36	1	2140	U
36	1	2158	A
36	1	2169	G
36	1	2170	U
36	1	2177	G
36	1	2184	U
36	1	2187	G
36	1	2188	A
36	1	2194	G
36	1	2195	C
36	1	2198	A
36	1	2205	U
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2213	A
36	1	2223	A
36	1	2225	U
36	1	2228	A
36	1	2244	A
36	1	2245	C
36	1	2246	G
36	1	2249	G
36	1	2250	G

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Mol	Chain	Res	Type
36	1	2254	U
36	1	2255	A
36	1	2256	A
36	1	2258	U
36	1	2262	A
36	1	2272	G
36	1	2273	G
36	1	2279	A
36	1	2281	A
36	1	2282	U
36	1	2284	C
36	1	2298	U
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2319	U
36	1	2323	G
36	1	2334	U
36	1	2336	U
36	1	2360	C
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2388	U
36	1	2393	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2424	A
36	1	2435	G
36	1	2437	G
36	1	2444	C
36	1	2445	A

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Mol	Chain	Res	Type
36	1	2502	A
36	1	2503	G
36	1	2504	U
36	1	2507	C
36	1	2511	A
36	1	2514	U
36	1	2515	A
36	1	2519	A
36	1	2522	G
36	1	2523	A
36	1	2532	U
36	1	2533	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2549	G
36	1	2551	U
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2561	A
36	1	2567	C
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2581	U
36	1	2585	G
36	1	2586	G
36	1	2589	G
36	1	2590	A
36	1	2593	A
36	1	2594	C
36	1	2606	G
36	1	2607	G
36	1	2613	U

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Mol	Chain	Res	Type
36	1	2614	G
36	1	2622	C
36	1	2623	G
36	1	2637	A
36	1	2647	A
36	1	2652	U
36	1	2653	C
36	1	2656	A
36	1	2657	A
36	1	2674	A
36	1	2677	G
36	1	2681	U
36	1	2689	A
36	1	2690	G
36	1	2691	A
36	1	2694	A
36	1	2696	A
36	1	2699	G
36	1	2705	A
36	1	2707	C
36	1	2708	C
36	1	2712	U
36	1	2713	U
36	1	2714	G
36	1	2728	G
36	1	2729	U
36	1	2753	G
36	1	2755	C
36	1	2762	A
36	1	2764	C
36	1	2771	U
36	1	2772	C
36	1	2773	C
36	1	2777	G
36	1	2778	G
36	1	2780	A
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2810	C
36	1	2817	A

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Mol	Chain	Res	Type
36	1	2818	U
36	1	2825	C
36	1	2826	U
36	1	2839	G
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2849	C
36	1	2858	U
36	1	2860	U
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2878	G
36	1	2887	A
36	1	2889	C
36	1	2898	G
36	1	2899	C
36	1	2902	A
36	1	2923	U
36	1	2935	U
36	1	2936	A
36	1	2941	A
36	1	2942	C
36	1	2945	G
36	1	2947	G
36	1	2971	A
36	1	2974	U
36	1	2977	G
36	1	2983	C
36	1	2990	G
36	1	2992	U
36	1	2996	U
36	1	2997	G
36	1	3006	A
36	1	3012	A
36	1	3030	G
36	1	3037	U
36	1	3056	U
36	1	3057	U
36	1	3059	G
36	1	3078	U

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Mol	Chain	Res	Type
36	1	3079	U
36	1	3080	G
36	1	3085	G
36	1	3086	A
36	1	3092	C
36	1	3113	A
36	1	3122	A
36	1	3123	A
36	1	3130	A
36	1	3131	U
36	1	3134	A
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3164	C
36	1	3165	A
36	1	3168	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3185	U
36	1	3187	A
36	1	3196	U
36	1	3198	U
36	1	3207	U
36	1	3210	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3228	C
36	1	3229	G
36	1	3243	A
36	1	3245	A
36	1	3246	G
36	1	3247	G

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Mol	Chain	Res	Type
36	1	3253	G
36	1	3259	U
36	1	3270	U
36	1	3272	C
36	1	3274	A
36	1	3276	G
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3289	G
36	1	3293	U
36	1	3294	A
36	1	3304	U
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3328	G
36	1	3334	U
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3367	C
36	1	3369	G
36	1	3378	C
36	1	3382	U
36	1	3386	G
36	1	3389	U
37	3	7	G
37	3	9	C
37	3	19	C
37	3	22	A
37	3	42	A

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Mol	Chain	Res	Type
37	3	47	C
37	3	50	U
37	3	51	A
37	3	54	U
37	3	59	U
37	3	65	G
37	3	76	A
37	3	88	G
37	3	89	G
37	3	90	U
37	3	91	G
37	3	95	A
37	3	101	G
37	3	102	A
37	3	103	A
37	3	109	G
37	3	110	G
37	3	112	G
37	3	121	U
38	4	2	A
38	4	17	A
38	4	21	C
38	4	22	U
38	4	26	U
38	4	34	U
38	4	35	C
38	4	48	A
38	4	52	A
38	4	53	A
38	4	58	G
38	4	59	A
38	4	62	C
38	4	63	G
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U

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Mol	Chain	Res	Type
38	4	95	G
38	4	96	A
38	4	100	U
38	4	104	A
38	4	105	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	115	C
38	4	125	U
38	4	126	A
38	4	127	U
38	4	128	U
38	4	148	G
38	4	155	A
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	6	G
1	6	13	C
1	6	19	A
1	6	20	G
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	36	C
1	6	44	U
1	6	46	A
1	6	47	A
1	6	57	G
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	104	A

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Mol	Chain	Res	Type
1	6	114	C
1	6	124	A
1	6	126	A
1	6	127	G
1	6	129	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	144	U
1	6	145	A
1	6	146	U
1	6	153	G
1	6	158	U
1	6	159	U
1	6	166	C
1	6	178	U
1	6	185	U
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	195	G
1	6	196	G
1	6	197	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	222	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	240	U

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Mol	Chain	Res	Type
1	6	241	U
1	6	246	G
1	6	249	U
1	6	250	C
1	6	260	U
1	6	261	U
1	6	265	A
1	6	270	C
1	6	271	A
1	6	272	U
1	6	273	G
1	6	275	C
1	6	277	U
1	6	278	U
1	6	279	G
1	6	280	U
1	6	281	G
1	6	287	G
1	6	299	A
1	6	308	C
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	337	G
1	6	338	C
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	370	A
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	405	C
1	6	416	A
1	6	418	G
1	6	424	C
1	6	425	A

