



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 07:36 AM BST

PDB ID : 4U4Q
Title : Crystal structure of Homoharringtonine 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

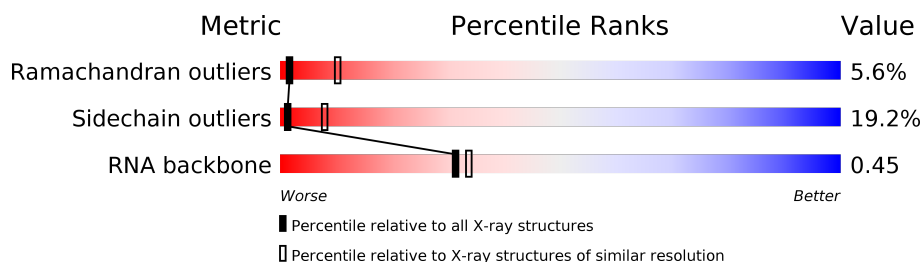
1 Overall quality at a glance

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)















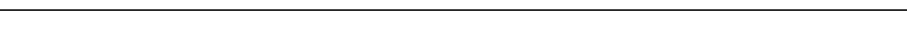




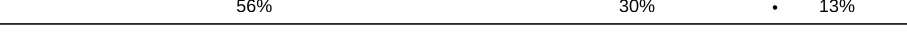





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	65% 27% 5% .
1	6	1800	65% 29% 6%
2	S0	251	62% 18% . 18%
2	s0	251	61% 20% . 18%
3	S1	254	59% 24% . 16%
3	s1	254	65% 19% . 15%
4	S2	253	68% 17% . 14%
4	s2	253	65% 19% . 14%




















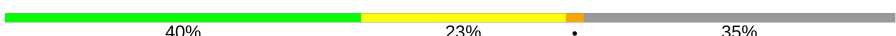





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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3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















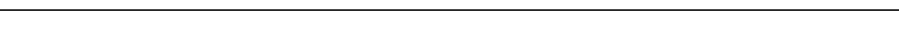




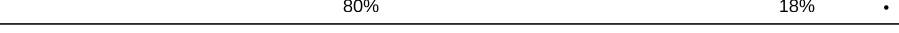





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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	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	 81% 18% .
56	N0	172	 78% 21% .
56	n0	172	 81% 19%
57	N1	159	 82% 17% .
57	n1	159	 82% 17% .
58	N2	120	 69% 14% 17%
58	n2	120	 66% 15% . 18%
59	N3	136	 84% 15% .
59	n3	136	 89% 10% .
60	N4	155	 54% 8% . 37%
60	n4	155	 70% 15% . 13%
61	N5	141	 65% 21% 14%
61	n5	141	 63% 20% . 15%
62	N6	126	 81% 17% ..
62	n6	126	 74% 25% .
63	N7	135	 79% 18% .
63	n7	135	 76% 21% .
64	N8	148	 78% 19% .
64	n8	148	 80% 18% .
65	N9	58	 79% 19% .
65	n9	58	 71% 26% .
66	O0	104	 79% 14% 7%
66	o0	104	 79% 17% .
67	O1	112	 76% 19% . .
67	o1	112	 72% 24% . .

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Mol	Chain	Length	Quality of chain
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	120	
70	o4	120	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	e0	62	

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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>39%7%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 411245 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
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	147	ALA	GLY	conflict	UNP P0CX47
c1	147	ALA	GLY	conflict	UNP P0CX47

- 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			

- 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				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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			
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	12	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			
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			

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

- 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			
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		0	0	0
			796	516	131	149				
58	n2	98	Total	C	N	O		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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	121	LYS	-	expression tag	UNP P87262
o4	121	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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				
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			

- Molecule 81 is a protein called Unknown protein chain 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 chain 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 chain 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	4	Total	Mg	0	0
			4	4		
85	m6	2	Total	Mg	0	0
			2	2		
85	n8	5	Total	Mg	0	0
			5	5		
85	o1	1	Total	Mg	0	0
			1	1		
85	N5	1	Total	Mg	0	0
			1	1		
85	6	147	Total	Mg	0	0
			147	147		
85	sM	2	Total	Mg	0	0
			2	2		
85	O4	1	Total	Mg	0	0
			1	1		
85	q1	1	Total	Mg	0	0
			1	1		
85	l3	3	Total	Mg	0	0
			3	3		
85	M1	2	Total	Mg	0	0
			2	2		
85	n0	2	Total	Mg	0	0
			2	2		
85	d6	1	Total	Mg	0	0
			1	1		
85	C8	1	Total	Mg	0	0
			1	1		
85	O3	1	Total	Mg	0	0
			1	1		
85	S6	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L4	1	Total 1	Mg 1	0	0
85	l7	3	Total 3	Mg 3	0	0
85	M5	2	Total 2	Mg 2	0	0
85	c9	2	Total 2	Mg 2	0	0
85	S2	2	Total 2	Mg 2	0	0
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	M9	2	Total 2	Mg 2	0	0
85	q0	1	Total 1	Mg 1	0	0
85	o4	2	Total 2	Mg 2	0	0
85	M0	3	Total 3	Mg 3	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	500	Total 500	Mg 500	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	s6	1	Total 1	Mg 1	0	0
85	l4	1	Total 1	Mg 1	0	0
85	1	466	Total 466	Mg 466	0	0
85	s4	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	S8	1	Total 1	Mg 1	0	0

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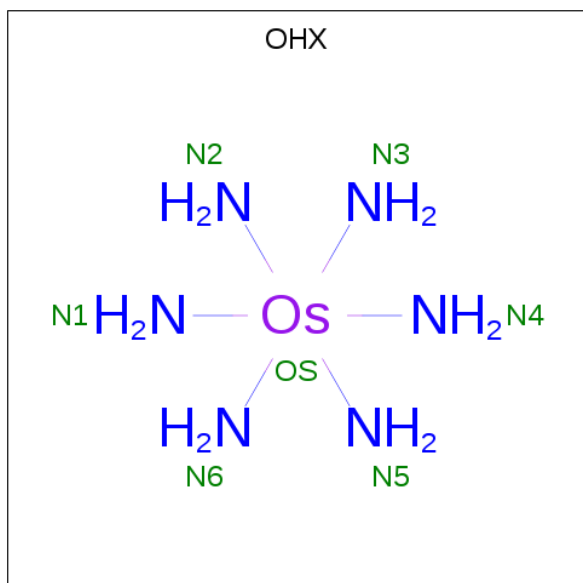
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	m1	2	Total 2	Mg 2	0	0
85	O2	1	Total 1	Mg 1	0	0
85	s9	1	Total 1	Mg 1	0	0
85	o3	2	Total 2	Mg 2	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	2	Total 2	Mg 2	0	0
85	N8	6	Total 6	Mg 6	0	0
85	4	23	Total 23	Mg 23	0	0
85	n6	2	Total 2	Mg 2	0	0
85	S4	2	Total 2	Mg 2	0	0
85	L2	2	Total 2	Mg 2	0	0
85	o7	1	Total 1	Mg 1	0	0
85	l5	1	Total 1	Mg 1	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	5	Total 5	Mg 5	0	0
85	L6	1	Total 1	Mg 1	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	c7	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	7	16	Total	Mg	0	0
			16	16		
85	n3	2	Total	Mg	0	0
			2	2		
85	L3	3	Total	Mg	0	0
			3	3		
85	2	121	Total	Mg	0	0
			121	121		
85	12	2	Total	Mg	0	0
			2	2		
85	8	15	Total	Mg	0	0
			15	15		
85	m0	1	Total	Mg	0	0
			1	1		
85	M6	1	Total	Mg	0	0
			1	1		
85	N0	1	Total	Mg	0	0
			1	1		
85	3	13	Total	Mg	0	0
			13	13		

- 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		

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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		
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		
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		
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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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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
86	1	1	Total	N	Os	0	0
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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
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
86	1	1	Total	N	Os	0	0
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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
86	1	1	Total	N	Os	0	0
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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	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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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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86	4	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
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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
			7	6	1		
86	M5	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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	N1	1	Total	N	Os	0	0
			7	6	1		
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
			7	6	1		
86	O9	1	Total	N	Os	0	0
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86	Q2	1	Total	N	Os	0	0
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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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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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			7	6	1		
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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		
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	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	7	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	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	13	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		

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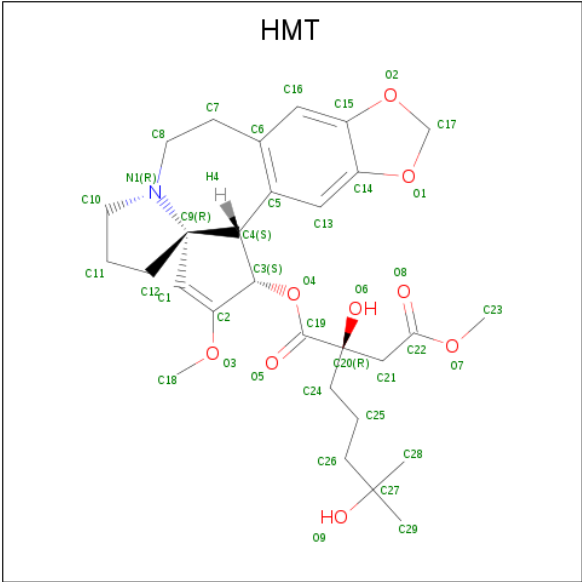
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l9	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	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		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	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	o9	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 1 1	0	0
87	D6	1	Total Zn 1 1	0	0
87	Q2	1	Total Zn 1 1	0	0
87	e1	1	Total Zn 1 1	0	0
87	Q3	1	Total Zn 1 1	0	0
87	D9	1	Total Zn 1 1	0	0
87	E1	1	Total Zn 1 1	0	0
87	Q0	1	Total Zn 1 1	0	0
87	d7	1	Total Zn 1 1	0	0
87	q3	1	Total Zn 1 1	0	0
87	d9	1	Total Zn 1 1	0	0
87	D7	1	Total Zn 1 1	0	0
87	d6	1	Total Zn 1 1	0	0
87	o7	1	Total Zn 1 1	0	0
87	O7	1	Total Zn 1 1	0	0
87	q2	1	Total Zn 1 1	0	0

- Molecule 88 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano
yl]cephalotaxine (three-letter code: HMT) (formula: C₂₉H₃₉NO₉).



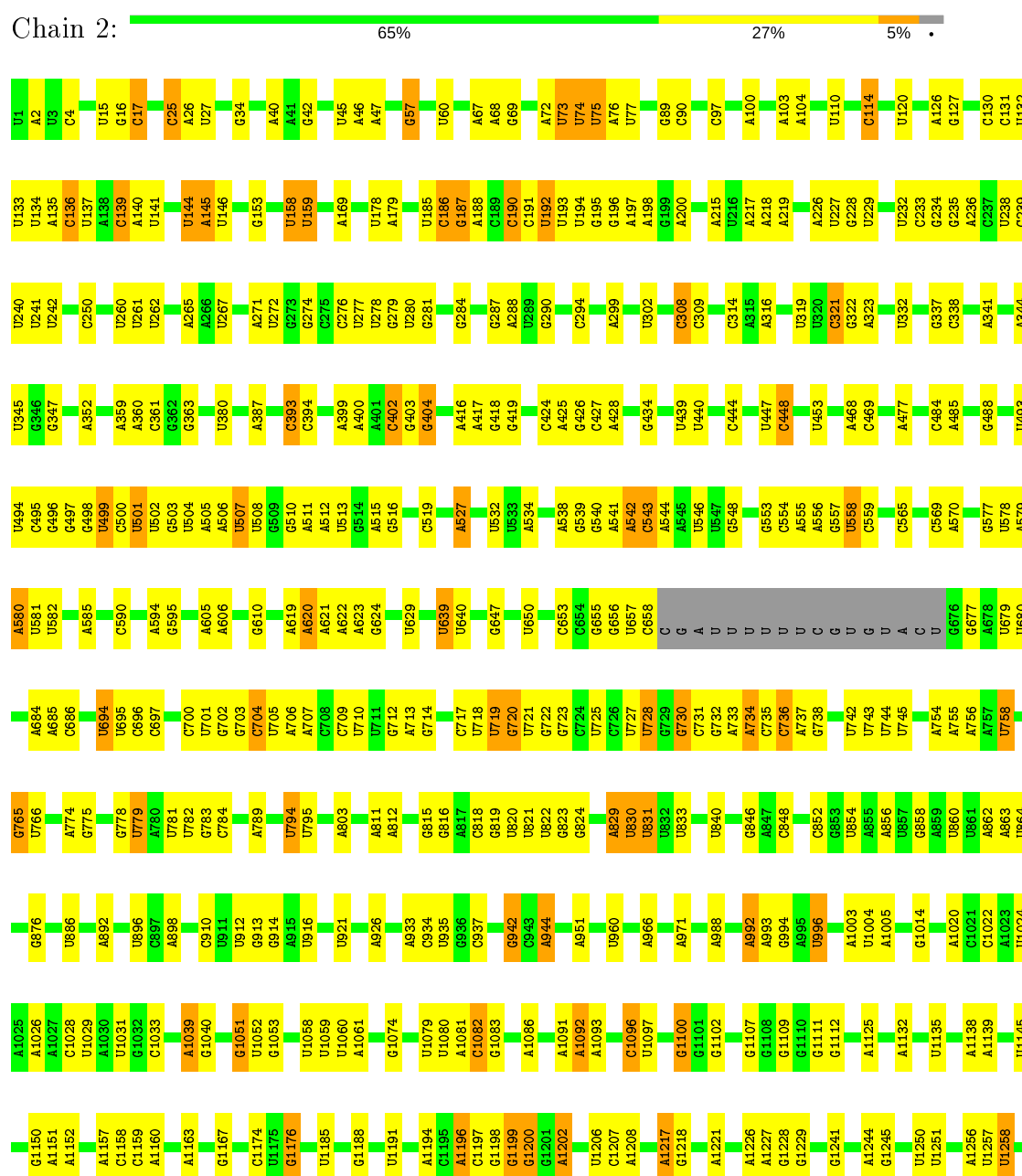
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	1	1	Total	C	N	O	0	0
			39	29	1	9		
88	5	1	Total	C	N	O	0	0
			39	29	1	9		

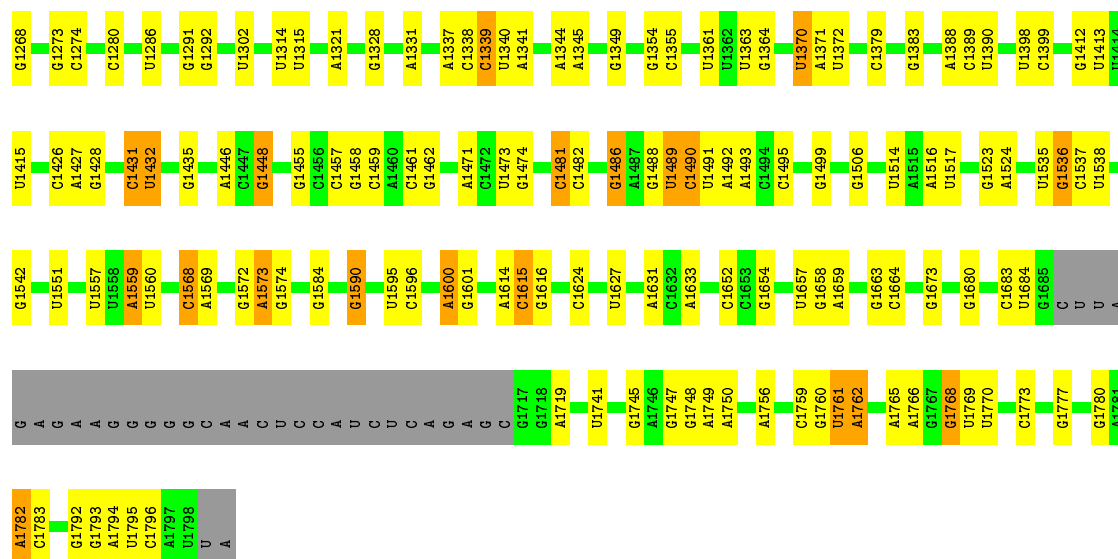
3 Residue-property plots

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.

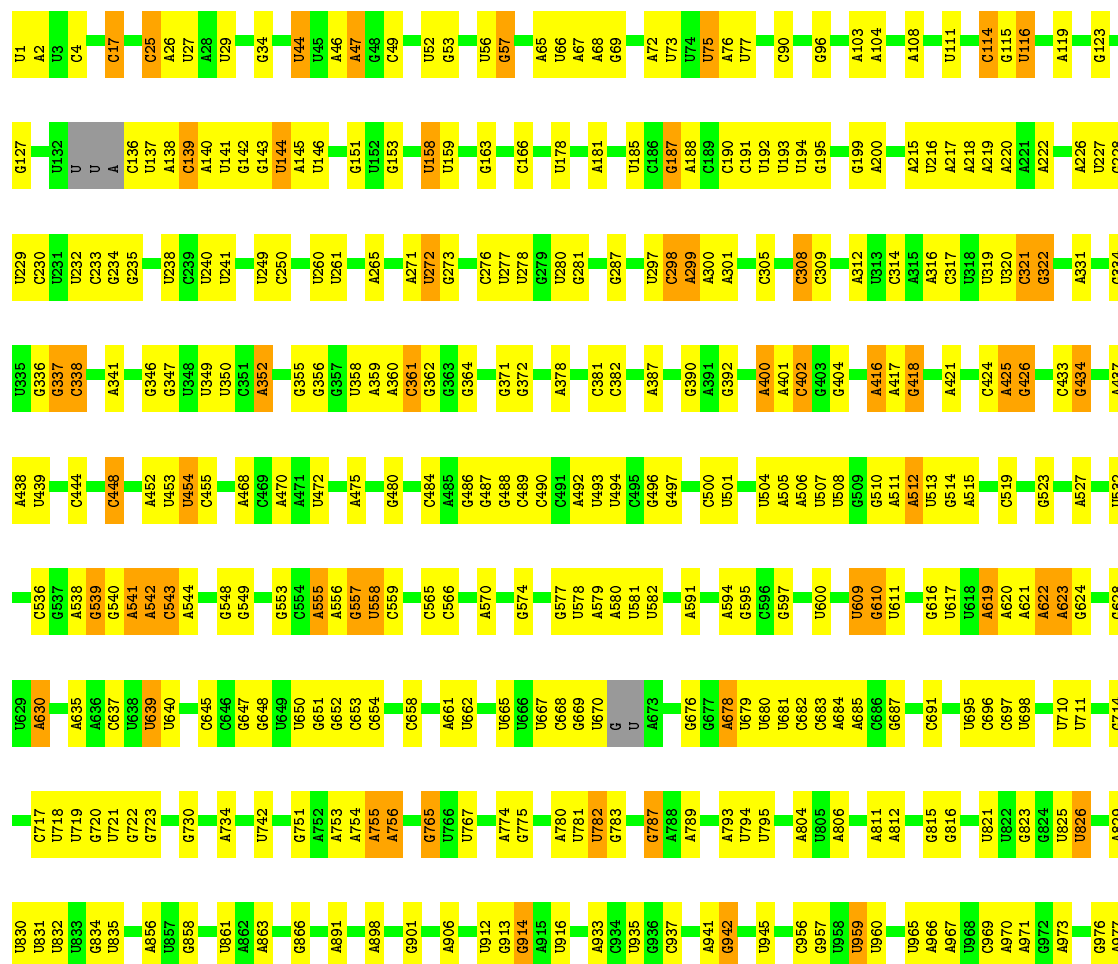
• Molecule 1: 18S ribosomal RNA

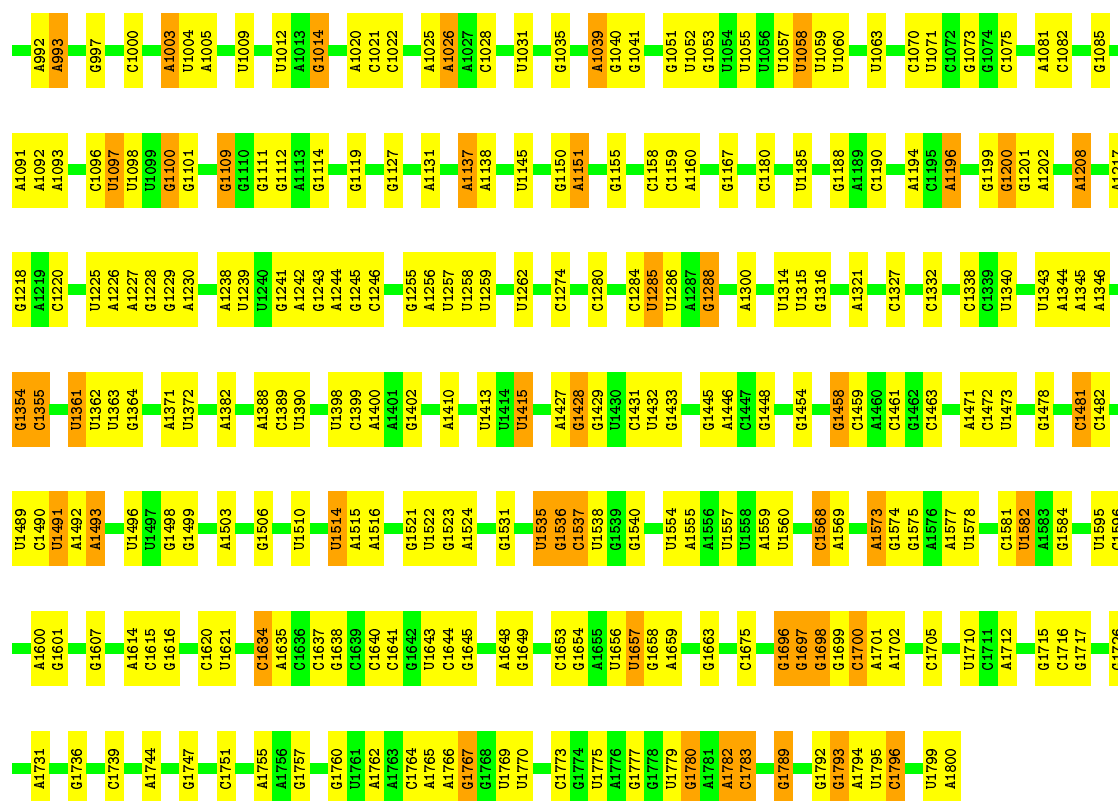




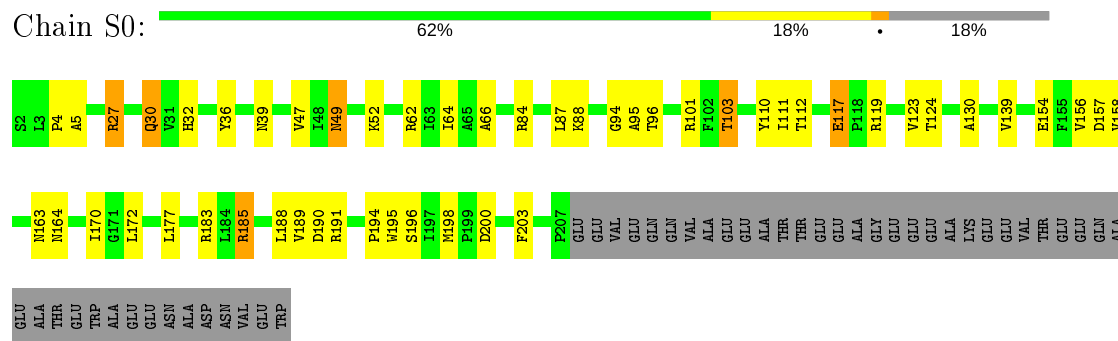
● Molecule 1: 18S ribosomal RNA

Chain 6: 65% 29% 6%

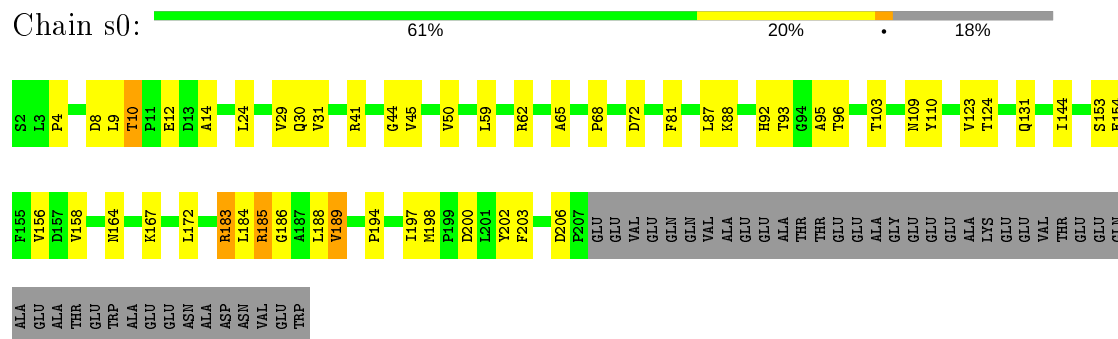




- Molecule 2: 40S ribosomal protein S0-A

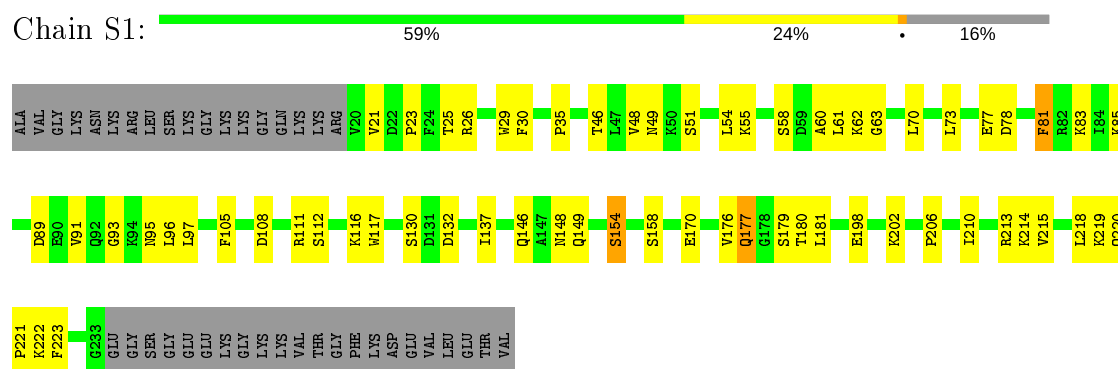


- Molecule 2: 40S ribosomal protein S0-A



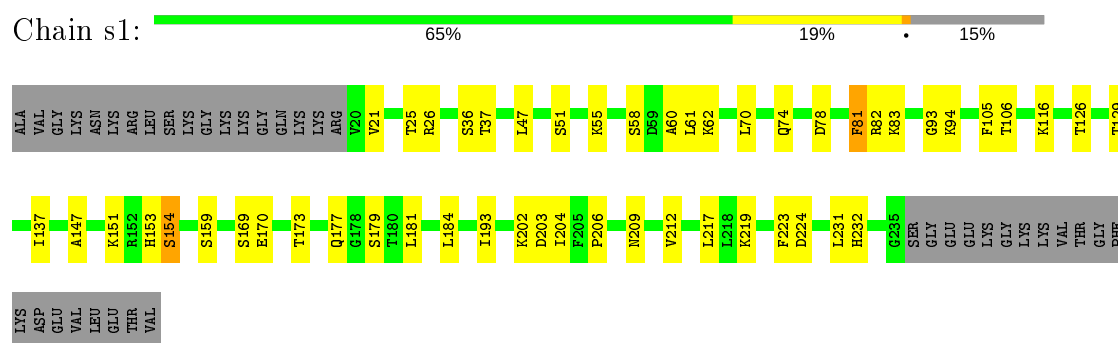
- Molecule 3: 40S ribosomal protein S1-A

Chain S1:



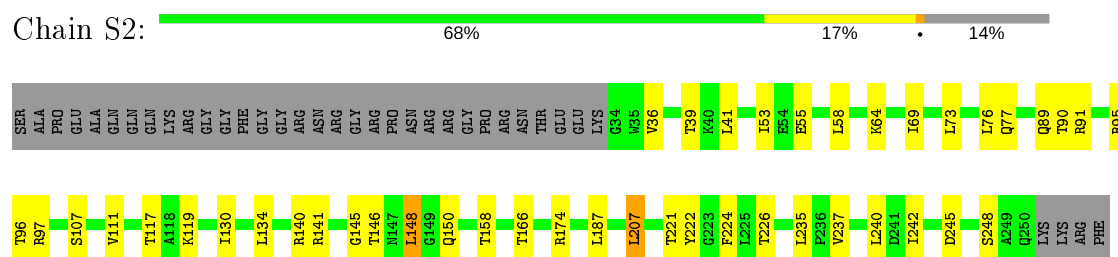
- Molecule 3: 40S ribosomal protein S1-A

Chain s1:



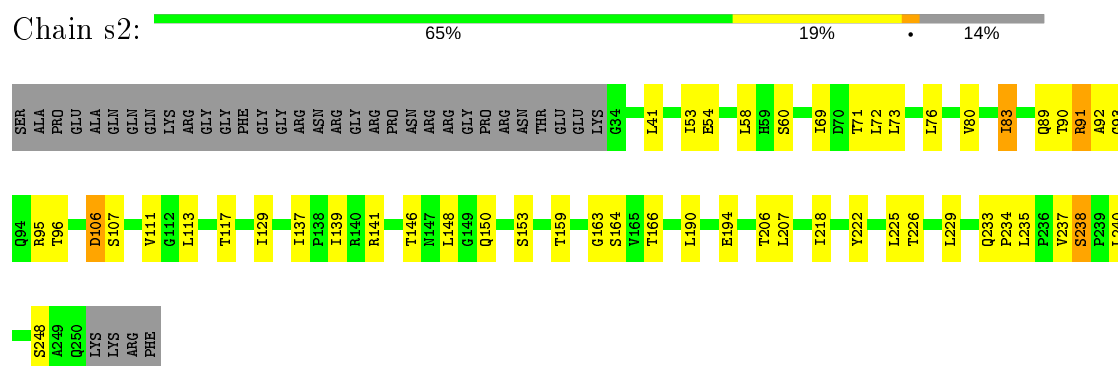
- Molecule 4: 40S ribosomal protein S2

Chain S2:



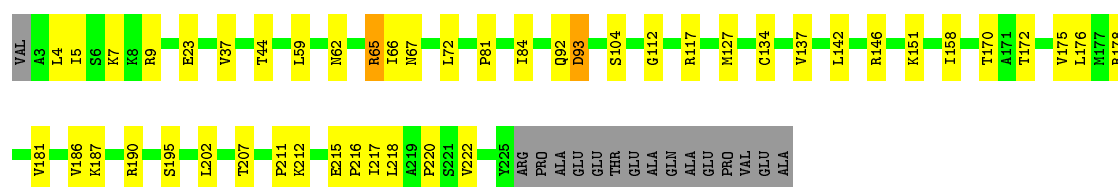
- Molecule 4: 40S ribosomal protein S2

Chain s2:



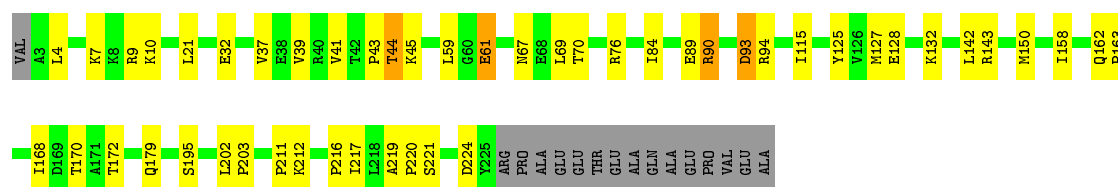
- Molecule 5: 40S ribosomal protein S3

Chain S3: 




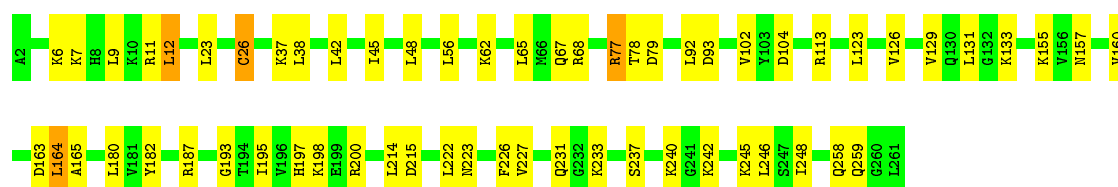
- Molecule 5: 40S ribosomal protein S3

Chain s3: 




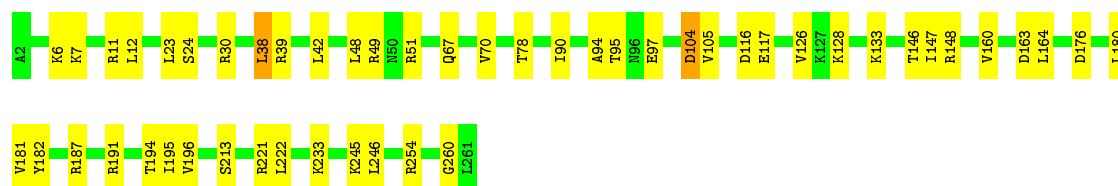
- Molecule 6: 40S ribosomal protein S4-A

Chain S4: 



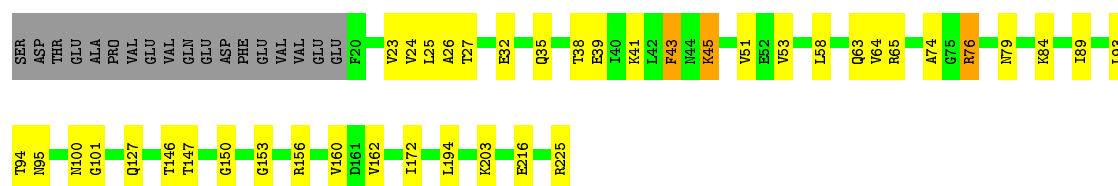
- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 



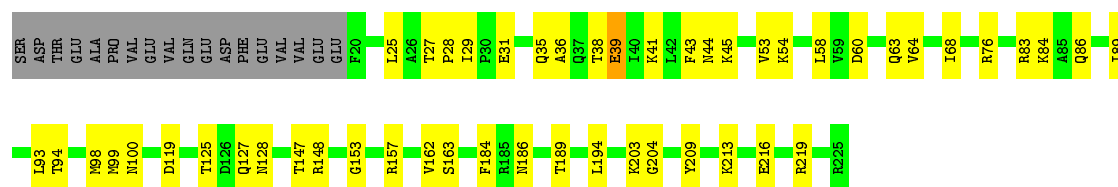
- Molecule 7: 40S ribosomal protein S5

Chain S5: 



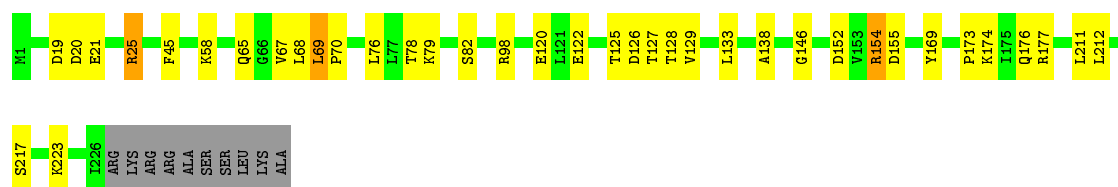
- Molecule 7: 40S ribosomal protein S5

Chain s5: 



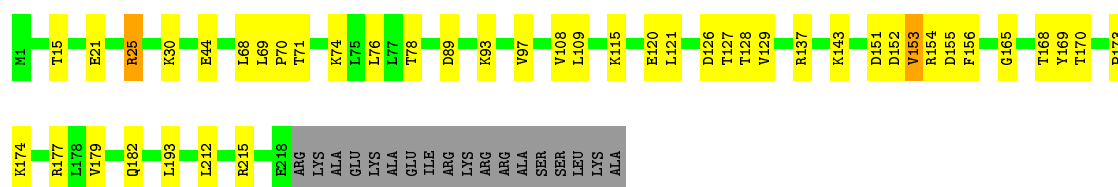
- Molecule 8: 40S ribosomal protein S6-A

Chain S6: 



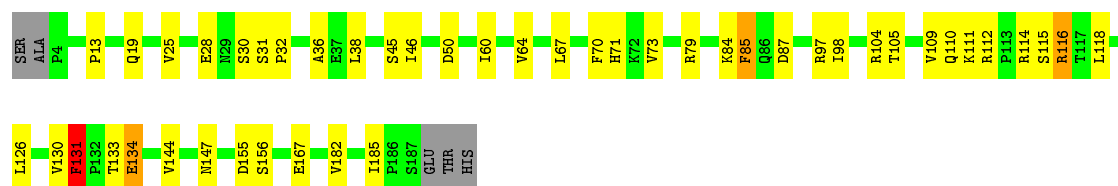
- Molecule 8: 40S ribosomal protein S6-A

Chain s6: 




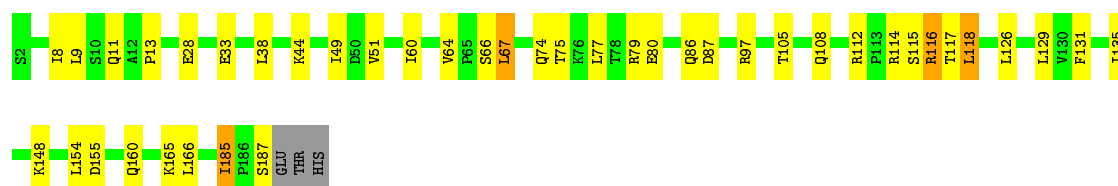
- Molecule 9: 40S ribosomal protein S7-A

Chain S7: 




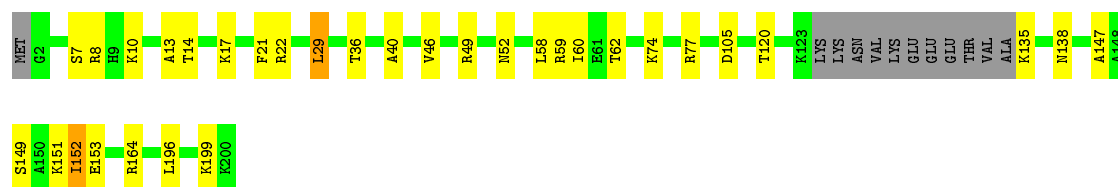
- Molecule 9: 40S ribosomal protein S7-A

Chain s7: 




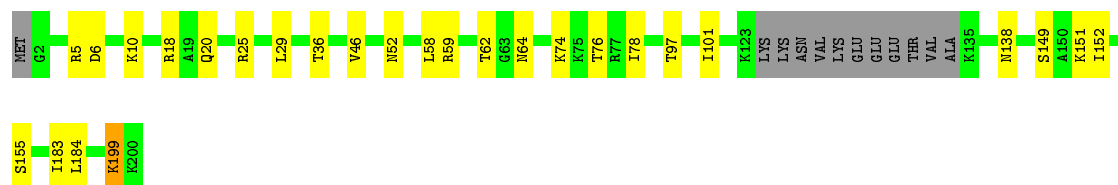
- Molecule 10: 40S ribosomal protein S8-A

Chain S8:  78% 15% 6%



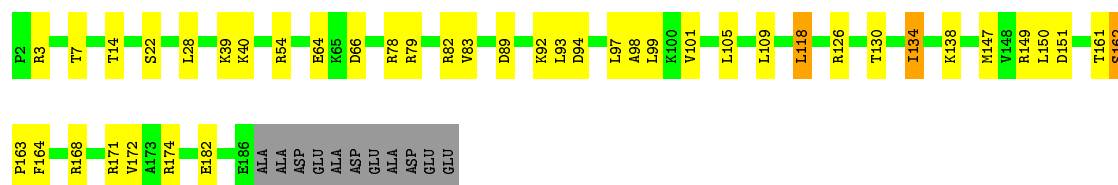
- Molecule 10: 40S ribosomal protein S8-A

Chain s8:  81% 13% 6%



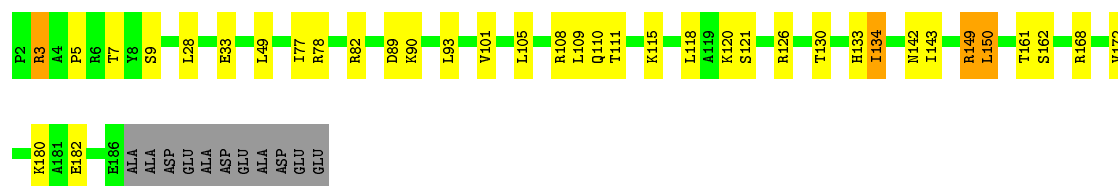
- Molecule 11: 40S ribosomal protein S9-A

Chain S9:  73% 20% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9:  76% 17% 6%



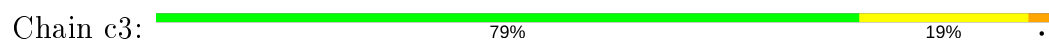
- Molecule 12: 40S ribosomal protein S10-A

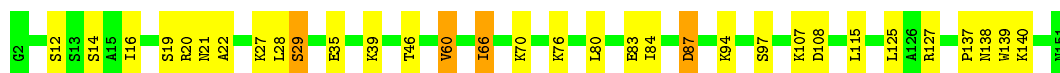
Chain C0:  71% 18% 9%



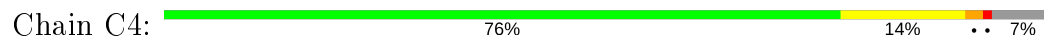
- Molecule 12: 40S ribosomal protein S10-A

Chain c0:  66% 23% 9%

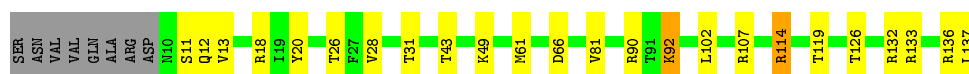
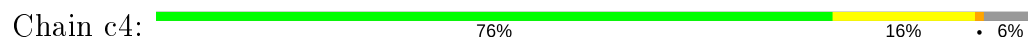




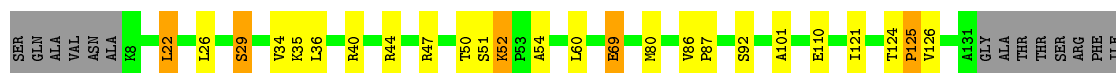
- Molecule 16: 40S ribosomal protein S14-A



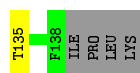
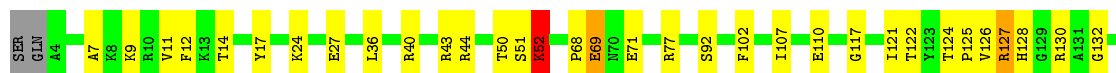
- Molecule 16: 40S ribosomal protein S14-A



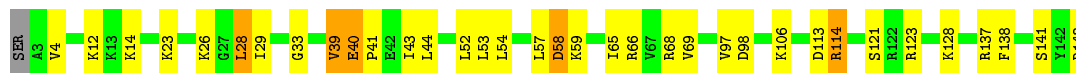
- Molecule 17: 40S ribosomal protein S15



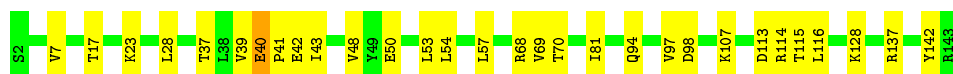
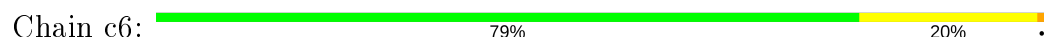
- Molecule 17: 40S ribosomal protein S15



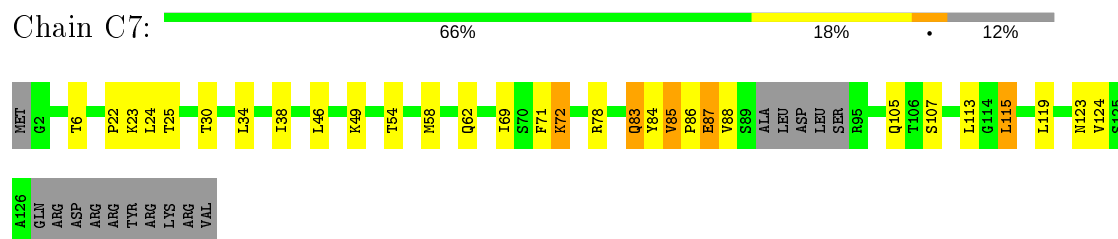
- Molecule 18: 40S ribosomal protein S16-A



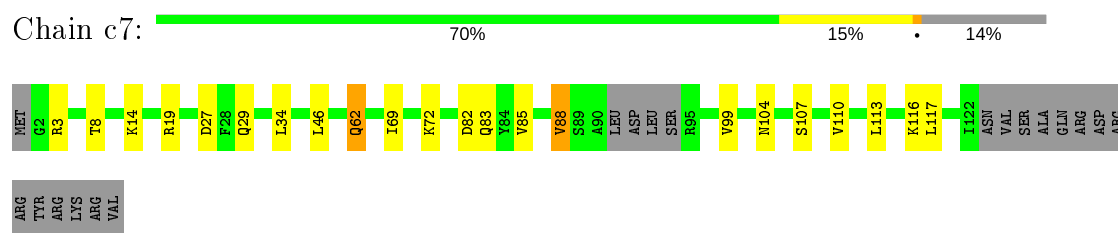
- Molecule 18: 40S ribosomal protein S16-A



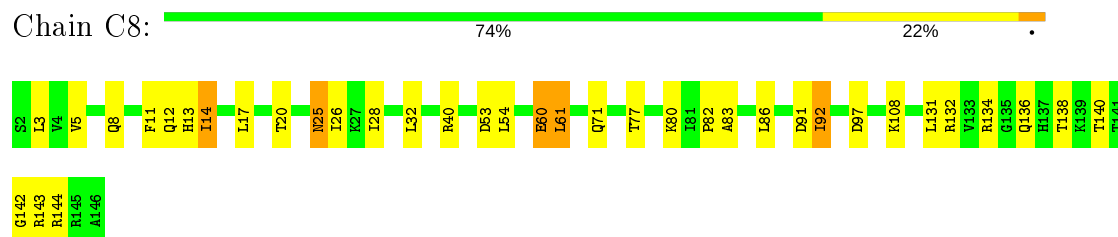
- Molecule 19: 40S ribosomal protein S17-A



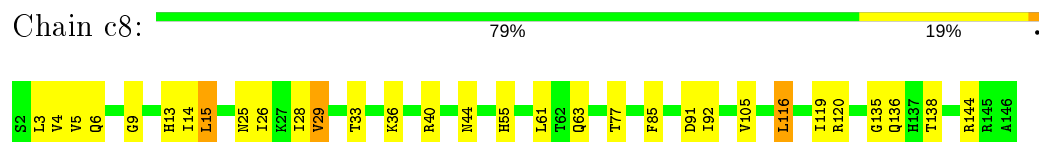
- Molecule 19: 40S ribosomal protein S17-A



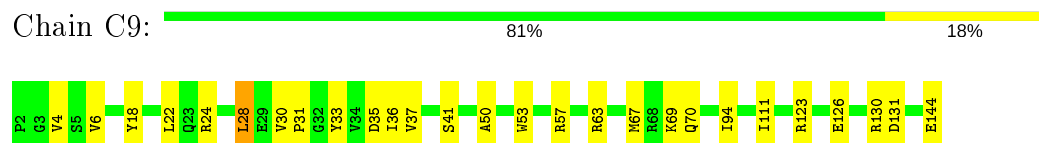
- Molecule 20: 40S ribosomal protein S18-A



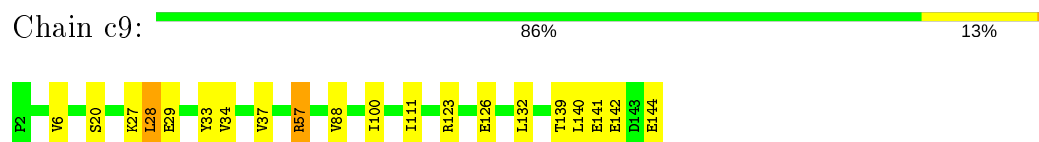
- Molecule 20: 40S ribosomal protein S18-A



- Molecule 21: 40S ribosomal protein S19-A

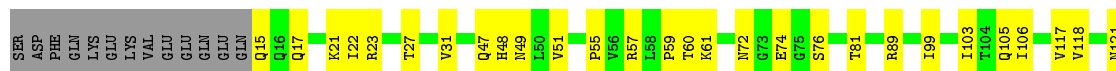


- Molecule 21: 40S ribosomal protein S19-A



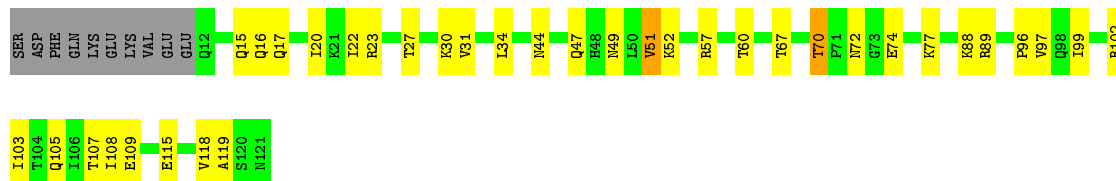
- Molecule 22: 40S ribosomal protein S20

Chain D0:  66% 23% 11%




- Molecule 22: 40S ribosomal protein S20

Chain d0:  62% 28% 8%



- Molecule 23: 40S ribosomal protein S21-A

Chain D1:  79% 17% 4%



- Molecule 23: 40S ribosomal protein S21-A

Chain d1:  80% 18% 2%




- Molecule 24: 40S ribosomal protein S22-A

Chain D2:  86% 12% 2%




- Molecule 24: 40S ribosomal protein S22-A

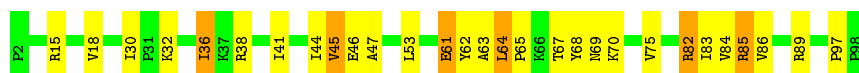
Chain d2:  88% 12% 0%



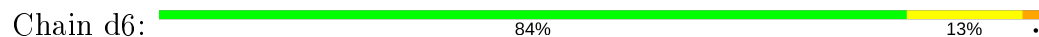
- Molecule 25: 40S ribosomal protein S23-A

Chain D3:  78% 19% 3%

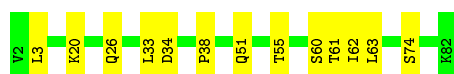
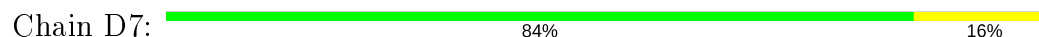




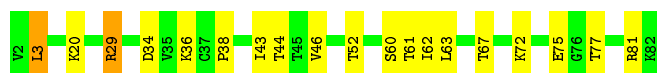
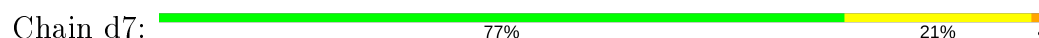
- Molecule 28: 40S ribosomal protein S26-B



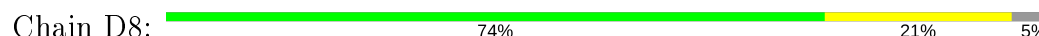
- Molecule 29: 40S ribosomal protein S27-A



- Molecule 29: 40S ribosomal protein S27-A



- Molecule 30: 40S ribosomal protein S28-A



- Molecule 30: 40S ribosomal protein S28-A



- Molecule 31: 40S ribosomal protein S29-A



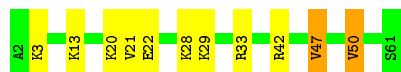
- Molecule 31: 40S ribosomal protein S29-A





- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 82% 15%



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 54% 36% 7%



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 57% 38%



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

Chain SR: 86% 14%



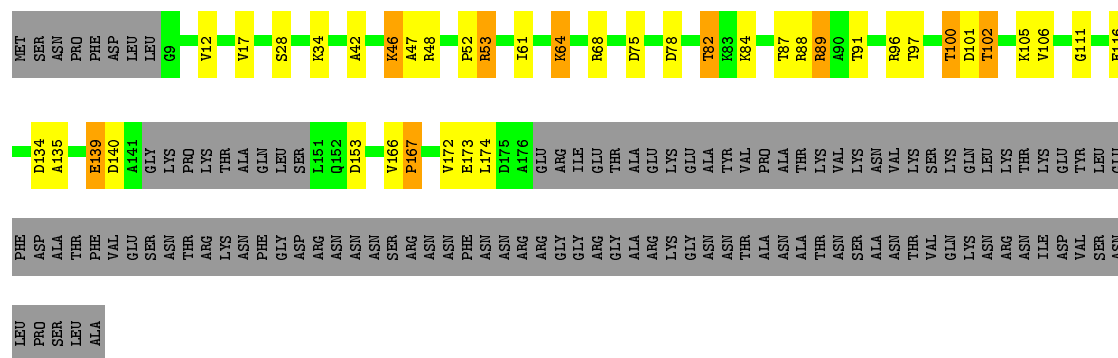
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 88% 12%

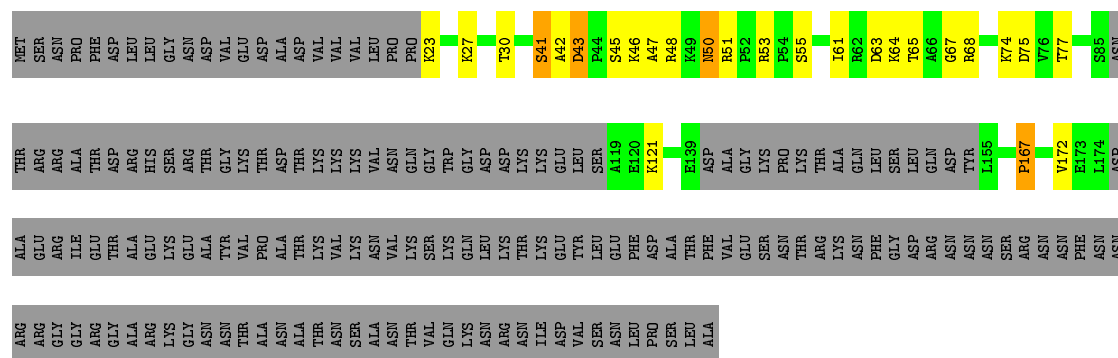


- Molecule 35: Suppressor protein STM1

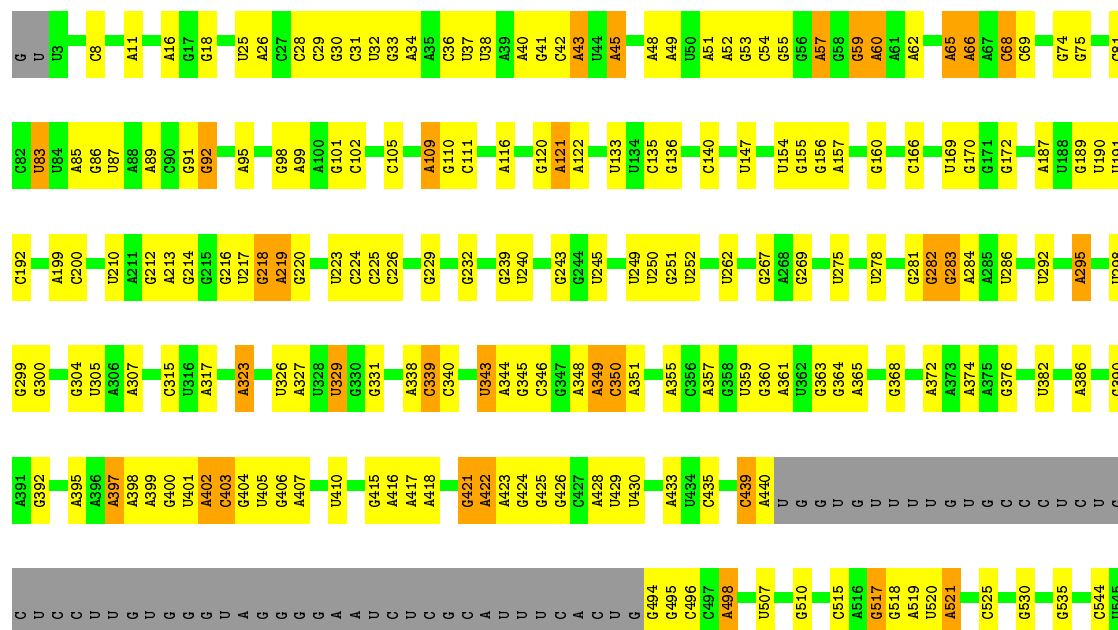
Chain SM: 44% 11% 42%



• Molecule 35: Suppressor protein STM1

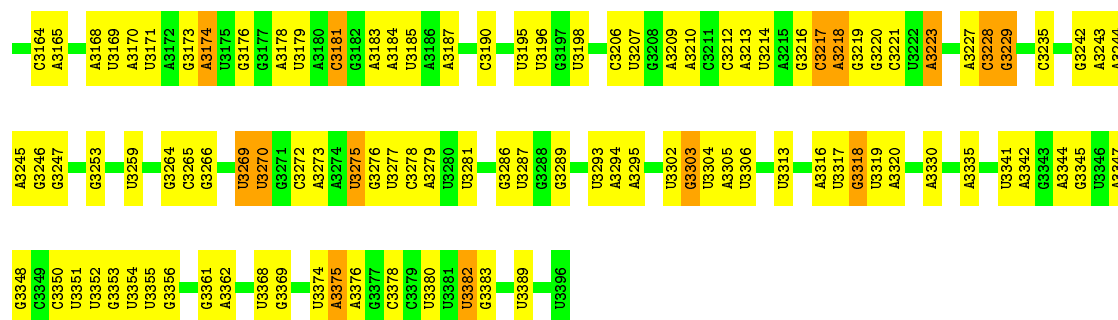


• Molecule 36: 25S ribosomal RNA

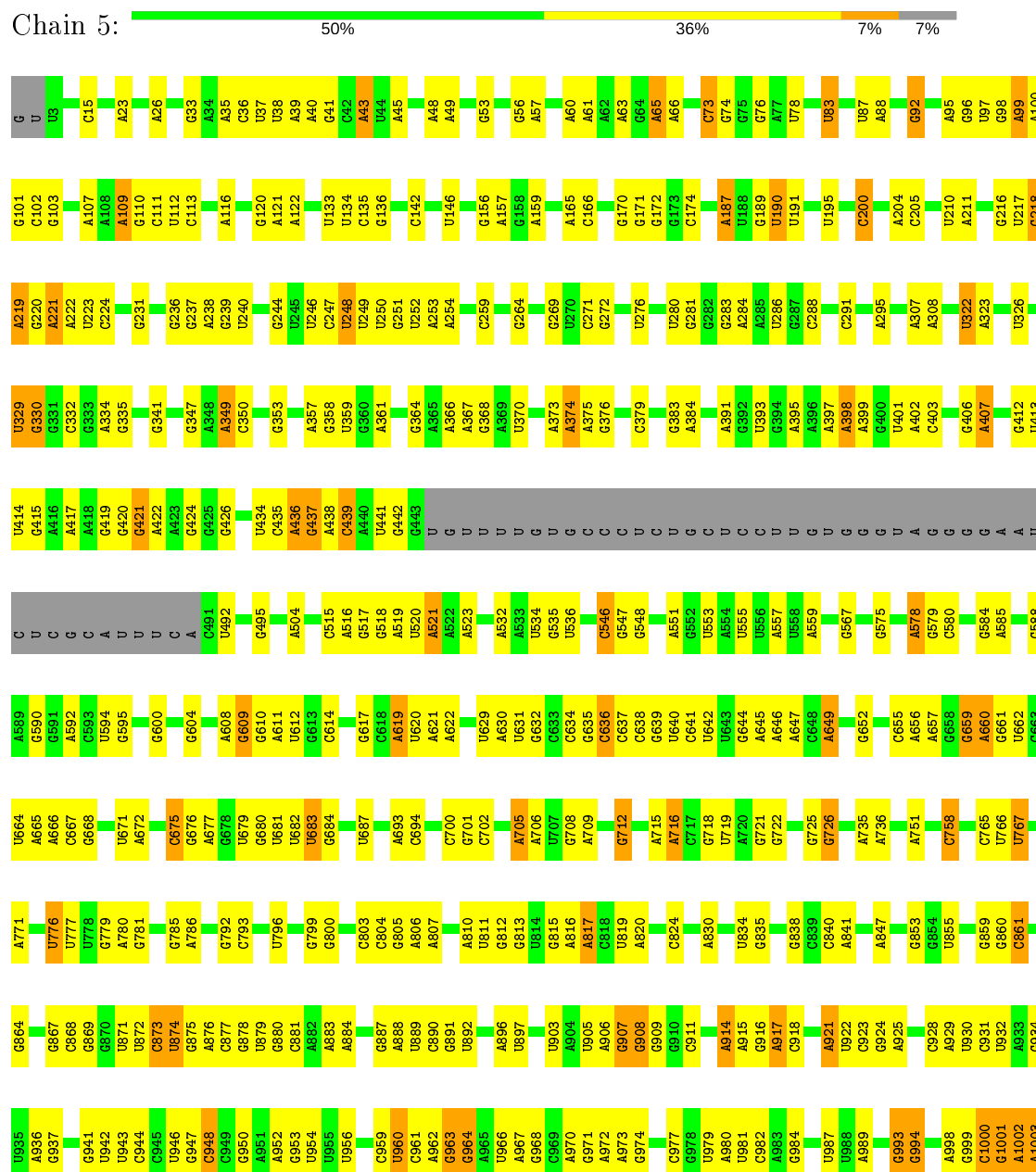


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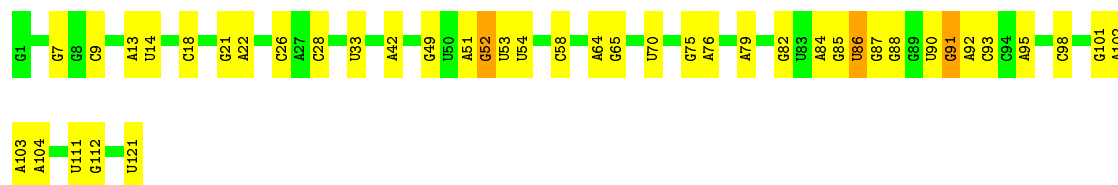


- Molecule 36: 25S ribosomal RNA

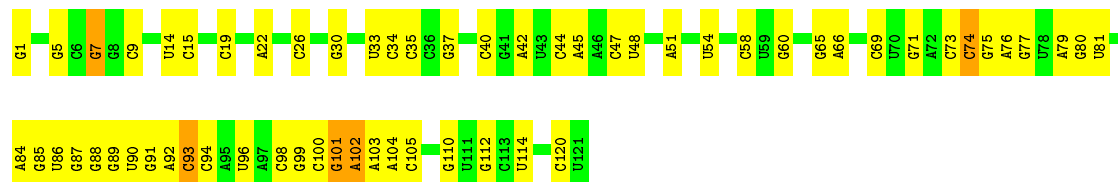




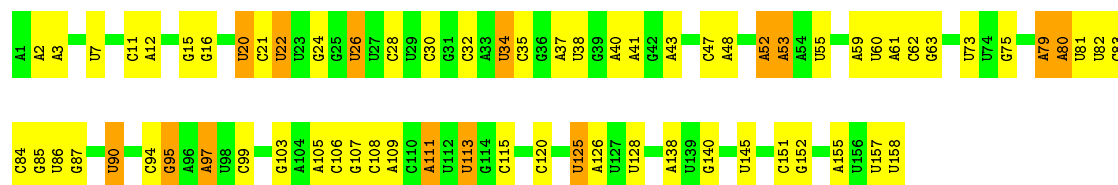
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G3378	A3186	G3286	G3108	U3013	A2941	A2872	C2798	G2706	C2627	G2530	G
	A3187	A3187	G3109	U3014	C2942	U2873	A2799	C2710	C2627	G2531	U
					G2943	G2874	G2800			U2532	G
					U2944	U2875	A2801	G2714	U2630	G2533	G
					A2945	C2876	A2802		U2631	G2534	A
					U2946	G2877	C2810	U2717	G2632		A
					G2947	C2878			U2633		C
					U2948	C2879	A2813	A2721	U2634		C
					U2949	U2880	G2814		A2635		U
					G2950	C2881	G2815	U2725	A2636		C
							G2816	C2726	A2637		U
							A2817	A2727	C2638		G
							U2818	G2728	G2639		G
							A2819	U2729	A2640		C
							G2820	G2730	A2641		C
							C2821	U2731	G2642		A
							U2822	G2732	G2643		G
							G2823	A2733	C2644		U
							A2824		A2645		G
							C2825	A2743	A2646		U
							U2826		G2647		G
							A2827	A2746	G2648		A
							G2828	U2752	G2651		A
							C2829	G2753	U2652		A
							U2830	G2754	C2653		U
							G2831	G2755	A2654		A
							U2832	C2756	A2655		C
							A2833	U2757	G2656		C
							C2834	A2758	G2660		U
							U2835		G2661		C
							G2836	A2762	U2662		A
							A2837	C2764	G2663		C
							U2838		A2674		U
							C2839	U2763	G2677		U
							U2840	C2764	A2678		A
							G2841				C
							U2842	U2767	G2677		U
							C2843		A2678		U
							U2844	C2772			A
							A2845	C2773	U2681		A
							G2846	U2774	C2682		U
							U2847	G2775	U2683		U
							C2848	U2776	C2684		U
							A2849	G2777	C2685		A
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							U2851	A2779	U2688		G
							C2852		A2689		A
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							G2856	U2783	A2691		G
							U2857		A2692		G
							C2858	G2787	C2693		U
							U2859		A2694		G
							G2860	A2790	A2695		U
							U2861	G2791	A2696		A
							A2865	A2792	A2697		A
							U2866	G2793	G2700		G
							G2869	G2794	G2700		U
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							C2997				A
							A3000				A
							G3003				A
							U3004				A
							C3005				A
							A3006				A
							G3007				A
							U3008				



- Molecule 37: 5S ribosomal RNA



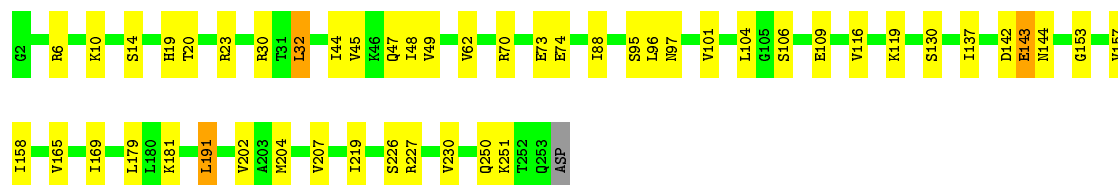
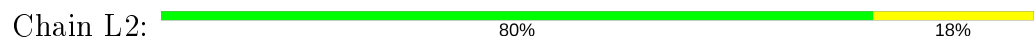
- Molecule 38: 5.8S ribosomal RNA



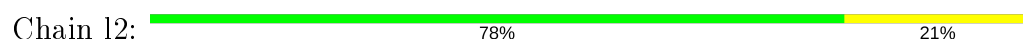
- Molecule 38: 5.8S ribosomal RNA

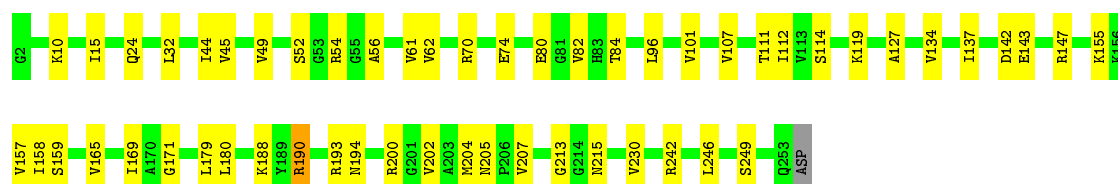


- Molecule 39: 60S ribosomal protein L2-A



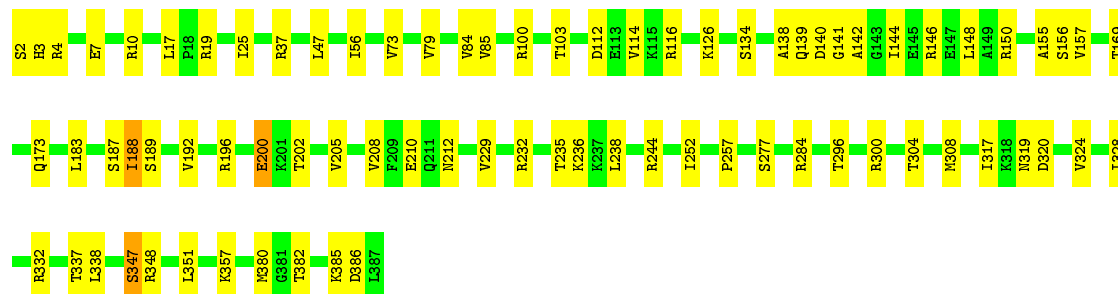
- Molecule 39: 60S ribosomal protein L2-A





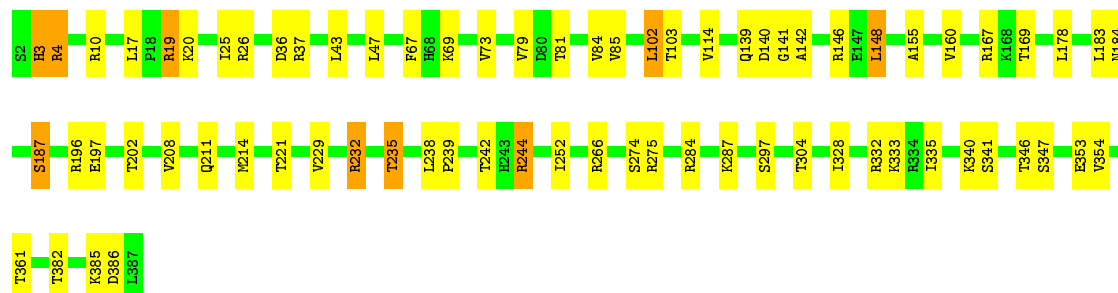
- Molecule 40: 60S ribosomal protein L3

Chain L3: 80% 19% .



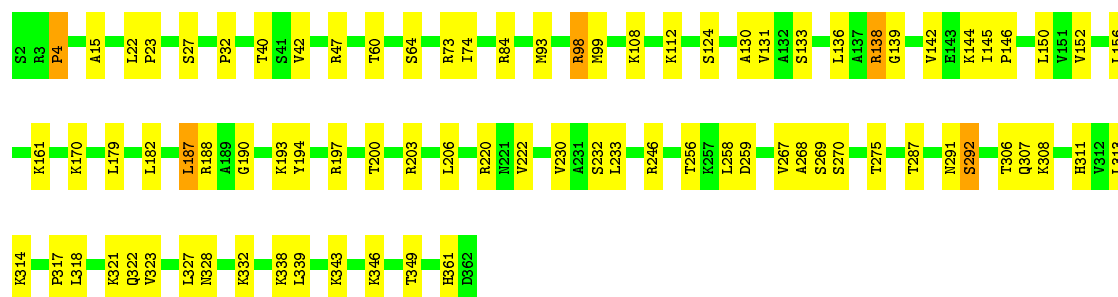
- Molecule 40: 60S ribosomal protein L3

Chain l3: 81% 16% .



- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 77% 22% .



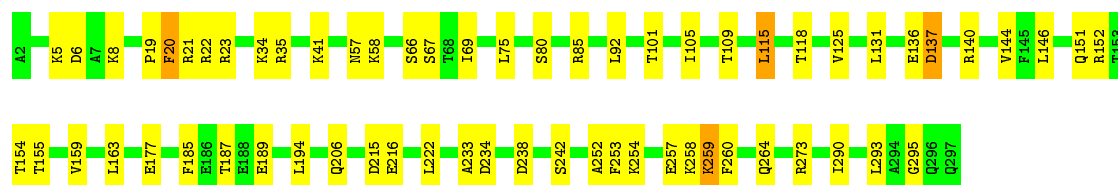
- Molecule 41: 60S ribosomal protein L4-A

Chain l4: 81% 17% .



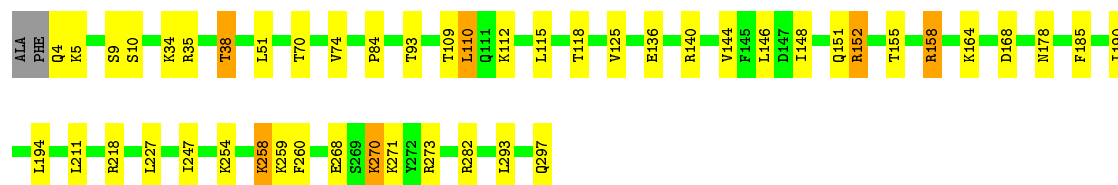
- Molecule 42: 60S ribosomal protein L5

Chain L5: 79% 20% .



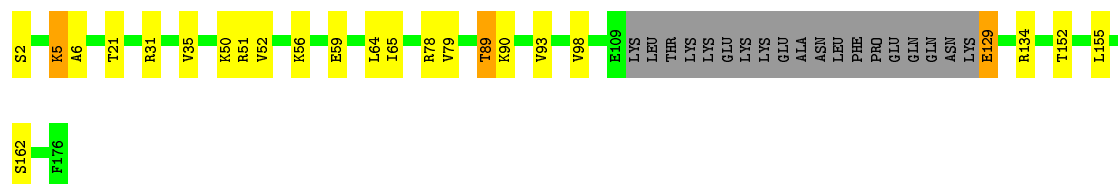
- Molecule 42: 60S ribosomal protein L5

Chain l5: 83% 14% ..



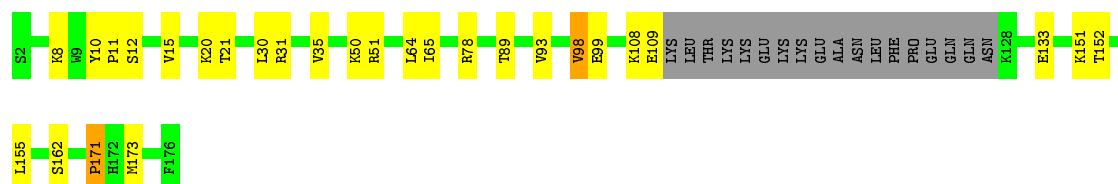
- Molecule 43: 60S ribosomal protein L6-A

Chain L6: 75% 12% . 11%

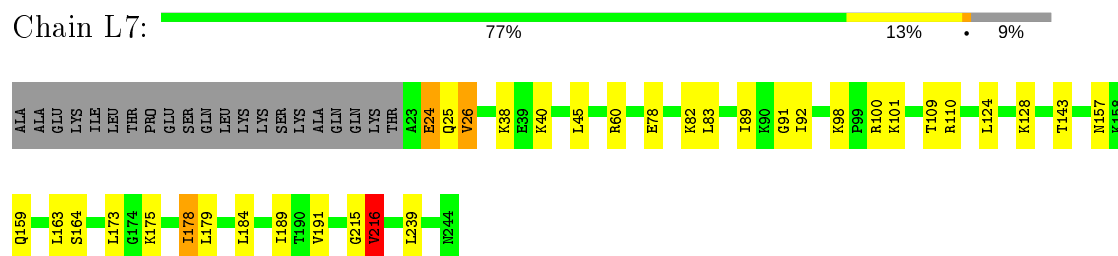


- Molecule 43: 60S ribosomal protein L6-A

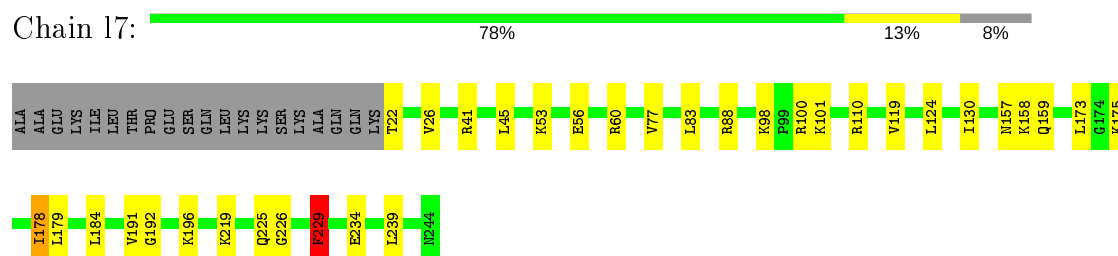
Chain l6: 74% 15% . 10%



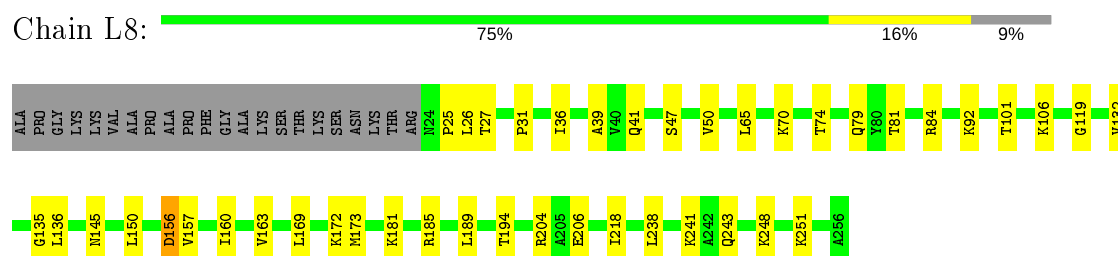
- Molecule 44: 60S ribosomal protein L7-A



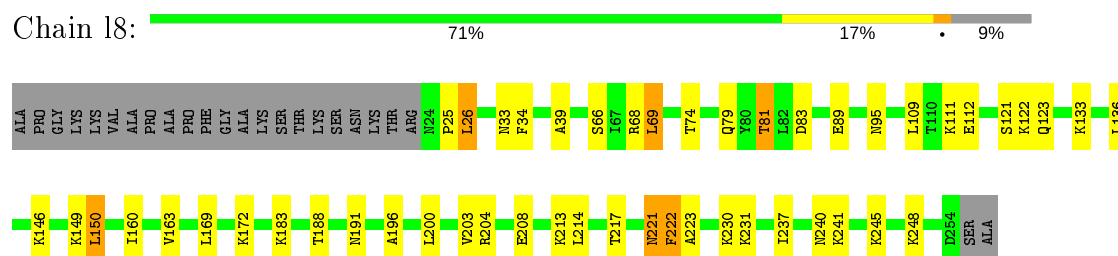
- Molecule 44: 60S ribosomal protein L7-A



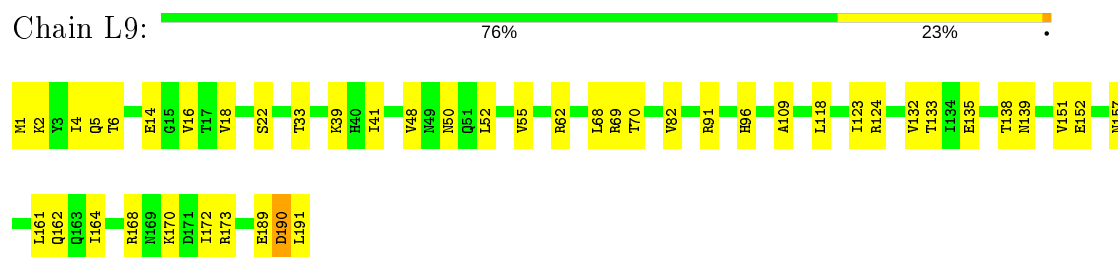
- Molecule 45: 60S ribosomal protein L8-A



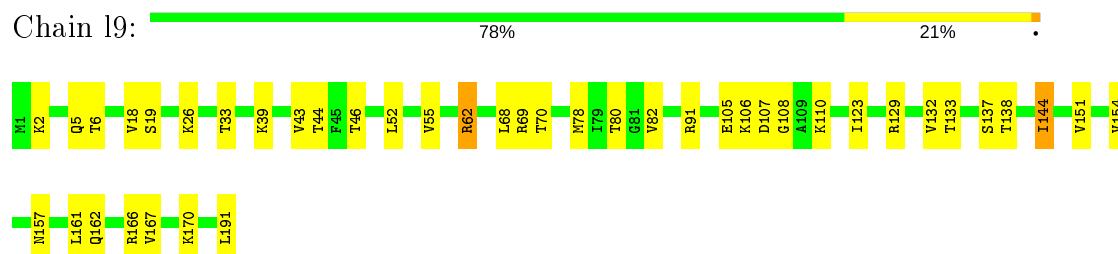
- Molecule 45: 60S ribosomal protein L8-A



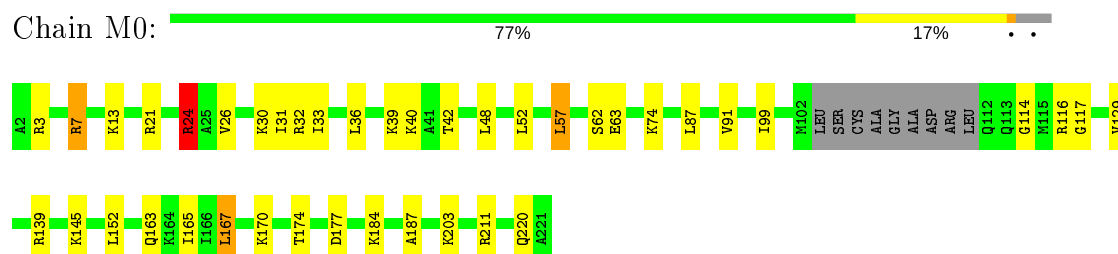
- Molecule 46: 60S ribosomal protein L9-A



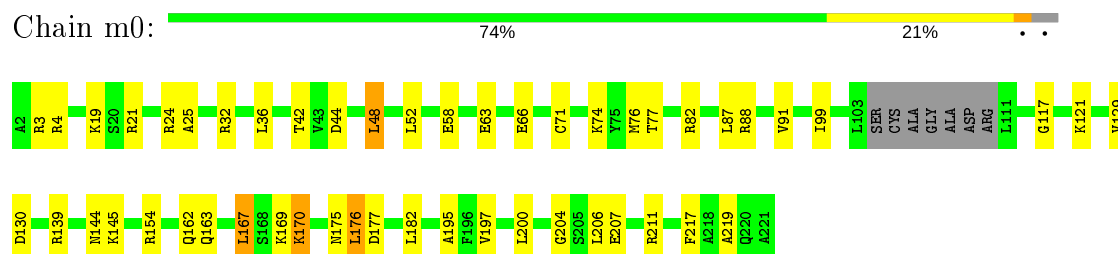
- Molecule 46: 60S ribosomal protein L9-A



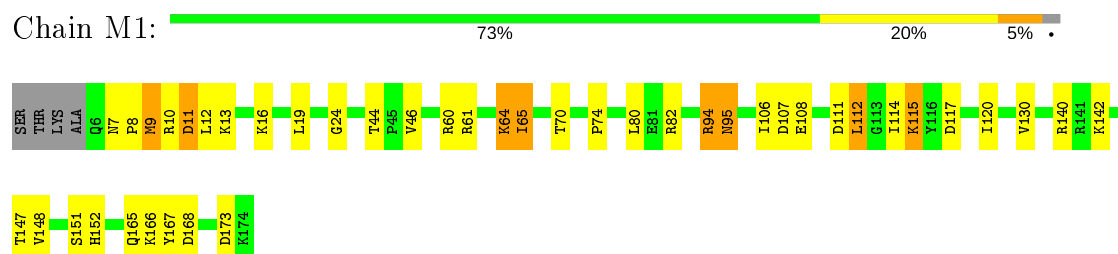
- Molecule 47: 60S ribosomal protein L10



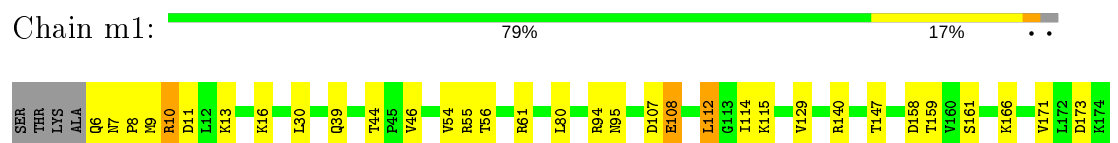
- Molecule 47: 60S ribosomal protein L10




- Molecule 48: 60S ribosomal protein L11-B

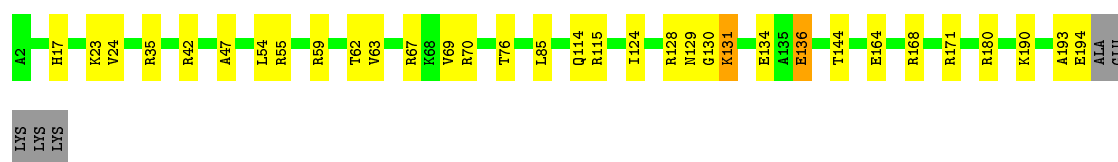


- Molecule 48: 60S ribosomal protein L11-B




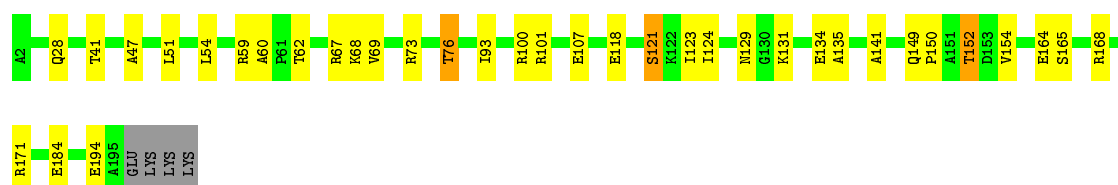
- Molecule 49: 60S ribosomal protein L13-A

Chain M3:  81% 16% ..




- Molecule 49: 60S ribosomal protein L13-A

Chain m3:  80% 17% ..




