



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 07:52 PM BST

PDB ID : 4U55
Title : Crystal structure of Cryptopleurine bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.20 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

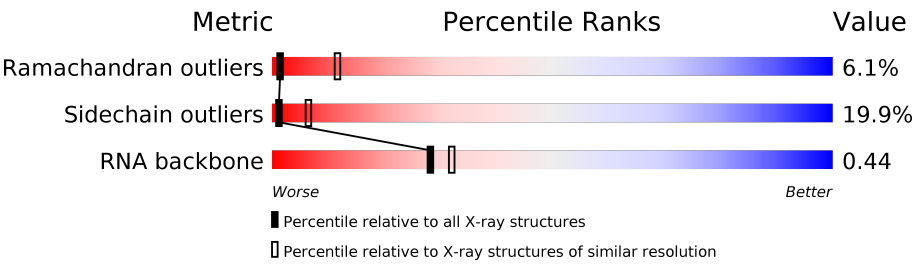
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)















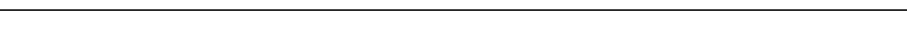




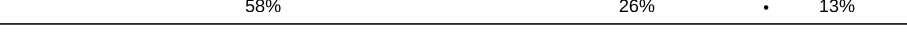





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	<div><div>62%</div><div>30%</div><div>6%</div><div>.</div></div>
1	6	1800	<div><div>64%</div><div>31%</div><div>5%</div></div>
2	S0	251	<div><div>65%</div><div>17%</div><div>.</div><div>18%</div></div>
2	s0	251	<div><div>62%</div><div>18%</div><div>.</div><div>18%</div></div>
3	S1	254	<div><div>60%</div><div>22%</div><div>.</div><div>16%</div></div>
3	s1	254	<div><div>66%</div><div>18%</div><div>.</div><div>15%</div></div>
4	S2	253	<div><div>68%</div><div>16%</div><div>.</div><div>14%</div></div>
4	s2	253	<div><div>63%</div><div>21%</div><div>.</div><div>14%</div></div>















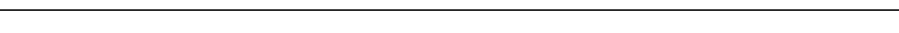




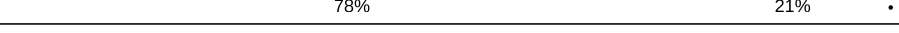
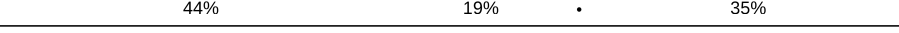




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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3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










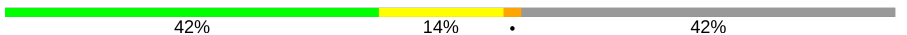

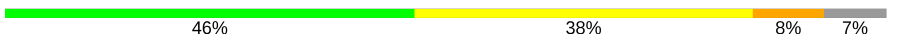
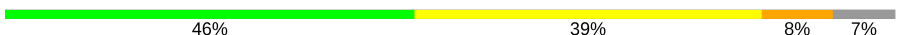












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Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107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















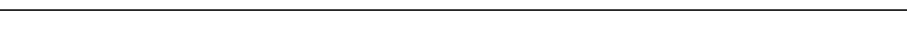




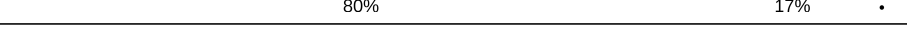





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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	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	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	

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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	p0	311	<div><div></div><div>38%8%54%</div></div>
82	m2	160	<div><div></div><div>93%6%</div></div>
83	p1	47	<div><div></div><div>100%</div></div>
84	p2	46	<div><div></div><div>100%</div></div>

2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			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			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			679	402	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	13	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	14	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	15	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	16	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	17	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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			
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			
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 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	p0	143	Total	C	N	O	S	0	0	0
			1076	686	192	195	3			

- Molecule 82 is a protein called Unknown protein chain m2.

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

- 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	3	Total	Mg	0	0
			3	3		
85	m6	1	Total	Mg	0	0
			1	1		
85	n8	4	Total	Mg	0	0
			4	4		
85	q3	1	Total	Mg	0	0
			1	1		
85	o1	1	Total	Mg	0	0
			1	1		
85	N5	1	Total	Mg	0	0
			1	1		
85	6	148	Total	Mg	0	0
			148	148		
85	sM	2	Total	Mg	0	0
			2	2		
85	O4	1	Total	Mg	0	0
			1	1		
85	m5	2	Total	Mg	0	0
			2	2		
85	l3	1	Total	Mg	0	0
			1	1		
85	M1	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	d6	1	Total 1	Mg 1	0	0
85	2	125	Total 125	Mg 125	0	0
85	n0	2	Total 2	Mg 2	0	0
85	L4	1	Total 1	Mg 1	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	1	Total 1	Mg 1	0	0
85	c9	1	Total 1	Mg 1	0	0
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	o4	2	Total 2	Mg 2	0	0
85	M9	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	M0	3	Total 3	Mg 3	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	505	Total 505	Mg 505	0	0
85	L5	2	Total 2	Mg 2	0	0
85	O7	3	Total 3	Mg 3	0	0
85	s6	1	Total 1	Mg 1	0	0
85	Q2	1	Total 1	Mg 1	0	0

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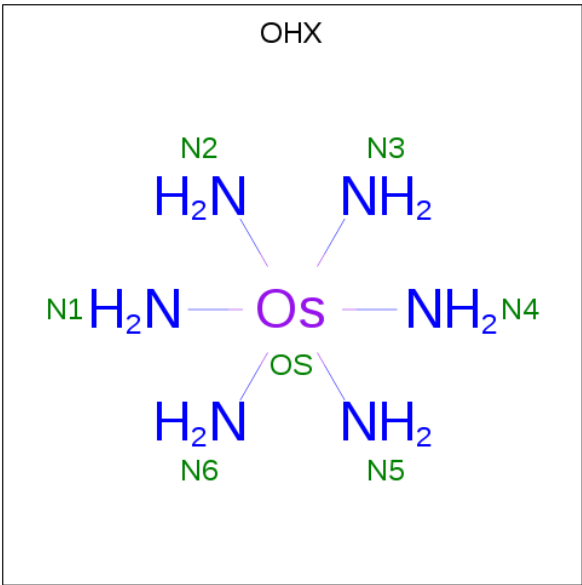
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	d4	1	Total 1	Mg 1	0	0
85	n9	1	Total 1	Mg 1	0	0
85	1	469	Total 469	Mg 469	0	0
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	1	Total 1	Mg 1	0	0
85	O2	1	Total 1	Mg 1	0	0
85	o7	1	Total 1	Mg 1	0	0
85	o3	1	Total 1	Mg 1	0	0
85	d3	1	Total 1	Mg 1	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	2	Total 2	Mg 2	0	0
85	4	21	Total 21	Mg 21	0	0
85	n6	1	Total 1	Mg 1	0	0
85	S4	1	Total 1	Mg 1	0	0
85	L2	1	Total 1	Mg 1	0	0
85	m1	1	Total 1	Mg 1	0	0
85	l5	2	Total 2	Mg 2	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	5	Total 5	Mg 5	0	0
85	N8	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	s1	1	Total 1	Mg 1	0	0
85	l9	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
85	7	17	Total 17	Mg 17	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	3	Total 3	Mg 3	0	0
85	O5	1	Total 1	Mg 1	0	0
85	N6	2	Total 2	Mg 2	0	0
85	8	14	Total 14	Mg 14	0	0
85	l4	1	Total 1	Mg 1	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0
85	m0	1	Total 1	Mg 1	0	0
85	3	14	Total 14	Mg 14	0	0

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



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		

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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		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	C1	1	Total	N	Os	0	0
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86	C3	1	Total	N	Os	0	0
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86	C5	1	Total	N	Os	0	0
			7	6	1		
86	C8	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	SR	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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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	L4	1	Total	N	Os	0	0
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86	M5	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M9	1	Total	N	Os	0	0
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86	N9	1	Total	N	Os	0	0
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86	O2	1	Total	N	Os	0	0
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86	O9	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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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	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	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		

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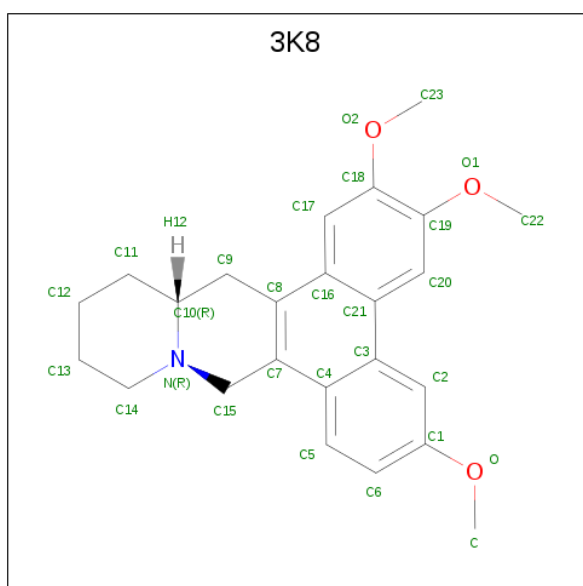
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
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	m9	1	Total	N	Os	0	0
			7	6	1		
86	n1	1	Total	N	Os	0	0
			7	6	1		

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

- Molecule 87 is (14aR)-2,3,6-trimethoxy-11,12,13,14,14a,15-hexahydro-9H-dibenzo[f,h]pyrido [1,2-b]isoquinoline (three-letter code: 3K8) (formula: C₂₄H₂₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
87	2	1	Total	C	N	O	0	0
			28	24	1	3		
87	6	1	Total	C	N	O	0	0
			28	24	1	3		

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	q0	1	Total	Zn	0	0
			1	1		
88	D6	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		