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Mol	Chain	Res	Type
1	6	426	G
1	6	434	G
1	6	439	U
1	6	444	C
1	6	448	C
1	6	477	A
1	6	478	A
1	6	484	C
1	6	485	A
1	6	486	G
1	6	487	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	496	G
1	6	497	G
1	6	499	U
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	507	U
1	6	508	U
1	6	510	G
1	6	511	A
1	6	515	A
1	6	519	C
1	6	527	A
1	6	528	U
1	6	536	C
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G

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Mol	Chain	Res	Type
1	6	551	G
1	6	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	565	C
1	6	566	C
1	6	570	A
1	6	571	G
1	6	574	G
1	6	577	G
1	6	579	A
1	6	580	A
1	6	581	U
1	6	582	U
1	6	591	A
1	6	594	A
1	6	595	G
1	6	602	U
1	6	609	U
1	6	611	U
1	6	617	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	630	A
1	6	639	U
1	6	640	U
1	6	644	C
1	6	650	U
1	6	651	G
1	6	652	G
1	6	653	C
1	6	658	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C

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Mol	Chain	Res	Type
1	6	669	G
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	680	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C
1	6	695	U
1	6	697	C
1	6	698	U
1	6	699	U
1	6	709	C
1	6	710	U
1	6	711	U
1	6	715	U
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	723	G
1	6	730	G
1	6	739	G
1	6	751	G
1	6	753	A
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	774	A
1	6	775	G
1	6	779	U
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G

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Mol	Chain	Res	Type
1	6	789	A
1	6	792	U
1	6	793	A
1	6	794	U
1	6	806	A
1	6	811	A
1	6	812	A
1	6	814	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	822	U
1	6	823	G
1	6	825	U
1	6	826	U
1	6	828	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	846	G
1	6	847	A
1	6	856	A
1	6	860	U
1	6	861	U
1	6	863	A
1	6	898	A
1	6	904	G
1	6	906	A
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	959	U
1	6	960	U
1	6	962	C
1	6	970	A
1	6	971	A

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Mol	Chain	Res	Type
1	6	985	G
1	6	992	A
1	6	996	U
1	6	998	A
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1021	C
1	6	1026	A
1	6	1028	C
1	6	1039	A
1	6	1040	G
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1073	G
1	6	1081	A
1	6	1082	C
1	6	1091	A
1	6	1092	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1138	A
1	6	1139	A
1	6	1150	G
1	6	1151	A
1	6	1154	G
1	6	1155	G
1	6	1158	C
1	6	1160	A
1	6	1167	G
1	6	1179	G
1	6	1185	U
1	6	1191	U
1	6	1193	A
1	6	1194	A
1	6	1196	A

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Mol	Chain	Res	Type
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1203	A
1	6	1208	A
1	6	1217	A
1	6	1218	G
1	6	1219	A
1	6	1220	C
1	6	1227	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1240	U
1	6	1241	G
1	6	1242	A
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1259	U
1	6	1262	U
1	6	1275	A
1	6	1286	U
1	6	1314	U
1	6	1315	U
1	6	1321	A
1	6	1337	A
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1348	A
1	6	1354	G
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G

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Mol	Chain	Res	Type
1	6	1370	U
1	6	1371	A
1	6	1372	U
1	6	1388	A
1	6	1390	U
1	6	1391	A
1	6	1396	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1413	U
1	6	1414	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1429	G
1	6	1431	C
1	6	1433	G
1	6	1445	G
1	6	1446	A
1	6	1447	C
1	6	1448	G
1	6	1454	G
1	6	1458	G
1	6	1459	C
1	6	1461	C
1	6	1471	A
1	6	1482	C
1	6	1486	G
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1496	U
1	6	1506	G
1	6	1513	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G

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Mol	Chain	Res	Type
1	6	1523	G
1	6	1524	A
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1554	U
1	6	1555	A
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1571	C
1	6	1573	A
1	6	1574	G
1	6	1575	G
1	6	1582	U
1	6	1584	G
1	6	1590	G
1	6	1601	G
1	6	1613	U
1	6	1616	G
1	6	1619	C
1	6	1621	U
1	6	1622	G
1	6	1637	C
1	6	1657	U
1	6	1658	G
1	6	1682	U
1	6	1683	C
1	6	1696	G
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1727	G

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Mol	Chain	Res	Type
1	6	1736	G
1	6	1742	U
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	16	A
36	5	24	G
36	5	26	A
36	5	33	G
36	5	38	U
36	5	40	A
36	5	43	A
36	5	44	U
36	5	49	A
36	5	56	G
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	72	C
36	5	73	C
36	5	76	G
36	5	83	U
36	5	88	A
36	5	92	G
36	5	93	C
36	5	99	A
36	5	109	A

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Mol	Chain	Res	Type
36	5	110	G
36	5	111	C
36	5	113	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	142	C
36	5	150	A
36	5	156	G
36	5	157	A
36	5	165	A
36	5	166	C
36	5	170	G
36	5	171	G
36	5	173	G
36	5	174	C
36	5	180	C
36	5	182	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	202	G
36	5	210	U
36	5	211	A
36	5	213	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	224	C
36	5	234	G
36	5	236	G
36	5	237	G
36	5	238	A
36	5	239	G
36	5	240	U
36	5	241	G
36	5	244	G

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Mol	Chain	Res	Type
36	5	245	U
36	5	247	C
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	257	U
36	5	258	G
36	5	259	C
36	5	269	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	315	C
36	5	323	A
36	5	329	U
36	5	330	G
36	5	334	A
36	5	343	U
36	5	349	A
36	5	350	C
36	5	352	A
36	5	375	A
36	5	376	G
36	5	382	U
36	5	395	A
36	5	397	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	417	A
36	5	421	G
36	5	422	A
36	5	425	G
36	5	436	A
36	5	437	G
36	5	439	C
36	5	440	A

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Mol	Chain	Res	Type
36	5	441	U
36	5	442	G
36	5	492	U
36	5	495	G
36	5	520	U
36	5	521	A
36	5	531	G
36	5	535	G
36	5	542	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	551	A
36	5	552	G
36	5	553	U
36	5	555	U
36	5	556	U
36	5	557	A
36	5	559	A
36	5	560	G
36	5	578	A
36	5	579	G
36	5	589	A
36	5	592	A
36	5	600	G
36	5	604	G
36	5	608	A
36	5	609	G
36	5	610	G
36	5	611	A
36	5	619	A
36	5	620	U
36	5	621	A
36	5	622	A
36	5	636	C
36	5	639	G
36	5	640	U
36	5	647	A
36	5	649	A
36	5	653	A
36	5	657	A
36	5	660	A