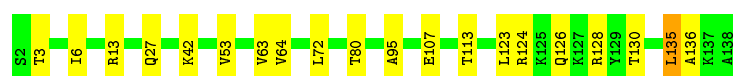
- Molecule 50: 60S ribosomal protein L14-A

Chain M4:  80% 18% ...




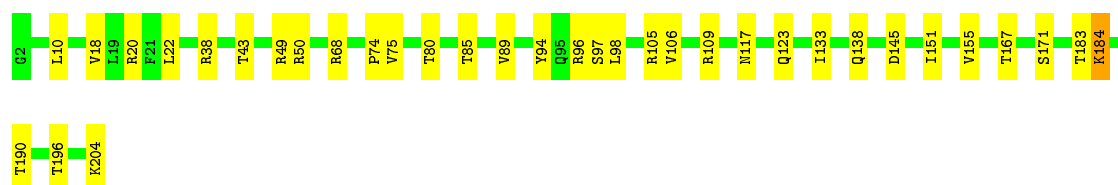
- Molecule 50: 60S ribosomal protein L14-A

Chain m4:  85% 14% .




- Molecule 51: 60S ribosomal protein L15-A

Chain M5:  83% 17%

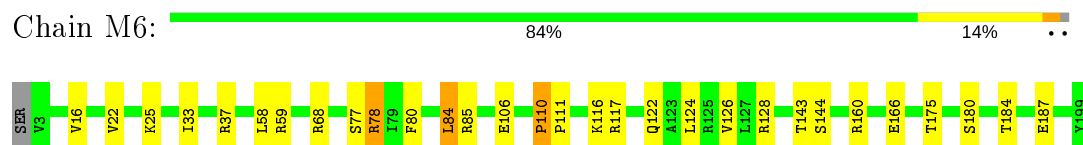


- Molecule 51: 60S ribosomal protein L15-A

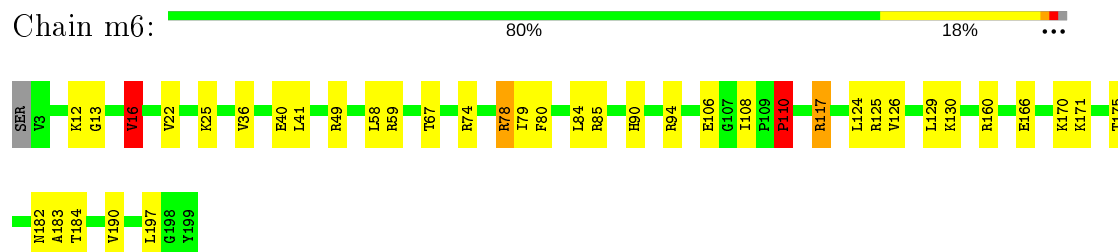
Chain m5:  85% 14% .



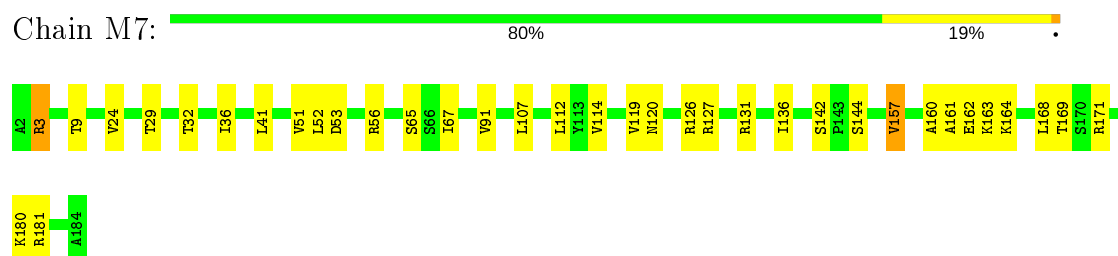
- Molecule 52: 60S ribosomal protein L16-A



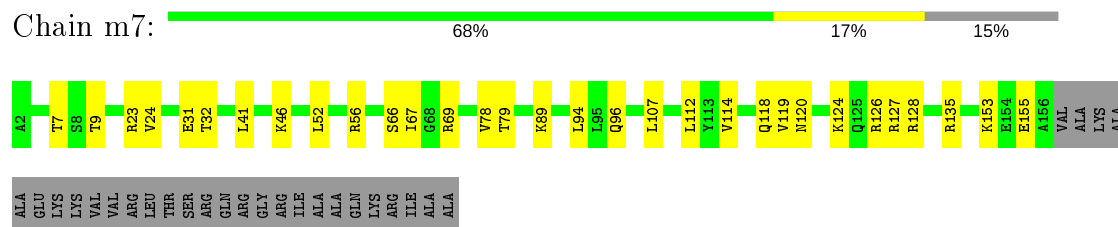
- Molecule 52: 60S ribosomal protein L16-A



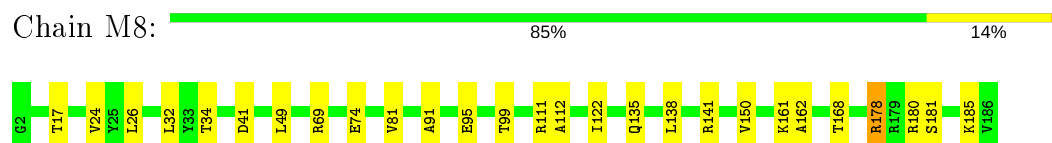
- Molecule 53: 60S ribosomal protein L17-A



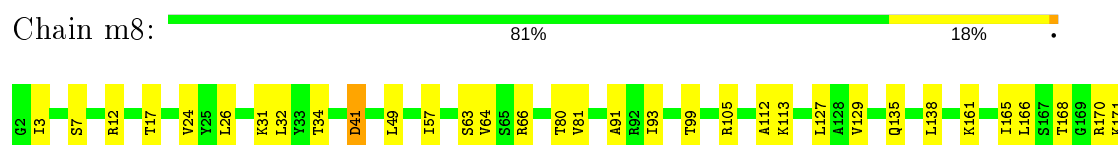
- Molecule 53: 60S ribosomal protein L17-A



- Molecule 54: 60S ribosomal protein L18-A



- Molecule 54: 60S ribosomal protein L18-A





- Molecule 55: 60S ribosomal protein L19-A

Chain M9: 85% 15%



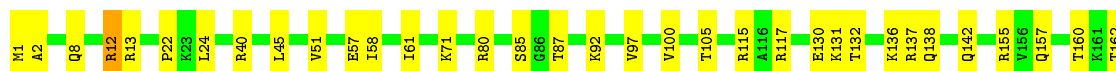
- Molecule 55: 60S ribosomal protein L19-A

Chain m9: 81% 18%



- Molecule 56: 60S ribosomal protein L20-A

Chain N0: 78% 21%



- Molecule 56: 60S ribosomal protein L20-A

Chain n0: 81% 19%

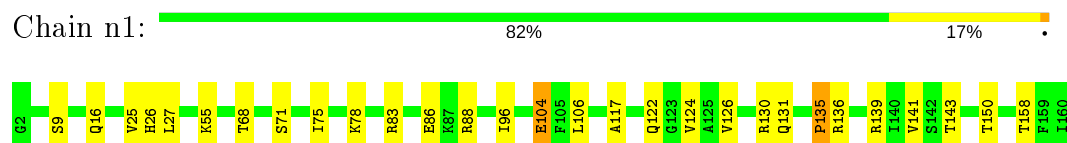


- Molecule 57: 60S ribosomal protein L21-A

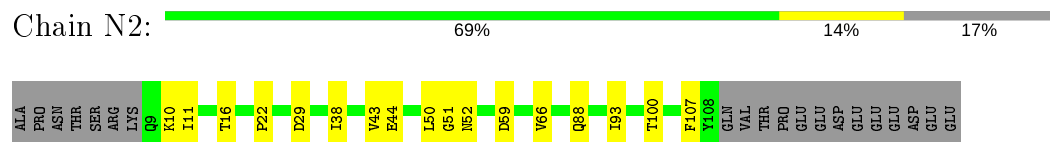
Chain N1: 82% 17%



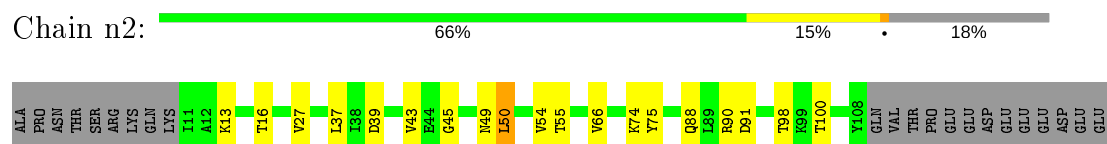
- Molecule 57: 60S ribosomal protein L21-A



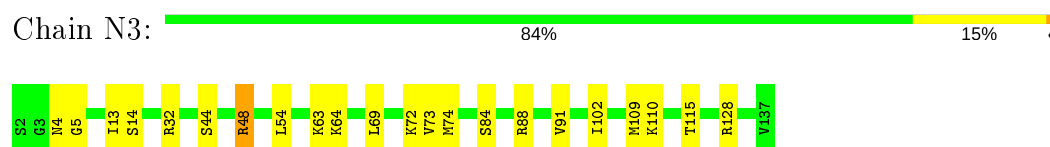
- Molecule 58: 60S ribosomal protein L22-A



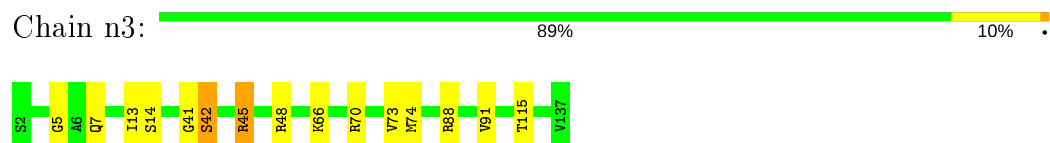
- Molecule 58: 60S ribosomal protein L22-A



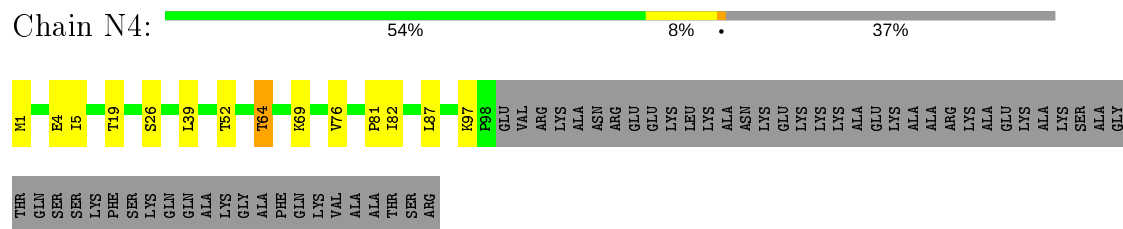
- Molecule 59: 60S ribosomal protein L23-A



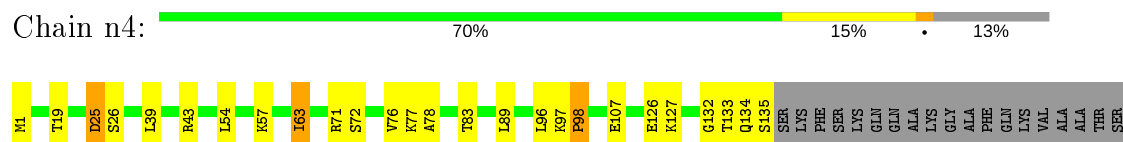
- Molecule 59: 60S ribosomal protein L23-A



- Molecule 60: 60S ribosomal protein L24-A

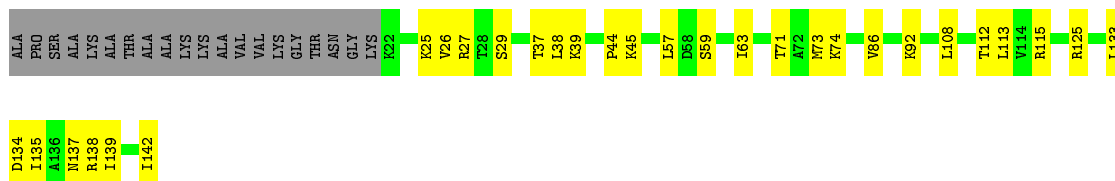


- Molecule 60: 60S ribosomal protein L24-A

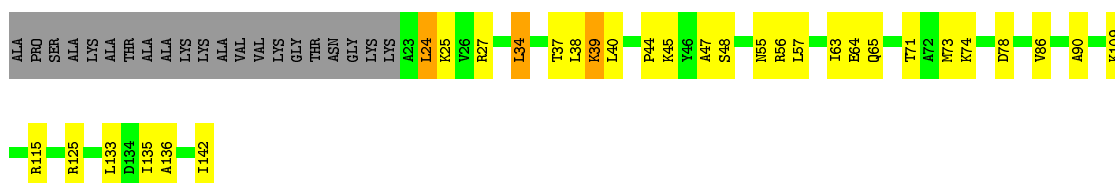


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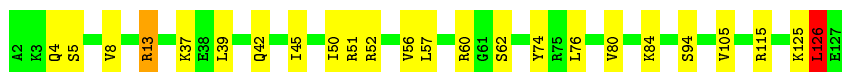
- Molecule 61: 60S ribosomal protein L25

Chain N5:  65% 21% 14%

- Molecule 61: 60S ribosomal protein L25

Chain n5:  63% 20% 15%


- Molecule 62: 60S ribosomal protein L26-A

Chain N6:  81% 17% ..

- Molecule 62: 60S ribosomal protein L26-A

Chain n6:  74% 25% .


- Molecule 63: 60S ribosomal protein L27-A

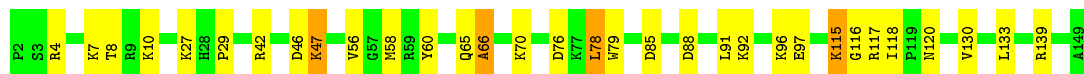
Chain N7:  79% 18% .

- Molecule 63: 60S ribosomal protein L27-A

Chain n7:  76% 21% .

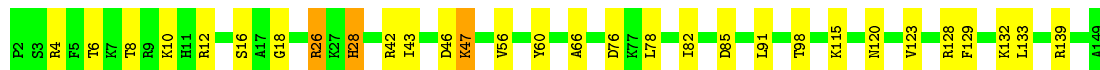
- Molecule 64: 60S ribosomal protein L28

Chain N8:  78% 19% .




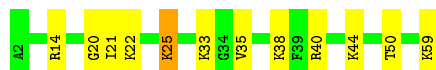
- Molecule 64: 60S ribosomal protein L28

Chain n8:  80% 18% .



- Molecule 65: 60S ribosomal protein L29

Chain N9:  79% 19% .




- Molecule 65: 60S ribosomal protein L29

Chain n9:  71% 26% .




- Molecule 66: 60S ribosomal protein L30

Chain O0:  79% 14% 7%




- Molecule 66: 60S ribosomal protein L30

Chain o0:  79% 17% .



- Molecule 67: 60S ribosomal protein L31-A

Chain O1:  76% 19% . .




- Molecule 67: 60S ribosomal protein L31-A

Chain o1:  72% 24%




- Molecule 68: 60S ribosomal protein L32

Chain O2:  84% 15%



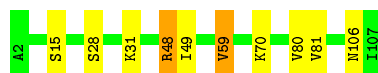
- Molecule 68: 60S ribosomal protein L32

Chain o2:  77% 20%




- Molecule 69: 60S ribosomal protein L33-A

Chain O3:  91% 8%




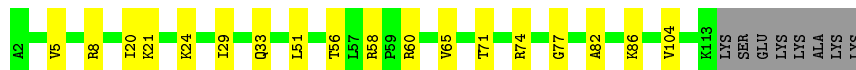
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:  85% 15%



- Molecule 70: 60S ribosomal protein L34-A

Chain O4:  78% 15% 7%




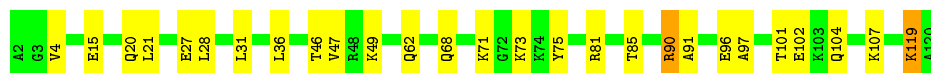
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:  74% 18% 7%




- Molecule 71: 60S ribosomal protein L35-A

Chain O5:  77% 21%



- Molecule 71: 60S ribosomal protein L35-A

Chain o5:  77% 23%



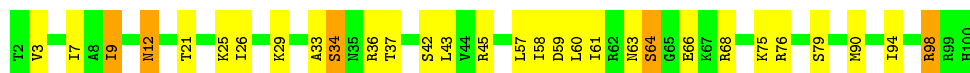
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:  74% 22%



- Molecule 72: 60S ribosomal protein L36-A

Chain o6:  70% 25% 5%




- Molecule 73: 60S ribosomal protein L37-A

Chain O7:  80% 17%



- Molecule 73: 60S ribosomal protein L37-A

Chain o7:  80% 18%




- Molecule 74: 60S ribosomal protein L38

Chain O8:  74% 26%




- Molecule 74: 60S ribosomal protein L38

Chain o8:  78% 22%




- Molecule 75: 60S ribosomal protein L39

Chain O9:  80% 20%




- Molecule 75: 60S ribosomal protein L39

Chain o9:  80% 18% .



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  77% 21% .



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  71% 27% .



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  68% 28% .




- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  68% 32%




- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  76% 22%




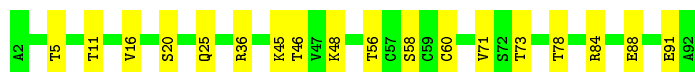
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  83% 15%




- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  80% 20%



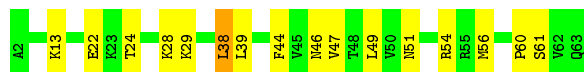
- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  88% 12%



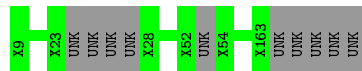
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:  74% 24%




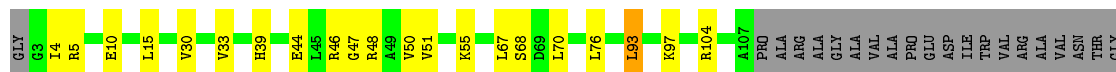
- Molecule 81: Unknown protein chain m2

Chain m2:  94% 6%



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0:  39% 7% 54%



[illegible]

- Molecule 83: Unknown protein chain p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 84: Unknown protein chain p2

Chain p2:  100%

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	436.25Å 286.92Å 303.84Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	49.69 – 3.00	Depositor
% Data completeness (in resolution range)	98.8 (49.69-3.00)	Depositor
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.208 , 0.255	Depositor
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.180	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411245	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: HMT, 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	0.68	1/41698 (0.0%)	1.25	264/64972 (0.4%)
1	6	0.84	11/42765 (0.0%)	1.37	434/66634 (0.7%)
2	S0	0.46	0/1617	0.68	0/2215
2	s0	0.48	0/1623	0.70	0/2222
3	S1	0.37	0/1735	0.64	0/2335
3	s1	0.50	0/1748	0.66	0/2352
4	S2	0.48	0/1665	0.65	0/2263
4	s2	0.57	0/1665	0.75	0/2263
5	S3	0.47	0/1759	0.64	0/2368
5	s3	0.41	0/1759	0.60	0/2368
6	S4	0.45	0/2109	0.70	0/2839
6	s4	0.55	0/2109	0.78	1/2839 (0.0%)
7	S5	0.37	0/1629	0.58	0/2202
7	s5	0.45	0/1629	0.64	0/2202
8	S6	0.46	0/1823	0.64	0/2439
8	s6	0.56	0/1779	0.70	0/2379
9	S7	0.42	0/1506	0.64	1/2028 (0.0%)
9	s7	0.47	0/1516	0.67	1/2043 (0.0%)
10	S8	0.51	0/1514	0.72	1/2021 (0.0%)
10	s8	0.62	0/1514	0.76	1/2021 (0.0%)
11	S9	0.46	0/1519	0.63	0/2035
11	s9	0.53	0/1519	0.74	2/2035 (0.1%)
12	C0	0.42	0/790	0.69	1/1069 (0.1%)
12	c0	0.36	0/777	0.64	3/1049 (0.3%)
13	C1	0.58	1/1240 (0.1%)	0.67	0/1675
13	c1	0.65	1/1194 (0.1%)	0.78	1/1610 (0.1%)
14	C2	0.37	0/900	0.63	0/1224
14	c2	0.30	0/900	0.56	0/1224
15	C3	0.48	0/1215	0.67	2/1638 (0.1%)
15	c3	0.59	0/1215	0.71	0/1638
16	C4	0.39	0/901	0.65	0/1217
16	c4	0.54	0/960	0.76	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.43	0/998	0.65	0/1341
17	c5	0.49	0/1060	0.70	0/1426
18	C6	0.43	0/1125	0.69	3/1510 (0.2%)
18	c6	0.48	0/1131	0.67	0/1518
19	C7	0.44	0/935	0.63	0/1254
19	c7	0.49	0/914	0.72	0/1224
20	C8	0.42	0/1211	0.61	0/1628
20	c8	0.49	0/1211	0.71	2/1628 (0.1%)
21	C9	0.40	0/1130	0.59	0/1517
21	c9	0.49	0/1130	0.66	1/1517 (0.1%)
22	D0	0.44	0/865	0.63	0/1169
22	d0	0.48	0/892	0.66	0/1205
23	D1	0.45	0/693	0.64	0/935
23	d1	0.52	0/693	0.72	0/935
24	D2	0.49	0/1038	0.69	2/1395 (0.1%)
24	d2	0.60	0/1038	0.74	1/1395 (0.1%)
25	D3	0.62	0/1139	0.75	1/1518 (0.1%)
25	d3	0.70	0/1139	0.83	1/1518 (0.1%)
26	D4	0.44	0/1087	0.63	1/1449 (0.1%)
26	d4	0.55	0/1087	0.71	0/1449
27	D5	0.39	0/571	0.69	0/768
27	d5	0.41	0/566	0.63	0/761
28	D6	0.45	0/782	0.66	0/1047
28	d6	0.55	0/782	0.71	0/1047
29	D7	0.43	0/620	0.66	0/838
29	d7	0.50	0/620	0.75	1/838 (0.1%)
30	D8	0.36	0/499	0.59	0/670
30	d8	0.44	0/499	0.67	0/670
31	D9	0.47	0/452	0.72	1/600 (0.2%)
31	d9	0.48	0/452	0.64	0/600
32	E0	0.48	0/483	0.63	0/643
33	E1	0.45	0/577	0.77	0/770
33	e1	0.39	0/619	0.74	1/822 (0.1%)
34	SR	0.36	0/2494	0.58	0/3393
34	sR	0.37	0/2495	0.55	0/3395
35	SM	0.54	1/1113 (0.1%)	0.79	4/1502 (0.3%)
35	sM	0.49	0/683	0.70	1/923 (0.1%)
36	1	1.11	100/75394 (0.1%)	1.65	1834/117545 (1.6%)
36	5	1.17	147/75414 (0.2%)	1.69	1950/117575 (1.7%)
37	3	0.90	2/2883 (0.1%)	1.41	33/4491 (0.7%)
37	7	1.15	8/2883 (0.3%)	1.71	80/4491 (1.8%)
38	4	1.06	4/3746 (0.1%)	1.62	86/5832 (1.5%)
38	8	0.98	1/3746 (0.0%)	1.47	39/5832 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.73	0/1948	0.85	2/2617 (0.1%)
39	l2	0.75	1/1946 (0.1%)	0.90	3/2614 (0.1%)
40	L3	0.74	1/3146 (0.0%)	0.83	0/4228
40	l3	0.85	0/3146	0.93	11/4228 (0.3%)
41	L4	0.82	0/2800	0.96	7/3790 (0.2%)
41	l4	0.75	0/2800	0.90	3/3790 (0.1%)
42	L5	0.57	0/2425	0.69	0/3271
42	l5	0.74	0/2408	0.82	2/3248 (0.1%)
43	L6	0.76	0/1260	0.81	0/1694
43	l6	0.80	0/1269	0.87	2/1705 (0.1%)
44	L7	0.79	0/1821	0.89	2/2451 (0.1%)
44	l7	0.87	0/1828	0.89	1/2461 (0.0%)
45	L8	0.57	0/1836	0.70	2/2481 (0.1%)
45	l8	0.53	0/1795	0.67	1/2429 (0.0%)
46	L9	0.66	0/1539	0.77	0/2073
46	l9	0.80	0/1539	0.86	0/2073
47	M0	0.74	0/1741	0.84	4/2335 (0.2%)
47	m0	0.76	0/1758	0.86	3/2358 (0.1%)
48	M1	0.50	0/1374	0.71	1/1842 (0.1%)
48	m1	0.63	0/1374	0.82	1/1842 (0.1%)
49	M3	0.74	0/1568	0.85	0/2106
49	m3	0.71	0/1573	0.85	0/2113
50	M4	0.74	0/1068	0.84	1/1438 (0.1%)
50	m4	0.81	0/1074	0.82	0/1446
51	M5	0.75	0/1757	0.85	0/2354
51	m5	0.67	0/1757	0.82	0/2354
52	M6	0.89	1/1585 (0.1%)	0.91	4/2128 (0.2%)
52	m6	1.01	5/1585 (0.3%)	0.99	8/2128 (0.4%)
53	M7	0.80	0/1443	0.89	2/1944 (0.1%)
53	m7	0.90	0/1250	0.89	1/1683 (0.1%)
54	M8	0.82	0/1465	0.89	2/1965 (0.1%)
54	m8	0.75	0/1465	0.93	2/1965 (0.1%)
55	M9	0.55	0/1538	0.66	0/2050
55	m9	0.65	0/1538	0.70	1/2050 (0.0%)
56	N0	0.77	0/1481	0.89	0/1990
56	n0	0.86	0/1481	0.89	1/1990 (0.1%)
57	N1	0.76	0/1300	0.80	0/1743
57	n1	0.88	1/1300 (0.1%)	0.86	1/1743 (0.1%)
58	N2	0.43	0/812	0.62	0/1099
58	n2	0.51	0/794	0.66	0/1076
59	N3	0.72	0/1018	0.83	1/1369 (0.1%)
59	n3	0.83	0/1018	0.94	3/1369 (0.2%)
60	N4	0.55	0/712	0.67	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.68	0/1052	0.74	0/1398
61	N5	0.63	0/979	0.78	0/1321
61	n5	0.66	0/974	0.79	1/1314 (0.1%)
62	N6	0.70	0/1004	0.88	2/1341 (0.1%)
62	n6	0.69	0/1004	0.81	0/1341
63	N7	0.53	0/1118	0.68	1/1497 (0.1%)
63	n7	0.50	0/1118	0.67	0/1497
64	N8	0.80	0/1204	0.92	4/1612 (0.2%)
64	n8	0.76	0/1204	0.91	2/1612 (0.1%)
65	N9	0.76	0/473	0.81	0/629
65	n9	0.84	0/473	0.98	0/629
66	O0	0.50	0/751	0.67	0/1008
66	o0	0.54	0/775	0.68	0/1040
67	O1	0.62	0/890	0.68	0/1196
67	o1	0.80	0/897	0.87	1/1205 (0.1%)
68	O2	0.82	0/1041	0.85	0/1394
68	o2	0.85	0/1041	0.93	1/1394 (0.1%)
69	O3	0.91	0/868	0.92	2/1168 (0.2%)
69	o3	0.95	0/868	0.86	0/1168
70	O4	0.59	0/890	0.83	2/1189 (0.2%)
70	o4	0.60	0/890	0.80	0/1189
71	O5	0.72	0/978	0.82	1/1301 (0.1%)
71	o5	0.58	0/974	0.71	0/1297
72	O6	0.65	0/778	0.81	1/1034 (0.1%)
72	o6	0.61	0/777	0.72	0/1033
73	O7	0.81	0/696	0.94	2/923 (0.2%)
73	o7	0.76	0/696	0.90	1/923 (0.1%)
74	O8	0.53	0/618	0.64	0/826
74	o8	0.46	0/614	0.67	0/822
75	O9	0.79	1/443 (0.2%)	0.87	1/588 (0.2%)
75	o9	0.75	0/443	0.87	1/588 (0.2%)
76	Q0	0.78	0/423	0.81	0/562
76	q0	0.94	0/423	0.94	2/562 (0.4%)
77	Q1	0.57	0/234	1.04	1/300 (0.3%)
77	q1	0.82	0/234	1.05	1/300 (0.3%)
78	Q2	0.94	1/860 (0.1%)	0.84	0/1136
78	q2	0.82	1/860 (0.1%)	0.83	0/1136
79	Q3	0.72	0/701	0.83	0/934
79	q3	0.72	0/701	0.80	0/934
80	e0	0.54	0/499	0.72	0/665
82	p0	0.45	0/1092	0.62	0/1474
All	All	0.88	289/430074 (0.1%)	1.31	4853/631364 (0.8%)

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
5	s3	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
11	s9	0	1
16	C4	0	1
17	c5	0	1
18	c6	0	2
19	C7	0	2
22	d0	0	1
25	d3	0	1
27	D5	0	2
27	d5	0	1
33	E1	0	1
39	L2	0	1
39	l2	0	2
42	l5	0	2
43	L6	0	3
43	l6	0	1
44	l7	0	2
45	l8	0	1
48	M1	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	2
60	n4	0	1
62	n6	0	1
63	n7	0	1
64	n8	0	3
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
All	All	0	45

All (289) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	16.24	2.09	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-11.04	1.29	1.38
36	1	3181	C	N3-C4	-10.76	1.26	1.33
78	q2	17	CYS	CB-SG	10.62	2.00	1.82
36	5	1152	G	C2-N3	-9.57	1.25	1.32
36	5	1152	G	N9-C8	7.75	1.43	1.37
36	5	960	U	N1-C2	7.57	1.45	1.38
36	5	2726	C	N3-C4	-7.48	1.28	1.33
36	5	1152	G	N3-C4	-7.45	1.30	1.35
36	5	1304	A	N3-C4	7.37	1.39	1.34
36	5	953	G	C5-C4	-7.20	1.33	1.38
57	n1	104	GLU	CB-CG	7.13	1.65	1.52
36	5	1158	A	C5-C6	-7.10	1.34	1.41
36	5	2243	A	N3-C4	-7.06	1.30	1.34
36	5	934	G	N7-C5	-7.03	1.35	1.39
36	5	1149	G	N9-C8	-7.01	1.32	1.37
36	1	34	A	N9-C4	-6.90	1.33	1.37
13	C1	128	CYS	CB-SG	-6.87	1.70	1.82
36	5	1874	A	N9-C4	-6.85	1.33	1.37
52	m6	80	PHE	CB-CG	-6.83	1.39	1.51
36	1	659	G	N1-C2	-6.81	1.32	1.37
36	1	1141	C	N1-C6	-6.75	1.33	1.37
36	1	2761	G	N9-C8	-6.74	1.33	1.37
1	6	1659	A	N9-C4	-6.71	1.33	1.37
36	5	2954	U	C4-O4	6.65	1.28	1.23
36	5	1332	A	N3-C4	-6.57	1.30	1.34
38	4	28	C	N1-C6	-6.56	1.33	1.37
36	1	1858	A	N7-C5	-6.55	1.35	1.39
36	5	636	C	N1-C6	-6.54	1.33	1.37
36	5	2138	A	N7-C5	-6.53	1.35	1.39
36	5	2386	A	N7-C5	-6.51	1.35	1.39
36	5	970	A	N9-C4	-6.50	1.33	1.37
36	5	3084	C	N1-C6	-6.50	1.33	1.37
36	5	420	G	N7-C5	-6.50	1.35	1.39
36	5	420	G	N9-C8	-6.48	1.33	1.37
36	5	1370	G	N9-C8	-6.46	1.33	1.37
36	5	2147	A	C5-C6	-6.45	1.35	1.41
36	5	2954	U	N1-C2	6.45	1.44	1.38
36	1	2617	U	N3-C4	-6.43	1.32	1.38
36	5	1152	G	C5-C6	-6.42	1.35	1.42
36	5	2335	G	C5-C4	-6.40	1.33	1.38
36	1	338	A	N7-C5	-6.40	1.35	1.39
36	1	931	C	N3-C4	-6.39	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N1-C2	6.35	1.42	1.37
36	5	657	A	C5-C6	-6.33	1.35	1.41
36	1	1394	A	N9-C4	-6.27	1.34	1.37
36	1	2147	A	N9-C4	-6.23	1.34	1.37
36	5	2280	A	N9-C4	-6.23	1.34	1.37
1	6	1744	A	N9-C4	-6.22	1.34	1.37
36	5	649	A	C5-C6	-6.22	1.35	1.41
36	5	420	G	C5-C4	-6.21	1.34	1.38
36	1	343	U	N3-C4	-6.19	1.32	1.38
36	5	1429	G	N9-C4	-6.18	1.33	1.38
36	5	36	C	N1-C2	-6.18	1.33	1.40
36	5	2358	A	N9-C4	-6.17	1.34	1.37
38	4	28	C	N3-C4	-6.17	1.29	1.33
36	1	1392	G	C5-C4	-6.14	1.34	1.38
36	5	1847	A	N9-C4	-6.13	1.34	1.37
36	1	931	C	N1-C6	-6.13	1.33	1.37
36	5	1851	G	N7-C5	-6.13	1.35	1.39
36	5	1370	G	C6-N1	-6.12	1.35	1.39
36	1	1452	A	N9-C4	-6.12	1.34	1.37
36	5	2942	C	N1-C6	-6.12	1.33	1.37
36	1	368	G	N7-C5	-6.11	1.35	1.39
36	1	1119	C	N3-C4	-6.08	1.29	1.33
36	5	2813	A	N7-C5	-6.07	1.35	1.39
36	1	653	A	C5-C6	-6.07	1.35	1.41
36	1	1335	C	N1-C6	-6.06	1.33	1.37
36	5	2971	A	N9-C4	6.05	1.41	1.37
36	5	1115	G	N1-C2	-6.05	1.32	1.37
38	4	28	C	C4-C5	-6.03	1.38	1.43
36	1	661	G	N7-C5	-6.02	1.35	1.39
1	6	65	A	N9-C4	-6.02	1.34	1.37
36	1	1429	G	C5-C4	-6.01	1.34	1.38
36	5	947	G	N3-C4	-6.01	1.31	1.35
36	1	1103	A	N7-C5	5.97	1.42	1.39
36	1	189	G	N7-C5	-5.96	1.35	1.39
36	1	2419	A	N9-C4	-5.96	1.34	1.37
36	5	1902	G	C5-C4	-5.94	1.34	1.38
13	c1	128	CYS	CB-SG	-5.94	1.72	1.81
36	5	953	G	N7-C5	-5.94	1.35	1.39
36	1	2147	A	N3-C4	-5.93	1.31	1.34
36	5	2988	C	N3-C4	-5.92	1.29	1.33
36	1	1382	G	C5-C4	-5.89	1.34	1.38
36	1	1159	A	C6-N1	-5.88	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2280	A	N3-C4	-5.88	1.31	1.34
36	1	910	G	N7-C5	-5.88	1.35	1.39
36	1	1308	A	N7-C5	-5.87	1.35	1.39
36	5	1103	A	N9-C4	5.87	1.41	1.37
1	6	17	C	N3-C4	-5.87	1.29	1.33
36	5	3047	U	C2-N3	-5.86	1.33	1.37
36	1	2714	G	N9-C4	-5.85	1.33	1.38
36	1	2793	G	C2-N3	-5.84	1.28	1.32
1	6	1119	G	N7-C5	-5.84	1.35	1.39
36	1	800	G	C2-N3	-5.83	1.28	1.32
36	5	3052	G	C2-N3	-5.83	1.28	1.32
36	1	1103	A	N9-C4	5.82	1.41	1.37
36	5	2704	A	C5-C6	-5.81	1.35	1.41
36	5	2302	G	N1-C2	-5.81	1.33	1.37
36	5	2823	G	C5-C6	-5.80	1.36	1.42
36	1	2281	A	N9-C4	-5.80	1.34	1.37
36	5	970	A	N3-C4	-5.79	1.31	1.34
36	5	1199	C	N1-C6	-5.79	1.33	1.37
37	7	96	U	C4-O4	-5.79	1.19	1.23
40	L3	200	GLU	CG-CD	5.79	1.60	1.51
36	5	1177	G	N3-C4	-5.78	1.31	1.35
36	5	1159	A	N9-C4	-5.77	1.34	1.37
36	1	984	G	N7-C5	-5.76	1.35	1.39
36	1	936	A	N9-C4	-5.76	1.34	1.37
36	5	1200	A	N3-C4	-5.75	1.31	1.34
36	1	1367	G	N7-C5	-5.74	1.35	1.39
36	1	2385	G	N9-C4	-5.74	1.33	1.38
36	5	971	G	C5-C4	-5.74	1.34	1.38
36	5	426	G	C5-C4	-5.72	1.34	1.38
36	1	2867	C	N3-C4	-5.71	1.29	1.33
1	6	437	A	N9-C4	-5.69	1.34	1.37
36	5	3076	C	N3-C4	-5.69	1.29	1.33
36	5	2860	U	C4-O4	5.68	1.28	1.23
36	1	1164	G	C6-N1	-5.68	1.35	1.39
36	1	1377	G	N1-C2	-5.68	1.33	1.37
1	6	337	G	C2-N3	5.67	1.37	1.32
36	5	1432	C	N1-C6	-5.67	1.33	1.37
36	5	1110	U	C2-N3	-5.66	1.33	1.37
37	7	96	U	N3-C4	-5.65	1.33	1.38
36	5	3245	A	N9-C4	-5.64	1.34	1.37
36	5	934	G	C5-C4	-5.63	1.34	1.38
36	5	36	C	N1-C6	-5.63	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2636	A	C5-C6	-5.62	1.35	1.41
1	2	992	A	N9-C4	-5.61	1.34	1.37
36	5	917	A	C6-N1	-5.61	1.31	1.35
36	1	2837	A	C5-C6	-5.61	1.36	1.41
36	5	1152	G	C8-N7	5.61	1.34	1.30
36	1	2836	C	N3-C4	-5.60	1.30	1.33
36	5	2978	U	N1-C2	5.59	1.43	1.38
36	1	2977	G	C5-C4	-5.58	1.34	1.38
36	1	588	G	N7-C5	-5.58	1.35	1.39
52	m6	40	GLU	CG-CD	5.58	1.60	1.51
36	5	973	A	N7-C5	-5.58	1.35	1.39
36	5	2122	G	C5-C4	-5.56	1.34	1.38
36	5	2375	G	C6-N1	-5.56	1.35	1.39
36	1	1133	A	N9-C4	-5.55	1.34	1.37
36	1	943	U	C2-N3	-5.54	1.33	1.37
36	1	33	G	N7-C5	-5.52	1.35	1.39
36	5	2824	G	N7-C5	-5.52	1.35	1.39
36	1	895	A	C5-C6	-5.51	1.36	1.41
36	5	984	G	N7-C5	-5.51	1.35	1.39
36	5	2993	G	C5-C6	-5.50	1.36	1.42
37	7	94	C	N1-C6	-5.49	1.33	1.37
36	5	609	G	C2-N3	-5.48	1.28	1.32
36	1	2726	C	N3-C4	-5.48	1.30	1.33
36	5	3042	U	N3-C4	-5.47	1.33	1.38
36	5	3259	U	N1-C2	-5.47	1.33	1.38
36	5	706	A	N9-C4	-5.47	1.34	1.37
36	1	658	G	N9-C8	-5.47	1.34	1.37
36	1	2984	C	N3-C4	-5.46	1.30	1.33
36	5	2389	C	N3-C4	-5.45	1.30	1.33
36	5	1103	A	C5-C4	5.45	1.42	1.38
36	1	2971	A	N9-C4	5.45	1.41	1.37
36	1	2946	A	N7-C5	-5.44	1.35	1.39
36	5	1309	U	N1-C2	-5.44	1.33	1.38
36	1	969	C	N1-C6	-5.44	1.33	1.37
36	1	716	A	C5-C6	-5.44	1.36	1.41
36	5	1328	C	N1-C6	-5.44	1.33	1.37
36	1	651	G	N1-C2	-5.42	1.33	1.37
52	m6	78	ARG	CZ-NH1	5.41	1.40	1.33
36	5	2860	U	N3-C4	5.41	1.43	1.38
36	5	2372	A	N7-C5	-5.40	1.36	1.39
36	1	2169	G	C5-C6	5.39	1.47	1.42
36	5	2815	G	C5-C4	-5.39	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	424	G	N1-C2	-5.38	1.33	1.37
36	1	1429	G	N9-C8	-5.38	1.34	1.37
37	7	93	C	N3-C4	-5.38	1.30	1.33
36	1	421	G	N1-C2	-5.37	1.33	1.37
36	5	367	A	N9-C4	-5.36	1.34	1.37
35	SM	134	ASP	CA-C	5.35	1.66	1.52
36	5	891	G	C5-C4	-5.35	1.34	1.38
36	1	3305	A	C6-N1	-5.34	1.31	1.35
36	5	1879	A	C5-C6	-5.34	1.36	1.41
36	5	1886	A	N3-C4	-5.33	1.31	1.34
36	5	2330	C	N1-C6	-5.33	1.33	1.37
36	5	2364	G	N7-C5	-5.33	1.36	1.39
36	5	642	U	C2-N3	-5.32	1.34	1.37
36	5	2830	G	N3-C4	-5.32	1.31	1.35
36	5	2303	A	N9-C4	-5.32	1.34	1.37
36	1	2877	G	N7-C5	-5.31	1.36	1.39
36	5	1143	A	N9-C4	-5.31	1.34	1.37
36	1	2406	C	N1-C6	-5.30	1.33	1.37
36	1	985	U	N1-C2	-5.29	1.33	1.38
36	1	1147	G	N9-C8	-5.29	1.34	1.37
36	1	2649	A	N9-C4	5.29	1.41	1.37
75	O9	2	ALA	CA-CB	-5.29	1.41	1.52
36	5	2697	A	N7-C5	-5.29	1.36	1.39
36	5	3107	U	C2-N3	-5.29	1.34	1.37
36	5	2953	U	C4-O4	5.28	1.27	1.23
36	5	2383	C	N1-C6	-5.28	1.33	1.37
36	1	2162	U	C4-O4	-5.28	1.19	1.23
36	5	636	C	N3-C4	-5.28	1.30	1.33
36	5	2954	U	C4-C5	5.28	1.48	1.43
36	5	2993	G	N1-C2	-5.27	1.33	1.37
36	1	795	G	C5-C4	-5.26	1.34	1.38
36	1	815	G	N3-C4	-5.26	1.31	1.35
36	5	88	A	N9-C4	-5.26	1.34	1.37
36	5	642	U	N1-C2	-5.25	1.33	1.38
36	1	402	A	N3-C4	-5.25	1.31	1.34
1	6	308	C	N3-C4	-5.25	1.30	1.33
36	5	2412	G	N7-C5	-5.25	1.36	1.39
37	7	87	G	N7-C5	-5.25	1.36	1.39
36	5	947	G	N1-C2	-5.24	1.33	1.37
36	5	2971	A	N7-C5	5.24	1.42	1.39
36	1	2364	G	N3-C4	-5.24	1.31	1.35
52	m6	16	VAL	CB-CG2	-5.24	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1582	C	N1-C6	5.23	1.40	1.37
36	5	368	G	C6-N1	-5.23	1.35	1.39
36	5	631	U	C2-N3	-5.22	1.34	1.37
1	6	623	A	N9-C4	-5.22	1.34	1.37
36	1	1364	C	N1-C6	-5.21	1.34	1.37
36	5	635	G	C5-C4	-5.21	1.34	1.38
36	5	966	U	N3-C4	-5.21	1.33	1.38
36	5	3143	C	N1-C6	-5.20	1.34	1.37
36	5	1195	A	N3-C4	-5.20	1.31	1.34
36	5	1117	G	C5-C4	-5.19	1.34	1.38
37	7	96	U	C4-C5	-5.19	1.38	1.43
36	5	3004	C	N1-C6	-5.19	1.34	1.37
36	5	2874	G	N3-C4	-5.18	1.31	1.35
36	1	1606	U	N1-C2	-5.17	1.33	1.38
37	7	88	G	C6-N1	-5.17	1.35	1.39
38	8	7	U	N1-C6	-5.17	1.33	1.38
36	5	2351	U	N3-C4	-5.16	1.33	1.38
36	5	875	G	C6-N1	-5.15	1.35	1.39
36	5	36	C	C4-C5	-5.15	1.38	1.43
36	5	2646	C	N1-C6	-5.15	1.34	1.37
36	1	407	A	C5-C6	-5.14	1.36	1.41
36	5	934	G	C5-C6	-5.14	1.37	1.42
37	3	82	G	C6-N1	-5.14	1.35	1.39
36	1	48	A	N7-C5	-5.13	1.36	1.39
37	3	95	A	C5-C6	-5.13	1.36	1.41
36	1	2333	C	N3-C4	-5.12	1.30	1.33
36	1	892	U	C2-N3	-5.12	1.34	1.37
39	l2	213	GLY	C-O	5.11	1.31	1.23
52	M6	80	PHE	CB-CG	-5.11	1.42	1.51
1	6	321	C	N1-C2	5.10	1.45	1.40
36	1	92	G	C5-C4	-5.10	1.34	1.38
36	1	1660	C	N1-C6	-5.09	1.34	1.37
36	5	3362	A	N9-C4	-5.09	1.34	1.37
36	5	3008	A	N9-C4	-5.09	1.34	1.37
36	5	1311	G	C5-C4	-5.08	1.34	1.38
36	5	1331	U	C4-O4	-5.08	1.19	1.23
36	5	2987	A	N7-C5	-5.08	1.36	1.39
52	m6	40	GLU	CD-OE1	5.08	1.31	1.25
36	5	1113	G	N3-C4	-5.08	1.31	1.35
36	5	877	C	N1-C6	5.08	1.40	1.37
36	1	2952	G	N9-C4	-5.07	1.33	1.38
36	1	630	A	N7-C5	-5.07	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2605	G	C5-C4	-5.07	1.34	1.38
36	5	952	A	N9-C4	-5.07	1.34	1.37
36	1	85	A	N9-C4	-5.07	1.34	1.37
36	1	155	G	N9-C4	5.07	1.42	1.38
1	6	163	G	N3-C4	-5.07	1.31	1.35
36	1	667	C	N3-C4	-5.07	1.30	1.33
36	1	1427	U	C2-N3	-5.07	1.34	1.37
36	5	1476	G	N9-C4	-5.07	1.33	1.38
36	5	1324	U	C2-N3	-5.07	1.34	1.37
36	1	1335	C	N3-C4	-5.06	1.30	1.33
36	5	2856	G	N7-C5	-5.06	1.36	1.39
36	5	2136	C	N1-C6	-5.06	1.34	1.37
38	4	11	C	C4-C5	-5.06	1.39	1.43
36	5	417	A	C5-C4	-5.06	1.35	1.38
36	5	2943	G	N7-C5	-5.06	1.36	1.39
36	1	2642	A	N9-C4	-5.05	1.34	1.37
36	5	1304	A	N9-C8	-5.05	1.33	1.37
36	1	1326	A	N9-C4	-5.05	1.34	1.37
36	5	2419	A	P-O5'	5.05	1.64	1.59
36	5	652	G	N7-C5	-5.05	1.36	1.39
36	1	339	C	N3-C4	-5.04	1.30	1.33
36	1	635	G	C5-C6	-5.04	1.37	1.42
36	1	1404	G	N9-C8	-5.04	1.34	1.37
36	5	424	G	C5-C4	-5.04	1.34	1.38
36	5	962	A	C5-C4	-5.03	1.35	1.38
36	1	2982	A	N9-C8	-5.03	1.33	1.37
36	5	1432	C	C4-C5	-5.03	1.39	1.43
36	1	3362	A	N7-C5	-5.02	1.36	1.39
36	5	1489	A	N7-C5	-5.02	1.36	1.39
36	1	635	G	C5-C4	-5.02	1.34	1.38
36	5	3209	A	C5-C4	5.02	1.42	1.38
36	1	421	G	C5-C4	-5.02	1.34	1.38
36	1	343	U	C2-N3	-5.00	1.34	1.37
36	5	2354	C	N1-C6	-5.00	1.34	1.37
37	7	88	G	N1-C2	-5.00	1.33	1.37
36	1	323	A	N9-C4	-5.00	1.34	1.37