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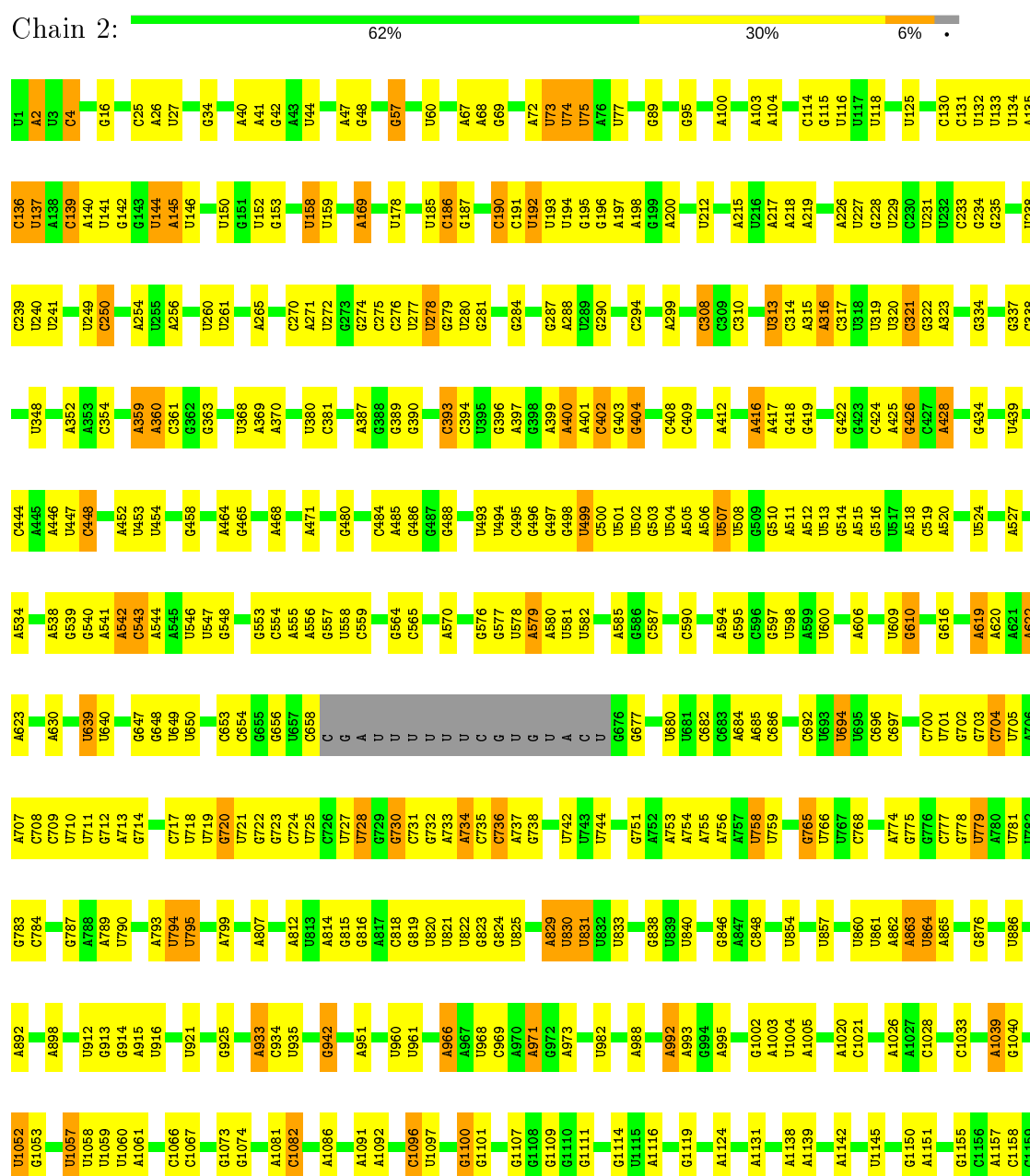
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	e1	1	Total 1	Zn 1	0	0
88	Q3	1	Total 1	Zn 1	0	0
88	D9	1	Total 1	Zn 1	0	0
88	E1	1	Total 1	Zn 1	0	0
88	Q0	1	Total 1	Zn 1	0	0
88	d7	1	Total 1	Zn 1	0	0
88	q3	1	Total 1	Zn 1	0	0
88	d9	1	Total 1	Zn 1	0	0
88	D7	1	Total 1	Zn 1	0	0
88	d6	1	Total 1	Zn 1	0	0
88	o7	1	Total 1	Zn 1	0	0
88	O7	1	Total 1	Zn 1	0	0
88	q2	1	Total 1	Zn 1	0	0

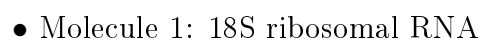
3 Residue-property plots

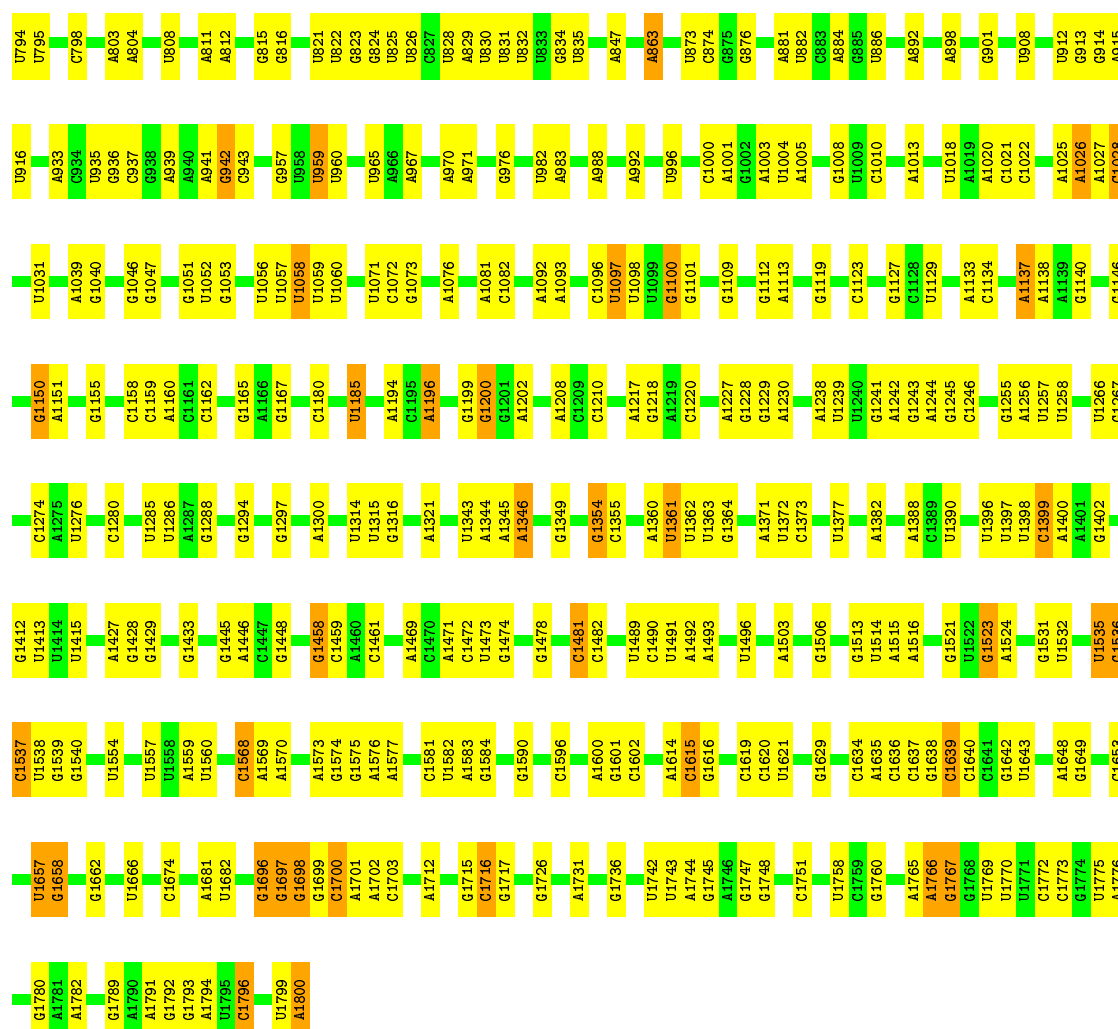
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