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Mol	Chain	Res	Type
36	5	661	G
36	5	662	U
36	5	677	A
36	5	681	U
36	5	690	A
36	5	705	A
36	5	712	G
36	5	715	A
36	5	716	A
36	5	719	U
36	5	720	A
36	5	722	G
36	5	724	U
36	5	725	G
36	5	736	A
36	5	737	G
36	5	750	G
36	5	766	U
36	5	767	U
36	5	776	U
36	5	777	U
36	5	781	G
36	5	785	G
36	5	786	A
36	5	806	A
36	5	817	A
36	5	830	A
36	5	859	G
36	5	861	C
36	5	874	U
36	5	879	U
36	5	881	C
36	5	891	G
36	5	894	G
36	5	895	A
36	5	896	A
36	5	897	U
36	5	907	G
36	5	908	G
36	5	910	G
36	5	914	A
36	5	916	G

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Mol	Chain	Res	Type
36	5	917	A
36	5	919	U
36	5	921	A
36	5	923	C
36	5	924	G
36	5	937	G
36	5	944	C
36	5	959	C
36	5	960	U
36	5	977	C
36	5	979	U
36	5	983	A
36	5	993	G
36	5	994	G
36	5	997	A
36	5	1001	G
36	5	1002	A
36	5	1003	A
36	5	1006	A
36	5	1010	G
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1028	U
36	5	1029	G
36	5	1032	C
36	5	1033	U
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1050	U
36	5	1052	U
36	5	1064	A
36	5	1065	A
36	5	1071	U
36	5	1072	G
36	5	1081	U

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Mol	Chain	Res	Type
36	5	1082	U
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1117	G
36	5	1129	A
36	5	1131	G
36	5	1144	U
36	5	1147	G
36	5	1153	A
36	5	1159	A
36	5	1160	C
36	5	1166	G
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1192	C
36	5	1193	A
36	5	1196	C
36	5	1200	A
36	5	1201	C
36	5	1209	G
36	5	1222	G
36	5	1232	C
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1243	G
36	5	1244	A
36	5	1245	A
36	5	1246	G
36	5	1254	C
36	5	1258	U
36	5	1259	A
36	5	1262	G

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Mol	Chain	Res	Type
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1281	G
36	5	1285	G
36	5	1305	U
36	5	1307	G
36	5	1309	U
36	5	1313	G
36	5	1321	G
36	5	1329	U
36	5	1330	A
36	5	1332	A
36	5	1348	U
36	5	1349	G
36	5	1350	A
36	5	1352	A
36	5	1353	U
36	5	1356	U
36	5	1375	G
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1389	G
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1424	C
36	5	1425	U
36	5	1431	G
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1456	A
36	5	1461	A
36	5	1481	A
36	5	1482	A
36	5	1490	A
36	5	1495	U

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Mol	Chain	Res	Type
36	5	1500	G
36	5	1501	U
36	5	1502	C
36	5	1503	A
36	5	1508	C
36	5	1519	G
36	5	1527	C
36	5	1536	G
36	5	1541	G
36	5	1544	G
36	5	1553	U
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1564	U
36	5	1565	G
36	5	1566	A
36	5	1567	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1589	A
36	5	1593	A
36	5	1605	A
36	5	1620	U
36	5	1625	A
36	5	1629	U
36	5	1633	C
36	5	1635	G
36	5	1638	A

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Mol	Chain	Res	Type
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1651	U
36	5	1685	C
36	5	1687	U
36	5	1701	C
36	5	1713	G
36	5	1716	U
36	5	1717	U
36	5	1721	U
36	5	1722	U
36	5	1725	C
36	5	1736	G
36	5	1750	A
36	5	1751	G
36	5	1752	A
36	5	1760	A
36	5	1761	C
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1767	C
36	5	1769	G
36	5	1770	G
36	5	1778	G
36	5	1780	G
36	5	1795	U
36	5	1797	A
36	5	1810	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1820	U
36	5	1821	U
36	5	1839	A
36	5	1841	A
36	5	1842	A
36	5	1845	G

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Mol	Chain	Res	Type
36	5	1846	C
36	5	1848	G
36	5	1849	C
36	5	1850	A
36	5	1864	A
36	5	1866	C
36	5	1869	C
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1893	A
36	5	1906	G
36	5	1908	A
36	5	1935	G
36	5	1947	G
36	5	1952	G
36	5	2101	C
36	5	2102	U
36	5	2112	U
36	5	2113	A
36	5	2120	A
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2139	A
36	5	2144	A
36	5	2158	A
36	5	2169	G
36	5	2187	G
36	5	2188	A
36	5	2189	U
36	5	2198	A
36	5	2199	G
36	5	2201	G
36	5	2205	U
36	5	2207	A
36	5	2209	U
36	5	2210	G
36	5	2222	A
36	5	2223	A
36	5	2225	U
36	5	2231	C

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Mol	Chain	Res	Type
36	5	2239	G
36	5	2244	A
36	5	2250	G
36	5	2251	G
36	5	2252	A
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2258	U
36	5	2264	U
36	5	2270	A
36	5	2273	G
36	5	2274	U
36	5	2278	C
36	5	2279	A
36	5	2280	A
36	5	2281	A
36	5	2282	U
36	5	2288	G
36	5	2297	U
36	5	2298	U
36	5	2306	C
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2333	C
36	5	2334	U
36	5	2336	U
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2388	U
36	5	2392	C
36	5	2393	G
36	5	2397	A
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2410	U

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Mol	Chain	Res	Type
36	5	2411	U
36	5	2418	G
36	5	2420	C
36	5	2435	G
36	5	2436	U
36	5	2439	A
36	5	2440	G
36	5	2441	A
36	5	2443	A
36	5	2444	C
36	5	2504	U
36	5	2505	U
36	5	2506	U
36	5	2507	C
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2514	U
36	5	2515	A
36	5	2523	A
36	5	2524	A
36	5	2525	G
36	5	2526	C
36	5	2530	G
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2541	U
36	5	2543	U
36	5	2549	G
36	5	2552	C
36	5	2555	G
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2585	G

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Mol	Chain	Res	Type
36	5	2586	G
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2614	G
36	5	2619	G
36	5	2625	C
36	5	2639	G
36	5	2652	U
36	5	2654	C
36	5	2656	A
36	5	2674	A
36	5	2677	G
36	5	2681	U
36	5	2689	A
36	5	2690	G
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2700	G
36	5	2714	G
36	5	2726	C
36	5	2728	G
36	5	2729	U
36	5	2734	A
36	5	2739	A
36	5	2749	G
36	5	2752	U
36	5	2753	G
36	5	2762	A
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2783	U
36	5	2787	G
36	5	2796	G
36	5	2799	A
36	5	2800	G
36	5	2801	A