All (4853) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	26.65	141.93	128.60
36	5	1152	G	N3-C4-N9	-25.57	110.66	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	C2-N3-C4	-18.36	102.72	111.90
36	5	2818	U	O5'-P-OP1	-17.90	89.22	110.70
36	5	1116	G	O5'-P-OP1	-16.32	91.01	105.70
36	5	874	U	O5'-P-OP1	-16.28	91.05	105.70
36	5	1152	G	N3-C2-N2	-16.19	108.57	119.90
36	5	1419	A	O5'-P-OP2	-15.91	91.38	105.70
36	1	1104	G	O5'-P-OP1	-15.19	92.03	105.70
36	5	2373	A	O5'-P-OP2	-15.18	92.04	105.70
36	1	1495	U	C5-C6-N1	-14.64	115.38	122.70
36	5	1152	G	C8-N9-C1'	14.16	145.40	127.00
36	1	1308	A	O5'-P-OP2	-14.05	93.06	105.70
1	6	1773	C	N3-C4-C5	-14.02	116.29	121.90
36	5	1152	G	C5-N7-C8	-13.56	97.52	104.30
36	5	2297	U	O5'-P-OP2	-13.46	93.59	105.70
36	1	802	C	O5'-P-OP1	-13.44	93.60	105.70
36	5	3245	A	C5-N7-C8	-13.43	97.19	103.90
36	5	398	A	O5'-P-OP2	-13.42	93.62	105.70
36	5	437	G	C8-N9-C4	-13.39	101.04	106.40
36	5	3245	A	N7-C8-N9	13.32	120.46	113.80
36	5	2726	C	C5-C4-N4	12.89	129.22	120.20
36	1	2936	A	O5'-P-OP1	-12.79	94.19	105.70
36	5	1152	G	N1-C6-O6	12.67	127.50	119.90
36	5	1152	G	C4-N9-C1'	-12.61	110.10	126.50
1	6	1634	C	C2-N1-C1'	12.51	132.56	118.80
36	5	1308	A	O5'-P-OP1	-12.45	94.50	105.70
36	5	2403	G	O5'-P-OP2	-12.26	94.67	105.70
36	1	2714	G	N3-C4-C5	12.23	134.71	128.60
36	5	3245	A	C2-N3-C4	-12.08	104.56	110.60
36	5	1313	G	O5'-P-OP2	-12.04	94.87	105.70
36	1	2617	U	C5-C6-N1	-12.00	116.70	122.70
36	1	2621	G	N3-C2-N2	-11.87	111.59	119.90
36	5	636	C	C6-N1-C2	11.82	125.03	120.30
36	1	2617	U	C5-C4-O4	11.82	132.99	125.90
36	1	2822	U	O5'-P-OP1	-11.76	95.12	105.70
36	5	1304	A	N1-C6-N6	11.76	125.65	118.60
36	5	948	C	C6-N1-C2	11.74	125.00	120.30
36	1	282	G	O5'-P-OP1	-11.62	95.24	105.70
36	5	1304	A	C5-C6-N6	-11.62	114.41	123.70
36	1	1308	A	C8-N9-C4	-11.61	101.16	105.80
36	5	2923	U	O5'-P-OP1	-11.59	95.27	105.70
36	5	3245	A	N1-C6-N6	11.44	125.47	118.60
36	5	1307	G	P-O3'-C3'	11.19	133.13	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	11	C	C5-C6-N1	11.19	126.59	121.00
38	4	11	C	C6-N1-C2	-11.18	115.83	120.30
36	5	1879	A	N1-C6-N6	11.10	125.26	118.60
36	5	2704	A	O5'-P-OP1	-11.08	95.73	105.70
36	5	2290	C	C6-N1-C2	11.03	124.71	120.30
36	5	3245	A	C6-C5-N7	-11.01	124.59	132.30
36	5	2928	C	C6-N1-C2	-11.00	115.90	120.30
36	5	641	C	N1-C2-O2	-11.00	112.30	118.90
36	5	2726	C	C6-N1-C2	-10.93	115.93	120.30
36	5	2824	G	O5'-P-OP2	-10.92	95.87	105.70
1	6	163	G	N3-C4-N9	-10.84	119.50	126.00
36	1	1381	A	O5'-P-OP2	10.84	123.70	110.70
36	1	517	G	C8-N9-C4	-10.78	102.09	106.40
36	5	922	U	N3-C2-O2	-10.76	114.67	122.20
36	5	2375	G	N1-C6-O6	-10.73	113.46	119.90
36	5	2634	U	C2-N3-C4	-10.72	120.57	127.00
36	1	639	G	N1-C6-O6	10.72	126.33	119.90
36	1	218	G	O5'-P-OP2	-10.67	96.10	105.70
36	1	2397	A	N1-C6-N6	10.60	124.96	118.60
36	1	2846	U	N3-C2-O2	-10.57	114.80	122.20
36	5	2726	C	N3-C4-N4	-10.53	110.63	118.00
36	5	1152	G	N1-C2-N2	10.52	125.67	116.20
36	1	3362	A	O4'-C1'-N9	10.51	116.61	108.20
36	1	2169	G	N1-C6-O6	-10.48	113.61	119.90
36	1	28	C	N3-C4-C5	10.46	126.08	121.90
36	1	1389	G	C4-C5-N7	10.46	114.98	110.80
36	1	406	G	O4'-C1'-N9	10.44	116.55	108.20
36	1	1389	G	C5-C6-O6	-10.43	122.34	128.60
37	7	93	C	O5'-P-OP2	-10.41	96.33	105.70
37	7	87	G	N1-C6-O6	10.41	126.14	119.90
36	1	645	A	C6-N1-C2	-10.39	112.37	118.60
36	1	3278	C	N1-C2-O2	10.39	125.13	118.90
36	1	2871	G	O5'-P-OP2	-10.32	96.42	105.70
1	6	1773	C	C6-N1-C2	-10.31	116.18	120.30
36	1	1495	U	C4-C5-C6	10.29	125.88	119.70
36	1	2617	U	N3-C4-O4	-10.27	112.21	119.40
36	1	3306	U	N3-C4-O4	-10.26	112.22	119.40
1	6	453	U	N3-C2-O2	-10.23	115.04	122.20
36	5	2389	C	C6-N1-C2	10.21	124.39	120.30
36	5	652	G	O5'-P-OP2	-10.19	96.53	105.70
1	6	1773	C	N3-C4-N4	10.19	125.13	118.00
36	5	877	C	N3-C4-C5	10.18	125.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	SM	135	ALA	N-CA-CB	10.17	124.33	110.10
36	1	1365	G	C8-N9-C4	-10.17	102.33	106.40
36	1	2726	C	N3-C4-N4	-10.17	110.88	118.00
36	5	1110	U	N1-C2-O2	10.16	129.91	122.80
36	1	1308	A	N7-C8-N9	10.15	118.88	113.80
36	5	1190	A	C8-N9-C4	-10.14	101.74	105.80
1	6	453	U	N1-C2-O2	10.13	129.89	122.80
36	1	880	G	N1-C6-O6	-10.11	113.83	119.90
1	6	44	U	N1-C2-O2	-10.11	115.72	122.80
36	5	437	G	N7-C8-N9	10.09	118.15	113.10
36	5	1208	U	C5-C4-O4	10.09	131.96	125.90
36	1	1365	G	N3-C4-C5	-10.07	123.56	128.60
1	6	402	C	O5'-P-OP2	-10.06	96.64	105.70
36	1	2846	U	C5-C4-O4	10.05	131.93	125.90
36	5	437	G	N9-C4-C5	10.04	109.42	105.40
36	5	881	C	O5'-P-OP2	-10.03	96.67	105.70
36	5	2389	C	N3-C4-C5	10.03	125.91	121.90
36	5	3078	U	N3-C2-O2	-10.03	115.18	122.20
36	1	776	U	C4-C5-C6	10.00	125.70	119.70
36	1	339	C	OP1-P-OP2	-9.99	104.61	119.60
36	5	1208	U	N3-C2-O2	-9.95	115.23	122.20
37	7	35	C	C6-N1-C2	9.95	124.28	120.30
36	5	2366	C	C6-N1-C2	-9.93	116.33	120.30
36	1	1216	C	C6-N1-C2	-9.90	116.34	120.30
36	5	2389	C	C5-C6-N1	-9.89	116.05	121.00
37	7	90	U	N3-C4-C5	9.87	120.52	114.60
36	1	3057	U	N3-C2-O2	-9.87	115.29	122.20
36	5	2634	U	N3-C4-C5	9.86	120.52	114.60
36	5	424	G	C5-C6-O6	-9.84	122.69	128.60
36	5	2392	C	N3-C4-C5	9.83	125.83	121.90
36	1	2827	U	C5-C4-O4	9.83	131.80	125.90
36	5	2186	U	O5'-P-OP2	-9.81	96.87	105.70
1	2	553	G	N1-C6-O6	9.79	125.77	119.90
36	1	1838	G	N1-C6-O6	9.78	125.77	119.90
36	1	1492	G	C5-N7-C8	9.78	109.19	104.30
36	5	2678	A	N1-C6-N6	-9.78	112.73	118.60
36	1	776	U	N1-C2-N3	9.77	120.76	114.90
36	5	1452	A	N1-C6-N6	9.76	124.46	118.60
36	5	2136	C	C6-N1-C2	9.75	124.20	120.30
36	5	2234	G	C5-C6-O6	-9.74	122.76	128.60
36	1	1409	G	N1-C6-O6	-9.71	114.07	119.90
1	2	639	U	N3-C2-O2	-9.67	115.43	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	922	U	N1-C2-O2	9.66	129.56	122.80
36	1	2923	U	O5'-P-OP1	-9.66	97.01	105.70
36	5	793	C	N1-C2-O2	-9.66	113.11	118.90
36	1	1902	G	C5-C6-O6	-9.64	122.82	128.60
36	5	2331	C	N3-C4-C5	-9.64	118.04	121.90
36	5	3214	U	N3-C2-O2	-9.63	115.46	122.20
36	5	1792	C	O5'-P-OP2	-9.63	97.03	105.70
36	1	3306	U	C5-C4-O4	9.62	131.67	125.90
36	1	3181	C	C5-C4-N4	9.59	126.91	120.20
36	1	2797	C	O5'-P-OP1	-9.57	97.08	105.70
36	1	1346	G	O5'-P-OP2	-9.57	97.08	105.70
1	6	1773	C	N1-C2-O2	-9.57	113.16	118.90
36	1	521	A	N1-C6-N6	9.56	124.34	118.60
36	1	1556	C	C2-N1-C1'	9.53	129.28	118.80
38	4	22	U	C5-C6-N1	-9.53	117.94	122.70
36	1	1153	A	O5'-P-OP1	-9.52	97.13	105.70
36	1	2359	C	N1-C2-O2	-9.50	113.20	118.90
36	5	2611	U	C5-C6-N1	-9.49	117.95	122.70
36	5	1520	G	C5-C6-O6	-9.48	122.91	128.60
36	5	2389	C	O5'-P-OP1	-9.44	97.20	105.70
36	1	716	A	N1-C6-N6	9.42	124.25	118.60
36	5	776	U	N3-C2-O2	-9.41	115.61	122.20
36	5	1101	G	N3-C2-N2	9.40	126.48	119.90
36	5	2726	C	N3-C2-O2	-9.39	115.33	121.90
36	1	2406	C	C6-N1-C2	9.38	124.05	120.30
36	1	640	U	C5-C4-O4	-9.38	120.28	125.90
36	1	1450	G	O5'-P-OP1	-9.37	97.27	105.70
36	1	942	U	C5-C4-O4	-9.35	120.29	125.90
36	5	2618	G	N3-C4-N9	9.35	131.61	126.00
36	1	2726	C	N3-C2-O2	-9.32	115.38	121.90
36	1	2215	A	C8-N9-C4	9.31	109.52	105.80
36	5	2395	G	O5'-P-OP2	-9.29	97.34	105.70
36	5	3154	C	N1-C2-O2	9.28	124.47	118.90
36	5	2632	G	O5'-P-OP1	-9.28	97.35	105.70
36	1	1149	G	N1-C6-O6	9.28	125.47	119.90
36	1	1484	U	P-O3'-C3'	9.27	130.83	119.70
36	1	1452	A	C8-N9-C4	9.26	109.50	105.80
1	2	321	C	C6-N1-C2	-9.26	116.60	120.30
36	5	622	A	N1-C6-N6	9.25	124.15	118.60
1	6	448	C	C6-N1-C2	-9.24	116.60	120.30
36	5	3245	A	C4-C5-N7	9.24	115.32	110.70
36	1	2818	U	O5'-P-OP1	-9.23	97.39	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2572	C	N1-C2-O2	9.22	124.43	118.90
36	5	2836	C	C4-C5-C6	9.22	122.01	117.40
36	1	2144	A	C5-C6-N6	-9.22	116.32	123.70
36	1	2617	U	N1-C2-N3	9.20	120.42	114.90
1	6	609	U	C5-C4-O4	9.17	131.41	125.90
36	1	421	G	C5-C6-O6	-9.17	123.10	128.60
36	1	3181	C	N3-C4-N4	-9.17	111.58	118.00
36	5	88	A	C8-N9-C4	9.16	109.47	105.80
36	1	517	G	N7-C8-N9	9.16	117.68	113.10
36	1	1495	U	N1-C2-N3	9.16	120.39	114.90
36	5	2334	U	N3-C2-O2	-9.16	115.79	122.20
36	5	384	A	C8-N9-C4	9.15	109.46	105.80
36	1	2363	A	N1-C6-N6	-9.14	113.11	118.60
36	1	2642	A	C6-N1-C2	9.14	124.09	118.60
38	4	113	U	C5-C4-O4	9.11	131.37	125.90
36	5	2858	U	N3-C2-O2	-9.09	115.83	122.20
36	1	439	C	N1-C2-O2	9.07	124.34	118.90
36	1	1216	C	O5'-P-OP2	-9.07	97.54	105.70
36	5	922	U	N3-C4-O4	-9.05	113.06	119.40
36	1	716	A	N9-C4-C5	-9.04	102.18	105.80
38	4	109	A	N1-C6-N6	9.04	124.02	118.60
36	1	155	G	N3-C4-C5	-9.03	124.08	128.60
36	5	2978	U	O4'-C1'-N1	9.03	115.42	108.20
36	5	1548	C	N1-C2-O2	-9.03	113.48	118.90
36	5	1369	A	N1-C6-N6	9.02	124.01	118.60
36	5	2362	C	O5'-P-OP2	-8.99	97.61	105.70
36	5	406	G	O4'-C1'-N9	8.99	115.39	108.20
36	5	2385	G	O5'-P-OP1	-8.99	97.61	105.70
36	1	3344	A	N7-C8-N9	8.97	118.29	113.80
36	5	2823	G	C4-C5-N7	8.97	114.39	110.80
36	1	339	C	N3-C2-O2	-8.97	115.62	121.90
36	5	2930	A	N1-C6-N6	-8.97	113.22	118.60
36	1	585	A	C8-N9-C4	8.96	109.38	105.80
36	1	2176	U	N3-C2-O2	-8.96	115.93	122.20
36	1	2714	G	C2-N3-C4	-8.96	107.42	111.90
36	1	1831	U	N3-C2-O2	-8.94	115.94	122.20
36	5	1403	C	C6-N1-C2	8.94	123.88	120.30
1	2	402	C	C6-N1-C2	8.93	123.87	120.30
36	5	1200	A	C8-N9-C4	-8.92	102.23	105.80
36	1	2355	G	N1-C6-O6	8.91	125.25	119.90
36	5	1879	A	C6-C5-N7	-8.91	126.06	132.30
36	5	2930	A	N9-C4-C5	8.91	109.36	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	979	U	C6-N1-C2	-8.90	115.66	121.00
1	6	1634	C	C6-N1-C1'	-8.90	110.12	120.80
36	5	1158	A	N1-C6-N6	8.90	123.94	118.60
36	5	222	A	O5'-P-OP2	-8.90	97.69	105.70
37	3	86	U	C2-N3-C4	-8.89	121.67	127.00
36	1	2693	C	C6-N1-C2	8.89	123.86	120.30
36	5	2973	G	C8-N9-C4	-8.89	102.84	106.40
36	1	3278	C	N3-C2-O2	-8.88	115.68	121.90
36	1	407	A	O5'-P-OP2	-8.88	97.71	105.70
36	1	1495	U	C2-N3-C4	-8.87	121.68	127.00
36	5	922	U	C2-N3-C4	-8.87	121.68	127.00
36	1	2617	U	C4-C5-C6	8.85	125.01	119.70
36	1	1381	A	O5'-P-OP1	-8.84	97.74	105.70
36	1	2942	C	N1-C2-O2	-8.84	113.60	118.90
36	1	2714	G	N3-C4-N9	-8.84	120.70	126.00
36	5	1060	U	N3-C4-O4	-8.84	113.22	119.40
36	5	2865	U	C5-C6-N1	8.84	127.12	122.70
36	5	590	G	C5-C6-O6	-8.83	123.30	128.60
36	5	1152	G	C4-C5-N7	8.83	114.33	110.80
36	5	2354	C	N1-C2-O2	-8.83	113.60	118.90
36	5	1298	C	C6-N1-C2	-8.82	116.77	120.30
36	5	3362	A	C2-N3-C4	-8.82	106.19	110.60
1	2	73	U	O4'-C1'-N1	8.82	115.26	108.20
36	1	3057	U	C5-C4-O4	8.82	131.19	125.90
36	1	655	C	C6-N1-C2	-8.82	116.77	120.30
36	1	2283	G	N1-C6-O6	8.81	125.19	119.90
36	5	2351	U	N3-C2-O2	-8.81	116.03	122.20
36	5	1844	C	C6-N1-C2	-8.80	116.78	120.30
36	1	304	G	N3-C2-N2	-8.80	113.74	119.90
36	1	895	A	C2-N3-C4	-8.80	106.20	110.60
36	1	2870	C	C2-N1-C1'	-8.80	109.12	118.80
36	5	960	U	N3-C4-C5	8.80	119.88	114.60
36	1	365	A	N1-C6-N6	8.78	123.87	118.60
1	6	1657	U	O5'-P-OP2	-8.78	97.80	105.70
36	5	1902	G	C5-C6-O6	-8.78	123.33	128.60
36	5	1513	G	C8-N9-C4	-8.77	102.89	106.40
1	6	44	U	N3-C2-O2	8.76	128.33	122.20
36	5	1452	A	N9-C4-C5	-8.76	102.30	105.80
36	1	2836	C	C5-C4-N4	8.75	126.33	120.20
36	1	1216	C	C5-C6-N1	8.75	125.37	121.00
36	1	1405	U	N3-C4-C5	8.74	119.84	114.60
36	5	1213	G	C5-C6-O6	-8.74	123.36	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	966	U	N3-C2-O2	-8.74	116.08	122.20
36	1	1196	C	C6-N1-C2	8.74	123.80	120.30
36	1	120	G	C8-N9-C4	8.73	109.89	106.40
36	5	952	A	N1-C6-N6	8.73	123.84	118.60
36	5	2398	A	N1-C6-N6	-8.73	113.36	118.60
36	1	802	C	N3-C2-O2	-8.73	115.79	121.90
1	6	144	U	N3-C2-O2	-8.72	116.09	122.20
37	3	86	U	C5-C4-O4	-8.72	120.67	125.90
36	5	189	G	N1-C6-O6	-8.72	114.67	119.90
36	5	1119	C	N3-C4-C5	8.71	125.39	121.90
36	1	709	A	C8-N9-C4	8.71	109.28	105.80
1	6	57	G	O5'-P-OP2	-8.71	97.86	105.70
36	5	3012	A	C8-N9-C4	8.70	109.28	105.80
36	5	96	G	O5'-P-OP2	-8.69	97.88	105.70
36	5	3245	A	C8-N9-C4	-8.68	102.33	105.80
36	1	2358	A	C8-N9-C4	8.68	109.27	105.80
36	1	895	A	N1-C6-N6	8.64	123.78	118.60
36	1	1301	A	O5'-P-OP1	-8.63	97.93	105.70
36	1	2617	U	N3-C2-O2	-8.63	116.16	122.20
36	5	437	G	N3-C2-N2	-8.63	113.86	119.90
1	6	362	G	O5'-P-OP2	-8.63	97.94	105.70
36	5	3041	U	N3-C2-O2	8.61	128.22	122.20
36	5	3200	G	N1-C6-O6	8.60	125.06	119.90
36	1	1389	G	N9-C4-C5	-8.59	101.96	105.40
36	5	1306	G	C5-C6-O6	-8.59	123.45	128.60
36	5	3212	C	N1-C2-O2	-8.59	113.75	118.90
36	1	2850	G	C6-C5-N7	-8.58	125.25	130.40
52	m6	78	ARG	NE-CZ-NH2	-8.58	116.01	120.30
36	5	2383	C	N3-C4-C5	-8.57	118.47	121.90
36	5	2899	C	C6-N1-C2	-8.57	116.87	120.30
36	1	2886	U	C5-C4-O4	-8.56	120.76	125.90
38	8	80	A	N7-C8-N9	8.55	118.08	113.80
36	1	958	C	C2-N3-C4	-8.55	115.62	119.90
36	5	1842	A	O5'-P-OP2	-8.55	98.00	105.70
36	5	2899	C	N1-C2-N3	8.55	125.18	119.20
36	5	1304	A	N9-C4-C5	-8.54	102.38	105.80
36	5	3078	U	N1-C2-O2	8.54	128.78	122.80
36	1	3362	A	N7-C8-N9	8.53	118.07	113.80
36	5	3362	A	N1-C2-N3	8.54	133.57	129.30
36	5	3123	A	C8-N9-C4	8.53	109.21	105.80
36	5	3218	A	N1-C6-N6	8.53	123.72	118.60
36	5	835	G	O4'-C1'-N9	8.52	115.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3041	U	C5-C4-O4	-8.52	120.79	125.90
36	5	2644	C	O5'-P-OP1	-8.52	98.04	105.70
36	5	3185	U	O5'-P-OP2	-8.51	98.04	105.70
36	1	1495	U	N1-C2-O2	-8.51	116.84	122.80
36	5	1308	A	O5'-P-OP2	8.51	120.91	110.70
36	1	645	A	N3-C4-C5	-8.51	120.84	126.80
1	6	1700	C	C2-N1-C1'	8.51	128.16	118.80
38	4	79	A	C8-N9-C4	-8.51	102.40	105.80
36	1	2144	A	N1-C6-N6	8.50	123.70	118.60
36	5	3214	U	C5-C4-O4	8.49	131.00	125.90
1	6	371	G	C6-C5-N7	-8.48	125.31	130.40
36	5	2377	G	C8-N9-C4	8.47	109.79	106.40
36	1	2621	G	N1-C6-O6	8.46	124.98	119.90
36	1	895	A	O5'-P-OP1	-8.46	98.09	105.70
36	1	2836	C	C6-N1-C2	-8.45	116.92	120.30
36	5	1101	G	N1-C6-O6	-8.44	114.84	119.90
1	6	337	G	C6-C5-N7	-8.43	125.34	130.40
36	5	1548	C	N3-C2-O2	8.43	127.80	121.90
36	1	1164	G	N1-C6-O6	-8.42	114.85	119.90
36	1	2870	C	C6-N1-C1'	8.42	130.90	120.80
36	5	2398	A	C5-N7-C8	8.41	108.11	103.90
36	5	2797	C	N1-C2-O2	-8.41	113.85	118.90
36	5	3245	A	N1-C2-N3	8.41	133.50	129.30
37	7	40	C	N1-C2-O2	-8.41	113.86	118.90
1	6	1700	C	N1-C2-O2	8.40	123.94	118.90
36	1	2627	C	C6-N1-C2	8.40	123.66	120.30
38	8	80	A	C8-N9-C4	-8.39	102.44	105.80
36	5	1304	A	N3-C4-N9	8.39	134.11	127.40
36	5	1897	G	N1-C6-O6	8.39	124.94	119.90
36	5	2632	G	N1-C6-O6	-8.38	114.87	119.90
36	5	636	C	C5-C6-N1	-8.38	116.81	121.00
36	5	2928	C	N3-C2-O2	-8.37	116.04	121.90
36	1	1303	A	C8-N9-C4	8.37	109.15	105.80
36	1	2393	G	O5'-P-OP2	-8.36	98.17	105.70
36	1	893	C	C6-N1-C2	-8.36	116.96	120.30
36	5	1208	U	N1-C2-N3	8.35	119.91	114.90
36	1	2827	U	N3-C4-O4	-8.35	113.56	119.40
36	5	1113	G	O5'-P-OP1	-8.35	98.19	105.70
36	5	1452	A	C5-C6-N6	-8.35	117.02	123.70
36	5	426	G	C8-N9-C4	8.34	109.74	106.40
36	1	2884	C	N3-C4-C5	8.34	125.24	121.90
36	1	1389	G	N1-C6-O6	8.34	124.90	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2823	G	N1-C6-O6	8.34	124.90	119.90
36	1	895	A	C5-N7-C8	-8.33	99.73	103.90
36	5	869	G	N1-C6-O6	-8.33	114.90	119.90
36	5	1239	C	C5-C6-N1	8.33	125.17	121.00
36	5	424	G	N3-C4-N9	8.32	130.99	126.00
36	1	895	A	C4-C5-N7	8.32	114.86	110.70
36	1	3181	C	N3-C2-O2	-8.32	116.08	121.90
36	1	880	G	C5-C6-O6	8.31	133.58	128.60
36	5	3362	A	N1-C6-N6	8.30	123.58	118.60
36	5	2148	U	N1-C2-O2	-8.29	117.00	122.80
36	5	2272	G	O4'-C1'-N9	8.28	114.83	108.20
1	6	371	G	N3-C4-N9	8.28	130.97	126.00
36	1	659	G	N3-C2-N2	8.28	125.69	119.90
36	1	25	U	N1-C2-O2	-8.27	117.01	122.80
36	1	931	C	C5-C6-N1	-8.27	116.86	121.00
36	1	1404	G	C8-N9-C4	8.27	109.71	106.40
36	5	1788	C	C6-N1-C2	-8.27	116.99	120.30
36	5	2858	U	N1-C2-O2	8.27	128.59	122.80
36	1	1902	G	C4-C5-N7	8.26	114.11	110.80
36	1	3362	A	C6-C5-N7	-8.26	126.52	132.30
36	1	2619	G	O5'-P-OP1	-8.25	98.27	105.70
36	5	2392	C	C2-N3-C4	-8.25	115.78	119.90
36	5	890	C	O5'-P-OP2	-8.25	98.28	105.70
36	1	2373	A	O5'-P-OP1	-8.24	98.28	105.70
36	1	1197	A	N1-C6-N6	8.24	123.54	118.60
36	1	2572	C	C2-N1-C1'	8.24	127.86	118.80
36	1	2144	A	N9-C4-C5	-8.23	102.51	105.80
36	5	2870	C	N3-C4-C5	8.23	125.19	121.90
36	1	2726	C	C5-C4-N4	8.22	125.95	120.20
36	5	1110	U	N3-C2-O2	-8.22	116.45	122.20
36	5	2823	G	C5-C6-O6	-8.22	123.67	128.60
36	5	1208	U	N3-C4-O4	-8.22	113.65	119.40
1	2	453	U	C2-N1-C1'	8.21	127.56	117.70
36	5	2287	C	O5'-P-OP2	-8.21	98.31	105.70
36	1	2376	G	C5-N7-C8	-8.21	100.20	104.30
36	1	922	U	C5-C6-N1	8.20	126.80	122.70
1	2	1096	C	N1-C2-O2	8.20	123.82	118.90
36	5	2764	C	C5-C4-N4	-8.20	114.46	120.20
38	4	113	U	N1-C2-N3	8.20	119.82	114.90
36	5	2385	G	N1-C6-O6	8.20	124.82	119.90
36	1	949	C	C4-C5-C6	8.19	121.50	117.40
36	5	931	C	C2-N3-C4	-8.19	115.81	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	908	G	O4'-C1'-N9	-8.18	101.65	108.20
36	1	2850	G	C5-C6-O6	-8.18	123.69	128.60
36	5	2889	C	C2-N3-C4	-8.18	115.81	119.90
36	5	218	G	O5'-P-OP2	-8.18	98.34	105.70
36	5	968	G	O5'-P-OP1	-8.18	98.34	105.70
36	5	2278	C	C4-C5-C6	-8.17	113.31	117.40
36	5	942	U	C5-C4-O4	-8.17	121.00	125.90
1	6	1100	G	N3-C4-C5	-8.17	124.52	128.60
36	1	650	C	N1-C2-O2	-8.16	114.00	118.90
36	1	984	G	N3-C2-N2	8.16	125.61	119.90
36	1	2836	C	C4-C5-C6	8.16	121.48	117.40
36	5	361	A	N1-C6-N6	-8.16	113.70	118.60
36	1	885	U	C5-C6-N1	-8.15	118.62	122.70
36	1	1405	U	C6-N1-C2	8.15	125.89	121.00
36	5	546	C	N1-C2-O2	8.15	123.79	118.90
38	8	92	A	O5'-P-OP1	-8.15	98.36	105.70
36	1	2942	C	N3-C2-O2	8.15	127.61	121.90
37	7	77	G	O5'-P-OP1	8.15	120.48	110.70
36	5	1372	C	C6-N1-C2	8.14	123.56	120.30
36	5	2877	G	N9-C4-C5	8.14	108.66	105.40
36	5	3103	A	C5-C6-N1	8.14	121.77	117.70
36	1	1307	G	N1-C6-O6	-8.14	115.02	119.90
36	5	2815	G	C8-N9-C4	8.14	109.66	106.40
36	1	350	C	C6-N1-C2	-8.14	117.05	120.30
36	1	1377	G	N3-C2-N2	8.13	125.59	119.90
1	6	1	U	C2-N1-C1'	8.13	127.45	117.70
1	6	1026	A	O5'-P-OP1	-8.12	98.39	105.70
36	5	92	G	C5-C6-N1	8.12	115.56	111.50
36	1	1118	C	C6-N1-C2	-8.12	117.05	120.30
36	1	2996	U	C2-N1-C1'	8.12	127.44	117.70
36	5	1842	A	O5'-P-OP1	8.12	120.44	110.70
1	2	1280	C	N3-C4-C5	-8.11	118.66	121.90
36	1	3214	U	N3-C2-O2	-8.11	116.52	122.20
1	6	1075	C	N1-C2-O2	-8.11	114.03	118.90
36	1	2915	U	N1-C2-O2	-8.11	117.13	122.80
36	5	1292	C	C6-N1-C2	8.11	123.54	120.30
1	2	1039	A	O4'-C1'-N9	8.10	114.68	108.20
36	1	339	C	N3-C4-N4	-8.10	112.33	118.00
36	5	817	A	O5'-P-OP1	-8.10	98.41	105.70
36	5	2142	A	C5-C6-N1	8.09	121.75	117.70
36	5	1587	A	O5'-P-OP1	-8.09	98.42	105.70
36	1	651	G	N3-C4-C5	-8.09	124.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2409	G	N1-C6-O6	-8.09	115.05	119.90
1	6	114	C	N1-C2-O2	8.08	123.75	118.90
36	1	802	C	O5'-P-OP2	8.08	120.40	110.70
38	8	111	A	N1-C6-N6	8.08	123.45	118.60
1	6	65	A	C2-N3-C4	-8.07	106.56	110.60
36	1	1310	G	N1-C6-O6	-8.07	115.06	119.90
36	1	1367	G	N1-C6-O6	8.07	124.74	119.90
36	1	2400	G	N3-C2-N2	-8.07	114.25	119.90
36	5	2389	C	C2-N3-C4	-8.07	115.87	119.90
36	5	2420	C	C6-N1-C2	8.07	123.53	120.30
36	5	3209	A	O4'-C1'-N9	8.07	114.65	108.20
36	1	1495	U	C2-N1-C1'	-8.06	108.03	117.70
36	5	2524	A	O4'-C1'-N9	8.06	114.65	108.20
36	1	661	G	C8-N9-C4	-8.06	103.18	106.40
36	5	934	G	N1-C6-O6	8.05	124.73	119.90
36	1	999	G	C5-C6-O6	-8.05	123.77	128.60
36	5	2874	G	C5-C6-N1	-8.05	107.47	111.50
36	5	1160	C	C2-N1-C1'	-8.04	109.96	118.80
36	1	681	U	C5-C4-O4	-8.03	121.08	125.90
1	2	57	G	O5'-P-OP2	-8.02	98.48	105.70
36	1	2176	U	N1-C2-O2	8.02	128.41	122.80
36	5	887	G	N3-C2-N2	8.02	125.51	119.90
36	1	28	C	C6-N1-C2	8.01	123.50	120.30
36	5	637	C	N1-C2-O2	-8.01	114.09	118.90
36	1	1316	C	N3-C4-N4	8.00	123.60	118.00
38	4	32	C	N1-C2-O2	-8.00	114.10	118.90
31	D9	36	LEU	CA-CB-CG	7.99	133.68	115.30
38	4	109	A	C5-C6-N6	-7.99	117.31	123.70
1	6	321	C	N3-C2-O2	-7.99	116.31	121.90
36	5	2375	G	C5-C6-O6	7.99	133.39	128.60
36	1	2764	C	C6-N1-C2	-7.98	117.11	120.30
1	6	973	A	O5'-P-OP2	-7.97	98.53	105.70
36	1	339	C	C5-C4-N4	7.96	125.78	120.20
36	1	797	U	O5'-P-OP2	7.96	120.25	110.70
36	1	984	G	N1-C2-N2	-7.96	109.04	116.20
36	5	2935	U	O5'-P-OP2	-7.96	98.54	105.70
36	5	948	C	C5-C6-N1	-7.96	117.02	121.00
36	1	942	U	C2-N3-C4	-7.95	122.23	127.00
36	1	2867	C	N3-C4-C5	7.95	125.08	121.90
36	1	2411	U	N3-C4-O4	-7.95	113.84	119.40
1	6	941	A	N1-C6-N6	-7.94	113.83	118.60
36	1	1141	C	C4-C5-C6	7.94	121.37	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2634	U	C2-N3-C4	-7.94	122.24	127.00
36	1	785	G	C5-C6-N1	7.93	115.47	111.50
36	1	2385	G	N3-C4-C5	7.93	132.56	128.60
36	5	92	G	C2-N3-C4	7.93	115.86	111.90
36	5	2927	C	OP2-P-O3'	7.92	122.63	105.20
36	5	960	U	N1-C2-O2	7.92	128.35	122.80
1	6	1782	A	C8-N9-C4	-7.92	102.63	105.80
36	5	3382	U	C2-N1-C1'	7.92	127.20	117.70
44	17	229	PHE	CB-CG-CD1	7.92	126.34	120.80
1	6	1654	G	O5'-P-OP2	-7.91	98.58	105.70
36	5	804	C	N3-C4-C5	-7.91	118.74	121.90
36	1	1911	A	N1-C6-N6	7.91	123.34	118.60
36	1	2621	G	N1-C2-N2	7.91	123.32	116.20
36	5	1126	G	C8-N9-C4	-7.91	103.24	106.40
36	1	2572	C	N1-C2-O2	7.91	123.64	118.90
36	5	2334	U	O5'-P-OP2	-7.91	98.58	105.70
1	6	1537	C	C6-N1-C2	-7.90	117.14	120.30
36	5	366	A	N1-C6-N6	7.90	123.34	118.60
36	1	2414	G	N3-C2-N2	-7.90	114.37	119.90
36	1	3228	C	N3-C2-O2	-7.89	116.38	121.90
36	5	1108	U	O5'-P-OP2	-7.89	98.60	105.70
36	5	2993	G	C4-C5-N7	7.88	113.95	110.80
36	1	637	C	C2-N3-C4	-7.88	115.96	119.90
1	2	453	U	N3-C2-O2	-7.88	116.68	122.20
36	1	2874	G	N9-C4-C5	7.88	108.55	105.40
1	6	1641	C	N1-C2-O2	-7.88	114.17	118.90
36	1	1365	G	C2-N3-C4	7.87	115.84	111.90
1	6	542	A	O4'-C1'-N9	7.87	114.50	108.20
36	1	2850	G	C4-C5-N7	7.87	113.95	110.80
36	1	2414	G	N1-C6-O6	7.87	124.62	119.90
1	6	609	U	N3-C2-O2	-7.87	116.69	122.20
36	1	2850	G	N1-C6-O6	7.86	124.62	119.90
36	1	1428	A	N1-C6-N6	7.86	123.31	118.60
36	5	2899	C	N3-C2-O2	-7.86	116.40	121.90
36	5	3362	A	C5-N7-C8	-7.86	99.97	103.90
36	1	1138	U	N3-C2-O2	-7.85	116.70	122.20
36	1	1405	U	C2-N3-C4	-7.85	122.29	127.00
36	5	2815	G	N7-C8-N9	-7.85	109.17	113.10
36	1	2359	C	C2-N3-C4	-7.84	115.98	119.90
36	5	2764	C	N3-C4-C5	7.83	125.03	121.90
36	5	2147	A	N1-C6-N6	7.83	123.30	118.60
1	6	308	C	C2-N3-C4	-7.83	115.98	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	776	U	N1-C2-N3	7.83	119.60	114.90
36	5	2572	C	C2-N1-C1'	7.83	127.41	118.80
36	5	2870	C	C2-N1-C1'	-7.82	110.20	118.80
36	5	216	G	C5-C6-O6	-7.82	123.91	128.60
36	5	922	U	N1-C2-N3	7.81	119.59	114.90
38	8	16	G	N1-C6-O6	7.81	124.59	119.90
36	1	2606	G	N3-C2-N2	7.81	125.37	119.90
40	l3	102	LEU	CA-CB-CG	7.80	133.24	115.30
1	2	1560	U	N3-C2-O2	-7.80	116.74	122.20
36	1	421	G	C4-C5-N7	7.80	113.92	110.80
36	5	3095	U	N3-C2-O2	-7.79	116.74	122.20
36	1	3362	A	C5-N7-C8	-7.79	100.00	103.90
36	1	2409	G	N3-C2-N2	7.78	125.35	119.90
53	M7	3	ARG	NE-CZ-NH2	-7.78	116.41	120.30
36	5	3362	A	C6-C5-N7	-7.78	126.86	132.30
1	6	630	A	C2-N3-C4	-7.77	106.71	110.60
1	2	74	U	O5'-P-OP1	-7.77	98.70	105.70
36	1	2960	C	O5'-P-OP2	-7.77	98.71	105.70
38	4	120	C	N1-C2-O2	-7.77	114.24	118.90
36	5	2618	G	C5-C6-N1	7.76	115.38	111.50
37	7	101	G	N1-C6-O6	7.76	124.56	119.90
36	1	2283	G	N3-C2-N2	-7.76	114.47	119.90
36	5	974	G	N3-C4-C5	-7.75	124.72	128.60
1	2	1096	C	N3-C2-O2	-7.75	116.47	121.90
36	5	2255	A	O5'-P-OP1	-7.75	98.72	105.70
36	5	2980	U	N3-C2-O2	-7.75	116.77	122.20
36	5	2985	C	C5-C6-N1	7.75	124.88	121.00
36	1	2165	G	O5'-P-OP2	-7.75	98.73	105.70
36	1	957	C	O5'-P-OP2	-7.75	98.73	105.70
1	6	308	C	C5-C6-N1	-7.75	117.13	121.00
36	5	1918	C	O5'-P-OP2	-7.74	98.73	105.70
36	1	1858	A	N1-C6-N6	7.74	123.24	118.60
36	1	3362	A	N1-C6-N6	7.74	123.24	118.60
1	2	639	U	N1-C2-O2	7.74	128.22	122.80
36	1	1145	G	N1-C6-O6	7.74	124.54	119.90
36	5	3190	C	C6-N1-C2	-7.74	117.21	120.30
36	1	1127	G	N1-C6-O6	7.73	124.54	119.90
36	5	2872	A	O5'-P-OP1	7.73	119.98	110.70
36	1	1103	A	O5'-P-OP2	7.73	119.98	110.70
36	5	776	U	C5-C6-N1	-7.73	118.83	122.70
1	6	543	C	N1-C2-O2	7.73	123.54	118.90
1	2	75	U	N1-C2-O2	7.72	128.21	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	47	A	O5'-P-OP1	-7.72	98.75	105.70
36	5	2726	C	N1-C2-N3	7.72	124.60	119.20
36	5	341	G	C5-C6-O6	-7.71	123.97	128.60
36	1	1116	G	O5'-P-OP1	-7.71	98.76	105.70
36	1	2885	C	C6-N1-C2	7.71	123.39	120.30
36	1	278	U	N1-C2-O2	-7.71	117.40	122.80
1	2	139	C	P-O3'-C3'	7.70	128.94	119.70
36	1	1669	C	C6-N1-C2	7.70	123.38	120.30
36	1	1434	G	N1-C6-O6	7.70	124.52	119.90
36	1	1443	G	C8-N9-C4	-7.69	103.32	106.40
36	1	651	G	N3-C4-N9	7.68	130.61	126.00
36	5	676	G	N9-C4-C5	7.68	108.47	105.40
36	5	3052	G	N3-C4-N9	-7.68	121.39	126.00
36	1	1367	G	C5-C6-O6	-7.68	123.99	128.60
36	1	2640	A	C6-N1-C2	-7.68	113.99	118.60
36	5	2531	C	N1-C2-O2	7.68	123.51	118.90
36	1	421	G	N3-C4-N9	7.67	130.60	126.00
36	1	350	C	N3-C2-O2	-7.67	116.53	121.90
36	1	2633	U	OP1-P-O3'	7.67	122.07	105.20
36	1	2996	U	C6-N1-C1'	-7.66	110.47	121.20
38	4	113	U	C4-C5-C6	7.66	124.30	119.70
37	7	37	G	C5-C6-O6	-7.66	124.00	128.60
36	1	1556	C	C6-N1-C2	-7.66	117.24	120.30
36	5	1897	G	C4-C5-N7	7.66	113.86	110.80
36	5	2402	A	N9-C4-C5	7.66	108.86	105.80
36	1	2812	C	C5-C6-N1	-7.66	117.17	121.00
1	6	1085	G	O5'-P-OP1	-7.65	98.81	105.70
36	1	344	A	N1-C6-N6	-7.65	114.01	118.60
36	1	1116	G	C8-N9-C4	-7.65	103.34	106.40
36	5	2148	U	N3-C2-O2	7.65	127.55	122.20
36	5	3052	G	N9-C4-C5	7.64	108.46	105.40
36	1	2886	U	N3-C4-O4	7.64	124.75	119.40
36	5	934	G	C6-C5-N7	-7.63	125.82	130.40
36	5	3218	A	C4-C5-N7	7.63	114.51	110.70
36	1	716	A	C4-C5-N7	7.62	114.51	110.70
1	6	1634	C	C6-N1-C2	-7.61	117.26	120.30
36	1	979	U	N3-C2-O2	-7.61	116.88	122.20
36	1	3217	C	N3-C2-O2	-7.61	116.58	121.90
36	5	840	C	C6-N1-C2	-7.60	117.26	120.30
36	1	2621	G	O5'-P-OP1	7.60	119.82	110.70
36	1	1589	A	O4'-C1'-N9	-7.60	102.12	108.20
1	6	609	U	N3-C4-O4	-7.60	114.08	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	922	U	C5-C6-N1	-7.60	118.90	122.70
36	1	3217	C	C2-N1-C1'	7.59	127.16	118.80
1	6	139	C	N3-C2-O2	-7.59	116.58	121.90
1	6	558	U	N1-C2-O2	7.59	128.12	122.80
36	1	895	A	C6-C5-N7	-7.59	126.99	132.30
36	1	2397	A	C5-C6-N6	-7.59	117.63	123.70
36	5	709	A	O5'-P-OP1	-7.59	98.87	105.70
36	1	2642	A	C5-C6-N1	-7.59	113.91	117.70
36	5	3218	A	C5-N7-C8	-7.59	100.11	103.90
18	C6	40	GLU	C-N-CD	-7.59	103.91	120.60
1	6	337	G	C4-N9-C1'	7.59	136.36	126.50
36	5	622	A	N9-C4-C5	-7.59	102.77	105.80
36	5	908	G	C5-C6-O6	-7.59	124.05	128.60
36	5	1879	A	C4-C5-N7	7.58	114.49	110.70
36	5	2871	G	O5'-P-OP2	-7.58	98.88	105.70
41	L4	327	LEU	CA-CB-CG	7.58	132.74	115.30
1	6	194	U	C2-N1-C1'	7.58	126.80	117.70
36	5	921	A	O5'-P-OP2	-7.58	98.88	105.70
36	1	2601	A	C8-N9-C4	7.58	108.83	105.80
36	5	2403	G	O5'-P-OP1	7.58	119.79	110.70
36	1	958	C	N3-C4-C5	7.58	124.93	121.90
1	6	1657	U	N1-C2-O2	7.57	128.10	122.80
36	1	2305	G	C5-C6-O6	-7.57	124.06	128.60
36	1	3318	G	C4-N9-C1'	7.57	136.34	126.50
36	5	1710	C	C6-N1-C2	7.57	123.33	120.30
36	1	2798	C	N3-C4-C5	-7.56	118.87	121.90
36	5	2278	C	C5-C6-N1	7.56	124.78	121.00
1	6	1634	C	N1-C2-O2	7.56	123.44	118.90
36	1	2131	A	O5'-P-OP2	-7.56	98.90	105.70
1	6	858	G	O4'-C1'-N9	7.56	114.25	108.20
36	5	2872	A	O5'-P-OP2	-7.56	98.90	105.70
36	1	3306	U	N3-C2-O2	-7.55	116.91	122.20
36	1	2606	G	N1-C2-N2	-7.55	109.40	116.20
38	4	113	U	C5-C6-N1	-7.55	118.92	122.70
36	5	546	C	N3-C2-O2	-7.55	116.61	121.90
36	5	1209	G	N1-C6-O6	-7.55	115.37	119.90
36	1	2808	A	N1-C6-N6	7.55	123.13	118.60
37	7	87	G	C5-C6-O6	-7.55	124.07	128.60
36	5	1113	G	C2-N3-C4	-7.54	108.13	111.90
36	5	2142	A	C6-N1-C2	-7.54	114.07	118.60
36	5	2421	U	N1-C2-N3	7.54	119.42	114.90
36	5	2870	C	C6-N1-C1'	7.54	129.85	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2400	G	O5'-P-OP1	-7.54	98.92	105.70
1	2	558	U	N1-C2-O2	7.53	128.07	122.80
36	1	645	A	C5-C6-N1	7.53	121.47	117.70
36	1	1312	C	N1-C2-O2	-7.53	114.38	118.90
36	1	1445	U	C2-N3-C4	-7.53	122.48	127.00
36	5	934	G	C4-N9-C1'	7.53	136.29	126.50
36	1	835	G	O4'-C1'-N9	7.53	114.22	108.20
36	1	2359	C	N3-C4-C5	7.52	124.91	121.90
36	5	2113	A	C8-N9-C4	7.52	108.81	105.80
36	5	2956	A	O5'-P-OP1	-7.52	98.93	105.70
36	1	1849	C	N1-C2-O2	-7.52	114.39	118.90
36	1	1149	G	C5-C6-O6	-7.52	124.09	128.60
36	5	2246	G	O5'-P-OP2	7.52	119.72	110.70
36	5	1483	G	O4'-C1'-N9	7.52	114.21	108.20
36	1	1902	G	N1-C6-O6	7.51	124.41	119.90
1	6	1473	U	N3-C2-O2	-7.51	116.94	122.20
36	1	2302	G	C5-C6-O6	7.51	133.11	128.60
1	6	1634	C	C5-C6-N1	7.51	124.75	121.00
36	5	2796	G	O5'-P-OP2	-7.51	98.94	105.70
36	5	358	G	O5'-P-OP2	-7.50	98.95	105.70
36	5	1134	G	O5'-P-OP2	-7.50	98.95	105.70
36	5	2398	A	N7-C8-N9	-7.50	110.05	113.80
1	6	782	U	N3-C2-O2	-7.50	116.95	122.20
36	5	2426	U	N1-C2-O2	7.50	128.05	122.80
1	6	371	G	C5-C6-O6	-7.49	124.11	128.60
36	5	3092	C	O4'-C1'-N1	7.49	114.19	108.20
36	5	3216	G	O5'-P-OP2	-7.49	98.96	105.70
36	1	1197	A	C5-C6-N6	-7.49	117.71	123.70
36	5	3306	U	O5'-P-OP2	-7.49	98.96	105.70
36	1	357	A	O5'-P-OP2	-7.48	98.97	105.70
36	5	2954	U	N3-C2-O2	-7.48	116.96	122.20
36	5	929	A	O5'-P-OP2	-7.48	98.97	105.70
10	S8	29	LEU	CA-CB-CG	7.48	132.50	115.30
36	5	3154	C	C2-N1-C1'	7.48	127.03	118.80
36	5	2371	G	N9-C4-C5	-7.47	102.41	105.40
36	1	282	G	C8-N9-C4	-7.47	103.41	106.40
36	1	648	C	O5'-P-OP1	-7.47	98.98	105.70
36	5	942	U	N3-C4-O4	7.46	124.62	119.40
36	1	2869	U	O5'-P-OP1	-7.46	98.99	105.70
36	5	971	G	N7-C8-N9	-7.46	109.37	113.10
36	1	2418	G	OP1-P-O3'	7.46	121.61	105.20
36	1	2870	C	N3-C4-N4	-7.46	112.78	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2617	U	C2-N3-C4	-7.45	122.53	127.00
36	5	56	G	N1-C6-O6	-7.45	115.43	119.90
36	5	2189	U	O5'-P-OP1	-7.45	98.99	105.70
36	1	155	G	N3-C4-N9	7.45	130.47	126.00
38	4	20	U	C5-C6-N1	-7.45	118.98	122.70
36	5	1367	G	C8-N9-C1'	-7.45	117.32	127.00
1	6	609	U	N1-C2-N3	7.44	119.36	114.90
36	5	3014	U	C5-C4-O4	-7.44	121.44	125.90
36	5	2618	G	C6-N1-C2	-7.44	120.64	125.10
36	5	419	G	C5-C6-O6	-7.43	124.14	128.60
36	5	1309	U	O5'-P-OP1	-7.43	99.01	105.70
36	5	2619	G	C5-C6-O6	-7.43	124.14	128.60
36	1	368	G	C6-C5-N7	-7.43	125.94	130.40
36	5	3047	U	N1-C2-O2	7.43	128.00	122.80
37	7	90	U	C6-N1-C2	7.43	125.46	121.00
36	5	1004	U	N1-C2-O2	7.43	128.00	122.80
36	5	2302	G	N1-C6-O6	-7.43	115.44	119.90
36	1	1604	G	C4-N9-C1'	7.42	136.15	126.50
36	1	2389	C	N3-C4-C5	7.42	124.87	121.90
36	5	2421	U	N1-C2-O2	-7.42	117.61	122.80
36	1	2640	A	C8-N9-C4	-7.42	102.83	105.80
36	5	1897	G	C5-C6-O6	-7.41	124.16	128.60
36	5	3309	G	N3-C4-C5	-7.41	124.90	128.60
36	5	987	U	O5'-P-OP1	-7.40	99.04	105.70
37	7	101	G	C6-C5-N7	-7.40	125.96	130.40
1	2	542	A	O4'-C1'-N9	7.40	114.12	108.20
36	1	3057	U	N3-C4-O4	-7.40	114.22	119.40
36	1	1443	G	N7-C8-N9	7.39	116.80	113.10
36	1	2403	G	O5'-P-OP2	-7.39	99.05	105.70
36	5	1152	G	C4-C5-C6	-7.39	114.36	118.80
36	5	776	U	C4-C5-C6	7.39	124.13	119.70
36	1	2417	U	C2-N3-C4	-7.39	122.57	127.00
36	1	2874	G	C8-N9-C4	-7.39	103.44	106.40
36	5	420	G	N3-C4-N9	7.38	130.43	126.00
36	5	984	G	C4-C5-C6	7.38	123.23	118.80
36	5	1468	A	N1-C6-N6	7.38	123.03	118.60
36	5	1886	A	O5'-P-OP2	-7.38	99.06	105.70
43	16	173	MET	CB-CG-SD	-7.38	90.27	112.40
1	2	453	U	N1-C2-O2	7.37	127.96	122.80
36	1	1520	G	C4-C5-N7	-7.37	107.85	110.80
36	5	3178	A	O5'-P-OP1	-7.37	99.07	105.70
36	1	2808	A	N9-C4-C5	-7.37	102.85	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2758	A	C8-N9-C4	-7.37	102.85	105.80
36	1	510	G	N1-C6-O6	7.36	124.32	119.90
1	6	163	G	C2-N3-C4	-7.36	108.22	111.90
36	1	1911	A	C5-C6-N6	-7.36	117.81	123.70
37	3	103	A	N1-C6-N6	7.36	123.02	118.60
36	5	2823	G	N9-C4-C5	-7.36	102.46	105.40
1	2	577	G	C4-C5-N7	7.36	113.74	110.80
36	5	1876	U	C5-C6-N1	7.36	126.38	122.70
1	2	1596	C	N1-C2-O2	7.35	123.31	118.90
38	4	103	G	N3-C4-C5	-7.35	124.92	128.60
36	5	2957	G	C5-C6-O6	-7.35	124.19	128.60
1	6	321	C	N1-C2-O2	7.35	123.31	118.90
36	5	2874	G	C5-C6-O6	7.35	133.01	128.60
36	1	1904	C	C5-C6-N1	7.35	124.67	121.00
36	1	2376	G	C4-C5-N7	7.34	113.74	110.80
36	5	805	G	C8-N9-C4	7.34	109.34	106.40
36	1	2383	C	C6-N1-C2	7.34	123.24	120.30
36	1	931	C	C6-N1-C2	7.34	123.24	120.30
1	6	119	A	C2-N3-C4	-7.33	106.93	110.60
1	6	866	G	C8-N9-C4	7.33	109.33	106.40
36	5	335	G	N1-C6-O6	-7.33	115.50	119.90
36	1	521	A	N9-C4-C5	-7.33	102.87	105.80
36	1	2777	G	C5-C6-O6	7.33	133.00	128.60
36	5	2115	G	N1-C6-O6	7.33	124.30	119.90
1	2	17	C	O5'-P-OP2	-7.32	99.11	105.70
36	1	2327	U	O5'-P-OP1	-7.32	99.11	105.70
36	1	3382	U	N1-C2-O2	7.32	127.93	122.80
36	5	966	U	C6-N1-C2	-7.32	116.61	121.00
12	C0	88	PRO	N-CA-CB	7.32	112.09	103.30
36	5	2231	C	O4'-C1'-N1	7.32	114.06	108.20
36	5	2147	A	C5-C6-N6	-7.32	117.84	123.70
36	1	1429	G	N3-C4-C5	-7.32	124.94	128.60
36	5	1083	G	O5'-P-OP1	-7.32	99.11	105.70
36	5	2281	A	C8-N9-C4	7.31	108.73	105.80
73	o7	65	ARG	NE-CZ-NH1	7.31	123.96	120.30
36	1	101	G	O4'-C1'-N9	7.31	114.05	108.20
36	1	307	A	O5'-P-OP2	-7.31	99.12	105.70
36	1	859	G	N3-C4-N9	7.31	130.39	126.00
36	5	1149	G	N3-C4-C5	-7.31	124.95	128.60
36	1	807	A	N1-C6-N6	7.30	122.98	118.60
36	5	3052	G	C4-C5-N7	-7.30	107.88	110.80
36	5	994	G	N3-C4-N9	7.30	130.38	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1004	U	N3-C2-O2	-7.30	117.09	122.20
36	5	1016	C	O5'-P-OP1	-7.30	99.13	105.70
36	1	54	C	N3-C4-C5	7.30	124.82	121.90
36	5	640	U	N1-C2-O2	-7.30	117.69	122.80
36	5	1370	G	N1-C6-O6	-7.29	115.52	119.90
36	1	1445	U	N1-C2-O2	-7.29	117.69	122.80
36	1	641	C	O4'-C1'-N1	7.29	114.03	108.20
36	1	984	G	C6-C5-N7	-7.29	126.03	130.40
36	1	1160	C	C2-N3-C4	7.29	123.55	119.90
38	8	96	A	C8-N9-C4	7.29	108.72	105.80
36	5	914	A	C2-N3-C4	-7.29	106.95	110.60
36	5	932	U	C5-C4-O4	-7.29	121.53	125.90
36	1	2899	C	C2-N1-C1'	7.29	126.82	118.80
36	5	2396	G	C8-N9-C4	-7.29	103.48	106.40
1	6	1031	U	C6-N1-C2	7.29	125.37	121.00
36	5	2948	C	N3-C4-C5	7.29	124.81	121.90
36	1	45	A	O5'-P-OP1	-7.28	99.15	105.70
36	5	645	A	C6-N1-C2	-7.28	114.23	118.60
36	5	2132	C	C6-N1-C2	-7.28	117.39	120.30
36	1	364	G	C5-C6-O6	-7.28	124.23	128.60
37	7	7	G	O5'-P-OP1	7.28	119.43	110.70
36	1	942	U	OP1-P-OP2	-7.27	108.69	119.60
36	1	979	U	N1-C2-N3	7.27	119.26	114.90
36	5	3107	U	OP2-P-O3'	7.27	121.20	105.20
36	5	3050	U	C5-C4-O4	7.27	130.26	125.90
36	5	641	C	C2-N3-C4	-7.27	116.27	119.90
36	5	1405	U	C5-C6-N1	-7.27	119.07	122.70
36	5	1316	C	N3-C4-N4	7.26	123.08	118.00
36	5	668	G	N1-C6-O6	-7.26	115.54	119.90
36	5	909	G	N1-C6-O6	-7.26	115.55	119.90
36	1	2397	A	C6-C5-N7	-7.26	127.22	132.30
36	5	875	G	N1-C6-O6	-7.25	115.55	119.90
36	1	859	G	N9-C4-C5	-7.25	102.50	105.40
1	6	438	A	O5'-P-OP1	-7.25	99.17	105.70
52	m6	94	ARG	NE-CZ-NH1	-7.25	116.67	120.30
36	1	2987	A	N1-C6-N6	7.25	122.95	118.60
1	6	957	G	N1-C6-O6	7.25	124.25	119.90
41	14	339	LEU	CA-CB-CG	7.25	131.97	115.30
1	6	957	G	C5-C6-N1	-7.25	107.88	111.50
1	2	110	U	N3-C2-O2	-7.24	117.13	122.20
36	1	2728	G	C2-N3-C4	7.24	115.52	111.90
36	5	2351	U	C6-N1-C2	-7.24	116.66	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1192	C	N1-C2-O2	7.24	123.24	118.90
38	4	108	C	N1-C2-O2	-7.24	114.56	118.90
36	5	2790	A	O5'-P-OP2	-7.24	99.19	105.70
36	5	2947	G	C8-N9-C4	7.24	109.30	106.40
36	5	3197	G	N3-C2-N2	-7.24	114.83	119.90
1	6	1614	A	N1-C6-N6	7.23	122.94	118.60
1	2	1596	C	N3-C2-O2	-7.23	116.84	121.90
36	1	2142	A	C6-N1-C2	-7.23	114.26	118.60
1	6	163	G	N3-C4-C5	7.23	132.21	128.60
36	5	1926	C	C6-N1-C2	7.23	123.19	120.30
36	1	2937	G	C8-N9-C4	7.22	109.29	106.40
1	6	163	G	N9-C4-C5	7.22	108.29	105.40
36	5	3026	G	C5-C6-O6	-7.22	124.27	128.60
36	1	2861	U	O5'-P-OP2	7.21	119.36	110.70
36	5	1001	G	O5'-P-OP1	-7.21	99.21	105.70
36	5	1316	C	C6-N1-C2	-7.21	117.41	120.30
36	1	1113	G	N9-C4-C5	7.21	108.28	105.40
36	1	2621	G	O5'-P-OP2	-7.21	99.21	105.70
36	5	347	G	N1-C6-O6	7.21	124.23	119.90
36	1	681	U	N3-C4-O4	7.21	124.45	119.40
36	1	2936	A	N1-C6-N6	-7.21	114.28	118.60
36	1	2150	G	C8-N9-C4	-7.21	103.52	106.40
36	5	2881	C	C6-N1-C2	7.21	123.18	120.30
36	1	1164	G	C5-C6-O6	7.20	132.92	128.60
24	d2	93	LEU	CA-CB-CG	7.20	131.87	115.30
36	1	3108	G	N1-C6-O6	-7.20	115.58	119.90
1	6	1789	G	N3-C4-N9	7.20	130.32	126.00
38	4	113	U	N3-C2-O2	-7.20	117.16	122.20
1	6	308	C	N3-C4-N4	-7.20	112.96	118.00
52	M6	78	ARG	NE-CZ-NH1	7.19	123.90	120.30
36	5	934	G	C5-C6-O6	-7.19	124.28	128.60
36	5	700	C	C6-N1-C2	7.19	123.18	120.30
36	5	2136	C	C5-C6-N1	-7.19	117.40	121.00
36	1	2339	C	C6-N1-C2	-7.19	117.42	120.30
36	1	2979	U	C5-C6-N1	-7.18	119.11	122.70
15	C3	22	ALA	C-N-CD	-7.18	104.80	120.60
36	5	3362	A	O4'-C1'-N9	7.18	113.95	108.20
36	5	3047	U	N3-C2-O2	-7.18	117.17	122.20
40	l3	4	ARG	NE-CZ-NH1	7.18	123.89	120.30
36	1	639	G	C5-C6-O6	-7.18	124.29	128.60
36	5	925	A	C8-N9-C4	7.17	108.67	105.80
37	3	88	G	N1-C6-O6	-7.17	115.60	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2827	U	C5-C6-N1	-7.17	119.11	122.70
36	1	1520	G	C5-N7-C8	7.17	107.89	104.30
1	2	1773	C	N3-C4-C5	-7.17	119.03	121.90
36	1	2846	U	N3-C4-O4	-7.17	114.38	119.40
36	1	1405	U	C5-C6-N1	-7.16	119.12	122.70
36	1	3183	A	N1-C6-N6	7.16	122.90	118.60
36	1	659	G	N1-C2-N2	-7.16	109.75	116.20
36	1	3108	G	C5-C6-O6	7.16	132.90	128.60
36	1	645	A	N3-C4-N9	7.16	133.13	127.40
36	1	2714	G	C5-N7-C8	-7.16	100.72	104.30
36	1	2983	C	N3-C4-N4	-7.16	112.99	118.00
36	5	984	G	N3-C4-C5	-7.16	125.02	128.60
36	5	2948	C	N3-C4-N4	-7.16	112.99	118.00
36	1	1858	A	C6-C5-N7	-7.16	127.29	132.30
36	5	546	C	C6-N1-C2	-7.16	117.44	120.30
36	5	3049	A	C8-N9-C4	7.16	108.66	105.80
36	5	984	G	C6-C5-N7	-7.16	126.11	130.40
36	5	2630	C	N1-C2-O2	-7.16	114.61	118.90
36	1	2935	U	O5'-P-OP2	-7.16	99.26	105.70
36	5	2948	C	C4-C5-C6	-7.16	113.82	117.40
36	1	793	C	N1-C2-O2	-7.15	114.61	118.90
36	1	2728	G	C5-C6-O6	-7.15	124.31	128.60
1	6	390	G	O5'-P-OP2	-7.15	99.26	105.70
36	5	283	G	C5-C6-O6	-7.15	124.31	128.60
36	5	2678	A	C5-C6-N6	7.15	129.42	123.70
36	1	1547	G	N7-C8-N9	-7.15	109.53	113.10
36	1	2936	A	O5'-P-OP2	7.15	119.28	110.70
36	5	1117	G	O5'-P-OP1	-7.14	99.27	105.70
36	1	226	C	N3-C4-C5	-7.14	119.04	121.90
36	1	2863	G	N3-C2-N2	7.14	124.90	119.90
36	5	880	G	C4-N9-C1'	-7.14	117.22	126.50
36	5	1116	G	C4-C5-N7	-7.14	107.94	110.80
36	5	2377	G	N7-C8-N9	-7.14	109.53	113.10
36	1	2162	U	N3-C4-C5	7.14	118.88	114.60
36	1	3344	A	C5-N7-C8	-7.14	100.33	103.90
1	6	1127	G	N1-C2-N3	7.14	128.18	123.90
36	1	1429	G	N3-C4-N9	7.13	130.28	126.00
36	1	1909	A	C8-N9-C4	7.13	108.65	105.80
36	5	877	C	C4-C5-C6	-7.13	113.83	117.40
36	5	644	G	C8-N9-C4	-7.13	103.55	106.40
1	6	782	U	N1-C2-O2	7.13	127.79	122.80
36	5	2813	A	C4-C5-C6	7.13	120.56	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	m1	112	LEU	CA-CB-CG	7.13	131.69	115.30
36	1	498	A	O5'-P-OP2	-7.12	99.29	105.70
36	5	1006	A	O5'-P-OP2	-7.12	99.29	105.70
36	5	2296	A	C5-C6-N6	-7.12	118.00	123.70
36	5	2411	U	C2-N3-C4	-7.12	122.73	127.00
36	5	361	A	C2-N3-C4	7.12	114.16	110.60
36	1	681	U	N1-C2-O2	-7.12	117.82	122.80
1	2	1745	G	O5'-P-OP2	-7.12	99.30	105.70
36	5	2989	U	C5-C6-N1	-7.12	119.14	122.70
36	1	2283	G	C5-C6-O6	-7.11	124.33	128.60
36	5	2572	C	N3-C2-O2	-7.11	116.92	121.90
36	5	1154	A	N1-C2-N3	-7.11	125.75	129.30
36	5	53	G	O5'-P-OP2	-7.11	99.30	105.70
36	5	3012	A	O5'-P-OP2	-7.11	99.30	105.70
37	3	90	U	C5-C4-O4	-7.11	121.64	125.90
36	5	2639	G	N1-C6-O6	7.11	124.16	119.90
36	5	712	G	O5'-P-OP2	-7.10	99.31	105.70
36	5	2345	A	N1-C6-N6	7.10	122.86	118.60
36	5	2411	U	N3-C4-C5	7.10	118.86	114.60
1	2	1600	A	C2-N3-C4	-7.10	107.05	110.60
36	5	3343	G	N3-C4-N9	7.10	130.26	126.00
36	1	646	A	N1-C2-N3	7.10	132.85	129.30
36	1	1428	A	C5-C6-N6	-7.09	118.03	123.70
36	1	1528	G	O5'-P-OP1	-7.09	99.32	105.70
36	1	1007	U	C5-C4-O4	-7.09	121.64	125.90
36	1	1421	G	C8-N9-C4	7.09	109.24	106.40
36	5	1112	A	O5'-P-OP1	-7.09	99.32	105.70
1	6	610	G	C8-N9-C1'	-7.09	117.78	127.00
36	1	1113	G	N3-C2-N2	-7.09	114.94	119.90
36	1	2942	C	C6-N1-C2	7.09	123.14	120.30
36	1	666	A	N1-C6-N6	-7.09	114.35	118.60
36	5	1311	G	O5'-P-OP2	-7.09	99.32	105.70
36	1	29	C	C6-N1-C2	7.08	123.13	120.30
36	5	2299	A	O5'-P-OP2	-7.08	99.33	105.70
36	1	2412	G	C8-N9-C4	-7.08	103.57	106.40
36	1	406	G	O5'-P-OP2	-7.08	99.33	105.70
36	1	1137	C	O5'-P-OP2	-7.08	99.33	105.70
36	1	2818	U	C5-C6-N1	7.08	126.24	122.70
36	5	1329	U	C2-N3-C4	-7.08	122.75	127.00
36	5	439	C	C4-C5-C6	7.07	120.94	117.40
36	1	709	A	N7-C8-N9	-7.07	110.26	113.80
36	1	2169	G	C6-C5-N7	7.07	134.64	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	32	C	N3-C4-C5	7.07	124.73	121.90
36	5	609	G	N3-C2-N2	-7.07	114.95	119.90
36	5	2145	A	N1-C2-N3	7.07	132.84	129.30
1	6	1145	U	N1-C2-O2	-7.06	117.86	122.80
36	1	2359	C	C5-C4-N4	-7.06	115.26	120.20
1	6	1645	G	N1-C6-O6	-7.06	115.67	119.90
36	5	2986	U	C5-C4-O4	-7.06	121.66	125.90
36	1	329	U	N1-C2-N3	7.06	119.13	114.90
36	1	1142	G	C5-C6-N1	7.06	115.03	111.50
36	1	1437	C	C6-N1-C2	-7.05	117.48	120.30
1	6	308	C	C2-N1-C1'	-7.05	111.04	118.80
1	6	957	G	N3-C2-N2	-7.05	114.97	119.90
36	1	672	A	N1-C6-N6	7.05	122.83	118.60
36	5	1169	A	C5-C6-N1	-7.05	114.18	117.70
36	1	426	G	N3-C4-N9	7.04	130.23	126.00
36	1	2634	U	N1-C2-N3	7.04	119.12	114.90
1	6	301	A	O5'-P-OP2	-7.04	99.36	105.70
1	6	453	U	C5-C4-O4	7.04	130.12	125.90
36	5	1152	G	C5-C6-O6	-7.04	124.38	128.60
36	5	694	C	C6-N1-C2	-7.04	117.48	120.30
36	5	1848	G	C5-C6-O6	-7.04	124.38	128.60
36	5	3060	C	N1-C2-O2	-7.03	114.68	118.90
36	1	1852	G	N1-C6-O6	7.03	124.12	119.90
1	6	163	G	C8-N9-C4	-7.03	103.59	106.40
36	1	770	G	O4'-C1'-N9	7.03	113.82	108.20
36	1	2831	G	N1-C6-O6	7.03	124.12	119.90
36	1	1849	C	N3-C2-O2	7.03	126.82	121.90
36	1	2643	A	C8-N9-C4	7.03	108.61	105.80
36	5	200	C	C2-N3-C4	7.03	123.41	119.90
36	1	3036	G	N3-C4-C5	-7.02	125.09	128.60
1	2	1747	G	N1-C6-O6	7.02	124.11	119.90
36	1	1279	C	C6-N1-C2	-7.02	117.49	120.30
50	M4	135	LEU	CA-CB-CG	7.02	131.45	115.30
1	6	1581	C	N3-C4-C5	7.02	124.71	121.90
36	5	1316	C	N1-C2-O2	-7.02	114.69	118.90
1	6	1657	U	C5-C6-N1	7.02	126.21	122.70
36	5	1190	A	N7-C8-N9	7.01	117.31	113.80
36	5	1328	C	N3-C4-C5	-7.01	119.09	121.90
36	1	580	C	N1-C2-O2	-7.01	114.69	118.90
36	5	216	G	N1-C6-O6	7.01	124.11	119.90
38	4	109	A	N9-C4-C5	-7.01	103.00	105.80
36	5	889	U	N3-C4-C5	7.00	118.80	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2957	G	N1-C6-O6	7.00	124.10	119.90
36	5	1879	A	C5-C6-N6	-7.00	118.10	123.70
36	1	2393	G	C5-C6-O6	-7.00	124.40	128.60
36	5	1158	A	C5-C6-N6	-7.00	118.10	123.70
36	5	1592	G	C8-N9-C4	-7.00	103.60	106.40
36	5	2891	U	N3-C4-C5	7.00	118.80	114.60
36	1	946	U	N3-C2-O2	-7.00	117.30	122.20
36	5	1878	G	C4-N9-C1'	7.00	135.60	126.50
1	6	1739	C	N1-C2-O2	-7.00	114.70	118.90
36	5	2371	G	C8-N9-C4	6.99	109.20	106.40
1	6	795	U	N3-C2-O2	-6.99	117.31	122.20
36	5	523	A	N1-C6-N6	-6.99	114.41	118.60
36	5	907	G	N9-C4-C5	-6.99	102.61	105.40
1	6	337	G	C8-N9-C1'	-6.99	117.92	127.00
36	5	3285	C	C2-N1-C1'	6.99	126.49	118.80
36	1	805	G	C8-N9-C4	6.99	109.19	106.40
36	1	1489	A	N1-C6-N6	6.99	122.79	118.60
36	1	573	C	C2-N3-C4	-6.98	116.41	119.90
36	1	968	G	C2-N3-C4	6.98	115.39	111.90
36	5	609	G	N1-C6-O6	6.98	124.09	119.90
36	5	2145	A	C6-N1-C2	-6.98	114.41	118.60
36	1	1394	A	OP2-P-O3'	6.98	120.55	105.20
1	2	1389	C	N1-C2-O2	6.98	123.09	118.90
36	1	33	G	N1-C6-O6	6.97	124.08	119.90
36	5	2366	C	C5-C6-N1	6.97	124.49	121.00
1	2	507	U	C2-N1-C1'	6.97	126.06	117.70
36	1	939	U	C2-N1-C1'	-6.97	109.33	117.70
36	5	2234	G	C8-N9-C4	6.97	109.19	106.40
36	1	922	U	N3-C2-O2	-6.97	117.32	122.20
36	1	2874	G	N1-C2-N3	6.96	128.08	123.90
1	6	1581	C	C6-N1-C2	6.96	123.08	120.30
36	5	869	G	C5-C6-N1	6.96	114.98	111.50
36	5	2398	A	C4-C5-N7	-6.96	107.22	110.70
36	1	936	A	N1-C6-N6	6.96	122.77	118.60
36	5	39	A	C8-N9-C4	6.96	108.58	105.80
36	5	1158	A	C4-C5-N7	6.96	114.18	110.70
39	12	190	ARG	NE-CZ-NH1	-6.96	116.82	120.30
36	5	1321	G	N1-C6-O6	6.95	124.07	119.90
36	5	1520	G	N1-C6-O6	6.95	124.07	119.90
36	5	3183	A	N1-C6-N6	6.95	122.77	118.60
35	SM	134	ASP	CB-CA-C	-6.95	96.50	110.40
59	n3	45	ARG	NE-CZ-NH1	-6.95	116.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2362	C	N1-C2-O2	6.95	123.07	118.90
36	5	2117	A	N1-C6-N6	-6.95	114.43	118.60
36	5	2869	U	C2-N1-C1'	6.95	126.03	117.70
36	5	3136	G	C6-C5-N7	-6.95	126.23	130.40
36	1	940	G	C5-C6-N1	6.94	114.97	111.50
36	1	1604	G	N3-C4-C5	-6.94	125.13	128.60
1	6	1075	C	N3-C2-O2	6.94	126.76	121.90
36	1	2606	G	C6-C5-N7	-6.93	126.24	130.40
36	1	1147	G	C5-N7-C8	6.93	107.77	104.30
36	1	2659	G	N1-C6-O6	6.93	124.06	119.90
1	6	942	G	C8-N9-C4	-6.93	103.63	106.40
36	5	804	C	C4-C5-C6	6.93	120.86	117.40
36	5	2978	U	N3-C2-O2	-6.92	117.35	122.20
36	1	859	G	C6-C5-N7	-6.92	126.25	130.40
36	1	1891	A	C8-N9-C4	6.92	108.57	105.80
36	1	3069	G	O5'-P-OP2	-6.92	99.47	105.70
36	1	116	A	O4'-C1'-N9	6.92	113.73	108.20
37	7	74	C	N1-C2-O2	-6.91	114.75	118.90
36	5	3339	A	N1-C6-N6	6.91	122.75	118.60
36	1	407	A	N1-C6-N6	6.91	122.75	118.60
1	6	1535	U	N3-C2-O2	-6.91	117.36	122.20
36	5	3211	C	C6-N1-C2	6.91	123.06	120.30
36	5	2286	U	N3-C2-O2	-6.91	117.36	122.20
36	5	672	A	C8-N9-C4	-6.90	103.04	105.80
36	5	3052	G	C5-C6-O6	6.90	132.74	128.60
36	1	1434	G	C5-C6-O6	-6.90	124.46	128.60
1	6	371	G	N1-C6-O6	6.90	124.04	119.90
36	5	868	C	C6-N1-C2	6.90	123.06	120.30
36	5	2211	U	C4-C5-C6	6.90	123.84	119.70
36	5	2823	G	C6-C5-N7	-6.90	126.26	130.40
36	5	2871	G	N3-C4-C5	-6.90	125.15	128.60
1	2	1761	U	C6-N1-C2	-6.89	116.86	121.00
36	1	2986	U	N1-C2-N3	6.89	119.04	114.90
36	5	580	C	C6-N1-C2	-6.89	117.54	120.30
36	1	859	G	C8-N9-C1'	-6.89	118.04	127.00
36	5	2606	G	C8-N9-C4	-6.89	103.65	106.40
36	5	1324	U	C5-C6-N1	-6.88	119.26	122.70
36	5	3245	A	C5-C6-N1	-6.88	114.26	117.70
36	1	3374	U	C5-C4-O4	-6.88	121.77	125.90
36	5	2979	U	O5'-P-OP1	-6.88	99.51	105.70
36	1	66	A	O5'-P-OP1	-6.88	99.51	105.70
36	5	2757	U	N3-C2-O2	-6.88	117.39	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2305	G	C6-C5-N7	-6.88	126.28	130.40
36	1	2818	U	O5'-P-OP2	-6.88	99.51	105.70
36	1	1115	G	C8-N9-C4	-6.87	103.65	106.40
36	5	36	C	C5-C6-N1	6.87	124.44	121.00
36	5	2168	A	O5'-P-OP2	-6.87	99.52	105.70
36	1	1182	A	O5'-P-OP1	-6.87	99.52	105.70
36	1	3209	A	N1-C6-N6	6.87	122.72	118.60
1	2	192	U	C2-N1-C1'	6.87	125.94	117.70
36	1	2305	G	N1-C6-O6	6.87	124.02	119.90
36	5	636	C	N3-C4-C5	6.87	124.65	121.90
36	5	2393	G	C2-N3-C4	6.87	115.33	111.90
36	5	1101	G	C5-C6-O6	6.87	132.72	128.60
36	1	922	U	C5-C4-O4	6.86	130.02	125.90
36	5	3080	G	N1-C6-O6	6.86	124.02	119.90
36	1	2714	G	C4-C5-N7	6.86	113.54	110.80
36	1	1131	G	C8-N9-C4	6.86	109.14	106.40
36	5	1884	A	OP2-P-O3'	6.86	120.28	105.20
36	1	3344	A	C2-N3-C4	-6.85	107.17	110.60
1	6	977	A	N1-C6-N6	6.85	122.71	118.60
1	6	308	C	C6-N1-C1'	6.85	129.02	120.80
37	7	45	A	O5'-P-OP2	-6.85	99.53	105.70
36	5	3092	C	N1-C2-O2	6.85	123.01	118.90
36	5	1178	G	OP2-P-O3'	6.85	120.26	105.20
36	5	2931	C	C5-C4-N4	-6.84	115.41	120.20
36	1	278	U	N1-C2-N3	6.84	119.00	114.90
1	6	158	U	P-O3'-C3'	6.84	127.91	119.70
36	1	3184	A	O5'-P-OP1	-6.84	99.55	105.70
36	5	3027	A	N9-C4-C5	-6.84	103.06	105.80
36	1	2329	C	O5'-P-OP2	-6.84	99.55	105.70
36	1	2777	G	C8-N9-C4	-6.84	103.67	106.40
36	1	3344	A	C8-N9-C4	-6.83	103.07	105.80
38	4	30	C	O5'-P-OP1	-6.83	99.55	105.70
36	1	1492	G	N7-C8-N9	-6.83	109.68	113.10
36	5	884	A	C2-N3-C4	-6.83	107.19	110.60
36	5	1049	C	N3-C4-C5	6.83	124.63	121.90
36	5	1370	G	N3-C2-N2	6.83	124.68	119.90
36	5	2794	G	C5-C6-N1	6.83	114.91	111.50
36	5	2813	A	C8-N9-C4	-6.83	103.07	105.80
36	5	3368	U	C2-N1-C1'	-6.83	109.51	117.70
36	1	2144	A	N3-C4-N9	6.82	132.86	127.40
36	1	2305	G	N3-C4-N9	6.82	130.09	126.00
36	1	3242	G	C8-N9-C4	6.82	109.13	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2138	A	C2-N3-C4	-6.82	107.19	110.60
36	5	1365	G	C6-C5-N7	-6.82	126.31	130.40
35	SM	167	PRO	N-CA-CB	6.82	111.48	103.30
37	7	40	C	N3-C2-O2	6.82	126.67	121.90
36	1	939	U	N1-C2-O2	-6.82	118.03	122.80
36	1	1367	G	C6-C5-N7	-6.82	126.31	130.40
1	2	1652	C	C6-N1-C2	-6.81	117.57	120.30
36	5	38	U	C5-C4-O4	-6.81	121.81	125.90
37	7	79	A	N1-C6-N6	6.81	122.69	118.60
36	1	577	C	N1-C2-O2	-6.81	114.81	118.90
36	1	1409	G	C5-C6-O6	6.81	132.69	128.60
36	5	971	G	C5-N7-C8	6.81	107.70	104.30
36	1	1516	C	N1-C2-O2	-6.81	114.81	118.90
36	5	892	U	N3-C4-O4	-6.81	114.64	119.40
36	5	368	G	C5-C6-O6	6.80	132.68	128.60
38	4	43	A	O5'-P-OP1	-6.80	99.58	105.70
36	5	37	U	N1-C2-N3	6.80	118.98	114.90
36	5	1152	G	C5-C6-N1	-6.80	108.10	111.50
1	2	934	C	C2-N1-C1'	6.80	126.28	118.80
36	1	984	G	N3-C4-N9	6.79	130.08	126.00
36	5	1805	C	C6-N1-C2	6.79	123.02	120.30
36	1	2978	U	O4'-C1'-N1	6.79	113.63	108.20
36	5	934	G	C8-N9-C1'	-6.79	118.17	127.00
38	4	37	A	C8-N9-C4	-6.79	103.08	105.80
36	1	716	A	C5-C6-N6	-6.78	118.27	123.70
36	1	2397	A	C4-C5-N7	6.78	114.09	110.70
1	6	421	A	N1-C6-N6	6.78	122.67	118.60
1	6	452	A	N1-C6-N6	6.78	122.67	118.60
36	1	65	A	P-O3'-C3'	6.78	127.83	119.70
36	1	1197	A	N9-C4-C5	-6.78	103.09	105.80
36	1	1421	G	N7-C8-N9	-6.78	109.71	113.10
36	5	952	A	O5'-P-OP2	-6.78	99.60	105.70
36	5	1170	A	N1-C6-N6	6.78	122.67	118.60
36	1	782	U	N3-C4-C5	6.78	118.67	114.60
1	2	704	C	N1-C2-O2	6.77	122.97	118.90
36	1	1127	G	C5-C6-O6	-6.77	124.54	128.60
36	5	83	U	N3-C2-O2	-6.77	117.46	122.20
37	7	37	G	N3-C4-N9	6.77	130.06	126.00
36	1	961	C	C5-C6-N1	-6.77	117.62	121.00
36	5	800	G	C8-N9-C4	6.77	109.11	106.40
36	1	1838	G	C6-C5-N7	-6.76	126.34	130.40
36	1	3143	C	N1-C2-O2	-6.76	114.84	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	349	U	O5'-P-OP2	-6.76	99.61	105.70
1	6	1568	C	C6-N1-C2	-6.76	117.59	120.30
36	5	2704	A	N1-C6-N6	6.76	122.66	118.60
1	2	507	U	N1-C2-O2	6.76	127.53	122.80
36	1	30	G	N1-C6-O6	-6.76	115.84	119.90
36	1	421	G	N9-C4-C5	-6.76	102.70	105.40
36	1	2276	G	C8-N9-C4	-6.76	103.70	106.40
36	5	2404	A	N1-C6-N6	6.76	122.66	118.60
36	1	959	C	N3-C4-C5	6.76	124.60	121.90
36	5	2113	A	N7-C8-N9	-6.76	110.42	113.80
36	1	573	C	C5-C6-N1	-6.75	117.62	121.00
36	1	2867	C	C5-C6-N1	-6.75	117.62	121.00
36	5	357	A	O5'-P-OP2	-6.75	99.62	105.70
36	1	2642	A	N1-C2-N3	-6.75	125.92	129.30
1	6	1514	U	N3-C4-O4	-6.75	114.67	119.40
36	5	3260	G	C5-C6-O6	6.75	132.65	128.60
36	5	660	A	N7-C8-N9	-6.75	110.42	113.80
1	2	558	U	N3-C2-O2	-6.75	117.48	122.20
36	1	921	A	O4'-C1'-N9	-6.75	102.80	108.20
36	1	2376	G	N7-C8-N9	6.75	116.47	113.10
36	5	3049	A	N7-C8-N9	-6.75	110.43	113.80
36	5	1209	G	N9-C4-C5	6.75	108.10	105.40
20	c8	15	LEU	CA-CB-CG	6.74	130.81	115.30
36	5	45	A	C6-N1-C2	-6.74	114.56	118.60
36	1	2247	G	N1-C6-O6	6.74	123.94	119.90
1	6	350	U	C5-C6-N1	-6.74	119.33	122.70
36	5	2794	G	C5-C6-O6	-6.74	124.56	128.60
37	7	110	G	O5'-P-OP2	-6.73	99.64	105.70
36	1	1103	A	O5'-P-OP1	-6.73	99.64	105.70
36	5	2884	C	C5-C4-N4	-6.73	115.49	120.20
36	1	1153	A	N1-C6-N6	6.73	122.64	118.60
36	1	1312	C	N3-C2-O2	6.73	126.61	121.90
1	6	558	U	N3-C2-O2	-6.73	117.49	122.20
36	5	424	G	C2-N3-C4	6.73	115.27	111.90
36	5	1888	U	C2-N3-C4	-6.73	122.96	127.00
36	1	911	C	C2-N3-C4	-6.73	116.53	119.90
36	1	701	G	N3-C2-N2	-6.73	115.19	119.90
36	5	384	A	N7-C8-N9	-6.73	110.44	113.80
36	5	1876	U	C6-N1-C2	-6.73	116.97	121.00
36	1	1161	G	O5'-P-OP1	-6.72	99.65	105.70
36	5	1738	C	N1-C2-O2	-6.72	114.87	118.90
36	5	2869	U	N1-C2-O2	6.72	127.51	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	797	U	OP1-P-OP2	-6.72	109.52	119.60
36	1	2322	C	N3-C4-C5	6.72	124.59	121.90
36	5	3141	A	N1-C2-N3	6.72	132.66	129.30
36	1	639	G	O5'-P-OP1	6.72	118.76	110.70
36	1	1492	G	C4-C5-N7	-6.72	108.11	110.80
36	5	2327	U	C5-C6-N1	-6.72	119.34	122.70
1	6	858	G	C4-C5-N7	6.72	113.49	110.80
1	6	371	G	N9-C4-C5	-6.71	102.71	105.40
36	5	2965	U	N1-C2-O2	-6.71	118.10	122.80
36	1	3382	U	N3-C2-O2	-6.71	117.50	122.20
36	1	917	A	N1-C6-N6	-6.71	114.58	118.60
36	5	2142	A	OP1-P-O3'	6.71	119.96	105.20
36	1	42	C	C6-N1-C2	-6.71	117.62	120.30
36	1	397	A	O4'-C1'-N9	6.71	113.57	108.20
36	5	861	C	C6-N1-C2	6.71	122.98	120.30
36	5	1898	G	O4'-C1'-N9	6.71	113.56	108.20
36	5	2330	C	O5'-P-OP2	-6.70	99.67	105.70
38	8	100	U	C2-N1-C1'	6.70	125.74	117.70
37	7	89	G	N3-C2-N2	6.70	124.59	119.90
1	6	1596	C	N3-C2-O2	-6.70	117.21	121.90
62	N6	13	ARG	NE-CZ-NH2	-6.70	116.95	120.30
36	5	1200	A	N9-C4-C5	6.70	108.48	105.80
36	1	2642	A	C8-N9-C4	6.70	108.48	105.80
36	1	281	G	N3-C2-N2	-6.69	115.21	119.90
38	4	109	A	C4-C5-N7	6.69	114.05	110.70
36	5	420	G	C5-C6-O6	-6.69	124.58	128.60
36	1	1296	C	C6-N1-C2	-6.69	117.62	120.30
36	1	1366	A	C5-N7-C8	-6.69	100.56	103.90
36	5	2133	U	N3-C4-O4	-6.69	114.72	119.40
36	5	2350	C	O5'-P-OP1	6.69	118.73	110.70
36	5	3141	A	C4-C5-C6	6.69	120.34	117.00
37	3	95	A	N1-C6-N6	6.69	122.61	118.60
36	5	1370	G	N1-C2-N2	-6.69	110.18	116.20
36	5	2234	G	N9-C4-C5	-6.69	102.72	105.40
36	1	1116	G	C6-C5-N7	-6.69	126.39	130.40
36	1	2244	A	O5'-P-OP1	6.69	118.73	110.70
1	6	1145	U	N3-C4-O4	6.69	124.08	119.40
36	1	3101	G	N1-C6-O6	-6.68	115.89	119.90
36	1	2874	G	C4-C5-N7	-6.68	108.13	110.80
36	5	1370	G	N3-C4-N9	6.68	130.01	126.00
36	5	1452	A	C8-N9-C4	6.68	108.47	105.80
36	1	796	U	OP2-P-O3'	6.67	119.89	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1405	U	C2-N3-C4	-6.67	123.00	127.00
36	5	2622	C	N3-C4-C5	-6.67	119.23	121.90
38	8	19	C	N3-C4-C5	-6.67	119.23	121.90
36	1	426	G	C8-N9-C1'	-6.67	118.33	127.00
38	4	47	C	N3-C2-O2	-6.67	117.23	121.90
36	5	838	G	C5-C6-O6	6.67	132.60	128.60
36	1	648	C	C2-N1-C1'	6.67	126.14	118.80
36	1	1134	G	C5-C6-O6	-6.67	124.60	128.60
36	5	2350	C	N1-C2-O2	-6.67	114.90	118.90
36	1	1373	A	O5'-P-OP2	-6.66	99.71	105.70
36	1	3217	C	N1-C2-O2	6.66	122.90	118.90
36	1	283	G	O4'-C1'-N9	-6.66	102.87	108.20
36	1	890	C	C6-N1-C2	-6.66	117.64	120.30
36	5	2133	U	N3-C4-C5	6.66	118.59	114.60
36	1	2859	U	C4-C5-C6	6.66	123.69	119.70
1	6	1100	G	N3-C4-N9	6.66	129.99	126.00
36	1	651	G	C8-N9-C1'	-6.65	118.35	127.00
36	5	905	U	O5'-P-OP2	-6.65	99.71	105.70
52	M6	84	LEU	CB-CG-CD2	-6.65	99.69	111.00
36	5	1003	A	C8-N9-C4	6.65	108.46	105.80
36	5	2757	U	N1-C2-N3	6.65	118.89	114.90
36	1	3368	U	C2-N1-C1'	-6.65	109.72	117.70
36	1	785	G	C2-N3-C4	6.65	115.22	111.90
38	4	20	U	N3-C4-C5	6.65	118.59	114.60
36	1	938	C	C6-N1-C2	-6.65	117.64	120.30
36	5	922	U	C5-C4-O4	6.65	129.89	125.90
36	1	2827	U	C2-N1-C1'	-6.64	109.73	117.70
36	5	2772	C	P-O3'-C3'	6.64	127.67	119.70
36	5	3218	A	C6-C5-N7	-6.64	127.65	132.30
36	5	952	A	C5-C6-N6	-6.64	118.39	123.70
36	5	2980	U	N1-C2-N3	6.64	118.89	114.90
36	5	1452	A	C4-C5-N7	6.64	114.02	110.70
36	1	43	A	C8-N9-C4	6.64	108.46	105.80
36	5	2758	A	N9-C4-C5	6.64	108.46	105.80
36	5	2877	G	C4-C5-N7	-6.64	108.14	110.80
40	l3	19	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	6	352	A	OP2-P-O3'	6.64	119.80	105.20
36	5	332	C	N3-C2-O2	-6.64	117.25	121.90
36	5	2211	U	N3-C2-O2	-6.64	117.55	122.20
36	5	2836	C	C5-C6-N1	-6.64	117.68	121.00
36	1	1617	G	C8-N9-C4	6.63	109.05	106.40
36	5	1592	G	C5-C6-N1	-6.63	108.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3218	A	P-O3'-C3'	6.63	127.66	119.70
36	1	1332	A	N7-C8-N9	6.63	117.12	113.80
36	1	908	G	C8-N9-C1'	-6.63	118.38	127.00
36	1	3266	G	C8-N9-C4	-6.63	103.75	106.40
1	2	728	U	C2-N1-C1'	6.63	125.66	117.70
36	1	1130	A	C2-N3-C4	6.63	113.92	110.60
36	1	1389	G	C6-C5-N7	-6.63	126.42	130.40
36	5	2326	A	C8-N9-C4	6.63	108.45	105.80
36	5	3210	A	N1-C6-N6	-6.63	114.62	118.60
36	5	2849	C	C5-C6-N1	6.63	124.31	121.00
36	5	217	U	OP1-P-O3'	6.62	119.78	105.20
36	1	422	A	N1-C6-N6	-6.62	114.63	118.60
36	1	2634	U	C5-C6-N1	-6.62	119.39	122.70
1	6	308	C	N1-C2-N3	6.62	123.84	119.20
36	5	3101	G	N1-C6-O6	-6.62	115.93	119.90
1	6	1100	G	C6-N1-C2	-6.62	121.13	125.10
36	5	1130	A	C2-N3-C4	6.62	113.91	110.60
36	5	2300	G	N1-C6-O6	-6.62	115.93	119.90
1	6	1537	C	N3-C4-C5	-6.62	119.25	121.90
1	2	830	U	N3-C2-O2	-6.62	117.57	122.20
36	5	2869	U	C6-N1-C1'	-6.62	111.94	121.20
1	2	1082	C	N1-C2-O2	6.61	122.87	118.90
36	1	281	G	N9-C4-C5	6.61	108.05	105.40
36	1	1124	U	C5-C6-N1	6.61	126.01	122.70
36	1	1440	G	O5'-P-OP1	-6.61	99.75	105.70
36	1	2866	U	N1-C2-O2	-6.61	118.17	122.80
36	5	2693	C	N3-C4-C5	6.61	124.54	121.90
36	1	1396	C	C6-N1-C2	6.61	122.94	120.30
36	5	932	U	N3-C4-O4	6.61	124.03	119.40
1	2	1022	C	N3-C4-C5	6.61	124.54	121.90
36	1	200	C	N1-C2-O2	6.61	122.86	118.90
1	6	542	A	O5'-P-OP1	-6.61	99.75	105.70
36	5	1335	C	N3-C2-O2	6.61	126.52	121.90
36	5	2950	G	O4'-C1'-N9	6.61	113.48	108.20
36	1	1353	U	N3-C2-O2	-6.60	117.58	122.20
36	1	1709	C	N1-C2-O2	-6.60	114.94	118.90
47	M0	57	LEU	CA-CB-CG	6.60	130.49	115.30
36	5	92	G	N1-C6-O6	-6.60	115.94	119.90
36	5	2412	G	N3-C4-C5	-6.60	125.30	128.60
1	2	144	U	N3-C2-O2	-6.60	117.58	122.20
1	2	1745	G	C5-C6-O6	-6.60	124.64	128.60
36	1	1310	G	C5-C6-O6	6.60	132.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3027	A	C8-N9-C4	6.60	108.44	105.80
36	5	3362	A	C4-C5-N7	6.60	114.00	110.70
36	1	585	A	N7-C8-N9	-6.59	110.50	113.80
36	5	272	G	N1-C6-O6	6.59	123.86	119.90
36	1	702	C	C2-N3-C4	-6.59	116.61	119.90
36	5	1112	A	C4-C5-C6	6.59	120.30	117.00
36	5	1721	U	N1-C2-O2	6.59	127.41	122.80
36	5	3377	G	N1-C6-O6	6.59	123.85	119.90
1	2	1652	C	C5-C6-N1	6.59	124.29	121.00
36	1	2643	A	N9-C4-C5	-6.59	103.17	105.80
36	5	92	G	N3-C4-C5	-6.59	125.31	128.60
36	5	3309	G	C4-N9-C1'	6.59	135.06	126.50
36	5	1902	G	O5'-P-OP1	-6.58	99.77	105.70
36	5	2372	A	P-O3'-C3'	6.58	127.60	119.70
36	1	81	C	C2-N3-C4	-6.58	116.61	119.90
36	1	2620	G	C8-N9-C4	6.58	109.03	106.40
36	5	159	A	C8-N9-C4	6.58	108.43	105.80
36	5	1832	C	N3-C4-C5	6.58	124.53	121.90
36	1	304	G	N1-C2-N2	6.58	122.12	116.20
37	7	26	C	C4-C5-C6	6.58	120.69	117.40
36	1	2179	C	N3-C4-C5	6.58	124.53	121.90
36	5	1420	C	OP2-P-O3'	6.58	119.67	105.20
42	15	152	ARG	NE-CZ-NH1	6.58	123.59	120.30
36	5	2370	G	C5-C6-N1	6.57	114.79	111.50
36	5	2618	G	N3-C4-C5	-6.57	125.31	128.60
36	5	2849	C	N3-C4-C5	-6.57	119.27	121.90
36	1	1003	A	N1-C6-N6	6.57	122.54	118.60
36	1	1514	G	O5'-P-OP1	-6.57	99.79	105.70
36	1	1904	C	C6-N1-C2	-6.57	117.67	120.30
36	5	2660	G	O5'-P-OP2	-6.57	99.79	105.70
1	2	553	G	C6-C5-N7	-6.57	126.46	130.40
1	6	272	U	P-O3'-C3'	6.57	127.58	119.70
36	5	2234	G	N1-C6-O6	6.57	123.84	119.90
36	5	3362	A	N7-C8-N9	6.57	117.08	113.80
1	2	1125	A	O5'-P-OP1	-6.57	99.79	105.70
36	1	961	C	C6-N1-C2	6.57	122.93	120.30
36	5	1306	G	N1-C6-O6	6.57	123.84	119.90
1	2	1462	G	N1-C6-O6	6.57	123.84	119.90
37	7	93	C	N3-C2-O2	-6.57	117.31	121.90
36	5	1298	C	N1-C2-O2	-6.56	114.96	118.90
36	5	2630	C	O5'-P-OP1	-6.56	99.79	105.70
36	5	2915	U	C2-N3-C4	-6.56	123.06	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3103	A	O5'-P-OP2	-6.56	99.80	105.70
36	5	859	G	N3-C4-C5	-6.56	125.32	128.60
36	1	644	G	C8-N9-C4	-6.56	103.78	106.40
36	1	960	U	N1-C2-O2	-6.56	118.21	122.80
36	5	871	U	C5-C4-O4	6.56	129.84	125.90
36	5	3228	C	N3-C2-O2	-6.56	117.31	121.90
1	2	1462	G	N9-C4-C5	-6.56	102.78	105.40
36	5	1152	G	N7-C8-N9	6.56	116.38	113.10
36	5	1410	U	O5'-P-OP2	-6.56	99.80	105.70
36	5	393	U	C6-N1-C2	-6.56	117.07	121.00
36	5	2142	A	OP1-P-OP2	-6.56	109.77	119.60
36	1	2976	A	N1-C6-N6	-6.55	114.67	118.60
38	4	20	U	N3-C4-O4	-6.55	114.81	119.40
36	1	2397	A	N9-C4-C5	-6.55	103.18	105.80
1	6	1600	A	N9-C1'-C2'	6.55	122.51	114.00
69	O3	48	ARG	NE-CZ-NH2	-6.55	117.03	120.30
36	1	1300	G	C5-C6-O6	-6.54	124.67	128.60
36	1	1391	C	OP1-P-OP2	6.54	129.42	119.60
36	1	2145	A	O5'-P-OP2	-6.54	99.81	105.70
36	5	661	G	C8-N9-C4	-6.54	103.78	106.40
36	1	1329	U	N1-C1'-C2'	-6.54	104.81	112.00
36	1	357	A	C5-N7-C8	-6.54	100.63	103.90
36	1	2627	C	C5-C6-N1	-6.54	117.73	121.00
1	6	455	C	N1-C2-O2	-6.54	114.98	118.90
36	1	2173	U	N1-C2-O2	-6.54	118.22	122.80
36	5	2993	G	C5-C6-O6	-6.54	124.68	128.60
1	2	992	A	N3-C4-C5	6.54	131.38	126.80
36	1	2247	G	C5-C6-O6	-6.54	124.68	128.60
36	1	1168	U	OP1-P-OP2	-6.53	109.80	119.60
36	1	3090	U	C5-C4-O4	-6.53	121.98	125.90
1	2	402	C	N3-C2-O2	6.53	126.47	121.90
36	1	651	G	C5-N7-C8	6.53	107.56	104.30
36	5	578	A	O5'-P-OP2	6.53	118.54	110.70
36	1	2601	A	N7-C8-N9	-6.53	110.53	113.80
38	4	95	G	N3-C4-C5	6.53	131.86	128.60
36	5	1312	C	C6-N1-C2	-6.53	117.69	120.30
1	6	623	A	O5'-P-OP1	-6.53	99.83	105.70
36	5	925	A	N7-C8-N9	-6.53	110.54	113.80
36	5	1212	A	O5'-P-OP2	-6.53	99.83	105.70
36	5	2660	G	C8-N9-C4	6.53	109.01	106.40
36	1	1113	G	C8-N9-C4	-6.52	103.79	106.40
36	5	2631	U	OP1-P-O3'	6.52	119.55	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2630	C	C5-C4-N4	-6.52	115.63	120.20
36	1	2777	G	N9-C4-C5	6.52	108.01	105.40
36	1	639	G	N9-C1'-C2'	-6.52	104.83	112.00
36	1	721	G	C6-C5-N7	-6.52	126.49	130.40
36	1	2169	G	C4-C5-N7	-6.52	108.19	110.80
36	1	2628	A	C8-N9-C4	-6.52	103.19	105.80
37	7	104	A	N1-C6-N6	6.52	122.51	118.60
36	5	2928	C	N3-C4-C5	-6.52	119.29	121.90
36	5	3308	C	N1-C2-O2	-6.52	114.99	118.90
1	6	1025	A	N1-C6-N6	6.51	122.51	118.60
36	5	807	A	C5-N7-C8	-6.51	100.64	103.90
36	5	2164	A	N1-C6-N6	6.51	122.51	118.60
36	1	1556	C	N3-C2-O2	-6.51	117.34	121.90
36	5	1185	C	C6-N1-C2	-6.51	117.69	120.30
36	5	2797	C	N3-C2-O2	6.51	126.46	121.90
36	5	2902	A	N1-C6-N6	6.51	122.51	118.60
1	6	194	U	N1-C2-O2	6.51	127.36	122.80
36	5	954	U	C5-C6-N1	6.51	125.95	122.70
36	1	970	A	C5-N7-C8	-6.51	100.65	103.90
36	5	3009	G	O5'-P-OP1	-6.51	99.84	105.70
36	5	1926	C	N1-C2-O2	-6.50	115.00	118.90
41	14	187	LEU	CA-CB-CG	6.50	130.26	115.30
36	1	2938	G	OP1-P-OP2	6.50	129.35	119.60
36	5	2383	C	N3-C4-N4	6.50	122.55	118.00
36	1	1820	U	P-O3'-C3'	6.50	127.50	119.70
36	1	1838	G	N9-C4-C5	-6.50	102.80	105.40
36	1	941	G	C8-N9-C4	-6.49	103.80	106.40
36	5	864	G	OP2-P-O3'	6.49	119.48	105.20
1	6	1600	A	C2-N3-C4	-6.49	107.36	110.60
36	5	994	G	N3-C2-N2	6.49	124.44	119.90
36	5	1301	A	N1-C6-N6	6.49	122.50	118.60
36	5	99	A	C8-N9-C4	6.49	108.39	105.80
36	5	2294	U	C2-N3-C4	-6.49	123.11	127.00
36	1	2400	G	N1-C6-O6	6.49	123.79	119.90
36	5	2899	C	O5'-P-OP1	6.49	118.48	110.70
36	1	2298	U	O4'-C1'-N1	6.49	113.39	108.20
36	1	60	A	C8-N9-C4	6.48	108.39	105.80
38	4	94	C	C6-N1-C2	6.48	122.89	120.30
1	6	453	U	C2-N1-C1'	6.48	125.48	117.70
36	5	1112	A	N3-C4-C5	-6.48	122.26	126.80
36	5	1434	G	C8-N9-C4	-6.48	103.81	106.40
36	1	2693	C	N3-C4-C5	6.48	124.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1330	A	OP1-P-OP2	-6.48	109.88	119.60
36	5	2884	C	C2-N1-C1'	6.48	125.93	118.80
38	8	19	C	C4-C5-C6	6.48	120.64	117.40
1	2	1273	G	O4'-C1'-N9	6.48	113.38	108.20
36	5	629	U	O5'-P-OP2	-6.48	99.87	105.70
38	4	32	C	C2-N3-C4	-6.48	116.66	119.90
36	1	2249	G	N3-C4-N9	6.47	129.88	126.00
36	5	811	U	C5-C4-O4	-6.47	122.02	125.90
1	2	1339	C	P-O3'-C3'	6.47	127.46	119.70
36	5	280	U	C5-C4-O4	-6.47	122.02	125.90
1	6	1560	U	N3-C2-O2	-6.47	117.67	122.20
36	5	2352	A	N1-C2-N3	6.47	132.53	129.30
36	1	645	A	C2-N3-C4	6.46	113.83	110.60
36	1	3362	A	N1-C2-N3	6.46	132.53	129.30
36	1	3122	A	O5'-P-OP1	-6.46	99.89	105.70
36	5	3301	U	C6-N1-C2	6.46	124.88	121.00
36	1	818	C	N3-C2-O2	-6.46	117.38	121.90
36	1	1852	G	C5-C6-O6	-6.46	124.72	128.60
54	M8	178	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	6	1100	G	C4-N9-C1'	6.46	134.90	126.50
36	1	2314	U	C6-N1-C2	6.46	124.87	121.00
36	5	1116	G	N3-C4-C5	-6.46	125.37	128.60
36	5	3101	G	O5'-P-OP1	-6.46	99.89	105.70
36	1	3228	C	N1-C2-O2	6.45	122.77	118.90
36	5	2405	C	N3-C2-O2	-6.45	117.38	121.90
36	5	3048	A	O5'-P-OP2	-6.45	99.89	105.70
36	1	646	A	O5'-P-OP2	-6.45	99.89	105.70
36	1	1433	A	C8-N9-C4	-6.45	103.22	105.80
36	1	1171	G	C4-C5-N7	6.45	113.38	110.80
36	5	2231	C	C2-N1-C1'	6.45	125.89	118.80
36	5	2606	G	C5-C6-O6	6.45	132.47	128.60
1	2	831	U	C2-N1-C1'	6.45	125.44	117.70
36	1	1881	A	C8-N9-C4	6.45	108.38	105.80
36	1	2850	G	N9-C4-C5	-6.45	102.82	105.40
1	2	136	C	C6-N1-C2	-6.45	117.72	120.30
36	1	339	C	N1-C2-O2	6.45	122.77	118.90
36	5	1316	C	N3-C4-C5	-6.45	119.32	121.90
36	5	2821	C	C6-N1-C2	-6.45	117.72	120.30
36	1	1182	A	C8-N9-C4	6.44	108.38	105.80
36	5	2818	U	C5-C4-O4	-6.44	122.03	125.90
36	5	2953	U	C4-C5-C6	6.44	123.56	119.70
36	5	860	G	O5'-P-OP2	-6.44	99.90	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	931	C	C2-N3-C4	-6.44	116.68	119.90
36	5	2643	A	N1-C6-N6	6.44	122.46	118.60
36	1	1794	G	O5'-P-OP2	-6.44	99.91	105.70
36	1	2383	C	C5-C6-N1	-6.44	117.78	121.00
36	1	2850	G	N3-C4-N9	6.44	129.86	126.00
36	5	853	G	N1-C6-O6	6.44	123.76	119.90
36	5	2606	G	N9-C4-C5	6.44	107.97	105.40
36	5	1126	G	N9-C4-C5	6.43	107.97	105.40
36	1	1949	G	O5'-P-OP1	-6.43	99.91	105.70
36	1	2402	A	C8-N9-C4	-6.43	103.23	105.80
77	Q1	9	ARG	NE-CZ-NH1	6.43	123.52	120.30
36	1	635	G	C5-C6-O6	-6.43	124.74	128.60
36	1	918	C	N1-C2-O2	-6.43	115.04	118.90
36	1	1898	G	C5-C6-O6	-6.43	124.74	128.60
36	1	2968	G	C4-C5-N7	6.43	113.37	110.80
36	5	45	A	C5-C6-N1	6.43	120.92	117.70
36	5	434	U	O5'-P-OP1	6.43	118.42	110.70
47	M0	24	ARG	NE-CZ-NH1	6.43	123.51	120.30
36	5	2890	A	N1-C6-N6	6.43	122.46	118.60
36	1	664	U	C5-C6-N1	-6.42	119.49	122.70
52	m6	125	ARG	NE-CZ-NH1	-6.42	117.09	120.30
36	5	1902	G	N1-C6-O6	6.42	123.75	119.90
36	1	1124	U	C4-C5-C6	-6.42	115.85	119.70
36	1	1864	A	C8-N9-C4	6.42	108.37	105.80
36	1	3216	G	N1-C6-O6	-6.42	116.05	119.90
36	5	776	U	C2-N3-C4	-6.42	123.15	127.00
36	1	2144	A	C8-N9-C4	6.42	108.37	105.80
36	5	1313	G	N1-C6-O6	6.42	123.75	119.90
36	1	1140	G	N3-C2-N2	6.42	124.39	119.90
36	1	1316	C	C5-C4-N4	-6.41	115.71	120.20
36	1	1433	A	C2-N3-C4	6.41	113.81	110.60
36	1	2550	U	C5-C4-O4	6.41	129.75	125.90
36	1	2874	G	C5-C6-O6	6.41	132.45	128.60
36	1	2345	A	N1-C6-N6	6.41	122.44	118.60
36	1	934	G	C4-N9-C1'	6.41	134.83	126.50
36	1	2944	U	C5-C4-O4	-6.41	122.06	125.90
36	5	1434	G	O5'-P-OP2	-6.41	99.93	105.70
47	M0	167	LEU	CA-CB-CG	6.41	130.03	115.30
36	5	1612	A	O5'-P-OP1	-6.41	99.94	105.70
36	5	3080	G	C6-C5-N7	-6.41	126.56	130.40
36	1	931	C	N3-C4-C5	6.40	124.46	121.90
36	5	2700	G	C5-C6-O6	-6.40	124.76	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2358	A	C2-N3-C4	-6.40	107.40	110.60
36	1	3270	U	O5'-P-OP1	-6.40	99.94	105.70
36	5	56	G	C6-C5-N7	6.40	134.24	130.40
36	1	1141	C	C6-N1-C2	-6.39	117.74	120.30
1	6	1793	G	O5'-P-OP1	-6.39	99.94	105.70
37	7	80	G	N3-C4-C5	-6.39	125.40	128.60
38	8	84	C	C6-N1-C2	-6.39	117.74	120.30
1	2	110	U	N1-C2-O2	6.39	127.27	122.80
73	O7	65	ARG	NE-CZ-NH1	6.39	123.50	120.30
36	5	972	A	OP2-P-O3'	6.39	119.26	105.20
36	1	86	G	C5-C6-N1	6.39	114.69	111.50
36	1	2712	U	N3-C2-O2	-6.39	117.73	122.20
36	1	2958	A	C5-C6-N1	6.39	120.90	117.70
1	6	1000	C	C4-C5-C6	6.39	120.60	117.40
36	5	931	C	N3-C4-C5	6.39	124.46	121.90
36	5	2393	G	O5'-P-OP2	-6.39	99.95	105.70
1	6	767	U	N3-C2-O2	-6.39	117.73	122.20
1	6	1700	C	C6-N1-C1'	-6.39	113.13	120.80
36	5	519	A	N1-C6-N6	6.39	122.43	118.60
36	5	2334	U	N1-C2-N3	6.39	118.73	114.90
36	1	1419	A	O4'-C1'-N9	6.38	113.31	108.20
36	1	2298	U	C5-C4-O4	6.38	129.73	125.90
36	5	1051	U	N3-C4-C5	6.38	118.43	114.60
36	5	1909	A	C8-N9-C4	6.38	108.35	105.80
36	1	1429	G	C5-N7-C8	6.38	107.49	104.30
36	1	2979	U	C2-N3-C4	-6.38	123.17	127.00
36	5	671	U	N3-C2-O2	6.38	126.67	122.20
36	5	2187	G	N9-C4-C5	-6.38	102.85	105.40
38	4	40	A	N1-C6-N6	6.38	122.43	118.60
36	5	1403	C	C5-C6-N1	-6.38	117.81	121.00
36	5	63	A	N1-C6-N6	6.38	122.43	118.60
36	5	2639	G	C6-C5-N7	-6.38	126.58	130.40
36	1	1907	C	N3-C4-C5	-6.38	119.35	121.90
36	1	2154	U	C5-C4-O4	-6.37	122.08	125.90
36	1	800	G	C5-C6-N1	-6.37	108.31	111.50
36	1	1144	U	C5-C6-N1	-6.37	119.51	122.70
36	1	1556	C	N1-C2-O2	6.37	122.72	118.90
36	5	3308	C	C4-C5-C6	6.37	120.58	117.40
1	2	1495	C	O5'-P-OP1	-6.37	99.97	105.70
36	1	1122	U	N3-C4-C5	6.37	118.42	114.60
36	1	2983	C	C5-C6-N1	-6.37	117.81	121.00
36	5	1879	A	C5-N7-C8	-6.37	100.72	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1923	C	C6-N1-C2	6.37	122.85	120.30
36	1	2356	A	C5-C6-N6	-6.37	118.61	123.70
36	1	2943	G	N3-C2-N2	6.37	124.36	119.90
36	5	931	C	C5-C6-N1	-6.37	117.82	121.00
36	5	1380	G	O5'-P-OP2	-6.37	99.97	105.70
36	5	1124	U	C4-C5-C6	-6.37	115.88	119.70
1	2	1773	C	C6-N1-C2	-6.36	117.75	120.30
36	5	3154	C	N3-C2-O2	-6.36	117.45	121.90
36	1	1907	C	C6-N1-C2	-6.36	117.75	120.30
1	2	1568	C	P-O3'-C3'	6.36	127.33	119.70
36	1	1475	A	C8-N9-C4	6.36	108.34	105.80
36	1	2250	G	O5'-P-OP1	-6.36	99.97	105.70
36	5	3260	G	C4-C5-N7	-6.36	108.26	110.80
36	1	2244	A	C8-N9-C4	6.36	108.34	105.80
36	1	2977	G	N7-C8-N9	-6.36	109.92	113.10
1	2	1761	U	C5-C4-O4	6.36	129.71	125.90
36	5	1838	G	N3-C2-N2	-6.36	115.45	119.90
36	1	1122	U	N3-C4-O4	-6.35	114.95	119.40
36	1	62	A	C2-N3-C4	6.35	113.78	110.60
37	3	103	A	C5-C6-N6	-6.35	118.62	123.70
36	5	2849	C	N1-C2-O2	-6.35	115.09	118.90
36	1	2302	G	N1-C6-O6	-6.35	116.09	119.90
36	1	2927	C	OP2-P-O3'	6.35	119.17	105.20
37	7	100	C	C6-N1-C2	6.35	122.84	120.30
36	1	1094	U	C5-C6-N1	6.35	125.87	122.70
1	6	362	G	C4-N9-C1'	6.35	134.75	126.50
36	5	1402	C	C2-N3-C4	-6.35	116.73	119.90
36	1	1427	U	N3-C2-O2	-6.34	117.76	122.20
1	6	416	A	N1-C6-N6	6.34	122.41	118.60
36	5	1119	C	OP2-P-O3'	6.34	119.16	105.20
36	1	91	G	N1-C6-O6	6.34	123.70	119.90
36	1	1147	G	C4-C5-N7	-6.34	108.26	110.80
36	1	2417	U	N1-C2-O2	-6.34	118.36	122.80
36	1	3362	A	C4-C5-N7	6.34	113.87	110.70
36	5	2383	C	C4-C5-C6	6.34	120.57	117.40
1	2	1096	C	C2-N1-C1'	6.34	125.77	118.80
36	1	895	A	N7-C8-N9	6.34	116.97	113.80
36	1	2893	C	N3-C4-C5	6.34	124.44	121.90
1	6	542	A	P-O3'-C3'	6.34	127.31	119.70
1	6	352	A	N7-C8-N9	-6.34	110.63	113.80
36	1	1142	G	N3-C4-N9	6.33	129.80	126.00
38	4	125	U	C2-N1-C1'	6.33	125.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	24	G	C5-C6-O6	-6.33	124.80	128.60
36	1	821	U	N3-C2-O2	-6.33	117.77	122.20
36	1	2967	A	C8-N9-C4	6.33	108.33	105.80
35	sM	167	PRO	N-CA-CB	6.33	110.89	103.30
36	5	585	A	O5'-P-OP2	-6.33	100.00	105.70
36	5	622	A	C5-C6-N6	-6.33	118.64	123.70
1	2	1200	G	N1-C6-O6	6.33	123.70	119.90
36	1	2363	A	C5-C6-N6	6.33	128.76	123.70
36	5	3200	G	C5-C6-O6	-6.33	124.80	128.60
1	2	590	C	C6-N1-C2	-6.32	117.77	120.30
36	1	92	G	N9-C4-C5	-6.32	102.87	105.40
36	1	423	A	C8-N9-C4	-6.32	103.27	105.80
36	5	2873	U	C2-N3-C4	-6.32	123.21	127.00
36	5	3101	G	N1-C2-N2	-6.32	110.51	116.20
36	1	121	A	C8-N9-C4	6.32	108.33	105.80
36	1	2304	C	N3-C2-O2	-6.32	117.48	121.90
36	5	3092	C	N3-C4-C5	6.32	124.43	121.90
36	1	295	A	O5'-P-OP1	-6.32	100.02	105.70
36	1	1429	G	N3-C2-N2	6.32	124.32	119.90
36	5	1882	G	O5'-P-OP1	-6.32	100.02	105.70
36	5	2758	A	C2-N3-C4	6.32	113.76	110.60
1	2	554	C	N1-C2-O2	6.31	122.69	118.90
36	1	1429	G	C2-N3-C4	6.31	115.06	111.90
36	5	706	A	O5'-P-OP1	-6.31	100.02	105.70
36	5	1160	C	C6-N1-C1'	6.31	128.38	120.80
36	1	2359	C	N3-C2-O2	6.31	126.32	121.90
36	5	1200	A	C4-C5-C6	6.31	120.16	117.00
36	5	3026	G	N1-C6-O6	6.31	123.69	119.90
36	5	1489	A	N1-C6-N6	6.31	122.39	118.60
36	1	1331	U	O4'-C1'-N1	-6.31	103.15	108.20
36	5	2971	A	N9-C4-C5	-6.31	103.28	105.80
36	5	838	G	N1-C6-O6	-6.31	116.12	119.90
36	5	934	G	N3-C4-N9	6.31	129.78	126.00
36	5	435	C	O5'-P-OP1	6.31	118.27	110.70
36	5	2815	G	C5-N7-C8	6.31	107.45	104.30
36	1	81	C	N3-C4-C5	6.30	124.42	121.90
36	1	1154	A	C4-C5-C6	6.30	120.15	117.00
36	1	2846	U	N1-C2-N3	6.30	118.68	114.90
36	5	2889	C	N3-C2-O2	-6.30	117.49	121.90
36	1	1905	G	C2-N3-C4	6.30	115.05	111.90
36	5	424	G	C5-C6-N1	6.30	114.65	111.50
36	5	706	A	C8-N9-C4	6.30	108.32	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	507	U	N3-C2-O2	-6.30	117.79	122.20
36	1	2285	C	C5-C4-N4	-6.30	115.79	120.20
37	3	98	C	N3-C4-C5	-6.30	119.38	121.90
36	5	982	C	OP2-P-O3'	6.30	119.05	105.20
36	1	1520	G	C2-N3-C4	6.29	115.05	111.90
36	1	2679	A	O4'-C1'-N9	6.29	113.23	108.20
36	5	1331	U	C5-C4-O4	-6.29	122.12	125.90
37	7	37	G	N9-C4-C5	-6.29	102.88	105.40
36	5	810	A	O5'-P-OP1	-6.29	100.04	105.70
36	5	3115	C	N1-C2-O2	-6.29	115.12	118.90
36	1	941	G	N3-C4-C5	-6.29	125.45	128.60
36	5	2775	U	C5-C6-N1	-6.29	119.56	122.70
36	5	2954	U	N1-C2-O2	6.29	127.20	122.80
1	2	1202	A	C8-N9-C4	-6.29	103.28	105.80
36	1	517	G	N3-C4-C5	-6.29	125.45	128.60
36	1	2292	U	C2-N3-C4	-6.29	123.23	127.00
36	5	2948	C	OP1-P-OP2	-6.29	110.17	119.60
36	5	2412	G	N3-C4-N9	6.29	129.77	126.00
36	1	365	A	C5-C6-N6	-6.29	118.67	123.70
36	5	1440	G	N9-C4-C5	6.29	107.92	105.40
36	5	3103	A	C6-N1-C2	-6.29	114.83	118.60
36	1	661	G	C4-N9-C1'	6.28	134.67	126.50
36	1	1741	A	N1-C6-N6	6.28	122.37	118.60
36	5	840	C	N1-C2-N3	6.28	123.60	119.20
36	1	91	G	N3-C4-C5	6.28	131.74	128.60
36	1	609	G	O5'-P-OP2	-6.28	100.05	105.70
36	1	92	G	C8-N9-C4	6.28	108.91	106.40
1	6	421	A	C8-N9-C4	6.28	108.31	105.80
36	5	2645	G	N1-C6-O6	-6.28	116.13	119.90
9	S7	118	LEU	CA-CB-CG	6.28	129.74	115.30
36	5	1725	C	O4'-C1'-N1	6.28	113.22	108.20
36	1	350	C	N1-C2-O2	6.28	122.67	118.90
36	1	934	G	C8-N9-C1'	-6.28	118.84	127.00
52	M6	78	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	2	1432	U	C5-C6-N1	-6.28	119.56	122.70
36	1	2278	C	C5-C6-N1	6.28	124.14	121.00
38	4	48	A	C8-N9-C4	-6.28	103.29	105.80
36	5	2110	G	C4-C5-N7	6.28	113.31	110.80
36	5	2320	A	C2-N3-C4	-6.28	107.46	110.60
36	5	2954	U	C2-N1-C1'	6.27	125.23	117.70
36	1	1510	G	N3-C4-N9	6.27	129.76	126.00
36	1	2349	U	O5'-P-OP2	-6.27	100.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2760	C	N1-C2-O2	-6.27	115.14	118.90
36	5	881	C	C5-C6-N1	6.27	124.14	121.00
36	1	655	C	N1-C2-N3	6.27	123.59	119.20
36	1	52	A	O5'-P-OP2	-6.27	100.06	105.70
37	3	93	C	N3-C4-C5	6.27	124.41	121.90
1	6	1340	U	N3-C2-O2	-6.27	117.81	122.20
36	5	3187	A	N1-C6-N6	-6.27	114.84	118.60
36	5	3214	U	N3-C4-O4	-6.27	115.01	119.40
37	7	15	C	N3-C4-C5	6.26	124.41	121.90
36	5	881	C	C2-N3-C4	6.26	123.03	119.90
36	1	416	A	OP2-P-O3'	6.26	118.96	105.20
36	5	2623	G	N9-C4-C5	-6.25	102.90	105.40
36	5	3060	C	N3-C4-N4	6.25	122.38	118.00
36	5	3244	A	O5'-P-OP1	-6.25	100.07	105.70
1	2	992	A	C2-N3-C4	-6.25	107.47	110.60
36	5	2931	C	N3-C4-N4	6.25	122.38	118.00
36	5	3308	C	C2-N3-C4	-6.25	116.77	119.90
1	6	858	G	C4-N9-C1'	6.25	134.63	126.50
56	n0	40	ARG	NE-CZ-NH1	6.25	123.42	120.30
36	5	2113	A	C5-C6-N1	6.25	120.82	117.70
36	5	2157	G	O5'-P-OP1	-6.25	100.08	105.70
1	2	1748	G	N3-C4-N9	-6.25	122.25	126.00
36	1	3216	G	N9-C4-C5	6.25	107.90	105.40
44	L7	215	GLY	N-CA-C	-6.25	97.49	113.10
36	5	680	G	O5'-P-OP2	-6.25	100.08	105.70
36	1	2726	C	N1-C2-N3	6.24	123.57	119.20
36	5	3176	G	N3-C2-N2	-6.24	115.53	119.90
1	6	1640	C	C5-C4-N4	-6.24	115.83	120.20
36	5	200	C	C5-C6-N1	6.24	124.12	121.00
36	5	984	G	N1-C2-N2	-6.24	110.58	116.20
36	5	2865	U	C4-C5-C6	-6.24	115.96	119.70
36	5	2988	C	N3-C2-O2	-6.24	117.53	121.90
36	5	928	C	O5'-P-OP2	-6.24	100.09	105.70
36	5	2115	G	C5-C6-O6	-6.24	124.86	128.60
36	1	89	A	N3-C4-C5	-6.24	122.44	126.80
36	1	282	G	P-O3'-C3'	6.24	127.18	119.70
1	6	1779	U	N3-C2-O2	-6.23	117.84	122.20
36	1	668	G	N1-C6-O6	-6.23	116.16	119.90
36	1	232	G	N3-C4-C5	-6.23	125.48	128.60
36	1	2150	G	C5-C6-N1	-6.23	108.39	111.50
36	1	2968	G	C6-C5-N7	-6.23	126.66	130.40
36	5	1440	G	C4-C5-N7	-6.23	108.31	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2688	U	N1-C2-N3	-6.23	111.16	114.90
1	2	345	U	N1-C2-N3	6.23	118.64	114.90
36	1	2413	A	C8-N9-C4	6.22	108.29	105.80
36	5	1473	G	C8-N9-C4	6.22	108.89	106.40
37	7	1	G	C6-C5-N7	-6.22	126.67	130.40
36	1	405	U	C6-N1-C2	6.22	124.73	121.00
36	1	510	G	C5-C6-O6	-6.22	124.87	128.60
37	7	34	C	O5'-P-OP1	-6.22	100.10	105.70
38	4	97	A	C8-N9-C4	-6.22	103.31	105.80
36	5	2531	C	C2-N1-C1'	6.22	125.64	118.80
1	6	151	G	N3-C2-N2	-6.22	115.55	119.90
36	5	1425	U	C5-C4-O4	6.22	129.63	125.90
36	5	3142	A	O5'-P-OP1	-6.22	100.11	105.70
36	5	2945	G	C5-C6-O6	-6.21	124.87	128.60
1	6	542	A	N1-C6-N6	6.21	122.33	118.60
1	6	1747	G	O5'-P-OP2	-6.21	100.11	105.70
36	5	2966	G	C5-C6-O6	-6.21	124.87	128.60
1	2	159	U	N3-C2-O2	6.21	126.55	122.20
1	2	1615	C	C6-N1-C2	-6.21	117.81	120.30
36	1	2901	G	N1-C6-O6	6.21	123.63	119.90
36	5	1148	G	C8-N9-C4	6.21	108.89	106.40
36	1	1175	C	C2-N3-C4	-6.21	116.80	119.90
36	5	2861	U	O5'-P-OP2	6.21	118.15	110.70
36	1	3362	A	C4-N9-C1'	6.21	137.48	126.30
1	6	426	G	N3-C4-C5	-6.21	125.50	128.60
36	5	1434	G	C5-C6-N1	6.21	114.61	111.50
1	6	1614	A	C4-C5-N7	6.21	113.80	110.70
36	5	3154	C	C5-C6-N1	6.21	124.10	121.00
36	1	2679	A	C2-N3-C4	-6.21	107.50	110.60
36	1	428	A	N1-C6-N6	-6.20	114.88	118.60
36	1	721	G	N1-C6-O6	6.20	123.62	119.90
36	1	1338	C	N3-C4-C5	-6.20	119.42	121.90
36	5	374	A	P-O3'-C3'	6.20	127.14	119.70
36	5	834	U	N3-C4-C5	6.20	118.32	114.60
1	2	694	U	C2-N1-C1'	6.20	125.14	117.70
36	1	2640	A	C5-C6-N1	6.20	120.80	117.70
36	5	652	G	C4-C5-C6	6.20	122.52	118.80
36	5	2919	A	N1-C6-N6	-6.20	114.88	118.60
36	5	2350	C	OP1-P-OP2	-6.19	110.31	119.60
36	5	2941	A	O5'-P-OP2	-6.19	100.12	105.70
36	1	640	U	C2-N3-C4	-6.19	123.29	127.00
36	5	2831	G	N3-C4-C5	-6.19	125.50	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2891	U	N3-C4-O4	-6.19	115.07	119.40
38	8	21	C	N3-C4-C5	-6.19	119.42	121.90
36	5	102	C	N3-C4-N4	6.19	122.33	118.00
36	5	2904	U	C5-C6-N1	-6.19	119.61	122.70
36	5	3040	A	C8-N9-C4	6.19	108.28	105.80
1	6	1009	U	C5-C6-N1	-6.19	119.61	122.70
36	5	3308	C	N1-C2-N3	6.19	123.53	119.20
1	6	1000	C	C2-N3-C4	-6.18	116.81	119.90
36	5	2914	G	C8-N9-C1'	-6.18	118.96	127.00
36	1	521	A	C5-C6-N6	-6.18	118.75	123.70
36	5	1438	U	C6-N1-C2	-6.18	117.29	121.00
36	5	2278	C	N1-C2-O2	6.18	122.61	118.90
36	5	928	C	N3-C2-O2	-6.18	117.57	121.90
36	5	2296	A	N7-C8-N9	6.18	116.89	113.80
1	6	1697	G	N3-C4-C5	-6.18	125.51	128.60
36	5	1314	C	N3-C4-C5	6.18	124.37	121.90
1	2	1331	A	N1-C6-N6	-6.18	114.89	118.60
36	1	636	C	N3-C2-O2	-6.18	117.58	121.90
36	5	2637	A	N1-C6-N6	6.18	122.31	118.60
36	1	300	G	O5'-P-OP1	-6.18	100.14	105.70
1	6	558	U	C2-N1-C1'	6.18	125.11	117.70
36	5	617	G	N9-C4-C5	-6.18	102.93	105.40
36	5	2717	U	N1-C2-N3	6.17	118.60	114.90
36	1	2860	U	C5-C6-N1	6.17	125.79	122.70
36	1	1604	G	C8-N9-C1'	-6.17	118.98	127.00
36	1	1837	U	N3-C2-O2	6.17	126.52	122.20
1	6	116	U	C6-N1-C2	-6.17	117.30	121.00
36	5	630	A	C2-N3-C4	-6.17	107.52	110.60
36	5	1628	C	C6-N1-C2	-6.17	117.83	120.30
36	5	2970	C	C6-N1-C2	6.17	122.77	120.30
36	1	2572	C	N3-C2-O2	-6.17	117.58	121.90
36	1	2957	G	C4-C5-N7	-6.17	108.33	110.80
1	6	114	C	N3-C2-O2	-6.17	117.58	121.90
36	5	2162	U	O5'-P-OP2	-6.17	100.15	105.70
36	1	2352	A	O5'-P-OP2	-6.17	100.15	105.70
36	1	2554	A	P-O3'-C3'	6.17	127.10	119.70
36	5	1205	A	O5'-P-OP2	-6.17	100.15	105.70
36	5	2134	G	C5-C6-O6	6.17	132.30	128.60
36	5	2337	C	C5-C4-N4	-6.17	115.88	120.20
36	1	2281	A	C2-N3-C4	-6.17	107.52	110.60
1	6	371	G	C4-C5-N7	6.17	113.27	110.80
36	1	2356	A	N1-C6-N6	6.16	122.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	767	U	C5-C4-O4	6.16	129.60	125.90
1	2	16	G	N3-C4-N9	6.16	129.70	126.00
1	2	1426	C	C4-C5-C6	-6.16	114.32	117.40
36	1	1308	A	O5'-P-OP1	6.16	118.09	110.70
36	5	2377	G	C5-N7-C8	6.16	107.38	104.30
36	5	2896	A	N1-C6-N6	-6.16	114.90	118.60
36	1	421	G	C5-C6-N1	6.16	114.58	111.50
36	1	1114	U	N3-C4-C5	6.16	118.30	114.60
36	1	2150	G	N9-C4-C5	6.16	107.86	105.40
36	5	1495	U	O4'-C1'-N1	6.16	113.13	108.20
36	5	3245	A	C4-C5-C6	6.16	120.08	117.00
36	1	1556	C	C6-N1-C1'	-6.16	113.41	120.80
36	1	3302	U	C6-N1-C2	6.16	124.69	121.00
38	4	94	C	N3-C4-C5	6.16	124.36	121.90
37	7	100	C	C5-C6-N1	-6.16	117.92	121.00
36	1	776	U	C5-C6-N1	-6.16	119.62	122.70
36	1	1377	G	N1-C6-O6	-6.16	116.21	119.90
36	5	1780	G	N1-C6-O6	-6.16	116.21	119.90
36	1	2409	G	N1-C2-N2	-6.15	110.66	116.20
1	6	421	A	N9-C4-C5	-6.15	103.34	105.80
36	5	2816	G	O4'-C1'-N9	6.15	113.12	108.20
36	1	2816	G	O4'-C1'-N9	6.15	113.12	108.20
1	6	426	G	C4-N9-C1'	6.15	134.50	126.50
36	5	1662	G	C5-C6-N1	-6.15	108.42	111.50
36	5	3195	U	OP1-P-O3'	6.15	118.73	105.20
38	8	16	G	O5'-P-OP2	-6.15	100.17	105.70
63	N7	135	ARG	NE-CZ-NH2	6.15	123.37	120.30
36	5	78	U	O5'-P-OP1	-6.15	100.17	105.70
36	5	1010	G	O5'-P-OP2	-6.15	100.17	105.70
36	5	2419	A	C8-N9-C4	-6.15	103.34	105.80
36	5	283	G	C4-C5-N7	6.15	113.26	110.80
1	2	942	G	C8-N9-C4	-6.14	103.94	106.40
36	5	665	A	N1-C6-N6	6.14	122.29	118.60
36	5	2285	C	C6-N1-C2	-6.14	117.84	120.30
38	8	8	C	O5'-P-OP2	-6.14	100.17	105.70
36	1	2192	C	O5'-P-OP2	-6.14	100.17	105.70
1	6	1568	C	C2-N1-C1'	6.14	125.56	118.80
36	5	1444	G	C5-C6-O6	-6.14	124.92	128.60
1	2	75	U	C2-N1-C1'	6.14	125.07	117.70
36	5	43	A	O5'-P-OP1	-6.14	100.17	105.70
36	5	1104	G	C6-C5-N7	-6.14	126.72	130.40
1	6	1111	G	C6-C5-N7	-6.14	126.72	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2403	G	O5'-P-OP1	6.14	118.06	110.70
1	6	1614	A	C5-N7-C8	-6.14	100.83	103.90
1	2	1241	G	O4'-C1'-N9	6.14	113.11	108.20
36	1	2424	A	N1-C6-N6	6.14	122.28	118.60
36	5	436	A	N7-C8-N9	6.14	116.87	113.80
1	6	1600	A	C5-N7-C8	-6.13	100.83	103.90
36	5	880	G	C8-N9-C1'	6.13	134.98	127.00
37	7	30	G	N3-C4-C5	-6.13	125.53	128.60
36	1	640	U	N3-C4-O4	6.13	123.69	119.40
36	1	2606	G	N3-C4-N9	6.13	129.68	126.00
36	1	3218	A	C8-N9-C4	-6.13	103.35	105.80
36	5	383	G	C8-N9-C4	6.13	108.85	106.40
36	5	1879	A	N7-C8-N9	6.13	116.87	113.80
36	5	41	G	N1-C6-O6	6.13	123.58	119.90
1	2	1258	U	N3-C2-O2	-6.13	117.91	122.20
36	1	968	G	N3-C4-C5	-6.13	125.54	128.60
36	1	1510	G	C6-C5-N7	-6.13	126.72	130.40
36	1	2727	A	C2-N3-C4	6.13	113.66	110.60
36	5	1440	G	C5-C6-O6	6.13	132.28	128.60
36	5	2310	U	N1-C2-O2	6.13	127.09	122.80
36	1	1362	G	C8-N9-C4	6.13	108.85	106.40
36	5	2858	U	C2-N1-C1'	6.13	125.05	117.70
36	1	1846	C	O5'-P-OP1	-6.12	100.19	105.70
38	4	61	A	C5-C6-N6	-6.12	118.80	123.70
36	5	3195	U	P-O3'-C3'	6.12	127.05	119.70
37	7	1	G	C4-N9-C1'	6.12	134.46	126.50
1	2	158	U	P-O3'-C3'	6.12	127.05	119.70
36	5	1184	A	N1-C6-N6	-6.12	114.93	118.60
36	5	2678	A	N9-C4-C5	6.12	108.25	105.80
36	1	922	U	C4-C5-C6	-6.12	116.03	119.70
36	1	1832	C	C5-C6-N1	-6.12	117.94	121.00
1	6	543	C	N3-C2-O2	-6.12	117.62	121.90
11	s9	3	ARG	NE-CZ-NH2	6.12	123.36	120.30
36	5	2402	A	N1-C6-N6	-6.12	114.93	118.60
36	5	2550	U	C5-C4-O4	6.12	129.57	125.90
36	5	3020	U	N3-C4-O4	6.12	123.68	119.40
36	1	60	A	N9-C4-C5	-6.12	103.35	105.80
1	6	1644	C	O5'-P-OP2	-6.12	100.20	105.70
36	5	329	U	C6-N1-C2	6.12	124.67	121.00
36	5	1132	C	O5'-P-OP1	-6.12	100.20	105.70
36	5	2639	G	C5-C6-O6	-6.12	124.93	128.60
36	5	2908	G	N9-C4-C5	6.12	107.85	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	821	U	C5-C4-O4	6.11	129.57	125.90
36	1	1307	G	OP1-P-O3'	6.11	118.65	105.20
36	1	2834	G	C4-C5-N7	6.11	113.25	110.80
36	1	3209	A	C5-C6-N1	-6.11	114.64	117.70
36	1	3368	U	N1-C2-O2	-6.11	118.52	122.80
36	1	3380	U	O5'-P-OP2	-6.11	100.20	105.70
36	5	1403	C	N3-C4-C5	6.11	124.34	121.90
36	1	351	A	OP1-P-OP2	6.11	128.77	119.60
36	1	1297	C	O5'-P-OP1	-6.11	100.20	105.70
1	2	448	C	C6-N1-C2	-6.11	117.86	120.30
36	1	25	U	N1-C2-N3	6.11	118.57	114.90
1	6	65	A	N1-C6-N6	6.11	122.27	118.60
36	5	3368	U	C5-C6-N1	-6.11	119.64	122.70
36	1	349	A	OP2-P-O3'	6.11	118.64	105.20
36	1	1138	U	C2-N3-C4	-6.11	123.33	127.00
36	1	1154	A	N3-C4-C5	-6.11	122.53	126.80
36	5	639	G	O5'-P-OP1	6.11	118.03	110.70
36	5	644	G	N3-C4-C5	-6.11	125.55	128.60
36	5	2204	C	N3-C4-N4	-6.11	113.72	118.00
36	5	3153	U	N1-C2-O2	6.11	127.08	122.80
36	5	1507	G	O5'-P-OP1	-6.11	100.21	105.70
1	2	577	G	C5-N7-C8	-6.10	101.25	104.30
1	2	647	G	N3-C4-N9	-6.10	122.34	126.00
36	1	776	U	C5-C4-O4	6.10	129.56	125.90
36	5	584	G	C4-C5-N7	-6.10	108.36	110.80
36	5	2634	U	C5-C4-O4	-6.10	122.24	125.90
36	5	2368	A	N1-C6-N6	-6.10	114.94	118.60
38	8	111	A	C5-N7-C8	-6.10	100.85	103.90
36	1	3178	A	N1-C6-N6	6.10	122.26	118.60
37	7	35	C	C5-C6-N1	-6.10	117.95	121.00
36	5	359	U	OP1-P-OP2	-6.10	110.46	119.60
36	1	345	G	O5'-P-OP2	-6.09	100.22	105.70
36	1	2169	G	C5-C6-O6	6.09	132.26	128.60
36	5	800	G	N9-C4-C5	-6.09	102.96	105.40
36	5	1409	G	OP2-P-O3'	6.09	118.61	105.20
36	5	2211	U	N1-C2-N3	6.09	118.56	114.90
36	5	2249	G	N3-C4-C5	-6.09	125.55	128.60
36	1	1133	A	C5-C6-N6	-6.09	118.83	123.70
37	7	77	G	O5'-P-OP2	-6.09	100.22	105.70
36	1	659	G	N3-C4-N9	6.09	129.66	126.00
36	1	1340	G	N3-C2-N2	6.09	124.16	119.90
36	5	3306	U	C5-C4-O4	-6.09	122.25	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2293	C	N3-C4-N4	6.09	122.26	118.00
36	1	2893	C	C2-N3-C4	-6.09	116.86	119.90
38	4	20	U	C2-N3-C4	-6.09	123.35	127.00
36	5	999	G	N1-C6-O6	-6.09	116.25	119.90
36	1	2176	U	C5-C4-O4	6.09	129.55	125.90
36	1	2836	C	N3-C4-N4	-6.09	113.74	118.00
1	6	1514	U	C5-C4-O4	6.09	129.55	125.90
1	2	192	U	N1-C2-O2	6.08	127.06	122.80
36	5	612	U	O5'-P-OP1	-6.08	100.22	105.70
36	5	2943	G	C6-C5-N7	-6.08	126.75	130.40
36	5	1365	G	N1-C6-O6	6.08	123.55	119.90
36	5	2947	G	N9-C4-C5	-6.08	102.97	105.40
36	5	2980	U	C6-N1-C2	-6.08	117.35	121.00
36	1	1305	U	N1-C2-O2	6.08	127.06	122.80
36	1	2692	A	N1-C6-N6	6.08	122.25	118.60
36	5	2524	A	N9-C1'-C2'	6.08	121.91	114.00
36	5	3093	C	C6-N1-C2	6.08	122.73	120.30
1	2	1273	G	C2-N3-C4	6.08	114.94	111.90
36	1	1902	G	N9-C4-C5	-6.08	102.97	105.40
36	1	2812	C	C6-N1-C2	6.08	122.73	120.30
36	5	751	A	O5'-P-OP2	-6.08	100.23	105.70
36	1	586	C	C6-N1-C2	6.08	122.73	120.30
36	1	1419	A	O5'-P-OP2	-6.08	100.23	105.70
1	6	647	G	N3-C4-N9	-6.08	122.35	126.00
36	5	946	U	O5'-P-OP2	-6.08	100.23	105.70
36	5	3150	A	N1-C6-N6	6.08	122.25	118.60
1	6	194	U	N3-C2-O2	-6.08	117.95	122.20
36	1	2915	U	C5-C4-O4	-6.08	122.25	125.90
1	6	1663	G	O5'-P-OP2	-6.08	100.23	105.70
1	2	75	U	N3-C2-O2	-6.07	117.95	122.20
36	1	721	G	C4-C5-N7	6.07	113.23	110.80
36	1	2366	C	C5-C6-N1	6.07	124.04	121.00
36	1	2836	C	N1-C2-N3	6.07	123.45	119.20
36	5	419	G	N3-C4-N9	6.07	129.64	126.00
38	8	7	U	O5'-P-OP2	-6.07	100.23	105.70
36	1	803	C	C5-C6-N1	-6.07	117.96	121.00
36	5	2334	U	C2-N3-C4	-6.07	123.36	127.00
36	1	92	G	O5'-P-OP1	-6.07	100.24	105.70
36	1	907	G	N3-C2-N2	6.07	124.15	119.90
36	1	1307	G	C6-C5-N7	6.07	134.04	130.40
1	6	639	U	C2-N1-C1'	6.07	124.98	117.70
36	1	2314	U	N1-C2-N3	-6.07	111.26	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2514	U	O5'-P-OP1	-6.07	100.24	105.70
36	5	3101	G	C5-C6-O6	6.07	132.24	128.60
1	2	944	A	C8-N9-C4	6.07	108.23	105.80
36	5	2155	G	C8-N9-C4	6.07	108.83	106.40
36	5	1901	A	O5'-P-OP2	-6.06	100.24	105.70
36	1	37	U	C4-C5-C6	6.06	123.34	119.70
36	1	1484	U	OP2-P-O3'	6.06	118.54	105.20
1	6	418	G	C4-C5-N7	6.06	113.22	110.80
36	5	189	G	C5-C6-O6	6.06	132.24	128.60
36	5	941	G	N1-C6-O6	-6.06	116.26	119.90
1	6	1653	C	C6-N1-C2	-6.06	117.88	120.30
12	c0	83	PRO	N-CA-CB	6.06	110.57	103.30
1	2	580	A	C8-N9-C4	-6.06	103.38	105.80
36	1	2937	G	N7-C8-N9	-6.05	110.07	113.10
37	7	84	A	C4-C5-C6	6.05	120.03	117.00
36	5	1607	U	O5'-P-OP1	-6.05	100.25	105.70
36	1	1307	G	N9-C4-C5	6.05	107.82	105.40
36	5	2700	G	C4-C5-N7	6.05	113.22	110.80
1	2	1051	G	P-O3'-C3'	6.05	126.96	119.70
1	2	1200	G	N3-C2-N2	-6.05	115.67	119.90
36	5	641	C	C2-N1-C1'	-6.05	112.15	118.80
36	5	907	G	O5'-P-OP1	-6.05	100.26	105.70
36	5	1413	G	N1-C6-O6	-6.05	116.27	119.90
36	5	2618	G	N1-C2-N2	-6.05	110.75	116.20
72	O6	76	ARG	NE-CZ-NH1	-6.05	117.28	120.30
36	1	2756	C	C6-N1-C2	-6.05	117.88	120.30
36	1	939	U	O5'-P-OP2	-6.04	100.26	105.70
70	O4	51	LEU	CA-CB-CG	6.04	129.20	115.30
36	1	590	G	C4-C5-N7	6.04	113.22	110.80
36	1	1130	A	C8-N9-C4	-6.04	103.38	105.80
38	4	125	U	N1-C2-O2	6.04	127.03	122.80
36	5	2345	A	C5-C6-N6	-6.04	118.87	123.70
36	1	2731	U	C5-C6-N1	6.04	125.72	122.70
36	5	2296	A	C5-C6-N1	6.04	120.72	117.70
1	2	1486	G	C5-N7-C8	-6.04	101.28	104.30
36	1	658	G	C8-N9-C4	6.04	108.81	106.40
36	1	999	G	C4-C5-N7	6.04	113.22	110.80
1	6	352	A	N1-C6-N6	-6.04	114.98	118.60
36	5	2794	G	N3-C4-N9	6.04	129.62	126.00
36	5	799	G	C6-N1-C2	-6.04	121.48	125.10
36	5	1170	A	N9-C4-C5	-6.04	103.39	105.80
36	1	651	G	C4-N9-C1'	6.03	134.34	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3277	U	N3-C2-O2	-6.03	117.98	122.20
1	6	1340	U	N1-C2-O2	6.03	127.02	122.80
36	1	959	C	C6-N1-C2	6.03	122.71	120.30
36	5	1434	G	C2-N3-C4	6.03	114.92	111.90
36	5	1925	U	C5-C4-O4	-6.03	122.28	125.90
36	1	2823	G	OP1-P-O3'	6.03	118.46	105.20
36	5	612	U	O5'-P-OP2	6.03	117.93	110.70
36	5	878	G	C8-N9-C4	-6.03	103.99	106.40
36	1	1489	A	C5-C6-N6	-6.03	118.88	123.70
36	5	909	G	C5-N7-C8	6.03	107.31	104.30
36	1	3318	G	C8-N9-C1'	-6.03	119.17	127.00
1	6	362	G	C8-N9-C1'	-6.02	119.17	127.00
1	2	1749	A	N1-C6-N6	6.02	122.21	118.60
36	1	1002	A	C8-N9-C4	6.02	108.21	105.80
36	5	890	C	O5'-P-OP1	6.02	117.93	110.70
41	L4	138	ARG	NE-CZ-NH2	-6.02	117.29	120.30
38	4	38	U	N3-C2-O2	-6.02	117.99	122.20
36	5	1375	G	C8-N9-C4	-6.02	103.99	106.40
36	1	338	A	OP2-P-O3'	6.02	118.44	105.20
36	5	984	G	N3-C4-N9	6.02	129.61	126.00
36	1	645	A	N1-C2-N3	6.02	132.31	129.30
1	6	362	G	N3-C4-N9	6.02	129.61	126.00
12	c0	97	PRO	N-CA-CB	6.02	110.52	103.30
36	5	792	G	O5'-P-OP1	-6.02	100.28	105.70
36	5	2943	G	O5'-P-OP2	-6.02	100.29	105.70
36	1	344	A	N1-C2-N3	-6.01	126.29	129.30
36	1	435	C	C6-N1-C2	6.01	122.71	120.30
36	5	3054	U	N3-C4-O4	6.01	123.61	119.40
1	2	610	G	N1-C6-O6	6.01	123.51	119.90
36	1	282	G	C2'-C3'-O3'	6.01	123.32	113.70
36	5	2622	C	C6-N1-C2	-6.01	117.89	120.30
36	1	1145	G	C5-C6-O6	-6.01	124.99	128.60
36	5	413	U	N3-C4-O4	6.01	123.61	119.40
59	n3	5	GLY	N-CA-C	-6.01	98.07	113.10
36	1	32	U	N1-C2-O2	-6.01	118.59	122.80
36	1	407	A	C4-C5-N7	6.01	113.70	110.70
36	1	997	A	C4-C5-C6	6.01	120.00	117.00
36	1	1115	G	N7-C8-N9	6.01	116.11	113.10
36	1	1334	U	N3-C4-C5	-6.01	111.00	114.60
36	1	1429	G	N7-C8-N9	-6.01	110.10	113.10
36	5	2112	U	O5'-P-OP1	-6.01	100.29	105.70
36	5	2973	G	N7-C8-N9	6.01	116.11	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	811	U	C5-C6-N1	-6.01	119.70	122.70
36	5	1112	A	C2-N3-C4	6.01	113.60	110.60
36	1	345	G	N3-C4-C5	-6.01	125.60	128.60
1	6	425	A	N1-C6-N6	-6.01	115.00	118.60
36	1	1269	U	C2-N1-C1'	6.00	124.91	117.70
36	5	2834	G	O5'-P-OP2	-6.00	100.30	105.70
36	5	2293	C	N3-C4-C5	6.00	124.30	121.90
37	7	90	U	N3-C4-O4	-6.00	115.20	119.40
36	5	1891	A	O5'-P-OP2	-6.00	100.30	105.70
36	5	2310	U	C2-N1-C1'	6.00	124.90	117.70
38	8	33	A	N1-C6-N6	6.00	122.20	118.60
36	1	2726	C	C2-N3-C4	-6.00	116.90	119.90
36	5	2300	G	C5-C6-N1	6.00	114.50	111.50
36	1	2891	U	C5-C4-O4	-6.00	122.30	125.90
36	5	417	A	OP2-P-O3'	6.00	118.40	105.20
36	5	834	U	C6-N1-C2	6.00	124.60	121.00
36	5	2915	U	N3-C4-C5	6.00	118.20	114.60
36	5	2983	C	O5'-P-OP1	-6.00	100.30	105.70
36	1	790	U	C5-C4-O4	6.00	129.50	125.90
36	1	1304	A	O5'-P-OP1	-6.00	100.31	105.70
36	5	662	U	N3-C4-O4	-6.00	115.20	119.40
36	5	1335	C	N1-C2-O2	-6.00	115.30	118.90
36	5	810	A	C2-N3-C4	5.99	113.60	110.60
38	8	113	U	C2-N1-C1'	5.99	124.89	117.70
36	5	649	A	C5-C6-N6	-5.99	118.91	123.70
36	5	1115	G	C5-C6-O6	5.99	132.19	128.60
36	5	107	A	C2-N3-C4	5.99	113.59	110.60
36	5	758	C	O5'-P-OP2	-5.99	100.31	105.70
36	5	1148	G	N9-C4-C5	-5.99	103.00	105.40
36	5	1604	G	C8-N9-C1'	-5.99	119.21	127.00
1	2	404	G	C8-N9-C4	5.99	108.80	106.40
69	O3	48	ARG	NE-CZ-NH1	5.99	123.29	120.30
36	5	1149	G	C4-C5-N7	-5.99	108.41	110.80
36	5	2621	G	N1-C6-O6	5.99	123.49	119.90
36	1	3005	A	N1-C6-N6	-5.99	115.01	118.60
36	5	1367	G	C4-N9-C1'	5.99	134.28	126.50
36	1	3228	C	C2-N1-C1'	5.99	125.38	118.80
1	6	371	G	C8-N9-C1'	-5.99	119.22	127.00
36	5	516	A	C8-N9-C4	5.99	108.19	105.80
25	d3	33	LEU	CA-CB-CG	-5.98	101.54	115.30
36	5	101	G	O4'-C1'-N9	5.98	112.99	108.20
1	2	1573	A	P-O3'-C3'	5.98	126.88	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1858	A	C5-C6-N6	-5.98	118.92	123.70
36	5	684	G	C6-C5-N7	-5.98	126.81	130.40
36	1	2631	U	N3-C4-O4	-5.98	115.22	119.40
36	5	1154	A	C2-N3-C4	5.98	113.59	110.60
36	5	1198	C	N3-C2-O2	-5.98	117.72	121.90
1	2	74	U	O4'-C1'-N1	5.98	112.98	108.20
1	2	736	C	C5-C6-N1	5.98	123.99	121.00
36	5	1788	C	C5-C6-N1	5.98	123.99	121.00
36	5	2191	U	N3-C4-O4	-5.98	115.22	119.40
1	6	305	C	N1-C2-O2	-5.97	115.31	118.90
1	6	309	C	O5'-P-OP1	-5.97	100.32	105.70
36	5	646	A	O5'-P-OP1	5.97	117.87	110.70
36	5	888	A	C2-N3-C4	-5.97	107.61	110.60
36	1	278	U	N3-C4-O4	5.97	123.58	119.40
36	1	1064	A	O4'-C1'-N9	-5.97	103.42	108.20
36	1	2984	C	N3-C2-O2	-5.97	117.72	121.90
1	6	767	U	OP1-P-O3'	5.97	118.34	105.20
36	5	1710	C	C5-C6-N1	-5.97	118.01	121.00
36	5	2281	A	O4'-C1'-N9	5.97	112.98	108.20
36	1	952	A	C8-N9-C4	-5.97	103.41	105.80
36	5	1371	G	C5-N7-C8	5.97	107.28	104.30
36	5	2916	U	OP1-P-O3'	5.97	118.33	105.20
36	1	979	U	O4'-C1'-N1	5.97	112.97	108.20
36	1	1324	U	O5'-P-OP1	5.97	117.86	110.70
36	1	1926	C	N1-C2-O2	-5.97	115.32	118.90
36	5	2323	G	N9-C4-C5	5.97	107.79	105.40
36	1	1360	C	C6-N1-C2	5.96	122.69	120.30
36	5	291	C	N3-C4-N4	-5.96	113.82	118.00
36	5	2372	A	C8-N9-C4	-5.96	103.41	105.80
36	1	2298	U	N3-C4-O4	-5.96	115.23	119.40
36	1	2651	G	C4-C5-N7	-5.96	108.42	110.80
1	6	1751	C	C6-N1-C2	5.96	122.69	120.30
36	5	638	C	C2-N3-C4	-5.96	116.92	119.90
36	5	1112	A	N3-C4-N9	5.96	132.17	127.40
36	1	2385	G	C4-N9-C1'	-5.96	118.75	126.50
36	1	1365	G	N9-C4-C5	5.96	107.78	105.40
36	1	2140	U	O5'-P-OP2	-5.96	100.34	105.70
36	1	2409	G	C5-C6-O6	5.96	132.17	128.60
36	5	1156	C	N1-C2-O2	-5.96	115.33	118.90
36	5	1926	C	N3-C2-O2	5.96	126.07	121.90
36	1	915	A	C8-N9-C4	-5.95	103.42	105.80
36	1	2243	A	O5'-P-OP2	-5.95	100.34	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	614	C	O5'-P-OP2	-5.95	100.34	105.70
36	1	2393	G	C8-N9-C4	5.95	108.78	106.40
1	6	337	G	N3-C4-N9	5.95	129.57	126.00
1	6	453	U	N3-C4-O4	-5.95	115.23	119.40
36	5	2250	G	N1-C6-O6	-5.95	116.33	119.90
38	8	111	A	C6-C5-N7	-5.95	128.13	132.30
1	2	1206	U	N3-C4-O4	5.95	123.56	119.40
36	5	2302	G	C5-C6-O6	5.95	132.17	128.60
36	5	2607	G	OP2-P-O3'	5.95	118.28	105.20
39	L2	191	LEU	CA-CB-CG	-5.94	101.63	115.30
36	1	1435	A	OP1-P-OP2	-5.94	110.69	119.60
36	1	1450	G	O5'-P-OP2	5.94	117.83	110.70
36	5	906	A	C6-N1-C2	-5.94	115.03	118.60
36	5	909	G	C4-C5-N7	-5.94	108.42	110.80
38	8	113	U	C5-C6-N1	5.94	125.67	122.70
36	1	2163	C	C5-C4-N4	5.94	124.36	120.20
36	1	2772	C	O4'-C1'-N1	5.94	112.95	108.20
36	5	2531	C	N3-C2-O2	-5.94	117.74	121.90
36	5	2662	G	N3-C4-C5	-5.94	125.63	128.60
36	1	682	U	N3-C4-C5	5.94	118.16	114.60
36	1	3217	C	C6-N1-C1'	-5.94	113.67	120.80
36	1	629	U	OP2-P-O3'	5.94	118.26	105.20
36	1	2350	C	C5-C6-N1	-5.94	118.03	121.00
36	5	1878	G	C8-N9-C1'	-5.94	119.28	127.00
38	8	55	U	N3-C4-O4	5.94	123.56	119.40
36	1	919	U	N1-C2-O2	5.94	126.95	122.80
36	1	1434	G	N7-C8-N9	5.94	116.07	113.10
36	1	350	C	O5'-P-OP1	-5.93	100.36	105.70
36	1	1848	G	O5'-P-OP1	-5.93	100.36	105.70
36	5	3027	A	N1-C6-N6	5.93	122.16	118.60
36	1	701	G	OP2-P-O3'	5.93	118.25	105.20
1	6	1777	G	N1-C6-O6	5.93	123.46	119.90
36	5	41	G	C4-C5-N7	5.93	113.17	110.80
36	5	1130	A	N1-C2-N3	-5.93	126.33	129.30
36	1	226	C	C6-N1-C2	-5.93	117.93	120.30
36	1	2964	G	O5'-P-OP2	-5.93	100.36	105.70
1	6	804	A	N1-C6-N6	5.93	122.16	118.60
36	5	2180	G	O5'-P-OP2	-5.93	100.36	105.70
37	7	90	U	C4-C5-C6	-5.93	116.14	119.70
36	1	962	A	N9-C4-C5	5.93	108.17	105.80
36	1	392	G	C5-C6-O6	-5.93	125.04	128.60
36	1	658	G	C8-N9-C1'	-5.93	119.30	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1112	A	C5-N7-C8	-5.93	100.94	103.90
1	6	1643	U	C2-N3-C4	-5.93	123.44	127.00
36	5	805	G	N9-C4-C5	-5.93	103.03	105.40
36	1	1902	G	C6-C5-N7	-5.92	126.85	130.40
36	5	1307	G	N1-C6-O6	-5.92	116.34	119.90
36	5	2843	U	N3-C2-O2	-5.92	118.05	122.20
36	5	2878	G	C5-C6-N1	5.92	114.46	111.50
37	7	80	G	N3-C4-N9	5.92	129.56	126.00
37	7	98	C	O5'-P-OP2	-5.92	100.37	105.70
36	1	278	U	C6-N1-C2	-5.92	117.45	121.00
36	1	1931	U	C2-N1-C1'	-5.92	110.59	117.70
36	1	2397	A	C5-N7-C8	-5.92	100.94	103.90
36	1	109	A	N1-C6-N6	-5.92	115.05	118.60
36	5	2611	U	C4-C5-C6	5.92	123.25	119.70
36	1	1295	G	N1-C6-O6	-5.92	116.35	119.90
36	1	2305	G	C8-N9-C1'	-5.92	119.31	127.00
36	1	905	U	O5'-P-OP2	-5.92	100.37	105.70
36	5	1604	G	N3-C4-N9	5.92	129.55	126.00
36	5	2663	G	O5'-P-OP2	-5.92	100.38	105.70
36	1	2621	G	N9-C4-C5	5.92	107.77	105.40
36	1	1098	A	C8-N9-C4	-5.91	103.44	105.80
36	1	3375	A	C8-N9-C4	-5.91	103.44	105.80
36	5	271	C	C6-N1-C2	5.91	122.67	120.30
36	1	2797	C	N3-C4-C5	-5.91	119.53	121.90
36	5	2928	C	C2-N1-C1'	5.91	125.30	118.80
36	1	1159	A	O4'-C1'-N9	5.91	112.93	108.20
36	1	1169	A	OP2-P-O3'	5.91	118.20	105.20
37	3	93	C	C6-N1-C2	5.91	122.66	120.30
36	5	909	G	C5-C6-O6	5.91	132.15	128.60
68	o2	47	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	2	1174	C	N1-C2-O2	5.91	122.44	118.90
1	2	1196	A	P-O3'-C3'	5.91	126.79	119.70
36	1	399	A	O5'-P-OP1	-5.91	100.38	105.70
36	1	1351	U	N1-C2-O2	5.91	126.94	122.80
36	1	1581	C	N1-C2-O2	5.91	122.45	118.90
36	5	2293	C	N1-C2-O2	5.91	122.44	118.90
36	1	1175	C	O5'-P-OP1	-5.91	100.39	105.70
36	1	2550	U	N1-C2-N3	5.91	118.44	114.90
38	4	41	A	N1-C2-N3	5.91	132.25	129.30
1	6	1634	C	N3-C2-O2	-5.91	117.77	121.90
36	5	693	A	O5'-P-OP2	5.91	117.79	110.70
36	5	2873	U	O5'-P-OP2	-5.91	100.38	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2991	A	C8-N9-C4	-5.91	103.44	105.80
36	1	806	A	O4'-C1'-N9	-5.90	103.48	108.20
36	1	816	A	OP2-P-O3'	5.90	118.18	105.20
36	1	3269	U	C5-C4-O4	5.90	129.44	125.90
1	6	1097	U	P-O3'-C3'	5.90	126.78	119.70
38	8	8	C	C6-N1-C2	-5.90	117.94	120.30
36	1	910	G	C5-C6-N1	-5.90	108.55	111.50
40	l3	275	ARG	NE-CZ-NH1	-5.90	117.35	120.30
36	5	1390	A	C8-N9-C4	-5.90	103.44	105.80
36	5	2836	C	C2-N3-C4	-5.90	116.95	119.90
1	2	1486	G	N7-C8-N9	5.90	116.05	113.10
36	1	220	G	C5-C6-O6	-5.90	125.06	128.60
36	1	2187	G	C5-C6-N1	-5.90	108.55	111.50
36	1	2658	G	C8-N9-C4	5.90	108.76	106.40
36	1	2861	U	O5'-P-OP1	-5.90	100.39	105.70
36	1	2941	A	O4'-C1'-N9	-5.90	103.48	108.20
1	2	1462	G	C5-C6-O6	-5.90	125.06	128.60
1	6	858	G	C6-C5-N7	-5.90	126.86	130.40
36	5	39	A	N9-C4-C5	-5.89	103.44	105.80
36	1	1307	G	P-O3'-C3'	5.89	126.77	119.70
36	5	2164	A	C6-C5-N7	-5.89	128.18	132.30
36	1	25	U	N3-C4-O4	5.89	123.52	119.40
36	1	217	U	OP1-P-O3'	5.89	118.16	105.20
36	1	282	G	N3-C4-C5	-5.89	125.66	128.60
36	1	3048	A	O5'-P-OP2	-5.89	100.40	105.70
1	6	619	A	OP2-P-O3'	5.89	118.16	105.20
36	5	2314	U	N3-C4-O4	5.89	123.52	119.40
36	5	2648	G	OP1-P-O3'	5.89	118.16	105.20
1	6	111	U	N1-C2-N3	5.89	118.43	114.90
36	5	2993	G	C5-C6-N1	5.89	114.44	111.50
36	5	3309	G	N3-C4-N9	5.89	129.53	126.00
36	1	33	G	O5'-P-OP2	-5.89	100.40	105.70
1	6	901	G	C4-C5-N7	5.89	113.16	110.80
36	5	2283	G	C5-C6-O6	-5.89	125.07	128.60
36	5	2660	G	N9-C4-C5	-5.89	103.05	105.40
36	1	636	C	C2-N1-C1'	5.88	125.27	118.80
1	6	1773	C	C4-C5-C6	5.88	120.34	117.40
43	l6	30	LEU	CA-CB-CG	5.88	128.83	115.30
76	q0	111	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	2	1560	U	C5-C4-O4	5.88	129.43	125.90
36	1	41	G	OP2-P-O3'	5.88	118.14	105.20
36	1	3013	U	O5'-P-OP2	-5.88	100.41	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1328	C	C4-C5-C6	5.88	120.34	117.40
36	1	681	U	N3-C2-O2	5.88	126.32	122.20
1	2	554	C	N3-C4-C5	-5.88	119.55	121.90
36	1	3183	A	C5-C6-N6	-5.88	119.00	123.70
36	5	666	A	N1-C6-N6	-5.88	115.07	118.60
36	5	3126	C	C4-C5-C6	-5.88	114.46	117.40
1	2	1762	A	C8-N9-C4	5.88	108.15	105.80
36	1	2628	A	C6-N1-C2	-5.88	115.07	118.60
36	1	3265	C	C6-N1-C2	5.88	122.65	120.30
37	3	88	G	N3-C4-C5	-5.88	125.66	128.60
1	6	993	A	O5'-P-OP2	-5.88	100.41	105.70
36	5	1107	C	OP2-P-O3'	5.88	118.13	105.20
36	1	200	C	C2-N1-C1'	5.88	125.26	118.80
37	3	86	U	N1-C2-O2	-5.88	118.69	122.80
73	O7	5	THR	C-N-CD	5.88	140.74	128.40
36	5	875	G	O5'-P-OP1	5.88	117.75	110.70
36	1	959	C	C5-C4-N4	-5.87	116.09	120.20
36	1	1397	C	N3-C4-C5	5.87	124.25	121.90
36	1	2244	A	N7-C8-N9	-5.87	110.86	113.80
1	6	299	A	O5'-P-OP2	-5.87	100.41	105.70
36	5	1208	U	O5'-P-OP1	-5.87	100.42	105.70
36	5	2278	C	N3-C4-C5	5.87	124.25	121.90
1	2	1328	G	C8-N9-C4	5.87	108.75	106.40
36	1	281	G	C6-N1-C2	-5.87	121.58	125.10
36	1	668	G	N9-C4-C5	5.87	107.75	105.40
1	6	371	G	C4-N9-C1'	5.87	134.13	126.50
36	5	718	G	N3-C4-C5	-5.87	125.67	128.60
36	1	1131	G	N9-C4-C5	-5.87	103.05	105.40
1	6	1280	C	N3-C4-C5	-5.87	119.55	121.90
36	5	3200	G	C6-C5-N7	-5.87	126.88	130.40
36	1	1117	G	O5'-P-OP1	-5.87	100.42	105.70
36	5	2753	G	N3-C2-N2	-5.87	115.79	119.90
36	1	1060	U	C5-C6-N1	-5.87	119.77	122.70
36	1	1299	U	C5-C6-N1	-5.87	119.77	122.70
36	5	1206	G	C5-C6-O6	5.87	132.12	128.60
36	5	2110	G	C5-C6-O6	-5.87	125.08	128.60
36	1	1442	U	N3-C2-O2	5.86	126.30	122.20
36	1	2139	A	N1-C6-N6	-5.86	115.08	118.60
36	5	1316	C	C4-C5-C6	5.86	120.33	117.40
36	5	2866	U	OP1-P-O3'	5.86	118.10	105.20
36	1	1445	U	C5-C4-O4	-5.86	122.38	125.90
36	1	2314	U	O5'-P-OP2	-5.86	100.42	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2598	G	C2-N3-C4	5.86	114.83	111.90
36	5	655	C	C6-N1-C2	-5.86	117.95	120.30
36	1	1112	A	N1-C6-N6	5.86	122.12	118.60
36	1	3059	G	C4-C5-N7	-5.86	108.46	110.80
36	5	666	A	O5'-P-OP1	-5.86	100.43	105.70
37	7	87	G	N3-C2-N2	-5.86	115.80	119.90
1	2	145	A	C8-N9-C4	-5.86	103.46	105.80
1	6	756	A	C8-N9-C4	-5.86	103.46	105.80
36	5	3212	C	C2-N3-C4	-5.86	116.97	119.90
36	1	3181	C	C4-C5-C6	5.86	120.33	117.40
38	4	111	A	N1-C6-N6	5.86	122.11	118.60
36	5	2138	A	C5-C6-N1	-5.86	114.77	117.70
47	m0	88	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	2	1654	G	O5'-P-OP2	-5.85	100.43	105.70
36	5	1461	A	N1-C6-N6	-5.85	115.09	118.60
36	5	2869	U	N3-C2-O2	-5.85	118.10	122.20
1	2	728	U	N1-C2-O2	5.85	126.90	122.80
36	1	1481	A	C4-N9-C1'	5.85	136.84	126.30
36	1	2293	C	C5-C4-N4	-5.85	116.10	120.20
36	5	2757	U	C6-N1-C2	-5.85	117.49	121.00
36	1	1301	A	N1-C6-N6	5.85	122.11	118.60
36	1	2698	G	O5'-P-OP1	-5.85	100.44	105.70
1	6	75	U	O4'-C1'-N1	5.85	112.88	108.20
36	5	3012	A	N9-C4-C5	-5.85	103.46	105.80
36	5	3123	A	N7-C8-N9	-5.85	110.88	113.80
36	1	2821	C	O5'-P-OP2	5.85	117.72	110.70
36	1	3344	A	N1-C2-N3	5.85	132.22	129.30
1	6	1765	A	N1-C6-N6	-5.85	115.09	118.60
1	6	1775	U	C5-C6-N1	-5.85	119.78	122.70
36	5	820	A	C8-N9-C4	-5.85	103.46	105.80
36	5	1119	C	C2-N3-C4	-5.85	116.98	119.90
36	5	2353	G	C5-C6-O6	-5.85	125.09	128.60
1	2	734	A	OP1-P-O3'	5.84	118.06	105.20
36	1	780	A	N1-C2-N3	5.84	132.22	129.30
36	1	964	G	OP2-P-O3'	5.84	118.06	105.20
1	6	144	U	N1-C2-N3	5.84	118.41	114.90
1	2	1761	U	N3-C2-O2	-5.84	118.11	122.20
38	4	90	U	N1-C2-O2	-5.84	118.71	122.80
36	5	1008	U	C2-N1-C1'	-5.84	110.69	117.70
36	1	343	U	N1-C2-N3	5.84	118.41	114.90
36	1	2411	U	N3-C4-C5	5.84	118.10	114.60
36	1	3244	A	O4'-C1'-N9	-5.84	103.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	973	A	N1-C6-N6	5.84	122.10	118.60
36	5	1149	G	C2-N3-C4	5.84	114.82	111.90
36	5	2407	C	O5'-P-OP2	-5.84	100.44	105.70
36	5	2942	C	N3-C4-N4	5.84	122.09	118.00
36	5	3040	A	N7-C8-N9	-5.84	110.88	113.80
36	1	1150	A	C5-C6-N1	5.84	120.62	117.70
36	1	1400	G	O5'-P-OP2	-5.84	100.44	105.70
36	1	1436	U	N3-C2-O2	5.84	126.29	122.20
36	1	2870	C	C4-C5-C6	-5.84	114.48	117.40
64	n8	12	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	6	1472	C	N1-C2-O2	-5.84	115.40	118.90
36	5	2405	C	C2-N3-C4	-5.84	116.98	119.90
36	5	2627	C	C2-N3-C4	-5.84	116.98	119.90
36	5	3145	C	C6-N1-C2	5.84	122.64	120.30
36	1	2146	C	N3-C4-C5	5.84	124.23	121.90
36	5	341	G	N1-C6-O6	5.84	123.40	119.90
36	5	1128	U	C2-N3-C4	-5.84	123.50	127.00
36	5	1431	G	C4-C5-N7	-5.84	108.47	110.80
36	5	2351	U	C5-C4-O4	5.84	129.40	125.90
36	5	3055	U	C5-C4-O4	-5.84	122.40	125.90
36	1	943	U	N1-C2-O2	5.83	126.89	122.80
36	1	519	A	N1-C6-N6	5.83	122.10	118.60
36	1	1669	C	N3-C2-O2	5.83	125.98	121.90
36	1	2281	A	C5-C6-N1	-5.83	114.78	117.70
36	5	2335	G	N3-C4-C5	-5.83	125.68	128.60
1	6	577	G	C4-C5-N7	5.83	113.13	110.80
36	5	1373	A	O5'-P-OP2	-5.83	100.45	105.70
36	5	3006	A	C8-N9-C4	-5.83	103.47	105.80
36	1	907	G	N3-C4-C5	-5.83	125.69	128.60
36	1	1510	G	N9-C4-C5	-5.83	103.07	105.40
36	1	2865	U	C5-C4-O4	-5.83	122.40	125.90
36	5	41	G	C5-C6-O6	-5.83	125.10	128.60
36	5	2343	C	N3-C4-N4	-5.83	113.92	118.00
1	2	1022	C	C2-N3-C4	-5.83	116.99	119.90
36	1	939	U	N3-C2-O2	5.82	126.28	122.20
36	1	225	C	C4-C5-C6	5.82	120.31	117.40
36	1	2403	G	OP1-P-O3'	5.82	118.01	105.20
36	5	3343	G	N9-C4-C5	-5.82	103.07	105.40
1	2	287	G	O4'-C1'-N9	5.82	112.86	108.20
1	2	736	C	C2-N1-C1'	5.82	125.20	118.80
36	5	2780	A	N1-C6-N6	5.82	122.09	118.60
36	1	2930	A	O4'-C1'-N9	5.82	112.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2996	U	C5-C4-O4	-5.82	122.41	125.90
36	1	2121	G	N1-C6-O6	-5.82	116.41	119.90
1	6	418	G	O5'-P-OP1	-5.82	100.46	105.70
1	6	1536	G	O5'-P-OP1	-5.82	100.46	105.70
1	6	1640	C	O5'-P-OP2	-5.82	100.46	105.70
36	5	1604	G	C4-N9-C1'	5.82	134.06	126.50
36	5	1911	A	N1-C6-N6	5.82	122.09	118.60
36	1	3090	U	N1-C2-O2	-5.82	118.73	122.80
1	6	1503	A	C2-N3-C4	-5.82	107.69	110.60
36	5	103	G	N3-C4-N9	-5.82	122.51	126.00
36	5	283	G	C5-N7-C8	-5.82	101.39	104.30
36	5	1163	A	N1-C6-N6	-5.82	115.11	118.60
36	1	498	A	C8-N9-C4	-5.81	103.47	105.80
36	1	859	G	C4-N9-C1'	5.81	134.06	126.50
36	5	859	G	C2-N3-C4	5.81	114.81	111.90
36	1	2847	A	O5'-P-OP1	-5.81	100.47	105.70
1	6	755	A	N9-C1'-C2'	-5.81	105.61	112.00
36	5	424	G	N3-C4-C5	-5.81	125.69	128.60
36	5	1112	A	C4-N9-C1'	5.81	136.76	126.30
36	5	1169	A	C2-N3-C4	-5.81	107.69	110.60
36	5	2396	G	C6-N1-C2	-5.81	121.61	125.10
36	5	2816	G	C5-C6-O6	-5.81	125.11	128.60
36	1	2245	C	C6-N1-C2	-5.81	117.98	120.30
1	6	945	U	N3-C2-O2	-5.81	118.13	122.20
36	5	1496	C	C2-N1-C1'	5.81	125.19	118.80
36	1	348	A	OP2-P-O3'	5.81	117.98	105.20
36	1	1135	A	O5'-P-OP2	-5.81	100.47	105.70
36	1	2358	A	O5'-P-OP2	-5.81	100.47	105.70
36	5	883	A	O5'-P-OP2	5.81	117.67	110.70