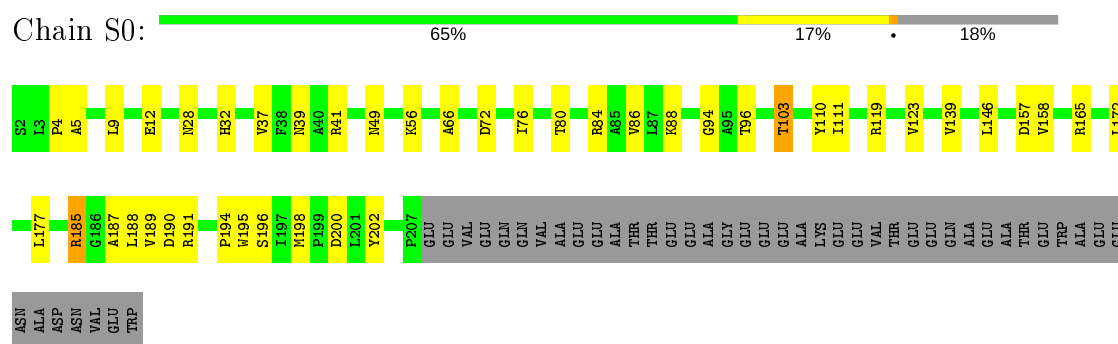
- Molecule 1: 18S ribosomal RNA



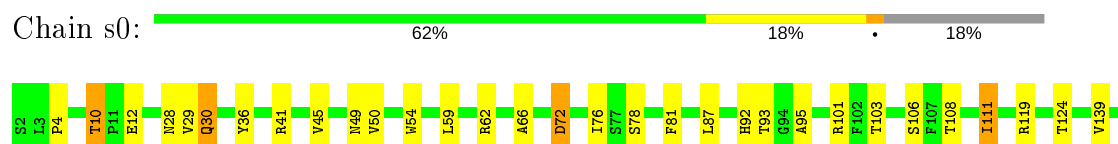


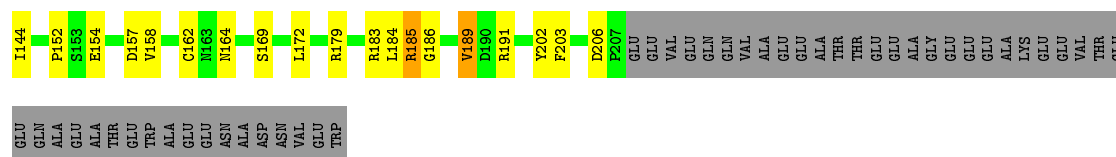


- Molecule 2: 40S ribosomal protein S0-A

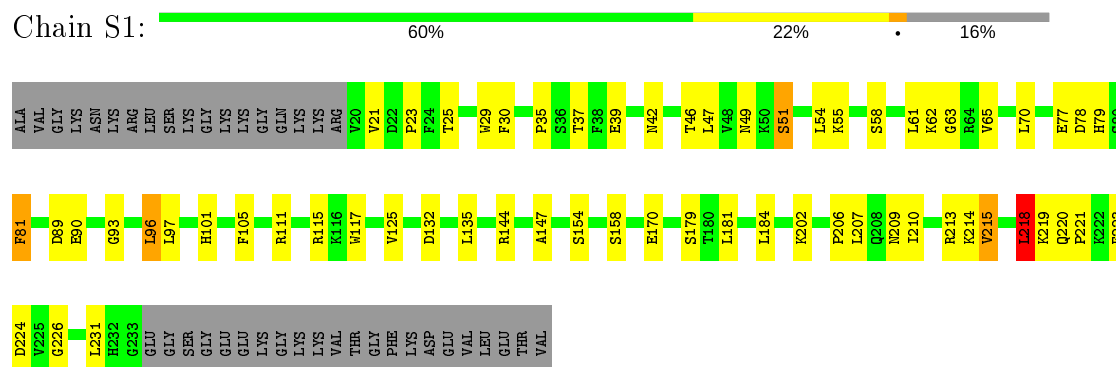


- Molecule 2: 40S ribosomal protein S0-A

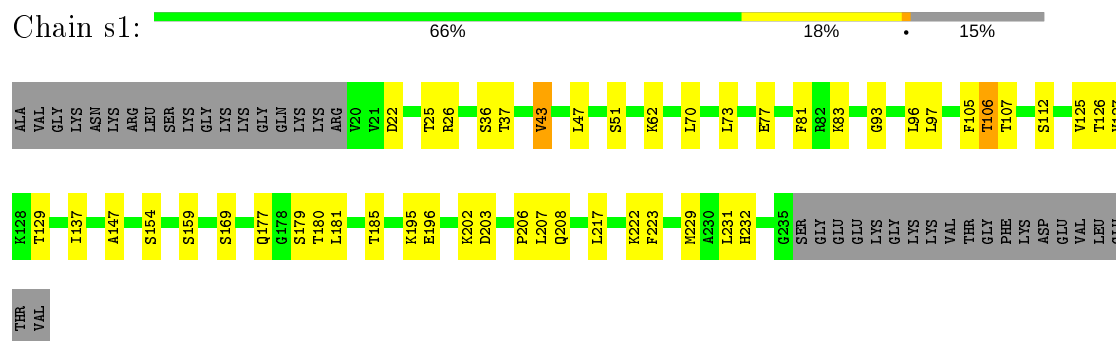




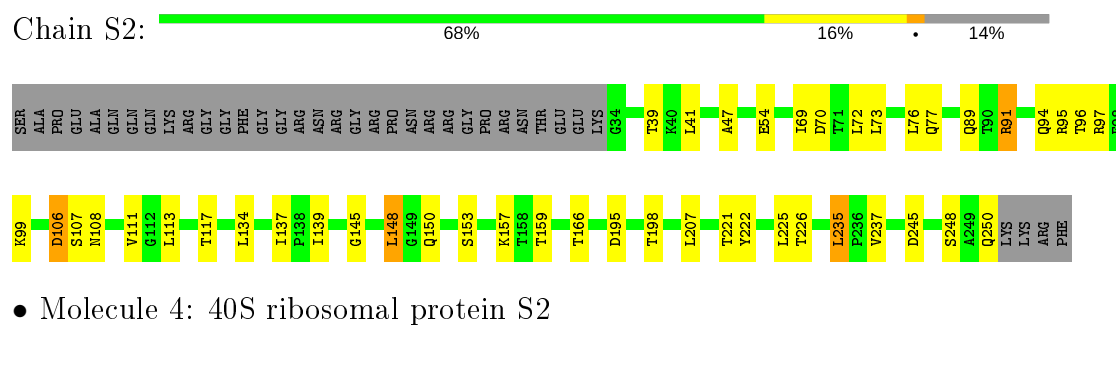
• Molecule 3: 40S ribosomal protein S1-A



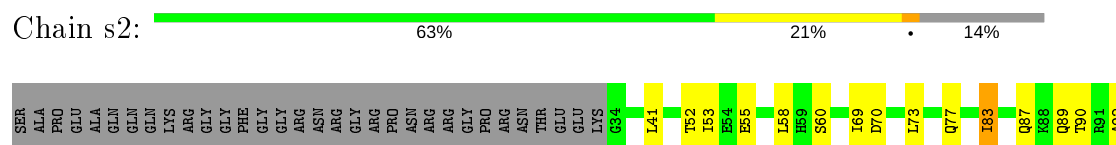
• Molecule 3: 40S ribosomal protein S1-A

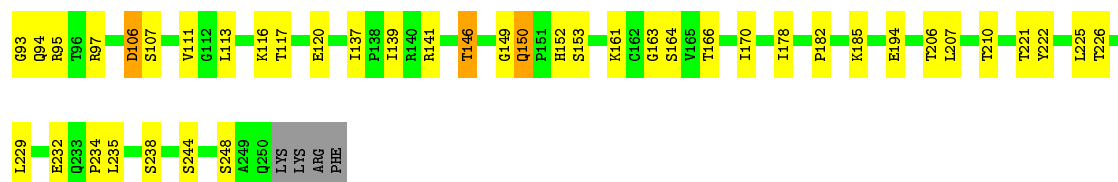


• Molecule 4: 40S ribosomal protein S2



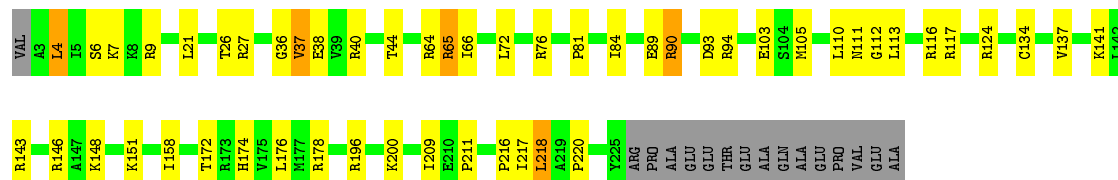
• Molecule 4: 40S ribosomal protein S2





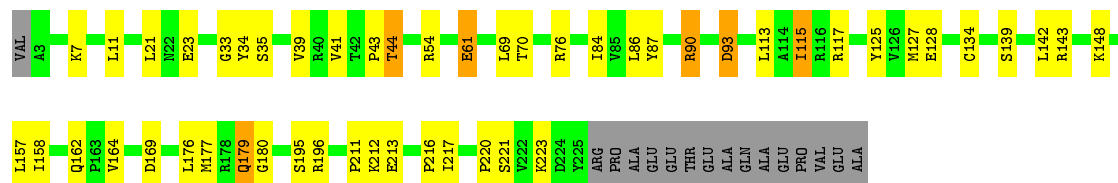
- Molecule 5: 40S ribosomal protein S3

Chain S3: 72% 20% 7%



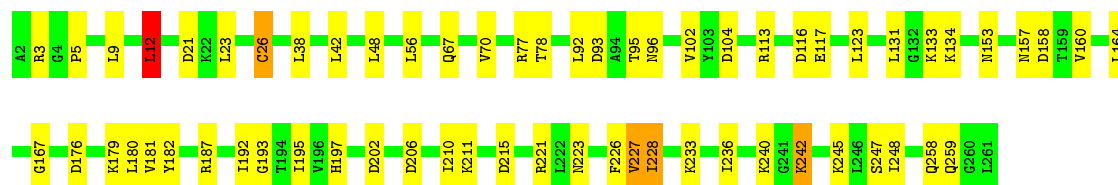
- Molecule 5: 40S ribosomal protein S3

Chain s3: 72% 19% 7%



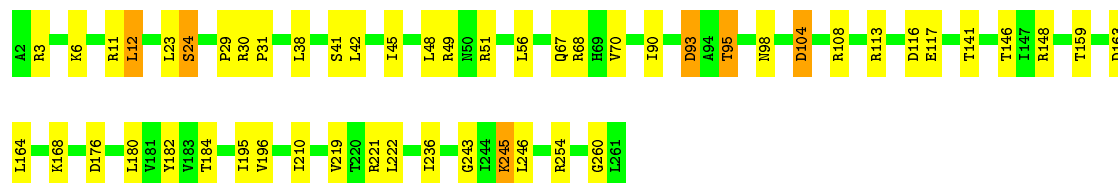
- Molecule 6: 40S ribosomal protein S4-A

Chain S4: 76% 22% 2%



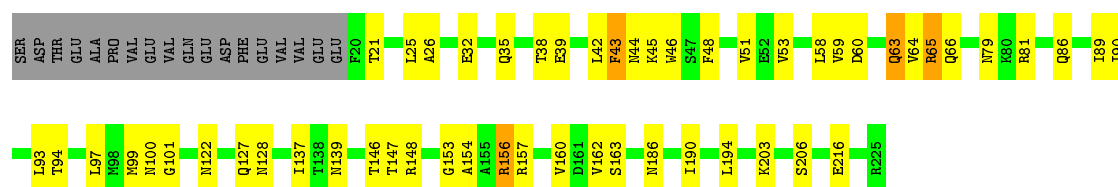
- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 80% 18% 2%



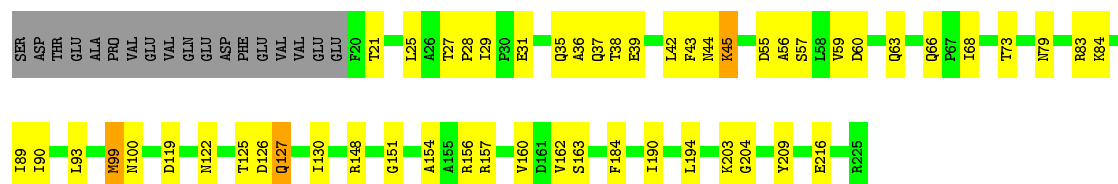
- Molecule 7: 40S ribosomal protein S5

Chain S5: 68% 22% 8%



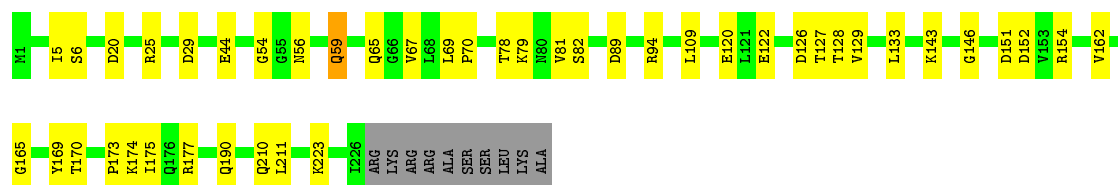
• Molecule 7: 40S ribosomal protein S5

Chain s5: 68% 22% 8%



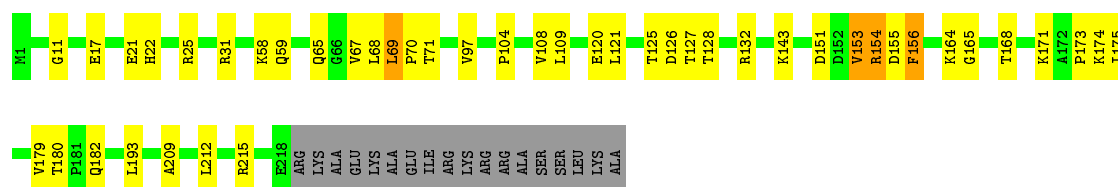
• Molecule 8: 40S ribosomal protein S6-A

Chain S6: 77% 18% 5%



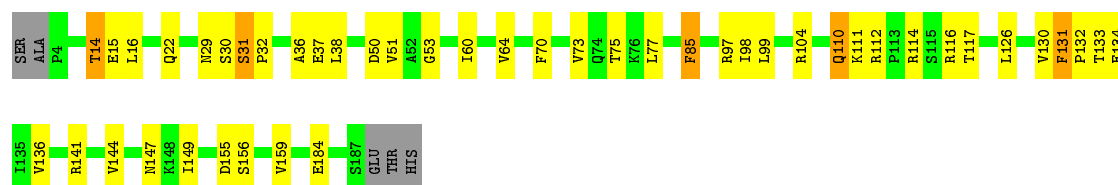
• Molecule 8: 40S ribosomal protein S6-A

Chain s6: 73% 17% 8%



• Molecule 9: 40S ribosomal protein S7-A

Chain S7: 73% 22% 5%



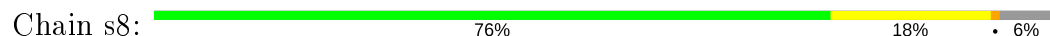
• Molecule 9: 40S ribosomal protein S7-A

Chain s7: 79% 17% 4%

- Molecule 10: 40S ribosomal protein S8-A



- Molecule 10: 40S ribosomal protein S8-A



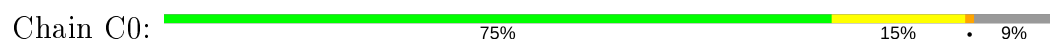
- Molecule 11: 40S ribosomal protein S9-A



- Molecule 11: 40S ribosomal protein S9-A

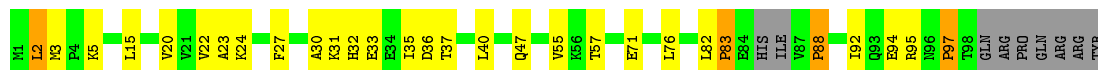


- Molecule 12: 40S ribosomal protein S10-A

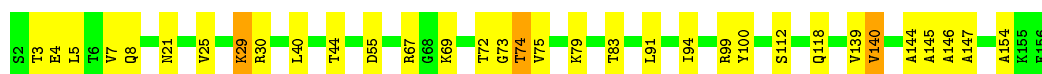
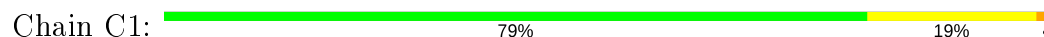