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Mol	Chain	Res	Type
36	5	2810	C
36	5	2814	G
36	5	2817	A
36	5	2818	U
36	5	2819	A
36	5	2821	C
36	5	2822	U
36	5	2829	U
36	5	2837	A
36	5	2838	A
36	5	2843	U
36	5	2845	A
36	5	2847	A
36	5	2853	A
36	5	2861	U
36	5	2871	G
36	5	2872	A
36	5	2887	A
36	5	2889	C
36	5	2896	A
36	5	2899	C
36	5	2904	U
36	5	2923	U
36	5	2928	C
36	5	2932	U
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2947	G
36	5	2955	U
36	5	2957	G
36	5	2971	A
36	5	2972	G
36	5	2983	C
36	5	2987	A
36	5	2990	G
36	5	2996	U
36	5	2997	G
36	5	3006	A
36	5	3012	A
36	5	3033	A
36	5	3049	A

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Mol	Chain	Res	Type
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3069	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3092	C
36	5	3104	U
36	5	3119	U
36	5	3122	A
36	5	3128	G
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3153	U
36	5	3154	C
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3159	C
36	5	3160	U
36	5	3163	A
36	5	3164	C
36	5	3165	A
36	5	3166	C
36	5	3167	A
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3177	G
36	5	3179	U
36	5	3180	A
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U

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Mol	Chain	Res	Type
36	5	3197	G
36	5	3198	U
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3227	A
36	5	3228	C
36	5	3229	G
36	5	3239	G
36	5	3243	A
36	5	3244	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3261	C
36	5	3263	G
36	5	3265	C
36	5	3268	A
36	5	3269	U
36	5	3270	U
36	5	3273	A
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3278	C
36	5	3279	A
36	5	3280	U
36	5	3282	U
36	5	3283	U
36	5	3285	C
36	5	3286	G
36	5	3287	U
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3313	U
36	5	3316	A
36	5	3317	U

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Mol	Chain	Res	Type
36	5	3319	U
36	5	3325	G
36	5	3335	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3350	C
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3355	U
36	5	3356	G
36	5	3358	U
36	5	3369	G
36	5	3378	C
36	5	3382	U
36	5	3383	G
36	5	3389	U
36	5	3390	G
36	5	3393	U
36	5	3396	U
37	7	11	A
37	7	22	A
37	7	27	A
37	7	33	U
37	7	42	A
37	7	54	U
37	7	55	A
37	7	58	C
37	7	60	G
37	7	64	A
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	99	G
37	7	101	G
37	7	102	A
37	7	103	A
37	7	110	G
37	7	112	G
37	7	115	G

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Mol	Chain	Res	Type
37	7	116	C
37	7	121	U
38	8	34	U
38	8	35	C
38	8	43	A
38	8	48	A
38	8	49	G
38	8	52	A
38	8	53	A
38	8	57	C
38	8	58	G
38	8	59	A
38	8	62	C
38	8	63	G
38	8	79	A
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	85	G
38	8	86	U
38	8	87	G
38	8	88	A
38	8	89	A
38	8	95	G
38	8	96	A
38	8	97	A
38	8	98	U
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	114	G
38	8	122	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	155	A
38	8	156	U
38	8	157	U
38	8	158	U

All (306) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	73	U
1	2	103	A
1	2	104	A
1	2	114	C
1	2	126	A
1	2	130	C
1	2	131	C
1	2	136	C
1	2	158	U
1	2	218	A
1	2	240	U
1	2	277	U
1	2	280	U
1	2	321	C
1	2	400	A
1	2	417	A
1	2	468	A
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	510	G
1	2	512	A
1	2	558	U
1	2	582	U
1	2	685	A
1	2	696	C
1	2	704	C
1	2	720	G
1	2	721	U
1	2	734	A
1	2	755	A
1	2	794	U
1	2	811	A
1	2	829	A
1	2	1058	U
1	2	1081	A
1	2	1137	A
1	2	1157	A
1	2	1196	A

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Mol	Chain	Res	Type
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1339	C
1	2	1344	A
1	2	1370	U
1	2	1371	A
1	2	1481	C
1	2	1490	C
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1657	U
1	2	1761	U
36	1	5	G
36	1	13	A
36	1	43	A
36	1	65	A
36	1	93	C
36	1	210	U
36	1	223	U
36	1	239	G
36	1	282	G
36	1	349	A
36	1	374	A
36	1	397	A
36	1	547	G
36	1	559	A
36	1	588	G
36	1	594	U
36	1	647	A
36	1	715	A
36	1	763	G
36	1	816	A
36	1	873	C
36	1	896	A
36	1	916	G
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G

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Mol	Chain	Res	Type
36	1	1103	A
36	1	1196	C
36	1	1222	G
36	1	1273	A
36	1	1307	G
36	1	1329	U
36	1	1348	U
36	1	1352	A
36	1	1355	A
36	1	1419	A
36	1	1481	A
36	1	1507	G
36	1	1554	U
36	1	1562	C
36	1	1582	C
36	1	1716	U
36	1	1765	U
36	1	1815	U
36	1	1820	U
36	1	1841	A
36	1	1842	A
36	1	1846	C
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2249	G
36	1	2281	A
36	1	2309	A
36	1	2372	A
36	1	2374	C
36	1	2400	G
36	1	2418	G
36	1	2513	U
36	1	2523	A
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2677	G
36	1	2689	A
36	1	2728	G

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Mol	Chain	Res	Type
36	1	2772	C
36	1	2801	A
36	1	2817	A
36	1	2818	U
36	1	2867	C
36	1	2887	A
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3195	U
36	1	3217	C
36	1	3218	A
36	1	3228	C
36	1	3242	G
36	1	3269	U
36	1	3275	U
36	1	3315	G
36	1	3316	A
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
37	3	49	G
37	3	86	U
38	4	80	A
38	4	85	G
38	4	111	A
38	4	125	U
1	6	25	C
1	6	66	U
1	6	114	C
1	6	139	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	218	A
1	6	240	U
1	6	259	U
1	6	272	U
1	6	277	U
1	6	280	U

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Mol	Chain	Res	Type
1	6	400	A
1	6	417	A
1	6	539	G
1	6	542	A
1	6	557	G
1	6	558	U
1	6	651	G
1	6	664	U
1	6	678	A
1	6	697	C
1	6	717	C
1	6	720	G
1	6	755	A
1	6	815	G
1	6	829	A
1	6	834	G
1	6	1051	G
1	6	1058	U
1	6	1097	U
1	6	1137	A
1	6	1207	C
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1431	C
1	6	1481	C
1	6	1489	U
1	6	1491	U
1	6	1523	G
1	6	1535	U
1	6	1568	C
1	6	1572	G
1	6	1573	A
1	6	1615	C
1	6	1620	C
1	6	1657	U
1	6	1696	G
1	6	1698	G
1	6	1700	C
36	5	40	A
36	5	43	A
36	5	93	C