36	5	1406	A	N1-C6-N6	5.81	122.08	118.60
36	5	1844	C	N3-C2-O2	-5.81	117.83	121.90
37	3	92	A	C2-N3-C4	-5.81	107.70	110.60
1	6	1657	U	C2-N1-C1'	5.81	124.67	117.70
36	1	2177	G	N3-C4-N9	5.80	129.48	126.00
36	1	2873	U	O5'-P-OP2	-5.80	100.47	105.70
36	5	721	G	C5-C6-N1	5.80	114.40	111.50
36	5	819	U	N1-C2-O2	-5.80	118.74	122.80
36	5	1390	A	N9-C4-C5	5.80	108.12	105.80
36	5	2886	U	C5-C4-O4	5.80	129.38	125.90
36	5	835	G	C5-C6-N1	5.80	114.40	111.50
36	5	2618	G	N9-C4-C5	-5.80	103.08	105.40
36	1	860	G	C8-N9-C4	5.80	108.72	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	908	G	N7-C8-N9	-5.80	110.20	113.10
36	1	2283	G	N1-C2-N2	5.80	121.42	116.20
36	5	1151	U	C5-C6-N1	5.80	125.60	122.70
36	1	1565	G	C8-N9-C4	-5.80	104.08	106.40
36	1	2874	G	C5-C6-N1	-5.80	108.60	111.50
36	5	1206	G	N9-C4-C5	5.80	107.72	105.40
36	5	2110	G	N9-C4-C5	-5.80	103.08	105.40
36	5	2404	A	N1-C2-N3	-5.80	126.40	129.30
36	5	2624	G	C6-C5-N7	-5.80	126.92	130.40
37	7	5	G	N9-C4-C5	-5.80	103.08	105.40
36	1	2631	U	C5-C6-N1	-5.80	119.80	122.70
36	5	200	C	C2-N1-C1'	5.80	125.18	118.80
36	5	280	U	N1-C2-O2	-5.80	118.74	122.80
36	5	956	U	C2-N3-C4	-5.80	123.52	127.00
36	1	1142	G	C5-C6-O6	-5.79	125.12	128.60
36	1	2883	U	N1-C2-O2	5.79	126.86	122.80
36	5	109	A	O5'-P-OP2	-5.79	100.48	105.70
1	2	831	U	C6-N1-C2	-5.79	117.52	121.00
36	1	1586	G	N3-C4-N9	5.79	129.48	126.00
36	5	3052	G	C8-N9-C1'	5.79	134.53	127.00
36	1	954	U	O5'-P-OP2	-5.79	100.49	105.70
37	3	91	G	C6-C5-N7	-5.79	126.92	130.40
36	5	2732	G	O5'-P-OP2	-5.79	100.49	105.70
1	2	734	A	P-O3'-C3'	5.79	126.65	119.70
36	1	2124	G	N1-C6-O6	5.79	123.37	119.90
36	1	2953	U	N1-C2-O2	-5.79	118.75	122.80
36	5	41	G	OP2-P-O3'	5.79	117.94	105.20
36	5	972	A	C4-C5-C6	5.79	119.89	117.00
36	5	2982	A	C8-N9-C4	5.79	108.12	105.80
36	5	3053	G	N1-C6-O6	5.79	123.37	119.90
37	7	105	C	N3-C2-O2	-5.79	117.85	121.90
36	5	812	G	C5-N7-C8	5.79	107.19	104.30
37	7	14	U	N3-C4-O4	-5.79	115.35	119.40
36	1	365	A	C6-C5-N7	-5.79	128.25	132.30
1	6	1751	C	C5-C6-N1	-5.79	118.11	121.00
36	5	815	G	C2-N3-C4	5.79	114.79	111.90
1	6	358	U	O5'-P-OP1	-5.78	100.50	105.70
36	1	2730	G	N3-C2-N2	-5.78	115.85	119.90
36	1	2984	C	C5-C4-N4	5.78	124.25	120.20
36	5	964	G	C8-N9-C4	-5.78	104.09	106.40
36	5	2814	G	C6-C5-N7	-5.78	126.93	130.40
36	5	609	G	C5-C6-O6	-5.78	125.13	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1764	C	C6-N1-C2	5.78	122.61	120.30
36	5	264	G	N1-C6-O6	5.78	123.37	119.90
36	1	1307	G	C5-C6-O6	5.78	132.07	128.60
36	1	1351	U	N3-C2-O2	-5.78	118.16	122.20
1	6	977	A	C5-C6-N6	-5.78	119.08	123.70
36	5	702	C	C6-N1-C2	-5.77	117.99	120.30
36	1	1152	G	C4-C5-N7	5.77	113.11	110.80
36	1	1307	G	C2'-C3'-O3'	5.77	122.94	113.70
36	1	317	A	O5'-P-OP2	-5.77	100.51	105.70
36	1	880	G	C4-C5-N7	-5.77	108.49	110.80
36	5	718	G	C8-N9-C4	-5.77	104.09	106.40
36	5	3052	G	N3-C2-N2	-5.77	115.86	119.90
36	1	404	G	C5-C6-N1	-5.77	108.62	111.50
36	1	1114	U	C4-C5-C6	-5.77	116.24	119.70
36	1	2944	U	O5'-P-OP1	-5.77	100.51	105.70
36	5	1465	A	N1-C2-N3	5.77	132.19	129.30
36	5	2710	C	N1-C2-O2	-5.77	115.44	118.90
36	5	3154	C	C6-N1-C2	-5.77	117.99	120.30
36	1	3206	C	C6-N1-C2	5.77	122.61	120.30
36	5	88	A	N7-C8-N9	-5.77	110.92	113.80
36	5	1306	G	C8-N9-C4	5.77	108.71	106.40
36	5	2633	U	C5-C6-N1	-5.77	119.82	122.70
36	5	2873	U	N1-C2-N3	5.77	118.36	114.90
36	1	155	G	N1-C6-O6	-5.76	116.44	119.90
36	5	2819	A	N1-C6-N6	-5.76	115.14	118.60
53	m7	135	ARG	NE-CZ-NH1	5.76	123.18	120.30
36	1	2190	U	OP2-P-O3'	5.76	117.88	105.20
36	5	640	U	N1-C2-N3	5.76	118.36	114.90
36	5	2273	G	C4-C5-N7	-5.76	108.50	110.80
36	5	2873	U	N1-C2-O2	-5.76	118.77	122.80
36	1	1366	A	N7-C8-N9	5.76	116.68	113.80
36	1	2952	G	C5-C6-N1	-5.76	108.62	111.50
36	5	1598	G	N1-C6-O6	-5.76	116.44	119.90
36	1	3057	U	N1-C2-N3	5.76	118.36	114.90
36	5	1635	G	N1-C6-O6	-5.76	116.44	119.90
36	5	2139	A	C5-C6-N6	5.76	128.31	123.70
36	5	2403	G	C2-N3-C4	5.76	114.78	111.90
36	5	2792	A	C8-N9-C4	-5.76	103.50	105.80
36	5	3109	G	N1-C6-O6	-5.76	116.44	119.90
1	6	1112	G	C5-C6-O6	-5.76	125.14	128.60
36	5	815	G	N3-C4-C5	-5.76	125.72	128.60
36	5	906	A	C5-C6-N1	5.76	120.58	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2273	G	C4-N9-C1'	-5.76	119.02	126.50
37	7	19	C	O5'-P-OP2	-5.76	100.52	105.70
36	1	3015	G	C5-C6-O6	-5.75	125.15	128.60
1	6	1355	C	C6-N1-C2	-5.75	118.00	120.30
36	5	1082	U	N1-C2-N3	5.75	118.35	114.90
36	5	1239	C	C6-N1-C2	-5.75	118.00	120.30
36	5	1331	U	N3-C4-C5	5.75	118.05	114.60
1	2	581	U	C2-N1-C1'	5.75	124.60	117.70
1	6	1	U	C6-N1-C1'	-5.75	113.15	121.20
36	5	2290	C	N3-C4-C5	5.75	124.20	121.90
36	5	2838	A	O5'-P-OP1	5.75	117.60	110.70
36	5	1138	U	O5'-P-OP2	-5.75	100.53	105.70
36	5	1331	U	N3-C2-O2	5.75	126.22	122.20
36	1	690	A	OP1-P-O3'	5.75	117.85	105.20
36	1	1335	C	N3-C2-O2	-5.75	117.88	121.90
36	1	2831	G	C5-C6-O6	-5.75	125.15	128.60
1	6	795	U	N1-C2-O2	5.75	126.82	122.80
36	5	682	U	C2-N1-C1'	-5.75	110.80	117.70
36	5	1317	A	C5-C6-N6	-5.75	119.10	123.70
36	5	2354	C	N3-C4-N4	5.75	122.02	118.00
36	1	2572	C	C6-N1-C1'	-5.75	113.91	120.80
36	1	2823	G	C4-C5-N7	-5.75	108.50	110.80
36	5	1127	G	C5-C6-N1	5.75	114.37	111.50
36	5	1141	C	C6-N1-C2	5.75	122.60	120.30
36	5	2161	G	N3-C2-N2	-5.75	115.88	119.90
1	2	393	C	N3-C4-C5	5.75	124.20	121.90
36	5	948	C	N3-C2-O2	5.75	125.92	121.90
36	5	948	C	C5-C4-N4	-5.75	116.18	120.20
37	3	79	A	N1-C2-N3	5.74	132.17	129.30
1	6	755	A	C3'-C2'-C1'	5.74	106.09	101.50
36	5	1156	C	C6-N1-C2	-5.74	118.00	120.30
36	5	1489	A	C4-C5-C6	5.74	119.87	117.00
36	1	1365	G	N1-C6-O6	-5.74	116.45	119.90
36	1	2276	G	N9-C4-C5	5.74	107.70	105.40
37	3	87	G	C8-N9-C4	5.74	108.70	106.40
36	1	851	C	C6-N1-C2	-5.74	118.00	120.30
36	1	3275	U	OP1-P-O3'	5.74	117.83	105.20
36	5	2865	U	N1-C2-N3	-5.74	111.45	114.90
36	1	1434	G	C5-N7-C8	-5.74	101.43	104.30
38	4	12	A	N1-C2-N3	-5.74	126.43	129.30
36	5	1369	A	N9-C4-C5	-5.74	103.50	105.80
1	2	187	G	OP1-P-O3'	5.74	117.82	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	878	G	N3-C4-C5	-5.74	125.73	128.60
36	1	1303	A	O5'-P-OP1	-5.74	100.54	105.70
36	1	2245	C	N3-C2-O2	-5.74	117.89	121.90
36	1	2798	C	C6-N1-C2	-5.74	118.01	120.30
64	N8	115	LYS	C-N-CA	-5.74	110.26	122.30
36	5	2295	A	C5-C6-N1	5.74	120.57	117.70
36	5	3005	A	O5'-P-OP2	-5.74	100.54	105.70
1	6	1389	C	C2-N1-C1'	5.73	125.11	118.80
1	6	1432	U	O4'-C1'-N1	5.73	112.79	108.20
36	5	609	G	N1-C2-N2	5.73	121.36	116.20
36	5	1002	A	O5'-P-OP2	-5.73	100.54	105.70
36	5	3052	G	C6-C5-N7	5.73	133.84	130.40
36	1	292	U	C5-C6-N1	-5.73	119.83	122.70
36	1	718	G	C4-C5-N7	5.73	113.09	110.80
36	1	1838	G	C5-C6-O6	-5.73	125.16	128.60
37	7	35	C	N3-C2-O2	5.73	125.91	121.90
36	1	869	G	N1-C6-O6	-5.73	116.46	119.90
1	6	321	C	C2-N1-C1'	5.73	125.10	118.80
1	6	1481	C	C6-N1-C2	-5.73	118.01	120.30
36	5	3136	G	C2-N3-C4	-5.73	109.04	111.90
36	1	2242	A	N9-C4-C5	5.73	108.09	105.80
36	1	68	C	OP2-P-O3'	5.73	117.80	105.20
36	1	1420	C	N1-C2-N3	5.73	123.21	119.20
36	5	2762	A	N1-C2-N3	-5.73	126.44	129.30
36	1	616	G	C5-C6-O6	-5.72	125.17	128.60
36	1	1163	A	OP1-P-OP2	5.72	128.19	119.60
36	1	1414	G	C5-C6-O6	-5.72	125.17	128.60
36	1	229	G	O5'-P-OP2	5.72	117.57	110.70
36	1	1151	U	N1-C2-N3	5.72	118.33	114.90
36	1	2863	G	N1-C2-N2	-5.72	111.05	116.20
36	5	987	U	N1-C2-N3	5.72	118.33	114.90
36	5	1608	C	N1-C2-O2	5.72	122.33	118.90
38	8	33	A	C5-C6-N6	-5.72	119.12	123.70
1	2	1761	U	P-O3'-C3'	5.72	126.56	119.70
36	1	637	C	C5-C6-N1	-5.72	118.14	121.00
36	5	672	A	N7-C8-N9	5.72	116.66	113.80
36	5	841	A	O5'-P-OP2	-5.72	100.55	105.70
36	5	2295	A	C5-C6-N6	-5.72	119.12	123.70
36	1	1843	C	N1-C2-O2	-5.72	115.47	118.90
36	5	1842	A	N9-C4-C5	-5.72	103.51	105.80
36	1	1102	A	OP1-P-O3'	5.72	117.77	105.20
36	1	2349	U	C5-C6-N1	-5.72	119.84	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1499	G	N3-C2-N2	5.72	123.90	119.90
40	13	244	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	2	831	U	C5-C6-N1	5.71	125.56	122.70
36	1	3264	G	O5'-P-OP1	-5.71	100.56	105.70
36	1	3361	G	N3-C4-C5	-5.71	125.74	128.60
1	6	1783	C	N1-C2-O2	5.71	122.33	118.90
36	5	903	U	N3-C2-O2	-5.71	118.20	122.20
37	7	40	C	C5-C4-N4	-5.71	116.20	120.20
1	2	720	G	OP1-P-O3'	5.71	117.77	105.20
36	1	1634	G	C8-N9-C4	-5.71	104.11	106.40
36	1	1364	C	N3-C4-C5	5.71	124.18	121.90
36	1	3362	A	C8-N9-C4	-5.71	103.52	105.80
1	6	400	A	N1-C6-N6	5.71	122.03	118.60
36	5	1512	U	N3-C2-O2	-5.71	118.20	122.20
36	1	2142	A	N3-C4-C5	-5.71	122.81	126.80
1	6	29	U	C5-C4-O4	5.71	129.32	125.90
36	5	1239	C	C2-N1-C1'	5.71	125.08	118.80
36	1	1507	G	N3-C2-N2	-5.71	115.91	119.90
36	1	3055	U	C5-C4-O4	-5.71	122.48	125.90
36	5	88	A	N9-C4-C5	-5.71	103.52	105.80
36	5	1725	C	C6-N1-C1'	5.71	127.65	120.80
36	1	2983	C	C2-N3-C4	-5.71	117.05	119.90
1	6	1188	G	N1-C6-O6	5.71	123.32	119.90
36	5	2940	A	C6-N1-C2	-5.71	115.18	118.60
36	5	2921	U	N1-C2-N3	5.70	118.32	114.90
36	1	2323	G	N3-C4-C5	-5.70	125.75	128.60
36	5	2836	C	O4'-C1'-N1	5.70	112.76	108.20
36	1	2818	U	C5'-C4'-O4'	-5.70	102.26	109.10
1	6	1478	G	C4-N9-C1'	5.70	133.91	126.50
36	5	1858	A	O4'-C1'-N9	5.70	112.76	108.20
36	1	2162	U	C4-C5-C6	-5.70	116.28	119.70
1	6	542	A	C6-C5-N7	-5.70	128.31	132.30
1	6	1473	U	C5-C4-O4	5.70	129.32	125.90
36	1	213	A	N9-C1'-C2'	-5.70	105.73	112.00
36	5	2354	C	N3-C2-O2	5.70	125.89	121.90
36	5	2904	U	C2-N3-C4	-5.70	123.58	127.00
36	1	2857	C	N3-C4-C5	5.70	124.18	121.90
36	5	2385	G	N3-C4-C5	5.70	131.45	128.60
37	7	37	G	N1-C6-O6	5.70	123.32	119.90
36	1	281	G	C2-N3-C4	5.69	114.75	111.90
36	1	1316	C	N1-C2-O2	-5.69	115.48	118.90
1	6	337	G	N3-C2-N2	5.69	123.89	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	967	A	C5-C6-N1	5.69	120.55	117.70
36	5	97	U	N3-C2-O2	5.69	126.19	122.20
36	5	3041	U	N1-C2-N3	-5.69	111.48	114.90
36	5	3215	A	C2-N3-C4	-5.69	107.75	110.60
37	7	9	C	N3-C4-C5	5.69	124.18	121.90
36	1	943	U	N3-C2-O2	-5.69	118.22	122.20
36	1	1907	C	C5-C6-N1	5.69	123.85	121.00
36	1	2281	A	N3-C4-C5	5.69	130.78	126.80
1	6	965	U	N1-C2-O2	5.69	126.78	122.80
1	6	1767	G	C4-N9-C1'	-5.69	119.10	126.50
36	5	308	A	O5'-P-OP2	-5.69	100.58	105.70
1	2	114	C	N1-C2-O2	-5.69	115.48	118.90
1	6	1739	C	C2-N1-C1'	-5.69	112.54	118.80
36	5	2632	G	N3-C2-N2	5.69	123.88	119.90
36	1	1836	C	N1-C2-O2	5.69	122.31	118.90
36	1	2899	C	OP2-P-O3'	5.69	117.72	105.20
36	1	199	A	O4'-C1'-N9	5.69	112.75	108.20
36	1	949	C	C5-C6-N1	-5.69	118.16	121.00
36	1	1053	A	C8-N9-C4	5.69	108.08	105.80
36	1	2787	G	C5-C6-N1	5.69	114.34	111.50
36	1	3305	A	N1-C6-N6	-5.69	115.19	118.60
36	5	1832	C	C6-N1-C2	5.69	122.58	120.30
36	5	2827	U	C5-C6-N1	-5.69	119.86	122.70
36	1	1152	G	O4'-C1'-N9	5.69	112.75	108.20
38	4	115	C	N3-C4-C5	5.69	124.17	121.90
1	2	830	U	N1-C2-O2	5.68	126.78	122.80
36	1	1425	U	N1-C2-N3	5.68	118.31	114.90
36	1	1464	G	O5'-P-OP2	-5.68	100.58	105.70
36	1	2833	A	C8-N9-C4	5.68	108.07	105.80
36	1	2891	U	C2-N3-C4	-5.68	123.59	127.00
36	5	38	U	C2-N3-C4	-5.68	123.59	127.00
36	5	1918	C	O5'-P-OP1	5.68	117.52	110.70
36	5	2180	G	C4-C5-N7	5.68	113.07	110.80
36	1	515	C	C5-C6-N1	5.68	123.84	121.00
36	5	2246	G	O5'-P-OP1	-5.68	100.59	105.70
36	1	2339	C	OP1-P-O3'	5.68	117.70	105.20
36	5	660	A	C2-N3-C4	5.68	113.44	110.60
36	1	2350	C	C2-N3-C4	-5.68	117.06	119.90
36	5	264	G	C6-C5-N7	-5.68	126.99	130.40
36	5	283	G	O4'-C1'-N9	-5.68	103.66	108.20
36	5	435	C	O5'-P-OP2	-5.68	100.59	105.70
38	8	140	G	C5-C6-N1	-5.68	108.66	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1160	C	N1-C2-N3	-5.68	115.22	119.20
36	1	3036	G	C4-N9-C1'	5.68	133.88	126.50
36	5	3126	C	N3-C4-C5	5.68	124.17	121.90
47	m0	167	LEU	CA-CB-CG	5.68	128.36	115.30
1	6	1697	G	N3-C4-N9	5.68	129.41	126.00
36	5	63	A	C5-C6-N6	-5.68	119.16	123.70
36	5	701	G	C4-C5-N7	-5.68	108.53	110.80
36	5	2820	A	O5'-P-OP1	5.68	117.51	110.70
1	2	380	U	N3-C2-O2	-5.67	118.23	122.20
38	4	16	G	O4'-C1'-N9	5.67	112.74	108.20
36	5	869	G	N3-C4-C5	-5.67	125.76	128.60
36	5	2385	G	C5-C6-O6	-5.67	125.20	128.60
36	1	517	G	C6-C5-N7	-5.67	127.00	130.40
36	1	585	A	O5'-P-OP2	-5.67	100.59	105.70
1	6	1582	U	C5-C6-N1	-5.67	119.86	122.70
1	6	1657	U	N3-C2-O2	-5.67	118.23	122.20
1	2	1559	A	O4'-C1'-N9	5.67	112.74	108.20
36	1	1335	C	C5-C6-N1	-5.67	118.16	121.00
36	1	2176	U	N3-C4-O4	-5.67	115.43	119.40
1	6	1109	G	C8-N9-C4	-5.67	104.13	106.40
36	5	1185	C	N3-C2-O2	-5.67	117.93	121.90
36	5	1927	G	C5-C6-O6	5.67	132.00	128.60
36	5	2364	G	C5-C6-O6	5.67	132.00	128.60
36	5	2662	G	C2-N3-C4	5.67	114.73	111.90
36	5	1213	G	C4-C5-N7	5.67	113.07	110.80
36	5	3218	A	C2-N3-C4	-5.67	107.77	110.60
1	2	308	C	N1-C2-O2	-5.67	115.50	118.90
36	1	1428	A	C4-C5-N7	5.67	113.53	110.70
1	6	1739	C	C6-N1-C1'	5.67	127.60	120.80
1	6	1782	A	N9-C4-C5	5.67	108.07	105.80
36	5	264	G	N3-C4-N9	5.67	129.40	126.00
36	5	1128	U	C5-C6-N1	-5.67	119.87	122.70
36	5	2249	G	P-O3'-C3'	5.67	126.50	119.70
36	1	1433	A	N3-C4-C5	-5.67	122.83	126.80
36	5	435	C	C2-N3-C4	-5.67	117.07	119.90
36	5	2550	U	N3-C2-O2	-5.67	118.23	122.20
36	5	2627	C	N3-C4-N4	-5.67	114.03	118.00
1	2	694	U	N1-C2-O2	5.66	126.77	122.80
36	1	1428	A	C6-C5-N7	-5.66	128.34	132.30
1	6	1700	C	N3-C2-O2	-5.66	117.94	121.90
36	5	100	A	N1-C6-N6	5.66	122.00	118.60
36	5	767	U	O4'-C1'-N1	5.66	112.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1436	U	C5-C4-O4	-5.66	122.50	125.90
36	5	3331	U	C5-C6-N1	-5.66	119.87	122.70
36	1	1420	C	C6-N1-C2	-5.66	118.03	120.30
36	5	1456	A	C8-N9-C4	5.66	108.06	105.80
36	1	2314	U	C5-C4-O4	-5.66	122.50	125.90
36	1	2712	U	C5-C4-O4	5.66	129.30	125.90
36	1	57	A	C5-C6-N1	-5.66	114.87	117.70
36	5	2930	A	O4'-C1'-N9	5.66	112.73	108.20
36	5	3017	A	N1-C6-N6	5.66	122.00	118.60
36	1	53	G	N9-C4-C5	-5.66	103.14	105.40
36	1	1405	U	N3-C2-O2	5.66	126.16	122.20
36	5	2296	A	C8-N9-C4	-5.66	103.54	105.80
36	5	2655	U	N3-C2-O2	5.66	126.16	122.20
76	q0	103	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	2	1490	C	C6-N1-C2	-5.66	118.04	120.30
36	1	424	G	N3-C2-N2	5.66	123.86	119.90
36	1	815	G	C4-C5-C6	5.66	122.19	118.80
36	1	1332	A	C8-N9-C4	-5.66	103.54	105.80
36	1	2134	G	OP1-P-OP2	-5.66	111.12	119.60
36	1	2375	G	O4'-C1'-N9	5.66	112.72	108.20
36	5	368	G	N9-C4-C5	5.66	107.66	105.40
36	5	2289	U	N1-C2-O2	5.66	126.76	122.80
36	1	426	G	C8-N9-C4	5.65	108.66	106.40
36	5	517	G	N3-C4-C5	-5.65	125.77	128.60
36	5	1381	A	O5'-P-OP1	-5.65	100.61	105.70
36	1	811	U	C4-C5-C6	5.65	123.09	119.70
36	1	940	G	N1-C6-O6	-5.65	116.51	119.90
36	1	1166	G	C8-N9-C4	5.65	108.66	106.40
1	6	1361	U	C2-N1-C1'	5.65	124.48	117.70
36	5	2746	A	C2-N3-C4	-5.65	107.77	110.60
37	7	1	G	N3-C4-N9	5.65	129.39	126.00
18	C6	28	LEU	CA-CB-CG	5.65	128.29	115.30
36	1	95	A	O5'-P-OP1	5.65	117.48	110.70
36	1	498	A	N1-C6-N6	-5.65	115.21	118.60
36	1	655	C	N3-C2-O2	-5.65	117.94	121.90
36	5	3012	A	N1-C6-N6	5.65	121.99	118.60
36	1	2870	C	C5-C4-N4	5.65	124.15	120.20
36	5	3135	U	O5'-P-OP1	-5.65	100.62	105.70
36	1	2355	G	C5-C6-O6	-5.65	125.21	128.60
36	1	2983	C	N3-C2-O2	-5.65	117.95	121.90
1	6	1614	A	O4'-C1'-N9	5.65	112.72	108.20
36	5	824	C	C6-N1-C2	-5.65	118.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	903	U	N1-C2-O2	5.65	126.75	122.80
38	4	99	C	C6-N1-C2	5.65	122.56	120.30
36	1	1340	G	N3-C4-N9	5.64	129.39	126.00
36	1	1916	U	C5-C6-N1	-5.64	119.88	122.70
36	1	2192	C	C4-C5-C6	5.64	120.22	117.40
36	5	1846	C	C2-N3-C4	-5.64	117.08	119.90
36	5	3228	C	N1-C2-O2	5.64	122.29	118.90
36	1	1199	C	C6-N1-C2	5.64	122.56	120.30
36	1	3302	U	C5-C6-N1	-5.64	119.88	122.70
36	5	964	G	N7-C8-N9	5.64	115.92	113.10
36	1	439	C	C2-N1-C1'	5.64	125.00	118.80
36	1	3174	A	C5-N7-C8	-5.64	101.08	103.90
36	5	642	U	O5'-P-OP2	-5.64	100.62	105.70
36	5	1547	G	O5'-P-OP1	-5.64	100.62	105.70
36	1	802	C	C6-N1-C2	-5.64	118.05	120.30
36	5	936	A	N9-C4-C5	5.64	108.06	105.80
36	1	91	G	C4-N9-C1'	-5.64	119.17	126.50
36	1	800	G	C4-C5-N7	-5.64	108.55	110.80
36	1	1141	C	N1-C2-N3	5.64	123.15	119.20
36	1	1392	G	C2-N3-C4	5.64	114.72	111.90
36	1	3045	G	C2-N3-C4	5.64	114.72	111.90
36	5	37	U	C6-N1-C2	-5.64	117.62	121.00
36	5	368	G	N1-C6-O6	-5.64	116.52	119.90
36	5	803	C	N1-C2-O2	-5.64	115.52	118.90
36	5	2988	C	N1-C2-O2	5.64	122.28	118.90
1	6	512	A	P-O3'-C3'	5.63	126.46	119.70
1	6	577	G	N7-C8-N9	5.63	115.92	113.10
36	1	815	G	C4-N9-C1'	5.63	133.82	126.50
36	1	1422	G	O5'-P-OP1	-5.63	100.63	105.70
36	1	2851	A	C8-N9-C4	5.63	108.05	105.80
1	2	321	C	N3-C2-O2	-5.63	117.96	121.90
36	1	934	G	N3-C4-N9	5.63	129.38	126.00
36	1	2996	U	N1-C2-O2	5.63	126.74	122.80
1	6	866	G	N7-C8-N9	-5.63	110.28	113.10
36	5	847	A	O5'-P-OP1	-5.63	100.63	105.70
36	5	908	G	N1-C6-O6	5.63	123.28	119.90
36	5	1371	G	C4-C5-N7	-5.63	108.55	110.80
36	5	1489	A	C6-C5-N7	-5.63	128.36	132.30
36	1	1308	A	C4-C5-C6	5.63	119.81	117.00
37	3	33	U	N3-C2-O2	-5.63	118.26	122.20
36	5	641	C	N1-C2-N3	5.63	123.14	119.20
36	5	2343	C	N3-C4-C5	5.63	124.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	368	G	N1-C6-O6	5.63	123.28	119.90
36	1	633	C	N1-C2-O2	-5.63	115.52	118.90
36	1	1428	A	C5-N7-C8	-5.63	101.09	103.90
36	1	2694	A	O5'-P-OP2	-5.63	100.63	105.70
36	1	2834	G	N3-C2-N2	5.63	123.84	119.90
1	6	364	G	C6-N1-C2	-5.63	121.72	125.10
36	1	659	G	OP2-P-O3'	5.63	117.58	105.20
36	1	1048	A	N1-C2-N3	-5.63	126.49	129.30
36	1	3344	A	O4'-C1'-N9	5.63	112.70	108.20
36	5	272	G	C5-C6-O6	-5.63	125.22	128.60
36	5	999	G	C5-C6-O6	5.63	131.98	128.60
36	5	3382	U	N3-C2-O2	-5.63	118.26	122.20
1	2	553	G	C5-C6-N1	-5.62	108.69	111.50
36	1	390	G	N1-C6-O6	-5.62	116.53	119.90
36	5	1483	G	O5'-P-OP1	-5.62	100.64	105.70
36	5	3217	C	C2-N1-C1'	-5.62	112.61	118.80
36	1	816	A	C2-N3-C4	5.62	113.41	110.60
1	6	17	C	N1-C2-O2	5.62	122.27	118.90
36	5	1452	A	C6-C5-N7	-5.62	128.36	132.30
36	5	1114	U	OP1-P-O3'	5.62	117.57	105.20
36	5	2426	U	N3-C2-O2	-5.62	118.27	122.20
36	5	2817	A	OP2-P-O3'	5.62	117.57	105.20
36	5	3368	U	N1-C2-O2	-5.62	118.86	122.80
36	1	2209	U	C5-C6-N1	5.62	125.51	122.70
36	1	1834	U	C5-C6-N1	-5.62	119.89	122.70
36	1	2163	C	N3-C4-N4	-5.62	114.07	118.00
36	1	2628	A	N9-C4-C5	5.62	108.05	105.80
1	6	1481	C	N3-C2-O2	-5.62	117.97	121.90
36	5	641	C	C6-N1-C1'	5.62	127.54	120.80
36	5	1101	G	N1-C2-N2	-5.62	111.14	116.20
36	5	1852	G	C8-N9-C4	-5.62	104.15	106.40
1	2	1291	G	N3-C4-N9	-5.62	122.63	126.00
36	1	697	A	O5'-P-OP1	-5.62	100.65	105.70
1	6	630	A	C5-C6-N1	-5.62	114.89	117.70
1	2	42	G	O5'-P-OP1	-5.61	100.65	105.70
36	1	3050	U	N1-C2-O2	5.61	126.73	122.80
36	1	3079	U	C2-N1-C1'	-5.61	110.96	117.70
38	4	103	G	C8-N9-C4	-5.61	104.16	106.40
1	6	355	G	N9-C4-C5	5.61	107.65	105.40
36	5	92	G	N3-C4-N9	5.61	129.37	126.00
36	5	221	A	C2-N3-C4	-5.61	107.79	110.60
36	1	425	G	C8-N9-C4	-5.61	104.16	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2710	C	N1-C2-O2	-5.61	115.53	118.90
38	4	145	U	N1-C2-N3	5.61	118.27	114.90
1	6	609	U	C5-C6-N1	-5.61	119.89	122.70
9	s7	118	LEU	CA-CB-CG	5.61	128.21	115.30
36	5	1060	U	N3-C4-C5	5.61	117.97	114.60
36	5	3208	G	N3-C4-C5	-5.61	125.79	128.60
36	1	782	U	C6-N1-C2	5.61	124.37	121.00
1	6	337	G	O4'-C1'-N9	-5.61	103.71	108.20
36	5	1481	A	P-O3'-C3'	5.61	126.43	119.70
36	1	2306	C	N3-C2-O2	-5.61	117.97	121.90
36	1	2887	A	C8-N9-C4	-5.61	103.56	105.80
36	5	2916	U	N1-C2-O2	-5.61	118.87	122.80
36	1	583	G	N3-C4-N9	-5.61	122.64	126.00
36	1	1138	U	N3-C4-C5	5.61	117.96	114.60
36	1	2334	U	OP2-P-O3'	5.61	117.53	105.20
36	5	2353	G	N1-C6-O6	5.61	123.27	119.90
36	5	2857	C	N3-C4-C5	5.61	124.14	121.90
36	5	3095	U	N1-C2-N3	5.61	118.26	114.90
52	m6	94	ARG	NE-CZ-NH2	5.61	123.10	120.30
36	1	1303	A	N7-C8-N9	-5.61	111.00	113.80
36	1	1487	G	N9-C4-C5	5.61	107.64	105.40
36	1	2946	A	OP1-P-OP2	-5.61	111.19	119.60
36	5	1200	A	OP1-P-O3'	5.61	117.53	105.20
36	1	716	A	C8-N9-C4	5.60	108.04	105.80
36	1	1103	A	P-O3'-C3'	5.60	126.42	119.70
1	6	755	A	O4'-C1'-N9	5.60	112.68	108.20
36	5	2706	G	O5'-P-OP1	5.60	117.42	110.70
1	2	186	C	C6-N1-C2	-5.60	118.06	120.30
36	1	2688	U	C6-N1-C2	5.60	124.36	121.00
1	6	1767	G	N3-C4-C5	5.60	131.40	128.60
52	M6	37	ARG	NE-CZ-NH1	-5.60	117.50	120.30
36	5	2282	U	C5-C6-N1	-5.60	119.90	122.70
38	8	111	A	C4-C5-N7	5.60	113.50	110.70
36	1	949	C	N1-C2-N3	5.60	123.12	119.20
36	1	984	G	N3-C4-C5	-5.60	125.80	128.60
36	1	1458	U	C5-C6-N1	-5.60	119.90	122.70
36	1	1605	A	N7-C8-N9	-5.60	111.00	113.80
36	1	2121	G	C5-C6-N1	5.60	114.30	111.50
36	5	942	U	N1-C2-O2	-5.60	118.88	122.80
38	8	4	C	C2-N3-C4	-5.60	117.10	119.90
36	1	1405	U	C5-C4-O4	-5.60	122.54	125.90
36	1	3265	C	N3-C4-C5	5.60	124.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1201	C	O5'-P-OP2	5.60	117.42	110.70
36	1	1008	U	C2-N1-C1'	-5.59	110.99	117.70
36	1	2309	A	O5'-P-OP1	-5.59	100.67	105.70
36	1	2973	G	N1-C6-O6	5.59	123.26	119.90
36	5	2317	A	O5'-P-OP2	-5.59	100.66	105.70
36	1	3229	G	C5-C6-O6	-5.59	125.24	128.60
1	6	194	U	C5-C6-N1	5.59	125.50	122.70
1	6	1596	C	N1-C2-O2	5.59	122.26	118.90
36	1	111	C	C6-N1-C2	5.59	122.54	120.30
36	1	363	G	C4-C5-N7	5.59	113.04	110.80
1	6	187	G	P-O3'-C3'	5.59	126.41	119.70
36	1	639	G	C6-C5-N7	-5.59	127.05	130.40
36	1	2920	U	C2-N3-C4	-5.59	123.65	127.00
36	5	1347	U	N3-C2-O2	5.59	126.11	122.20
36	5	2733	A	N1-C6-N6	5.59	121.95	118.60
36	5	2865	U	N1-C2-O2	5.59	126.71	122.80
1	2	1092	A	N1-C6-N6	5.59	121.95	118.60
36	1	1313	G	N1-C6-O6	5.59	123.25	119.90
36	1	1452	A	N7-C8-N9	-5.59	111.01	113.80
36	1	2964	G	OP1-P-O3'	5.59	117.49	105.20
36	5	349	A	OP2-P-O3'	5.59	117.49	105.20
36	5	3044	G	N3-C4-C5	-5.59	125.81	128.60
36	1	657	A	OP1-P-O3'	5.58	117.49	105.20
36	1	1127	G	O5'-P-OP1	-5.58	100.67	105.70
36	5	873	C	P-O3'-C3'	5.58	126.40	119.70
36	5	1844	C	N1-C2-N3	5.58	123.11	119.20
36	5	3084	C	C6-N1-C2	5.58	122.53	120.30
36	1	678	G	N1-C6-O6	5.58	123.25	119.90
36	1	2867	C	C6-N1-C2	5.58	122.53	120.30
1	6	553	G	N3-C4-N9	-5.58	122.65	126.00
12	c0	88	PRO	N-CA-CB	5.58	110.00	103.30
36	5	1178	G	C4-C5-N7	5.58	113.03	110.80
36	5	2394	G	C5-C6-N1	-5.58	108.71	111.50
36	1	1602	A	C8-N9-C4	5.58	108.03	105.80
36	1	2376	G	C6-C5-N7	-5.58	127.05	130.40
36	1	2632	G	C5-C6-N1	5.58	114.29	111.50
36	5	276	U	C5-C4-O4	-5.58	122.55	125.90
36	5	2157	G	C8-N9-C4	5.58	108.63	106.40
1	2	345	U	N3-C2-O2	-5.58	118.29	122.20
36	1	1127	G	N3-C4-C5	5.58	131.39	128.60
20	c8	116	LEU	CA-CB-CG	5.58	128.13	115.30
36	5	1402	C	C5-C6-N1	-5.58	118.21	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1881	A	OP1-P-OP2	5.58	127.97	119.60
36	1	2802	A	OP2-P-O3'	5.58	117.47	105.20
36	5	1365	G	C5-C6-O6	-5.58	125.25	128.60
36	5	1537	A	C8-N9-C4	5.58	108.03	105.80
37	7	5	G	C6-C5-N7	-5.58	127.05	130.40
36	1	1114	U	C6-N1-C2	5.58	124.34	121.00
36	1	3344	A	C6-C5-N7	-5.58	128.40	132.30
36	1	304	G	N9-C4-C5	5.57	107.63	105.40
36	1	1114	U	N1-C2-N3	-5.57	111.56	114.90
36	1	2356	A	N9-C4-C5	-5.57	103.57	105.80
36	5	960	U	C2-N3-C4	-5.57	123.66	127.00
36	5	2244	A	O5'-P-OP1	5.57	117.39	110.70
1	6	555	A	P-O3'-C3'	5.57	126.39	119.70
36	5	1166	G	C6-C5-N7	-5.57	127.06	130.40
37	7	86	U	N3-C2-O2	-5.57	118.30	122.20
1	2	1633	A	C8-N9-C4	-5.57	103.57	105.80
36	1	655	C	N3-C4-C5	-5.57	119.67	121.90
36	1	1100	U	N1-C2-O2	-5.57	118.90	122.80
36	1	1374	G	N3-C2-N2	5.57	123.80	119.90
36	1	2650	U	N1-C2-N3	5.57	118.24	114.90
1	2	1654	G	N3-C4-C5	-5.57	125.82	128.60
36	1	2162	U	N1-C2-O2	5.57	126.70	122.80
36	5	3288	G	C5-C6-N1	5.57	114.28	111.50
37	7	81	U	N3-C2-O2	-5.57	118.30	122.20
36	5	359	U	O5'-P-OP2	5.57	117.38	110.70
36	5	2187	G	N3-C4-N9	5.57	129.34	126.00
37	7	101	G	C4-C5-N7	5.57	113.03	110.80
1	2	1462	G	C8-N9-C4	5.57	108.63	106.40
36	1	2368	A	N1-C6-N6	-5.57	115.26	118.60
36	1	2987	A	C4-C5-C6	5.57	119.78	117.00
36	1	3361	G	N3-C4-N9	5.57	129.34	126.00
36	5	73	C	N1-C2-O2	-5.57	115.56	118.90
36	5	2601	A	N1-C6-N6	-5.57	115.26	118.60
36	5	2648	G	C5-C6-N1	5.57	114.28	111.50
36	1	53	G	C8-N9-C4	5.56	108.62	106.40
36	1	2867	C	C2-N3-C4	-5.56	117.12	119.90
36	5	1879	A	O5'-P-OP1	5.56	117.38	110.70
37	7	92	A	C8-N9-C4	5.56	108.03	105.80
1	2	1107	G	N1-C6-O6	5.56	123.24	119.90
36	1	800	G	N3-C2-N2	-5.56	116.01	119.90
38	4	53	A	C2-N3-C4	5.56	113.38	110.60
44	L7	216	VAL	N-CA-C	5.56	126.02	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	400	A	OP2-P-O3'	5.56	117.44	105.20
36	5	1158	A	C6-C5-N7	-5.56	128.41	132.30
36	1	1898	G	N1-C6-O6	5.56	123.24	119.90
36	1	423	A	N9-C4-C5	5.56	108.02	105.80
36	5	1521	G	C5-C6-O6	5.56	131.94	128.60
36	5	2400	G	C6-C5-N7	-5.56	127.06	130.40
36	1	795	G	O5'-P-OP1	-5.56	100.70	105.70
36	1	922	U	N3-C4-O4	-5.56	115.51	119.40
36	5	2852	C	C5-C4-N4	-5.56	116.31	120.20
36	1	323	A	C8-N9-C4	5.56	108.02	105.80
36	1	2899	C	C2-N3-C4	-5.56	117.12	119.90
36	5	1174	G	C8-N9-C1'	-5.56	119.78	127.00
36	5	2953	U	N3-C4-O4	5.56	123.29	119.40
1	2	394	C	N1-C2-O2	5.55	122.23	118.90
36	1	43	A	N3-C4-C5	5.55	130.69	126.80
36	1	1475	A	N7-C8-N9	-5.55	111.02	113.80
36	5	1419	A	O5'-P-OP1	5.55	117.36	110.70
36	5	3049	A	C6-N1-C2	5.55	121.93	118.60
36	1	2358	A	N7-C8-N9	-5.55	111.02	113.80
36	1	2637	A	O5'-P-OP1	-5.55	100.70	105.70
36	5	1364	C	OP2-P-O3'	5.55	117.42	105.20
36	5	874	U	C2-N1-C1'	-5.55	111.04	117.70
37	7	5	G	N1-C6-O6	5.55	123.23	119.90
1	2	996	U	C5-C6-N1	5.55	125.47	122.70
36	1	1831	U	N1-C2-O2	5.55	126.69	122.80
36	1	3362	A	C2-N3-C4	-5.55	107.83	110.60
1	6	610	G	C4-N9-C1'	5.55	133.71	126.50
38	8	19	C	N3-C4-N4	5.55	121.88	118.00
36	1	859	G	C4-C5-C6	5.55	122.13	118.80
36	1	1377	G	C5-C6-N1	5.55	114.27	111.50
36	1	494	G	N3-C4-N9	5.55	129.33	126.00
36	1	3382	U	C2-N1-C1'	5.55	124.36	117.70
1	6	1109	G	N9-C4-C5	5.55	107.62	105.40
36	5	1548	C	C2-N1-C1'	-5.55	112.70	118.80
36	1	2983	C	C5-C4-N4	5.54	124.08	120.20
36	5	960	U	C6-N1-C1'	-5.54	113.44	121.20
36	5	2311	G	C8-N9-C4	5.54	108.62	106.40
18	C6	40	GLU	C-N-CA	5.54	145.27	122.00
36	1	716	A	C6-C5-N7	-5.54	128.42	132.30
36	1	2522	G	C4-N9-C1'	5.54	133.70	126.50
36	1	2867	C	N3-C4-N4	-5.54	114.12	118.00
41	L4	197	ARG	NE-CZ-NH1	-5.54	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	347	G	C5-C6-O6	-5.54	125.28	128.60
36	5	1725	C	C5'-C4'-O4'	5.54	115.75	109.10
36	5	2369	G	C8-N9-C1'	-5.54	119.80	127.00
36	5	87	U	C5-C4-O4	5.54	129.22	125.90
36	5	660	A	C8-N9-C4	5.54	108.02	105.80
36	1	2984	C	N3-C4-N4	-5.54	114.12	118.00
1	6	555	A	C2'-C3'-O3'	5.54	122.56	113.70
36	5	98	G	C2-N3-C4	-5.54	109.13	111.90
36	5	977	C	C6-N1-C2	5.54	122.52	120.30
36	5	2114	C	OP1-P-OP2	5.54	127.91	119.60
36	5	2727	A	C8-N9-C4	-5.54	103.58	105.80
36	5	2971	A	C2-N3-C4	5.54	113.37	110.60
36	1	2355	G	N3-C2-N2	-5.54	116.02	119.90
36	5	878	G	C6-C5-N7	-5.54	127.08	130.40
36	1	32	U	N1-C2-N3	5.54	118.22	114.90
36	1	1149	G	N3-C2-N2	-5.54	116.02	119.90
36	1	1313	G	C6-C5-N7	-5.54	127.08	130.40
36	1	3081	C	C5-C6-N1	-5.54	118.23	121.00
36	5	504	A	C8-N9-C4	5.54	108.01	105.80
36	5	2801	A	C8-N9-C4	5.54	108.01	105.80
36	5	3007	U	C2-N3-C4	-5.54	123.68	127.00
36	1	3214	U	C5-C4-O4	5.53	129.22	125.90
38	4	140	G	C8-N9-C4	-5.53	104.19	106.40
1	6	1568	C	P-O3'-C3'	5.53	126.34	119.70
36	5	1181	U	O5'-P-OP1	-5.53	100.72	105.70
36	5	1513	G	N7-C8-N9	5.53	115.87	113.10
36	5	2976	A	C8-N9-C4	5.53	108.01	105.80
36	1	1443	G	C5-N7-C8	-5.53	101.53	104.30
36	1	2723	U	N3-C2-O2	5.53	126.07	122.20
1	6	1656	U	O5'-P-OP1	5.53	117.34	110.70
1	2	720	G	P-O3'-C3'	5.53	126.34	119.70
36	1	1385	C	C6-N1-C2	5.53	122.51	120.30
36	1	2940	A	C4-C5-C6	5.53	119.77	117.00
36	5	426	G	N9-C4-C5	-5.53	103.19	105.40
36	5	1359	C	N3-C4-N4	5.53	121.87	118.00
36	5	1848	G	C5-C6-N1	5.53	114.27	111.50
36	1	633	C	C5-C6-N1	-5.53	118.23	121.00
48	M1	112	LEU	CA-CB-CG	5.53	128.02	115.30
36	5	1902	G	C6-N1-C2	-5.53	121.78	125.10
36	1	36	C	N3-C4-C5	-5.53	119.69	121.90
36	1	1344	G	OP2-P-O3'	5.53	117.36	105.20
36	1	1430	U	C2-N3-C4	-5.53	123.68	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	3	98	C	N1-C2-O2	-5.53	115.58	118.90
36	5	2950	G	C4-C5-N7	5.53	113.01	110.80
36	5	3208	G	C5-C6-O6	-5.53	125.28	128.60
36	5	3392	U	N1-C2-N3	5.53	118.22	114.90
1	2	187	G	P-O3'-C3'	5.53	126.33	119.70
36	1	930	U	O5'-P-OP1	-5.53	100.73	105.70
70	O4	60	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	6	901	G	C5-C6-O6	-5.53	125.28	128.60
1	6	1058	U	OP1-P-O3'	5.53	117.35	105.20
38	8	127	U	O5'-P-OP1	-5.53	100.73	105.70
36	1	439	C	N3-C2-O2	-5.52	118.03	121.90
36	1	2646	C	C6-N1-C2	5.52	122.51	120.30
36	5	2996	U	N1-C2-O2	5.52	126.67	122.80
36	1	2406	C	N3-C4-C5	5.52	124.11	121.90
36	1	2899	C	C6-N1-C1'	-5.52	114.17	120.80
1	6	891	A	N1-C6-N6	5.52	121.91	118.60
36	1	329	U	C6-N1-C2	-5.52	117.69	121.00
36	1	1412	G	C5-C6-O6	5.52	131.91	128.60
36	5	619	A	N1-C6-N6	-5.52	115.29	118.60
1	2	719	U	C2-N1-C1'	5.52	124.32	117.70
36	5	2093	A	O4'-C1'-N9	5.52	112.61	108.20
36	5	2871	G	N3-C4-N9	5.52	129.31	126.00
36	5	3042	U	N3-C4-O4	-5.52	115.54	119.40
36	5	3215	A	N1-C6-N6	5.52	121.91	118.60
36	5	3218	A	C5-C6-N6	-5.52	119.28	123.70
1	2	25	C	P-O3'-C3'	5.52	126.32	119.70
36	1	3368	U	C6-N1-C1'	5.52	128.93	121.20
1	6	144	U	C6-N1-C2	-5.52	117.69	121.00
36	5	1213	G	N1-C6-O6	5.52	123.21	119.90
36	5	2888	U	N3-C4-O4	5.52	123.26	119.40
36	5	3003	G	OP1-P-OP2	-5.52	111.32	119.60
36	5	3142	A	O5'-P-OP2	5.52	117.32	110.70
36	5	3209	A	N7-C8-N9	5.52	116.56	113.80
36	1	1292	C	C6-N1-C2	5.52	122.51	120.30
36	1	3140	G	C5-C6-O6	-5.52	125.29	128.60
36	1	1300	G	C6-N1-C2	-5.51	121.79	125.10
36	1	1333	C	O5'-P-OP1	5.51	117.32	110.70
36	5	1196	C	N1-C2-O2	5.51	122.21	118.90
36	5	2392	C	C6-N1-C2	5.51	122.51	120.30
37	7	93	C	N3-C4-N4	-5.51	114.14	118.00
1	2	1596	C	C2-N1-C1'	5.51	124.86	118.80
36	1	2351	U	O5'-P-OP2	5.51	117.31	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	947	G	O5'-P-OP2	-5.51	100.74	105.70
24	D2	93	LEU	CA-CB-CG	5.51	127.98	115.30
36	1	345	G	N1-C6-O6	-5.51	116.59	119.90
36	1	830	A	N1-C6-N6	5.51	121.91	118.60
36	1	2527	G	N3-C4-N9	-5.51	122.69	126.00
38	4	3	A	C8-N9-C4	5.51	108.00	105.80
38	4	80	A	O5'-P-OP2	-5.51	100.74	105.70
1	6	1537	C	N1-C2-O2	-5.51	115.59	118.90
36	5	2348	A	N1-C2-N3	-5.51	126.54	129.30
36	5	2926	A	C8-N9-C4	-5.51	103.59	105.80
36	5	3343	G	N1-C2-N2	-5.51	111.24	116.20
37	7	89	G	N1-C6-O6	-5.51	116.59	119.90
36	1	2572	C	C6-N1-C2	-5.51	118.10	120.30
36	1	2987	A	C6-C5-N7	-5.51	128.44	132.30
1	6	858	G	C8-N9-C1'	-5.51	119.84	127.00
36	5	1158	A	N9-C4-C5	-5.51	103.60	105.80
36	5	2385	G	C4-C5-N7	5.51	113.00	110.80
36	5	2838	A	N1-C6-N6	5.51	121.91	118.60
1	2	1100	G	N3-C4-C5	-5.51	125.85	128.60
36	1	1329	U	O4'-C1'-N1	5.51	112.61	108.20
36	5	891	G	C2-N3-C4	5.51	114.65	111.90
36	1	105	C	C5-C4-N4	-5.51	116.35	120.20
1	6	696	C	O4'-C1'-N1	5.51	112.61	108.20
1	2	1145	U	N1-C2-O2	-5.50	118.95	122.80
36	1	1919	G	C8-N9-C4	-5.50	104.20	106.40
36	5	41	G	C5-N7-C8	-5.50	101.55	104.30
1	2	1339	C	C6-N1-C2	-5.50	118.10	120.30
36	1	60	A	N1-C6-N6	5.50	121.90	118.60
36	1	1433	A	C5-C6-N1	5.50	120.45	117.70
36	5	2335	G	C2-N3-C4	5.50	114.65	111.90
36	5	2941	A	N9-C4-C5	5.50	108.00	105.80
1	2	704	C	C2-N1-C1'	5.50	124.85	118.80
36	1	397	A	N1-C6-N6	-5.50	115.30	118.60
36	1	1315	U	C5-C6-N1	-5.50	119.95	122.70
36	1	2434	U	N3-C2-O2	-5.50	118.35	122.20
36	1	2611	U	C2-N3-C4	-5.50	123.70	127.00
36	5	358	G	O5'-P-OP1	5.50	117.30	110.70
36	5	2730	G	N1-C6-O6	5.50	123.20	119.90
36	1	2514	U	O5'-P-OP1	-5.50	100.75	105.70
36	5	2819	A	N1-C2-N3	-5.50	126.55	129.30
36	1	120	G	N9-C4-C5	-5.50	103.20	105.40
36	1	885	U	C2-N3-C4	-5.50	123.70	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1160	C	O5'-P-OP1	-5.50	100.75	105.70
36	1	1433	A	C5-C6-N6	-5.50	119.30	123.70
36	5	1083	G	OP1-P-OP2	5.50	127.85	119.60
36	5	1129	A	O5'-P-OP2	-5.50	100.75	105.70
1	6	577	G	C6-C5-N7	-5.50	127.10	130.40
36	5	111	C	C6-N1-C2	5.50	122.50	120.30
36	5	3050	U	N3-C4-O4	-5.50	115.55	119.40
36	1	1164	G	N3-C4-C5	-5.50	125.85	128.60
1	6	1003	A	C8-N9-C4	5.50	108.00	105.80
36	5	420	G	N3-C4-C5	-5.50	125.85	128.60
36	5	3335	A	N1-C6-N6	5.50	121.90	118.60
37	3	28	C	C5-C4-N4	-5.49	116.35	120.20
1	6	378	A	N1-C6-N6	5.49	121.90	118.60
36	5	1190	A	N9-C4-C5	5.49	108.00	105.80
36	5	2895	G	C5-N7-C8	5.49	107.05	104.30
36	1	1346	G	C2-N3-C4	-5.49	109.15	111.90
36	1	573	C	N3-C4-N4	-5.49	114.16	118.00
36	1	644	G	C4-C5-C6	5.49	122.09	118.80
36	1	2241	U	O5'-P-OP1	-5.49	100.76	105.70
36	1	2883	U	O5'-P-OP2	-5.49	100.76	105.70
36	5	982	C	C5-C6-N1	5.49	123.75	121.00
36	1	1411	C	N3-C4-C5	5.49	124.09	121.90
38	4	47	C	C2-N3-C4	-5.49	117.16	119.90
36	5	1160	C	C5-C4-N4	5.49	124.04	120.20
36	1	355	A	C2-N3-C4	-5.49	107.86	110.60
36	1	3054	U	C5-C6-N1	-5.49	119.96	122.70
36	5	973	A	C4-C5-C6	5.49	119.74	117.00
38	8	107	G	N1-C6-O6	5.49	123.19	119.90
24	D2	104	LEU	CA-CB-CG	5.49	127.92	115.30
36	1	2651	G	C6-C5-N7	5.49	133.69	130.40
1	6	1180	C	C6-N1-C2	-5.49	118.11	120.30
36	5	200	C	N3-C4-N4	5.49	121.84	118.00
36	5	366	A	C6-C5-N7	-5.49	128.46	132.30
36	5	1392	G	C8-N9-C4	5.49	108.59	106.40
37	7	102	A	C5-C6-N1	-5.49	114.96	117.70
1	2	992	A	C4-C5-C6	-5.48	114.26	117.00
36	5	1869	C	C6-N1-C2	5.48	122.49	120.30
36	5	2850	G	C5-C6-O6	-5.48	125.31	128.60
36	1	433	A	C2-N3-C4	5.48	113.34	110.60
36	1	1334	U	N3-C4-O4	5.48	123.24	119.40
38	4	140	G	N9-C4-C5	5.48	107.59	105.40
1	6	1127	G	C8-N9-C4	-5.48	104.21	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	42	C	N1-C2-N3	5.48	123.04	119.20
36	1	518	G	O4'-C1'-N9	5.48	112.58	108.20
36	1	714	G	N1-C2-N3	5.48	127.19	123.90
36	1	2725	U	C5-C6-N1	-5.48	119.96	122.70
36	5	989	A	N1-C6-N6	-5.48	115.31	118.60
36	5	1849	C	P-O3'-C3'	5.48	126.28	119.70
36	5	2377	G	N1-C6-O6	-5.48	116.61	119.90
36	5	2549	G	C6-C5-N7	-5.48	127.11	130.40
36	1	1171	G	C5-C6-O6	-5.48	125.31	128.60
1	6	139	C	N1-C2-O2	5.48	122.19	118.90
36	5	1051	U	C2-N3-C4	-5.48	123.71	127.00
36	5	2651	G	C8-N9-C4	5.48	108.59	106.40
1	2	1198	G	C8-N9-C4	-5.48	104.21	106.40
36	1	1125	U	OP2-P-O3'	5.48	117.25	105.20
36	1	1411	C	C2-N3-C4	-5.48	117.16	119.90
36	1	2719	U	N1-C2-N3	5.48	118.19	114.90
1	6	1783	C	C5-C4-N4	5.48	124.03	120.20
36	1	2343	C	N3-C4-C5	5.48	124.09	121.90
1	6	1726	G	OP2-P-O3'	5.48	117.25	105.20
1	2	190	C	O4'-C1'-N1	5.47	112.58	108.20
36	1	363	G	C5-C6-O6	-5.47	125.31	128.60
38	4	109	A	C5-N7-C8	-5.47	101.16	103.90
1	6	1100	G	C8-N9-C1'	-5.47	119.88	127.00
36	5	1213	G	C8-N9-C4	5.47	108.59	106.40
36	5	1897	G	C5-N7-C8	-5.47	101.56	104.30
36	5	2572	C	C6-N1-C1'	-5.47	114.23	120.80
36	5	2817	A	C2-N3-C4	5.47	113.34	110.60
37	7	87	G	C6-C5-N7	-5.47	127.12	130.40
36	1	331	G	C2-N3-C4	5.47	114.64	111.90
36	1	407	A	C5-N7-C8	-5.47	101.16	103.90
36	1	996	A	OP2-P-O3'	5.47	117.24	105.20
36	1	1653	G	C4-C5-N7	-5.47	108.61	110.80
36	1	2776	C	N1-C2-O2	-5.47	115.62	118.90
36	1	3375	A	C5'-C4'-C3'	-5.47	107.24	116.00
36	5	2908	G	N3-C2-N2	-5.47	116.07	119.90
37	7	69	C	C6-N1-C2	5.47	122.49	120.30
36	1	1855	U	N3-C2-O2	-5.47	118.37	122.20
36	5	220	G	O5'-P-OP2	-5.47	100.78	105.70
36	5	675	C	C5-C4-N4	-5.47	116.37	120.20
36	5	812	G	N7-C8-N9	-5.47	110.36	113.10
36	1	1911	A	C6-C5-N7	-5.47	128.47	132.30
1	2	794	U	P-O3'-C3'	5.47	126.26	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	922	U	C2-N3-C4	5.47	130.28	127.00
36	1	1510	G	C4-C5-N7	5.47	112.99	110.80
36	1	2646	C	C2-N3-C4	-5.47	117.17	119.90
1	6	144	U	O4'-C1'-N1	5.47	112.57	108.20
36	5	112	U	O4'-C1'-N1	5.47	112.57	108.20
36	5	1846	C	P-O3'-C3'	-5.47	113.14	119.70
36	5	2158	A	C5-C6-N1	5.47	120.43	117.70
36	5	2643	A	C5-C6-N6	-5.47	119.33	123.70
36	5	2837	A	O5'-P-OP1	-5.47	100.78	105.70
36	5	2931	C	N3-C2-O2	5.47	125.73	121.90
36	1	2787	G	C2-N3-C4	5.46	114.63	111.90
1	6	1288	G	O5'-P-OP2	-5.46	100.78	105.70
36	5	2296	A	C2-N3-C4	5.46	113.33	110.60
36	1	357	A	N7-C8-N9	5.46	116.53	113.80
1	6	402	C	O4'-C1'-N1	5.46	112.57	108.20
36	5	2215	A	C8-N9-C4	5.46	107.98	105.80
36	5	2426	U	N3-C4-O4	-5.46	115.58	119.40
1	2	186	C	C2-N1-C1'	5.46	124.81	118.80
1	6	297	U	C2-N1-C1'	5.46	124.25	117.70
36	5	216	G	N9-C4-C5	-5.46	103.22	105.40
36	5	1180	A	O4'-C1'-N9	-5.46	103.83	108.20
36	5	2830	G	N1-C2-N3	5.46	127.18	123.90
36	5	2988	C	C5-C6-N1	-5.46	118.27	121.00
36	1	2640	A	N9-C4-C5	5.46	107.98	105.80
36	5	2930	A	C6-C5-N7	5.46	136.12	132.30
1	2	992	A	N3-C4-N9	-5.46	123.03	127.40
36	1	1321	G	N9-C4-C5	5.46	107.58	105.40
36	1	2692	A	C5-C6-N6	-5.46	119.33	123.70
1	6	352	A	C8-N9-C4	5.46	107.98	105.80
1	6	1200	G	N3-C4-C5	5.46	131.33	128.60
36	5	1879	A	C8-N9-C4	-5.46	103.62	105.80
1	2	453	U	C6-N1-C1'	-5.46	113.56	121.20
36	1	405	U	N3-C4-C5	5.46	117.87	114.60
36	1	642	U	N1-C2-O2	5.46	126.62	122.80
36	1	1841	A	N1-C6-N6	-5.46	115.33	118.60
1	6	1775	U	C2-N3-C4	-5.46	123.73	127.00
36	5	2818	U	C2-N3-C4	-5.46	123.73	127.00
36	1	1505	C	N1-C2-O2	-5.46	115.63	118.90
1	6	334	G	C5-C6-N1	5.46	114.23	111.50
1	6	1127	G	C4-C5-C6	5.46	122.07	118.80
1	6	1783	C	N3-C2-O2	-5.46	118.08	121.90
36	1	345	G	C6-N1-C2	-5.45	121.83	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	s9	149	ARG	NE-CZ-NH1	5.45	123.03	120.30
36	5	281	G	N1-C6-O6	5.45	123.17	119.90
36	5	2283	G	C8-N9-C4	5.45	108.58	106.40
36	5	2323	G	C5-C6-O6	5.45	131.87	128.60
36	5	2411	U	C5-C4-O4	-5.45	122.63	125.90
1	2	1455	G	C5-C6-N1	-5.45	108.77	111.50
36	1	2884	C	C5-C4-N4	-5.45	116.38	120.20
36	5	799	G	C5-C6-N1	5.45	114.23	111.50
36	5	1592	G	N7-C8-N9	5.45	115.83	113.10
38	8	43	A	C8-N9-C4	-5.45	103.62	105.80
36	1	2763	U	N1-C2-O2	-5.45	118.98	122.80
36	1	2891	U	N1-C2-O2	-5.45	118.98	122.80
36	1	993	G	O4'-C1'-N9	5.45	112.56	108.20
36	5	2895	G	N3-C4-C5	-5.45	125.88	128.60
1	2	448	C	N3-C4-C5	-5.45	119.72	121.90
1	2	1777	G	C6-C5-N7	-5.45	127.13	130.40
36	1	343	U	C6-N1-C2	-5.45	117.73	121.00
36	1	498	A	N9-C4-C5	5.45	107.98	105.80
36	1	626	U	O5'-P-OP1	-5.45	100.80	105.70
36	1	1382	G	C8-N9-C4	5.45	108.58	106.40
36	1	1605	A	C8-N9-C4	5.45	107.98	105.80
36	1	2808	A	C6-C5-N7	-5.45	128.49	132.30
36	5	3078	U	C2-N1-C1'	5.45	124.23	117.70
36	5	3080	G	C4-C5-N7	5.45	112.98	110.80
36	1	1389	G	N3-C4-N9	5.44	129.27	126.00
36	1	3034	C	N1-C2-O2	5.44	122.17	118.90
36	5	617	G	C4-C5-N7	5.44	112.98	110.80
36	5	1901	A	C5-C6-N6	-5.44	119.34	123.70
36	5	2401	A	C8-N9-C4	-5.44	103.62	105.80
36	5	3354	U	N3-C2-O2	-5.44	118.39	122.20
36	1	2149	A	O5'-P-OP2	5.44	117.23	110.70
36	1	2281	A	C8-N9-C4	5.44	107.98	105.80
36	1	2918	G	OP1-P-OP2	5.44	127.76	119.60
36	5	1708	C	C6-N1-C2	5.44	122.48	120.30
36	1	1586	G	O5'-P-OP2	-5.44	100.80	105.70
36	1	2414	G	C5-C6-O6	-5.44	125.34	128.60
36	5	941	G	N9-C4-C5	5.44	107.58	105.40
36	5	1512	U	C5-C4-O4	5.44	129.16	125.90
36	5	2207	A	N1-C6-N6	5.44	121.86	118.60
36	5	2290	C	C5-C6-N1	-5.44	118.28	121.00
36	5	2371	G	C2-N3-C4	-5.44	109.18	111.90
36	5	2884	C	C6-N1-C1'	-5.44	114.27	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2939	G	C8-N9-C4	5.44	108.58	106.40
36	1	2814	G	C5-C6-O6	-5.44	125.34	128.60
36	1	2884	C	C6-N1-C2	5.44	122.48	120.30
36	5	407	A	C4-C5-C6	5.44	119.72	117.00
36	1	11	A	C8-N9-C4	5.44	107.97	105.80
36	1	2622	C	C6-N1-C2	-5.44	118.12	120.30
61	n5	34	LEU	CA-CB-CG	5.44	127.80	115.30
1	2	1258	U	C2-N1-C1'	5.43	124.22	117.70
15	C3	22	ALA	C-N-CA	5.43	144.82	122.00
36	1	909	G	O5'-P-OP2	5.43	117.22	110.70
36	1	2915	U	C2-N3-C4	-5.43	123.74	127.00
1	6	298	C	OP2-P-O3'	5.43	117.16	105.20
1	6	1039	A	O4'-C1'-N9	5.43	112.55	108.20
36	5	264	G	C5-C6-O6	-5.43	125.34	128.60
36	5	952	A	N9-C4-C5	-5.43	103.63	105.80
36	5	2110	G	N1-C6-O6	5.43	123.16	119.90
36	5	2340	U	N3-C4-C5	5.43	117.86	114.60
36	5	2819	A	N9-C4-C5	5.43	107.97	105.80
36	1	85	A	C2-N3-C4	-5.43	107.88	110.60
36	1	1004	U	N3-C2-O2	-5.43	118.40	122.20
36	1	1142	G	N3-C4-C5	-5.43	125.88	128.60
36	1	2627	C	C2-N3-C4	-5.43	117.18	119.90
36	5	95	A	C8-N9-C4	5.43	107.97	105.80
36	5	1426	C	N3-C4-C5	5.43	124.07	121.90
36	1	1604	G	N3-C4-N9	5.43	129.26	126.00
36	5	307	A	N9-C4-C5	5.43	107.97	105.80
36	5	415	G	N1-C6-O6	-5.43	116.64	119.90
36	5	1046	A	C4-C5-C6	5.43	119.72	117.00
36	5	1112	A	C6-N1-C2	-5.43	115.34	118.60
36	5	3137	C	N3-C4-N4	-5.43	114.20	118.00
1	6	300	A	C8-N9-C4	5.43	107.97	105.80
1	6	1058	U	P-O3'-C3'	5.43	126.22	119.70
36	5	1897	G	C6-C5-N7	-5.43	127.14	130.40
36	5	2618	G	N3-C2-N2	5.43	123.70	119.90
36	1	654	C	C6-N1-C2	5.43	122.47	120.30
36	1	2994	A	N1-C6-N6	5.43	121.86	118.60
36	5	379	C	C6-N1-C2	-5.43	118.13	120.30
36	5	2433	U	C6-N1-C2	5.43	124.26	121.00
36	5	2987	A	C4-C5-C6	5.43	119.71	117.00
1	2	794	U	N1-C2-O2	5.43	126.60	122.80
36	1	55	G	C8-N9-C4	5.43	108.57	106.40
36	1	400	G	O4'-C1'-N9	5.43	112.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1389	G	C5-N7-C8	-5.43	101.59	104.30
36	1	1487	G	N3-C4-N9	-5.43	122.74	126.00
36	5	1014	U	C6-N1-C1'	-5.43	113.60	121.20
36	5	2201	G	N3-C2-N2	5.43	123.70	119.90
36	5	2984	C	N3-C4-C5	5.43	124.07	121.90
36	5	3285	C	C5-C6-N1	5.43	123.71	121.00
1	2	1107	G	C6-C5-N7	-5.42	127.14	130.40
26	D4	74	LEU	CA-CB-CG	5.42	127.78	115.30
36	1	630	A	O5'-P-OP2	-5.42	100.82	105.70
36	1	3362	A	C5-C6-N6	-5.42	119.36	123.70
36	5	1390	A	N1-C6-N6	-5.42	115.35	118.60
36	1	351	A	OP1-P-O3'	5.42	117.13	105.20
36	1	1495	U	C6-N1-C1'	5.42	128.79	121.20
1	6	914	G	C4-C5-N7	5.42	112.97	110.80
36	5	1370	G	N3-C4-C5	-5.42	125.89	128.60
36	5	2624	G	C4-N9-C1'	5.42	133.55	126.50
36	5	2655	U	C6-N1-C2	5.42	124.25	121.00
1	2	308	C	C2-N1-C1'	-5.42	112.84	118.80
1	2	758	U	N3-C2-O2	-5.42	118.40	122.20
1	2	1768	G	C4-N9-C1'	-5.42	119.45	126.50
36	1	653	A	C4-C5-N7	5.42	113.41	110.70
36	1	1464	G	N1-C6-O6	-5.42	116.65	119.90
1	6	1274	C	C6-N1-C2	-5.42	118.13	120.30
36	5	2282	U	C6-N1-C2	5.42	124.25	121.00
36	5	2887	A	C4-C5-C6	5.42	119.71	117.00
36	5	834	U	N3-C2-O2	5.42	125.99	122.20
36	1	155	G	C2-N3-C4	5.42	114.61	111.90
38	4	7	U	N1-C2-N3	5.42	118.15	114.90
36	5	92	G	O5'-P-OP2	5.42	117.20	110.70
36	5	2688	U	OP1-P-O3'	5.42	117.12	105.20
36	1	1492	G	N3-C4-C5	-5.42	125.89	128.60
36	1	1498	A	C2-N3-C4	5.42	113.31	110.60
1	6	96	G	C5-C6-O6	5.42	131.85	128.60
36	5	967	A	O5'-P-OP2	-5.42	100.83	105.70
36	5	1440	G	N1-C6-O6	-5.42	116.65	119.90
36	5	2930	A	C8-N9-C1'	5.42	137.45	127.70
37	7	37	G	C6-C5-N7	-5.42	127.15	130.40
36	1	2869	U	OP2-P-O3'	5.42	117.11	105.20
38	4	26	U	N3-C2-O2	-5.42	118.41	122.20
38	4	32	C	N3-C2-O2	5.42	125.69	121.90
36	5	2634	U	N1-C2-N3	5.42	118.15	114.90
36	5	3277	U	C5-C6-N1	5.42	125.41	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	499	U	P-O3'-C3'	5.41	126.19	119.70
36	5	1206	G	C4-C5-N7	-5.41	108.63	110.80
36	5	1496	C	C5-C6-N1	5.41	123.71	121.00
36	5	2618	G	C5-C6-O6	-5.41	125.35	128.60
36	5	2989	U	C6-N1-C2	5.41	124.25	121.00
1	2	159	U	C6-N1-C2	5.41	124.25	121.00
36	1	392	G	N1-C6-O6	5.41	123.15	119.90
36	1	2373	A	C5'-C4'-O4'	-5.41	102.61	109.10
36	5	807	A	C4-C5-N7	5.41	113.41	110.70
36	5	3382	U	N1-C2-O2	5.41	126.59	122.80
36	1	2607	G	O5'-P-OP1	5.41	117.19	110.70
38	4	40	A	C5-C6-N6	-5.41	119.37	123.70
36	5	2632	G	C5-C6-O6	5.41	131.85	128.60
52	m6	78	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	2	1370	U	P-O3'-C3'	5.41	126.19	119.70
36	1	87	U	N1-C2-N3	5.41	118.15	114.90
36	1	404	G	C8-N9-C4	5.41	108.56	106.40
36	1	1344	G	C8-N9-C4	5.41	108.56	106.40
36	1	1547	G	C8-N9-C4	5.41	108.56	106.40
38	4	79	A	N7-C8-N9	5.41	116.50	113.80
1	6	372	G	C2-N3-C4	5.41	114.60	111.90
36	5	283	G	N1-C6-O6	5.41	123.14	119.90
40	l3	232	ARG	NE-CZ-NH2	-5.41	117.59	120.30
36	5	1791	C	C2-N1-C1'	5.41	124.75	118.80
37	7	81	U	N1-C2-O2	5.41	126.58	122.80
36	1	999	G	OP2-P-O3'	5.41	117.09	105.20
36	1	1733	G	C6-C5-N7	-5.41	127.16	130.40
37	3	70	U	O5'-P-OP2	-5.41	100.83	105.70
1	6	25	C	C6-N1-C2	-5.41	118.14	120.30
1	6	1796	C	N3-C4-N4	-5.41	114.22	118.00
36	5	37	U	C4-C5-C6	5.41	122.94	119.70
36	5	952	A	C6-C5-N7	-5.41	128.52	132.30
36	1	2965	U	C2-N3-C4	-5.40	123.76	127.00
36	5	2172	A	N1-C6-N6	5.40	121.84	118.60
36	5	2512	C	C5-C6-N1	5.40	123.70	121.00
36	1	361	A	N1-C6-N6	-5.40	115.36	118.60
36	1	1820	U	N3-C2-O2	-5.40	118.42	122.20
36	1	2384	A	C5-C6-N6	-5.40	119.38	123.70
36	1	2385	G	C8-N9-C4	5.40	108.56	106.40
1	6	1137	A	N7-C8-N9	-5.40	111.10	113.80
36	5	725	G	O5'-P-OP2	-5.40	100.84	105.70
36	5	2303	A	C2-N3-C4	-5.40	107.90	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3109	G	N9-C4-C5	5.40	107.56	105.40
36	5	3134	A	O5'-P-OP2	-5.40	100.84	105.70
38	4	11	C	C4-C5-C6	-5.40	114.70	117.40
38	4	108	C	N3-C2-O2	5.40	125.68	121.90
1	6	53	G	N3-C4-C5	-5.40	125.90	128.60
1	6	317	C	C2-N3-C4	-5.40	117.20	119.90
36	5	705	A	O5'-P-OP1	5.40	117.18	110.70
36	5	2945	G	C6-C5-N7	-5.40	127.16	130.40
36	5	3141	A	C6-N1-C2	-5.40	115.36	118.60
36	1	1431	G	N3-C4-C5	-5.40	125.90	128.60
38	4	22	U	C6-N1-C2	5.40	124.24	121.00
36	1	683	U	N1-C2-O2	-5.40	119.02	122.80
36	5	3028	G	O5'-P-OP1	-5.40	100.84	105.70
36	5	3098	G	O5'-P-OP2	-5.40	100.84	105.70
1	2	1782	A	C8-N9-C4	-5.40	103.64	105.80
36	1	386	A	N1-C6-N6	5.40	121.84	118.60
36	1	1297	C	C6-N1-C2	5.40	122.46	120.30
36	5	993	G	O4'-C1'-N9	5.40	112.52	108.20
36	5	3374	U	N3-C4-C5	5.40	117.84	114.60
36	1	960	U	C2-N1-C1'	-5.39	111.23	117.70
36	1	2859	U	N1-C2-N3	5.39	118.14	114.90
1	6	355	G	C8-N9-C4	-5.39	104.24	106.40
36	5	61	A	N1-C2-N3	5.39	132.00	129.30
36	5	2396	G	N3-C4-C5	-5.39	125.90	128.60
36	5	2661	G	N3-C4-C5	-5.39	125.90	128.60
77	q1	12	ARG	NE-CZ-NH1	-5.39	117.60	120.30
36	1	496	C	O5'-P-OP2	5.39	117.17	110.70
36	1	3111	U	N3-C4-O4	-5.39	115.62	119.40
36	5	414	U	N3-C4-O4	5.39	123.17	119.40
36	5	2350	C	N1-C2-N3	5.39	122.97	119.20
36	5	2878	G	OP1-P-OP2	-5.39	111.51	119.60
64	n8	28	HIS	N-CA-C	5.39	125.56	111.00
36	1	2585	G	N3-C4-C5	-5.39	125.91	128.60
36	1	2651	G	C5-C6-O6	5.39	131.84	128.60
36	1	2865	U	N3-C4-C5	5.39	117.83	114.60
1	2	581	U	C5-C6-N1	5.39	125.39	122.70
36	1	2378	C	C2-N3-C4	-5.39	117.20	119.90
6	s4	38	LEU	CA-CB-CG	5.39	127.70	115.30
36	5	1834	U	OP1-P-O3'	5.39	117.06	105.20
36	5	3133	C	C6-N1-C2	-5.39	118.14	120.30
37	7	1	G	C8-N9-C1'	-5.39	119.99	127.00
40	l3	20	LYS	CD-CE-NZ	-5.39	99.30	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2206	G	C5-C6-O6	-5.39	125.37	128.60
1	6	346	G	C8-N9-C4	-5.39	104.25	106.40
36	5	2643	A	N9-C4-C5	-5.39	103.64	105.80
1	2	1014	G	C8-N9-C4	-5.39	104.25	106.40
1	2	1432	U	C6-N1-C2	5.39	124.23	121.00
36	1	788	C	C2-N1-C1'	-5.39	112.87	118.80
36	1	2344	U	C5-C6-N1	-5.39	120.01	122.70
37	3	104	A	N1-C6-N6	-5.39	115.37	118.60
36	5	1841	A	C4-C5-C6	5.39	119.69	117.00
36	5	3214	U	N1-C2-N3	5.39	118.13	114.90
36	1	912	G	N3-C2-N2	-5.38	116.13	119.90
36	1	1112	A	C5-C6-N6	-5.38	119.39	123.70
36	1	1200	A	OP1-P-O3'	5.38	117.04	105.20
36	1	1906	G	OP1-P-O3'	5.38	117.05	105.20
36	1	2278	C	C4-C5-C6	-5.38	114.71	117.40
36	5	1304	A	C6-C5-N7	-5.38	128.53	132.30
36	5	2416	U	N1-C2-N3	5.38	118.13	114.90
36	1	346	C	C5-C6-N1	-5.38	118.31	121.00
36	1	1124	U	N3-C4-C5	5.38	117.83	114.60
36	1	1172	G	N1-C6-O6	5.38	123.13	119.90
36	1	2385	G	N3-C4-N9	-5.38	122.77	126.00
36	5	65	A	O5'-P-OP2	-5.38	100.86	105.70
36	5	2128	C	C2-N3-C4	-5.38	117.21	119.90
36	5	2396	G	N9-C4-C5	5.38	107.55	105.40
36	5	3259	U	C5'-C4'-O4'	-5.38	102.64	109.10
1	2	16	G	C6-C5-N7	-5.38	127.17	130.40
36	1	660	A	N1-C2-N3	-5.38	126.61	129.30
36	1	1160	C	N1-C2-O2	5.38	122.13	118.90
36	1	1294	A	N9-C4-C5	5.38	107.95	105.80
36	1	1300	G	N3-C4-C5	-5.38	125.91	128.60
1	6	1698	G	P-O3'-C3'	5.38	126.16	119.70
36	5	414	U	C5-C4-O4	-5.38	122.67	125.90
36	5	2721	A	O5'-P-OP1	-5.38	100.86	105.70
36	5	3354	U	C6-N1-C2	-5.38	117.77	121.00
36	1	936	A	P-O3'-C3'	5.38	126.15	119.70
36	1	1184	A	OP2-P-O3'	5.38	117.03	105.20
36	5	436	A	C4-N9-C1'	5.38	135.98	126.30
36	5	1430	U	C6-N1-C2	5.38	124.23	121.00
36	5	1846	C	C5-C6-N1	-5.38	118.31	121.00
36	5	2843	U	C2-N1-C1'	5.38	124.15	117.70
36	1	2773	C	O5'-P-OP2	-5.38	100.86	105.70
1	6	782	U	C2-N1-C1'	5.38	124.15	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2606	G	OP1-P-O3'	5.38	117.02	105.20
36	5	2898	G	N7-C8-N9	-5.38	110.41	113.10
36	5	3148	U	C5-C4-O4	-5.38	122.67	125.90
1	2	1773	C	N3-C4-N4	5.37	121.76	118.00
36	1	1655	G	N3-C4-N9	5.37	129.22	126.00
36	1	1834	U	N1-C2-N3	5.37	118.12	114.90
36	1	2646	C	C5-C4-N4	-5.37	116.44	120.20
36	1	2793	G	OP1-P-OP2	-5.37	111.54	119.60
1	6	455	C	N3-C4-N4	5.37	121.76	118.00
1	6	628	G	O5'-P-OP2	-5.37	100.86	105.70
29	d7	29	ARG	NE-CZ-NH1	5.37	122.99	120.30
36	5	853	G	C5-C6-O6	-5.37	125.38	128.60
36	5	2416	U	C6-N1-C2	-5.37	117.78	121.00
36	1	1081	U	C2-N1-C1'	5.37	124.14	117.70
36	1	1345	G	OP2-P-O3'	5.37	117.02	105.20
62	N6	126	LEU	CA-CB-CG	5.37	127.65	115.30
1	6	557	G	N1-C6-O6	-5.37	116.68	119.90
1	6	1675	C	C5-C4-N4	-5.37	116.44	120.20
36	5	1014	U	C2-N1-C1'	5.37	124.15	117.70
36	5	1166	G	C2-N3-C4	-5.37	109.21	111.90
36	5	2362	C	C5-C6-N1	5.37	123.69	121.00
36	1	2800	G	C6-N1-C2	-5.37	121.88	125.10
36	1	3174	A	N7-C8-N9	5.37	116.48	113.80
1	2	1274	C	C4-C5-C6	5.37	120.08	117.40
36	1	2169	G	C2-N3-C4	5.37	114.58	111.90
1	6	549	G	N3-C4-N9	-5.37	122.78	126.00
36	1	907	G	O4'-C1'-N9	5.37	112.49	108.20
1	6	1503	A	O4'-C1'-N9	5.37	112.49	108.20
36	5	3333	G	O5'-P-OP2	-5.37	100.87	105.70
36	1	1376	C	C4-C5-C6	5.37	120.08	117.40
36	5	264	G	N9-C4-C5	-5.37	103.25	105.40
36	5	1146	C	C5-C4-N4	-5.37	116.44	120.20
36	5	1927	G	N1-C6-O6	-5.37	116.68	119.90
36	5	2310	U	N3-C2-O2	-5.37	118.44	122.20
36	1	1004	U	N1-C2-O2	5.36	126.56	122.80
36	5	48	A	O5'-P-OP1	-5.36	100.87	105.70
36	5	436	A	C6-C5-N7	-5.36	128.54	132.30
36	5	1310	G	N1-C6-O6	-5.36	116.68	119.90
37	3	28	C	N3-C4-N4	5.36	121.75	118.00
36	1	361	A	O5'-P-OP1	-5.36	100.88	105.70
36	1	2764	C	C5-C6-N1	5.36	123.68	121.00
36	5	2412	G	C6-C5-N7	-5.36	127.18	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	66	A	O5'-P-OP1	-5.36	100.88	105.70
36	1	2325	G	N1-C6-O6	-5.36	116.69	119.90
37	7	47	C	N1-C2-O2	-5.36	115.69	118.90
36	1	1427	U	N1-C2-O2	5.36	126.55	122.80
36	1	2349	U	N3-C4-O4	-5.36	115.65	119.40
37	3	88	G	N3-C4-N9	5.36	129.21	126.00
38	4	32	C	C2-N1-C1'	-5.36	112.91	118.80
38	4	125	U	C6-N1-C1'	-5.36	113.70	121.20
36	5	88	A	C6-N1-C2	5.36	121.81	118.60
36	5	3304	U	N1-C2-O2	-5.36	119.05	122.80
36	5	3369	G	C2-N3-C4	5.36	114.58	111.90
36	1	55	G	N7-C8-N9	-5.36	110.42	113.10
36	1	1115	G	C4-N9-C1'	5.36	133.46	126.50
36	1	2135	U	N3-C4-C5	5.36	117.81	114.60
38	4	90	U	N3-C2-O2	5.36	125.95	122.20
1	6	352	A	N1-C2-N3	-5.36	126.62	129.30
36	5	3146	G	N3-C2-N2	5.36	123.65	119.90
38	8	63	G	N1-C6-O6	-5.36	116.69	119.90
36	1	653	A	N9-C4-C5	-5.35	103.66	105.80
36	1	917	A	C5-C6-N6	5.35	127.98	123.70
36	1	3109	G	O5'-P-OP2	5.35	117.12	110.70
1	6	1614	A	C6-C5-N7	-5.35	128.55	132.30
36	5	1901	A	N3-C4-N9	5.35	131.68	127.40
36	1	1168	U	O5'-P-OP1	5.35	117.12	110.70
36	1	1741	A	C6-C5-N7	-5.35	128.55	132.30
36	1	2383	C	C2-N3-C4	-5.35	117.22	119.90
36	1	2526	C	C2-N1-C1'	5.35	124.69	118.80
36	5	929	A	C8-N9-C4	5.35	107.94	105.80
36	5	2309	A	O5'-P-OP1	-5.35	100.88	105.70
36	5	2653	C	C6-N1-C2	-5.35	118.16	120.30
38	8	103	G	N3-C4-N9	5.35	129.21	126.00
36	1	282	G	N7-C8-N9	5.35	115.78	113.10
36	1	908	G	C8-N9-C4	5.35	108.54	106.40
38	4	52	A	C8-N9-C4	-5.35	103.66	105.80
1	6	1773	C	C5-C6-N1	5.35	123.68	121.00
36	5	998	A	OP1-P-OP2	-5.35	111.57	119.60
36	5	2326	A	OP2-P-O3'	5.35	116.97	105.20
36	5	2373	A	OP1-P-O3'	5.35	116.97	105.20
36	1	200	C	C6-N1-C1'	-5.35	114.38	120.80
36	1	1490	A	N1-C6-N6	5.35	121.81	118.60
36	1	2541	U	P-O3'-C3'	5.35	126.12	119.70
36	5	2211	U	C5-C4-O4	5.35	129.11	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	876	A	N1-C6-N6	5.35	121.81	118.60
36	1	1832	C	N3-C2-O2	-5.35	118.16	121.90
36	5	994	G	N3-C4-C5	-5.35	125.93	128.60
36	5	2942	C	C5-C4-N4	-5.35	116.46	120.20
45	18	69	LEU	CA-CB-CG	5.35	127.60	115.30
1	2	858	G	N1-C6-O6	-5.35	116.69	119.90
36	1	859	G	N3-C2-N2	5.35	123.64	119.90
1	6	1640	C	C2-N1-C1'	5.35	124.68	118.80
36	5	2685	C	N1-C2-O2	-5.35	115.69	118.90
36	1	785	G	N1-C6-O6	-5.34	116.69	119.90
36	1	1506	A	N1-C6-N6	-5.34	115.39	118.60
36	5	322	U	C5-C4-O4	-5.34	122.69	125.90
36	5	518	G	O4'-C1'-N9	5.34	112.48	108.20
36	5	1343	A	O5'-P-OP2	-5.34	100.89	105.70
36	5	2392	C	C5-C6-N1	-5.34	118.33	121.00
36	5	2395	G	C5-C6-O6	-5.34	125.39	128.60
1	2	590	C	C2-N1-C1'	5.34	124.68	118.80
36	1	2885	C	N3-C4-C5	5.34	124.04	121.90
36	1	2984	C	C6-N1-C2	-5.34	118.16	120.30
36	1	3057	U	C6-N1-C2	-5.34	117.80	121.00
36	5	813	G	C5-C6-O6	-5.34	125.39	128.60
36	5	915	A	OP1-P-OP2	5.34	127.61	119.60
36	5	1097	G	N9-C4-C5	-5.34	103.26	105.40
75	o9	45	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	2	730	G	C4-N9-C1'	5.34	133.44	126.50
36	1	968	G	C8-N9-C4	-5.34	104.26	106.40
36	5	667	C	C6-N1-C2	5.34	122.44	120.30
36	5	1113	G	C5-C6-N1	-5.34	108.83	111.50
1	2	1024	U	OP2-P-O3'	5.34	116.94	105.20
1	6	1151	A	N1-C6-N6	-5.34	115.40	118.60
36	1	3140	G	N3-C4-N9	5.34	129.20	126.00
1	6	787	G	N3-C4-C5	-5.34	125.93	128.60
21	c9	57	ARG	NE-CZ-NH1	5.34	122.97	120.30
36	5	534	U	N3-C2-O2	-5.34	118.47	122.20
36	5	2372	A	OP1-P-O3'	5.34	116.94	105.20
36	5	2877	G	C8-N9-C4	-5.34	104.27	106.40
36	5	3089	C	C6-N1-C2	-5.34	118.17	120.30
1	6	1012	U	C5-C4-O4	-5.33	122.70	125.90
36	5	3048	A	OP1-P-OP2	5.33	127.60	119.60
36	1	1439	U	OP1-P-O3'	5.33	116.93	105.20
36	1	2320	A	C2-N3-C4	-5.33	107.93	110.60
36	1	2407	C	N1-C2-O2	-5.33	115.70	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2977	G	C8-N9-C4	5.33	108.53	106.40
36	1	3036	G	N3-C4-N9	5.33	129.20	126.00
1	6	115	G	C5-C6-O6	-5.33	125.40	128.60
36	5	1110	U	N3-C4-O4	-5.33	115.67	119.40
36	5	2874	G	N9-C4-C5	5.33	107.53	105.40
37	3	95	A	N9-C4-C5	-5.33	103.67	105.80
38	4	151	C	C4-C5-C6	5.33	120.07	117.40
36	5	1521	G	N1-C6-O6	-5.33	116.70	119.90
36	1	275	U	N3-C2-O2	5.33	125.93	122.20
1	6	1014	G	C5-C6-O6	5.33	131.80	128.60
36	1	743	C	C6-N1-C2	5.33	122.43	120.30
36	1	2853	A	C8-N9-C4	-5.33	103.67	105.80
1	6	1777	G	C5-C6-O6	-5.33	125.40	128.60
33	e1	100	LEU	CA-CB-CG	5.33	127.55	115.30
36	5	205	C	N3-C4-C5	5.33	124.03	121.90
36	5	954	U	C2-N3-C4	5.33	130.20	127.00
36	5	2434	U	C5-C6-N1	-5.33	120.03	122.70
36	5	2889	C	N1-C2-N3	5.33	122.93	119.20
36	5	3147	G	N1-C2-N3	5.33	127.10	123.90
36	1	2861	U	N3-C2-O2	-5.33	118.47	122.20
36	1	911	C	N3-C4-C5	5.33	124.03	121.90
36	1	2372	A	O5'-P-OP2	-5.33	100.91	105.70
36	1	2863	G	N1-C6-O6	-5.33	116.70	119.90
36	1	2911	A	C4-C5-C6	-5.33	114.34	117.00
36	5	779	G	C6-C5-N7	-5.33	127.20	130.40
36	5	1177	G	C2-N3-C4	5.33	114.56	111.90
39	12	190	ARG	NE-CZ-NH2	5.33	122.96	120.30
36	1	1466	G	N3-C4-N9	5.32	129.19	126.00
36	1	2993	G	N3-C4-N9	5.32	129.19	126.00
1	6	577	G	C5-N7-C8	-5.32	101.64	104.30
1	6	581	U	C2-N1-C1'	-5.32	111.31	117.70
36	5	326	U	N3-C2-O2	5.32	125.93	122.20
1	6	678	A	P-O3'-C3'	5.32	126.09	119.70
36	5	219	A	C5-C6-N1	-5.32	115.04	117.70
36	5	1115	G	N1-C6-O6	-5.32	116.71	119.90
36	5	3197	G	C8-N9-C4	-5.32	104.27	106.40
36	5	2134	G	N1-C6-O6	-5.32	116.71	119.90
1	6	826	U	C5-C6-N1	5.32	125.36	122.70
36	5	220	G	N3-C2-N2	5.32	123.62	119.90
1	2	89	G	C8-N9-C4	5.32	108.53	106.40
36	1	34	A	C5-N7-C8	-5.32	101.24	103.90
36	1	2345	A	O5'-P-OP1	5.32	117.08	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2859	U	N3-C4-C5	-5.32	111.41	114.60
36	1	2929	C	C6-N1-C2	-5.32	118.17	120.30
1	6	1535	U	N1-C2-O2	5.32	126.52	122.80
36	5	2772	C	OP2-P-O3'	5.32	116.90	105.20
36	5	3343	G	N3-C2-N2	5.32	123.62	119.90
1	2	1572	G	N9-C4-C5	-5.32	103.27	105.40
36	1	382	U	N1-C2-O2	-5.32	119.08	122.80
36	1	633	C	C6-N1-C2	5.32	122.43	120.30
36	1	1483	G	C5-C6-N1	5.32	114.16	111.50
36	1	2836	C	N3-C2-O2	-5.32	118.18	121.90
38	4	151	C	N3-C4-C5	-5.32	119.77	121.90
36	5	1116	G	N9-C4-C5	5.32	107.53	105.40
36	5	1332	A	C6-N1-C2	-5.32	115.41	118.60
36	1	970	A	N7-C8-N9	5.31	116.46	113.80
1	6	1697	G	C2-N3-C4	5.31	114.56	111.90
36	5	1285	G	C8-N9-C4	5.31	108.53	106.40
36	5	2352	A	O5'-P-OP2	-5.31	100.92	105.70
1	2	942	G	N3-C4-C5	-5.31	125.94	128.60
36	1	1127	G	N1-C2-N2	5.31	120.98	116.20
36	1	2394	G	N1-C6-O6	-5.31	116.71	119.90
36	5	288	C	N3-C4-C5	5.31	124.03	121.90
36	5	1376	C	C2-N3-C4	-5.31	117.24	119.90
36	5	2135	U	C5-C4-O4	-5.31	122.71	125.90
40	13	26	ARG	NE-CZ-NH1	-5.31	117.64	120.30
36	5	1886	A	N1-C2-N3	-5.31	126.64	129.30
36	1	2524	A	O4'-C1'-N9	5.31	112.45	108.20
36	5	911	C	C2-N3-C4	-5.31	117.25	119.90
36	5	934	G	N3-C4-C5	-5.31	125.94	128.60
36	5	2351	U	N3-C4-O4	-5.31	115.68	119.40
36	1	1421	G	C5-N7-C8	5.31	106.95	104.30
36	1	1447	G	C6-N1-C2	-5.31	121.92	125.10
38	4	73	U	N3-C4-O4	-5.31	115.69	119.40
36	5	1075	A	O4'-C1'-N9	-5.31	103.95	108.20
36	5	2113	A	O4'-C1'-N9	-5.31	103.95	108.20
37	7	44	C	OP2-P-O3'	5.31	116.88	105.20
55	m9	105	LEU	CA-CB-CG	5.31	127.51	115.30
36	1	1206	G	O5'-P-OP2	-5.31	100.92	105.70
36	1	2846	U	N1-C2-O2	5.31	126.51	122.80
36	1	3181	C	C5-C6-N1	-5.31	118.35	121.00
36	5	1506	A	N9-C4-C5	5.31	107.92	105.80
1	2	610	G	C8-N9-C1'	-5.30	120.10	127.00
36	1	908	G	N3-C2-N2	-5.30	116.19	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1377	G	C4-C5-N7	5.30	112.92	110.80
36	1	2623	G	N3-C2-N2	5.30	123.61	119.90
36	1	2714	G	C4-C5-C6	-5.30	115.62	118.80
36	1	2960	C	N3-C4-C5	5.30	124.02	121.90
1	6	1537	C	C6-N1-C1'	5.30	127.17	120.80
36	5	426	G	OP2-P-O3'	5.30	116.87	105.20
36	5	867	G	N9-C4-C5	-5.30	103.28	105.40
36	5	1056	U	OP2-P-O3'	5.30	116.87	105.20
36	5	1112	A	C8-N9-C1'	-5.30	118.15	127.70
36	5	1238	C	P-O3'-C3'	5.30	126.06	119.70
36	5	2758	A	O4'-C1'-N9	5.30	112.44	108.20
36	5	2909	U	N1-C2-O2	-5.30	119.09	122.80
1	2	1765	A	O5'-P-OP1	-5.30	100.93	105.70
36	1	993	G	O5'-P-OP2	-5.30	100.93	105.70
36	5	1430	U	C5-C6-N1	-5.30	120.05	122.70
36	5	2228	A	C8-N9-C4	-5.30	103.68	105.80
1	2	1600	A	N1-C6-N6	5.30	121.78	118.60
36	1	1110	U	OP2-P-O3'	5.30	116.86	105.20
36	1	1152	G	OP1-P-OP2	5.30	127.55	119.60
36	1	1294	A	N1-C6-N6	-5.30	115.42	118.60
36	1	1415	U	C5-C6-N1	-5.30	120.05	122.70
36	1	1481	A	C8-N9-C1'	-5.30	118.16	127.70
36	1	2953	U	N1-C2-N3	5.30	118.08	114.90
36	1	3139	A	C5'-C4'-O4'	-5.30	102.74	109.10
36	5	2743	A	C8-N9-C4	5.30	107.92	105.80
36	1	421	G	C2-N3-C4	5.30	114.55	111.90
36	1	1447	G	C5-C6-O6	-5.30	125.42	128.60
36	1	2381	G	N1-C6-O6	-5.30	116.72	119.90
36	1	2589	G	C2-N3-C4	-5.30	109.25	111.90
38	4	20	U	C2-N1-C1'	-5.30	111.34	117.70
38	4	95	G	C4-N9-C1'	-5.30	119.61	126.50
1	6	331	A	C2-N3-C4	-5.30	107.95	110.60
36	5	1170	A	N3-C4-N9	5.30	131.64	127.40
36	5	2852	C	C2-N3-C4	-5.30	117.25	119.90
37	7	85	G	OP1-P-OP2	-5.30	111.65	119.60
40	l3	232	ARG	NE-CZ-NH1	5.30	122.95	120.30
36	5	2905	U	N1-C2-N3	5.30	118.08	114.90
36	1	53	G	O5'-P-OP2	-5.30	100.93	105.70
36	1	2618	G	N1-C6-O6	-5.30	116.72	119.90
36	1	2930	A	N9-C4-C5	5.30	107.92	105.80
1	6	1777	G	C4-C5-N7	5.30	112.92	110.80
36	5	1908	A	C2-N3-C4	5.30	113.25	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2842	U	C5-C4-O4	-5.30	122.72	125.90
36	5	2870	C	N3-C4-N4	-5.30	114.29	118.00
36	5	2994	A	N1-C6-N6	5.30	121.78	118.60
36	5	3309	G	C8-N9-C4	-5.30	104.28	106.40
36	1	2646	C	C5-C6-N1	-5.29	118.35	121.00
1	6	139	C	C6-N1-C2	-5.29	118.18	120.30
36	5	810	A	N1-C2-N3	-5.29	126.65	129.30
36	5	1710	C	N3-C4-C5	5.29	124.02	121.90
1	2	1448	G	O5'-P-OP1	-5.29	100.94	105.70
36	1	410	U	N1-C2-N3	5.29	118.08	114.90
36	1	609	G	N3-C4-C5	-5.29	125.95	128.60
36	1	776	U	N3-C4-C5	-5.29	111.42	114.60
36	1	949	C	C2-N3-C4	-5.29	117.25	119.90
36	1	2630	C	N3-C4-N4	5.29	121.70	118.00
38	4	15	G	N7-C8-N9	-5.29	110.45	113.10
36	5	637	C	C2-N3-C4	-5.29	117.25	119.90
36	5	1805	C	N3-C4-C5	5.29	124.02	121.90
36	5	2332	A	C8-N9-C4	5.29	107.92	105.80
36	1	644	G	C6-C5-N7	-5.29	127.22	130.40
1	6	1767	G	C8-N9-C4	5.29	108.52	106.40
36	5	636	C	C5-C4-N4	-5.29	116.50	120.20
36	5	2928	C	C4-C5-C6	5.29	120.05	117.40
1	2	543	C	N3-C2-O2	-5.29	118.20	121.90
36	5	1910	A	N1-C2-N3	-5.29	126.66	129.30
1	2	1600	A	N9-C4-C5	-5.29	103.69	105.80
36	5	379	C	N3-C4-C5	-5.29	119.78	121.90
36	5	683	U	O5'-P-OP2	-5.29	100.94	105.70
36	5	2187	G	C6-C5-N7	-5.29	127.23	130.40
36	5	2985	C	C2-N3-C4	5.29	122.55	119.90
36	1	2281	A	C6-N1-C2	5.29	121.77	118.60
36	5	1492	G	N3-C2-N2	5.29	123.60	119.90
1	2	1217	A	O4'-C1'-N9	-5.29	103.97	108.20
36	5	2349	U	N3-C2-O2	-5.29	118.50	122.20
36	5	2351	U	N1-C2-O2	5.29	126.50	122.80
36	5	3049	A	N1-C2-N3	-5.29	126.66	129.30
1	2	629	U	C6-N1-C2	5.28	124.17	121.00
36	1	1741	A	C2-N3-C4	-5.28	107.96	110.60
39	L2	6	ARG	NE-CZ-NH1	-5.28	117.66	120.30
36	5	1201	C	C6-N1-C2	-5.28	118.19	120.30
36	1	843	A	C2-N3-C4	-5.28	107.96	110.60
1	6	337	G	N7-C8-N9	5.28	115.74	113.10
36	5	1124	U	C5-C6-N1	5.28	125.34	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	992	A	C5-N7-C8	-5.28	101.26	103.90
36	1	38	U	C5-C6-N1	5.28	125.34	122.70
36	1	1507	G	N1-C6-O6	5.28	123.07	119.90
36	1	2603	G	N3-C2-N2	5.28	123.60	119.90
36	1	1442	U	C5-C4-O4	-5.28	122.73	125.90
36	1	2620	G	C5-C6-O6	-5.28	125.43	128.60
36	1	3303	G	N9-C4-C5	-5.28	103.29	105.40
36	5	1592	G	C4-C5-C6	5.28	121.97	118.80
36	5	3092	C	C6-N1-C2	5.28	122.41	120.30
1	2	527	A	C8-N9-C4	-5.28	103.69	105.80
36	1	641	C	N3-C4-C5	5.28	124.01	121.90
36	1	954	U	C6-N1-C2	-5.28	117.83	121.00
36	1	2371	G	O5'-P-OP2	-5.28	100.95	105.70
1	6	338	C	C6-N1-C2	-5.28	118.19	120.30
53	M7	131	ARG	NE-CZ-NH1	-5.28	117.66	120.30
36	5	1605	A	O4'-C1'-N9	5.28	112.42	108.20
36	5	1846	C	N3-C4-C5	5.28	124.01	121.90
36	5	1906	G	OP1-P-O3'	5.28	116.81	105.20
36	5	2231	C	C6-N1-C1'	-5.28	114.47	120.80
36	5	281	G	C5-C6-O6	-5.27	125.44	128.60
36	5	419	G	N3-C4-C5	-5.27	125.96	128.60
36	1	220	G	N1-C6-O6	5.27	123.06	119.90
36	1	1175	C	N3-C4-C5	5.27	124.01	121.90
36	5	1899	G	C8-N9-C4	-5.27	104.29	106.40
36	5	2401	A	O5'-P-OP2	-5.27	100.96	105.70
36	1	2309	A	OP1-P-OP2	5.27	127.51	119.60
36	1	2827	U	N3-C2-O2	-5.27	118.51	122.20
36	1	3145	C	OP2-P-O3'	5.27	116.80	105.20
38	4	37	A	N7-C8-N9	5.27	116.44	113.80
1	6	355	G	N3-C2-N2	-5.27	116.21	119.90
36	5	1794	G	O4'-C1'-N9	-5.27	103.98	108.20
36	5	2176	U	C2-N1-C1'	5.27	124.03	117.70
37	7	75	G	N1-C6-O6	5.27	123.06	119.90
36	1	1906	G	C4-N9-C1'	5.27	133.35	126.50
1	6	434	G	N7-C8-N9	-5.27	110.47	113.10
1	6	541	A	P-O3'-C3'	-5.27	113.38	119.70
36	5	687	U	C6-N1-C2	5.27	124.16	121.00
36	5	1198	C	C2-N3-C4	-5.27	117.27	119.90
36	5	2991	A	N9-C4-C5	5.27	107.91	105.80
36	5	3101	G	N3-C2-N2	5.27	123.59	119.90
36	5	3186	A	N1-C6-N6	-5.27	115.44	118.60
36	1	1368	U	C2-N3-C4	-5.27	123.84	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2927	C	P-O3'-C3'	5.27	126.02	119.70
36	5	107	A	N1-C6-N6	-5.27	115.44	118.60
36	5	1420	C	C2-N1-C1'	-5.27	113.00	118.80
36	5	2407	C	N3-C4-N4	5.27	121.69	118.00
36	5	2978	U	N1-C2-O2	5.27	126.49	122.80
36	1	2169	G	C5-C6-N1	5.26	114.13	111.50
36	1	2417	U	C5-C6-N1	-5.26	120.07	122.70
1	6	52	U	N3-C2-O2	-5.26	118.52	122.20
36	5	889	U	C4-C5-C6	-5.26	116.54	119.70
36	5	1085	A	C2-N3-C4	-5.26	107.97	110.60
36	5	1307	G	C2'-C3'-O3'	5.26	122.12	113.70
36	5	1506	A	C8-N9-C4	-5.26	103.69	105.80
36	5	2181	C	N3-C4-C5	5.26	124.01	121.90
36	5	2684	C	C6-N1-C2	-5.26	118.19	120.30
36	1	1858	A	C4-C5-N7	5.26	113.33	110.70
36	5	88	A	N3-C4-C5	5.26	130.48	126.80
36	5	861	C	N3-C2-O2	5.26	125.58	121.90
36	5	2137	U	OP1-P-OP2	-5.26	111.71	119.60
36	5	3328	G	N1-C6-O6	-5.26	116.74	119.90
36	1	267	G	C2-N3-C4	-5.26	109.27	111.90
36	1	364	G	C5-C6-N1	5.26	114.13	111.50
36	1	782	U	C4-C5-C6	-5.26	116.54	119.70
1	6	1415	U	N1-C2-O2	5.26	126.48	122.80
36	5	2602	G	O5'-P-OP2	-5.26	100.97	105.70
36	5	2880	U	C6-N1-C2	-5.26	117.84	121.00
36	5	3334	U	N1-C2-N3	5.26	118.06	114.90
36	1	876	A	C5-C6-N6	-5.26	119.50	123.70
36	1	3044	G	N1-C2-N2	-5.26	111.47	116.20
36	5	660	A	C5-N7-C8	5.26	106.53	103.90
36	5	1723	A	C5-C6-N1	5.26	120.33	117.70
36	5	2420	C	N3-C4-C5	5.26	124.00	121.90
36	1	648	C	C6-N1-C2	-5.25	118.20	120.30
36	1	651	G	N1-C2-N2	-5.25	111.47	116.20
1	6	123	G	C8-N9-C4	-5.25	104.30	106.40
36	5	516	A	N9-C4-C5	-5.25	103.70	105.80
36	1	583	G	N3-C2-N2	-5.25	116.22	119.90
36	1	1513	G	C6-N1-C2	-5.25	121.95	125.10
36	1	2215	A	N7-C8-N9	-5.25	111.17	113.80
36	5	2127	U	N1-C2-N3	5.25	118.05	114.90
36	5	2202	C	C5-C4-N4	-5.25	116.52	120.20
36	5	2314	U	C5-C4-O4	-5.25	122.75	125.90
1	2	1481	C	C6-N1-C2	-5.25	118.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	83	U	C5-C4-O4	-5.25	122.75	125.90
36	1	1791	C	N1-C2-O2	-5.25	115.75	118.90
47	M0	152	LEU	CA-CB-CG	-5.25	103.22	115.30
36	5	2849	C	N3-C2-O2	5.25	125.58	121.90
36	1	958	C	N3-C2-O2	-5.25	118.22	121.90
36	1	1911	A	C4-C5-N7	5.25	113.33	110.70
1	6	1463	C	C6-N1-C2	5.25	122.40	120.30
36	5	2371	G	N3-C2-N2	5.25	123.58	119.90
36	1	1834	U	C4-C5-C6	5.25	122.85	119.70
36	1	1837	U	N1-C2-O2	-5.25	119.13	122.80
36	1	2762	A	N7-C8-N9	-5.25	111.18	113.80
36	1	3044	G	N3-C2-N2	5.25	123.57	119.90
38	4	34	U	C5-C4-O4	-5.25	122.75	125.90
1	6	1114	G	O4'-C1'-N9	5.25	112.40	108.20
36	5	584	G	N9-C4-C5	5.25	107.50	105.40
36	5	1387	G	N3-C2-N2	-5.25	116.23	119.90
36	5	2115	G	O5'-P-OP1	-5.25	100.98	105.70
1	2	1082	C	C2-N1-C1'	5.25	124.57	118.80
36	1	963	G	C5-C6-O6	-5.25	125.45	128.60
36	1	2827	U	C6-N1-C1'	5.25	128.55	121.20
36	1	327	A	C8-N9-C4	5.25	107.90	105.80
57	n1	106	LEU	CA-CB-CG	-5.25	103.24	115.30
36	1	896	A	C5-C6-N1	5.24	120.32	117.70
36	1	1407	A	C8-N9-C4	5.24	107.90	105.80
36	1	1527	C	O5'-P-OP1	-5.24	100.98	105.70
36	1	2273	G	C8-N9-C4	5.24	108.50	106.40
36	1	2306	C	N1-C2-O2	5.24	122.05	118.90
36	1	2632	G	O4'-C1'-N9	5.24	112.39	108.20
1	6	610	G	C8-N9-C4	5.24	108.50	106.40
1	6	1458	G	C4-N9-C1'	5.24	133.32	126.50
36	5	330	G	O5'-P-OP2	-5.24	100.98	105.70
36	5	1096	U	N1-C2-O2	-5.24	119.13	122.80
36	5	3392	U	N3-C4-O4	-5.24	115.73	119.40
1	2	323	A	O5'-P-OP2	-5.24	100.98	105.70
36	1	372	A	O5'-P-OP2	-5.24	100.98	105.70
36	1	677	A	O5'-P-OP2	5.24	116.99	110.70
36	1	1304	A	OP1-P-OP2	5.24	127.46	119.60
1	6	600	U	N3-C4-O4	5.24	123.07	119.40
36	5	2728	G	N9-C4-C5	5.24	107.50	105.40
36	1	2915	U	N1-C2-N3	5.24	118.04	114.90
38	4	107	G	OP1-P-O3'	5.24	116.73	105.20
1	6	512	A	C2'-C3'-O3'	5.24	122.09	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2273	G	C8-N9-C1'	5.24	133.81	127.00
36	5	2996	U	N1-C2-N3	-5.24	111.76	114.90
36	5	3202	G	C5-C6-O6	5.24	131.75	128.60
36	1	95	A	OP1-P-OP2	-5.24	111.74	119.60
36	1	1025	A	C8-N9-C4	-5.24	103.70	105.80
36	1	2853	A	N9-C4-C5	5.24	107.90	105.80
36	1	3269	U	O5'-P-OP2	-5.24	100.98	105.70
36	5	1879	A	C3'-C2'-C1'	5.24	105.69	101.50
36	5	1882	G	O5'-P-OP2	5.24	116.99	110.70
36	5	2957	G	N9-C4-C5	-5.24	103.31	105.40
36	5	2296	A	C5-N7-C8	-5.24	101.28	103.90
36	1	908	G	N1-C2-N2	5.24	120.91	116.20
1	6	597	G	O5'-P-OP2	-5.24	100.99	105.70
1	6	616	G	N9-C4-C5	5.24	107.50	105.40
36	5	2148	U	C2-N1-C1'	-5.24	111.42	117.70
36	5	2411	U	OP1-P-O3'	5.24	116.72	105.20
1	2	610	G	C5-C6-O6	-5.23	125.46	128.60
36	1	1269	U	N1-C2-O2	5.23	126.46	122.80
36	1	2338	C	OP1-P-O3'	5.23	116.72	105.20
1	6	390	G	C5-C6-O6	-5.23	125.46	128.60
36	5	63	A	N9-C4-C5	-5.23	103.71	105.80
36	5	1178	G	N1-C6-O6	5.23	123.04	119.90
1	2	569	C	O5'-P-OP1	-5.23	100.99	105.70
36	1	212	G	O4'-C1'-N9	5.23	112.39	108.20
36	1	1197	A	C4-C5-N7	5.23	113.32	110.70
36	1	2380	U	N3-C4-C5	5.23	117.74	114.60
36	5	1365	G	O4'-C1'-N9	-5.23	104.01	108.20
36	5	2150	G	C4-C5-N7	-5.23	108.71	110.80
36	5	2945	G	N1-C6-O6	5.23	123.04	119.90
1	6	1389	C	C6-N1-C1'	-5.23	114.52	120.80
36	5	1166	G	N1-C6-O6	5.23	123.04	119.90
36	5	2941	A	C4-C5-N7	-5.23	108.08	110.70
36	5	3096	C	C5-C4-N4	-5.23	116.54	120.20
36	5	3306	U	N3-C2-O2	5.23	125.86	122.20
54	m8	105	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	2	294	C	C6-N1-C2	5.23	122.39	120.30
36	1	730	C	C6-N1-C2	5.23	122.39	120.30
37	3	52	G	N1-C6-O6	-5.23	116.76	119.90
42	15	110	LEU	CA-CB-CG	5.23	127.33	115.30
1	2	1280	C	C6-N1-C2	-5.23	118.21	120.30
36	1	1164	G	C8-N9-C4	-5.23	104.31	106.40
36	1	3044	G	N3-C4-N9	5.23	129.14	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	M8	111	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	6	336	G	C8-N9-C4	5.23	108.49	106.40
36	5	2975	U	N1-C2-O2	5.23	126.46	122.80
36	5	3060	C	C5-C4-N4	-5.23	116.54	120.20
1	2	694	U	N3-C2-O2	-5.23	118.54	122.20
36	1	803	C	C4-C5-C6	5.23	120.01	117.40
36	5	195	U	O5'-P-OP2	-5.23	101.00	105.70
1	6	1600	A	C4-C5-N7	5.22	113.31	110.70
36	5	1660	C	C6-N1-C2	-5.22	118.21	120.30
36	5	1668	G	N3-C4-C5	-5.22	125.99	128.60
36	5	2848	G	C6-C5-N7	-5.22	127.27	130.40
36	5	665	A	N9-C4-C5	-5.22	103.71	105.80
36	5	892	U	N3-C4-C5	5.22	117.73	114.60
1	2	501	U	P-O3'-C3'	5.22	125.96	119.70
36	1	695	C	N3-C4-C5	5.22	123.99	121.90
36	1	702	C	N3-C4-C5	5.22	123.99	121.90
36	1	1517	G	O5'-P-OP1	5.22	116.96	110.70
36	5	771	A	C8-N9-C4	5.22	107.89	105.80
1	2	1132	A	N1-C6-N6	-5.22	115.47	118.60
36	5	424	G	N9-C4-C5	-5.22	103.31	105.40
36	5	1157	G	OP2-P-O3'	5.22	116.68	105.20
36	5	2287	C	N1-C2-O2	-5.22	115.77	118.90
36	5	2648	G	C2-N3-C4	5.22	114.51	111.90
36	5	2704	A	OP2-P-O3'	5.22	116.68	105.20
36	5	3208	G	C6-C5-N7	-5.22	127.27	130.40
36	1	812	G	O5'-P-OP2	-5.22	101.00	105.70
36	1	1711	C	C6-N1-C2	-5.22	118.21	120.30
36	1	2850	G	C8-N9-C1'	-5.22	120.22	127.00
36	1	2857	C	C5-C4-N4	-5.22	116.55	120.20
36	1	3362	A	C4-C5-C6	5.22	119.61	117.00
1	6	858	G	C5-N7-C8	-5.22	101.69	104.30
1	6	937	C	N1-C2-O2	-5.22	115.77	118.90
1	6	1119	G	C8-N9-C4	-5.22	104.31	106.40
36	5	187	A	OP1-P-OP2	-5.22	111.78	119.60
36	5	948	C	C2-N3-C4	-5.22	117.29	119.90
36	5	960	U	N3-C2-O2	-5.22	118.55	122.20
36	5	1738	C	N3-C2-O2	5.22	125.55	121.90
36	5	2273	G	C6-C5-N7	5.22	133.53	130.40
36	1	818	C	C6-N1-C2	-5.21	118.21	120.30
36	1	961	C	C2-N3-C4	-5.21	117.29	119.90
36	1	1864	A	N9-C4-C5	-5.21	103.71	105.80
36	5	412	G	OP1-P-OP2	-5.21	111.78	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1487	G	N3-C4-C5	-5.21	125.99	128.60
36	5	2364	G	N9-C4-C5	5.21	107.49	105.40
36	5	2398	A	C8-N9-C4	5.21	107.89	105.80
1	2	90	C	C6-N1-C2	-5.21	118.22	120.30
1	2	934	C	C6-N1-C1'	-5.21	114.54	120.80
36	1	346	C	N1-C2-O2	-5.21	115.77	118.90
38	4	61	A	C5-C6-N1	5.21	120.31	117.70
36	5	2767	U	N3-C4-O4	-5.21	115.75	119.40
1	2	704	C	N3-C2-O2	-5.21	118.25	121.90
36	1	86	G	O5'-P-OP2	-5.21	101.01	105.70
41	L4	98	ARG	NE-CZ-NH2	5.21	122.91	120.30
36	5	716	A	O4'-C1'-N9	-5.21	104.03	108.20
36	5	1329	U	C5-C6-N1	-5.21	120.09	122.70
1	2	1112	G	N1-C6-O6	5.21	123.03	119.90
36	1	2349	U	C2-N3-C4	-5.21	123.87	127.00
36	5	2640	A	C2-N3-C4	-5.21	108.00	110.60
59	n3	42	SER	N-CA-C	5.21	125.07	111.00
37	3	88	G	C5-N7-C8	5.21	106.90	104.30
38	4	60	U	N1-C2-N3	5.21	118.03	114.90
36	5	726	G	N1-C6-O6	5.21	123.03	119.90
36	5	824	C	N3-C2-O2	-5.21	118.25	121.90
36	5	1864	A	C5-C6-N6	-5.21	119.53	123.70
36	5	2280	A	OP2-P-O3'	5.21	116.66	105.20
1	2	1551	U	C5-C4-O4	-5.21	122.78	125.90
36	1	547	G	P-O3'-C3'	5.21	125.95	119.70
36	1	1338	C	N1-C2-O2	-5.21	115.78	118.90
36	1	1365	G	C4-N9-C1'	5.21	133.27	126.50
36	1	3041	U	C6-N1-C2	-5.21	117.88	121.00
36	5	923	C	C6-N1-C2	5.21	122.38	120.30
36	5	2965	U	N3-C2-O2	5.21	125.84	122.20
36	1	92	G	C5-C6-N1	5.21	114.10	111.50
36	5	963	G	C8-N9-C4	5.21	108.48	106.40
36	1	2942	C	N3-C4-C5	5.20	123.98	121.90
1	6	416	A	C2-N3-C4	-5.20	108.00	110.60
1	6	1493	A	C8-N9-C4	-5.20	103.72	105.80
37	7	42	A	C5-C6-N6	-5.20	119.54	123.70
38	8	105	A	C8-N9-C4	5.20	107.88	105.80
36	1	1166	G	N1-C6-O6	5.20	123.02	119.90
1	6	1491	U	P-O3'-C3'	5.20	125.94	119.70
36	5	1313	G	C5-C6-N1	-5.20	108.90	111.50
36	5	2950	G	C5-C6-O6	-5.20	125.48	128.60
36	5	3374	U	N3-C4-O4	-5.20	115.76	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	m0	48	LEU	CA-CB-CG	5.20	127.27	115.30
36	1	3303	G	C8-N9-C4	5.20	108.48	106.40
1	6	1777	G	O5'-P-OP1	-5.20	101.02	105.70
36	5	421	G	OP1-P-O3'	5.20	116.64	105.20
36	5	652	G	N3-C4-C5	-5.20	126.00	128.60
36	5	679	U	C5-C4-O4	5.20	129.02	125.90
36	5	812	G	C5-C6-O6	5.20	131.72	128.60
36	5	2630	C	N3-C2-O2	5.20	125.54	121.90
67	o1	90	PHE	CB-CA-C	-5.20	100.00	110.40
1	2	16	G	N3-C2-N2	5.20	123.54	119.90
36	1	950	G	N3-C2-N2	5.20	123.54	119.90
36	1	1466	G	N9-C4-C5	-5.20	103.32	105.40
36	1	2643	A	N1-C6-N6	5.20	121.72	118.60
1	6	337	G	C4-C5-C6	5.20	121.92	118.80
36	1	1406	A	C5-C6-N6	-5.20	119.54	123.70
36	5	875	G	N3-C4-C5	-5.20	126.00	128.60
36	5	2987	A	C8-N9-C4	5.20	107.88	105.80
1	2	192	U	C5-C6-N1	5.20	125.30	122.70
36	1	1137	C	C5-C4-N4	-5.20	116.56	120.20
36	5	1731	A	N1-C2-N3	5.20	131.90	129.30
36	5	2824	G	C5-C6-O6	-5.20	125.48	128.60
36	5	2939	G	N7-C8-N9	-5.20	110.50	113.10
36	1	896	A	C2-N3-C4	5.19	113.20	110.60
36	1	1366	A	C8-N9-C4	-5.19	103.72	105.80
1	6	1000	C	C2-N1-C1'	5.19	124.51	118.80
36	5	1716	U	P-O3'-C3'	5.19	125.93	119.70
36	5	3055	U	N3-C4-O4	5.19	123.04	119.40
36	1	909	G	C5-C6-O6	-5.19	125.48	128.60
36	1	1114	U	N1-C2-O2	5.19	126.44	122.80
36	1	1507	G	C5-C6-O6	-5.19	125.48	128.60
1	6	1663	G	O5'-P-OP1	5.19	116.93	110.70
36	5	2898	G	O4'-C1'-N9	-5.19	104.05	108.20
36	5	3287	U	N1-C2-O2	5.19	126.43	122.80
36	1	1433	A	O4'-C1'-N9	-5.19	104.05	108.20
59	N3	48	ARG	NE-CZ-NH1	5.19	122.89	120.30
64	N8	116	GLY	N-CA-C	5.19	126.08	113.10
36	5	87	U	N3-C4-O4	-5.19	115.77	119.40
36	5	2849	C	N3-C4-N4	5.19	121.63	118.00
36	5	2947	G	C5-C6-O6	-5.19	125.48	128.60
36	1	418	A	C2-N3-C4	-5.19	108.00	110.60
1	2	192	U	N3-C2-O2	-5.19	118.57	122.20
36	1	102	C	N1-C2-O2	-5.19	115.79	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	639	G	N9-C4-C5	-5.19	103.33	105.40
36	5	1075	A	C8-N9-C4	5.19	107.88	105.80
36	5	1297	C	N1-C2-O2	-5.19	115.79	118.90
36	1	898	U	N1-C2-O2	5.19	126.43	122.80
36	1	1780	G	N1-C6-O6	5.19	123.01	119.90
36	1	2731	U	OP2-P-O3'	5.19	116.61	105.20
36	5	567	G	N1-C6-O6	5.19	123.01	119.90
36	5	3050	U	N3-C2-O2	-5.19	118.57	122.20
36	1	2642	A	N3-C4-C5	5.18	130.43	126.80
36	1	2728	G	C5-C6-N1	5.18	114.09	111.50
37	3	95	A	C6-C5-N7	-5.18	128.67	132.30
1	6	433	C	OP2-P-O3'	5.18	116.61	105.20
36	5	956	U	C5-C6-N1	-5.18	120.11	122.70
36	5	2825	C	C6-N1-C2	5.18	122.37	120.30
36	5	3335	A	C5-C6-N6	-5.18	119.55	123.70
36	1	33	G	C6-C5-N7	-5.18	127.29	130.40
36	1	2101	C	P-O3'-C3'	5.18	125.92	119.70
36	1	2819	A	C2-N3-C4	5.18	113.19	110.60
36	1	3227	A	OP2-P-O3'	5.18	116.60	105.20
36	5	45	A	C5-C6-N6	-5.18	119.56	123.70
36	5	1347	U	N1-C2-O2	-5.18	119.17	122.80
36	5	2661	G	N3-C4-N9	5.18	129.11	126.00
37	7	105	C	C5-C4-N4	5.18	123.83	120.20
1	2	469	C	N1-C2-O2	-5.18	115.79	118.90
1	2	620	A	C8-N9-C4	-5.18	103.73	105.80
36	1	2360	C	C6-N1-C2	-5.18	118.23	120.30
38	4	60	U	C2-N3-C4	-5.18	123.89	127.00
36	1	942	U	N3-C4-O4	5.18	123.03	119.40
45	L8	189	LEU	CA-CB-CG	5.18	127.21	115.30
64	N8	29	PRO	C-N-CA	-5.18	111.42	122.30
36	5	1000	C	O4'-C1'-N1	5.18	112.34	108.20
36	5	1371	G	N1-C6-O6	-5.18	116.79	119.90
36	5	1491	A	N1-C6-N6	5.18	121.71	118.60
36	5	2300	G	N3-C2-N2	5.18	123.53	119.90
1	2	499	U	C3'-C2'-C1'	5.18	105.64	101.50
38	4	26	U	N3-C4-O4	-5.18	115.78	119.40
71	O5	36	LEU	CA-CB-CG	5.18	127.21	115.30
36	1	632	G	C5-C6-O6	5.18	131.71	128.60
36	1	2797	C	C5-C4-N4	5.18	123.82	120.20
1	6	1022	C	C2-N3-C4	-5.18	117.31	119.90
1	6	1354	G	C4-N9-C1'	5.18	133.23	126.50
36	5	953	G	N9-C4-C5	5.18	107.47	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2550	U	N3-C2-O2	-5.17	118.58	122.20
36	5	204	A	N1-C6-N6	-5.17	115.50	118.60
36	5	590	G	C4-C5-N7	5.17	112.87	110.80
36	5	936	A	C8-N9-C4	-5.17	103.73	105.80
36	5	1152	G	C8-N9-C4	-5.17	104.33	106.40
36	5	2408	U	O5'-P-OP2	-5.17	101.04	105.70
36	5	2541	U	C2-N1-C1'	5.17	123.91	117.70
36	5	3386	G	O5'-P-OP2	-5.17	101.04	105.70
52	m6	84	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	2	1615	C	N3-C2-O2	-5.17	118.28	121.90
36	1	720	A	C2-N3-C4	5.17	113.19	110.60
36	1	2623	G	N1-C2-N2	-5.17	111.54	116.20
1	6	1607	G	C4-C5-N7	-5.17	108.73	110.80
36	5	662	U	C5-C4-O4	5.17	129.00	125.90
36	5	1406	A	C5-C6-N6	-5.17	119.56	123.70
36	5	1449	A	C4-C5-C6	5.17	119.59	117.00
36	1	2401	A	C4-N9-C1'	-5.17	116.99	126.30
36	1	2723	U	C6-N1-C2	5.17	124.10	121.00
1	6	1332	C	N1-C2-O2	5.17	122.00	118.90
36	5	43	A	N1-C6-N6	5.17	121.70	118.60
36	5	950	G	N1-C6-O6	-5.17	116.80	119.90
36	5	1518	U	N3-C2-O2	-5.17	118.58	122.20
36	5	2388	U	OP2-P-O3'	5.17	116.58	105.20
36	5	2398	A	C5-C6-N6	5.17	127.84	123.70
36	5	2411	U	C5-C6-N1	-5.17	120.11	122.70
36	5	2938	G	C5-C6-N1	5.17	114.09	111.50
37	7	120	C	C6-N1-C2	5.17	122.37	120.30
36	1	1796	G	C8-N9-C4	-5.17	104.33	106.40
36	1	1815	U	P-O3'-C3'	5.17	125.90	119.70
36	1	2343	C	C2-N3-C4	-5.17	117.31	119.90
36	1	2637	A	N1-C6-N6	5.17	121.70	118.60
36	5	2633	U	OP1-P-O3'	5.17	116.58	105.20
36	1	360	G	C8-N9-C4	5.17	108.47	106.40
36	1	907	G	N3-C4-N9	5.17	129.10	126.00
36	1	1442	U	O5'-P-OP2	5.17	116.90	110.70
36	5	1822	C	C6-N1-C2	5.17	122.37	120.30
36	5	2345	A	C6-C5-N7	-5.17	128.68	132.30
36	5	2362	C	C4-C5-C6	-5.17	114.81	117.40
54	m8	127	LEU	CA-CB-CG	5.17	127.19	115.30
36	1	637	C	N3-C4-C5	5.17	123.97	121.90
36	1	833	G	N1-C6-O6	-5.17	116.80	119.90
36	1	889	U	C6-N1-C2	5.17	124.10	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1112	A	C4-C5-N7	5.17	113.28	110.70
36	1	1520	G	N7-C8-N9	-5.17	110.52	113.10
36	1	2349	U	N3-C2-O2	-5.17	118.58	122.20
37	3	85	G	OP2-P-O3'	5.17	116.57	105.20
1	6	1648	A	N1-C6-N6	5.17	121.70	118.60
36	5	248	U	C2-N1-C1'	5.17	123.90	117.70
36	5	1203	A	N1-C6-N6	5.17	121.70	118.60
36	5	2207	A	C6-C5-N7	-5.17	128.68	132.30
36	1	1415	U	N3-C2-O2	-5.17	118.58	122.20
1	6	635	A	OP2-P-O3'	5.17	116.56	105.20
1	2	1102	G	C2-N3-C4	5.16	114.48	111.90
1	2	1431	C	C6-N1-C2	5.16	122.36	120.30
36	1	45	A	N7-C8-N9	-5.16	111.22	113.80
36	1	636	C	O4'-C1'-N1	-5.16	104.07	108.20
36	1	809	G	N9-C4-C5	-5.16	103.33	105.40
36	1	810	A	OP1-P-OP2	-5.16	111.86	119.60
36	1	911	C	O5'-P-OP2	5.16	116.89	110.70
36	1	2923	U	O5'-P-OP2	5.16	116.90	110.70
38	4	97	A	N9-C4-C5	5.16	107.86	105.80
36	5	634	C	N3-C4-C5	5.16	123.97	121.90
36	5	994	G	N1-C2-N2	-5.16	111.55	116.20
37	7	37	G	C4-C5-N7	5.16	112.86	110.80
36	1	847	A	N1-C6-N6	5.16	121.70	118.60
36	1	1781	C	N1-C2-O2	-5.16	115.80	118.90
1	6	356	G	N1-C6-O6	-5.16	116.80	119.90
1	2	1747	G	C8-N9-C4	5.16	108.46	106.40
36	1	31	C	C2-N3-C4	-5.16	117.32	119.90
36	1	37	U	C5-C6-N1	-5.16	120.12	122.70
36	1	878	G	OP1-P-O3'	5.16	116.55	105.20
36	5	97	U	N1-C2-N3	-5.16	111.80	114.90
36	5	437	G	N1-C2-N3	5.16	127.00	123.90
36	5	2623	G	C8-N9-C4	5.16	108.46	106.40
36	5	2937	G	C5-C6-O6	-5.16	125.50	128.60
1	2	779	U	O4'-C1'-N1	5.16	112.33	108.20
36	1	878	G	C5-C6-N1	-5.16	108.92	111.50
36	1	1199	C	C2-N3-C4	-5.16	117.32	119.90
36	1	2374	C	C6-N1-C2	-5.16	118.24	120.30
36	5	796	U	C4-C5-C6	5.16	122.80	119.70
36	5	1435	A	C5-C6-N6	-5.16	119.57	123.70
36	5	2836	C	OP2-P-O3'	5.16	116.55	105.20
36	5	1665	C	N3-C4-C5	5.16	123.96	121.90
36	1	1909	A	N1-C2-N3	5.16	131.88	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	392	G	O4'-C1'-N9	5.16	112.33	108.20
36	5	200	C	N3-C4-C5	-5.16	119.84	121.90
36	5	665	A	C5-C6-N6	-5.16	119.58	123.70
36	5	2595	A	C5-C6-N6	5.16	127.82	123.70
36	5	2754	G	N3-C4-N9	5.16	129.09	126.00
25	D3	111	GLY	N-CA-C	-5.15	100.21	113.10
36	1	2787	G	N3-C4-C5	-5.15	126.02	128.60
36	5	216	G	C4-C5-N7	5.15	112.86	110.80
36	5	2140	U	N1-C2-N3	5.15	117.99	114.90
36	5	2941	A	N1-C6-N6	-5.15	115.51	118.60
36	5	3035	A	C8-N9-C4	5.15	107.86	105.80
36	1	66	A	O5'-P-OP2	5.15	116.88	110.70
36	1	2629	U	C5-C6-N1	5.15	125.28	122.70
36	1	2983	C	O4'-C1'-N1	5.15	112.32	108.20
36	1	3213	A	N1-C6-N6	5.15	121.69	118.60
37	3	75	G	N9-C4-C5	5.15	107.46	105.40
36	5	800	G	N3-C4-N9	5.15	129.09	126.00
36	5	963	G	N7-C8-N9	-5.15	110.52	113.10
36	1	1177	G	C5-C6-O6	-5.15	125.51	128.60
36	1	2130	G	C5-C6-O6	5.15	131.69	128.60
36	1	3151	U	O5'-P-OP2	-5.15	101.06	105.70
1	6	765	G	C8-N9-C4	5.15	108.46	106.40
1	6	956	C	C6-N1-C2	5.15	122.36	120.30
1	6	1478	G	C8-N9-C1'	-5.15	120.31	127.00
1	6	1675	C	N3-C4-N4	5.15	121.61	118.00
36	5	1116	G	OP2-P-O3'	5.15	116.53	105.20
36	5	1190	A	C4-N9-C1'	5.15	135.57	126.30
1	2	829	A	P-O3'-C3'	5.15	125.88	119.70
35	SM	134	ASP	CB-CG-OD2	5.15	122.93	118.30
36	1	359	U	C4-C5-C6	5.15	122.79	119.70
36	1	1403	C	C5-C4-N4	-5.15	116.60	120.20
38	4	61	A	N9-C4-C5	-5.15	103.74	105.80
36	5	2908	G	C8-N9-C4	-5.15	104.34	106.40
36	5	3136	G	N1-C2-N2	-5.15	111.57	116.20
36	1	1047	A	C8-N9-C4	5.15	107.86	105.80
36	1	2916	U	OP1-P-O3'	5.15	116.53	105.20
1	6	1473	U	C2-N1-C1'	5.15	123.88	117.70
36	5	1056	U	C5-C6-N1	5.15	125.27	122.70
36	5	1178	G	C6-C5-N7	-5.15	127.31	130.40
36	5	2889	C	N3-C4-C5	5.15	123.96	121.90
36	5	2944	U	N3-C4-C5	5.15	117.69	114.60
1	6	687	G	N3-C4-N9	-5.15	122.91	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	35	A	N1-C6-N6	5.15	121.69	118.60
36	5	520	U	N1-C2-O2	-5.15	119.20	122.80
36	1	2915	U	N3-C4-O4	5.14	123.00	119.40
36	5	368	G	C4-C5-N7	-5.14	108.74	110.80
36	5	1131	G	N1-C6-O6	5.14	122.99	119.90
1	2	344	A	N1-C6-N6	-5.14	115.51	118.60
1	2	1258	U	N1-C2-O2	5.14	126.40	122.80
1	2	1268	G	O5'-P-OP2	-5.14	101.07	105.70
36	1	1164	G	C4-N9-C1'	5.14	133.19	126.50
36	1	2696	A	N1-C6-N6	-5.14	115.52	118.60
41	L4	187	LEU	CA-CB-CG	5.14	127.13	115.30
1	6	56	U	C5-C4-O4	-5.14	122.81	125.90
1	6	523	G	N1-C6-O6	-5.14	116.81	119.90
36	5	671	U	C6-N1-C2	5.14	124.09	121.00
36	5	1337	A	C2-N3-C4	5.14	113.17	110.60
36	5	1417	G	N3-C4-C5	-5.14	126.03	128.60
36	5	2433	U	C5-C6-N1	-5.14	120.13	122.70
36	5	2914	G	N3-C4-N9	5.14	129.09	126.00
36	5	3080	G	N9-C4-C5	-5.14	103.34	105.40
36	5	3328	G	N3-C4-C5	-5.14	126.03	128.60
36	1	909	G	O5'-P-OP1	-5.14	101.07	105.70
36	1	2889	C	O5'-P-OP1	-5.14	101.07	105.70
1	6	1410	A	N1-C6-N6	5.14	121.68	118.60
36	5	2399	A	N1-C2-N3	5.14	131.87	129.30
36	1	968	G	C5-C6-N1	5.14	114.07	111.50
36	1	1054	A	O5'-P-OP2	-5.14	101.08	105.70
36	1	3318	G	C6-C5-N7	-5.14	127.32	130.40
39	12	242	ARG	NE-CZ-NH2	-5.14	117.73	120.30
36	1	155	G	C5-C6-N1	5.14	114.07	111.50
36	5	3351	U	N3-C2-O2	-5.14	118.60	122.20
36	1	216	G	C6-C5-N7	-5.14	127.32	130.40
36	1	2640	A	N3-C4-C5	-5.14	123.20	126.80
36	5	374	A	OP1-P-O3'	5.14	116.50	105.20
36	5	1316	C	N1-C2-N3	5.14	122.80	119.20
36	1	751	A	N1-C6-N6	-5.13	115.52	118.60
36	1	1391	C	C2-N3-C4	-5.13	117.33	119.90
36	1	2966	G	C5-C6-N1	5.13	114.07	111.50
36	5	952	A	C4-C5-N7	5.13	113.27	110.70
36	5	3287	U	N3-C2-O2	-5.13	118.61	122.20
36	1	395	A	C8-N9-C4	-5.13	103.75	105.80
36	5	1403	C	C2-N3-C4	-5.13	117.33	119.90
1	2	15	U	C6-N1-C2	-5.13	117.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2796	G	OP1-P-O3'	5.13	116.49	105.20
36	5	190	U	N3-C2-O2	-5.13	118.61	122.20
36	5	1496	C	OP1-P-OP2	-5.13	111.90	119.60
36	5	2400	G	OP2-P-O3'	5.13	116.49	105.20
36	1	2917	G	C2-N3-C4	5.13	114.47	111.90
36	1	3275	U	C6-N1-C2	-5.13	117.92	121.00
36	5	1868	G	N9-C4-C5	-5.13	103.35	105.40
38	8	126	A	OP1-P-O3'	5.13	116.49	105.20
1	2	553	G	C5-C6-O6	-5.13	125.52	128.60
36	1	1142	G	OP1-P-OP2	5.13	127.29	119.60
36	5	2383	C	N1-C2-O2	-5.13	115.82	118.90
37	7	34	C	C6-N1-C2	-5.13	118.25	120.30
1	2	1176	G	N1-C6-O6	5.13	122.98	119.90
1	2	1302	U	C6-N1-C2	-5.13	117.92	121.00
36	1	798	G	N3-C2-N2	-5.13	116.31	119.90
36	1	1911	A	C5-N7-C8	-5.13	101.34	103.90
36	5	840	C	N3-C2-O2	-5.13	118.31	121.90
36	5	1327	C	N3-C4-N4	-5.13	114.41	118.00
36	5	1465	A	C2-N3-C4	-5.13	108.04	110.60
36	5	1855	U	N1-C2-N3	5.13	117.98	114.90
36	5	2697	A	C4-C5-C6	5.12	119.56	117.00
1	2	944	A	N9-C4-C5	-5.12	103.75	105.80
36	1	678	G	C5-C6-O6	-5.12	125.53	128.60
1	6	914	G	C5-C6-O6	-5.12	125.53	128.60
1	6	1201	G	O5'-P-OP1	-5.12	101.09	105.70
36	5	517	G	N3-C4-N9	5.12	129.07	126.00
36	5	2133	U	OP2-P-O3'	5.12	116.47	105.20
1	2	794	U	OP1-P-O3'	5.12	116.47	105.20
36	1	37	U	N1-C2-N3	5.12	117.97	114.90
36	1	59	G	C6-N1-C2	5.12	128.17	125.10
36	1	2123	G	C5-C6-O6	-5.12	125.53	128.60
36	1	2993	G	N3-C2-N2	5.12	123.48	119.90
36	5	2234	G	C6-N1-C2	-5.12	122.03	125.10
38	8	24	G	N1-C6-O6	-5.12	116.83	119.90
36	5	1213	G	N9-C4-C5	-5.12	103.35	105.40
36	5	1336	U	OP2-P-O3'	5.12	116.46	105.20
37	7	71	G	OP2-P-O3'	5.12	116.47	105.20
1	2	380	U	N1-C2-O2	5.12	126.38	122.80
36	1	2688	U	C5-C4-O4	-5.12	122.83	125.90
36	5	1261	G	O4'-C1'-N9	5.12	112.30	108.20
36	1	1661	G	O5'-P-OP2	-5.12	101.09	105.70
52	m6	58	LEU	CB-CG-CD2	-5.12	102.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2281	A	P-O3'-C3'	-5.12	113.56	119.70
36	1	2619	G	OP1-P-OP2	5.12	127.27	119.60
1	6	1285	U	N3-C2-O2	-5.12	118.62	122.20
36	5	2283	G	O5'-P-OP2	-5.12	101.09	105.70
1	2	1462	G	C4-C5-N7	5.11	112.84	110.80
36	1	910	G	C4-C5-C6	5.11	121.87	118.80
36	1	3190	C	N3-C4-C5	5.11	123.94	121.90
1	6	1573	A	P-O3'-C3'	5.11	125.83	119.70
1	6	1780	G	C8-N9-C4	5.11	108.45	106.40
36	5	974	G	N3-C4-N9	5.11	129.07	126.00
36	5	1838	G	OP1-P-O3'	5.11	116.45	105.20
36	5	2144	A	O5'-P-OP2	-5.11	101.10	105.70
36	5	2930	A	N3-C4-N9	-5.11	123.31	127.40
36	1	424	G	N1-C2-N2	-5.11	111.60	116.20
36	1	1669	C	C5-C4-N4	-5.11	116.62	120.20
36	1	2879	C	N3-C2-O2	5.11	125.48	121.90
36	1	1385	C	C2-N1-C1'	-5.11	113.18	118.80
36	1	2174	G	N7-C8-N9	5.11	115.66	113.10
36	1	2249	G	N3-C2-N2	5.11	123.48	119.90
36	1	2624	G	C5-C6-O6	-5.11	125.53	128.60
36	1	2698	G	OP1-P-OP2	5.11	127.27	119.60
36	5	974	G	C5-C6-N1	5.11	114.06	111.50
36	5	1493	G	O4'-C1'-N9	5.11	112.29	108.20
36	5	2851	A	C8-N9-C4	5.11	107.84	105.80
36	5	1379	G	C8-N9-C4	5.11	108.44	106.40
36	1	214	G	N1-C6-O6	5.11	122.97	119.90
36	1	1157	G	OP2-P-O3'	5.11	116.44	105.20
36	1	2383	C	C5-C4-N4	-5.11	116.62	120.20
36	1	3302	U	N3-C4-O4	-5.11	115.82	119.40
37	3	88	G	C5-C6-O6	5.11	131.66	128.60
1	6	1200	G	N3-C4-N9	-5.11	122.94	126.00
36	5	1004	U	C5-C6-N1	5.11	125.25	122.70
36	5	3049	A	C5-N7-C8	5.11	106.45	103.90
1	2	186	C	C5-C6-N1	5.11	123.55	121.00
36	1	140	C	OP2-P-O3'	5.11	116.43	105.20
36	1	2215	A	N9-C4-C5	-5.11	103.76	105.80
36	1	2987	A	C5-C6-N6	-5.11	119.61	123.70
36	5	2369	G	C8-N9-C4	5.11	108.44	106.40
36	5	2623	G	N3-C4-N9	5.11	129.06	126.00
36	5	3214	U	N1-C2-O2	5.11	126.37	122.80
1	2	558	U	C2-N1-C1'	5.10	123.83	117.70
1	2	1595	U	O4'-C1'-N1	5.10	112.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	609	G	C5-C6-N1	5.10	114.05	111.50
36	5	515	C	C5-C4-N4	-5.10	116.63	120.20
36	5	1319	G	OP2-P-O3'	5.10	116.43	105.20
36	5	2109	U	N1-C2-N3	5.10	117.96	114.90
36	1	709	A	N9-C4-C5	-5.10	103.76	105.80
37	3	58	C	C6-N1-C2	-5.10	118.26	120.30
75	O9	13	MET	CB-CG-SD	-5.10	97.09	112.40
1	6	382	C	C2-N3-C4	-5.10	117.35	119.90
1	6	402	C	C5-C6-N1	-5.10	118.45	121.00
36	5	982	C	C6-N1-C2	-5.10	118.26	120.30
36	5	1112	A	C6-C5-N7	-5.10	128.73	132.30
38	8	77	A	C8-N9-C4	5.10	107.84	105.80
36	1	818	C	N1-C2-O2	5.10	121.96	118.90
36	1	1786	G	N1-C6-O6	-5.10	116.84	119.90
36	5	2280	A	C2-N3-C4	-5.10	108.05	110.60
36	1	880	G	N9-C4-C5	5.10	107.44	105.40
36	1	2817	A	OP2-P-O3'	5.10	116.42	105.20
1	6	1131	A	C6-C5-N7	-5.10	128.73	132.30
10	s8	5	ARG	NE-CZ-NH2	-5.10	117.75	120.30
36	5	1328	C	C6-N1-C2	-5.10	118.26	120.30
36	5	2338	C	N1-C2-O2	-5.10	115.84	118.90
36	5	2888	U	C5-C4-O4	-5.10	122.84	125.90
36	1	658	G	C4-C5-C6	5.10	121.86	118.80
36	1	920	A	OP1-P-O3'	5.10	116.41	105.20
36	1	1466	G	N3-C2-N2	5.10	123.47	119.90
36	5	719	U	N1-C2-O2	5.10	126.37	122.80
36	5	3007	U	C5-C6-N1	-5.10	120.15	122.70
40	l3	19	ARG	NE-CZ-NH1	5.10	122.85	120.30
36	1	1794	G	OP1-P-OP2	5.10	127.24	119.60
1	6	108	A	C6-N1-C2	-5.10	115.54	118.60
1	6	1145	U	N3-C4-C5	-5.10	111.54	114.60
1	2	447	U	C6-N1-C2	-5.09	117.94	121.00
1	2	1600	A	P-O3'-C3'	5.09	125.81	119.70
36	1	1793	C	C2-N3-C4	-5.09	117.35	119.90
36	1	1823	A	C4-C5-C6	5.09	119.55	117.00
36	1	2989	U	N1-C2-N3	5.09	117.96	114.90
1	6	622	A	N1-C6-N6	-5.09	115.54	118.60
1	6	1696	G	C3'-C2'-C1'	5.09	105.58	101.50
36	5	639	G	N1-C6-O6	5.09	122.96	119.90
36	5	779	G	N1-C6-O6	5.09	122.96	119.90
36	5	1192	C	C5-C4-N4	-5.09	116.63	120.20
36	5	2293	C	C4-C5-C6	-5.09	114.85	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2572	C	C6-N1-C2	-5.09	118.26	120.30
36	5	3041	U	C6-N1-C2	5.09	124.06	121.00
36	1	403	C	C2-N3-C4	5.09	122.45	119.90
36	1	1123	U	C4-C5-C6	5.09	122.75	119.70
1	6	639	U	N3-C2-O2	-5.09	118.64	122.20
1	6	1119	G	O5'-P-OP2	-5.09	101.12	105.70
36	5	1370	G	C8-N9-C4	5.09	108.44	106.40
36	5	2392	C	C2-N1-C1'	-5.09	113.20	118.80
36	5	2818	U	C5'-C4'-O4'	-5.09	102.99	109.10
36	5	2881	C	N3-C2-O2	5.09	125.46	121.90
36	1	8	C	C6-N1-C2	5.09	122.34	120.30
36	1	346	C	C2-N3-C4	-5.09	117.36	119.90
36	1	2424	A	C5-N7-C8	-5.09	101.36	103.90
1	6	111	U	C6-N1-C2	-5.09	117.95	121.00
1	6	1327	C	N1-C2-O2	5.09	121.95	118.90
36	5	676	G	C8-N9-C4	-5.09	104.36	106.40
1	2	728	U	N3-C2-O2	-5.09	118.64	122.20
1	2	765	G	O4'-C1'-N9	-5.09	104.13	108.20
36	5	358	G	N1-C6-O6	5.09	122.95	119.90
36	5	2329	C	N3-C4-C5	5.09	123.94	121.90
37	7	79	A	C5-N7-C8	-5.09	101.36	103.90
36	1	909	G	C8-N9-C4	5.09	108.44	106.40
36	1	2624	G	N1-C6-O6	5.09	122.95	119.90
41	L4	328	ASN	N-CA-C	5.09	124.73	111.00
1	6	1354	G	C8-N9-C4	-5.09	104.36	106.40
36	5	1216	C	N1-C2-O2	-5.09	115.85	118.90
36	5	1304	A	O5'-P-OP1	-5.09	101.12	105.70
36	5	2704	A	C4-C5-N7	5.09	113.24	110.70
38	8	5	U	N1-C2-O2	-5.09	119.24	122.80
36	1	815	G	N1-C6-O6	5.08	122.95	119.90
36	1	1484	U	C2-N1-C1'	5.08	123.80	117.70
36	1	2582	C	N1-C2-O2	5.08	121.95	118.90
36	5	373	A	C8-N9-C4	5.08	107.83	105.80
36	5	701	G	C5-C6-O6	5.08	131.65	128.60
1	2	610	G	C4-N9-C1'	5.08	133.11	126.50
36	1	805	G	N9-C4-C5	-5.08	103.37	105.40
36	1	2249	G	N3-C4-C5	-5.08	126.06	128.60
36	1	2305	G	N9-C4-C5	-5.08	103.37	105.40
1	6	1300	A	O5'-P-OP1	-5.08	101.12	105.70
36	5	335	G	C5-C6-O6	5.08	131.65	128.60
36	5	907	G	C4-C5-N7	5.08	112.83	110.80
36	5	1617	G	C5-C6-O6	-5.08	125.55	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1868	G	C6-C5-N7	-5.08	127.35	130.40
36	1	859	G	N1-C2-N2	-5.08	111.63	116.20
36	1	1162	U	C2-N1-C1'	5.08	123.80	117.70
36	1	1935	G	N3-C2-N2	5.08	123.46	119.90
1	6	454	U	O5'-P-OP2	-5.08	101.13	105.70
1	6	539	G	C5-C6-O6	-5.08	125.55	128.60
36	5	907	G	C8-N9-C4	5.08	108.43	106.40
36	5	1367	G	C4-C5-C6	5.08	121.85	118.80
37	7	74	C	N3-C2-O2	5.08	125.46	121.90
36	1	1372	C	C5-C6-N1	-5.08	118.46	121.00
36	5	649	A	N1-C6-N6	5.08	121.65	118.60
36	5	1341	U	C5-C4-O4	5.08	128.95	125.90
36	1	262	U	N3-C2-O2	5.08	125.75	122.20
36	1	797	U	O5'-P-OP1	-5.08	101.13	105.70
36	1	893	C	C5-C6-N1	5.08	123.54	121.00
36	1	1664	G	N1-C6-O6	-5.08	116.85	119.90
1	6	90	C	N3-C4-C5	5.08	123.93	121.90
1	6	1208	A	O4'-C1'-N9	5.08	112.26	108.20
36	5	632	G	O5'-P-OP2	-5.08	101.13	105.70
36	5	871	U	OP2-P-O3'	5.08	116.37	105.20
36	5	892	U	C2-N1-C1'	-5.08	111.61	117.70
36	5	1331	U	C6-N1-C2	5.08	124.05	121.00
36	5	2198	A	C5-C6-N6	-5.08	119.64	123.70
36	5	2996	U	C6-N1-C2	5.08	124.05	121.00
36	5	3330	A	C5-C6-N1	5.08	120.24	117.70
36	1	1105	A	C8-N9-C4	5.08	107.83	105.80
41	L4	139	GLY	N-CA-C	-5.08	100.41	113.10
1	6	361	C	C5-C6-N1	5.08	123.54	121.00
1	2	852	C	C5-C6-N1	5.08	123.54	121.00
36	1	2407	C	C5-C4-N4	-5.08	116.65	120.20
36	1	3090	U	N3-C2-O2	5.08	125.75	122.20
1	6	362	G	N3-C4-C5	-5.08	126.06	128.60
36	5	664	U	C6-N1-C2	-5.08	117.95	121.00
36	5	2403	G	OP1-P-O3'	5.08	116.36	105.20
36	1	815	G	C6-C5-N7	-5.07	127.36	130.40
36	1	818	C	C5-C4-N4	5.07	123.75	120.20
36	1	1528	G	OP1-P-OP2	5.07	127.21	119.60
36	1	2406	C	C5-C4-N4	-5.07	116.65	120.20
36	1	3059	G	N1-C6-O6	-5.07	116.86	119.90
38	4	21	C	C2-N1-C1'	-5.07	113.22	118.80
1	6	312	A	N1-C6-N6	-5.07	115.56	118.60
1	6	472	U	N1-C2-N3	5.07	117.94	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2395	G	C4-C5-N7	5.07	112.83	110.80
36	5	2524	A	C4-N9-C1'	5.07	135.43	126.30
37	3	84	A	C5-C6-N6	-5.07	119.64	123.70
38	4	113	U	C6-N1-C1'	5.07	128.30	121.20
36	5	659	G	P-O3'-C3'	5.07	125.79	119.70
36	5	2840	C	OP1-P-OP2	-5.07	111.99	119.60
1	2	1659	A	O5'-P-OP1	-5.07	101.14	105.70
36	1	758	C	N3-C4-N4	5.07	121.55	118.00
36	1	1112	A	C6-C5-N7	-5.07	128.75	132.30
36	1	2800	G	O5'-P-OP1	5.07	116.78	110.70
36	1	3057	U	N1-C2-O2	5.07	126.35	122.80
1	6	364	G	N3-C4-C5	-5.07	126.06	128.60
1	6	1649	G	N3-C2-N2	5.07	123.45	119.90
36	5	2631	U	N3-C4-C5	5.07	117.64	114.60
36	5	2940	A	O5'-P-OP2	-5.07	101.14	105.70
36	1	1200	A	C2-N3-C4	5.07	113.13	110.60
36	5	872	U	C5-C6-N1	5.07	125.23	122.70
36	1	2133	U	OP1-P-OP2	-5.07	112.00	119.60
36	5	2880	U	C5-C6-N1	5.07	125.23	122.70
36	5	2938	G	OP2-P-O3'	5.07	116.35	105.20
1	2	1745	G	N1-C6-O6	5.07	122.94	119.90
36	1	1380	G	O5'-P-OP2	-5.07	101.14	105.70
36	1	1492	G	N3-C4-N9	5.07	129.04	126.00
36	1	1800	A	C2-N3-C4	5.07	113.13	110.60
1	6	434	G	C8-N9-C4	5.07	108.43	106.40
36	5	575	G	N3-C4-C5	-5.07	126.07	128.60
36	5	1226	G	N9-C4-C5	-5.07	103.37	105.40
36	5	2725	U	N3-C4-C5	5.07	117.64	114.60
36	5	3143	C	N1-C2-O2	-5.07	115.86	118.90
36	5	3243	A	OP2-P-O3'	5.07	116.34	105.20
40	13	148	LEU	CB-CG-CD2	-5.07	102.39	111.00
36	1	813	G	N3-C4-N9	5.06	129.04	126.00
36	1	2697	A	C2-N3-C4	-5.06	108.07	110.60
1	6	581	U	N1-C2-O2	-5.06	119.25	122.80
36	5	1408	G	N9-C4-C5	5.06	107.42	105.40
36	5	1782	U	N1-C2-O2	-5.06	119.26	122.80
1	2	440	U	O5'-P-OP1	-5.06	101.14	105.70
36	1	515	C	C2-N3-C4	5.06	122.43	119.90
36	1	2943	G	N1-C6-O6	-5.06	116.86	119.90
36	5	812	G	C4-C5-N7	-5.06	108.78	110.80
36	5	971	G	C4-C5-N7	-5.06	108.78	110.80
36	5	2802	A	N1-C2-N3	-5.06	126.77	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3047	U	C5-C6-N1	-5.06	120.17	122.70
36	1	574	U	C5-C6-N1	-5.06	120.17	122.70
36	1	911	C	C5-C6-N1	-5.06	118.47	121.00
36	1	930	U	O5'-P-OP2	5.06	116.77	110.70
36	1	2142	A	OP1-P-OP2	-5.06	112.01	119.60
36	1	2407	C	N3-C4-N4	5.06	121.54	118.00
36	5	2978	U	P-O3'-C3'	5.06	125.77	119.70
36	1	430	U	C5-C6-N1	-5.06	120.17	122.70
36	1	972	A	C8-N9-C4	5.06	107.82	105.80
36	1	1368	U	C5-C4-O4	-5.06	122.86	125.90
1	6	959	U	O4'-C1'-N1	-5.06	104.15	108.20
1	6	1020	A	C8-N9-C4	-5.06	103.78	105.80
36	5	1170	A	C8-N9-C4	5.06	107.82	105.80
36	5	1919	G	N1-C6-O6	5.06	122.94	119.90
36	5	2728	G	O4'-C1'-N9	5.06	112.25	108.20
36	5	2994	A	C4-C5-C6	5.06	119.53	117.00
36	1	2273	G	N7-C8-N9	-5.06	110.57	113.10
36	1	2730	G	N3-C4-N9	-5.06	122.97	126.00
1	6	1757	G	C8-N9-C4	5.06	108.42	106.40
36	5	918	C	C5-C6-N1	5.06	123.53	121.00
36	5	3000	A	C8-N9-C4	5.06	107.82	105.80
36	1	1179	A	N1-C2-N3	5.06	131.83	129.30
36	1	1332	A	OP2-P-O3'	5.06	116.32	105.20
36	1	2304	C	C6-N1-C2	-5.06	118.28	120.30
1	6	1498	G	O5'-P-OP2	-5.06	101.15	105.70
13	c1	120	GLY	N-CA-C	-5.06	100.46	113.10
36	5	391	A	C8-N9-C4	5.06	107.82	105.80
36	5	1113	G	N3-C4-N9	-5.06	122.97	126.00
36	5	1209	G	C8-N9-C4	-5.06	104.38	106.40
36	5	2358	A	N3-C4-C5	5.06	130.34	126.80
36	5	2851	A	N7-C8-N9	-5.06	111.27	113.80
36	1	48	A	O4'-C1'-N9	5.05	112.24	108.20
36	1	1151	U	C6-N1-C2	-5.05	117.97	121.00
36	1	2638	C	C6-N1-C2	5.05	122.32	120.30
36	5	3285	C	C6-N1-C2	-5.05	118.28	120.30
38	8	54	A	C5-N7-C8	-5.05	101.37	103.90
36	1	2865	U	OP2-P-O3'	5.05	116.32	105.20
38	4	55	U	C2-N3-C4	-5.05	123.97	127.00
36	5	23	A	C5-C6-N6	-5.05	119.66	123.70
36	5	361	A	C4-C5-N7	-5.05	108.17	110.70
1	2	1560	U	N3-C4-O4	-5.05	115.86	119.40
36	1	802	C	N1-C2-O2	5.05	121.93	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1306	G	O5'-P-OP1	-5.05	101.15	105.70
36	1	2787	G	C5-C6-O6	-5.05	125.57	128.60
36	1	3223	A	N1-C6-N6	-5.05	115.57	118.60
1	6	1131	A	N1-C6-N6	5.05	121.63	118.60
1	6	1196	A	C8-N9-C4	5.05	107.82	105.80
36	5	521	A	C8-N9-C4	5.05	107.82	105.80
36	5	1852	G	N9-C4-C5	5.05	107.42	105.40
36	5	2172	A	C2-N3-C4	-5.05	108.07	110.60
1	2	1748	G	C5-C6-O6	5.05	131.63	128.60
36	1	3212	C	C6-N1-C2	5.05	122.32	120.30
1	6	937	C	C6-N1-C2	-5.05	118.28	120.30
36	5	2335	G	C6-N1-C2	-5.05	122.07	125.10
36	5	2409	G	O5'-P-OP2	-5.05	101.16	105.70
36	5	3309	G	C8-N9-C1'	-5.05	120.44	127.00
36	1	3181	C	N1-C2-N3	5.05	122.73	119.20
36	1	627	U	N1-C2-O2	-5.05	119.27	122.80
36	1	1780	G	C5-C6-O6	-5.05	125.57	128.60
36	5	329	U	C5-C6-N1	-5.05	120.18	122.70
36	5	1082	U	C6-N1-C2	-5.05	117.97	121.00
36	5	1112	A	C5-C6-N6	-5.05	119.66	123.70
36	5	1604	G	N3-C4-C5	-5.05	126.08	128.60
36	5	1902	G	N3-C2-N2	-5.05	116.37	119.90
36	5	2823	G	N3-C4-N9	5.05	129.03	126.00
36	5	3014	U	C2-N3-C4	-5.05	123.97	127.00
36	1	2355	G	C6-C5-N7	-5.04	127.37	130.40
38	4	41	A	C4-C5-C6	5.04	119.52	117.00
36	5	722	G	C8-N9-C4	-5.04	104.38	106.40
1	2	1426	C	N3-C4-C5	5.04	123.92	121.90
1	2	1745	G	N3-C4-N9	5.04	129.03	126.00
36	1	281	G	C5-C6-N1	5.04	114.02	111.50
36	1	374	A	C6-N1-C2	5.04	121.63	118.60
36	1	775	A	N1-C6-N6	5.04	121.63	118.60
36	1	934	G	C6-C5-N7	-5.04	127.37	130.40
36	1	2297	U	P-O3'-C3'	5.04	125.75	119.70
36	1	2837	A	N7-C8-N9	-5.04	111.28	113.80
1	6	352	A	C6-C5-N7	5.04	135.83	132.30
1	6	1190	C	C6-N1-C2	5.04	122.32	120.30
36	5	1456	A	C5-C6-N1	-5.04	115.18	117.70
36	5	2895	G	C4-C5-N7	-5.04	108.78	110.80
41	14	327	LEU	CA-CB-CG	5.04	126.90	115.30
1	2	937	C	C6-N1-C2	-5.04	118.28	120.30
36	1	2606	G	N9-C4-C5	-5.04	103.38	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	706	A	OP2-P-O3'	5.04	116.29	105.20
36	5	1077	U	N3-C4-C5	5.04	117.62	114.60
36	5	2290	C	C5-C4-N4	-5.04	116.67	120.20
36	5	3154	C	C2-N3-C4	5.04	122.42	119.90
36	1	1832	C	N3-C4-N4	-5.04	114.47	118.00
38	8	125	U	C2-N1-C1'	5.04	123.75	117.70
1	2	1199	G	O5'-P-OP2	-5.04	101.17	105.70
36	1	2362	C	N3-C2-O2	-5.04	118.37	121.90
36	1	2621	G	OP1-P-OP2	-5.04	112.04	119.60
36	1	2799	A	OP2-P-O3'	5.04	116.28	105.20
36	1	2846	U	C6-N1-C2	-5.04	117.98	121.00
37	3	111	U	O5'-P-OP1	-5.04	101.17	105.70
1	6	591	A	O5'-P-OP2	-5.04	101.17	105.70
1	6	1595	U	O4'-C1'-N1	5.04	112.23	108.20
36	5	1352	A	P-O3'-C3'	5.04	125.75	119.70
36	5	1487	G	C2-N3-C4	5.04	114.42	111.90
36	5	1671	C	O5'-P-OP1	-5.04	101.17	105.70
36	5	2648	G	N3-C4-C5	-5.04	126.08	128.60
36	5	2892	A	N9-C4-C5	5.04	107.82	105.80
37	7	105	C	N1-C2-O2	5.04	121.92	118.90
36	1	583	G	N9-C4-C5	5.04	107.42	105.40
36	1	2404	A	O5'-P-OP1	5.04	116.74	110.70
36	1	2970	C	C6-N1-C2	5.04	122.31	120.30
36	5	2297	U	OP1-P-OP2	5.04	127.16	119.60
36	5	3377	G	C5-C6-O6	-5.04	125.58	128.60
36	1	51	A	N1-C6-N6	5.04	121.62	118.60
36	1	267	G	O4'-C1'-N9	-5.04	104.17	108.20
1	6	1035	G	C8-N9-C4	5.04	108.41	106.40
1	6	1522	U	O4'-C1'-N1	5.04	112.23	108.20
36	5	875	G	C5-C6-N1	5.04	114.02	111.50
36	5	1048	A	OP1-P-O3'	5.04	116.28	105.20
36	5	1064	A	O4'-C1'-N9	-5.04	104.17	108.20
36	5	1152	G	N9-C4-C5	5.04	107.41	105.40
37	7	79	A	C5-C6-N6	-5.04	119.67	123.70
36	1	649	A	C6-N1-C2	-5.03	115.58	118.60
36	1	1855	U	N1-C2-N3	5.03	117.92	114.90
36	1	2828	G	N3-C4-C5	-5.03	126.08	128.60
36	5	57	A	OP2-P-O3'	5.03	116.27	105.20
36	5	335	G	O5'-P-OP2	5.03	116.74	110.70
36	5	873	C	OP2-P-O3'	5.03	116.27	105.20
36	5	981	U	C5-C6-N1	5.03	125.22	122.70
36	5	1145	G	N9-C4-C5	5.03	107.41	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1369	A	C5-C6-N6	-5.03	119.67	123.70
36	5	3101	G	C8-N9-C1'	-5.03	120.46	127.00
36	1	718	G	N3-C4-C5	5.03	131.12	128.60
36	5	1371	G	OP2-P-O3'	5.03	116.27	105.20
36	5	2754	G	N3-C4-C5	-5.03	126.08	128.60
36	5	3260	G	N9-C4-C5	5.03	107.41	105.40
36	5	3369	G	N1-C6-O6	-5.03	116.88	119.90
37	7	48	U	N1-C2-O2	-5.03	119.28	122.80
36	1	1060	U	N1-C2-O2	-5.03	119.28	122.80
36	1	1360	C	C5-C6-N1	-5.03	118.48	121.00
36	1	2398	A	C4-C5-C6	5.03	119.52	117.00
36	1	3302	U	N3-C4-C5	5.03	117.62	114.60
1	6	1208	A	C8-N9-C4	-5.03	103.79	105.80
36	5	195	U	N1-C2-N3	5.03	117.92	114.90
36	5	1112	A	O5'-P-OP2	5.03	116.74	110.70
36	5	1436	U	C2-N1-C1'	5.03	123.74	117.70
36	5	2938	G	C2-N3-C4	5.03	114.42	111.90
36	1	69	C	N1-C2-O2	-5.03	115.88	118.90
36	1	219	A	N1-C2-N3	5.03	131.81	129.30
36	1	2323	G	N3-C4-N9	5.03	129.02	126.00
36	5	719	U	C5-C6-N1	5.03	125.22	122.70
36	1	218	G	OP1-P-OP2	5.03	127.14	119.60
36	1	2901	G	C5-C6-O6	-5.03	125.58	128.60
1	6	1035	G	N3-C2-N2	5.03	123.42	119.90
36	5	364	G	C4-C5-N7	5.03	112.81	110.80
36	5	1049	C	C4-C5-C6	-5.03	114.89	117.40
36	5	1330	A	C2-N3-C4	5.03	113.11	110.60
36	5	2700	G	C5-C6-N1	5.03	114.01	111.50
1	2	606	A	O4'-C1'-N9	5.03	112.22	108.20
1	2	1741	U	C5-C6-N1	-5.03	120.19	122.70
36	1	345	G	OP1-P-OP2	5.03	127.14	119.60
36	1	350	C	C5-C6-N1	5.03	123.51	121.00
36	1	2883	U	O5'-P-OP1	5.03	116.73	110.70
1	2	1590	G	N1-C6-O6	-5.02	116.89	119.90
36	1	656	A	O5'-P-OP1	-5.02	101.18	105.70
36	1	2356	A	C4-C5-N7	5.02	113.21	110.70
1	6	17	C	N3-C2-O2	-5.02	118.38	121.90
36	5	657	A	N1-C6-N6	5.02	121.61	118.60
36	5	876	A	OP2-P-O3'	5.02	116.25	105.20
36	5	2250	G	C5-C6-O6	5.02	131.62	128.60
38	8	54	A	N1-C6-N6	5.02	121.61	118.60
36	1	18	G	OP2-P-O3'	5.02	116.25	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1313	G	C4-C5-N7	5.02	112.81	110.80
36	1	1404	G	N7-C8-N9	-5.02	110.59	113.10
36	1	1529	A	C2-N3-C4	-5.02	108.09	110.60
36	1	2600	C	N1-C2-O2	5.02	121.91	118.90
36	1	2945	G	N1-C6-O6	5.02	122.91	119.90
45	L8	65	LEU	CA-CB-CG	5.02	126.85	115.30
36	5	407	A	N1-C6-N6	5.02	121.61	118.60
36	5	2361	A	OP2-P-O3'	5.02	116.25	105.20
37	7	92	A	N9-C4-C5	-5.02	103.79	105.80
1	2	1654	G	C6-N1-C2	-5.02	122.09	125.10
36	1	894	G	OP1-P-O3'	5.02	116.25	105.20
36	5	915	A	N3-C4-C5	-5.02	123.28	126.80
36	5	2947	G	N3-C4-N9	5.02	129.01	126.00
36	1	1547	G	C5-N7-C8	5.02	106.81	104.30
36	1	2406	C	O5'-P-OP1	-5.02	101.18	105.70
36	5	146	U	C5-C6-N1	-5.02	120.19	122.70
36	5	2207	A	N7-C8-N9	5.02	116.31	113.80
36	5	3209	A	C8-N9-C4	-5.02	103.79	105.80
36	1	948	C	C5-C6-N1	-5.02	118.49	121.00
36	1	1201	C	N3-C4-N4	5.02	121.51	118.00
36	1	1860	G	N1-C6-O6	-5.02	116.89	119.90
36	1	2367	A	C4-C5-C6	5.02	119.51	117.00
1	6	532	U	OP2-P-O3'	5.02	116.24	105.20
36	5	308	A	O5'-P-OP1	5.02	116.72	110.70
36	5	439	C	N3-C4-C5	-5.02	119.89	121.90
36	5	984	G	C8-N9-C4	-5.02	104.39	106.40
36	5	2315	G	O5'-P-OP1	-5.02	101.18	105.70
36	5	2333	C	C5-C4-N4	-5.02	116.69	120.20
1	2	136	C	C5-C6-N1	5.02	123.51	121.00
1	2	1389	C	C2-N1-C1'	5.02	124.32	118.80
36	1	1351	U	C2-N1-C1'	5.02	123.72	117.70
36	1	2361	A	C6-N1-C2	-5.02	115.59	118.60
36	5	2356	A	C5-C6-N6	5.02	127.71	123.70
1	2	1489	U	C2-N1-C1'	5.01	123.72	117.70
36	1	429	U	N3-C4-C5	5.01	117.61	114.60
36	1	1364	C	C6-N1-C2	5.01	122.31	120.30
36	1	3112	G	C4-C5-N7	5.01	112.81	110.80
36	5	2350	C	C4-C5-C6	5.01	119.91	117.40
36	5	3076	C	N3-C4-C5	5.01	123.91	121.90
36	5	3275	U	C6-N1-C1'	5.01	128.22	121.20
37	7	42	A	C6-N1-C2	-5.01	115.59	118.60
52	m6	117	ARG	CG-CD-NE	-5.01	101.27	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1533	U	C5-C4-O4	-5.01	122.89	125.90
36	5	936	A	N1-C6-N6	-5.01	115.59	118.60
1	2	1536	G	C4-N9-C1'	5.01	133.01	126.50
36	1	52	A	OP1-P-O3'	5.01	116.23	105.20
36	1	646	A	C8-N9-C4	-5.01	103.80	105.80
36	1	1120	A	OP2-P-O3'	5.01	116.22	105.20
36	1	1882	G	O5'-P-OP1	-5.01	101.19	105.70
36	1	2137	U	C6-N1-C1'	-5.01	114.19	121.20
36	1	2958	A	OP2-P-O3'	5.01	116.23	105.20
36	1	3036	G	C8-N9-C4	-5.01	104.39	106.40
38	4	73	U	N1-C2-O2	5.01	126.31	122.80
36	5	43	A	O4'-C1'-N9	5.01	112.21	108.20
36	5	353	G	C4-N9-C1'	-5.01	119.98	126.50
36	5	536	U	C5-C6-N1	-5.01	120.19	122.70
36	5	1304	A	C8-N9-C4	5.01	107.80	105.80
36	5	1438	U	N1-C2-N3	5.01	117.91	114.90
36	5	2402	A	C5-C6-N6	5.01	127.71	123.70
36	5	2704	A	OP1-P-OP2	5.01	127.12	119.60
36	1	98	G	OP2-P-O3'	5.01	116.22	105.20
36	1	433	A	N3-C4-C5	-5.01	123.29	126.80
36	1	1831	U	C6-N1-C2	-5.01	118.00	121.00
36	1	2279	A	N9-C4-C5	-5.01	103.80	105.80
36	1	2571	U	N3-C2-O2	-5.01	118.69	122.20
64	N8	66	ALA	N-CA-C	-5.01	97.47	111.00
1	6	1700	C	C5-C6-N1	5.01	123.50	121.00
36	5	645	A	N3-C4-C5	-5.01	123.29	126.80
1	2	73	U	OP1-P-O3'	5.01	116.22	105.20
36	1	3043	C	N3-C4-N4	-5.01	114.49	118.00
1	6	47	A	N1-C2-N3	-5.01	126.80	129.30
36	5	1657	C	O4'-C1'-N1	5.01	112.21	108.20
36	5	1916	U	N3-C2-O2	-5.01	118.69	122.20
36	1	326	U	O5'-P-OP2	-5.01	101.19	105.70
36	1	340	C	C6-N1-C2	-5.01	118.30	120.30
36	1	2305	G	C4-N9-C1'	5.01	133.01	126.50
36	1	2659	G	C5-C6-O6	-5.01	125.60	128.60
36	1	3318	G	N3-C4-C5	-5.01	126.10	128.60
36	5	426	G	C2-N3-C4	5.01	114.40	111.90
36	5	930	U	OP1-P-O3'	5.01	116.21	105.20
36	5	1299	U	O5'-P-OP2	-5.01	101.19	105.70
36	5	2334	U	O5'-P-OP1	5.01	116.71	110.70
36	5	2944	U	OP2-P-O3'	5.01	116.22	105.20
1	2	1033	C	N3-C2-O2	-5.00	118.40	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2968	G	N1-C2-N2	-5.00	111.70	116.20
36	5	420	G	C6-C5-N7	-5.00	127.40	130.40
36	5	2619	G	C4-C5-N7	5.00	112.80	110.80
1	2	1145	U	N3-C4-O4	5.00	122.90	119.40
36	1	66	A	C8-N9-C4	5.00	107.80	105.80
36	1	282	G	N3-C2-N2	5.00	123.40	119.90
36	1	407	A	O5'-P-OP1	5.00	116.70	110.70
36	1	415	G	N1-C6-O6	-5.00	116.90	119.90
36	1	718	G	C5-N7-C8	-5.00	101.80	104.30
36	1	776	U	C6-N1-C2	-5.00	118.00	121.00
36	1	1119	C	C5-C6-N1	-5.00	118.50	121.00
36	1	3275	U	C5-C6-N1	5.00	125.20	122.70
1	6	1114	G	N3-C4-C5	-5.00	126.10	128.60
1	6	1428	G	O5'-P-OP1	-5.00	101.20	105.70
36	5	1931	U	O5'-P-OP2	-5.00	101.20	105.70
1	2	347	G	C8-N9-C4	-5.00	104.40	106.40
1	2	1273	G	N3-C4-C5	-5.00	126.10	128.60
36	1	1315	U	N3-C2-O2	-5.00	118.70	122.20
1	6	322	G	O5'-P-OP1	-5.00	101.20	105.70
36	5	1880	U	O5'-P-OP2	5.00	116.70	110.70
36	5	3186	A	N9-C4-C5	5.00	107.80	105.80