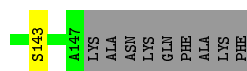
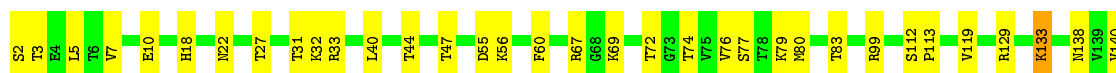
- Molecule 12: 40S ribosomal protein S10-A



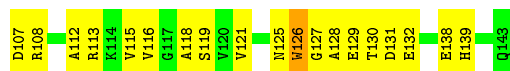
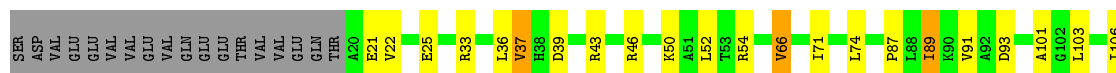
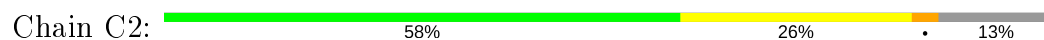
- Molecule 13: 40S ribosomal protein S11-A



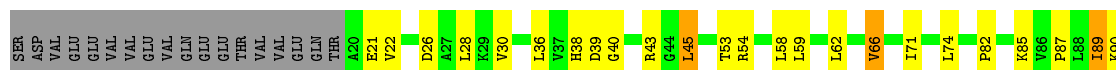
- Molecule 13: 40S ribosomal protein S11-A



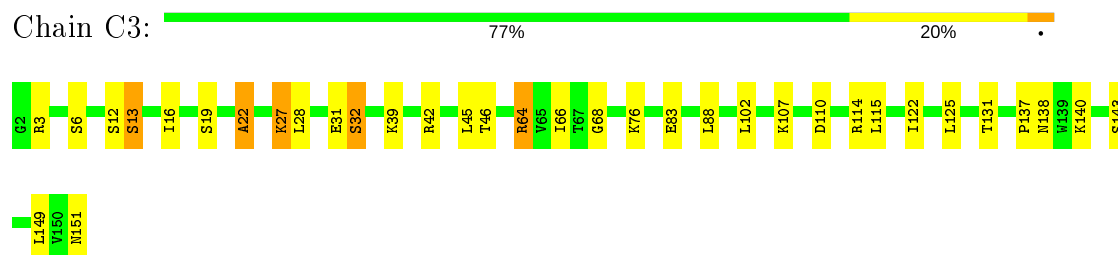
- Molecule 14: 40S ribosomal protein S12



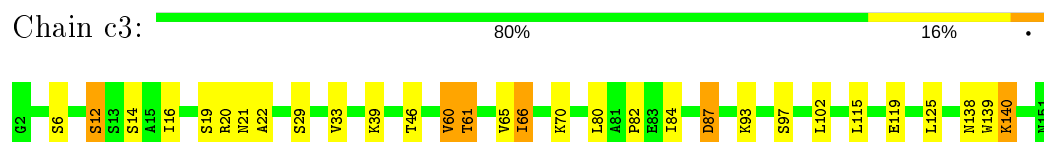
- Molecule 14: 40S ribosomal protein S12



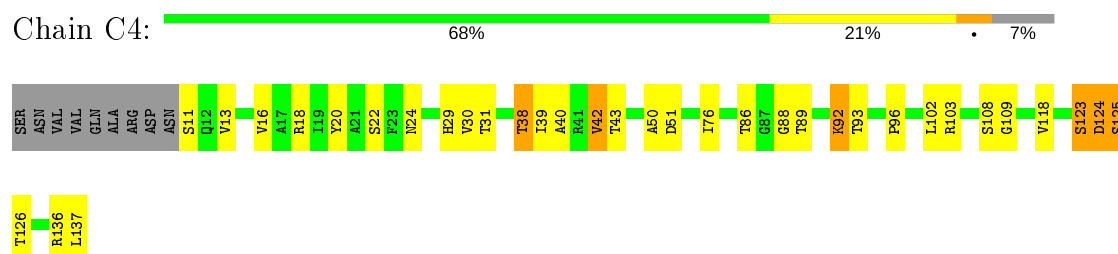
- Molecule 15: 40S ribosomal protein S13



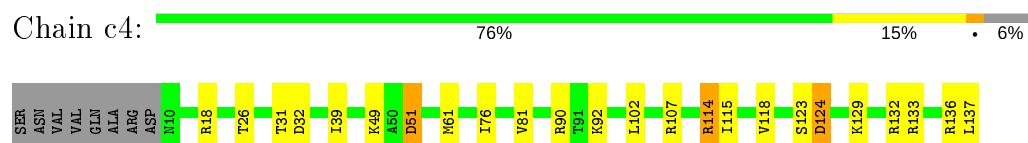
- Molecule 15: 40S ribosomal protein S13



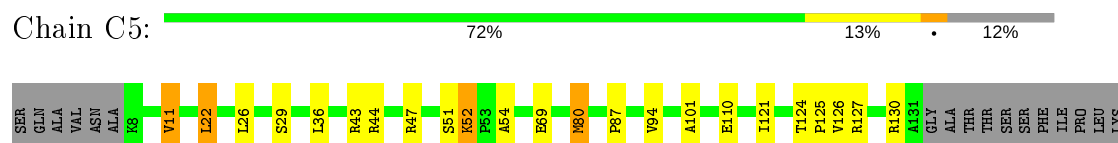
- Molecule 16: 40S ribosomal protein S14-A



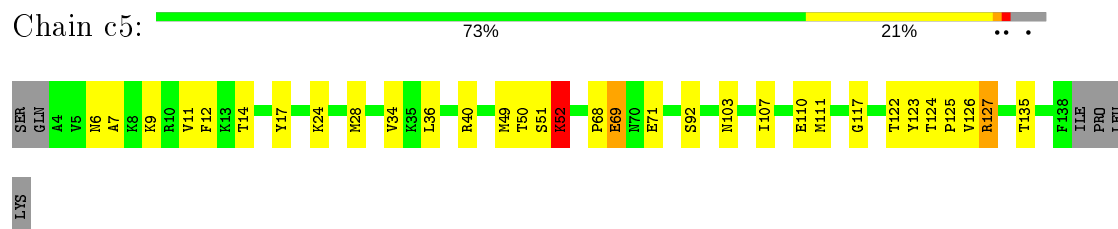
- Molecule 16: 40S ribosomal protein S14-A




- Molecule 17: 40S ribosomal protein S15

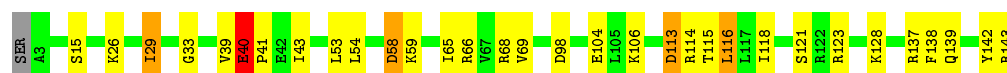


- Molecule 17: 40S ribosomal protein S15




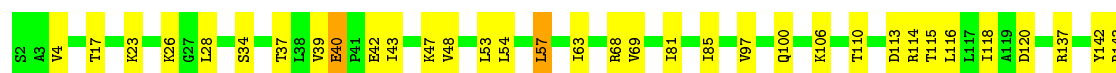
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:  77% 19% ..



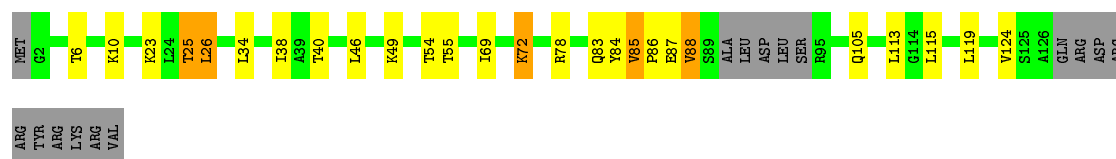
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:  76% 23% .



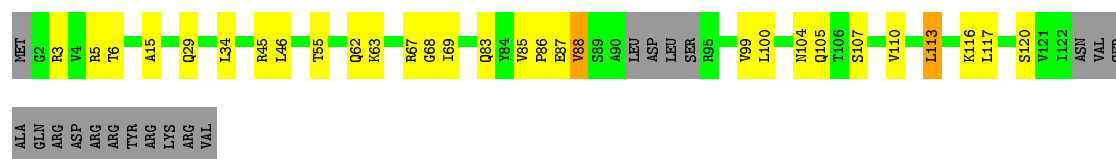
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:  69% 15% . 12%



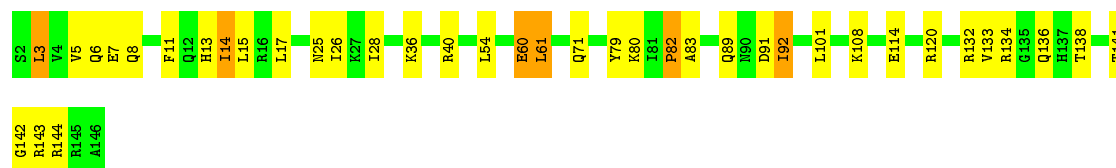
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:  65% 20% . 14%



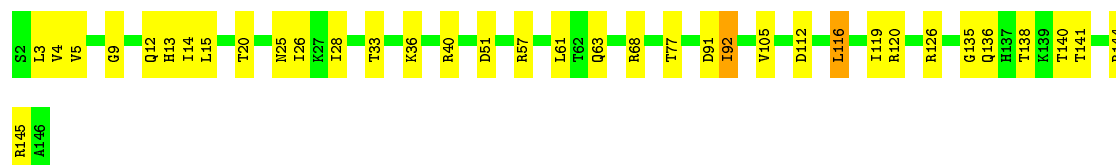
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:  73% 23% .

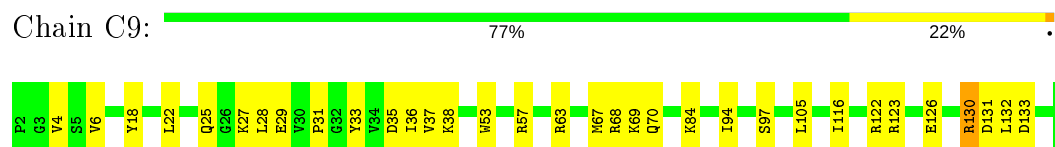


- Molecule 20: 40S ribosomal protein S18-A

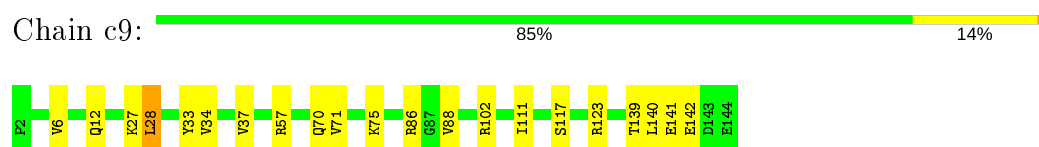
Chain c8:  75% 23% .