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Mol	Chain	Res	Type
36	5	210	U
36	5	223	U
36	5	238	A
36	5	374	A
36	5	397	A
36	5	557	A
36	5	588	G
36	5	594	U
36	5	647	A
36	5	659	G
36	5	715	A
36	5	735	A
36	5	765	C
36	5	766	U
36	5	816	A
36	5	896	A
36	5	908	G
36	5	916	G
36	5	960	U
36	5	978	G
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1181	U
36	5	1192	C
36	5	1236	G
36	5	1238	C
36	5	1239	C
36	5	1241	U
36	5	1284	C
36	5	1329	U
36	5	1331	U
36	5	1348	U
36	5	1352	A
36	5	1355	A
36	5	1392	G
36	5	1434	G
36	5	1481	A
36	5	1507	G
36	5	1554	U

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Mol	Chain	Res	Type
36	5	1560	G
36	5	1643	A
36	5	1716	U
36	5	1815	U
36	5	1816	A
36	5	1846	C
36	5	1879	A
36	5	2101	C
36	5	2112	U
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2281	A
36	5	2372	A
36	5	2374	C
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2539	C
36	5	2585	G
36	5	2593	A
36	5	2728	G
36	5	2752	U
36	5	2772	C
36	5	2801	A
36	5	2818	U
36	5	2820	A
36	5	2887	A
36	5	2896	A
36	5	2971	A
36	5	2996	U
36	5	3055	U
36	5	3056	U
36	5	3078	U
36	5	3121	U
36	5	3154	C
36	5	3167	A
36	5	3177	G
36	5	3195	U
36	5	3228	C
36	5	3242	G

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Mol	Chain	Res	Type
36	5	3246	G
36	5	3269	U
36	5	3275	U
36	5	3289	G
36	5	3340	G
36	5	3354	U
36	5	3357	U
37	7	49	G
38	8	84	C
38	8	111	A
38	8	113	U
38	8	126	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2562 ligands modelled in this entry, 1429 are monoatomic - leaving 1133 for Mogul analysis.