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
33	E1	105	TYR	Peptide
39	L2	19	HIS	Peptide
43	L6	129	GLU	Peptide
43	L6	51	ARG	Peptide
43	L6	89	THR	Peptide
48	M1	64	LYS	Peptide
52	M6	110	PRO	Peptide
56	N0	12	ARG	Peptide
56	N0	22	PRO	Peptide
65	N9	20	GLY	Peptide
67	O1	5	LYS	Peptide

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Mol	Chain	Res	Type	Group
9	S7	131	PHE	Peptide
10	S8	147	ALA	Peptide
17	c5	52	LYS	Peptide
18	c6	40	GLU	Peptide
18	c6	41	PRO	Peptide
22	d0	70	THR	Peptide
25	d3	44	GLY	Peptide
27	d5	85	LYS	Peptide
39	l2	143	GLU	Peptide
39	l2	171	GLY	Peptide
42	l5	270	LYS	Peptide
42	l5	271	LYS	Peptide
43	l6	51	ARG	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
45	l8	221	ASN	Peptide
52	m6	110	PRO	Peptide
60	n4	78	ALA	Peptide
62	n6	111	LEU	Peptide
63	n7	5	LEU	Peptide
64	n8	18	GLY	Peptide
64	n8	26	ARG	Peptide
64	n8	66	ALA	Peptide
65	n9	19	ASN	Peptide
67	o1	64	VAL	Peptide
5	s3	203	PRO	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide
11	s9	89	ASP	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	33 (16%)	26 (13%)	0	1
2	s0	204/251 (81%)	148 (72%)	33 (16%)	23 (11%)	0	2
3	S1	212/254 (84%)	147 (69%)	38 (18%)	27 (13%)	0	1
3	s1	214/254 (84%)	176 (82%)	22 (10%)	16 (8%)	1	5
4	S2	215/253 (85%)	179 (83%)	26 (12%)	10 (5%)	2	14
4	s2	215/253 (85%)	179 (83%)	25 (12%)	11 (5%)	2	12
5	S3	221/239 (92%)	178 (80%)	29 (13%)	14 (6%)	1	7
5	s3	221/239 (92%)	178 (80%)	27 (12%)	16 (7%)	1	5
6	S4	258/260 (99%)	206 (80%)	39 (15%)	13 (5%)	2	12
6	s4	258/260 (99%)	214 (83%)	30 (12%)	14 (5%)	2	11
7	S5	204/224 (91%)	160 (78%)	26 (13%)	18 (9%)	1	3
7	s5	204/224 (91%)	162 (79%)	27 (13%)	15 (7%)	1	5
8	S6	224/236 (95%)	194 (87%)	19 (8%)	11 (5%)	2	13
8	s6	216/236 (92%)	187 (87%)	19 (9%)	10 (5%)	2	14
9	S7	182/189 (96%)	134 (74%)	28 (15%)	20 (11%)	0	2
9	s7	184/189 (97%)	141 (77%)	33 (18%)	10 (5%)	2	11
10	S8	184/200 (92%)	159 (86%)	13 (7%)	12 (6%)	1	7
10	s8	184/200 (92%)	159 (86%)	20 (11%)	5 (3%)	5	26
11	S9	183/196 (93%)	152 (83%)	21 (12%)	10 (6%)	2	10
11	s9	183/196 (93%)	142 (78%)	33 (18%)	8 (4%)	2	15
12	C0	94/105 (90%)	71 (76%)	13 (14%)	10 (11%)	0	2
12	c0	92/105 (88%)	64 (70%)	14 (15%)	14 (15%)	0	1
13	C1	153/155 (99%)	123 (80%)	18 (12%)	12 (8%)	1	4
13	c1	144/155 (93%)	120 (83%)	15 (10%)	9 (6%)	1	7
14	C2	122/142 (86%)	68 (56%)	28 (23%)	26 (21%)	0	0
14	c2	122/142 (86%)	69 (57%)	31 (25%)	22 (18%)	0	0
15	C3	148/150 (99%)	125 (84%)	15 (10%)	8 (5%)	2	11
15	c3	148/150 (99%)	114 (77%)	24 (16%)	10 (7%)	1	6
16	C4	125/136 (92%)	91 (73%)	22 (18%)	12 (10%)	0	3
16	c4	126/136 (93%)	104 (82%)	15 (12%)	7 (6%)	2	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	C5	122/141 (86%)	85 (70%)	26 (21%)	11 (9%)	1	3
17	c5	133/141 (94%)	93 (70%)	22 (16%)	18 (14%)	0	1
18	C6	139/142 (98%)	113 (81%)	16 (12%)	10 (7%)	1	5
18	c6	140/142 (99%)	117 (84%)	16 (11%)	7 (5%)	2	12
19	C7	116/136 (85%)	90 (78%)	14 (12%)	12 (10%)	0	2
19	c7	113/136 (83%)	88 (78%)	18 (16%)	7 (6%)	1	8
20	C8	143/145 (99%)	112 (78%)	20 (14%)	11 (8%)	1	5
20	c8	143/145 (99%)	112 (78%)	22 (15%)	9 (6%)	1	7
21	C9	141/143 (99%)	119 (84%)	17 (12%)	5 (4%)	3	20
21	c9	141/143 (99%)	118 (84%)	19 (14%)	4 (3%)	5	25
22	D0	105/120 (88%)	83 (79%)	14 (13%)	8 (8%)	1	5
22	d0	108/120 (90%)	83 (77%)	15 (14%)	10 (9%)	0	3
23	D1	85/87 (98%)	63 (74%)	14 (16%)	8 (9%)	0	3
23	d1	85/87 (98%)	70 (82%)	12 (14%)	3 (4%)	3	20
24	D2	127/129 (98%)	109 (86%)	17 (13%)	1 (1%)	19	57
24	d2	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	6	29
25	D3	142/144 (99%)	109 (77%)	21 (15%)	12 (8%)	1	4
25	d3	142/144 (99%)	128 (90%)	8 (6%)	6 (4%)	3	16
26	D4	132/134 (98%)	108 (82%)	14 (11%)	10 (8%)	1	5
26	d4	132/134 (98%)	108 (82%)	15 (11%)	9 (7%)	1	6
27	D5	68/107 (64%)	43 (63%)	14 (21%)	11 (16%)	0	1
27	d5	67/107 (63%)	55 (82%)	7 (10%)	5 (8%)	1	5
28	D6	95/97 (98%)	58 (61%)	19 (20%)	18 (19%)	0	0
28	d6	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	1	4
29	D7	79/81 (98%)	67 (85%)	8 (10%)	4 (5%)	2	12
29	d7	79/81 (98%)	66 (84%)	7 (9%)	6 (8%)	1	5
30	D8	61/66 (92%)	51 (84%)	7 (12%)	3 (5%)	2	13
30	d8	61/66 (92%)	46 (75%)	8 (13%)	7 (12%)	0	2
31	D9	51/55 (93%)	43 (84%)	6 (12%)	2 (4%)	3	17
31	d9	51/55 (93%)	42 (82%)	5 (10%)	4 (8%)	1	4
32	E0	58/60 (97%)	47 (81%)	7 (12%)	4 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	E1	69/76 (91%)	36 (52%)	15 (22%)	18 (26%)	0	0
33	e1	74/76 (97%)	34 (46%)	20 (27%)	20 (27%)	0	0
34	SR	316/318 (99%)	277 (88%)	27 (8%)	12 (4%)	3	18
34	sR	316/318 (99%)	270 (85%)	36 (11%)	10 (3%)	4	22
35	SM	155/273 (57%)	113 (73%)	18 (12%)	24 (16%)	0	1
35	sM	98/273 (36%)	64 (65%)	20 (20%)	14 (14%)	0	1
39	L2	250/253 (99%)	225 (90%)	17 (7%)	8 (3%)	4	22
39	l2	250/253 (99%)	211 (84%)	33 (13%)	6 (2%)	6	29
40	L3	384/386 (100%)	336 (88%)	31 (8%)	17 (4%)	2	15
40	l3	384/386 (100%)	341 (89%)	31 (8%)	12 (3%)	4	23
41	L4	359/361 (99%)	293 (82%)	46 (13%)	20 (6%)	2	10
41	l4	359/361 (99%)	305 (85%)	35 (10%)	19 (5%)	2	11
42	L5	294/296 (99%)	245 (83%)	31 (10%)	18 (6%)	1	8
42	l5	292/296 (99%)	259 (89%)	23 (8%)	10 (3%)	3	20
43	L6	152/175 (87%)	135 (89%)	14 (9%)	3 (2%)	7	34
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	5	27
44	L7	220/243 (90%)	198 (90%)	14 (6%)	8 (4%)	3	19
44	l7	221/243 (91%)	199 (90%)	19 (9%)	3 (1%)	11	43
45	L8	231/255 (91%)	189 (82%)	34 (15%)	8 (4%)	3	20
45	l8	229/255 (90%)	183 (80%)	26 (11%)	20 (9%)	1	3
46	L9	189/191 (99%)	168 (89%)	15 (8%)	6 (3%)	4	22
46	l9	189/191 (99%)	174 (92%)	9 (5%)	6 (3%)	4	22
47	M0	207/220 (94%)	179 (86%)	20 (10%)	8 (4%)	3	17
47	m0	209/220 (95%)	168 (80%)	30 (14%)	11 (5%)	2	11
48	M1	167/173 (96%)	132 (79%)	17 (10%)	18 (11%)	0	2
48	m1	167/173 (96%)	140 (84%)	16 (10%)	11 (7%)	1	6
49	M3	191/198 (96%)	156 (82%)	28 (15%)	7 (4%)	3	19
49	m3	192/198 (97%)	156 (81%)	22 (12%)	14 (7%)	1	5
50	M4	134/137 (98%)	116 (87%)	10 (8%)	8 (6%)	1	9
50	m4	135/137 (98%)	121 (90%)	11 (8%)	3 (2%)	6	31
51	M5	201/203 (99%)	186 (92%)	10 (5%)	5 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	m5	201/203 (99%)	181 (90%)	13 (6%)	7 (4%)	3	20
52	M6	195/198 (98%)	180 (92%)	12 (6%)	3 (2%)	10	42
52	m6	195/198 (98%)	174 (89%)	16 (8%)	5 (3%)	5	27
53	M7	181/183 (99%)	153 (84%)	20 (11%)	8 (4%)	2	15
53	m7	153/183 (84%)	140 (92%)	11 (7%)	2 (1%)	12	45
54	M8	183/185 (99%)	157 (86%)	21 (12%)	5 (3%)	5	26
54	m8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	4	21
55	M9	186/188 (99%)	161 (87%)	23 (12%)	2 (1%)	14	50
55	m9	186/188 (99%)	163 (88%)	22 (12%)	1 (0%)	29	68
56	N0	170/172 (99%)	151 (89%)	14 (8%)	5 (3%)	4	24
56	n0	170/172 (99%)	154 (91%)	14 (8%)	2 (1%)	13	48
57	N1	157/159 (99%)	140 (89%)	12 (8%)	5 (3%)	4	22
57	n1	157/159 (99%)	139 (88%)	13 (8%)	5 (3%)	4	22
58	N2	98/120 (82%)	76 (78%)	15 (15%)	7 (7%)	1	5
58	n2	96/120 (80%)	82 (85%)	10 (10%)	4 (4%)	3	16
59	N3	134/136 (98%)	121 (90%)	11 (8%)	2 (2%)	10	42
59	n3	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	10	42
60	N4	96/155 (62%)	77 (80%)	12 (12%)	7 (7%)	1	5
60	n4	133/155 (86%)	110 (83%)	12 (9%)	11 (8%)	1	4
61	N5	119/141 (84%)	107 (90%)	9 (8%)	3 (2%)	5	28
61	n5	118/141 (84%)	96 (81%)	10 (8%)	12 (10%)	0	2
62	N6	124/126 (98%)	114 (92%)	7 (6%)	3 (2%)	6	29
62	n6	124/126 (98%)	110 (89%)	8 (6%)	6 (5%)	2	13
63	N7	133/135 (98%)	113 (85%)	12 (9%)	8 (6%)	1	9
63	n7	133/135 (98%)	104 (78%)	18 (14%)	11 (8%)	1	4
64	N8	146/148 (99%)	123 (84%)	13 (9%)	10 (7%)	1	6
64	n8	146/148 (99%)	121 (83%)	20 (14%)	5 (3%)	3	20
65	N9	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	3	19
65	n9	56/58 (97%)	41 (73%)	9 (16%)	6 (11%)	0	2
66	O0	95/104 (91%)	87 (92%)	8 (8%)	0	100	100
66	o0	98/104 (94%)	88 (90%)	9 (9%)	1 (1%)	15	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	O1	107/112 (96%)	98 (92%)	4 (4%)	5 (5%)	2	14
67	o1	107/112 (96%)	88 (82%)	15 (14%)	4 (4%)	3	19
68	O2	125/129 (97%)	112 (90%)	11 (9%)	2 (2%)	9	40
68	o2	125/129 (97%)	108 (86%)	12 (10%)	5 (4%)	3	17
69	O3	104/106 (98%)	96 (92%)	7 (7%)	1 (1%)	15	53
69	o3	104/106 (98%)	96 (92%)	7 (7%)	1 (1%)	15	53
70	O4	110/120 (92%)	100 (91%)	7 (6%)	3 (3%)	5	26
70	o4	110/120 (92%)	99 (90%)	7 (6%)	4 (4%)	3	19
71	O5	117/119 (98%)	103 (88%)	9 (8%)	5 (4%)	2	15
71	o5	117/119 (98%)	98 (84%)	14 (12%)	5 (4%)	2	15
72	O6	97/99 (98%)	76 (78%)	14 (14%)	7 (7%)	1	5
72	o6	97/99 (98%)	80 (82%)	9 (9%)	8 (8%)	1	4
73	O7	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	6	29
73	o7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	6	29
74	O8	75/77 (97%)	59 (79%)	14 (19%)	2 (3%)	5	26
74	o8	75/77 (97%)	63 (84%)	8 (11%)	4 (5%)	2	11
75	O9	48/50 (96%)	42 (88%)	5 (10%)	1 (2%)	7	33
75	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
76	Q0	50/52 (96%)	44 (88%)	4 (8%)	2 (4%)	3	17
76	q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	3	17
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
78	Q2	103/105 (98%)	83 (81%)	16 (16%)	4 (4%)	3	17
78	q2	103/105 (98%)	92 (89%)	8 (8%)	3 (3%)	4	24
79	Q3	89/91 (98%)	70 (79%)	16 (18%)	3 (3%)	3	20
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	14	50
80	e0	60/62 (97%)	44 (73%)	10 (17%)	6 (10%)	0	2
82	p0	139/311 (45%)	115 (83%)	19 (14%)	5 (4%)	3	19
All	All	22333/24143 (92%)	18550 (83%)	2534 (11%)	1249 (6%)	2	10