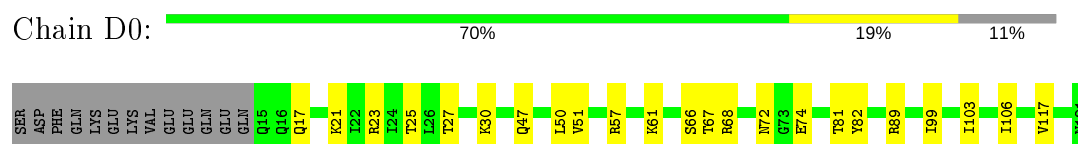
- Molecule 21: 40S ribosomal protein S19-A



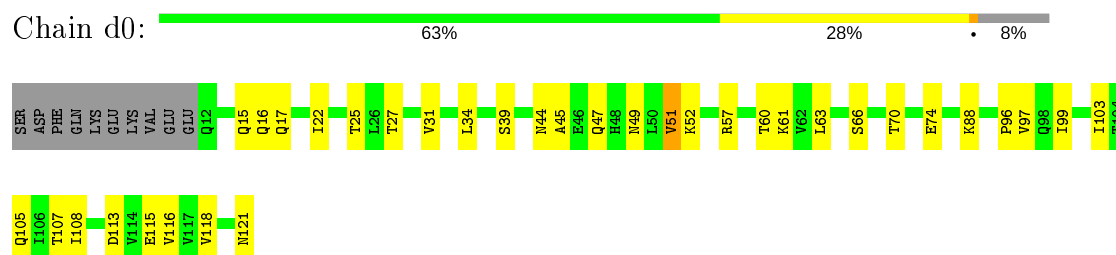
- Molecule 21: 40S ribosomal protein S19-A



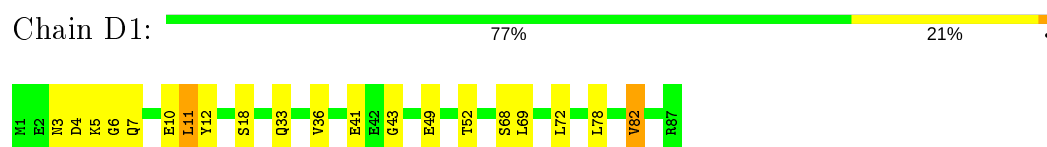
- Molecule 22: 40S ribosomal protein S20



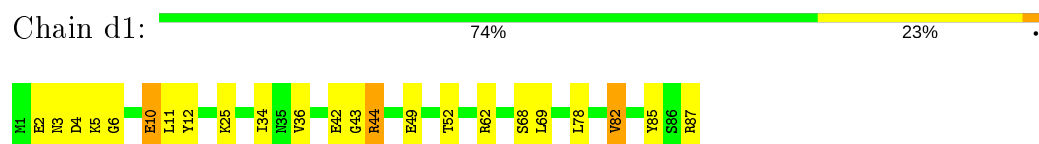
- Molecule 22: 40S ribosomal protein S20



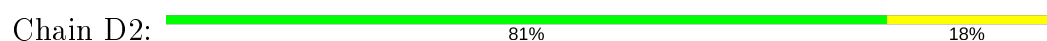
- Molecule 23: 40S ribosomal protein S21-A



- Molecule 23: 40S ribosomal protein S21-A

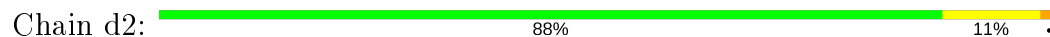


- Molecule 24: 40S ribosomal protein S22-A

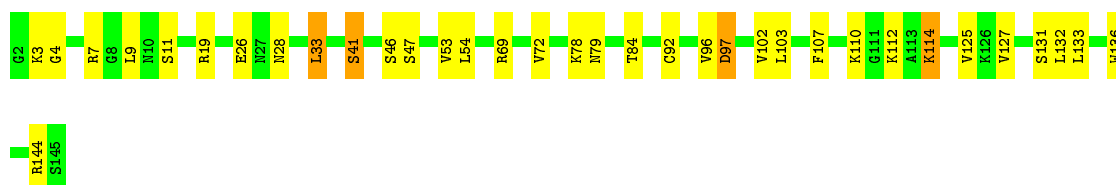
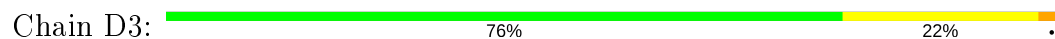




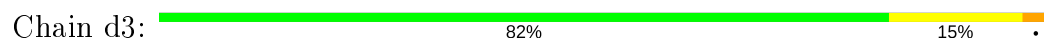
- Molecule 24: 40S ribosomal protein S22-A



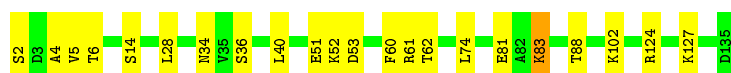
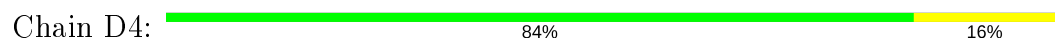
- Molecule 25: 40S ribosomal protein S23-A



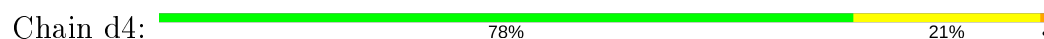
- Molecule 25: 40S ribosomal protein S23-A



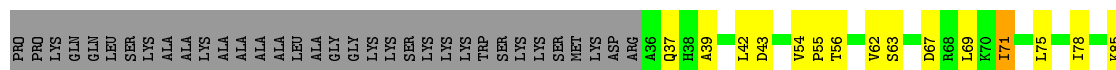
- Molecule 26: 40S ribosomal protein S24-A

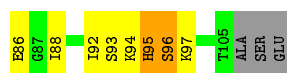


- Molecule 26: 40S ribosomal protein S24-A



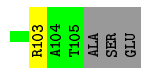
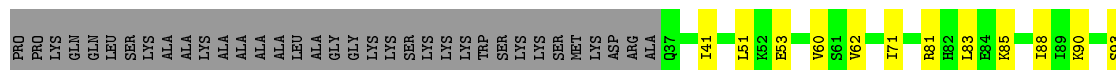
- Molecule 27: 40S ribosomal protein S25-A





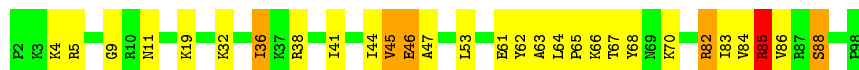
- Molecule 27: 40S ribosomal protein S25-A

Chain d5: 52% 12% 36%



- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 70% 24% 5%



- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 82% 16%



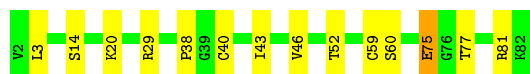
- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 81% 16%



- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 83% 16%



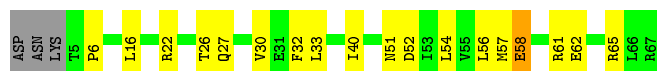
- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 67% 27% 5%



- Molecule 30: 40S ribosomal protein S28-A

Chain d8:  68% 26% • 5%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9:  75% 20% • •




- Molecule 31: 40S ribosomal protein S29-A

Chain d9:  69% 24% • •



- Molecule 32: 40S ribosomal protein S30-A

Chain E0:  82% 17% •



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:  53% 30% 11% 7%



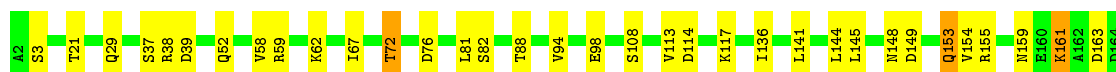
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:  57% 38% 5%



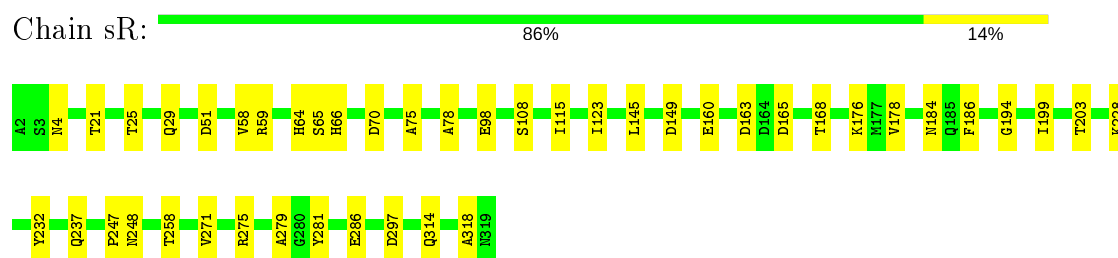
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:  80% 18% •



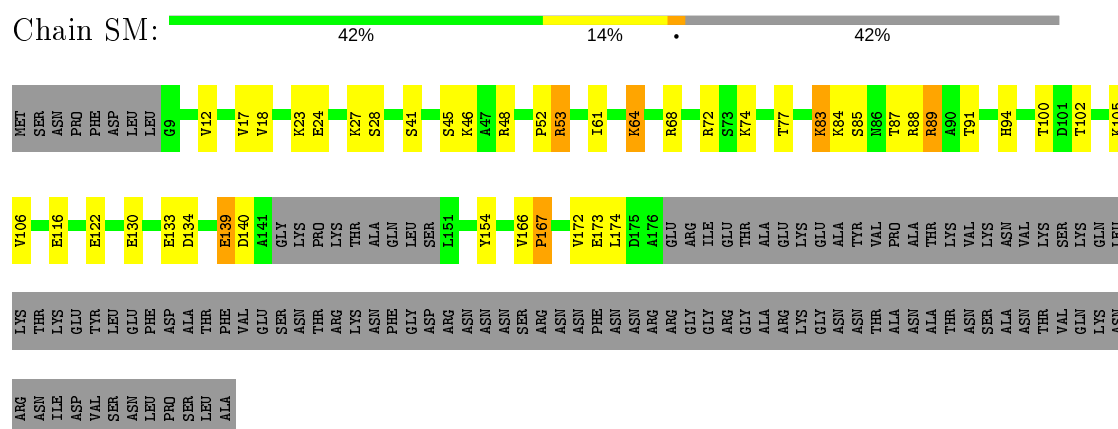
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



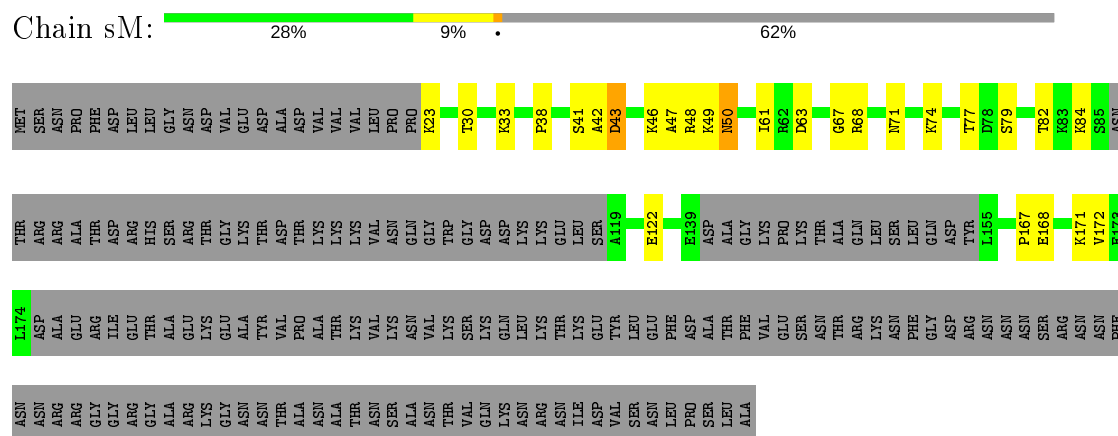
- Molecule 35: Suppressor protein STM1

Chain SM:



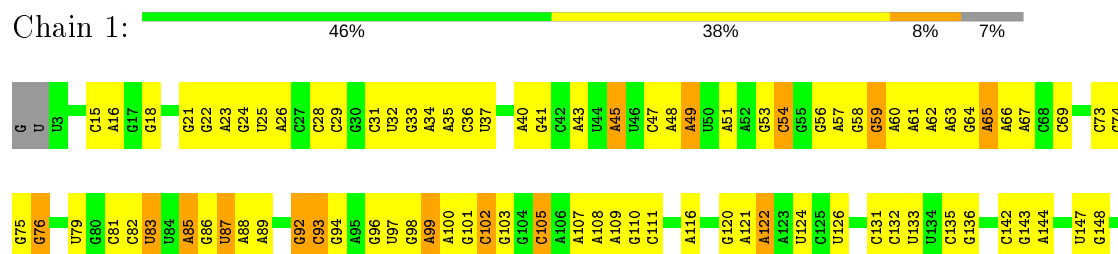
- Molecule 35: Suppressor protein STM1

Chain sM:



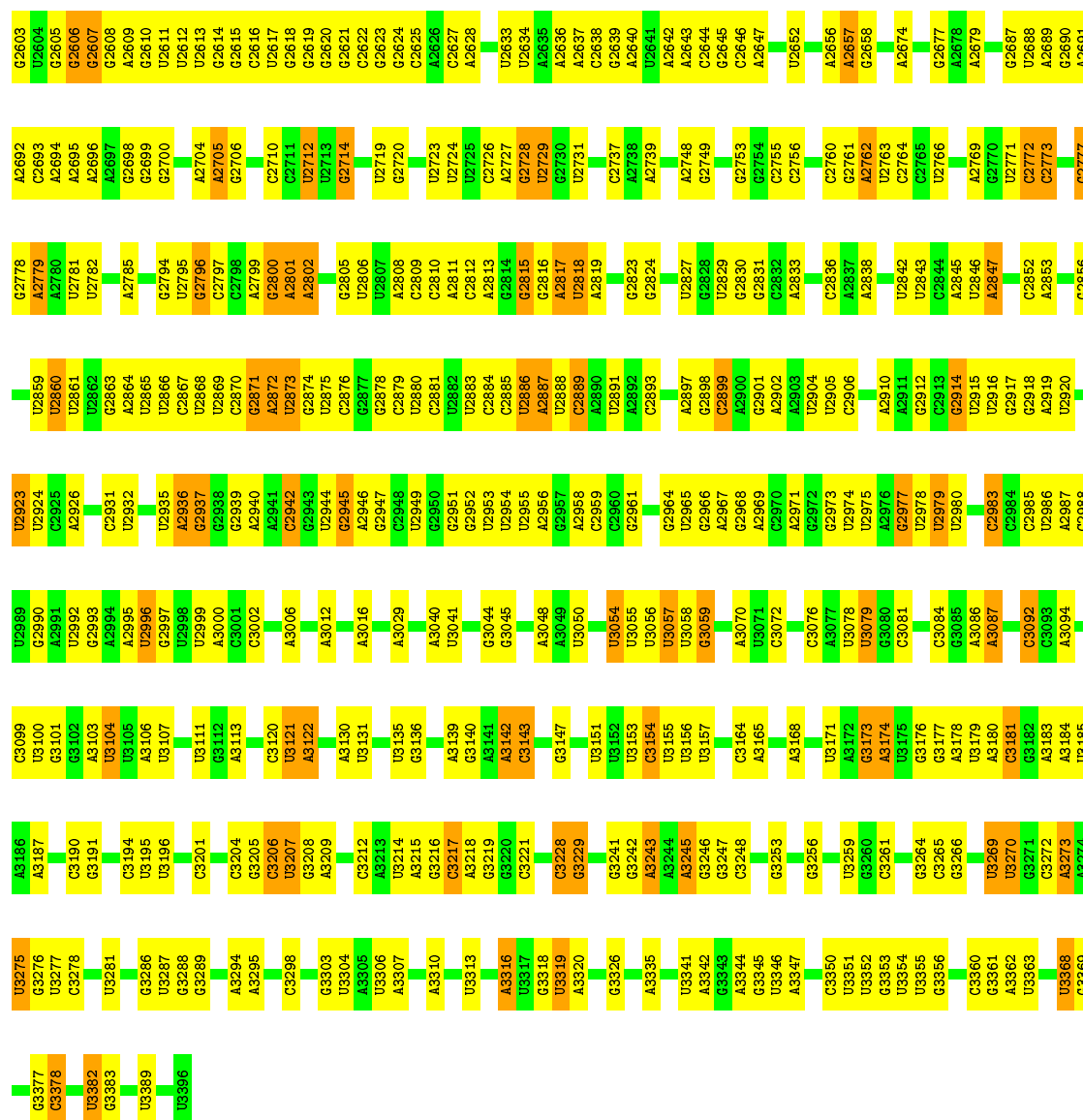
- Molecule 36: 25S ribosomal RNA

Chain 1:



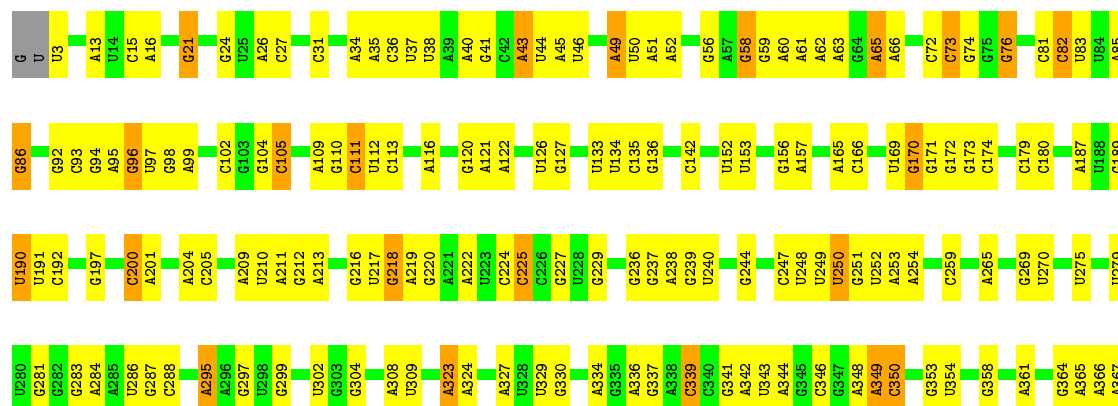
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C1137	U1138	G1139	G1140	C1141	G1142	A1143	U1144	G1145	C1146	U1147	G1148	G1149	A1150	U1151	U1152	A1153	C1154	C1155	C1156	G1157	A1158	U1159	C1160	G1161	G1164	A1165	G1166	U1167	G1171	U1172	U1173	C1174	C1175	U1176	G1177	G1178	A1179	U1180	U1181	A1182	C1185	G1186	C1187	U1188	C1189	A1190	U1191	C1192	A1193	G1194	A1195	U1196	A1197	C1198	U1199	A1200																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
G1059	U1060	A1061	G1062	G1063	A1064	A1065	C1069	U1070	U1071	G1072	U1081	U1082	G1083	G1087	A1093	U1094	U1095	U1096	G1097	A1098	A1102	A1103	G1104	A1105	G1106	C1107	U1108	U1109	A1112	G1113	U1114	G1115	G1116	G1117	C1118	C1119	A1120	U1121	U1122	U1123	U1124	U1125	G1126	G1127	U1128	A1129	A1130	G1131	A1132	A1133	G1134	A1135	A1136																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
C1201	A1202	A1203	A1204	G1207	U1208	G1209	U1210	C1211	G1212	G1213	C1216	A1217	U1218	A1221	G1222	A1225	G1226	C1227	C1232	G1233	G1236	G1237	U1241	G1242	C1243	A1244	A1245	G1246	U1247	G1248	G1249	U1258	A1259	G1262	A1263	G1264	U1265	G1266	U1267	G1268	U1269	A1270	C1271	G1272	A1273	A1274	A1278	C1279																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																</

G2503	G2364	A2281	U2193	C2118	G	G1902	A1816	C1693	U1572	G1497	U1425	G1357
U2504	G2365	U2282	G2194	G2118	U	U1903	G1817	A1696	G1576	A1498	U1425	G1362
A2511	C2366	G2283	C2197	G2121	A	C1904	U1818	A1696	A1577	A1503	A1428	A1363
U2514	A2367	C2284	U2200	G2122	A	G1905	U1819	G1905	C1578	U1504	G1429	C1364
A2515	A2368	U2285	G2201	G2123	C	U1906	U1820	U1716	C1579	C1505	U1430	C1365
A2519	G2369	C2287	G2202	G2124	G	C1907	U1821	U1717	A1580	A1506	G1431	A1366
A2520	G2370	G2290	C2202	A2125	G	U1911	C1822	A1723	C1581	G1507	C1432	G1367
U2521	G2371	G2291	U2205	G2130	C	U1912	U1827	U1724	C1582	C1508	U1433	U1368
G2522	A2372	C2293	C2206	G2131	U	U1916	A1835	C1726	A1583	G1507	A1434	A1369
A2523	G2373	U2294	U2207	C2132	A	C1917	C1836	C1725	G1586	U1510	A1435	G1370
U2527	G2374	A2295	A2208	U2133	U	U1918	U1837	G1733	U1587	G1513	U1436	G1371
G2532	A2376	A2296	U2209	G2134	G	G1919	G1838	G1733	A1588	G1514	C1437	C1372
U2533	G2377	U2297	G2210	U2135	U	U1929	A1839	A1741	U1589	U1438	U1438	A1373
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U2537	U2379	G2301	C2212	U2137	U	U1931	A1841	G1743	A1593	U1518	G1441	G1376
U2540	U2380	G2302	G2216	A2138	G	U1932	A1842	G1744	A1602	G1519	U1442	G1377
U2541	A2384	C2305	U2222	U2140	U	G1933	C1843	C1745	A1603	U1522	G1443	U1378
U2542	G2385	G2306	A2222	G2141	C	U1934	G1844	A1749	G1604	U1523	U1444	G1379
U2543	G2386	U2307	U2226	A2142	U	G1935	G1845	A1750	A1605	G1524	U1445	G1380
U2544	A2397	C2308	C2227	A2143	G	C1943	A1846	G1751	U1606	G1525	G1446	A1381
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U2546	G2399	U2310	C2231	A2145	C	U1950	C1848	C1762	A1612	C1527	U1448	C1385
U2547	G2400	G2311	U2241	C2151	G	U1951	A1850	U1763	A1617	G1528	A1450	A1386
U2548	A2401	A2313	A2242	U2153	U	C1952	G1851	U1764	G1617	A1529	A1453	G1387
U2549	G2402	U2314	C2243	A2158	A	G1953	C1852	U1765	A1619	C1531	U1454	G1389
U2550	A2403	G2315	A2244	U2159	C	U1954	U1853	G1766	G1620	U1532	U1455	U1392
U2551	C2405	G2316	U2245	C2152	C	U1955	C1854	C1767	A1621	A1533	A1456	A1393
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U2553	C2407	A2326	A2247	U2158	G	G	C1856	G1769	C1628	A1535	G1466	G1395
U2554	U2408	G2329	C2248	C2163	C	U	A1857	G1770	U1629	G1536	A1467	C1396
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U2560	G2414	G2335	U2250	A2168	A	C	U1877	U1795	A1654	U1554	A1475	C1403
U2561	C2415	U2336	C2257	G2174	C	G	G1878	G1796	G1655	U1555	G1476	C1404
U2562	U2416	C2337	A2256	U2175	U	U	A1879	A1797	A1656	C1556	U1477	U1405
U2563	U2417	U2338	C2257	U2176	C	A	U1880	A1800	C1657	U1557	G1480	A1406
U2564	G2418	A2343	U2263	G2177	C	G	A1883	U1801	G1658	A1558	A1481	U1407
U2565	A2419	U2351	U2268	A2178	A	C	A1886	A1804	U1659	G1561	U1482	G1412
U2566	C2422	A2352	C2272	C2179	G	U	A1891	G1807	C1663	C1562	G1485	G1413
U2567	G2425	G2353	U2273	A2183	C	C	U1896	G1808	U1670	U1564	G1486	G1414
U2568	U2426	G2354	U2102	U2184	C	G	G1897	A1809	G1677	G1565	A1489	U1415
U2569	U2427	U2355	G2111	A2188	U	U	G1898	A1810	U1683	U1567	G1492	A1418
U2570	U2428	A2356	U2112	U2191	C	G	G1899	A1814	A1683	U1568	G1493	A1419
U2571	U2429	U2357	U2113	C2192	U	G	G1900	A1815	U1683	U1569	U1494	U1420
U2572	U2430	U2358	C2114	C2192	C	C	U1901	A1815	U1683	U1570	U1495	G1421
U2573	U2431	U2359	C2114	C2192	U	C	U1902	A1815	U1683	U1571	U1496	C1422