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	$\# Z > 2$
86	OHX	6	2085	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	0,6,6	0.00	-	-		
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	0,6,6	0.00	-	-		
86	OHX	3	215	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4096	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	2	2149	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	6	2181	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	0,6,6	0.00	-	-		
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	6	2142	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		
86	OHX	c3	201	-	0,6,6	0.00	-	-		
86	OHX	5	4057	-	0,6,6	0.00	-	-		
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	5	4132	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	1	4082	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	5	3939	-	0,6,6	0.00	-	-		
86	OHX	5	4143	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	1	4072	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	1	4073	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	S9	201	-	0,6,6	0.00	-	-		
86	OHX	5	4100	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		
86	OHX	6	2206	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	5	4246	-	0,6,6	0.00	-	-		
86	OHX	1	4151	-	0,6,6	0.00	-	-		
86	OHX	2	2096	-	0,6,6	0.00	-	-		
86	OHX	1	4115	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		
86	OHX	L3	403	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
88	3J2	1	4209	-	28,30,30	1.57	5 (17%)	32,52,52	2.00	6 (18%)
86	OHX	8	217	-	0,6,6	0.00	-	-		
86	OHX	2	2121	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	2	2138	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	1	4037	-	0,6,6	0.00	-	-		
86	OHX	c8	203	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	5	4249	-	0,6,6	0.00	-	-		
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	6	2202	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
86	OHX	2	2073	-	0,6,6	0.00	-	-		
86	OHX	1	4145	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	o7	502	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	0,6,6	0.00	-	-		
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	n6	202	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	2	2106	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	5	4168	-	0,6,6	0.00	-	-		
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	5	4214	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	6	2089	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	1	4207	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	O7	105	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	5	4028	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	m0	303	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	0,6,6	0.00	-	-		
86	OHX	2	2122	-	0,6,6	0.00	-	-		
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	5	4047	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	5	3917	-	0,6,6	0.00	-	-		
86	OHX	6	2105	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		
86	OHX	1	3986	-	0,6,6	0.00	-	-		
86	OHX	1	3866	-	0,6,6	0.00	-	-		
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	5	4014	-	0,6,6	0.00	-	-		
86	OHX	m6	202	-	0,6,6	0.00	-	-		
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	6	2135	-	0,6,6	0.00	-	-		
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	0,6,6	0.00	-	-		
86	OHX	1	4158	-	0,6,6	0.00	-	-		
86	OHX	5	4003	-	0,6,6	0.00	-	-		
86	OHX	1	4156	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	6	2139	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	5	4234	86	0,6,6	0.00	-	-		
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	1	4098	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	5	3901	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	5	4036	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	1	3871	-	0,6,6	0.00	-	-		
86	OHX	1	4116	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		
86	OHX	6	2205	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	O2	201	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	6	2123	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		
88	3J2	5	4254	-	28,30,30	1.56	7 (25%)	32,52,52	1.75	8 (25%)
86	OHX	1	3869	-	0,6,6	0.00	-	-		
86	OHX	5	3915	-	0,6,6	0.00	-	-		
86	OHX	d4	201	-	0,6,6	0.00	-	-		
86	OHX	5	3952	-	0,6,6	0.00	-	-		
86	OHX	8	218	-	0,6,6	0.00	-	-		
86	OHX	8	216	-	0,6,6	0.00	-	-		
86	OHX	M6	202	-	0,6,6	0.00	-	-		
86	OHX	2	2102	-	0,6,6	0.00	-	-		
86	OHX	2	2126	-	0,6,6	0.00	-	-		
86	OHX	1	4020	-	0,6,6	0.00	-	-		
86	OHX	1	4087	-	0,6,6	0.00	-	-		
86	OHX	5	4211	-	0,6,6	0.00	-	-		
86	OHX	5	4124	-	0,6,6	0.00	-	-		
86	OHX	1	3942	-	0,6,6	0.00	-	-		
86	OHX	1	4170	-	0,6,6	0.00	-	-		
86	OHX	5	4252	-	0,6,6	0.00	-	-		
86	OHX	1	4175	-	0,6,6	0.00	-	-		
86	OHX	1	3870	-	0,6,6	0.00	-	-		
86	OHX	1	3898	-	0,6,6	0.00	-	-		
86	OHX	1	4180	-	0,6,6	0.00	-	-		
86	OHX	1	4052	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3929	-	0,6,6	0.00	-	-		
86	OHX	1	3997	-	0,6,6	0.00	-	-		
86	OHX	1	4004	-	0,6,6	0.00	-	-		
86	OHX	5	4248	-	0,6,6	0.00	-	-		
86	OHX	m7	206	-	0,6,6	0.00	-	-		
86	OHX	5	3972	-	0,6,6	0.00	-	-		
86	OHX	5	4241	-	0,6,6	0.00	-	-		
86	OHX	6	2177	-	0,6,6	0.00	-	-		
86	OHX	5	4236	-	0,6,6	0.00	-	-		
86	OHX	1	4084	-	0,6,6	0.00	-	-		
86	OHX	1	4186	-	0,6,6	0.00	-	-		
86	OHX	2	2054	-	0,6,6	0.00	-	-		
86	OHX	5	4092	-	0,6,6	0.00	-	-		
86	OHX	1	4150	-	0,6,6	0.00	-	-		
86	OHX	1	4200	-	0,6,6	0.00	-	-		
86	OHX	5	4089	-	0,6,6	0.00	-	-		
86	OHX	6	2191	-	0,6,6	0.00	-	-		
86	OHX	5	4154	-	0,6,6	0.00	-	-		
86	OHX	2	2134	-	0,6,6	0.00	-	-		
86	OHX	5	4178	-	0,6,6	0.00	-	-		
86	OHX	5	4073	-	0,6,6	0.00	-	-		
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	3	217	-	0,6,6	0.00	-	-		
86	OHX	5	4153	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	5	4055	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	4	223	-	0,6,6	0.00	-	-		
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	1	4191	-	0,6,6	0.00	-	-		
86	OHX	1	3868	-	0,6,6	0.00	-	-		
86	OHX	3	225	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	5	4018	-	0,6,6	0.00	-	-		
86	OHX	5	4142	-	0,6,6	0.00	-	-		
86	OHX	1	3928	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	0,6,6	0.00	-	-		
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	2	2039	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		
86	OHX	5	4126	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	6	2095	-	0,6,6	0.00	-	-		
86	OHX	13	404	-	0,6,6	0.00	-	-		
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	6	2074	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	q1	101	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	5	4235	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		
86	OHX	6	2082	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	4	225	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	s4	301	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	m8	201	-	0,6,6	0.00	-	-		
86	OHX	5	4222	-	0,6,6	0.00	-	-		
86	OHX	2	2028	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	5	3942	-	0,6,6	0.00	-	-		
86	OHX	8	219	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	0,6,6	0.00	-	-		
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	6	2203	-	0,6,6	0.00	-	-		
86	OHX	1	4065	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	1	4120	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	1	4083	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	2	2056	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	l3	403	-	0,6,6	0.00	-	-		
86	OHX	5	3900	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
86	OHX	C8	201	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	6	2195	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2147	86	0,6,6	0.00	-	-		
86	OHX	1	3917	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	5	4010	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	15	303	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		
86	OHX	2	2087	-	0,6,6	0.00	-	-		
86	OHX	2	2123	-	0,6,6	0.00	-	-		
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	1	4183	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	0,6,6	0.00	-	-		
86	OHX	1	4086	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	1	4035	-	0,6,6	0.00	-	-		
86	OHX	5	4253	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4081	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	L3	405	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	2	2172	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	0,6,6	0.00	-	-		
86	OHX	6	2116	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	5	4239	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		
86	OHX	6	2054	-	0,6,6	0.00	-	-		
86	OHX	5	4131	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		
86	OHX	5	3911	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	2	2094	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	5	4076	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	5	3982	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	5	4023	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	4	224	-	0,6,6	0.00	-	-		
86	OHX	14	402	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	0,6,6	0.00	-	-		
86	OHX	6	2137	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	1	4165	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	5	4149	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	1	3900	-	0,6,6	0.00	-	-		
86	OHX	2	2062	-	0,6,6	0.00	-	-		
86	OHX	1	4013	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		
86	OHX	5	4198	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	5	4247	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	0,6,6	0.00	-	-		
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	2	2035	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	6	2204	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	5	3955	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	5	3998	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	6	2196	-	0,6,6	0.00	-	-		
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	1	4091	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	5	4016	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	5	4161	-	0,6,6	0.00	-	-		
86	OHX	6	2198	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	0,6,6	0.00	-	-		
86	OHX	2	2024	-	0,6,6	0.00	-	-		
86	OHX	1	4053	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	5	4122	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	1	3873	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	1	3872	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		
86	OHX	s1	303	-	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	5	3924	-	0,6,6	0.00	-	-		
86	OHX	6	2174	-	0,6,6	0.00	-	-		
86	OHX	5	4228	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		
86	OHX	l5	302	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	0,6,6	0.00	-	-		
86	OHX	L3	404	-	0,6,6	0.00	-	-		
86	OHX	1	4045	-	0,6,6	0.00	-	-		
86	OHX	2	2144	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	7	220	-	0,6,6	0.00	-	-		
86	OHX	5	3988	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	2	2080	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	5	4232	-	0,6,6	0.00	-	-		
86	OHX	7	229	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	2	2180	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	2	2041	-	0,6,6	0.00	-	-		
86	OHX	M7	205	-	0,6,6	0.00	-	-		
86	OHX	7	219	-	0,6,6	0.00	-	-		
86	OHX	5	3913	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	6	2069	-	0,6,6	0.00	-	-		
86	OHX	1	4030	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	0,6,6	0.00	-	-		
86	OHX	1	4100	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	L4	403	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	Q2	502	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	s1	302	-	0,6,6	0.00	-	-		
86	OHX	2	2047	-	0,6,6	0.00	-	-		
86	OHX	O9	101	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	6	2093	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	M8	202	-	0,6,6	0.00	-	-		
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	2	2176	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	1	4000	86	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	m1	203	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	m9	201	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	1	4023	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4063	-	0,6,6	0.00	-	-		
86	OHX	1	3885	-	0,6,6	0.00	-	-		
86	OHX	5	3944	86	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	6	2050	-	0,6,6	0.00	-	-		
86	OHX	1	4153	-	0,6,6	0.00	-	-		
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	C1	201	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	5	4151	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	0,6,6	0.00	-	-		
86	OHX	M7	204	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		
86	OHX	5	3996	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	O3	202	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	2	2111	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	6	2187	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	o3	202	-	0,6,6	0.00	-	-		
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	1	4085	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		
86	OHX	1	4019	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	8	229	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	5	4251	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	6	2068	-	0,6,6	0.00	-	-		
86	OHX	6	2145	-	0,6,6	0.00	-	-		
86	OHX	5	4227	-	0,6,6	0.00	-	-		
86	OHX	2	2032	86	0,6,6	0.00	-	-		
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	1	4206	-	0,6,6	0.00	-	-		
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	0,6,6	0.00	-	-		
86	OHX	1	3998	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	1	3886	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	0,6,6	0.00	-	-		
86	OHX	5	4167	-	0,6,6	0.00	-	-		
86	OHX	M9	202	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	0,6,6	0.00	-	-		
86	OHX	5	3909	-	0,6,6	0.00	-	-		
86	OHX	1	4127	-	0,6,6	0.00	-	-		
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		
86	OHX	8	230	-	0,6,6	0.00	-	-		
86	OHX	1	3865	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	0,6,6	0.00	-	-		
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	1	4007	-	0,6,6	0.00	-	-		
86	OHX	C3	201	-	0,6,6	0.00	-	-		
86	OHX	2	2175	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	1	4025	-	0,6,6	0.00	-	-		
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	1	4008	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	5	3995	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	1	3967	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	5	4225	-	0,6,6	0.00	-	-		
86	OHX	5	4026	-	0,6,6	0.00	-	-		
86	OHX	1	3864	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	4	228	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		
86	OHX	1	4138	-	0,6,6	0.00	-	-		
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	6	2208	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		
86	OHX	5	3966	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	6	2207	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	7	222	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	4	237	-	0,6,6	0.00	-	-		
86	OHX	1	3978	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	1	4114	-	0,6,6	0.00	-	-		
86	OHX	1	4012	-	0,6,6	0.00	-	-		
86	OHX	M5	304	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	N9	102	-	0,6,6	0.00	-	-		
86	OHX	6	2075	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	1	3863	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	n3	202	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	5	4024	-	0,6,6	0.00	-	-		
86	OHX	2	2179	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	5	4045	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		
86	OHX	1	3934	-	0,6,6	0.00	-	-		
86	OHX	1	3891	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		
86	OHX	m5	305	-	0,6,6	0.00	-	-		
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
86	OHX	O7	104	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		
86	OHX	s8	303	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		
86	OHX	7	228	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	1	4208	-	0,6,6	0.00	-	-		
86	OHX	2	2170	-	0,6,6	0.00	-	-		
86	OHX	2	2163	-	0,6,6	0.00	-	-		
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	5	4217	-	0,6,6	0.00	-	-		
86	OHX	1	3947	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	5	4250	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4109	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	5	4097	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		
86	OHX	3	222	-	0,6,6	0.00	-	-		
86	OHX	5	4226	-	0,6,6	0.00	-	-		
86	OHX	6	2163	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	8	231	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	1	4014	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	5	4160	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	0,6,6	0.00	-	-		
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	M0	303	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		
86	OHX	5	3962	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	5	4175	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	1	4061	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	0,6,6	0.00	-	-		
86	OHX	4	236	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	1	3939	-	0,6,6	0.00	-	-		
86	OHX	6	2183	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	19	202	-	0,6,6	0.00	-	-		
86	OHX	5	3999	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	2	2178	-	0,6,6	0.00	-	-		
86	OHX	1	3957	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	1	3867	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	6	2151	-	0,6,6	0.00	-	-		
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		
86	OHX	2	2046	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	0,6,6	0.00	-	-		
86	OHX	5	3904	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
86	OHX	1	4009	-	0,6,6	0.00	-	-		
86	OHX	4	238	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	n9	102	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	1	3874	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	1	4168	86	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	15	304	-	0,6,6	0.00	-	-		
86	OHX	5	3945	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	1	3920	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	5	4125	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	1	3884	-	0,6,6	0.00	-	-		
86	OHX	6	2184	-	0,6,6	0.00	-	-		
86	OHX	5	3941	-	0,6,6	0.00	-	-		
86	OHX	5	4107	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	4	234	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3889	-	0,6,6	0.00	-	-		
86	OHX	6	2073	-	0,6,6	0.00	-	-		
86	OHX	5	4208	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	5	4038	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	5	4195	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		