All (1249) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	49	ASN
2	S0	66	ALA
2	S0	158	VAL
2	S0	185	ARG
2	S0	191	ARG
2	S0	203	PHE
3	S1	49	ASN
3	S1	58	SER
3	S1	63	GLY
3	S1	116	LYS
3	S1	148	ASN
3	S1	177	GLN
3	S1	179	SER
3	S1	206	PRO
3	S1	221	PRO
4	S2	148	LEU
5	S3	62	ASN
5	S3	65	ARG
5	S3	211	PRO
5	S3	212	LYS
5	S3	220	PRO
6	S4	26	CYS
6	S4	104	ASP
6	S4	164	LEU
7	S5	26	ALA
7	S5	35	GLN
7	S5	39	GLU
7	S5	63	GLN
7	S5	76	ARG
8	S6	20	ASP
8	S6	25	ARG
8	S6	154	ARG
8	S6	173	PRO
8	S6	174	LYS
9	S7	31	SER
9	S7	32	PRO
9	S7	64	VAL
9	S7	111	LYS
9	S7	112	ARG
9	S7	116	ARG
9	S7	131	PHE

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Mol	Chain	Res	Type
9	S7	133	THR
9	S7	134	GLU
9	S7	155	ASP
10	S8	22	ARG
10	S8	52	ASN
11	S9	98	ALA
11	S9	134	ILE
11	S9	164	PHE
12	C0	54	TYR
12	C0	60	SER
12	C0	64	TYR
12	C0	81	ASN
12	C0	87	VAL
12	C0	88	PRO
13	C1	7	VAL
13	C1	29	LYS
13	C1	95	PRO
13	C1	96	LYS
13	C1	147	ALA
14	C2	89	ILE
14	C2	93	ASP
14	C2	127	GLY
15	C3	22	ALA
15	C3	27	LYS
15	C3	138	ASN
16	C4	39	ILE
16	C4	124	ASP
16	C4	125	SER
17	C5	54	ALA
17	C5	125	PRO
17	C5	126	VAL
18	C6	40	GLU
18	C6	41	PRO
18	C6	59	LYS
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	124	VAL
20	C8	14	ILE
20	C8	60	GLU
20	C8	82	PRO
20	C8	91	ASP

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Mol	Chain	Res	Type
20	C8	92	ILE
21	C9	31	PRO
21	C9	53	TRP
22	D0	118	VAL
24	D2	83	ILE
25	D3	114	LYS
25	D3	131	SER
25	D3	137	LYS
26	D4	36	SER
27	D5	39	ALA
27	D5	43	ASP
27	D5	44	GLN
27	D5	71	ILE
27	D5	97	LYS
28	D6	18	VAL
28	D6	45	VAL
28	D6	65	PRO
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
29	D7	38	PRO
29	D7	62	ILE
32	E0	47	VAL
33	E1	98	VAL
33	E1	102	VAL
33	E1	103	LEU
33	E1	106	TYR
33	E1	128	ALA
34	SR	51	ASP
34	SR	161	LYS
34	SR	318	ALA
35	SM	52	PRO
35	SM	87	THR
35	SM	89	ARG
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
39	L2	250	GLN
40	L3	3	HIS
40	L3	4	ARG
40	L3	138	ALA
40	L3	140	ASP

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Mol	Chain	Res	Type
40	L3	300	ARG
40	L3	347	SER
40	L3	351	LEU
41	L4	130	ALA
41	L4	146	PRO
41	L4	268	ALA
41	L4	270	SER
41	L4	291	ASN
41	L4	317	PRO
41	L4	318	LEU
41	L4	338	LYS
42	L5	58	LYS
42	L5	233	ALA
42	L5	234	ASP
42	L5	258	LYS
43	L6	6	ALA
43	L6	98	VAL
44	L7	24	GLU
44	L7	26	VAL
44	L7	216	VAL
45	L8	25	PRO
45	L8	31	PRO
46	L9	50	ASN
46	L9	109	ALA
48	M1	8	PRO
48	M1	9	MET
48	M1	11	ASP
48	M1	74	PRO
48	M1	115	LYS
48	M1	165	GLN
49	M3	47	ALA
49	M3	129	ASN
50	M4	8	LYS
50	M4	9	ALA
50	M4	10	SER
51	M5	75	VAL
52	M6	111	PRO
53	M7	157	VAL
54	M8	41	ASP
54	M8	99	THR
55	M9	53	LYS
57	N1	159	PHE

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Mol	Chain	Res	Type
58	N2	44	GLU
58	N2	51	GLY
60	N4	64	THR
60	N4	81	PRO
61	N5	44	PRO
62	N6	84	LYS
63	N7	17	ARG
64	N8	76	ASP
67	O1	6	ASP
67	O1	7	VAL
67	O1	84	ASP
71	O5	91	ALA
71	O5	119	LYS
72	O6	33	ALA
75	O9	4	GLN
76	Q0	78	ILE
78	Q2	15	LYS
78	Q2	30	ALA
78	Q2	100	LYS
2	s0	4	PRO
2	s0	8	ASP
2	s0	164	ASN
2	s0	183	ARG
2	s0	185	ARG
2	s0	186	GLY
2	s0	206	ASP
3	s1	147	ALA
3	s1	154	SER
3	s1	206	PRO
3	s1	223	PHE
4	s2	92	ALA
5	s3	179	GLN
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
5	s3	221	SER
6	s4	95	THR
6	s4	195	ILE
6	s4	196	VAL
7	s5	28	PRO
7	s5	39	GLU

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Mol	Chain	Res	Type
7	s5	43	PHE
7	s5	54	LYS
7	s5	127	GLN
7	s5	184	PHE
7	s5	204	GLY
8	s6	153	VAL
8	s6	154	ARG
8	s6	173	PRO
8	s6	174	LYS
9	s7	64	VAL
9	s7	66	SER
9	s7	67	LEU
9	s7	74	GLN
9	s7	116	ARG
9	s7	131	PHE
9	s7	185	ILE
10	s8	62	THR
11	s9	118	LEU
11	s9	121	SER
12	c0	82	LEU
12	c0	83	PRO
12	c0	88	PRO
12	c0	97	PRO
13	c1	129	ARG
14	c2	22	VAL
14	c2	89	ILE
14	c2	131	ASP
15	c3	66	ILE
15	c3	87	ASP
15	c3	137	PRO
15	c3	139	TRP
16	c4	126	THR
16	c4	132	ARG
17	c5	9	LYS
17	c5	11	VAL
17	c5	51	SER
17	c5	52	LYS
17	c5	117	GLY
17	c5	125	PRO
17	c5	126	VAL
17	c5	127	ARG
17	c5	132	GLY

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Mol	Chain	Res	Type
18	c6	42	GLU
18	c6	116	LEU
19	c7	88	VAL
19	c7	104	ASN
19	c7	116	LYS
20	c8	92	ILE
21	c9	29	GLU
21	c9	33	TYR
22	d0	15	GLN
22	d0	17	GLN
22	d0	49	ASN
22	d0	51	VAL
22	d0	97	VAL
22	d0	118	VAL
24	d2	68	ARG
25	d3	128	SER
25	d3	131	SER
25	d3	138	GLU
26	d4	30	PRO
26	d4	33	ALA
26	d4	35	VAL
26	d4	52	LYS
27	d5	85	LYS
27	d5	104	ALA
29	d7	3	LEU
29	d7	38	PRO
29	d7	60	SER
29	d7	75	GLU
30	d8	61	ARG
31	d9	6	VAL
31	d9	7	TRP
80	e0	60	PRO
33	e1	79	LYS
33	e1	84	VAL
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	100	LEU
33	e1	102	VAL
33	e1	103	LEU
33	e1	106	TYR
34	sR	160	GLU

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Mol	Chain	Res	Type
34	sR	163	ASP
34	sR	165	ASP
34	sR	318	ALA
35	sM	47	ALA
35	sM	50	ASN
39	l2	24	GLN
39	l2	56	ALA
39	l2	96	LEU
39	l2	215	ASN
40	l3	3	HIS
40	l3	140	ASP
40	l3	155	ALA
40	l3	347	SER
41	l4	15	ALA
41	l4	90	PHE
41	l4	145	ILE
41	l4	302	ALA
41	l4	311	HIS
41	l4	329	PRO
41	l4	330	TYR
42	l5	5	LYS
42	l5	260	PHE
43	l6	98	VAL
45	l8	25	PRO
45	l8	26	LEU
45	l8	34	PHE
45	l8	121	SER
45	l8	123	GLN
47	m0	25	ALA
47	m0	170	LYS
47	m0	175	ASN
47	m0	207	GLU
48	m1	8	PRO
48	m1	9	MET
48	m1	10	ARG
48	m1	108	GLU
48	m1	115	LYS
49	m3	47	ALA
49	m3	93	ILE
49	m3	101	ARG
49	m3	121	SER
49	m3	134	GLU

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Mol	Chain	Res	Type
49	m3	152	THR
51	m5	183	THR
51	m5	187	ARG
52	m6	16	VAL
52	m6	110	PRO
54	m8	99	THR
56	n0	2	ALA
57	n1	136	ARG
59	n3	42	SER
60	n4	26	SER
60	n4	71	ARG
60	n4	76	VAL
60	n4	133	THR
61	n5	38	LEU
61	n5	44	PRO
61	n5	45	LYS
61	n5	55	ASN
62	n6	83	ASP
62	n6	84	LYS
62	n6	125	LYS
62	n6	126	LEU
63	n7	16	GLY
63	n7	17	ARG
63	n7	129	TRP
64	n8	76	ASP
65	n9	21	ILE
65	n9	23	LYS
65	n9	25	LYS
65	n9	39	PHE
66	o0	100	ILE
67	o1	5	LYS
67	o1	45	GLY
68	o2	4	LEU
68	o2	5	PRO
68	o2	27	ARG
69	o3	88	ASN
70	o4	79	SER
71	o5	119	LYS
72	o6	33	ALA
72	o6	63	ASN
72	o6	64	SER
72	o6	98	ARG

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Mol	Chain	Res	Type
74	o8	18	ALA
74	o8	19	ASP
82	p0	93	LEU
2	S0	5	ALA
2	S0	94	GLY
2	S0	95	ALA
2	S0	190	ASP
3	S1	60	ALA
3	S1	213	ARG
4	S2	107	SER
5	S3	81	PRO
5	S3	93	ASP
5	S3	216	PRO
6	S4	12	LEU
6	S4	195	ILE
7	S5	43	PHE
7	S5	74	ALA
7	S5	101	GLY
7	S5	150	GLY
7	S5	153	GLY
8	S6	122	GLU
9	S7	30	SER
9	S7	85	PHE
9	S7	156	SER
10	S8	59	ARG
10	S8	120	THR
10	S8	149	SER
10	S8	199	LYS
11	S9	150	LEU
12	C0	89	ALA
13	C1	6	THR
13	C1	55	ASP
13	C1	145	ALA
14	C2	21	GLU
14	C2	66	VAL
14	C2	83	GLU
14	C2	91	VAL
15	C3	12	SER
15	C3	28	LEU
15	C3	68	GLY
16	C4	40	ALA
16	C4	42	VAL

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Mol	Chain	Res	Type
16	C4	50	ALA
16	C4	123	SER
16	C4	126	THR
17	C5	80	MET
17	C5	101	ALA
18	C6	114	ARG
19	C7	6	THR
19	C7	24	LEU
19	C7	83	GLN
19	C7	115	LEU
20	C8	25	ASN
20	C8	61	LEU
20	C8	83	ALA
20	C8	144	ARG
22	D0	17	GLN
23	D1	2	GLU
23	D1	4	ASP
23	D1	11	LEU
23	D1	12	TYR
23	D1	49	GLU
25	D3	3	LYS
25	D3	70	LYS
25	D3	96	VAL
26	D4	4	ALA
26	D4	5	VAL
26	D4	34	ASN
27	D5	56	THR
27	D5	88	ILE
28	D6	46	GLU
28	D6	47	ALA
28	D6	63	ALA
28	D6	82	ARG
29	D7	63	LEU
31	D9	8	PHE
33	E1	84	VAL
33	E1	85	TYR
33	E1	111	GLU
33	E1	144	CYS
33	E1	145	HIS
34	SR	295	SER
35	SM	47	ALA
35	SM	102	THR

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Mol	Chain	Res	Type
35	SM	139	GLU
35	SM	153	ASP
39	L2	32	LEU
39	L2	251	LYS
40	L3	187	SER
41	L4	15	ALA
41	L4	131	VAL
41	L4	190	GLY
41	L4	311	HIS
42	L5	20	PHE
42	L5	57	ASN
42	L5	215	ASP
42	L5	252	ALA
42	L5	260	PHE
42	L5	295	GLY
44	L7	191	VAL
45	L8	36	ILE
45	L8	156	ASP
47	M0	24	ARG
47	M0	117	GLY
48	M1	24	GLY
48	M1	65	ILE
48	M1	94	ARG
48	M1	95	ASN
48	M1	151	SER
50	M4	112	LEU
51	M5	74	PRO
51	M5	184	LYS
52	M6	110	PRO
56	N0	2	ALA
56	N0	13	ARG
57	N1	124	VAL
58	N2	50	LEU
60	N4	87	LEU
61	N5	26	VAL
63	N7	18	TYR
63	N7	35	SER
63	N7	125	GLY
64	N8	47	LYS
64	N8	66	ALA
64	N8	79	TRP
64	N8	96	LYS