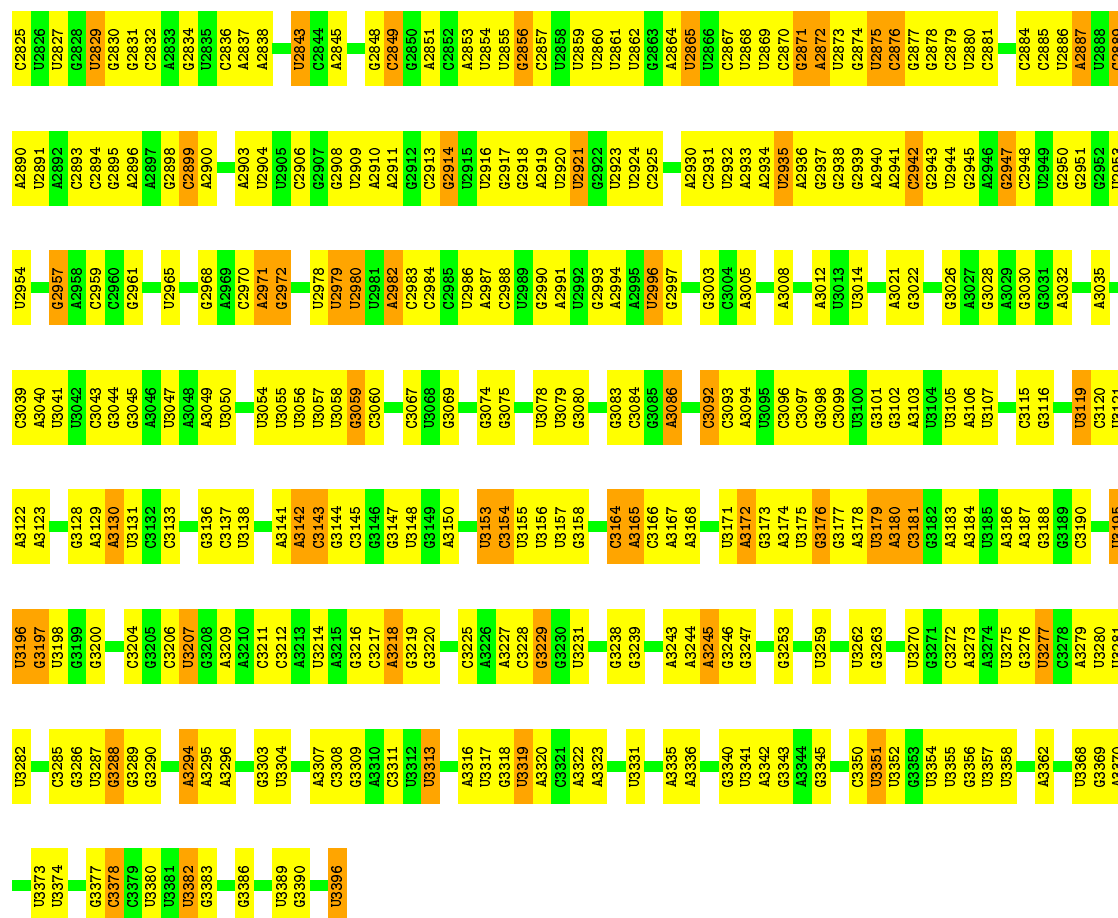
• Molecule 36: 25S ribosomal RNA

Chain 5: 46% 39% 8% 7%



G1517	U1436	G1357	C1284	C1189	U1041	G991	G800	A691	A619	U520	U	G368
U1518	C1437	G1365	G1285	A1190	U1122	G992	G801	A692	U620	A521	G	A369
G1519	U1438	C1366	A1286	U1191	C1045	C893	A801	A693	A521	A522	C	U370
U1522	U1445	G1365	G	C1192	A1046	G894	C802	A694	A622	A523	C	G371
U1523	A1446	G1366	U1293	G1194	U1126	A895	C803	C695	A630	U524	C	A374
A1524	G1447	U1368	U1294	A1195	G1127	A896	C804	C696	A631	C525	C	A375
C1527	G1450	A1369	G1295	C1196	U1128	U897	G805	A699	U632	G831	U	G376
G1528	C1451	G1370	C1296	A1197	U1129	U898	A807	A699	C633	G	G	G383
G1528	A1452	C1371	C1297	C1198	A1130	U903	U811	U704	G634	G535	C	U393
U1533	U1455	C1372	C1298	G1199	A1054	A904	U811	A705	G635	U	C	G394
A1534	A1456	A1373	U1299	A1200	A1055	G907	G815	U706	C636	G538	C	U395
A1535	A1456	G1374	G1300	C1201	U1056	G908	A816	G708	C637	C546	U	A396
G1536	G1376	C1375	A1301	A1202	C975	G909	A817	A709	G638	G547	U	A397
A1465	A1465	C1376	A1302	A1203	U979	G910	U817	U710	C639	G548	G	A398
G1466	G1466	G1379	A1304	A1205	A980	C911	U820	A711	U640	A551	U	A399
C1469	C1469	G1380	U1305	G1206	U981	G912	U821	G712	U642	U	G	G400
U1470	U1470	A1381	G1306	C982	A913	A914	G822	A715	U643	U555	G	U401
U1471	U1384	G1307	G1307	U1208	A915	A915	G826	A716	G644	U556	G	A402
U1472	C1385	A1308	U1309	U1210	G1147	G916	U826	C717	A645	U557	A	C403
C1548	G1473	C1386	U1310	U1211	G1148	A830	U821	G718	A646	U558	G	G404
U1549	G1474	G1387	G1311	A1212	G1149	A831	U822	U719	A647	A559	G	U405
A1475	A1475	C1312	G1312	U1151	A992	G832	G832	A720	C648	G560	G	G406
G1476	G1476	G1313	U1214	G1152	G993	U922	G833	G725	C650	C561	G	A407
G1480	G1480	U1314	G	G1222	G994	U923	U834	G726	G651	C562	A	U410
U1554	U1398	C1315	U1315	A1153	A998	G924	U835	A727	A653	U567	U	U411
A1482	A1399	A1316	A1317	A1154	G1001	A925	A836	G727	C654	G568	C	U414
G1483	G1400	A1317	G1400	C1156	G1002	A926	A837	G740	C655	U574	C	G415
U1484	A1407	G1318	G1319	A1157	A1003	C927	C838	C753	A656	G575	G	A416
G1486	G1408	C1320	C1320	A1158	A1004	A928	C839	C758	G657	C576	C	A417
U1494	G1416	U1329	U1329	A1159	U1004	A929	C840	U759	A578	C577	A	G420
U1495	U1417	A1330	U1330	G1161	G1005	U930	U841	U764	G421	A422	U	G421
C1496	C1418	U1331	U1331	U1162	A1006	C931	C861	C755	A423	A423	C	A422
C1497	A1419	U1332	G1332	U1163	G1010	G934	U865	U766	C586	G424	U	G424
A1498	C1420	G1335	C1335	A1167	U1094	U935	U866	C768	U669	U587	U	G425
A1499	G1421	C1339	C1339	U1168	A1098	A936	U869	G769	C670	G588	U	G426
G1496	G1422	U1501	U1501	A1169	A1099	U938	G870	G770	U671	A589	U	C427
C1502	C1423	G1340	G1340	A1170	U1100	U939	G870	U776	A672	G590	U	A428
A1503	C1424	G1344	G1344	G1171	G1101	G941	C873	U777	U673	G591	U	A436
A1503	U1425	G1344	G1344	G1172	A1102	U942	U874	U778	G676	A592	U	A437
A1506	U1426	U1348	U1348	G1173	A1103	U943	G875	G779	A677	G600	U	A438
G1507	A1428	A1259	A1259	G1174	G1104	C944	A876	A780	U678	G604	U	A439
C1508	C1429	A1350	A1350	G1175	G1021	G948	G878	G781	U679	U605	U	A440
A1509	U1430	U1351	U1351	U1177	G1024	C949	U879	G785	G680	G604	U	U507
A1513	A1431	A1352	A1352	A1179	A1025	G950	G880	A786	U681	U606	U	G510
G1514	C1432	U1353	U1353	U1180	U1110	A951	G881	G787	U682	C606	U	G511
A1515	A1433	G1354	G1354	U1181	A1112	A952	C882	G788	U683	A607	U	U512
C1516	G1434	A1355	A1355	A1182	G1113	U955	A883	C788	G609	G513	U	G513
G1592	A1587	U1588	U1588	U1183	U1114	U956	A884	C788	G610	G514	U	G514
G1592	A1588	A1588	A1588	U1184	G1115	C957	A888	C788	U687	A611	U	C515
G1592	A1589	A1589	A1589	U1185	G1116	C958	A888	C788	G688	G617	U	G518
G1592	A1590	A1590	A1590	U1186	G1117	C959	A888	C788	U689	C618	U	A519
G1592	A1591	A1591	A1591	U1187	G1118	U960	C890	C788	A690	C618	U	A519
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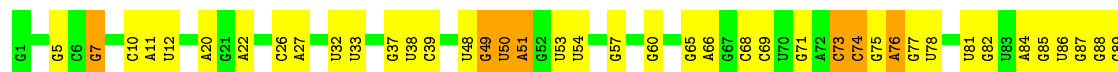
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A2743	G2579	G2652	G2579	G2606	A2363	G2435	C2128	C	A1911	C1844	U1737	A1594
A2748	G2584	A2656	G2584	G2607	G2364	U2436	G2128	G	A1912	G1845	C1738	U1595
U2752	G2585	G2661	G2585	G2608	G2365	G2437	A2131	C	A1913	C1846	G1745	G1598
G2753	G2586	G2664	G2586	G2609	G2366	A2438	C2132	C	A1847	A1847	A1750	G1599
G2754	U2587	C2664	G2587	G2610	A2367	G2440	U2133	U	C1849	C1849	G1751	G1604
G2755	U2588	C2664	G2588	G2611	A2368	A2441	G2134	U	A1850	A1850		
G2756	A2591	A2674	A2591	G2612	G2371	G2442	U2135	G	A1851	G1851		
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A2758	A2593	A2676	A2593	U2514	A2373	A2444	U2137	U	U1853	U1853		
U2759	U2597	G2677	U2597	U2515	G2374	A	A2138	A	C1854	C1854	A1760	A1612
G2760	G2598		G2598	G2512	G2375	U	A2139	U	U1855	U1855	A1761	
G2761	G2599		G2599	U2513	G2376	G	U2140	G	C1856	C1856	C1762	U1620
A2762	C2600		C2600	U2514	G2377	U	A2141	U	C1857	C1857	U1763	
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G2764	G2606		G2606	G2512	U2379	G	A2143	C	G1861	G1861	G1766	U1629
G2765	G2607		G2607	U2513	U2380	G	A2144	U			C1767	
C2772	G2608		G2608	U2514	G2381	U	A2145	U	A1864	A1864	G1770	
C2773	G2609		G2609	G2515	G2382	G	C2146	G	A1865	A1865		
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U2775	U2612		U2612	A2524	A2384	U	A2148	A	A1867	A1867	C1781	
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U2779	G2616		G2616	A2530	U2388	U	G2158	G	U1871	U1871	A1643	A1643
U2780	U2617		U2617	G2531	C2389	U	A2159	A	C1872	C1872	U1644	U1644
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U2802	G2639		G2639	U2560	U2410	U	U2181	U	G1903	G1903	U1717	U1717
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U2805	G2642		G2642	U2563	A2413	U	U2184	U	U1906	U1906	A1833	A1833
U2806	G2643		G2643	U2564	G2414	U	U2185	U	C1907	C1907	U1840	U1840
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U2809	G2646		G2646	U2567	G2417	U	U2188	U				
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U2812	G2649		G2649	U2570	G2420	U	U2191	U				
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U2818	G2655		G2655	U2576	G2426	U	U2197	U				
U2819	G2656		G2656	U2577	U2427	U	U2198	U				
U2820	G2657		G2657	U2578	G2428	U	U2199	U				
U2821	G2658		G2658	U2579	U2429	U	U2200	U				
U2822	G2659		G2659	U2580	G2430	U	U2201	U				
U2823	G2660		G2660	U2581	U2431	U	U2202	U				
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• Molecule 37: 5S ribosomal RNA