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
88	3J2	5	4254	-	-	0/2/65/65	0/5/5/5
88	3J2	1	4209	-	-	0/2/65/65	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4209	3J2	C4-C13	4.52	1.47	1.40
88	1	4209	3J2	C3-C1	4.40	1.57	1.51
88	5	4254	3J2	C4-C3	-4.14	1.34	1.39
88	5	4254	3J2	C4-C13	3.57	1.46	1.40
88	5	4254	3J2	C14-C13	-3.05	1.34	1.39
88	1	4209	3J2	C14-C13	-2.86	1.34	1.39
88	5	4254	3J2	C-C1	2.66	1.59	1.52
88	5	4254	3J2	O1-C3	2.20	1.38	1.35
88	5	4254	3J2	C14-C15	2.14	1.41	1.37
88	5	4254	3J2	C4-C5	-2.11	1.49	1.52
88	1	4209	3J2	O1-C3	2.03	1.37	1.35
88	1	4209	3J2	C10-C9	2.01	1.56	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4209	3J2	O6-C5-C6	-5.77	97.42	109.61
88	1	4209	3J2	O2-C11-C12	5.14	123.51	117.72
88	5	4254	3J2	C18-C8-C9	-4.85	99.90	108.96
88	1	4209	3J2	O1-C3-C1	-4.21	107.25	112.52

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	5	4254	3J2	O6-C5-C6	-4.13	100.89	109.61
88	1	4209	3J2	C18-C8-C9	-3.24	102.89	108.96
88	5	4254	3J2	C15-C14-C13	2.73	124.48	119.43
88	1	4209	3J2	C7-C12-C11	-2.69	99.05	106.85
88	5	4254	3J2	O1-C15-C14	-2.59	115.97	119.27
88	5	4254	3J2	C14-C13-C12	2.59	127.09	120.72
88	5	4254	3J2	C-C1-C2	2.56	116.29	110.31
88	5	4254	3J2	C7-C12-C11	-2.47	99.68	106.85
88	5	4254	3J2	C16-C12-C7	2.40	120.79	113.01
88	1	4209	3J2	C15-C14-C13	2.34	123.76	119.43