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Mol	Chain	Res	Type
70	O4	74	ARG
70	O4	77	GLY
71	O5	97	ALA
72	O6	27	SER
72	O6	28	TYR
72	O6	34	SER
73	O7	68	LYS
79	Q3	20	SER
79	Q3	58	SER
2	s0	14	ALA
2	s0	44	GLY
2	s0	95	ALA
2	s0	167	LYS
2	s0	184	LEU
2	s0	189	VAL
3	s1	26	ARG
3	s1	82	ARG
3	s1	93	GLY
4	s2	93	GLY
4	s2	107	SER
4	s2	163	GLY
5	s3	61	GLU
5	s3	76	ARG
5	s3	90	ARG
5	s3	195	SER
6	s4	12	LEU
6	s4	24	SER
6	s4	104	ASP
6	s4	163	ASP
6	s4	164	LEU
6	s4	245	LYS
7	s5	35	GLN
7	s5	36	ALA
7	s5	100	ASN
7	s5	209	TYR
8	s6	68	LEU
9	s7	155	ASP
10	s8	101	ILE
12	c0	30	ALA
12	c0	32	HIS
12	c0	92	ILE
12	c0	94	GLU

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Mol	Chain	Res	Type
13	c1	7	VAL
13	c1	114	ALA
13	c1	121	ASP
13	c1	144	ALA
14	c2	66	VAL
14	c2	82	PRO
14	c2	91	VAL
14	c2	93	ASP
14	c2	101	ALA
14	c2	118	ALA
14	c2	119	SER
15	c3	19	SER
15	c3	60	VAL
15	c3	108	ASP
15	c3	140	LYS
16	c4	92	LYS
17	c5	7	ALA
17	c5	17	TYR
17	c5	68	PRO
17	c5	135	THR
18	c6	39	VAL
18	c6	113	ASP
19	c7	99	VAL
20	c8	55	HIS
20	c8	91	ASP
21	c9	28	LEU
22	d0	52	LYS
23	d1	43	GLY
26	d4	53	ASP
26	d4	58	PHE
26	d4	78	SER
28	d6	13	LYS
28	d6	34	LYS
28	d6	58	VAL
28	d6	82	ARG
29	d7	20	LYS
29	d7	62	ILE
31	d9	16	LYS
80	e0	47	VAL
33	e1	136	LYS
33	e1	145	HIS
34	sR	4	ASN

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Mol	Chain	Res	Type
34	sR	161	LYS
35	sM	63	ASP
35	sM	67	GLY
35	sM	172	VAL
39	l2	127	ALA
39	l2	194	ASN
40	l3	142	ALA
40	l3	385	LYS
40	l3	386	ASP
41	l4	14	GLU
41	l4	232	SER
41	l4	342	LYS
42	l5	258	LYS
45	l8	81	THR
45	l8	122	LYS
45	l8	133	LYS
45	l8	203	VAL
45	l8	222	PHE
45	l8	223	ALA
45	l8	240	ASN
46	l9	144	ILE
47	m0	117	GLY
47	m0	204	GLY
47	m0	219	ALA
48	m1	94	ARG
49	m3	135	ALA
49	m3	141	ALA
49	m3	150	PRO
50	m4	135	LEU
51	m5	184	LYS
52	m6	13	GLY
53	m7	66	SER
53	m7	67	ILE
54	m8	41	ASP
54	m8	180	ARG
56	n0	133	ALA
57	n1	122	GLN
57	n1	135	PRO
58	n2	49	ASN
58	n2	91	ASP
60	n4	25	ASP
60	n4	63	ILE

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Mol	Chain	Res	Type
61	n5	24	LEU
61	n5	47	ALA
63	n7	56	LYS
63	n7	105	SER
63	n7	125	GLY
63	n7	128	GLN
63	n7	130	PHE
67	o1	83	GLU
68	o2	6	HIS
73	o7	86	ALA
76	q0	78	ILE
82	p0	47	GLY
2	S0	27	ARG
2	S0	30	GLN
2	S0	36	TYR
3	S1	35	PRO
3	S1	51	SER
3	S1	54	LEU
3	S1	62	LYS
3	S1	130	SER
3	S1	132	ASP
3	S1	154	SER
3	S1	158	SER
4	S2	207	LEU
4	S2	248	SER
5	S3	218	LEU
6	S4	77	ARG
7	S5	64	VAL
7	S5	95	ASN
7	S5	100	ASN
7	S5	127	GLN
8	S6	152	ASP
9	S7	73	VAL
9	S7	98	ILE
9	S7	115	SER
10	S8	13	ALA
10	S8	40	ALA
10	S8	105	ASP
10	S8	152	ILE
10	S8	153	GLU
11	S9	163	PRO
12	C0	94	GLU

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Mol	Chain	Res	Type
13	C1	146	ALA
13	C1	154	ALA
14	C2	87	PRO
14	C2	101	ALA
14	C2	107	ASP
14	C2	112	ALA
14	C2	119	SER
14	C2	131	ASP
15	C3	19	SER
16	C4	92	LYS
16	C4	127	ARG
17	C5	69	GLU
17	C5	87	PRO
18	C6	138	PHE
19	C7	72	LYS
20	C8	134	ARG
20	C8	142	GLY
23	D1	7	GLN
23	D1	10	GLU
25	D3	11	SER
25	D3	41	SER
25	D3	46	SER
25	D3	112	LYS
25	D3	128	SER
26	D4	47	VAL
26	D4	51	GLU
26	D4	60	PHE
28	D6	61	GLU
28	D6	62	TYR
28	D6	97	PRO
29	D7	51	GLN
33	E1	87	THR
33	E1	127	GLY
34	SR	98	GLU
35	SM	53	ARG
35	SM	88	ARG
35	SM	100	THR
35	SM	101	ASP
35	SM	173	GLU
39	L2	14	SER
39	L2	47	GLN
39	L2	143	GLU

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Mol	Chain	Res	Type
39	L2	144	ASN
40	L3	155	ALA
40	L3	348	ARG
40	L3	386	ASP
41	L4	361	HIS
42	L5	6	ASP
42	L5	21	ARG
42	L5	115	LEU
42	L5	137	ASP
42	L5	253	PHE
43	L6	5	LYS
44	L7	159	GLN
45	L8	39	ALA
45	L8	119	GLY
47	M0	187	ALA
47	M0	220	GLN
48	M1	108	GLU
48	M1	114	ILE
49	M3	131	LYS
49	M3	193	ALA
50	M4	29	ALA
50	M4	135	LEU
53	M7	160	ALA
53	M7	162	GLU
53	M7	163	LYS
54	M8	91	ALA
56	N0	130	GLU
59	N3	4	ASN
60	N4	97	LYS
64	N8	78	LEU
72	O6	3	VAL
74	O8	33	LYS
78	Q2	94	GLY
2	s0	10	THR
2	s0	81	PHE
2	s0	194	PRO
2	s0	200	ASP
2	s0	203	PHE
3	s1	129	THR
3	s1	179	SER
3	s1	209	ASN
3	s1	232	HIS

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Mol	Chain	Res	Type
4	s2	106	ASP
4	s2	234	PRO
5	s3	43	PRO
5	s3	45	LYS
5	s3	93	ASP
7	s5	60	ASP
7	s5	98	MET
8	s6	69	LEU
8	s6	70	PRO
8	s6	165	GLY
10	s8	199	LYS
11	s9	162	SER
12	c0	23	ALA
12	c0	31	LYS
12	c0	35	ILE
13	c1	133	LYS
14	c2	45	LEU
14	c2	58	LEU
14	c2	87	PRO
14	c2	108	ARG
16	c4	12	GLN
17	c5	14	THR
17	c5	50	THR
17	c5	128	HIS
19	c7	82	ASP
20	c8	44	ASN
22	d0	16	GLN
22	d0	96	PRO
23	d1	44	ARG
25	d3	70	LYS
26	d4	104	SER
27	d5	44	GLN
27	d5	87	GLY
28	d6	8	ASN
28	d6	47	ALA
28	d6	59	TYR
30	d8	65	ARG
31	d9	11	PRO
80	e0	38	LEU
33	e1	81	LYS
33	e1	112	GLY
33	e1	137	ASP

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Mol	Chain	Res	Type
33	e1	146	SER
34	sR	15	GLY
34	sR	141	LEU
35	sM	41	SER
35	sM	64	LYS
40	l3	187	SER
40	l3	235	THR
41	l4	146	PRO
41	l4	190	GLY
41	l4	233	LEU
42	l5	38	THR
42	l5	158	ARG
42	l5	178	ASN
42	l5	270	LYS
43	l6	10	TYR
43	l6	171	PRO
45	l8	39	ALA
45	l8	83	ASP
45	l8	112	GLU
45	l8	196	ALA
45	l8	237	ILE
47	m0	3	ARG
47	m0	82	ARG
47	m0	176	LEU
47	m0	195	ALA
48	m1	7	ASN
48	m1	39	GLN
49	m3	62	THR
49	m3	129	ASN
51	m5	76	PRO
51	m5	81	TYR
52	m6	183	ALA
57	n1	16	GLN
57	n1	117	ALA
58	n2	50	LEU
60	n4	77	LYS
61	n5	25	LYS
61	n5	48	SER
61	n5	136	ALA
64	n8	47	LYS
67	o1	47	ASP
70	o4	47	CYS

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Mol	Chain	Res	Type
71	o5	14	LYS
71	o5	40	SER
78	q2	78	LYS
82	p0	68	SER
2	S0	103	THR
2	S0	130	ALA
2	S0	139	VAL
2	S0	163	ASN
2	S0	189	VAL
2	S0	195	TRP
3	S1	23	PRO
3	S1	26	ARG
4	S2	91	ARG
4	S2	150	GLN
5	S3	44	THR
5	S3	195	SER
5	S3	217	ILE
6	S4	233	LYS
6	S4	245	LYS
7	S5	51	VAL
7	S5	58	LEU
8	S6	69	LEU
8	S6	70	PRO
8	S6	138	ALA
8	S6	146	GLY
9	S7	36	ALA
9	S7	84	LYS
9	S7	110	GLN
10	S8	10	LYS
12	C0	34	GLU
13	C1	113	PRO
14	C2	39	ASP
14	C2	68	GLU
14	C2	106	ILE
14	C2	108	ARG
14	C2	125	ASN
16	C4	18	ARG
16	C4	75	GLY
17	C5	29	SER
17	C5	51	SER
17	C5	52	LYS
18	C6	33	GLY

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Mol	Chain	Res	Type
18	C6	58	ASP
19	C7	87	GLU
19	C7	123	ASN
21	C9	28	LEU
21	C9	50	ALA
21	C9	69	LYS
26	D4	75	VAL
28	D6	32	LYS
28	D6	64	LEU
30	D8	36	THR
31	D9	20	GLN
33	E1	83	LYS
33	E1	86	THR
33	E1	100	LEU
33	E1	118	ARG
34	SR	3	SER
34	SR	28	GLY
34	SR	160	GLU
34	SR	237	GLN
35	SM	42	ALA
35	SM	46	LYS
35	SM	64	LYS
35	SM	111	GLY
41	L4	182	LEU
41	L4	232	SER
41	L4	233	LEU
41	L4	269	SER
42	L5	19	PRO
42	L5	125	VAL
42	L5	259	LYS
44	L7	163	LEU
45	L8	157	VAL
46	L9	96	HIS
46	L9	190	ASP
47	M0	7	ARG
48	M1	117	ASP
48	M1	152	HIS
48	M1	167	TYR
49	M3	76	THR
49	M3	130	GLY
49	M3	136	GLU
53	M7	161	ALA

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Mol	Chain	Res	Type
53	M7	169	THR
54	M8	112	ALA
54	M8	162	ALA
56	N0	167	ARG
57	N1	114	ALA
58	N2	11	ILE
58	N2	59	ASP
58	N2	107	PHE
61	N5	25	LYS
62	N6	126	LEU
63	N7	36	HIS
63	N7	102	GLU
63	N7	103	GLN
64	N8	117	ARG
65	N9	25	LYS
67	O1	53	PRO
67	O1	82	GLU
68	O2	68	PRO
69	O3	59	VAL
76	Q0	79	GLU
2	s0	92	HIS
2	s0	103	THR
4	s2	91	ARG
4	s2	150	GLN
4	s2	235	LEU
4	s2	238	SER
6	s4	90	ILE
6	s4	213	SER
6	s4	260	GLY
8	s6	152	ASP
9	s7	112	ARG
11	s9	120	LYS
11	s9	150	LEU
12	c0	3	MET
14	c2	103	LEU
14	c2	106	ILE
14	c2	107	ASP
14	c2	115	VAL
16	c4	11	SER
16	c4	90	ARG
17	c5	130	ARG
20	c8	61	LEU

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Mol	Chain	Res	Type
20	c8	135	GLY
24	d2	31	SER
27	d5	38	HIS
28	d6	46	GLU
30	d8	33	LEU
80	e0	54	ARG
80	e0	61	SER
33	e1	111	GLU
33	e1	131	PHE
35	sM	42	ALA
35	sM	43	ASP
35	sM	65	THR
35	sM	121	LYS
40	l3	141	GLY
40	l3	333	LYS
41	l4	142	VAL
44	l7	191	VAL
46	l9	2	LYS
46	l9	108	GLY
48	m1	114	ILE
49	m3	51	LEU
49	m3	60	ALA
50	m4	95	ALA
50	m4	136	ALA
54	m8	91	ALA
60	n4	72	SER
60	n4	83	THR
61	n5	39	LYS
61	n5	90	ALA
62	n6	91	ASN
63	n7	34	LYS
63	n7	103	GLN
64	n8	129	PHE
65	n9	24	PRO
68	o2	124	GLY
70	o4	82	ALA
71	o5	82	ALA
72	o6	12	ASN
72	o6	34	SER
73	o7	87	SER
78	q2	17	CYS
82	p0	198	PRO

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Mol	Chain	Res	Type
2	S0	164	ASN
2	S0	194	PRO
3	S1	81	PHE
4	S2	36	VAL
4	S2	235	LEU
5	S3	72	LEU
6	S4	157	ASN
6	S4	163	ASP
6	S4	165	ALA
6	S4	200	ARG
7	S5	45	LYS
7	S5	65	ARG
11	S9	118	LEU
11	S9	147	MET
12	C0	92	ILE
13	C1	4	GLU
14	C2	22	VAL
14	C2	128	ALA
17	C5	22	LEU
19	C7	23	LYS
22	D0	21	LYS
22	D0	49	ASN
23	D1	15	ARG
25	D3	40	SER
26	D4	95	GLY
26	D4	100	VAL
27	D5	38	HIS
27	D5	41	ILE
27	D5	55	PRO
28	D6	36	ILE
30	D8	35	ASP
30	D8	61	ARG
32	E0	13	LYS
32	E0	33	ARG
33	E1	110	ALA
33	E1	148	TYR
34	SR	194	GLY
35	SM	12	VAL
35	SM	174	LEU
40	L3	188	ILE
40	L3	317	ILE
40	L3	385	LYS

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Mol	Chain	Res	Type
41	L4	292	SER
46	L9	2	LYS
46	L9	39	LYS
47	M0	145	LYS
47	M0	211	ARG
48	M1	64	LYS
48	M1	111	ASP
50	M4	6	ILE
51	M5	94	TYR
51	M5	145	ASP
52	M6	16	VAL
53	M7	164	LYS
55	M9	3	ASN
57	N1	18	ASP
60	N4	69	LYS
63	N7	3	LYS
64	N8	27	LYS
64	N8	97	GLU
68	O2	127	ALA
70	O4	82	ALA
71	O5	90	ARG
72	O6	21	THR
73	O7	86	ALA
2	s0	65	ALA
3	s1	94	LYS
3	s1	106	THR
3	s1	224	ASP
5	s3	44	THR
6	s4	94	ALA
7	s5	29	ILE
8	s6	25	ARG
10	s8	52	ASN
10	s8	78	ILE
11	s9	168	ARG
12	c0	95	ARG
13	c1	5	LEU
13	c1	40	LEU
13	c1	55	ASP
14	c2	21	GLU
14	c2	39	ASP
14	c2	90	LYS
15	c3	22	ALA

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Mol	Chain	Res	Type
17	c5	69	GLU
18	c6	142	TYR
19	c7	62	GLN
20	c8	29	VAL
22	d0	119	ALA
23	d1	10	GLU
24	d2	56	HIS
25	d3	27	ASN
25	d3	101	GLU
26	d4	50	ALA
30	d8	6	PRO
30	d8	20	GLY
30	d8	57	MET
30	d8	62	GLU
80	e0	51	ASN
33	e1	86	THR
33	e1	124	PRO
34	sR	149	ASP
34	sR	186	PHE
35	sM	46	LYS
41	l4	5	GLN
41	l4	339	LEU
41	l4	352	ALA
42	l5	168	ASP
43	l6	11	PRO
44	l7	178	ILE
45	l8	69	LEU
46	l9	62	ARG
46	l9	167	VAL
48	m1	95	ASN
48	m1	173	ASP
49	m3	76	THR
51	m5	68	ARG
52	m6	90	HIS
54	m8	171	LYS
60	n4	132	GLY
61	n5	40	LEU
63	n7	104	PRO
64	n8	28	HIS
70	o4	78	GLY
74	o8	17	ARG
78	q2	33	ALA

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Mol	Chain	Res	Type
79	q3	51	ALA
82	p0	33	VAL
2	S0	117	GLU
2	S0	183	ARG
3	S1	93	GLY
3	S1	210	ILE
4	S2	39	THR
11	S9	126	ARG
14	C2	25	GLU
14	C2	75	VAL
14	C2	81	ASP
14	C2	82	PRO
15	C3	3	ARG
18	C6	113	ASP
22	D0	55	PRO
22	D0	106	ILE
27	D5	54	VAL
28	D6	53	LEU
35	SM	17	VAL
35	SM	82	THR
40	L3	142	ALA
44	L7	178	ILE
56	N0	24	LEU
62	N6	52	ARG
71	O5	75	TYR
72	O6	64	SER
74	O8	37	PRO
2	s0	68	PRO
2	s0	109	ASN
3	s1	60	ALA
3	s1	81	PHE
6	s4	30	ARG
11	s9	134	ILE
15	c3	29	SER
16	c4	114	ARG
18	c6	40	GLU
20	c8	14	ILE
21	c9	34	VAL
33	e1	110	ALA
35	sM	51	ARG
35	sM	167	PRO
40	l3	239	PRO

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Mol	Chain	Res	Type
41	l4	301	PRO
42	l5	9	SER
44	l7	229	PHE
45	l8	150	LEU
45	l8	188	THR
46	l9	110	LYS
51	m5	74	PRO
54	m8	112	ALA
64	n8	120	ASN
71	o5	84	LYS
5	S3	112	GLY
9	S7	13	PRO
22	D0	59	PRO
22	D0	117	VAL
44	L7	91	GLY
50	M4	36	VAL
57	N1	123	GLY
58	N2	22	PRO
79	Q3	71	VAL
20	c8	9	GLY
65	n9	37	PRO
72	o6	61	ILE
74	o8	37	PRO
3	S1	176	VAL
4	S2	145	GLY
11	S9	162	SER
14	C2	55	GLY
28	D6	75	VAL
41	L4	4	PRO
60	N4	76	VAL
65	N9	21	ILE
5	s3	219	ALA
41	l4	328	ASN
6	S4	193	GLY
18	C6	39	VAL
18	C6	97	VAL
34	SR	105	GLY
39	L2	153	GLY
40	L3	141	GLY
45	L8	135	GLY
4	s2	83	ILE
11	s9	5	PRO

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Mol	Chain	Res	Type
12	c0	4	PRO
14	c2	63	VAL
18	c6	97	VAL
19	c7	117	LEU
2	S0	64	ILE
3	S1	48	VAL
11	S9	168	ARG
14	C2	117	GLY
32	E0	50	VAL
34	SR	15	GLY
35	SM	172	VAL
47	M0	114	GLY
53	M7	51	VAL
59	N3	5	GLY
60	N4	82	ILE
64	N8	70	LYS
7	s5	153	GLY
9	s7	13	PRO
42	l5	125	VAL
58	n2	45	GLY
59	n3	41	GLY
60	n4	98	PRO
62	n6	85	VAL
72	o6	9	ILE
76	q0	80	PRO
3	S1	215	VAL
41	L4	23	PRO
5	s3	163	PRO
55	m9	77	GLY
40	L3	257	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%)	133 (81%)	31 (19%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	s0	165/209 (79%)	131 (79%)	34 (21%)	1	6
3	S1	191/223 (86%)	151 (79%)	40 (21%)	1	5
3	s1	192/223 (86%)	155 (81%)	37 (19%)	1	8
4	S2	176/204 (86%)	140 (80%)	36 (20%)	1	6
4	s2	176/204 (86%)	131 (74%)	45 (26%)	0	3
5	S3	182/194 (94%)	147 (81%)	35 (19%)	1	8
5	s3	182/194 (94%)	146 (80%)	36 (20%)	1	7
6	S4	221/221 (100%)	170 (77%)	51 (23%)	1	4
6	s4	221/221 (100%)	184 (83%)	37 (17%)	2	11
7	S5	173/190 (91%)	147 (85%)	26 (15%)	3	14
7	s5	173/190 (91%)	139 (80%)	34 (20%)	1	7
8	S6	188/201 (94%)	158 (84%)	30 (16%)	2	12
8	s6	187/201 (93%)	151 (81%)	36 (19%)	1	8
9	S7	165/169 (98%)	136 (82%)	29 (18%)	2	10
9	s7	165/169 (98%)	130 (79%)	35 (21%)	1	5
10	S8	150/161 (93%)	130 (87%)	20 (13%)	4	17
10	s8	150/161 (93%)	128 (85%)	22 (15%)	3	15
11	S9	158/165 (96%)	123 (78%)	35 (22%)	1	4
11	s9	158/165 (96%)	128 (81%)	30 (19%)	1	8
12	C0	77/98 (79%)	65 (84%)	12 (16%)	2	13
12	c0	73/98 (74%)	60 (82%)	13 (18%)	2	9
13	C1	129/136 (95%)	107 (83%)	22 (17%)	2	10
13	c1	129/136 (95%)	104 (81%)	25 (19%)	1	7
14	C2	88/118 (75%)	67 (76%)	21 (24%)	0	3
14	c2	88/118 (75%)	64 (73%)	24 (27%)	0	2
15	C3	127/127 (100%)	102 (80%)	25 (20%)	1	7
15	c3	127/127 (100%)	101 (80%)	26 (20%)	1	6
16	C4	81/104 (78%)	66 (82%)	15 (18%)	1	8
16	c4	97/104 (93%)	78 (80%)	19 (20%)	1	7
17	C5	101/117 (86%)	82 (81%)	19 (19%)	1	8
17	c5	103/117 (88%)	84 (82%)	19 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	C6	117/118 (99%)	89 (76%)	28 (24%)	0	3
18	c6	118/118 (100%)	96 (81%)	22 (19%)	1	8
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1	4
19	c7	92/124 (74%)	75 (82%)	17 (18%)	1	8
20	C8	128/128 (100%)	97 (76%)	31 (24%)	0	3
20	c8	128/128 (100%)	105 (82%)	23 (18%)	1	9
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	7
21	c9	115/115 (100%)	98 (85%)	17 (15%)	3	14
22	D0	100/113 (88%)	80 (80%)	20 (20%)	1	7
22	d0	103/113 (91%)	76 (74%)	27 (26%)	0	2
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	10
23	d1	74/74 (100%)	59 (80%)	15 (20%)	1	6
24	D2	110/110 (100%)	93 (84%)	17 (16%)	2	13
24	d2	110/110 (100%)	99 (90%)	11 (10%)	7	29
25	D3	119/119 (100%)	95 (80%)	24 (20%)	1	6
25	d3	119/119 (100%)	100 (84%)	19 (16%)	2	12
26	D4	112/112 (100%)	92 (82%)	20 (18%)	2	9
26	d4	112/112 (100%)	92 (82%)	20 (18%)	2	9
27	D5	61/88 (69%)	45 (74%)	16 (26%)	0	2
27	d5	61/88 (69%)	52 (85%)	9 (15%)	3	14
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1	6
28	d6	83/83 (100%)	72 (87%)	11 (13%)	4	17
29	D7	70/70 (100%)	61 (87%)	9 (13%)	4	19
29	d7	70/70 (100%)	56 (80%)	14 (20%)	1	7
30	D8	56/59 (95%)	45 (80%)	11 (20%)	1	7
30	d8	56/59 (95%)	44 (79%)	12 (21%)	1	5
31	D9	47/48 (98%)	41 (87%)	6 (13%)	4	19
31	d9	47/48 (98%)	36 (77%)	11 (23%)	1	4
32	E0	51/51 (100%)	42 (82%)	9 (18%)	2	10
33	E1	62/66 (94%)	48 (77%)	14 (23%)	1	4
33	e1	66/66 (100%)	49 (74%)	17 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	SR	260/261 (100%)	226 (87%)	34 (13%)	4	18
34	sR	260/261 (100%)	230 (88%)	30 (12%)	5	24
35	SM	97/228 (42%)	75 (77%)	22 (23%)	1	4
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	2
39	L2	193/195 (99%)	152 (79%)	41 (21%)	1	5
39	l2	192/195 (98%)	148 (77%)	44 (23%)	1	4
40	L3	319/322 (99%)	256 (80%)	63 (20%)	1	7
40	l3	321/322 (100%)	261 (81%)	60 (19%)	1	8
41	L4	288/288 (100%)	227 (79%)	61 (21%)	1	5
41	l4	288/288 (100%)	234 (81%)	54 (19%)	1	8
42	L5	244/244 (100%)	195 (80%)	49 (20%)	1	6
42	l5	243/244 (100%)	203 (84%)	40 (16%)	2	11
43	L6	134/152 (88%)	113 (84%)	21 (16%)	2	13
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	10
44	L7	186/204 (91%)	156 (84%)	30 (16%)	2	12
44	l7	187/204 (92%)	156 (83%)	31 (17%)	2	11
45	L8	187/207 (90%)	153 (82%)	34 (18%)	1	9
45	l8	177/207 (86%)	143 (81%)	34 (19%)	1	8
46	L9	171/171 (100%)	131 (77%)	40 (23%)	1	4
46	l9	171/171 (100%)	133 (78%)	38 (22%)	1	4
47	M0	177/186 (95%)	143 (81%)	34 (19%)	1	8
47	m0	179/186 (96%)	139 (78%)	40 (22%)	1	4
48	M1	147/150 (98%)	116 (79%)	31 (21%)	1	5
48	m1	147/150 (98%)	123 (84%)	24 (16%)	2	11
49	M3	154/158 (98%)	126 (82%)	28 (18%)	1	9
49	m3	154/158 (98%)	129 (84%)	25 (16%)	2	12
50	M4	107/108 (99%)	87 (81%)	20 (19%)	1	8
50	m4	108/108 (100%)	90 (83%)	18 (17%)	2	11
51	M5	175/175 (100%)	144 (82%)	31 (18%)	2	9
51	m5	175/175 (100%)	149 (85%)	26 (15%)	3	14
52	M6	160/161 (99%)	135 (84%)	25 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	m6	160/161 (99%)	130 (81%)	30 (19%)	1	8
53	M7	140/145 (97%)	112 (80%)	28 (20%)	1	7
53	m7	125/145 (86%)	97 (78%)	28 (22%)	1	4
54	M8	150/150 (100%)	129 (86%)	21 (14%)	3	16
54	m8	150/150 (100%)	122 (81%)	28 (19%)	1	8
55	M9	153/153 (100%)	126 (82%)	27 (18%)	2	10
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	4
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1	7
56	n0	156/156 (100%)	126 (81%)	30 (19%)	1	8
57	N1	136/136 (100%)	110 (81%)	26 (19%)	1	8
57	n1	136/136 (100%)	112 (82%)	24 (18%)	2	10
58	N2	87/106 (82%)	77 (88%)	10 (12%)	5	24
58	n2	85/106 (80%)	69 (81%)	16 (19%)	1	8
59	N3	104/104 (100%)	84 (81%)	20 (19%)	1	8
59	n3	104/104 (100%)	92 (88%)	12 (12%)	5	24
60	N4	57/129 (44%)	49 (86%)	8 (14%)	3	16
60	n4	100/129 (78%)	83 (83%)	17 (17%)	2	10
61	N5	104/117 (89%)	78 (75%)	26 (25%)	0	3
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	6
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1	6
62	n6	109/109 (100%)	82 (75%)	27 (25%)	0	3
63	N7	115/115 (100%)	92 (80%)	23 (20%)	1	7
63	n7	115/115 (100%)	90 (78%)	25 (22%)	1	5
64	N8	118/118 (100%)	96 (81%)	22 (19%)	1	8
64	n8	118/118 (100%)	95 (80%)	23 (20%)	1	7
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1	5
65	n9	46/46 (100%)	34 (74%)	12 (26%)	0	2
66	O0	81/87 (93%)	66 (82%)	15 (18%)	1	8
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1	6
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	4
67	o1	94/96 (98%)	71 (76%)	23 (24%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	O2	109/110 (99%)	92 (84%)	17 (16%)	2	13
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	4
69	O3	90/90 (100%)	80 (89%)	10 (11%)	6	25
69	o3	90/90 (100%)	75 (83%)	15 (17%)	2	11
70	O4	95/102 (93%)	82 (86%)	13 (14%)	3	17
70	o4	95/102 (93%)	74 (78%)	21 (22%)	1	4
71	O5	104/104 (100%)	81 (78%)	23 (22%)	1	4
71	o5	103/104 (99%)	81 (79%)	22 (21%)	1	5
72	O6	81/81 (100%)	59 (73%)	22 (27%)	0	2
72	o6	80/81 (99%)	53 (66%)	27 (34%)	0	1
73	O7	70/70 (100%)	55 (79%)	15 (21%)	1	5
73	o7	70/70 (100%)	55 (79%)	15 (21%)	1	5
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0	2
74	o8	67/68 (98%)	54 (81%)	13 (19%)	1	7
75	O9	45/45 (100%)	38 (84%)	7 (16%)	2	13
75	o9	45/45 (100%)	35 (78%)	10 (22%)	1	4
76	Q0	47/47 (100%)	36 (77%)	11 (23%)	1	4
76	q0	47/47 (100%)	35 (74%)	12 (26%)	0	3
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	0	3
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%)	61 (86%)	10 (14%)	3	16
80	e0	53/53 (100%)	42 (79%)	11 (21%)	1	5
82	p0	105/253 (42%)	86 (82%)	19 (18%)	1	9
All	All	18728/20241 (92%)	15139 (81%)	3589 (19%)	1	8

All (3589) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	27	ARG
2	S0	30	GLN

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Mol	Chain	Res	Type
2	S0	32	HIS
2	S0	47	VAL
2	S0	49	ASN
2	S0	52	LYS
2	S0	62	ARG
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	101	ARG
2	S0	103	THR
2	S0	110	TYR
2	S0	111	ILE
2	S0	112	THR
2	S0	117	GLU
2	S0	119	ARG
2	S0	123	VAL
2	S0	124	THR
2	S0	154	GLU
2	S0	156	VAL
2	S0	157	ASP
2	S0	170	ILE
2	S0	172	LEU
2	S0	177	LEU
2	S0	185	ARG
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	46	THR
3	S1	55	LYS
3	S1	61	LEU
3	S1	70	LEU
3	S1	73	LEU
3	S1	77	GLU
3	S1	78	ASP
3	S1	81	PHE
3	S1	83	LYS

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Mol	Chain	Res	Type
3	S1	85	LYS
3	S1	89	ASP
3	S1	91	VAL
3	S1	95	ASN
3	S1	96	LEU
3	S1	97	LEU
3	S1	105	PHE
3	S1	108	ASP
3	S1	111	ARG
3	S1	112	SER
3	S1	117	TRP
3	S1	137	ILE
3	S1	146	GLN
3	S1	149	GLN
3	S1	154	SER
3	S1	170	GLU
3	S1	177	GLN
3	S1	180	THR
3	S1	181	LEU
3	S1	198	GLU
3	S1	202	LYS
3	S1	214	LYS
3	S1	218	LEU
3	S1	219	LYS
3	S1	220	GLN
3	S1	222	LYS
3	S1	223	PHE
4	S2	41	LEU
4	S2	53	ILE
4	S2	55	GLU
4	S2	58	LEU
4	S2	64	LYS
4	S2	69	ILE
4	S2	73	LEU
4	S2	76	LEU
4	S2	77	GLN
4	S2	89	GLN
4	S2	90	THR
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	111	VAL

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Mol	Chain	Res	Type
4	S2	117	THR
4	S2	119	LYS
4	S2	130	ILE
4	S2	134	LEU
4	S2	140	ARG
4	S2	141	ARG
4	S2	146	THR
4	S2	148	LEU
4	S2	158	THR
4	S2	166	THR
4	S2	174	ARG
4	S2	187	LEU
4	S2	207	LEU
4	S2	221	THR
4	S2	222	TYR
4	S2	224	PHE
4	S2	226	THR
4	S2	237	VAL
4	S2	240	LEU
4	S2	242	ILE
4	S2	245	ASP
5	S3	4	LEU
5	S3	5	ILE
5	S3	7	LYS
5	S3	9	ARG
5	S3	23	GLU
5	S3	37	VAL
5	S3	59	LEU
5	S3	65	ARG
5	S3	66	ILE
5	S3	67	ASN
5	S3	84	ILE
5	S3	92	GLN
5	S3	93	ASP
5	S3	104	SER
5	S3	117	ARG
5	S3	127	MET
5	S3	134	CYS
5	S3	137	VAL
5	S3	142	LEU
5	S3	146	ARG
5	S3	151	LYS

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Mol	Chain	Res	Type
5	S3	158	ILE
5	S3	170	THR
5	S3	172	THR
5	S3	175	VAL
5	S3	176	LEU
5	S3	178	ARG
5	S3	181	VAL
5	S3	186	VAL
5	S3	187	LYS
5	S3	190	ARG
5	S3	202	LEU
5	S3	207	THR
5	S3	215	GLU
5	S3	222	VAL
6	S4	6	LYS
6	S4	7	LYS
6	S4	9	LEU
6	S4	11	ARG
6	S4	12	LEU
6	S4	23	LEU
6	S4	26	CYS
6	S4	37	LYS
6	S4	38	LEU
6	S4	42	LEU
6	S4	45	ILE
6	S4	48	LEU
6	S4	56	LEU
6	S4	62	LYS
6	S4	65	LEU
6	S4	67	GLN
6	S4	68	ARG
6	S4	77	ARG
6	S4	78	THR
6	S4	79	ASP
6	S4	92	LEU
6	S4	93	ASP
6	S4	102	VAL
6	S4	113	ARG
6	S4	123	LEU
6	S4	126	VAL
6	S4	129	VAL
6	S4	131	LEU

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Mol	Chain	Res	Type
6	S4	133	LYS
6	S4	155	LYS
6	S4	160	VAL
6	S4	164	LEU
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	197	HIS
6	S4	198	LYS
6	S4	214	LEU
6	S4	215	ASP
6	S4	222	LEU
6	S4	223	ASN
6	S4	226	PHE
6	S4	227	VAL
6	S4	231	GLN
6	S4	237	SER
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	248	ILE
6	S4	258	GLN
6	S4	259	GLN
7	S5	23	VAL
7	S5	24	VAL
7	S5	25	LEU
7	S5	27	THR
7	S5	32	GLU
7	S5	38	THR
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS
7	S5	53	VAL
7	S5	76	ARG
7	S5	79	ASN
7	S5	84	LYS
7	S5	89	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	146	THR
7	S5	147	THR
7	S5	156	ARG

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Mol	Chain	Res	Type
7	S5	160	VAL
7	S5	162	VAL
7	S5	172	ILE
7	S5	194	LEU
7	S5	203	LYS
7	S5	216	GLU
7	S5	225	ARG
8	S6	19	ASP
8	S6	21	GLU
8	S6	25	ARG
8	S6	45	PHE
8	S6	58	LYS
8	S6	65	GLN
8	S6	67	VAL
8	S6	68	LEU
8	S6	69	LEU
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	82	SER
8	S6	98	ARG
8	S6	120	GLU
8	S6	125	THR
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	129	VAL
8	S6	133	LEU
8	S6	154	ARG
8	S6	155	ASP
8	S6	169	TYR
8	S6	176	GLN
8	S6	177	ARG
8	S6	211	LEU
8	S6	212	LEU
8	S6	217	SER
8	S6	223	LYS
9	S7	19	GLN
9	S7	25	VAL
9	S7	28	GLU
9	S7	38	LEU
9	S7	45	SER

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Mol	Chain	Res	Type
9	S7	46	ILE
9	S7	50	ASP
9	S7	60	ILE
9	S7	67	LEU
9	S7	70	PHE
9	S7	71	HIS
9	S7	79	ARG
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG
9	S7	104	ARG
9	S7	105	THR
9	S7	109	VAL
9	S7	114	ARG
9	S7	116	ARG
9	S7	126	LEU
9	S7	130	VAL
9	S7	131	PHE
9	S7	134	GLU
9	S7	144	VAL
9	S7	147	ASN
9	S7	167	GLU
9	S7	182	VAL
9	S7	185	ILE
10	S8	7	SER
10	S8	8	ARG
10	S8	14	THR
10	S8	17	LYS
10	S8	21	PHE
10	S8	29	LEU
10	S8	36	THR
10	S8	46	VAL
10	S8	49	ARG
10	S8	58	LEU
10	S8	60	ILE
10	S8	62	THR
10	S8	74	LYS
10	S8	77	ARG
10	S8	135	LYS
10	S8	138	ASN
10	S8	151	LYS
10	S8	152	ILE

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Mol	Chain	Res	Type
10	S8	164	ARG
10	S8	196	LEU
11	S9	3	ARG
11	S9	7	THR
11	S9	14	THR
11	S9	22	SER
11	S9	28	LEU
11	S9	39	LYS
11	S9	40	LYS
11	S9	54	ARG
11	S9	64	GLU
11	S9	66	ASP
11	S9	78	ARG
11	S9	79	ARG
11	S9	82	ARG
11	S9	83	VAL
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	97	LEU
11	S9	99	LEU
11	S9	101	VAL
11	S9	105	LEU
11	S9	109	LEU
11	S9	118	LEU
11	S9	130	THR
11	S9	134	ILE
11	S9	138	LYS
11	S9	149	ARG
11	S9	151	ASP
11	S9	161	THR
11	S9	162	SER
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	182	GLU
12	C0	1	MET
12	C0	20	VAL
12	C0	27	PHE
12	C0	32	HIS
12	C0	55	VAL

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Mol	Chain	Res	Type
12	C0	56	LYS
12	C0	67	THR
12	C0	71	GLU
12	C0	76	LEU
12	C0	78	GLU
12	C0	81	ASN
12	C0	82	LEU
13	C1	8	GLN
13	C1	21	ASN
13	C1	29	LYS
13	C1	40	LEU
13	C1	43	LYS
13	C1	44	THR
13	C1	58	CYS
13	C1	63	LEU
13	C1	64	VAL
13	C1	67	ARG
13	C1	69	LYS
13	C1	74	THR
13	C1	79	LYS
13	C1	83	THR
13	C1	99	ARG
13	C1	109	VAL
13	C1	112	SER
13	C1	127	GLN
13	C1	128	CYS
13	C1	129	ARG
13	C1	131	ILE
13	C1	136	ARG
14	C2	28	LEU
14	C2	36	LEU
14	C2	37	VAL
14	C2	41	LEU
14	C2	43	ARG
14	C2	46	ARG
14	C2	50	LYS
14	C2	52	LEU
14	C2	54	ARG
14	C2	58	LEU
14	C2	61	VAL
14	C2	66	VAL
14	C2	71	ILE

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Mol	Chain	Res	Type
14	C2	86	VAL
14	C2	89	ILE
14	C2	103	LEU
14	C2	121	VAL
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	139	HIS
15	C3	3	ARG
15	C3	6	SER
15	C3	9	LYS
15	C3	16	ILE
15	C3	27	LYS
15	C3	39	LYS
15	C3	45	LEU
15	C3	56	ASP
15	C3	58	HIS
15	C3	62	GLN
15	C3	64	ARG
15	C3	66	ILE
15	C3	72	MET
15	C3	76	LYS
15	C3	83	GLU
15	C3	88	LEU
15	C3	94	LYS
15	C3	102	LEU
15	C3	114	ARG
15	C3	115	LEU
15	C3	125	LEU
15	C3	127	ARG
15	C3	134	VAL
15	C3	142	GLU
15	C3	151	ASN
16	C4	13	VAL
16	C4	14	PHE
16	C4	16	VAL
16	C4	20	TYR
16	C4	24	ASN
16	C4	29	HIS
16	C4	31	THR
16	C4	39	ILE
16	C4	42	VAL

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Mol	Chain	Res	Type
16	C4	92	LYS
16	C4	103	ARG
16	C4	123	SER
16	C4	129	LYS
16	C4	136	ARG
16	C4	137	LEU
17	C5	22	LEU
17	C5	26	LEU
17	C5	29	SER
17	C5	34	VAL
17	C5	35	LYS
17	C5	36	LEU
17	C5	40	ARG
17	C5	44	ARG
17	C5	47	ARG
17	C5	50	THR
17	C5	52	LYS
17	C5	60	LEU
17	C5	69	GLU
17	C5	86	VAL
17	C5	92	SER
17	C5	110	GLU
17	C5	121	ILE
17	C5	124	THR
17	C5	125	PRO
18	C6	4	VAL
18	C6	12	LYS
18	C6	14	LYS
18	C6	23	LYS
18	C6	26	LYS
18	C6	28	LEU
18	C6	29	ILE
18	C6	39	VAL
18	C6	43	ILE
18	C6	44	LEU
18	C6	52	LEU
18	C6	53	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	58	ASP
18	C6	65	ILE
18	C6	66	ARG

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Mol	Chain	Res	Type
18	C6	68	ARG
18	C6	69	VAL
18	C6	98	ASP
18	C6	106	LYS
18	C6	114	ARG
18	C6	121	SER
18	C6	123	ARG
18	C6	128	LYS
18	C6	137	ARG
18	C6	141	SER
18	C6	143	ARG
19	C7	25	THR
19	C7	30	THR
19	C7	34	LEU
19	C7	38	ILE
19	C7	46	LEU
19	C7	49	LYS
19	C7	54	THR
19	C7	58	MET
19	C7	62	GLN
19	C7	69	ILE
19	C7	71	PHE
19	C7	72	LYS
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	87	GLU
19	C7	105	GLN
19	C7	107	SER
19	C7	113	LEU
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	8	GLN
20	C8	11	PHE
20	C8	12	GLN
20	C8	13	HIS
20	C8	14	ILE
20	C8	17	LEU
20	C8	20	THR
20	C8	25	ASN

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Mol	Chain	Res	Type
20	C8	26	ILE
20	C8	28	ILE
20	C8	32	LEU
20	C8	40	ARG
20	C8	53	ASP
20	C8	54	LEU
20	C8	60	GLU
20	C8	61	LEU
20	C8	71	GLN
20	C8	77	THR
20	C8	80	LYS
20	C8	86	LEU
20	C8	92	ILE
20	C8	97	ASP
20	C8	108	LYS
20	C8	131	LEU
20	C8	132	ARG
20	C8	136	GLN
20	C8	138	THR
20	C8	140	THR
20	C8	143	ARG
21	C9	4	VAL
21	C9	6	VAL
21	C9	18	TYR
21	C9	22	LEU
21	C9	24	ARG
21	C9	28	LEU
21	C9	30	VAL
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	41	SER
21	C9	57	ARG
21	C9	63	ARG
21	C9	67	MET
21	C9	70	GLN
21	C9	94	ILE
21	C9	111	ILE
21	C9	123	ARG
21	C9	126	GLU
21	C9	130	ARG

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Mol	Chain	Res	Type
21	C9	131	ASP
21	C9	144	GLU
22	D0	15	GLN
22	D0	22	ILE
22	D0	23	ARG
22	D0	27	THR
22	D0	31	VAL
22	D0	47	GLN
22	D0	48	HIS
22	D0	51	VAL
22	D0	57	ARG
22	D0	60	THR
22	D0	61	LYS
22	D0	72	ASN
22	D0	74	GLU
22	D0	76	SER
22	D0	81	THR
22	D0	89	ARG
22	D0	99	ILE
22	D0	103	ILE
22	D0	105	GLN
22	D0	121	ASN
23	D1	3	ASN
23	D1	5	LYS
23	D1	7	GLN
23	D1	11	LEU
23	D1	18	SER
23	D1	25	LYS
23	D1	41	GLU
23	D1	49	GLU
23	D1	52	THR
23	D1	62	ARG
23	D1	69	LEU
23	D1	78	LEU
23	D1	80	LYS
24	D2	4	SER
24	D2	7	LEU
24	D2	22	LYS
24	D2	24	GLN
24	D2	25	VAL
24	D2	27	ILE
24	D2	53	ILE

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Mol	Chain	Res	Type
24	D2	65	LEU
24	D2	66	ASN
24	D2	81	VAL
24	D2	93	LEU
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR
24	D2	121	VAL
24	D2	129	VAL
25	D3	7	ARG
25	D3	9	LEU
25	D3	14	LYS
25	D3	16	ARG
25	D3	18	HIS
25	D3	19	ARG
25	D3	31	LYS
25	D3	41	SER
25	D3	62	LYS
25	D3	82	LYS
25	D3	84	THR
25	D3	96	VAL
25	D3	103	LEU
25	D3	107	PHE
25	D3	109	ARG
25	D3	110	LYS
25	D3	114	LYS
25	D3	117	ILE
25	D3	131	SER
25	D3	137	LYS
25	D3	138	GLU
25	D3	139	LYS
25	D3	140	LYS
25	D3	144	ARG
26	D4	17	LEU
26	D4	21	LYS
26	D4	29	HIS
26	D4	32	ARG
26	D4	34	ASN
26	D4	46	GLU
26	D4	47	VAL
26	D4	51	GLU

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Mol	Chain	Res	Type
26	D4	57	VAL
26	D4	61	ARG
26	D4	81	GLU
26	D4	96	LEU
26	D4	99	LYS
26	D4	102	LYS
26	D4	105	ARG
26	D4	123	LYS
26	D4	124	ARG
26	D4	127	LYS
26	D4	128	LYS
26	D4	129	VAL
27	D5	42	LEU
27	D5	48	ASP
27	D5	49	ARG
27	D5	50	ILE
27	D5	58	ARG
27	D5	59	TYR
27	D5	63	SER
27	D5	67	ASP
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	77	ARG
27	D5	85	LYS
27	D5	92	ILE
27	D5	95	HIS
27	D5	100	ILE
28	D6	15	ARG
28	D6	30	ILE
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	44	ILE
28	D6	45	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	67	THR
28	D6	68	TYR
28	D6	69	ASN
28	D6	70	LYS
28	D6	82	ARG

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Mol	Chain	Res	Type
28	D6	83	ILE
28	D6	85	ARG
28	D6	89	ARG
29	D7	3	LEU
29	D7	20	LYS
29	D7	26	GLN
29	D7	33	LEU
29	D7	34	ASP
29	D7	55	THR
29	D7	60	SER
29	D7	61	THR
29	D7	74	SER
30	D8	13	ILE
30	D8	14	LYS
30	D8	19	THR
30	D8	32	PHE
30	D8	33	LEU
30	D8	39	THR
30	D8	49	ARG
30	D8	51	ASN
30	D8	52	ASP
30	D8	58	GLU
30	D8	64	ARG
31	D9	9	SER
31	D9	19	ARG
31	D9	22	ARG
31	D9	30	LEU
31	D9	32	ARG
31	D9	36	LEU
32	E0	3	LYS
32	E0	20	LYS
32	E0	21	VAL
32	E0	22	GLU
32	E0	28	LYS
32	E0	29	LYS
32	E0	42	ARG
32	E0	47	VAL
32	E0	50	VAL
33	E1	86	THR
33	E1	89	LYS
33	E1	91	ILE
33	E1	97	LYS

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Mol	Chain	Res	Type
33	E1	106	TYR
33	E1	108	VAL
33	E1	113	LYS
33	E1	118	ARG
33	E1	120	GLU
33	E1	130	VAL
33	E1	139	LEU
33	E1	140	TYR
33	E1	147	VAL
33	E1	151	ASN
34	SR	6	VAL
34	SR	9	LEU
34	SR	29	GLN
34	SR	44	SER
34	SR	46	LYS
34	SR	48	THR
34	SR	52	GLN
34	SR	59	ARG
34	SR	76	ASP
34	SR	91	LEU
34	SR	109	ASP
34	SR	112	SER
34	SR	117	LYS
34	SR	136	ILE
34	SR	137	LYS
34	SR	141	LEU
34	SR	145	LEU
34	SR	149	ASP
34	SR	153	GLN
34	SR	165	ASP
34	SR	191	ASP
34	SR	193	ILE
34	SR	196	ASN
34	SR	199	ILE
34	SR	216	LYS
34	SR	222	LEU
34	SR	238	ASP
34	SR	248	ASN
34	SR	266	ASP
34	SR	268	GLN
34	SR	300	THR
34	SR	308	ASN

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Mol	Chain	Res	Type
34	SR	316	MET
34	SR	317	THR
35	SM	28	SER
35	SM	34	LYS
35	SM	46	LYS
35	SM	48	ARG
35	SM	53	ARG
35	SM	61	ILE
35	SM	64	LYS
35	SM	68	ARG
35	SM	75	ASP
35	SM	78	ASP
35	SM	82	THR
35	SM	84	LYS
35	SM	89	ARG
35	SM	91	THR
35	SM	96	ARG
35	SM	97	THR
35	SM	100	THR
35	SM	102	THR
35	SM	105	LYS
35	SM	106	VAL
35	SM	116	GLU
35	SM	139	GLU
39	L2	10	LYS
39	L2	20	THR
39	L2	23	ARG
39	L2	30	ARG
39	L2	32	LEU
39	L2	44	ILE
39	L2	45	VAL
39	L2	48	ILE
39	L2	49	VAL
39	L2	62	VAL
39	L2	70	ARG
39	L2	73	GLU
39	L2	74	GLU
39	L2	88	ILE
39	L2	95	SER
39	L2	96	LEU
39	L2	97	ASN
39	L2	101	VAL

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Mol	Chain	Res	Type
39	L2	104	LEU
39	L2	106	SER
39	L2	109	GLU
39	L2	116	VAL
39	L2	119	LYS
39	L2	130	SER
39	L2	137	ILE
39	L2	142	ASP
39	L2	143	GLU
39	L2	157	VAL
39	L2	158	ILE
39	L2	165	VAL
39	L2	169	ILE
39	L2	179	LEU
39	L2	181	LYS
39	L2	191	LEU
39	L2	202	VAL
39	L2	204	MET
39	L2	207	VAL
39	L2	219	ILE
39	L2	226	SER
39	L2	227	ARG
39	L2	230	VAL
40	L3	2	SER
40	L3	7	GLU
40	L3	10	ARG
40	L3	17	LEU
40	L3	19	ARG
40	L3	25	ILE
40	L3	37	ARG
40	L3	47	LEU
40	L3	56	ILE
40	L3	73	VAL
40	L3	79	VAL
40	L3	84	VAL
40	L3	85	VAL
40	L3	100	ARG
40	L3	103	THR
40	L3	112	ASP
40	L3	114	VAL
40	L3	116	ARG
40	L3	126	LYS

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Mol	Chain	Res	Type
40	L3	134	SER
40	L3	139	GLN
40	L3	144	ILE
40	L3	146	ARG
40	L3	148	LEU
40	L3	150	ARG
40	L3	156	SER
40	L3	157	VAL
40	L3	169	THR
40	L3	173	GLN
40	L3	183	LEU
40	L3	188	ILE
40	L3	189	SER
40	L3	192	VAL
40	L3	196	ARG
40	L3	200	GLU
40	L3	202	THR
40	L3	205	VAL
40	L3	208	VAL
40	L3	210	GLU
40	L3	212	ASN
40	L3	229	VAL
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	238	LEU
40	L3	244	ARG
40	L3	252	ILE
40	L3	277	SER
40	L3	284	ARG
40	L3	296	THR
40	L3	304	THR
40	L3	308	MET
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	347	SER
40	L3	357	LYS

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Mol	Chain	Res	Type
40	L3	380	MET
40	L3	382	THR
41	L4	4	PRO
41	L4	22	LEU
41	L4	27	SER
41	L4	32	PRO
41	L4	40	THR
41	L4	42	VAL
41	L4	47	ARG
41	L4	60	THR
41	L4	64	SER
41	L4	73	ARG
41	L4	74	ILE
41	L4	84	ARG
41	L4	93	MET
41	L4	98	ARG
41	L4	99	MET
41	L4	108	LYS
41	L4	112	LYS
41	L4	124	SER
41	L4	133	SER
41	L4	136	LEU
41	L4	138	ARG
41	L4	142	VAL
41	L4	144	LYS
41	L4	145	ILE
41	L4	150	LEU
41	L4	152	VAL
41	L4	156	LEU
41	L4	161	LYS
41	L4	170	LYS
41	L4	179	LEU
41	L4	187	LEU
41	L4	188	ARG
41	L4	193	LYS
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	206	LEU
41	L4	220	ARG
41	L4	222	VAL
41	L4	230	VAL

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Mol	Chain	Res	Type
41	L4	246	ARG
41	L4	256	THR
41	L4	258	LEU
41	L4	259	ASP
41	L4	267	VAL
41	L4	275	THR
41	L4	287	THR
41	L4	292	SER
41	L4	306	THR
41	L4	307	GLN
41	L4	308	LYS
41	L4	313	LEU
41	L4	314	LYS
41	L4	321	LYS
41	L4	322	GLN
41	L4	323	VAL
41	L4	332	LYS
41	L4	339	LEU
41	L4	343	LYS
41	L4	346	LYS
41	L4	349	THR
42	L5	5	LYS
42	L5	8	LYS
42	L5	20	PHE
42	L5	22	ARG
42	L5	23	ARG
42	L5	34	LYS
42	L5	35	ARG
42	L5	41	LYS
42	L5	66	SER
42	L5	67	SER
42	L5	69	ILE
42	L5	75	LEU
42	L5	80	SER
42	L5	85	ARG
42	L5	92	LEU
42	L5	101	THR
42	L5	105	ILE
42	L5	109	THR
42	L5	115	LEU
42	L5	118	THR
42	L5	131	LEU

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Mol	Chain	Res	Type
42	L5	136	GLU
42	L5	137	ASP
42	L5	140	ARG
42	L5	144	VAL
42	L5	146	LEU
42	L5	151	GLN
42	L5	152	ARG
42	L5	154	THR
42	L5	155	THR
42	L5	159	VAL
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE
42	L5	187	THR
42	L5	189	GLU
42	L5	194	LEU
42	L5	206	GLN
42	L5	216	GLU
42	L5	222	LEU
42	L5	238	ASP
42	L5	242	SER
42	L5	254	LYS
42	L5	257	GLU
42	L5	259	LYS
42	L5	264	GLN
42	L5	273	ARG
42	L5	290	ILE
42	L5	293	LEU
43	L6	2	SER
43	L6	5	LYS
43	L6	21	THR
43	L6	31	ARG
43	L6	35	VAL
43	L6	50	LYS
43	L6	52	VAL
43	L6	56	LYS
43	L6	59	GLU
43	L6	64	LEU
43	L6	65	ILE
43	L6	78	ARG
43	L6	79	VAL
43	L6	89	THR

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Mol	Chain	Res	Type
43	L6	90	LYS
43	L6	93	VAL
43	L6	129	GLU
43	L6	134	ARG
43	L6	152	THR
43	L6	155	LEU
43	L6	162	SER
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	38	LYS
44	L7	40	LYS
44	L7	45	LEU
44	L7	60	ARG
44	L7	78	GLU
44	L7	82	LYS
44	L7	83	LEU
44	L7	89	ILE
44	L7	92	ILE
44	L7	98	LYS
44	L7	100	ARG
44	L7	101	LYS
44	L7	109	THR
44	L7	110	ARG
44	L7	124	LEU
44	L7	128	LYS
44	L7	143	THR
44	L7	157	ASN
44	L7	164	SER
44	L7	173	LEU
44	L7	175	LYS
44	L7	178	ILE
44	L7	179	LEU
44	L7	184	LEU
44	L7	189	ILE
44	L7	216	VAL
44	L7	239	LEU
45	L8	26	LEU
45	L8	27	THR
45	L8	41	GLN
45	L8	47	SER
45	L8	50	VAL

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Mol	Chain	Res	Type
45	L8	70	LYS
45	L8	74	THR
45	L8	79	GLN
45	L8	81	THR
45	L8	84	ARG
45	L8	92	LYS
45	L8	101	THR
45	L8	106	LYS
45	L8	132	VAL
45	L8	136	LEU
45	L8	145	ASN
45	L8	150	LEU
45	L8	156	ASP
45	L8	160	ILE
45	L8	163	VAL
45	L8	169	LEU
45	L8	172	LYS
45	L8	173	MET
45	L8	181	LYS
45	L8	185	ARG
45	L8	194	THR
45	L8	204	ARG
45	L8	206	GLU
45	L8	218	ILE
45	L8	238	LEU
45	L8	241	LYS
45	L8	243	GLN
45	L8	248	LYS
45	L8	251	LYS
46	L9	1	MET
46	L9	4	ILE
46	L9	5	GLN
46	L9	6	THR
46	L9	14	GLU
46	L9	16	VAL
46	L9	18	VAL
46	L9	22	SER
46	L9	33	THR
46	L9	41	ILE
46	L9	48	VAL
46	L9	52	LEU
46	L9	55	VAL

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Mol	Chain	Res	Type
46	L9	62	ARG
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	82	VAL
46	L9	91	ARG
46	L9	118	LEU
46	L9	123	ILE
46	L9	124	ARG
46	L9	132	VAL
46	L9	133	THR
46	L9	135	GLU
46	L9	138	THR
46	L9	139	ASN
46	L9	151	VAL
46	L9	152	GLU
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	164	ILE
46	L9	168	ARG
46	L9	170	LYS
46	L9	172	ILE
46	L9	173	ARG
46	L9	189	GLU
46	L9	190	ASP
46	L9	191	LEU
47	M0	3	ARG
47	M0	7	ARG
47	M0	13	LYS
47	M0	21	ARG
47	M0	24	ARG
47	M0	26	VAL
47	M0	30	LYS
47	M0	31	ILE
47	M0	32	ARG
47	M0	33	ILE
47	M0	36	LEU
47	M0	39	LYS
47	M0	40	LYS
47	M0	42	THR
47	M0	48	LEU

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Mol	Chain	Res	Type
47	M0	52	LEU
47	M0	57	LEU
47	M0	62	SER
47	M0	63	GLU
47	M0	74	LYS
47	M0	87	LEU
47	M0	91	VAL
47	M0	99	ILE
47	M0	116	ARG
47	M0	129	VAL
47	M0	139	ARG
47	M0	163	GLN
47	M0	165	ILE
47	M0	167	LEU
47	M0	170	LYS
47	M0	174	THR
47	M0	177	ASP
47	M0	184	LYS
47	M0	203	LYS
48	M1	7	ASN
48	M1	9	MET
48	M1	10	ARG
48	M1	11	ASP
48	M1	12	LEU
48	M1	13	LYS
48	M1	16	LYS
48	M1	19	LEU
48	M1	44	THR
48	M1	46	VAL
48	M1	60	ARG
48	M1	61	ARG
48	M1	65	ILE
48	M1	70	THR
48	M1	80	LEU
48	M1	82	ARG
48	M1	94	ARG
48	M1	95	ASN
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	115	LYS
48	M1	120	ILE

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Mol	Chain	Res	Type
48	M1	130	VAL
48	M1	140	ARG
48	M1	142	LYS
48	M1	147	THR
48	M1	148	VAL
48	M1	166	LYS
48	M1	168	ASP
48	M1	173	ASP
49	M3	17	HIS
49	M3	23	LYS
49	M3	24	VAL
49	M3	35	ARG
49	M3	42	ARG
49	M3	54	LEU
49	M3	55	ARG
49	M3	59	ARG
49	M3	62	THR
49	M3	63	VAL
49	M3	67	ARG
49	M3	69	VAL
49	M3	70	ARG
49	M3	85	LEU
49	M3	114	GLN
49	M3	115	ARG
49	M3	124	ILE
49	M3	128	ARG
49	M3	131	LYS
49	M3	134	GLU
49	M3	136	GLU
49	M3	144	THR
49	M3	164	GLU
49	M3	168	ARG
49	M3	171	ARG
49	M3	180	ARG
49	M3	190	LYS
49	M3	194	GLU
50	M4	5	SER
50	M4	8	LYS
50	M4	15	VAL
50	M4	20	VAL
50	M4	27	GLN
50	M4	50	LYS

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Mol	Chain	Res	Type
50	M4	53	VAL
50	M4	63	VAL
50	M4	64	VAL
50	M4	66	THR
50	M4	72	LEU
50	M4	74	ARG
50	M4	90	VAL
50	M4	91	CYS
50	M4	92	GLU
50	M4	93	LYS
50	M4	102	LYS
50	M4	113	THR
50	M4	132	LYS
50	M4	135	LEU
51	M5	10	LEU
51	M5	18	VAL
51	M5	20	ARG
51	M5	22	LEU
51	M5	38	ARG
51	M5	43	THR
51	M5	49	ARG
51	M5	50	ARG
51	M5	68	ARG
51	M5	80	THR
51	M5	85	THR
51	M5	89	VAL
51	M5	96	ARG
51	M5	97	SER
51	M5	98	LEU
51	M5	105	ARG
51	M5	106	VAL
51	M5	109	ARG
51	M5	117	ASN
51	M5	123	GLN
51	M5	133	ILE
51	M5	138	GLN
51	M5	151	ILE
51	M5	155	VAL
51	M5	167	THR
51	M5	171	SER
51	M5	183	THR
51	M5	184	LYS

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Mol	Chain	Res	Type
51	M5	190	THR
51	M5	196	THR
51	M5	204	LYS
52	M6	22	VAL
52	M6	25	LYS
52	M6	33	ILE
52	M6	58	LEU
52	M6	59	ARG
52	M6	68	ARG
52	M6	77	SER
52	M6	78	ARG
52	M6	84	LEU
52	M6	85	ARG
52	M6	106	GLU
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	143	THR
52	M6	144	SER
52	M6	160	ARG
52	M6	166	GLU
52	M6	175	THR
52	M6	180	SER
52	M6	184	THR
52	M6	187	GLU
53	M7	3	ARG
53	M7	9	THR
53	M7	24	VAL
53	M7	29	THR
53	M7	32	THR
53	M7	36	ILE
53	M7	41	LEU
53	M7	52	LEU
53	M7	53	ASP
53	M7	56	ARG
53	M7	65	SER
53	M7	67	ILE
53	M7	91	VAL
53	M7	107	LEU

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Mol	Chain	Res	Type
53	M7	112	LEU
53	M7	114	VAL
53	M7	119	VAL
53	M7	120	ASN
53	M7	126	ARG
53	M7	127	ARG
53	M7	136	ILE
53	M7	142	SER
53	M7	144	SER
53	M7	157	VAL
53	M7	168	LEU
53	M7	171	ARG
53	M7	180	LYS
53	M7	181	ARG
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	69	ARG
54	M8	74	GLU
54	M8	81	VAL
54	M8	95	GLU
54	M8	122	ILE
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	150	VAL
54	M8	161	LYS
54	M8	168	THR
54	M8	178	ARG
54	M8	180	ARG
54	M8	181	SER
54	M8	185	LYS
55	M9	5	ARG
55	M9	10	LEU
55	M9	30	SER
55	M9	41	ILE
55	M9	43	LYS
55	M9	44	LEU
55	M9	46	LYS

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Mol	Chain	Res	Type
55	M9	51	VAL
55	M9	52	LYS
55	M9	55	VAL
55	M9	60	LYS
55	M9	71	ARG
55	M9	74	ARG
55	M9	86	GLU
55	M9	99	LEU
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	110	ARG
55	M9	130	ASN
55	M9	138	LEU
55	M9	144	GLN
55	M9	153	LYS
55	M9	164	LEU
55	M9	175	GLN
55	M9	180	LYS
55	M9	182	ASP
56	N0	1	MET
56	N0	8	GLN
56	N0	12	ARG
56	N0	40	ARG
56	N0	45	LEU
56	N0	51	VAL
56	N0	57	GLU
56	N0	58	ILE
56	N0	61	ILE
56	N0	71	LYS
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	131	LYS
56	N0	132	THR
56	N0	136	LYS

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Mol	Chain	Res	Type
56	N0	137	ARG
56	N0	138	GLN
56	N0	142	GLN
56	N0	155	ARG
56	N0	157	GLN
56	N0	160	THR
56	N0	162	THR
56	N0	166	LYS
56	N0	172	TYR
57	N1	9	SER
57	N1	16	GLN
57	N1	26	HIS
57	N1	27	LEU
57	N1	72	VAL
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	80	VAL
57	N1	83	ARG
57	N1	96	ILE
57	N1	97	LYS
57	N1	104	GLU
57	N1	106	LEU
57	N1	124	VAL
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	136	ARG
57	N1	139	ARG
57	N1	141	VAL
57	N1	144	GLU
57	N1	146	ASN
57	N1	149	GLN
57	N1	158	THR
57	N1	159	PHE
58	N2	10	LYS
58	N2	16	THR
58	N2	29	ASP
58	N2	38	ILE
58	N2	43	VAL
58	N2	52	ASN
58	N2	66	VAL

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Mol	Chain	Res	Type
58	N2	88	GLN
58	N2	93	ILE
58	N2	100	THR
59	N3	13	ILE
59	N3	14	SER
59	N3	32	ARG
59	N3	44	SER
59	N3	48	ARG
59	N3	54	LEU
59	N3	63	LYS
59	N3	64	LYS
59	N3	69	LEU
59	N3	72	LYS
59	N3	73	VAL
59	N3	74	MET
59	N3	84	SER
59	N3	88	ARG
59	N3	91	VAL
59	N3	102	ILE
59	N3	109	MET
59	N3	110	LYS
59	N3	115	THR
59	N3	128	ARG
60	N4	1	MET
60	N4	4	GLU
60	N4	5	ILE
60	N4	19	THR
60	N4	26	SER
60	N4	39	LEU
60	N4	52	THR
60	N4	64	THR
61	N5	27	ARG
61	N5	29	SER
61	N5	37	THR
61	N5	38	LEU
61	N5	39	LYS
61	N5	45	LYS
61	N5	57	LEU
61	N5	59	SER
61	N5	63	ILE
61	N5	71	THR
61	N5	73	MET

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Mol	Chain	Res	Type
61	N5	74	LYS
61	N5	86	VAL
61	N5	92	LYS
61	N5	108	LEU
61	N5	112	THR
61	N5	113	LEU
61	N5	115	ARG
61	N5	125	ARG
61	N5	133	LEU
61	N5	134	ASP
61	N5	135	ILE
61	N5	137	ASN
61	N5	138	ARG
61	N5	139	ILE
61	N5	142	ILE
62	N6	4	GLN
62	N6	5	SER
62	N6	8	VAL
62	N6	13	ARG
62	N6	37	LYS
62	N6	39	LEU
62	N6	42	GLN
62	N6	45	ILE
62	N6	50	ILE
62	N6	51	ARG
62	N6	56	VAL
62	N6	57	LEU
62	N6	60	ARG
62	N6	62	SER
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	94	SER
62	N6	105	VAL
62	N6	115	ARG
62	N6	125	LYS
62	N6	126	LEU
63	N7	14	VAL
63	N7	17	ARG
63	N7	24	VAL
63	N7	26	VAL
63	N7	27	LYS

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Mol	Chain	Res	Type
63	N7	30	ASP
63	N7	34	LYS
63	N7	46	ILE
63	N7	54	THR
63	N7	64	LYS
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	87	LEU
63	N7	102	GLU
63	N7	103	GLN
63	N7	107	ARG
63	N7	108	GLU
63	N7	109	GLU
63	N7	121	ARG
63	N7	127	ASN
63	N7	134	LEU
63	N7	135	ARG
64	N8	4	ARG
64	N8	7	LYS
64	N8	8	THR
64	N8	10	LYS
64	N8	42	ARG
64	N8	46	ASP
64	N8	47	LYS
64	N8	56	VAL
64	N8	58	MET
64	N8	60	TYR
64	N8	65	GLN
64	N8	78	LEU
64	N8	85	ASP
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	130	VAL
64	N8	133	LEU
64	N8	139	ARG
65	N9	14	ARG
65	N9	22	LYS

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Mol	Chain	Res	Type
65	N9	25	LYS
65	N9	33	LYS
65	N9	35	VAL
65	N9	38	LYS
65	N9	40	ARG
65	N9	44	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	9	SER
66	O0	14	LEU
66	O0	30	THR
66	O0	32	LYS
66	O0	34	LEU
66	O0	36	GLN
66	O0	39	SER
66	O0	40	LYS
66	O0	54	SER
66	O0	61	MET
66	O0	66	LYS
66	O0	75	ASN
66	O0	83	LYS
66	O0	100	ILE
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	31	ARG
67	O1	47	ASP
67	O1	55	LEU
67	O1	64	VAL
67	O1	68	GLU
67	O1	73	LEU
67	O1	76	SER
67	O1	79	ARG
67	O1	82	GLU
67	O1	84	ASP
67	O1	86	LYS
67	O1	96	VAL
67	O1	102	LYS
67	O1	106	THR

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Mol	Chain	Res	Type
67	O1	107	VAL
67	O1	110	GLU
68	O2	4	LEU
68	O2	19	ARG
68	O2	21	HIS
68	O2	33	ARG
68	O2	34	LYS
68	O2	41	VAL
68	O2	51	SER
68	O2	54	LYS
68	O2	62	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	76	VAL
68	O2	84	THR
68	O2	89	THR
68	O2	106	VAL
68	O2	125	ARG
68	O2	128	LEU
69	O3	15	SER
69	O3	28	SER
69	O3	31	LYS
69	O3	48	ARG
69	O3	49	ILE
69	O3	59	VAL
69	O3	70	LYS
69	O3	80	VAL
69	O3	81	VAL
69	O3	106	ASN
70	O4	5	VAL
70	O4	8	ARG
70	O4	20	ILE
70	O4	21	LYS
70	O4	24	LYS
70	O4	29	ILE
70	O4	33	GLN
70	O4	56	THR
70	O4	58	ARG
70	O4	65	VAL
70	O4	71	THR
70	O4	86	LYS
70	O4	104	VAL

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Mol	Chain	Res	Type
71	O5	4	VAL
71	O5	15	GLU
71	O5	20	GLN
71	O5	21	LEU
71	O5	27	GLU
71	O5	28	LEU
71	O5	31	LEU
71	O5	46	THR
71	O5	47	VAL
71	O5	49	LYS
71	O5	62	GLN
71	O5	68	GLN
71	O5	71	LYS
71	O5	73	LYS
71	O5	81	ARG
71	O5	85	THR
71	O5	90	ARG
71	O5	96	GLU
71	O5	101	THR
71	O5	102	GLU
71	O5	104	GLN
71	O5	107	LYS
71	O5	119	LYS
72	O6	11	LEU
72	O6	16	LYS
72	O6	18	THR
72	O6	21	THR
72	O6	26	ILE
72	O6	28	TYR
72	O6	34	SER
72	O6	36	ARG
72	O6	45	ARG
72	O6	52	PRO
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	62	ARG
72	O6	68	ARG
72	O6	76	ARG
72	O6	81	THR
72	O6	88	GLU
72	O6	89	GLU

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Mol	Chain	Res	Type
72	O6	90	MET
72	O6	97	SER
72	O6	99	ARG
73	O7	5	THR
73	O7	10	LYS
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	36	SER
73	O7	58	THR
73	O7	59	THR
73	O7	65	ARG
73	O7	67	LEU
73	O7	72	ARG
73	O7	80	THR
73	O7	84	SER
73	O7	85	LYS
74	O8	5	ILE
74	O8	12	LEU
74	O8	22	THR
74	O8	24	THR
74	O8	31	LEU
74	O8	32	ASN
74	O8	41	THR
74	O8	45	VAL
74	O8	46	ARG
74	O8	48	SER
74	O8	53	THR
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	69	LEU
74	O8	72	THR
74	O8	77	ARG
74	O8	78	LEU
75	O9	5	LYS
75	O9	21	ARG
75	O9	28	ARG
75	O9	29	LEU
75	O9	45	ARG
75	O9	47	THR

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Mol	Chain	Res	Type
75	O9	51	ILE
76	Q0	77	ILE
76	Q0	78	ILE
76	Q0	80	PRO
76	Q0	83	LYS
76	Q0	85	LEU
76	Q0	106	ARG
76	Q0	108	THR
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	127	LEU
77	Q1	4	LYS
77	Q1	6	ARG
77	Q1	9	ARG
77	Q1	11	ARG
77	Q1	13	LEU
77	Q1	16	LYS
77	Q1	17	ARG
77	Q1	19	LYS
78	Q2	8	ARG
78	Q2	13	LYS
78	Q2	17	CYS
78	Q2	26	THR
78	Q2	35	LEU
78	Q2	45	ARG
78	Q2	47	GLN
78	Q2	55	LYS
78	Q2	60	LYS
78	Q2	71	ARG
78	Q2	72	LEU
78	Q2	76	LYS
78	Q2	78	LYS
78	Q2	80	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	92	GLU
78	Q2	93	LEU
78	Q2	100	LYS
78	Q2	104	LEU
78	Q2	105	GLN

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Mol	Chain	Res	Type
79	Q3	5	THR
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	25	GLN
79	Q3	36	ARG
79	Q3	45	LYS
79	Q3	46	THR
79	Q3	48	LYS
79	Q3	56	THR
79	Q3	60	CYS
79	Q3	73	THR
79	Q3	78	THR
79	Q3	84	ARG
79	Q3	88	GLU
79	Q3	91	GLU
2	s0	9	LEU
2	s0	10	THR
2	s0	12	GLU
2	s0	24	LEU
2	s0	29	VAL
2	s0	30	GLN
2	s0	31	VAL
2	s0	41	ARG
2	s0	45	VAL
2	s0	50	VAL
2	s0	59	LEU
2	s0	62	ARG
2	s0	72	ASP
2	s0	87	LEU
2	s0	88	LYS
2	s0	93	THR
2	s0	96	THR
2	s0	110	TYR
2	s0	123	VAL
2	s0	124	THR
2	s0	131	GLN
2	s0	144	ILE
2	s0	153	SER
2	s0	154	GLU
2	s0	156	VAL
2	s0	158	VAL
2	s0	172	LEU

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Mol	Chain	Res	Type
2	s0	183	ARG
2	s0	185	ARG
2	s0	188	LEU
2	s0	189	VAL
2	s0	197	ILE
2	s0	198	MET
2	s0	202	TYR
3	s1	21	VAL
3	s1	25	THR
3	s1	36	SER
3	s1	37	THR
3	s1	47	LEU
3	s1	51	SER
3	s1	55	LYS
3	s1	58	SER
3	s1	61	LEU
3	s1	62	LYS
3	s1	70	LEU
3	s1	74	GLN
3	s1	78	ASP
3	s1	81	PHE
3	s1	83	LYS
3	s1	105	PHE
3	s1	116	LYS
3	s1	126	THR
3	s1	137	ILE
3	s1	151	LYS
3	s1	153	HIS
3	s1	154	SER
3	s1	159	SER
3	s1	169	SER
3	s1	170	GLU
3	s1	173	THR
3	s1	177	GLN
3	s1	181	LEU
3	s1	184	LEU
3	s1	193	ILE
3	s1	202	LYS
3	s1	203	ASP
3	s1	204	ILE
3	s1	212	VAL
3	s1	217	LEU

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Mol	Chain	Res	Type
3	s1	219	LYS
3	s1	231	LEU
4	s2	41	LEU
4	s2	53	ILE
4	s2	54	GLU
4	s2	58	LEU
4	s2	60	SER
4	s2	69	ILE
4	s2	71	THR
4	s2	72	LEU
4	s2	73	LEU
4	s2	76	LEU
4	s2	80	VAL
4	s2	83	ILE
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	95	ARG
4	s2	96	THR
4	s2	106	ASP
4	s2	111	VAL
4	s2	113	LEU
4	s2	117	THR
4	s2	129	ILE
4	s2	137	ILE
4	s2	139	ILE
4	s2	141	ARG
4	s2	146	THR
4	s2	148	LEU
4	s2	153	SER
4	s2	159	THR
4	s2	164	SER
4	s2	166	THR
4	s2	190	LEU
4	s2	194	GLU
4	s2	206	THR
4	s2	207	LEU
4	s2	218	ILE
4	s2	222	TYR
4	s2	225	LEU
4	s2	226	THR
4	s2	229	LEU

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Mol	Chain	Res	Type
4	s2	233	GLN
4	s2	237	VAL
4	s2	238	SER
4	s2	240	LEU
4	s2	248	SER
5	s3	4	LEU
5	s3	7	LYS
5	s3	9	ARG
5	s3	10	LYS
5	s3	21	LEU
5	s3	32	GLU
5	s3	37	VAL
5	s3	39	VAL
5	s3	41	VAL
5	s3	44	THR
5	s3	59	LEU
5	s3	61	GLU
5	s3	67	ASN
5	s3	69	LEU
5	s3	70	THR
5	s3	84	ILE
5	s3	89	GLU
5	s3	90	ARG
5	s3	93	ASP
5	s3	94	ARG
5	s3	115	ILE
5	s3	125	TYR
5	s3	127	MET
5	s3	128	GLU
5	s3	132	LYS
5	s3	142	LEU
5	s3	143	ARG
5	s3	150	MET
5	s3	158	ILE
5	s3	162	GLN
5	s3	168	ILE
5	s3	170	THR
5	s3	172	THR
5	s3	202	LEU
5	s3	212	LYS
5	s3	224	ASP
6	s4	6	LYS

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Mol	Chain	Res	Type
6	s4	7	LYS
6	s4	11	ARG
6	s4	23	LEU
6	s4	38	LEU
6	s4	39	ARG
6	s4	42	LEU
6	s4	48	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	67	GLN
6	s4	70	VAL
6	s4	78	THR
6	s4	97	GLU
6	s4	104	ASP
6	s4	105	VAL
6	s4	116	ASP
6	s4	117	GLU
6	s4	126	VAL
6	s4	128	LYS
6	s4	133	LYS
6	s4	146	THR
6	s4	147	ILE
6	s4	148	ARG
6	s4	160	VAL
6	s4	176	ASP
6	s4	180	LEU
6	s4	181	VAL
6	s4	182	TYR
6	s4	187	ARG
6	s4	191	ARG
6	s4	194	THR
6	s4	221	ARG
6	s4	222	LEU
6	s4	233	LYS
6	s4	246	LEU
6	s4	254	ARG
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU
7	s5	38	THR
7	s5	39	GLU
7	s5	41	LYS

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Mol	Chain	Res	Type
7	s5	45	LYS
7	s5	53	VAL
7	s5	58	LEU
7	s5	63	GLN
7	s5	64	VAL
7	s5	68	ILE
7	s5	76	ARG
7	s5	83	ARG
7	s5	84	LYS
7	s5	86	GLN
7	s5	89	ILE
7	s5	93	LEU
7	s5	94	THR
7	s5	119	ASP
7	s5	125	THR
7	s5	128	ASN
7	s5	147	THR
7	s5	148	ARG
7	s5	157	ARG
7	s5	162	VAL
7	s5	163	SER
7	s5	186	ASN
7	s5	189	THR
7	s5	194	LEU
7	s5	203	LYS
7	s5	213	LYS
7	s5	216	GLU
7	s5	219	ARG
8	s6	15	THR
8	s6	21	GLU
8	s6	25	ARG
8	s6	30	LYS
8	s6	44	GLU
8	s6	71	THR
8	s6	74	LYS
8	s6	76	LEU
8	s6	78	THR
8	s6	89	ASP
8	s6	93	LYS
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU

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Mol	Chain	Res	Type
8	s6	115	LYS
8	s6	120	GLU
8	s6	121	LEU
8	s6	126	ASP
8	s6	127	THR
8	s6	128	THR
8	s6	129	VAL
8	s6	137	ARG
8	s6	143	LYS
8	s6	151	ASP
8	s6	153	VAL
8	s6	155	ASP
8	s6	156	PHE
8	s6	168	THR
8	s6	169	TYR
8	s6	170	THR
8	s6	177	ARG
8	s6	179	VAL
8	s6	182	GLN
8	s6	193	LEU
8	s6	212	LEU
8	s6	215	ARG
9	s7	8	ILE
9	s7	9	LEU
9	s7	11	GLN
9	s7	28	GLU
9	s7	33	GLU
9	s7	38	LEU
9	s7	44	LYS
9	s7	49	ILE
9	s7	51	VAL
9	s7	60	ILE
9	s7	67	LEU
9	s7	75	THR
9	s7	77	LEU
9	s7	79	ARG
9	s7	80	GLU
9	s7	86	GLN
9	s7	87	ASP
9	s7	97	ARG
9	s7	105	THR
9	s7	108	GLN

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Mol	Chain	Res	Type
9	s7	114	ARG
9	s7	115	SER
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	126	LEU
9	s7	129	LEU
9	s7	135	ILE
9	s7	148	LYS
9	s7	154	LEU
9	s7	160	GLN
9	s7	165	LYS
9	s7	166	LEU
9	s7	185	ILE
9	s7	187	SER
10	s8	6	ASP
10	s8	10	LYS
10	s8	18	ARG
10	s8	20	GLN
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	46	VAL
10	s8	58	LEU
10	s8	59	ARG
10	s8	64	ASN
10	s8	74	LYS
10	s8	76	THR
10	s8	97	THR
10	s8	138	ASN
10	s8	149	SER
10	s8	151	LYS
10	s8	152	ILE
10	s8	155	SER
10	s8	183	ILE
10	s8	184	LEU
10	s8	199	LYS
11	s9	3	ARG
11	s9	7	THR
11	s9	9	SER
11	s9	28	LEU
11	s9	33	GLU

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Mol	Chain	Res	Type
11	s9	49	LEU
11	s9	77	ILE
11	s9	78	ARG
11	s9	82	ARG
11	s9	90	LYS
11	s9	93	LEU
11	s9	101	VAL
11	s9	105	LEU
11	s9	108	ARG
11	s9	109	LEU
11	s9	110	GLN
11	s9	111	THR
11	s9	115	LYS
11	s9	126	ARG
11	s9	130	THR
11	s9	133	HIS
11	s9	134	ILE
11	s9	142	ASN
11	s9	143	ILE
11	s9	149	ARG
11	s9	150	LEU
11	s9	161	THR
11	s9	172	VAL
11	s9	180	LYS
11	s9	182	GLU
12	c0	2	LEU
12	c0	5	LYS
12	c0	8	ARG
12	c0	13	GLN
12	c0	15	LEU
12	c0	20	VAL
12	c0	27	PHE
12	c0	36	ASP
12	c0	40	LEU
12	c0	47	GLN
12	c0	55	VAL
12	c0	57	THR
12	c0	71	GLU
13	c1	2	SER
13	c1	3	THR
13	c1	5	LEU
13	c1	10	GLU

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Mol	Chain	Res	Type
13	c1	22	ASN
13	c1	26	LYS
13	c1	30	ARG
13	c1	31	THR
13	c1	32	LYS
13	c1	33	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	47	THR
13	c1	60	PHE
13	c1	67	ARG
13	c1	74	THR
13	c1	76	VAL
13	c1	80	MET
13	c1	82	ARG
13	c1	83	THR
13	c1	122	ILE
13	c1	123	VAL
13	c1	129	ARG
13	c1	138	ASN
13	c1	140	VAL
14	c2	28	LEU
14	c2	36	LEU
14	c2	39	ASP
14	c2	43	ARG
14	c2	46	ARG
14	c2	52	LEU
14	c2	59	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	88	LEU
14	c2	89	ILE
14	c2	97	LEU
14	c2	103	LEU
14	c2	116	VAL
14	c2	121	VAL
14	c2	129	GLU
14	c2	132	GLU

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Mol	Chain	Res	Type
14	c2	136	ILE
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	21	ASN
15	c3	27	LYS
15	c3	28	LEU
15	c3	29	SER
15	c3	35	GLU
15	c3	39	LYS
15	c3	46	THR
15	c3	60	VAL
15	c3	66	ILE
15	c3	70	LYS
15	c3	76	LYS
15	c3	80	LEU
15	c3	83	GLU
15	c3	84	ILE
15	c3	87	ASP
15	c3	94	LYS
15	c3	97	SER
15	c3	107	LYS
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	138	ASN
16	c4	13	VAL
16	c4	18	ARG
16	c4	20	TYR
16	c4	26	THR
16	c4	28	VAL
16	c4	31	THR
16	c4	43	THR
16	c4	49	LYS
16	c4	61	MET
16	c4	66	ASP
16	c4	81	VAL
16	c4	92	LYS
16	c4	102	LEU

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Mol	Chain	Res	Type
16	c4	107	ARG
16	c4	114	ARG
16	c4	119	THR
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
17	c5	12	PHE
17	c5	24	LYS
17	c5	27	GLU
17	c5	36	LEU
17	c5	40	ARG
17	c5	43	ARG
17	c5	44	ARG
17	c5	52	LYS
17	c5	69	GLU
17	c5	71	GLU
17	c5	77	ARG
17	c5	92	SER
17	c5	102	PHE
17	c5	107	ILE
17	c5	110	GLU
17	c5	121	ILE
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	50	GLU
18	c6	53	LEU
18	c6	54	LEU
18	c6	57	LEU
18	c6	68	ARG
18	c6	69	VAL
18	c6	70	THR
18	c6	81	ILE
18	c6	94	GLN
18	c6	98	ASP

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Mol	Chain	Res	Type
18	c6	107	LYS
18	c6	114	ARG
18	c6	115	THR
18	c6	128	LYS
18	c6	137	ARG
19	c7	3	ARG
19	c7	8	THR
19	c7	14	LYS
19	c7	19	ARG
19	c7	27	ASP
19	c7	29	GLN
19	c7	34	LEU
19	c7	46	LEU
19	c7	62	GLN
19	c7	69	ILE
19	c7	72	LYS
19	c7	83	GLN
19	c7	85	VAL
19	c7	88	VAL
19	c7	107	SER
19	c7	110	VAL
19	c7	113	LEU
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	13	HIS
20	c8	15	LEU
20	c8	25	ASN
20	c8	26	ILE
20	c8	28	ILE
20	c8	29	VAL
20	c8	33	THR
20	c8	36	LYS
20	c8	40	ARG
20	c8	63	GLN
20	c8	77	THR
20	c8	85	PHE
20	c8	105	VAL
20	c8	116	LEU
20	c8	119	ILE
20	c8	120	ARG