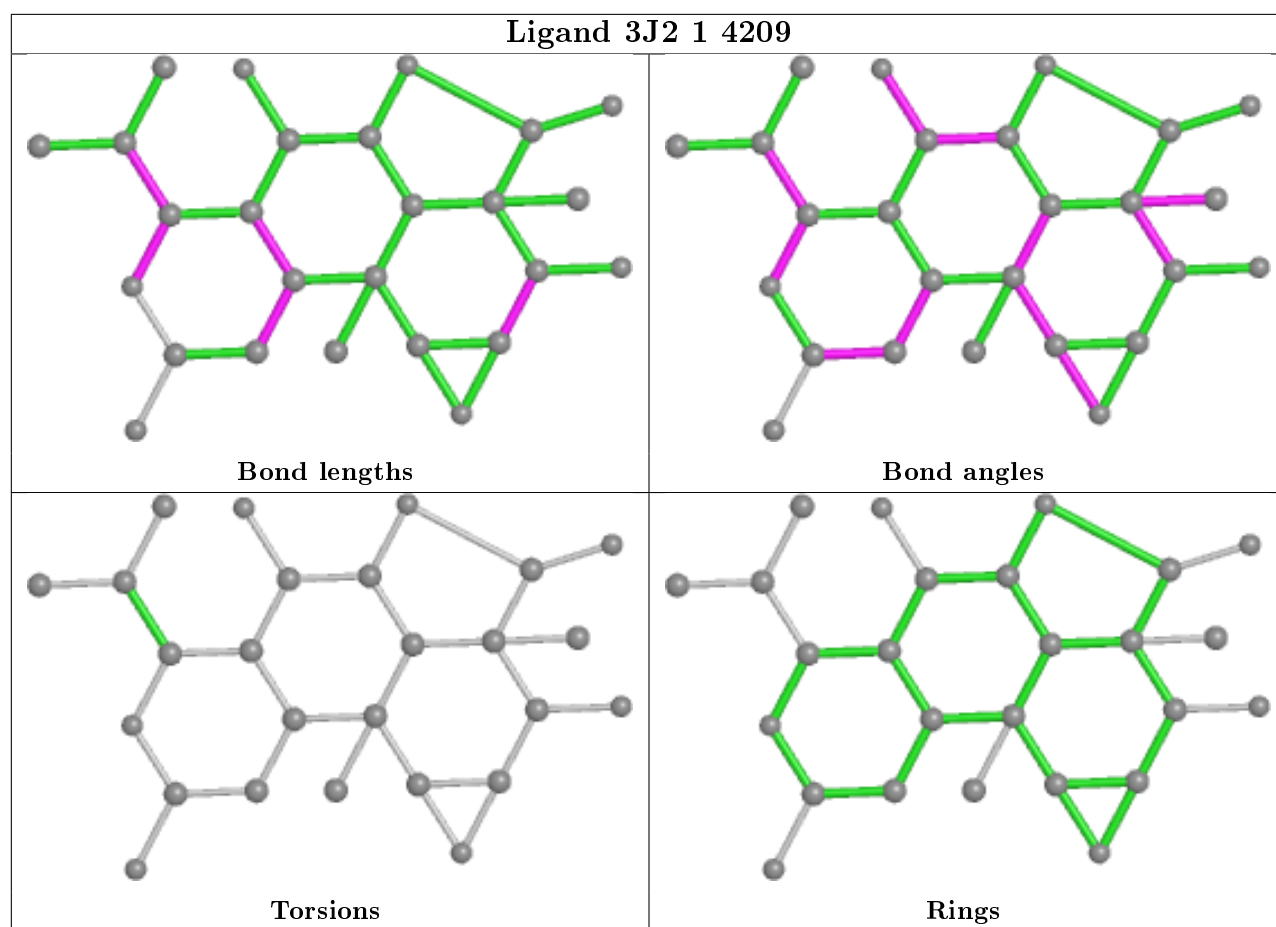
There are no chirality outliers.

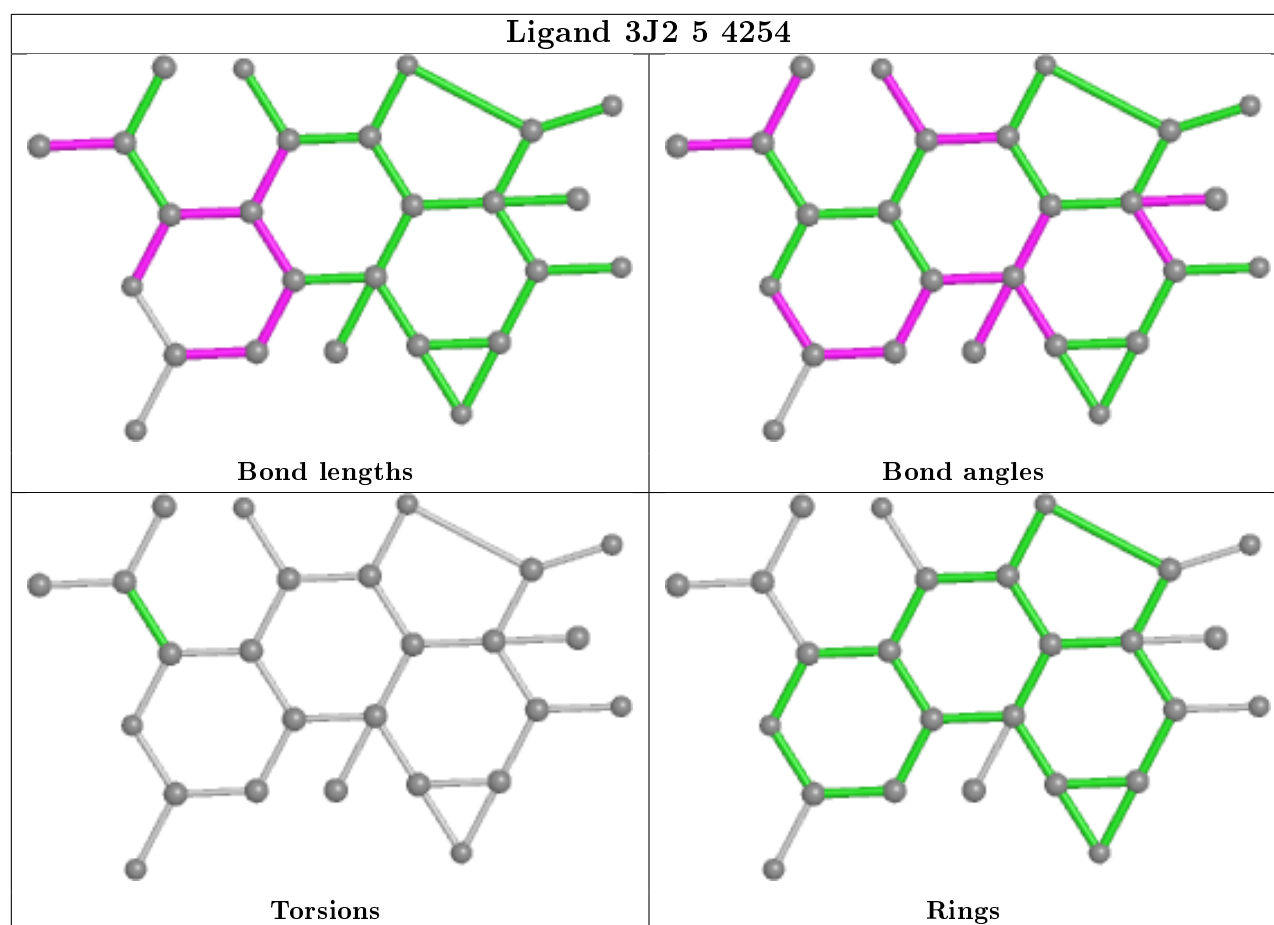
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.