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Mol	Chain	Res	Type
20	c8	136	GLN
20	c8	138	THR
20	c8	144	ARG
21	c9	6	VAL
21	c9	20	SER
21	c9	27	LYS
21	c9	28	LEU
21	c9	37	VAL
21	c9	57	ARG
21	c9	88	VAL
21	c9	100	ILE
21	c9	111	ILE
21	c9	123	ARG
21	c9	126	GLU
21	c9	132	LEU
21	c9	139	THR
21	c9	140	LEU
21	c9	141	GLU
21	c9	142	GLU
21	c9	144	GLU
22	d0	20	ILE
22	d0	22	ILE
22	d0	23	ARG
22	d0	27	THR
22	d0	30	LYS
22	d0	31	VAL
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	67	THR
22	d0	70	THR
22	d0	72	ASN
22	d0	74	GLU
22	d0	77	LYS
22	d0	88	LYS
22	d0	89	ARG
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE

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Mol	Chain	Res	Type
22	d0	105	GLN
22	d0	107	THR
22	d0	108	ILE
22	d0	109	GLU
22	d0	115	GLU
23	d1	2	GLU
23	d1	5	LYS
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	25	LYS
23	d1	32	VAL
23	d1	38	LYS
23	d1	49	GLU
23	d1	50	TYR
23	d1	52	THR
23	d1	68	SER
23	d1	69	LEU
23	d1	78	LEU
23	d1	81	ASN
24	d2	6	VAL
24	d2	7	LEU
24	d2	23	ARG
24	d2	24	GLN
24	d2	25	VAL
24	d2	26	LEU
24	d2	37	PHE
24	d2	65	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	105	THR
25	d3	9	LEU
25	d3	14	LYS
25	d3	16	ARG
25	d3	19	ARG
25	d3	20	ARG
25	d3	33	LEU
25	d3	40	SER
25	d3	66	SER
25	d3	73	ARG
25	d3	83	VAL
25	d3	84	THR

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Mol	Chain	Res	Type
25	d3	96	VAL
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	109	ARG
25	d3	131	SER
25	d3	133	LEU
25	d3	144	ARG
26	d4	5	VAL
26	d4	10	ARG
26	d4	14	SER
26	d4	21	LYS
26	d4	26	ASP
26	d4	34	ASN
26	d4	36	SER
26	d4	42	GLU
26	d4	43	LYS
26	d4	49	LYS
26	d4	51	GLU
26	d4	62	THR
26	d4	83	LYS
26	d4	88	THR
26	d4	92	VAL
26	d4	100	VAL
26	d4	102	LYS
26	d4	124	ARG
26	d4	128	LYS
26	d4	132	ARG
27	d5	41	ILE
27	d5	43	ASP
27	d5	46	LYS
27	d5	51	LEU
27	d5	53	GLU
27	d5	57	TYR
27	d5	60	VAL
27	d5	81	ARG
27	d5	88	ILE
28	d6	10	ARG
28	d6	12	LYS
28	d6	13	LYS
28	d6	25	ASN
28	d6	34	LYS

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Mol	Chain	Res	Type
28	d6	41	ILE
28	d6	55	GLU
28	d6	67	THR
28	d6	82	ARG
28	d6	85	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	29	ARG
29	d7	34	ASP
29	d7	36	LYS
29	d7	43	ILE
29	d7	44	THR
29	d7	46	VAL
29	d7	52	THR
29	d7	61	THR
29	d7	63	LEU
29	d7	67	THR
29	d7	72	LYS
29	d7	77	THR
29	d7	81	ARG
30	d8	16	LEU
30	d8	19	THR
30	d8	22	ARG
30	d8	28	VAL
30	d8	30	VAL
30	d8	32	PHE
30	d8	33	LEU
30	d8	39	THR
30	d8	52	ASP
30	d8	54	LEU
30	d8	62	GLU
30	d8	64	ARG
31	d9	4	GLU
31	d9	6	VAL
31	d9	10	HIS
31	d9	25	SER
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	39	CYS
31	d9	41	GLN
31	d9	44	ARG

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Mol	Chain	Res	Type
31	d9	54	LYS
80	e0	13	LYS
80	e0	22	GLU
80	e0	24	THR
80	e0	28	LYS
80	e0	29	LYS
80	e0	38	LEU
80	e0	39	LEU
80	e0	44	PHE
80	e0	46	ASN
80	e0	49	LEU
80	e0	56	MET
33	e1	80	ARG
33	e1	83	LYS
33	e1	87	THR
33	e1	90	LYS
33	e1	96	LYS
33	e1	99	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	107	LYS
33	e1	113	LYS
33	e1	120	GLU
33	e1	121	CYS
33	e1	134	ASN
33	e1	135	HIS
33	e1	140	TYR
33	e1	144	CYS
34	sR	21	THR
34	sR	25	THR
34	sR	29	GLN
34	sR	42	LEU
34	sR	58	VAL
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	100	TYR
34	sR	106	HIS

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Mol	Chain	Res	Type
34	sR	123	ILE
34	sR	145	LEU
34	sR	149	ASP
34	sR	157	VAL
34	sR	159	ASN
34	sR	168	THR
34	sR	176	LYS
34	sR	199	ILE
34	sR	228	LYS
34	sR	232	TYR
34	sR	275	ARG
34	sR	277	GLU
34	sR	286	GLU
34	sR	297	ASP
34	sR	309	VAL
34	sR	310	ILE
34	sR	312	VAL
35	sM	23	LYS
35	sM	27	LYS
35	sM	30	THR
35	sM	41	SER
35	sM	43	ASP
35	sM	45	SER
35	sM	48	ARG
35	sM	50	ASN
35	sM	53	ARG
35	sM	55	SER
35	sM	61	ILE
35	sM	68	ARG
35	sM	74	LYS
35	sM	75	ASP
35	sM	77	THR
39	l2	10	LYS
39	l2	15	ILE
39	l2	32	LEU
39	l2	44	ILE
39	l2	45	VAL
39	l2	49	VAL
39	l2	52	SER
39	l2	54	ARG
39	l2	61	VAL
39	l2	62	VAL

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Mol	Chain	Res	Type
39	12	70	ARG
39	12	74	GLU
39	12	80	GLU
39	12	82	VAL
39	12	84	THR
39	12	101	VAL
39	12	107	VAL
39	12	111	THR
39	12	112	ILE
39	12	114	SER
39	12	119	LYS
39	12	134	VAL
39	12	137	ILE
39	12	142	ASP
39	12	147	ARG
39	12	155	LYS
39	12	157	VAL
39	12	158	ILE
39	12	159	SER
39	12	165	VAL
39	12	169	ILE
39	12	179	LEU
39	12	180	LEU
39	12	188	LYS
39	12	190	ARG
39	12	193	ARG
39	12	200	ARG
39	12	202	VAL
39	12	204	MET
39	12	205	ASN
39	12	207	VAL
39	12	230	VAL
39	12	246	LEU
39	12	249	SER
40	13	3	HIS
40	13	4	ARG
40	13	10	ARG
40	13	17	LEU
40	13	19	ARG
40	13	25	ILE
40	13	36	ASP
40	13	37	ARG

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Mol	Chain	Res	Type
40	l3	43	LEU
40	l3	47	LEU
40	l3	67	PHE
40	l3	69	LYS
40	l3	73	VAL
40	l3	79	VAL
40	l3	81	THR
40	l3	84	VAL
40	l3	85	VAL
40	l3	102	LEU
40	l3	103	THR
40	l3	114	VAL
40	l3	139	GLN
40	l3	146	ARG
40	l3	148	LEU
40	l3	160	VAL
40	l3	167	ARG
40	l3	169	THR
40	l3	178	LEU
40	l3	183	LEU
40	l3	184	ASN
40	l3	187	SER
40	l3	196	ARG
40	l3	197	GLU
40	l3	202	THR
40	l3	208	VAL
40	l3	211	GLN
40	l3	214	MET
40	l3	221	THR
40	l3	229	VAL
40	l3	232	ARG
40	l3	235	THR
40	l3	238	LEU
40	l3	242	THR
40	l3	244	ARG
40	l3	252	ILE
40	l3	266	ARG
40	l3	274	SER
40	l3	284	ARG
40	l3	287	LYS
40	l3	297	SER
40	l3	304	THR

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Mol	Chain	Res	Type
40	l3	328	ILE
40	l3	332	ARG
40	l3	335	ILE
40	l3	340	LYS
40	l3	341	SER
40	l3	346	THR
40	l3	353	GLU
40	l3	354	VAL
40	l3	361	THR
40	l3	382	THR
41	l4	3	ARG
41	l4	27	SER
41	l4	47	ARG
41	l4	52	VAL
41	l4	53	SER
41	l4	55	LYS
41	l4	73	ARG
41	l4	90	PHE
41	l4	93	MET
41	l4	112	LYS
41	l4	118	LYS
41	l4	120	TYR
41	l4	122	THR
41	l4	129	THR
41	l4	144	LYS
41	l4	145	ILE
41	l4	148	ILE
41	l4	150	LEU
41	l4	151	VAL
41	l4	156	LEU
41	l4	169	LEU
41	l4	170	LYS
41	l4	179	LEU
41	l4	186	LYS
41	l4	187	LEU
41	l4	193	LYS
41	l4	200	THR
41	l4	201	GLN
41	l4	203	ARG
41	l4	206	LEU
41	l4	220	ARG
41	l4	222	VAL

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Mol	Chain	Res	Type
41	14	226	GLU
41	14	230	VAL
41	14	233	LEU
41	14	246	ARG
41	14	265	GLU
41	14	282	SER
41	14	283	THR
41	14	299	ILE
41	14	306	THR
41	14	307	GLN
41	14	313	LEU
41	14	314	LYS
41	14	319	LYS
41	14	323	VAL
41	14	327	LEU
41	14	333	VAL
41	14	338	LYS
41	14	339	LEU
41	14	347	THR
41	14	357	GLU
41	14	358	THR
41	14	359	LEU
42	15	4	GLN
42	15	10	SER
42	15	34	LYS
42	15	35	ARG
42	15	38	THR
42	15	51	LEU
42	15	70	THR
42	15	74	VAL
42	15	84	PRO
42	15	93	THR
42	15	109	THR
42	15	110	LEU
42	15	112	LYS
42	15	115	LEU
42	15	118	THR
42	15	136	GLU
42	15	140	ARG
42	15	144	VAL
42	15	146	LEU
42	15	148	ILE

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Mol	Chain	Res	Type
42	15	151	GLN
42	15	152	ARG
42	15	155	THR
42	15	158	ARG
42	15	164	LYS
42	15	185	PHE
42	15	190	ILE
42	15	194	LEU
42	15	211	LEU
42	15	218	ARG
42	15	227	LEU
42	15	247	ILE
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS
42	15	268	GLU
42	15	273	ARG
42	15	282	ARG
42	15	293	LEU
42	15	297	GLN
43	16	8	LYS
43	16	12	SER
43	16	15	VAL
43	16	20	LYS
43	16	21	THR
43	16	31	ARG
43	16	35	VAL
43	16	50	LYS
43	16	64	LEU
43	16	65	ILE
43	16	78	ARG
43	16	89	THR
43	16	93	VAL
43	16	98	VAL
43	16	99	GLU
43	16	108	LYS
43	16	109	GLU
43	16	133	GLU
43	16	151	LYS
43	16	152	THR
43	16	155	LEU
43	16	162	SER

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Mol	Chain	Res	Type
43	16	171	PRO
44	17	22	THR
44	17	26	VAL
44	17	41	ARG
44	17	45	LEU
44	17	53	LYS
44	17	56	GLU
44	17	60	ARG
44	17	77	VAL
44	17	83	LEU
44	17	88	ARG
44	17	98	LYS
44	17	100	ARG
44	17	101	LYS
44	17	110	ARG
44	17	119	VAL
44	17	124	LEU
44	17	130	ILE
44	17	157	ASN
44	17	158	LYS
44	17	159	GLN
44	17	173	LEU
44	17	175	LYS
44	17	178	ILE
44	17	179	LEU
44	17	184	LEU
44	17	196	LYS
44	17	219	LYS
44	17	225	GLN
44	17	229	PHE
44	17	234	GLU
44	17	239	LEU
45	18	26	LEU
45	18	33	ASN
45	18	66	SER
45	18	68	ARG
45	18	74	THR
45	18	79	GLN
45	18	81	THR
45	18	89	GLU
45	18	95	ASN
45	18	109	LEU

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Mol	Chain	Res	Type
45	18	111	LYS
45	18	136	LEU
45	18	146	LYS
45	18	149	LYS
45	18	150	LEU
45	18	160	ILE
45	18	163	VAL
45	18	169	LEU
45	18	172	LYS
45	18	183	LYS
45	18	191	ASN
45	18	200	LEU
45	18	204	ARG
45	18	208	GLU
45	18	213	LYS
45	18	214	LEU
45	18	217	THR
45	18	221	ASN
45	18	222	PHE
45	18	230	LYS
45	18	231	LYS
45	18	241	LYS
45	18	245	LYS
45	18	248	LYS
46	19	5	GLN
46	19	6	THR
46	19	18	VAL
46	19	19	SER
46	19	26	LYS
46	19	33	THR
46	19	39	LYS
46	19	43	VAL
46	19	44	THR
46	19	46	THR
46	19	52	LEU
46	19	55	VAL
46	19	62	ARG
46	19	68	LEU
46	19	69	ARG
46	19	70	THR
46	19	78	MET
46	19	80	THR

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Mol	Chain	Res	Type
46	l9	82	VAL
46	l9	91	ARG
46	l9	105	GLU
46	l9	106	LYS
46	l9	107	ASP
46	l9	123	ILE
46	l9	129	ARG
46	l9	132	VAL
46	l9	133	THR
46	l9	137	SER
46	l9	138	THR
46	l9	144	ILE
46	l9	151	VAL
46	l9	154	VAL
46	l9	157	ASN
46	l9	161	LEU
46	l9	162	GLN
46	l9	166	ARG
46	l9	170	LYS
46	l9	191	LEU
47	m0	4	ARG
47	m0	19	LYS
47	m0	21	ARG
47	m0	24	ARG
47	m0	32	ARG
47	m0	36	LEU
47	m0	42	THR
47	m0	44	ASP
47	m0	48	LEU
47	m0	52	LEU
47	m0	58	GLU
47	m0	63	GLU
47	m0	66	GLU
47	m0	71	CYS
47	m0	74	LYS
47	m0	76	MET
47	m0	77	THR
47	m0	87	LEU
47	m0	91	VAL
47	m0	99	ILE
47	m0	121	LYS
47	m0	129	VAL

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Mol	Chain	Res	Type
47	m0	130	ASP
47	m0	139	ARG
47	m0	144	ASN
47	m0	145	LYS
47	m0	154	ARG
47	m0	162	GLN
47	m0	163	GLN
47	m0	167	LEU
47	m0	169	LYS
47	m0	170	LYS
47	m0	176	LEU
47	m0	177	ASP
47	m0	182	LEU
47	m0	197	VAL
47	m0	200	LEU
47	m0	206	LEU
47	m0	211	ARG
47	m0	217	PHE
48	m1	6	GLN
48	m1	10	ARG
48	m1	11	ASP
48	m1	13	LYS
48	m1	16	LYS
48	m1	30	LEU
48	m1	44	THR
48	m1	46	VAL
48	m1	54	VAL
48	m1	55	ARG
48	m1	56	THR
48	m1	61	ARG
48	m1	80	LEU
48	m1	107	ASP
48	m1	108	GLU
48	m1	112	LEU
48	m1	129	VAL
48	m1	140	ARG
48	m1	147	THR
48	m1	158	ASP
48	m1	159	THR
48	m1	161	SER
48	m1	166	LYS
48	m1	171	VAL

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Mol	Chain	Res	Type
49	m3	28	GLN
49	m3	41	THR
49	m3	54	LEU
49	m3	59	ARG
49	m3	67	ARG
49	m3	68	LYS
49	m3	69	VAL
49	m3	73	ARG
49	m3	76	THR
49	m3	100	ARG
49	m3	107	GLU
49	m3	118	GLU
49	m3	121	SER
49	m3	123	ILE
49	m3	124	ILE
49	m3	131	LYS
49	m3	149	GLN
49	m3	152	THR
49	m3	154	VAL
49	m3	164	GLU
49	m3	165	SER
49	m3	168	ARG
49	m3	171	ARG
49	m3	184	GLU
49	m3	194	GLU
50	m4	3	THR
50	m4	6	ILE
50	m4	13	ARG
50	m4	27	GLN
50	m4	42	LYS
50	m4	53	VAL
50	m4	63	VAL
50	m4	64	VAL
50	m4	72	LEU
50	m4	80	THR
50	m4	107	GLU
50	m4	113	THR
50	m4	123	LEU
50	m4	124	ARG
50	m4	126	GLN
50	m4	128	ARG
50	m4	130	THR

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Mol	Chain	Res	Type
50	m4	135	LEU
51	m5	5	LYS
51	m5	7	LEU
51	m5	10	LEU
51	m5	15	GLN
51	m5	22	LEU
51	m5	24	ARG
51	m5	50	ARG
51	m5	67	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	105	ARG
51	m5	106	VAL
51	m5	135	VAL
51	m5	138	GLN
51	m5	153	ASP
51	m5	155	VAL
51	m5	171	SER
51	m5	176	LYS
51	m5	184	LYS
51	m5	190	THR
51	m5	204	LYS
52	m6	12	LYS
52	m6	16	VAL
52	m6	22	VAL
52	m6	25	LYS
52	m6	36	VAL
52	m6	41	LEU
52	m6	49	ARG
52	m6	59	ARG
52	m6	67	THR
52	m6	74	ARG
52	m6	78	ARG
52	m6	79	ILE
52	m6	85	ARG
52	m6	106	GLU
52	m6	108	ILE

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Mol	Chain	Res	Type
52	m6	110	PRO
52	m6	117	ARG
52	m6	124	LEU
52	m6	126	VAL
52	m6	129	LEU
52	m6	130	LYS
52	m6	160	ARG
52	m6	166	GLU
52	m6	170	LYS
52	m6	171	LYS
52	m6	175	THR
52	m6	182	ASN
52	m6	184	THR
52	m6	190	VAL
52	m6	197	LEU
53	m7	7	THR
53	m7	9	THR
53	m7	23	ARG
53	m7	24	VAL
53	m7	31	GLU
53	m7	32	THR
53	m7	41	LEU
53	m7	46	LYS
53	m7	52	LEU
53	m7	56	ARG
53	m7	69	ARG
53	m7	78	VAL
53	m7	79	THR
53	m7	89	LYS
53	m7	94	LEU
53	m7	96	GLN
53	m7	107	LEU
53	m7	112	LEU
53	m7	114	VAL
53	m7	118	GLN
53	m7	119	VAL
53	m7	120	ASN
53	m7	124	LYS
53	m7	126	ARG
53	m7	127	ARG
53	m7	128	ARG
53	m7	153	LYS

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Mol	Chain	Res	Type
53	m7	155	GLU
54	m8	3	ILE
54	m8	7	SER
54	m8	12	ARG
54	m8	17	THR
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	93	ILE
54	m8	113	LYS
54	m8	129	VAL
54	m8	135	GLN
54	m8	138	LEU
54	m8	161	LYS
54	m8	165	ILE
54	m8	166	LEU
54	m8	168	THR
54	m8	170	ARG
54	m8	178	ARG
55	m9	7	GLN
55	m9	8	LYS
55	m9	10	LEU
55	m9	17	VAL
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	52	LYS
55	m9	56	THR

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Mol	Chain	Res	Type
55	m9	57	VAL
55	m9	63	THR
55	m9	70	LYS
55	m9	74	ARG
55	m9	76	SER
55	m9	88	ARG
55	m9	91	SER
55	m9	99	LEU
55	m9	105	LEU
55	m9	106	LEU
55	m9	126	GLU
55	m9	127	SER
55	m9	138	LEU
55	m9	143	ILE
55	m9	152	GLU
55	m9	153	LYS
55	m9	162	ARG
55	m9	164	LEU
55	m9	167	ARG
55	m9	173	ARG
55	m9	177	VAL
56	n0	13	ARG
56	n0	17	GLU
56	n0	21	GLU
56	n0	23	LYS
56	n0	32	SER
56	n0	45	LEU
56	n0	50	LYS
56	n0	52	LYS
56	n0	53	LYS
56	n0	58	ILE
56	n0	60	SER
56	n0	80	ARG
56	n0	87	THR
56	n0	92	LYS
56	n0	97	VAL
56	n0	100	VAL
56	n0	104	GLU
56	n0	105	THR
56	n0	115	ARG
56	n0	117	ARG
56	n0	130	GLU

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Mol	Chain	Res	Type
56	n0	132	THR
56	n0	142	GLN
56	n0	148	LEU
56	n0	157	GLN
56	n0	160	THR
56	n0	162	THR
56	n0	166	LYS
56	n0	169	SER
56	n0	172	TYR
57	n1	9	SER
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	55	LYS
57	n1	68	THR
57	n1	71	SER
57	n1	75	ILE
57	n1	78	LYS
57	n1	83	ARG
57	n1	86	GLU
57	n1	88	ARG
57	n1	96	ILE
57	n1	104	GLU
57	n1	124	VAL
57	n1	126	VAL
57	n1	130	ARG
57	n1	131	GLN
57	n1	135	PRO
57	n1	139	ARG
57	n1	141	VAL
57	n1	143	THR
57	n1	150	THR
57	n1	158	THR
58	n2	13	LYS
58	n2	16	THR
58	n2	27	VAL
58	n2	37	LEU
58	n2	39	ASP
58	n2	43	VAL
58	n2	50	LEU
58	n2	54	VAL
58	n2	55	THR

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Mol	Chain	Res	Type
58	n2	66	VAL
58	n2	74	LYS
58	n2	75	TYR
58	n2	88	GLN
58	n2	90	ARG
58	n2	98	THR
58	n2	100	THR
59	n3	7	GLN
59	n3	13	ILE
59	n3	14	SER
59	n3	45	ARG
59	n3	48	ARG
59	n3	66	LYS
59	n3	70	ARG
59	n3	73	VAL
59	n3	74	MET
59	n3	88	ARG
59	n3	91	VAL
59	n3	115	THR
60	n4	1	MET
60	n4	19	THR
60	n4	25	ASP
60	n4	39	LEU
60	n4	43	ARG
60	n4	54	LEU
60	n4	57	LYS
60	n4	63	ILE
60	n4	89	LEU
60	n4	96	LEU
60	n4	97	LYS
60	n4	98	PRO
60	n4	107	GLU
60	n4	126	GLU
60	n4	127	LYS
60	n4	134	GLN
60	n4	135	SER
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	39	LYS
61	n5	56	ARG

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Mol	Chain	Res	Type
61	n5	57	LEU
61	n5	63	ILE
61	n5	64	GLU
61	n5	65	GLN
61	n5	71	THR
61	n5	73	MET
61	n5	74	LYS
61	n5	78	ASP
61	n5	86	VAL
61	n5	109	LYS
61	n5	115	ARG
61	n5	125	ARG
61	n5	133	LEU
61	n5	135	ILE
61	n5	142	ILE
62	n6	3	LYS
62	n6	4	GLN
62	n6	9	SER
62	n6	10	SER
62	n6	12	ARG
62	n6	13	ARG
62	n6	17	LYS
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	55	GLU
62	n6	57	LEU
62	n6	62	SER
62	n6	66	GLN
62	n6	70	ILE
62	n6	74	TYR
62	n6	76	LEU
62	n6	80	VAL
62	n6	83	ASP
62	n6	97	ILE
62	n6	105	VAL
62	n6	108	LYS
62	n6	120	GLN
62	n6	127	GLU

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Mol	Chain	Res	Type
63	n7	3	LYS
63	n7	14	VAL
63	n7	15	ARG
63	n7	17	ARG
63	n7	24	VAL
63	n7	26	VAL
63	n7	34	LYS
63	n7	46	ILE
63	n7	52	LYS
63	n7	65	ARG
63	n7	72	ILE
63	n7	81	LEU
63	n7	86	THR
63	n7	94	SER
63	n7	95	VAL
63	n7	98	THR
63	n7	99	GLU
63	n7	102	GLU
63	n7	103	GLN
63	n7	105	SER
63	n7	111	LYS
63	n7	121	ARG
63	n7	126	LYS
63	n7	134	LEU
63	n7	135	ARG
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	10	LYS
64	n8	16	SER
64	n8	26	ARG
64	n8	42	ARG
64	n8	43	ILE
64	n8	46	ASP
64	n8	47	LYS
64	n8	56	VAL
64	n8	60	TYR
64	n8	78	LEU
64	n8	82	ILE
64	n8	85	ASP
64	n8	91	LEU
64	n8	98	THR

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Mol	Chain	Res	Type
64	n8	115	LYS
64	n8	123	VAL
64	n8	128	ARG
64	n8	132	LYS
64	n8	133	LEU
64	n8	139	ARG
65	n9	14	ARG
65	n9	21	ILE
65	n9	22	LYS
65	n9	23	LYS
65	n9	26	THR
65	n9	33	LYS
65	n9	38	LYS
65	n9	50	THR
65	n9	52	LYS
65	n9	54	LEU
65	n9	58	LYS
65	n9	59	LYS
66	o0	6	SER
66	o0	8	GLU
66	o0	9	SER
66	o0	18	ILE
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	81	VAL
66	o0	86	ARG
66	o0	99	ASP
66	o0	103	THR
67	o1	6	ASP
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	28	ARG
67	o1	31	ARG

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Mol	Chain	Res	Type
67	o1	34	LYS
67	o1	44	MET
67	o1	46	THR
67	o1	55	LEU
67	o1	64	VAL
67	o1	76	SER
67	o1	84	ASP
67	o1	91	SER
67	o1	93	VAL
67	o1	98	VAL
67	o1	102	LYS
67	o1	104	LEU
67	o1	106	THR
67	o1	107	VAL
67	o1	110	GLU
67	o1	111	GLU
68	o2	4	LEU
68	o2	8	LYS
68	o2	16	LYS
68	o2	18	LYS
68	o2	19	ARG
68	o2	24	ARG
68	o2	27	ARG
68	o2	33	ARG
68	o2	35	GLN
68	o2	41	VAL
68	o2	51	SER
68	o2	54	LYS
68	o2	61	LYS
68	o2	71	HIS
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	89	THR
68	o2	91	THR
68	o2	95	GLU
68	o2	101	SER
68	o2	109	LEU
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	20	LYS

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Mol	Chain	Res	Type
69	o3	31	LYS
69	o3	49	ILE
69	o3	56	SER
69	o3	58	GLU
69	o3	59	VAL
69	o3	62	SER
69	o3	70	LYS
69	o3	78	SER
69	o3	84	THR
69	o3	86	ARG
69	o3	98	VAL
69	o3	106	ASN
69	o3	107	ILE
70	o4	5	VAL
70	o4	9	ARG
70	o4	20	ILE
70	o4	21	LYS
70	o4	24	LYS
70	o4	25	THR
70	o4	30	LEU
70	o4	31	ARG
70	o4	35	VAL
70	o4	47	CYS
70	o4	49	SER
70	o4	58	ARG
70	o4	65	VAL
70	o4	68	THR
70	o4	71	THR
70	o4	79	SER
70	o4	84	CYS
70	o4	86	LYS
70	o4	87	GLU
70	o4	88	ARG
70	o4	98	GLN
71	o5	15	GLU
71	o5	20	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	28	LEU
71	o5	36	LEU
71	o5	37	SER
71	o5	38	ARG

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Mol	Chain	Res	Type
71	o5	45	LYS
71	o5	47	VAL
71	o5	48	ARG
71	o5	62	GLN
71	o5	69	LEU
71	o5	79	ASP
71	o5	80	LEU
71	o5	81	ARG
71	o5	85	THR
71	o5	86	ARG
71	o5	89	ARG
71	o5	101	THR
71	o5	107	LYS
71	o5	113	GLN
72	o6	3	VAL
72	o6	7	ILE
72	o6	9	ILE
72	o6	12	ASN
72	o6	21	THR
72	o6	25	LYS
72	o6	26	ILE
72	o6	29	LYS
72	o6	34	SER
72	o6	36	ARG
72	o6	37	THR
72	o6	42	SER
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	64	SER
72	o6	66	GLU
72	o6	68	ARG
72	o6	75	LYS
72	o6	76	ARG
72	o6	79	SER
72	o6	90	MET
72	o6	94	ILE
72	o6	98	ARG
73	o7	3	LYS

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Mol	Chain	Res	Type
73	o7	11	ARG
73	o7	17	THR
73	o7	25	ARG
73	o7	33	THR
73	o7	36	SER
73	o7	44	THR
73	o7	45	ARG
73	o7	59	THR
73	o7	65	ARG
73	o7	67	LEU
73	o7	68	LYS
73	o7	72	ARG
73	o7	75	LYS
73	o7	80	THR
74	o8	5	ILE
74	o8	12	LEU
74	o8	24	THR
74	o8	41	THR
74	o8	45	VAL
74	o8	46	ARG
74	o8	50	SER
74	o8	53	THR
74	o8	61	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	72	THR
74	o8	78	LEU
75	o9	4	GLN
75	o9	11	GLN
75	o9	15	LYS
75	o9	21	ARG
75	o9	29	LEU
75	o9	41	ARG
75	o9	45	ARG
75	o9	47	THR
75	o9	48	LYS
75	o9	51	ILE
76	q0	78	ILE
76	q0	79	GLU
76	q0	83	LYS
76	q0	85	LEU
76	q0	87	SER

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Mol	Chain	Res	Type
76	q0	88	LYS
76	q0	106	ARG
76	q0	108	THR
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	127	LEU
77	q1	6	ARG
77	q1	9	ARG
77	q1	13	LEU
77	q1	14	LYS
77	q1	21	ARG
77	q1	23	ARG
77	q1	24	SER
78	q2	7	THR
78	q2	8	ARG
78	q2	20	HIS
78	q2	26	THR
78	q2	38	GLN
78	q2	61	LYS
78	q2	75	VAL
78	q2	78	LYS
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	93	LEU
78	q2	96	GLU
78	q2	100	LYS
78	q2	104	LEU
78	q2	105	GLN
79	q3	3	LYS
79	q3	20	SER
79	q3	24	ARG
79	q3	42	CYS
79	q3	48	LYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	81	SER
79	q3	90	VAL
82	p0	4	ILE
82	p0	5	ARG

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Mol	Chain	Res	Type
82	p0	10	GLU
82	p0	15	LEU
82	p0	30	VAL
82	p0	39	HIS
82	p0	44	GLU
82	p0	46	ARG
82	p0	48	ARG
82	p0	50	VAL
82	p0	51	VAL
82	p0	55	LYS
82	p0	67	LEU
82	p0	70	LEU
82	p0	76	LEU
82	p0	93	LEU
82	p0	97	LYS
82	p0	104	ARG
82	p0	185	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
3	S1	79	HIS
3	S1	149	GLN
3	S1	157	GLN
3	S1	177	GLN
5	S3	74	GLN
5	S3	179	GLN
7	S5	224	ASN
9	S7	74	GLN
12	C0	12	HIS
20	C8	25	ASN
20	C8	89	GLN
23	D1	74	GLN
23	D1	75	ASN
34	SR	195	HIS
39	L2	83	HIS
39	L2	132	ASN
39	L2	209	HIS
40	L3	139	GLN
41	L4	110	ASN
42	L5	81	HIS
44	L7	244	ASN

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Mol	Chain	Res	Type
47	M0	144	ASN
50	M4	62	GLN
56	N0	138	GLN
57	N1	26	HIS
69	O3	106	ASN
2	s0	23	HIS
7	s5	103	ASN
7	s5	104	ASN
7	s5	186	ASN
9	s7	71	HIS
9	s7	86	GLN
11	s9	110	GLN
11	s9	142	ASN
12	c0	32	HIS
20	c8	13	HIS
20	c8	25	ASN
22	d0	72	ASN
26	d4	22	GLN
26	d4	29	HIS
26	d4	34	ASN
80	e0	17	GLN
39	l2	50	HIS
40	l3	139	GLN
44	l7	80	GLN
44	l7	104	GLN
46	l9	50	ASN
47	m0	144	ASN
52	m6	90	HIS
55	m9	7	GLN
59	n3	4	ASN
64	n8	25	HIS
64	n8	44	ASN
64	n8	49	HIS
71	o5	20	GLN
75	o9	25	GLN
75	o9	50	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	481 (27%)	68 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	6	1793/1800 (99%)	463 (25%)	56 (3%)
36	1	3145/3396 (92%)	688 (21%)	83 (2%)
36	5	3145/3396 (92%)	647 (20%)	93 (2%)
37	3	120/121 (99%)	20 (16%)	4 (3%)
37	7	120/121 (99%)	19 (15%)	0
38	4	157/158 (99%)	35 (22%)	4 (2%)
38	8	157/158 (99%)	40 (25%)	3 (1%)
All	All	10384/10950 (94%)	2393 (23%)	311 (2%)

All (2393) 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	40	A
1	2	45	U
1	2	46	A
1	2	47	A
1	2	57	G
1	2	60	U
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	97	C
1	2	100	A
1	2	104	A
1	2	114	C
1	2	120	U
1	2	127	G
1	2	130	C
1	2	131	C

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Mol	Chain	Res	Type
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	140	A
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
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	188	A
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	215	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	233	C
1	2	234	G
1	2	235	G
1	2	236	A
1	2	238	U

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Mol	Chain	Res	Type
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U
1	2	250	C
1	2	260	U
1	2	261	U
1	2	262	U
1	2	265	A
1	2	267	U
1	2	271	A
1	2	272	U
1	2	274	G
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	299	A
1	2	302	U
1	2	308	C
1	2	309	C
1	2	314	C
1	2	316	A
1	2	319	U
1	2	321	C
1	2	322	G
1	2	332	U
1	2	337	G
1	2	338	C
1	2	341	A
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	363	G
1	2	387	A
1	2	393	C

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Mol	Chain	Res	Type
1	2	399	A
1	2	400	A
1	2	402	C
1	2	403	G
1	2	404	G
1	2	416	A
1	2	418	G
1	2	419	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	427	C
1	2	428	A
1	2	434	G
1	2	439	U
1	2	444	C
1	2	448	C
1	2	468	A
1	2	477	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

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Mol	Chain	Res	Type
1	2	516	G
1	2	519	C
1	2	527	A
1	2	532	U
1	2	534	A
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	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	570	A
1	2	578	U
1	2	579	A
1	2	580	A
1	2	585	A
1	2	594	A
1	2	595	G
1	2	605	A
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	655	G
1	2	656	G
1	2	657	U
1	2	658	C

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Mol	Chain	Res	Type
1	2	677	G
1	2	679	U
1	2	680	U
1	2	684	A
1	2	685	A
1	2	686	C
1	2	694	U
1	2	695	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	709	C
1	2	710	U
1	2	712	G
1	2	713	A
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

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Mol	Chain	Res	Type
1	2	742	U
1	2	743	U
1	2	744	U
1	2	745	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	758	U
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	789	A
1	2	794	U
1	2	795	U
1	2	803	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	833	U
1	2	840	U
1	2	846	G
1	2	848	C
1	2	854	U
1	2	856	A
1	2	860	U

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Mol	Chain	Res	Type
1	2	862	A
1	2	863	A
1	2	864	U
1	2	876	G
1	2	886	U
1	2	892	A
1	2	896	U
1	2	898	A
1	2	910	C
1	2	912	U
1	2	913	G
1	2	914	G
1	2	916	U
1	2	921	U
1	2	926	A
1	2	933	A
1	2	935	U
1	2	942	G
1	2	944	A
1	2	951	A
1	2	960	U
1	2	966	A
1	2	971	A
1	2	988	A
1	2	992	A
1	2	993	A
1	2	994	G
1	2	996	U
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1026	A
1	2	1028	C
1	2	1029	U
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

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Mol	Chain	Res	Type
1	2	1060	U
1	2	1061	A
1	2	1074	G
1	2	1079	U
1	2	1080	U
1	2	1082	C
1	2	1083	G
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1093	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1109	G
1	2	1111	G
1	2	1135	U
1	2	1138	A
1	2	1139	A
1	2	1150	G
1	2	1151	A
1	2	1152	A
1	2	1157	A
1	2	1158	C
1	2	1159	C
1	2	1160	A
1	2	1163	A
1	2	1167	G
1	2	1176	G
1	2	1185	U
1	2	1188	G
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G

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Mol	Chain	Res	Type
1	2	1221	A
1	2	1226	A
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1256	A
1	2	1257	U
1	2	1258	U
1	2	1286	U
1	2	1292	G
1	2	1314	U
1	2	1315	U
1	2	1321	A
1	2	1337	A
1	2	1338	C
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1349	G
1	2	1354	G
1	2	1355	C
1	2	1361	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	1388	A
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1412	G
1	2	1413	U
1	2	1415	U

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Mol	Chain	Res	Type
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1432	U
1	2	1435	G
1	2	1446	A
1	2	1448	G
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1461	C
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1482	C
1	2	1486	G
1	2	1488	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1499	G
1	2	1506	G
1	2	1514	U
1	2	1516	A
1	2	1517	U
1	2	1523	G
1	2	1524	A
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1542	G
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1574	G
1	2	1584	G
1	2	1590	G
1	2	1601	G
1	2	1614	A

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Mol	Chain	Res	Type
1	2	1616	G
1	2	1624	C
1	2	1627	U
1	2	1631	A
1	2	1657	U
1	2	1658	G
1	2	1663	G
1	2	1664	C
1	2	1673	G
1	2	1680	G
1	2	1683	C
1	2	1684	U
1	2	1719	A
1	2	1750	A
1	2	1756	A
1	2	1759	C
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1768	G
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	16	A
36	1	26	A
36	1	40	A
36	1	43	A
36	1	45	A
36	1	49	A
36	1	57	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A

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Mol	Chain	Res	Type
36	1	68	C
36	1	74	G
36	1	75	G
36	1	83	U
36	1	92	G
36	1	99	A
36	1	109	A
36	1	110	G
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	147	U
36	1	154	U
36	1	156	G
36	1	157	A
36	1	160	G
36	1	166	C
36	1	169	U
36	1	170	G
36	1	172	G
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	210	U
36	1	218	G
36	1	219	A
36	1	224	C
36	1	240	U
36	1	243	G
36	1	245	U
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	269	G
36	1	283	G
36	1	284	A
36	1	286	U
36	1	295	A

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Mol	Chain	Res	Type
36	1	298	U
36	1	299	G
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	376	G
36	1	397	A
36	1	398	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	417	A
36	1	421	G
36	1	422	A
36	1	439	C
36	1	440	A
36	1	495	G
36	1	498	A
36	1	507	U
36	1	517	G
36	1	520	U
36	1	521	A
36	1	525	C
36	1	530	G
36	1	535	G
36	1	544	C
36	1	546	C
36	1	547	G
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

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Mol	Chain	Res	Type
36	1	578	A
36	1	579	G
36	1	592	A
36	1	600	G
36	1	604	G
36	1	609	G
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A
36	1	636	C
36	1	639	G
36	1	642	U
36	1	644	G
36	1	649	A
36	1	658	G
36	1	660	A
36	1	661	G
36	1	677	A
36	1	681	U
36	1	691	A
36	1	705	A
36	1	708	G
36	1	712	G
36	1	715	A
36	1	716	A
36	1	720	A
36	1	726	G
36	1	758	C
36	1	763	G
36	1	764	U
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	781	G
36	1	785	G
36	1	786	A
36	1	804	C
36	1	806	A
36	1	817	A
36	1	830	A

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Mol	Chain	Res	Type
36	1	837	A
36	1	849	C
36	1	861	C
36	1	874	U
36	1	879	U
36	1	881	C
36	1	882	A
36	1	890	C
36	1	896	A
36	1	897	U
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	937	G
36	1	943	U
36	1	944	C
36	1	959	C
36	1	960	U
36	1	962	A
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	993	G
36	1	994	G
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1014	U
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

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Mol	Chain	Res	Type
36	1	1036	A
36	1	1037	C
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1063	G
36	1	1064	A
36	1	1065	A
36	1	1072	G
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1087	G
36	1	1088	U
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	1111	U
36	1	1116	G
36	1	1117	G
36	1	1121	U
36	1	1128	U
36	1	1131	G
36	1	1144	U
36	1	1153	A
36	1	1159	A
36	1	1168	U
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1191	U
36	1	1192	C
36	1	1193	A
36	1	1201	C
36	1	1209	G
36	1	1212	A
36	1	1213	G

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Mol	Chain	Res	Type
36	1	1216	C
36	1	1218	U
36	1	1222	G
36	1	1225	A
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1235	U
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1242	G
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1251	A
36	1	1258	U
36	1	1259	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	1278	A
36	1	1279	C
36	1	1285	G
36	1	1287	A
36	1	1292	C
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1323	G
36	1	1325	U
36	1	1330	A

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Mol	Chain	Res	Type
36	1	1333	C
36	1	1345	G
36	1	1348	U
36	1	1349	G
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	1379	G
36	1	1380	G
36	1	1386	A
36	1	1392	G
36	1	1399	A
36	1	1400	G
36	1	1405	U
36	1	1406	A
36	1	1418	A
36	1	1419	A
36	1	1425	U
36	1	1431	G
36	1	1434	G
36	1	1437	C
36	1	1446	A
36	1	1450	G
36	1	1455	U
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1490	A
36	1	1496	C
36	1	1503	A
36	1	1508	C
36	1	1528	G
36	1	1529	A
36	1	1555	U
36	1	1556	C
36	1	1558	A
36	1	1560	G
36	1	1561	G
36	1	1562	C

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Mol	Chain	Res	Type
36	1	1563	C
36	1	1564	U
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	1579	C
36	1	1580	A
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	1629	U
36	1	1639	C
36	1	1641	U
36	1	1642	A
36	1	1643	A
36	1	1644	C
36	1	1645	U
36	1	1651	U
36	1	1657	C
36	1	1683	A
36	1	1714	A
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1736	G
36	1	1741	A
36	1	1742	U
36	1	1750	A
36	1	1751	G
36	1	1760	A
36	1	1761	C
36	1	1762	C
36	1	1765	U
36	1	1766	G

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Mol	Chain	Res	Type
36	1	1767	C
36	1	1770	G
36	1	1775	G
36	1	1780	G
36	1	1781	C
36	1	1797	A
36	1	1805	C
36	1	1809	A
36	1	1810	A
36	1	1812	G
36	1	1814	A
36	1	1816	A
36	1	1817	G
36	1	1818	U
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1834	U
36	1	1838	G
36	1	1839	A
36	1	1840	U
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	1850	A
36	1	1855	U
36	1	1863	G
36	1	1864	A
36	1	1871	U
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1901	A
36	1	1906	G
36	1	1908	A
36	1	1935	G
36	1	1948	G
36	1	1951	C
36	1	1952	G

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Mol	Chain	Res	Type
36	1	1953	G
36	1	1954	G
36	1	2094	C
36	1	2101	C
36	1	2102	U
36	1	2107	A
36	1	2112	U
36	1	2113	A
36	1	2121	G
36	1	2122	G
36	1	2130	G
36	1	2131	A
36	1	2134	G
36	1	2140	U
36	1	2144	A
36	1	2158	A
36	1	2165	G
36	1	2169	G
36	1	2170	U
36	1	2177	G
36	1	2188	A
36	1	2192	C
36	1	2193	U
36	1	2194	G
36	1	2205	U
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2223	A
36	1	2228	A
36	1	2244	A
36	1	2249	G
36	1	2250	G
36	1	2255	A
36	1	2256	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	2288	G

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Mol	Chain	Res	Type
36	1	2298	U
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2315	G
36	1	2319	U
36	1	2330	C
36	1	2334	U
36	1	2336	U
36	1	2341	A
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2393	G
36	1	2395	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	2443	A
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2504	U
36	1	2511	A
36	1	2513	U
36	1	2514	U
36	1	2515	A
36	1	2519	A
36	1	2522	G
36	1	2523	A
36	1	2525	G

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Mol	Chain	Res	Type
36	1	2526	C
36	1	2530	G
36	1	2532	U
36	1	2533	G
36	1	2534	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	2547	A
36	1	2548	C
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2561	A
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	2576	G
36	1	2581	U
36	1	2585	G
36	1	2586	G
36	1	2593	A
36	1	2594	C
36	1	2602	G
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2626	A
36	1	2629	U
36	1	2637	A
36	1	2652	U
36	1	2656	A
36	1	2672	G
36	1	2674	A

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Mol	Chain	Res	Type
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	2702	A
36	1	2705	A
36	1	2714	G
36	1	2728	G
36	1	2729	U
36	1	2752	U
36	1	2753	G
36	1	2762	A
36	1	2771	U
36	1	2772	C
36	1	2773	C
36	1	2777	G
36	1	2778	G
36	1	2779	A
36	1	2787	G
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2810	C
36	1	2814	G
36	1	2816	G
36	1	2817	A
36	1	2818	U
36	1	2819	A
36	1	2829	U
36	1	2834	G
36	1	2836	C
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2847	A
36	1	2849	C
36	1	2860	U

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Mol	Chain	Res	Type
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2875	U
36	1	2883	U
36	1	2887	A
36	1	2889	C
36	1	2899	C
36	1	2900	A
36	1	2910	A
36	1	2914	G
36	1	2923	U
36	1	2927	C
36	1	2935	U
36	1	2936	A
36	1	2942	C
36	1	2944	U
36	1	2945	G
36	1	2947	G
36	1	2971	A
36	1	2974	U
36	1	2979	U
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	3040	A
36	1	3049	A
36	1	3050	U
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3080	G
36	1	3083	G
36	1	3086	A
36	1	3087	A
36	1	3092	C

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Mol	Chain	Res	Type
36	1	3113	A
36	1	3119	U
36	1	3122	A
36	1	3128	G
36	1	3130	A
36	1	3131	U
36	1	3139	A
36	1	3141	A
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3153	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	3169	U
36	1	3170	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	3220	G
36	1	3221	C
36	1	3223	A
36	1	3228	C
36	1	3229	G
36	1	3235	C

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Mol	Chain	Res	Type
36	1	3243	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3269	U
36	1	3270	U
36	1	3272	C
36	1	3273	A
36	1	3275	U
36	1	3276	G
36	1	3279	A
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	3295	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	3330	A
36	1	3335	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3348	G
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	3369	G
36	1	3375	A

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Mol	Chain	Res	Type
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
37	3	7	G
37	3	9	C
37	3	13	A
37	3	14	U
37	3	18	C
37	3	21	G
37	3	22	A
37	3	26	C
37	3	42	A
37	3	51	A
37	3	53	U
37	3	54	U
37	3	64	A
37	3	65	G
37	3	76	A
37	3	91	G
37	3	101	G
37	3	102	A
37	3	112	G
37	3	121	U
38	4	2	A
38	4	20	U
38	4	22	U
38	4	26	U
38	4	34	U
38	4	35	C
38	4	52	A
38	4	53	A
38	4	59	A
38	4	62	C
38	4	63	G
38	4	75	G
38	4	79	A
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C

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Mol	Chain	Res	Type
38	4	84	C
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	97	A
38	4	105	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	125	U
38	4	126	A
38	4	128	U
38	4	138	A
38	4	152	G
38	4	155	A
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	17	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	44	U
1	6	46	A
1	6	47	A
1	6	49	C
1	6	57	G
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	103	A
1	6	104	A
1	6	114	C
1	6	116	U

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Mol	Chain	Res	Type
1	6	127	G
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	142	G
1	6	143	G
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	181	A
1	6	185	U
1	6	187	G
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	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	229	U
1	6	230	C
1	6	232	U
1	6	233	C
1	6	234	G
1	6	235	G

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Mol	Chain	Res	Type
1	6	238	U
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	260	U
1	6	261	U
1	6	265	A
1	6	271	A
1	6	272	U
1	6	273	G
1	6	276	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	281	G
1	6	287	G
1	6	298	C
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	341	A
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	381	C
1	6	387	A
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	418	G
1	6	424	C

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Mol	Chain	Res	Type
1	6	425	A
1	6	426	G
1	6	434	G
1	6	439	U
1	6	444	C
1	6	448	C
1	6	454	U
1	6	468	A
1	6	470	A
1	6	475	A
1	6	480	G
1	6	484	C
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	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	512	A
1	6	513	U
1	6	514	G
1	6	515	A
1	6	519	C
1	6	527	A
1	6	536	C
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A

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Mol	Chain	Res	Type
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	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	574	G
1	6	578	U
1	6	579	A
1	6	580	A
1	6	582	U
1	6	594	A
1	6	595	G
1	6	609	U
1	6	610	G
1	6	611	U
1	6	617	U
1	6	619	A
1	6	620	A
1	6	621	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	630	A
1	6	637	C
1	6	639	U
1	6	640	U
1	6	645	C
1	6	648	G
1	6	650	U
1	6	651	G
1	6	652	G
1	6	653	C
1	6	654	C
1	6	658	C
1	6	661	A

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Mol	Chain	Res	Type
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
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	710	U
1	6	711	U
1	6	714	G
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	734	A
1	6	742	U
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	780	A
1	6	781	U
1	6	782	U

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Mol	Chain	Res	Type
1	6	783	G
1	6	787	G
1	6	789	A
1	6	793	A
1	6	794	U
1	6	806	A
1	6	811	A
1	6	812	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	823	G
1	6	825	U
1	6	826	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	856	A
1	6	861	U
1	6	863	A
1	6	898	A
1	6	906	A
1	6	912	U
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	966	A
1	6	969	C
1	6	970	A
1	6	971	A
1	6	976	G
1	6	992	A
1	6	993	A
1	6	997	G

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Mol	Chain	Res	Type
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1014	G
1	6	1021	C
1	6	1026	A
1	6	1028	C
1	6	1039	A
1	6	1040	G
1	6	1041	G
1	6	1052	U
1	6	1053	G
1	6	1055	U
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1063	U
1	6	1070	C
1	6	1071	U
1	6	1073	G
1	6	1082	C
1	6	1091	A
1	6	1092	A
1	6	1093	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1101	G
1	6	1109	G
1	6	1138	A
1	6	1150	G
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1167	G
1	6	1185	U
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	1208	A
1	6	1217	A
1	6	1218	G
1	6	1220	C
1	6	1225	U
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1238	A
1	6	1239	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	1284	C
1	6	1285	U
1	6	1286	U
1	6	1288	G
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1338	C
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	1355	C
1	6	1361	U

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Mol	Chain	Res	Type
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1371	A
1	6	1372	U
1	6	1382	A
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1413	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1429	G
1	6	1433	G
1	6	1445	G
1	6	1446	A
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	1481	C
1	6	1482	C
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	1510	U
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A

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Mol	Chain	Res	Type
1	6	1531	G
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	1573	A
1	6	1574	G
1	6	1575	G
1	6	1577	A
1	6	1578	U
1	6	1582	U
1	6	1584	G
1	6	1601	G
1	6	1615	C
1	6	1616	G
1	6	1621	U
1	6	1634	C
1	6	1635	A
1	6	1637	C
1	6	1638	G
1	6	1657	U
1	6	1658	G
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	1705	C
1	6	1710	U
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1731	A

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Mol	Chain	Res	Type
1	6	1736	G
1	6	1755	A
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	1789	G
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	26	A
36	5	33	G
36	5	40	A
36	5	43	A
36	5	49	A
36	5	60	A
36	5	65	A
36	5	66	A
36	5	73	C
36	5	74	G
36	5	76	G
36	5	83	U
36	5	92	G
36	5	99	A
36	5	109	A
36	5	110	G
36	5	113	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	133	U

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Mol	Chain	Res	Type
36	5	134	U
36	5	135	C
36	5	136	G
36	5	142	C
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	172	G
36	5	174	C
36	5	187	A
36	5	190	U
36	5	191	U
36	5	200	C
36	5	210	U
36	5	211	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	224	C
36	5	231	G
36	5	236	G
36	5	237	G
36	5	238	A
36	5	239	G
36	5	240	U
36	5	244	G
36	5	246	U
36	5	247	C
36	5	248	U
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	259	C
36	5	269	G
36	5	284	A
36	5	286	U

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Mol	Chain	Res	Type
36	5	295	A
36	5	322	U
36	5	323	A
36	5	329	U
36	5	330	G
36	5	334	A
36	5	349	A
36	5	350	C
36	5	370	U
36	5	375	A
36	5	376	G
36	5	395	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	407	A
36	5	421	G
36	5	422	A
36	5	436	A
36	5	437	G
36	5	438	A
36	5	439	C
36	5	441	U
36	5	442	G
36	5	492	U
36	5	495	G
36	5	521	A
36	5	532	A
36	5	535	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	551	A
36	5	553	U
36	5	555	U
36	5	557	A
36	5	559	A
36	5	578	A
36	5	579	G
36	5	592	A

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Mol	Chain	Res	Type
36	5	594	U
36	5	595	G
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	636	C
36	5	649	A
36	5	656	A
36	5	660	A
36	5	675	C
36	5	677	A
36	5	681	U
36	5	683	U
36	5	705	A
36	5	708	G
36	5	712	G
36	5	715	A
36	5	716	A
36	5	726	G
36	5	735	A
36	5	736	A
36	5	758	C
36	5	765	C
36	5	766	U
36	5	767	U
36	5	776	U
36	5	777	U
36	5	780	A
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	855	U
36	5	861	C

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Mol	Chain	Res	Type
36	5	874	U
36	5	879	U
36	5	896	A
36	5	897	U
36	5	907	G
36	5	908	G
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	924	G
36	5	937	G
36	5	943	U
36	5	944	C
36	5	948	C
36	5	959	C
36	5	960	U
36	5	961	C
36	5	963	G
36	5	964	G
36	5	979	U
36	5	980	A
36	5	993	G
36	5	994	G
36	5	1000	C
36	5	1001	G
36	5	1002	A
36	5	1003	A
36	5	1006	A
36	5	1010	G
36	5	1014	U
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	1027	A
36	5	1028	U
36	5	1029	G

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Mol	Chain	Res	Type
36	5	1034	U
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1071	U
36	5	1072	G
36	5	1081	U
36	5	1082	U
36	5	1088	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	1131	G
36	5	1152	G
36	5	1153	A
36	5	1156	C
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	1191	U
36	5	1192	C
36	5	1193	A
36	5	1197	A
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

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Mol	Chain	Res	Type
36	5	1241	U
36	5	1242	G
36	5	1243	G
36	5	1245	A
36	5	1246	G
36	5	1252	A
36	5	1258	U
36	5	1259	A
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1268	G
36	5	1281	G
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1312	C
36	5	1313	G
36	5	1330	A
36	5	1332	A
36	5	1348	U
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1354	G
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1434	G
36	5	1437	C
36	5	1443	G
36	5	1446	A

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Mol	Chain	Res	Type
36	5	1450	G
36	5	1481	A
36	5	1482	A
36	5	1490	A
36	5	1495	U
36	5	1502	C
36	5	1503	A
36	5	1508	C
36	5	1519	G
36	5	1528	G
36	5	1536	G
36	5	1541	G
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	1565	G
36	5	1566	A
36	5	1567	U
36	5	1569	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	1580	A
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1589	A
36	5	1600	U
36	5	1601	U
36	5	1619	A
36	5	1620	U
36	5	1629	U
36	5	1632	A

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Mol	Chain	Res	Type
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1657	C
36	5	1683	A
36	5	1687	U
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1725	C
36	5	1741	A
36	5	1750	A
36	5	1751	G
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1767	C
36	5	1770	G
36	5	1780	G
36	5	1793	C
36	5	1794	G
36	5	1797	A
36	5	1809	A
36	5	1810	A
36	5	1813	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	1846	C
36	5	1847	A
36	5	1848	G
36	5	1849	C
36	5	1850	A

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Mol	Chain	Res	Type
36	5	1876	U
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1884	A
36	5	1893	A
36	5	1906	G
36	5	1908	A
36	5	1932	A
36	5	1935	G
36	5	1947	G
36	5	1953	G
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2110	G
36	5	2111	G
36	5	2112	U
36	5	2113	A
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2144	A
36	5	2158	A
36	5	2169	G
36	5	2170	U
36	5	2184	U
36	5	2187	G
36	5	2188	A
36	5	2198	A
36	5	2205	U
36	5	2210	G
36	5	2223	A
36	5	2225	U
36	5	2228	A
36	5	2229	A
36	5	2231	C
36	5	2244	A
36	5	2250	G
36	5	2253	G
36	5	2255	A
36	5	2256	A

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Mol	Chain	Res	Type
36	5	2257	C
36	5	2258	U
36	5	2273	G
36	5	2276	G
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	2298	U
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2334	U
36	5	2336	U
36	5	2366	C
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	2394	G
36	5	2397	A
36	5	2401	A
36	5	2403	G
36	5	2404	A
36	5	2411	U
36	5	2418	G
36	5	2435	G
36	5	2436	U
36	5	2437	G
36	5	2438	A
36	5	2439	A
36	5	2440	G
36	5	2441	A
36	5	2443	A
36	5	2504	U
36	5	2505	U

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Mol	Chain	Res	Type
36	5	2506	U
36	5	2507	C
36	5	2508	U
36	5	2511	A
36	5	2512	C
36	5	2514	U
36	5	2515	A
36	5	2518	C
36	5	2522	G
36	5	2523	A
36	5	2526	C
36	5	2530	G
36	5	2531	C
36	5	2532	U
36	5	2534	G
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2549	G
36	5	2552	C
36	5	2555	G
36	5	2562	A
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2571	U
36	5	2573	G
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2586	G
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2610	G
36	5	2614	G
36	5	2631	U
36	5	2637	A

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Mol	Chain	Res	Type
36	5	2639	G
36	5	2652	U
36	5	2656	A
36	5	2674	A
36	5	2677	G
36	5	2681	U
36	5	2683	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	2728	G
36	5	2729	U
36	5	2752	U
36	5	2753	G
36	5	2755	C
36	5	2762	A
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
36	5	2810	C
36	5	2814	G
36	5	2817	A
36	5	2818	U
36	5	2839	G
36	5	2840	C
36	5	2843	U
36	5	2845	A
36	5	2849	C
36	5	2853	A
36	5	2871	G
36	5	2872	A

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Mol	Chain	Res	Type
36	5	2874	G
36	5	2875	U
36	5	2887	A
36	5	2889	C
36	5	2896	A
36	5	2899	C
36	5	2902	A
36	5	2904	U
36	5	2912	G
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2947	G
36	5	2954	U
36	5	2957	G
36	5	2971	A
36	5	2972	G
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3092	C
36	5	3093	C
36	5	3102	G
36	5	3104	U
36	5	3119	U
36	5	3122	A
36	5	3123	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3153	U

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Mol	Chain	Res	Type
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3159	C
36	5	3164	C
36	5	3165	A
36	5	3168	A
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3178	A
36	5	3179	U
36	5	3180	A
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
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	3242	G
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	3270	U
36	5	3273	A
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3279	A
36	5	3280	U

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Mol	Chain	Res	Type
36	5	3281	U
36	5	3282	U
36	5	3285	C
36	5	3286	G
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3313	U
36	5	3315	G
36	5	3316	A
36	5	3317	U
36	5	3319	U
36	5	3330	A
36	5	3331	U
36	5	3332	U
36	5	3333	G
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	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	3394	U
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	33	U
37	7	51	A
37	7	54	U
37	7	58	C

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Mol	Chain	Res	Type
37	7	60	G
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	91	G
37	7	93	C
37	7	99	G
37	7	101	G
37	7	102	A
37	7	103	A
37	7	112	G
37	7	114	U
38	8	21	C
38	8	24	G
38	8	34	U
38	8	35	C
38	8	46	G
38	8	48	A
38	8	51	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	80	A
38	8	81	U
38	8	83	C
38	8	84	C
38	8	86	U
38	8	87	G
38	8	88	A
38	8	95	G
38	8	96	A
38	8	97	A
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A

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Mol	Chain	Res	Type
38	8	113	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	130	C
38	8	137	C
38	8	138	A
38	8	152	G
38	8	156	U
38	8	157	U
38	8	158	U

All (311) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	73	U
1	2	74	U
1	2	103	A
1	2	126	A
1	2	130	C
1	2	131	C
1	2	133	U
1	2	139	C
1	2	144	U
1	2	158	U
1	2	187	G
1	2	217	A
1	2	218	A
1	2	232	U
1	2	240	U
1	2	278	U
1	2	280	U
1	2	400	A
1	2	417	A
1	2	468	A
1	2	484	C
1	2	497	G
1	2	499	U
1	2	501	U

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Mol	Chain	Res	Type
1	2	503	G
1	2	512	A
1	2	555	A
1	2	558	U
1	2	582	U
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	734	A
1	2	755	A
1	2	781	U
1	2	782	U
1	2	794	U
1	2	811	A
1	2	815	G
1	2	829	A
1	2	913	G
1	2	1051	G
1	2	1058	U
1	2	1081	A
1	2	1150	G
1	2	1157	A
1	2	1196	A
1	2	1207	C
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	1481	C
1	2	1489	U
1	2	1490	C
1	2	1517	U
1	2	1568	C
1	2	1573	A
1	2	1600	A
1	2	1615	C
1	2	1657	U
1	2	1761	U
36	1	43	A

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Mol	Chain	Res	Type
36	1	65	A
36	1	169	U
36	1	210	U
36	1	223	U
36	1	239	G
36	1	282	G
36	1	283	G
36	1	397	A
36	1	547	G
36	1	588	G
36	1	594	U
36	1	620	U
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
36	1	1103	A
36	1	1196	C
36	1	1273	A
36	1	1307	G
36	1	1317	A
36	1	1329	U
36	1	1352	A
36	1	1355	A
36	1	1419	A
36	1	1484	U
36	1	1507	G
36	1	1554	U
36	1	1562	C
36	1	1716	U
36	1	1815	U
36	1	1816	A
36	1	1820	U
36	1	1841	A
36	1	1846	C

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Mol	Chain	Res	Type
36	1	1849	C
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2227	C
36	1	2281	A
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2418	G
36	1	2513	U
36	1	2522	G
36	1	2525	G
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2704	A
36	1	2728	G
36	1	2772	C
36	1	2801	A
36	1	2818	U
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3139	A
36	1	3169	U
36	1	3195	U
36	1	3207	U
36	1	3218	A
36	1	3228	C
36	1	3269	U
36	1	3275	U
36	1	3303	G
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
37	3	13	A
37	3	49	G

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Mol	Chain	Res	Type
37	3	52	G
37	3	86	U
38	4	82	U
38	4	85	G
38	4	111	A
38	4	125	U
1	6	25	C
1	6	66	U
1	6	76	A
1	6	103	A
1	6	114	C
1	6	136	C
1	6	139	C
1	6	145	A
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	272	U
1	6	280	U
1	6	400	A
1	6	417	A
1	6	512	A
1	6	542	A
1	6	543	C
1	6	555	A
1	6	557	G
1	6	558	U
1	6	651	G
1	6	667	U
1	6	678	A
1	6	697	C
1	6	717	C
1	6	755	A
1	6	811	A
1	6	829	A
1	6	834	G
1	6	914	G
1	6	1051	G
1	6	1058	U
1	6	1081	A

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Mol	Chain	Res	Type
1	6	1097	U
1	6	1137	A
1	6	1227	A
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	1535	U
1	6	1568	C
1	6	1573	A
1	6	1615	C
1	6	1620	C
1	6	1637	C
1	6	1657	U
1	6	1696	G
1	6	1698	G
1	6	1700	C
36	5	43	A
36	5	210	U
36	5	223	U
36	5	238	A
36	5	374	A
36	5	397	A
36	5	546	C
36	5	588	G
36	5	647	A
36	5	659	G
36	5	715	A
36	5	726	G
36	5	735	A
36	5	765	C
36	5	816	A
36	5	873	C
36	5	896	A
36	5	908	G
36	5	916	G
36	5	993	G
36	5	1027	A
36	5	1064	A

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Mol	Chain	Res	Type
36	5	1081	U
36	5	1152	G
36	5	1181	U
36	5	1192	C
36	5	1199	C
36	5	1236	G
36	5	1238	C
36	5	1241	U
36	5	1307	G
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1370	G
36	5	1392	G
36	5	1434	G
36	5	1481	A
36	5	1514	G
36	5	1554	U
36	5	1560	G
36	5	1580	A
36	5	1716	U
36	5	1815	U
36	5	1816	A
36	5	1819	U
36	5	1846	C
36	5	1849	C
36	5	1878	G
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	2257	C
36	5	2281	A
36	5	2372	A
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2531	C

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Mol	Chain	Res	Type
36	5	2539	C
36	5	2682	C
36	5	2714	G
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2817	A
36	5	2818	U
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	3195	U
36	5	3207	U
36	5	3218	A
36	5	3228	C
36	5	3259	U
36	5	3275	U
36	5	3289	G
36	5	3303	G
36	5	3330	A
36	5	3340	G
36	5	3341	U
36	5	3357	U
38	8	34	U
38	8	111	A
38	8	126	A

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2562 ligands modelled in this entry, 1427 are monoatomic - leaving 1135 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	2095	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	1	4153	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	0,6,6	0.00	-	-		
86	OHX	2	2179	-	0,6,6	0.00	-	-		
86	OHX	2	2172	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	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	2121	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	L3	404	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		
88	HMT	1	4217	-	40,43,43	1.09	1 (2%)	41,66,66	0.75	2 (4%)
86	OHX	5	3901	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		
86	OHX	6	2085	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	0,6,6	0.00	-	-		
86	OHX	5	4225	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	1	3871	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	o2	201	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	1	4208	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	5	3942	-	0,6,6	0.00	-	-		
86	OHX	6	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	4014	-	0,6,6	0.00	-	-		
86	OHX	d4	201	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	O7	105	-	0,6,6	0.00	-	-		
86	OHX	s9	202	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	0,6,6	0.00	-	-		
86	OHX	5	4198	-	0,6,6	0.00	-	-		
86	OHX	5	3952	-	0,6,6	0.00	-	-		
86	OHX	5	4235	-	0,6,6	0.00	-	-		
86	OHX	6	2093	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	s1	302	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	1	4037	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	1	4115	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	5	4246	-	0,6,6	0.00	-	-		
86	OHX	l3	404	-	0,6,6	0.00	-	-		
86	OHX	m5	301	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	5	4252	-	0,6,6	0.00	-	-		
86	OHX	1	4004	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		
86	OHX	5	4248	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	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	3966	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	1	4116	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	5	4125	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	0,6,6	0.00	-	-		
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	1	3867	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	Q2	502	-	0,6,6	0.00	-	-		
86	OHX	5	4016	-	0,6,6	0.00	-	-		
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		
86	OHX	8	216	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	6	2105	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	7	217	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	2	2035	-	0,6,6	0.00	-	-		
86	OHX	5	4073	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	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	2122	-	0,6,6	0.00	-	-		
86	OHX	1	4156	-	0,6,6	0.00	-	-		
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	5	4232	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	O2	202	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	0,6,6	0.00	-	-		
86	OHX	2	2180	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		
86	OHX	1	3929	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	1	4150	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	m7	206	-	0,6,6	0.00	-	-		
86	OHX	8	229	-	0,6,6	0.00	-	-		
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	1	4191	-	0,6,6	0.00	-	-		
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	2	2163	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	5	3998	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	4	234	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	l3	406	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	1	4210	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	1	3884	-	0,6,6	0.00	-	-		
86	OHX	1	4019	-	0,6,6	0.00	-	-		
86	OHX	5	4250	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	1	4213	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	6	2205	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	8	230	-	0,6,6	0.00	-	-		
86	OHX	M7	207	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	o7	503	-	0,6,6	0.00	-	-		
86	OHX	5	4195	-	0,6,6	0.00	-	-		
86	OHX	L3	405	-	0,6,6	0.00	-	-		
86	OHX	5	4149	-	0,6,6	0.00	-	-		
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	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	2178	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	2	2028	-	0,6,6	0.00	-	-		
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	2	2106	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	5	4092	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	14	402	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	0,6,6	0.00	-	-		
86	OHX	2	2032	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	1	3873	-	0,6,6	0.00	-	-		
86	OHX	5	4178	-	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	2	2170	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	6	2145	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	5	4239	-	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	4038	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	M5	303	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	1	4091	-	0,6,6	0.00	-	-		
86	OHX	5	4131	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	5	4126	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	6	2135	-	0,6,6	0.00	-	-		
86	OHX	6	2198	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	n3	203	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	0,6,6	0.00	-	-		
86	OHX	5	3944	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	2	2054	-	0,6,6	0.00	-	-		
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	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	4010	-	0,6,6	0.00	-	-		
86	OHX	5	4132	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	5	3982	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	1	3886	-	0,6,6	0.00	-	-		
86	OHX	6	2202	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	6	2191	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	1	4009	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	1	4183	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	6	2163	-	0,6,6	0.00	-	-		
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	1	4180	-	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	4065	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
86	OHX	C8	202	-	0,6,6	0.00	-	-		
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		
86	OHX	5	3917	-	0,6,6	0.00	-	-		
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	5	4089	-	0,6,6	0.00	-	-		
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	2	2111	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	s8	303	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	1	4020	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	m8	201	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	n3	204	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	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	3917	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	0,6,6	0.00	-	-		
86	OHX	C3	201	-	0,6,6	0.00	-	-		
86	OHX	4	238	-	0,6,6	0.00	-	-		
86	OHX	1	4086	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		
86	OHX	m6	203	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		
86	OHX	1	3874	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	l3	405	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	1	4114	-	0,6,6	0.00	-	-		
86	OHX	s4	302	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	5	4142	-	0,6,6	0.00	-	-		
86	OHX	4	228	-	0,6,6	0.00	-	-		
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	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	3924	-	0,6,6	0.00	-	-		
86	OHX	5	4254	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	1	3898	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	1	4100	-	0,6,6	0.00	-	-		
86	OHX	5	4211	-	0,6,6	0.00	-	-		
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	1	4082	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	5	3995	-	0,6,6	0.00	-	-		
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	5	4234	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		
86	OHX	m0	303	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
86	OHX	1	4084	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		
86	OHX	2	2023	-	0,6,6	0.00	-	-		
86	OHX	1	4175	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		
86	OHX	5	3945	86	0,6,6	0.00	-	-		
86	OHX	3	214	-	0,6,6	0.00	-	-		
86	OHX	6	2174	-	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	2142	-	0,6,6	0.00	-	-		
86	OHX	2	2056	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	0,6,6	0.00	-	-		
86	OHX	5	4055	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	1	4216	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	1	3947	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	1	3986	-	0,6,6	0.00	-	-		
86	OHX	1	4200	-	0,6,6	0.00	-	-		
86	OHX	6	2050	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	M7	206	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	2	2073	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		
86	OHX	5	4208	-	0,6,6	0.00	-	-		
86	OHX	1	4063	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		
86	OHX	1	4158	-	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	2151	-	0,6,6	0.00	-	-		
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	5	4241	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	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	3978	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	2	2039	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	5	4175	-	0,6,6	0.00	-	-		
86	OHX	1	3998	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	5	4096	-	0,6,6	0.00	-	-		
86	OHX	2	2144	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	5	4122	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	5	4236	86	0,6,6	0.00	-	-		
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	1	3967	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	1	4214	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	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	4160	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	6	2195	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	5	4253	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	6	2075	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	0,6,6	0.00	-	-		
86	OHX	1	4211	-	0,6,6	0.00	-	-		
86	OHX	1	4206	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		
86	OHX	1	3928	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	0,6,6	0.00	-	-		
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	1	3997	-	0,6,6	0.00	-	-		
86	OHX	N9	101	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	6	2068	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	5	4097	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	2	2138	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	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	4098	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	5	4251	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		
86	OHX	4	224	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		
86	OHX	c3	201	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	2	2102	-	0,6,6	0.00	-	-		
86	OHX	2	2022	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	5	3909	-	0,6,6	0.00	-	-		
86	OHX	1	4168	-	0,6,6	0.00	-	-		
86	OHX	1	3869	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	L4	402	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	5	4023	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	1	4085	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	8	218	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		
86	OHX	m4	201	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	6	2203	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	6	2123	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	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	4168	-	0,6,6	0.00	-	-		
86	OHX	2	2047	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	2	2126	-	0,6,6	0.00	-	-		
86	OHX	5	4047	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	5	4247	-	0,6,6	0.00	-	-		
86	OHX	1	4083	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	3	222	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	1	4138	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	5	4214	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	1	4109	-	0,6,6	0.00	-	-		
86	OHX	1	4151	-	0,6,6	0.00	-	-		
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		
86	OHX	o3	203	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	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	4028	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	6	2184	-	0,6,6	0.00	-	-		
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		
86	OHX	1	3872	-	0,6,6	0.00	-	-		
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	5	3972	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	1	3868	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	4	225	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	1	4000	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	1	4012	-	0,6,6	0.00	-	-		
86	OHX	5	3962	-	0,6,6	0.00	-	-		
86	OHX	5	3911	-	0,6,6	0.00	-	-		
86	OHX	6	2177	-	0,6,6	0.00	-	-		
86	OHX	M8	201	-	0,6,6	0.00	-	-		
86	OHX	6	2073	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	N1	201	-	0,6,6	0.00	-	-		
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	0,6,6	0.00	-	-		
86	OHX	5	4107	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	1	4186	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	2	2024	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	2	2096	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	5	4249	-	0,6,6	0.00	-	-		
86	OHX	5	4026	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	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	4100	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
86	OHX	m1	203	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	1	3900	-	0,6,6	0.00	-	-		
86	OHX	2	2176	-	0,6,6	0.00	-	-		
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	6	2206	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	6	2196	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	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	4120	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	15	304	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	1	3870	-	0,6,6	0.00	-	-		
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	1	4061	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	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	1	4073	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	5	4045	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	1	4035	-	0,6,6	0.00	-	-		
86	OHX	6	2089	-	0,6,6	0.00	-	-		
86	OHX	5	4226	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	5	4076	-	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	2054	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	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	3955	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	6	2048	-	0,6,6	0.00	-	-		
86	OHX	5	3999	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	1	4007	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	1	3889	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	5	4036	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	1	4053	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	5	4154	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	8	219	-	0,6,6	0.00	-	-		
86	OHX	4	236	-	0,6,6	0.00	-	-		
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		
86	OHX	5	4057	-	0,6,6	0.00	-	-		
86	OHX	1	4072	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		
86	OHX	O3	202	-	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	2175	-	0,6,6	0.00	-	-		
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	4	237	-	0,6,6	0.00	-	-		
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	8	217	-	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	3913	-	0,6,6	0.00	-	-		
86	OHX	2	2080	-	0,6,6	0.00	-	-		
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	2	2147	-	0,6,6	0.00	-	-		
86	OHX	5	3904	-	0,6,6	0.00	-	-		
86	OHX	5	3915	-	0,6,6	0.00	-	-		
86	OHX	M9	203	-	0,6,6	0.00	-	-		
86	OHX	2	2134	-	0,6,6	0.00	-	-		
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	3	217	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	6	2082	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		
86	OHX	1	4081	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	5	4153	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	7	228	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	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	2139	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	5	4018	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	1	4215	-	0,6,6	0.00	-	-		
86	OHX	1	4170	-	0,6,6	0.00	-	-		
86	OHX	5	4003	-	0,6,6	0.00	-	-		
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	1	3957	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	1	4207	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	2	2123	-	0,6,6	0.00	-	-		
86	OHX	1	3942	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	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	222	-	0,6,6	0.00	-	-		
86	OHX	1	4052	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	M0	304	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	5	4161	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	5	4228	-	0,6,6	0.00	-	-		
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	5	4217	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		
86	OHX	5	4222	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	2	2087	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	2	2149	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	1	4087	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		
86	OHX	5	4167	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	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	2046	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	3	215	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		
86	OHX	1	4212	-	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	5	4024	-	0,6,6	0.00	-	-		
86	OHX	1	4045	-	0,6,6	0.00	-	-		
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	6	2181	-	0,6,6	0.00	-	-		
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	0,6,6	0.00	-	-		
86	OHX	7	219	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	6	2187	-	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	1	4025	-	0,6,6	0.00	-	-		
86	OHX	15	303	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	6	2137	-	0,6,6	0.00	-	-		
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	c8	201	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	1	4014	-	0,6,6	0.00	-	-		
86	OHX	1	3885	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	n9	101	-	0,6,6	0.00	-	-		
86	OHX	l9	202	-	0,6,6	0.00	-	-		
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	1	4023	-	0,6,6	0.00	-	-		
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	o9	101	-	0,6,6	0.00	-	-		
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	6	2204	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	5	4151	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	6	2074	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		
86	OHX	l5	302	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	0,6,6	0.00	-	-		
86	OHX	5	4124	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	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	4127	-	0,6,6	0.00	-	-		
86	OHX	O7	104	-	0,6,6	0.00	-	-		
86	OHX	1	4145	-	0,6,6	0.00	-	-		
86	OHX	5	3941	-	0,6,6	0.00	-	-		
88	HMT	5	4255	-	40,43,43	0.55	0	41,66,66	0.77	2 (4%)
86	OHX	5	4227	-	0,6,6	0.00	-	-		
86	OHX	2	2094	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		
86	OHX	2	2041	-	0,6,6	0.00	-	-		
86	OHX	1	4008	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	1	4209	-	0,6,6	0.00	-	-		
86	OHX	1	3920	-	0,6,6	0.00	-	-		
86	OHX	O9	101	-	0,6,6	0.00	-	-		
86	OHX	1	4165	-	0,6,6	0.00	-	-		
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	5	3996	-	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	HMT	5	4255	-	-	4/27/74/74	0/5/5/5
88	HMT	1	4217	-	-	8/27/74/74	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4217	HMT	C4-C3	-5.87	1.46	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	5	4255	HMT	C25-C26-C27	-2.37	106.74	115.75
88	1	4217	HMT	C20-C21-C22	2.26	121.06	114.09
88	5	4255	HMT	C18-O3-C2	-2.24	112.77	116.52
88	1	4217	HMT	C8-C7-C6	-2.01	109.13	114.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

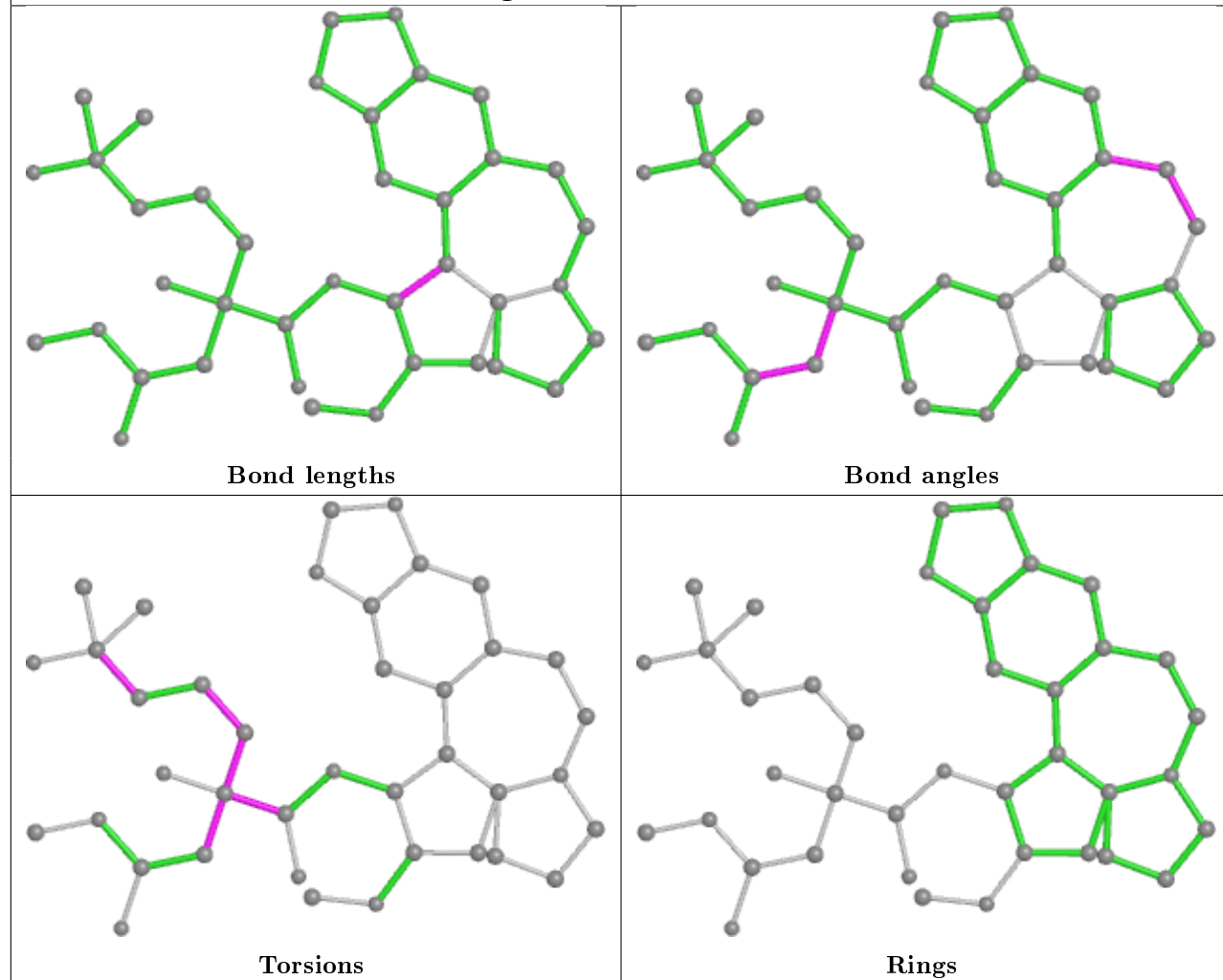
Mol	Chain	Res	Type	Atoms
88	1	4217	HMT	C19-C20-C24-C25
88	1	4217	HMT	C21-C20-C24-C25
88	1	4217	HMT	O6-C20-C24-C25
88	5	4255	HMT	C25-C26-C27-O9
88	1	4217	HMT	C20-C24-C25-C26
88	5	4255	HMT	C25-C26-C27-C28
88	1	4217	HMT	C25-C26-C27-C28
88	5	4255	HMT	C24-C25-C26-C27
88	5	4255	HMT	C25-C26-C27-C29
88	1	4217	HMT	C19-C20-C21-C22
88	1	4217	HMT	C25-C26-C27-O9
88	1	4217	HMT	O4-C19-C20-C21

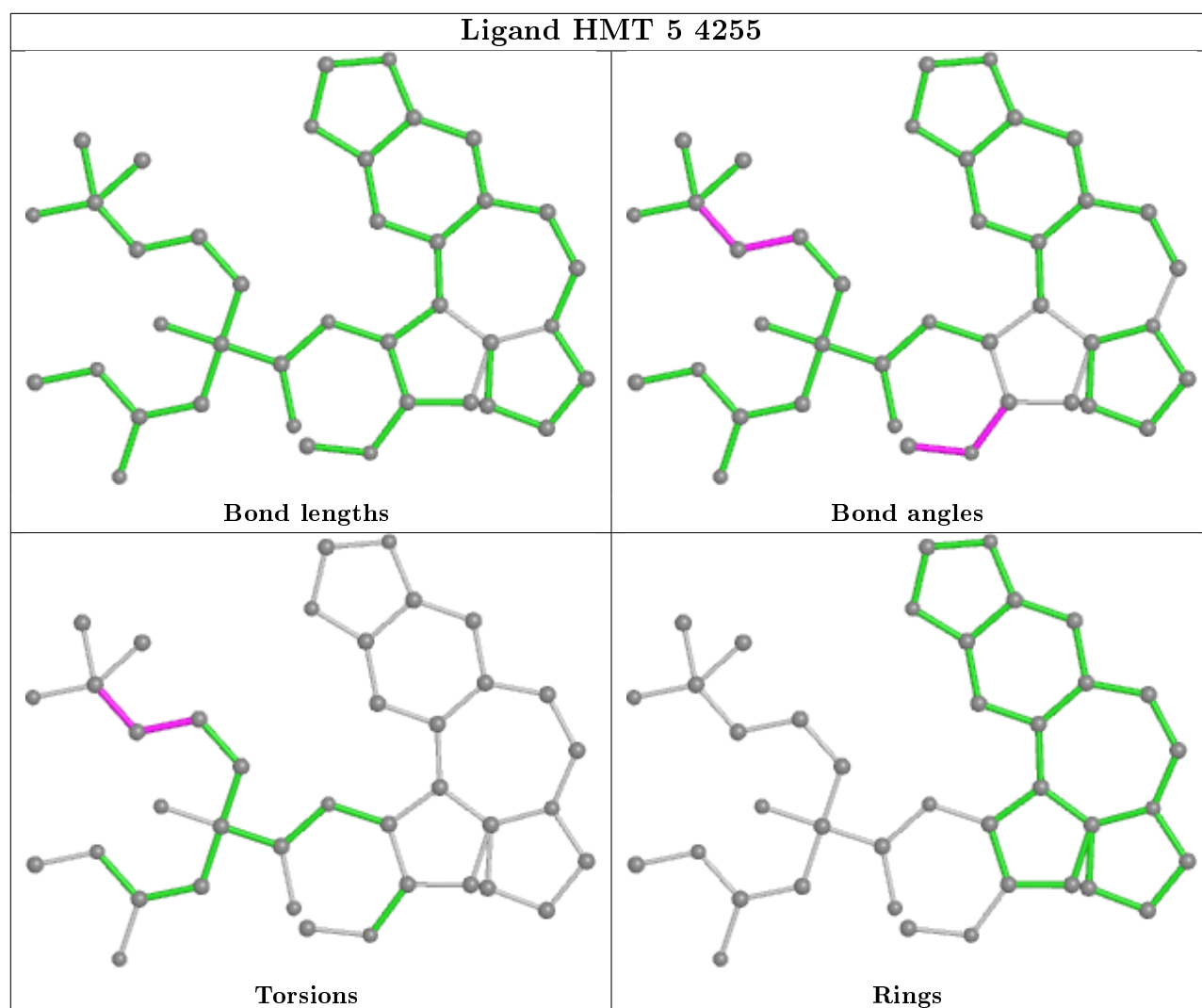
There are no ring outliers.

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.

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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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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