• Molecule 37: 5S ribosomal RNA

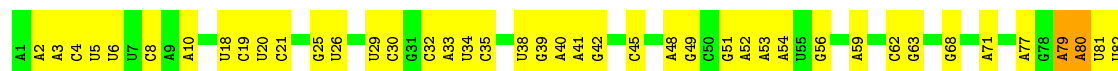


• Molecule 38: 5.8S ribosomal RNA





- Molecule 38: 5.8S ribosomal RNA



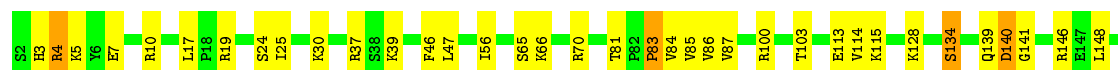
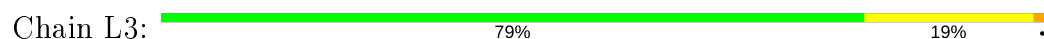
- Molecule 39: 60S ribosomal protein L2-A



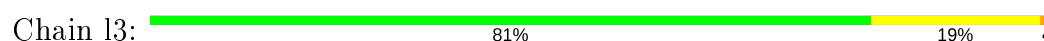
- Molecule 39: 60S ribosomal protein L2-A

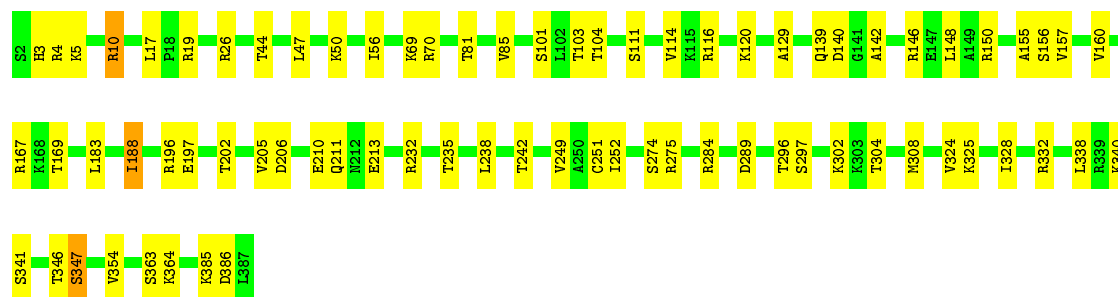


- Molecule 40: 60S ribosomal protein L3



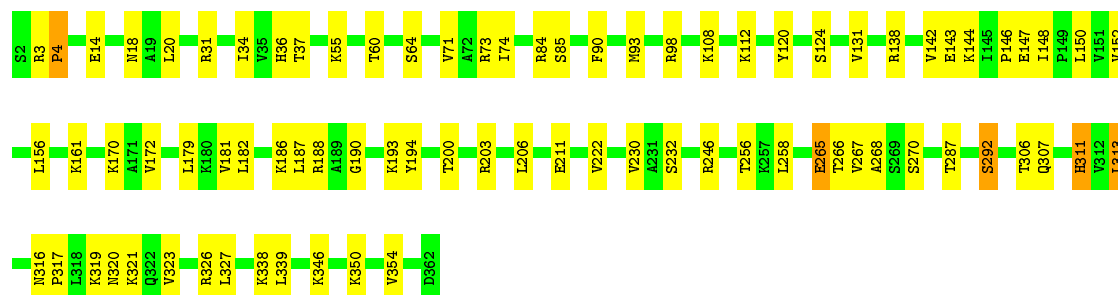
- Molecule 40: 60S ribosomal protein L3





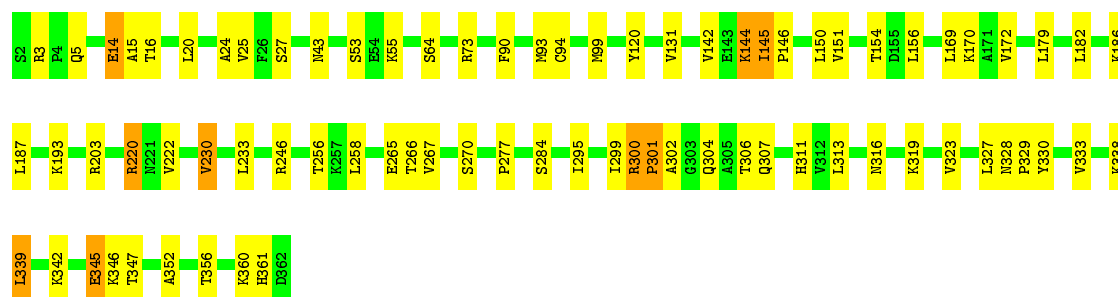
- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 78% 21% .



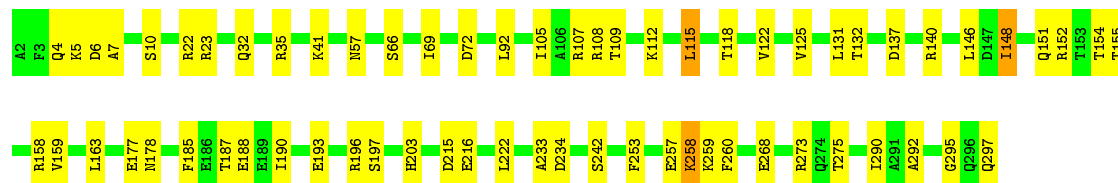
- Molecule 41: 60S ribosomal protein L4-A

Chain l4: 78% 19% .



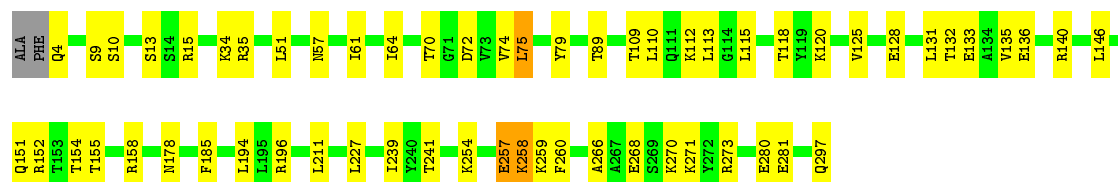
- Molecule 42: 60S ribosomal protein L5

Chain L5: 78% 21% .



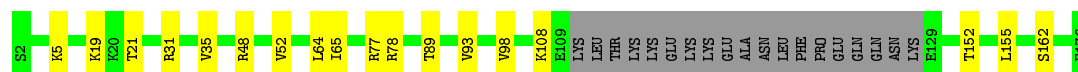
- Molecule 42: 60S ribosomal protein L5

Chain l5: 79% 19% ..



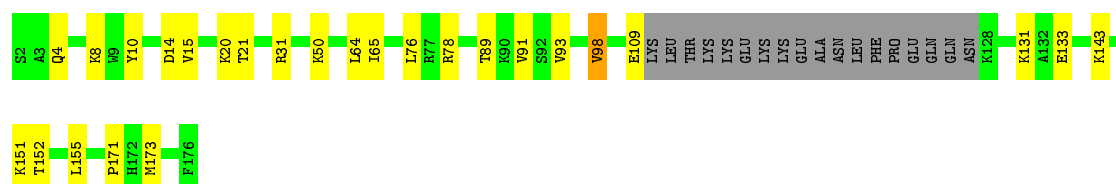
- Molecule 43: 60S ribosomal protein L6-A

Chain L6: 79% 10% 11%



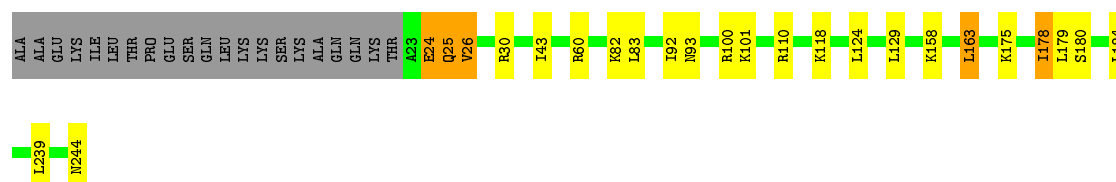
- Molecule 43: 60S ribosomal protein L6-A

Chain L6: 75% 14% 10%



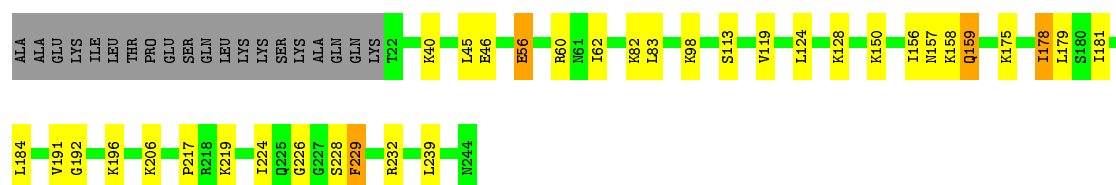
- Molecule 44: 60S ribosomal protein L7-A

Chain L7: 81% 8% 9%



- Molecule 44: 60S ribosomal protein L7-A

Chain L7: 77% 13% 8%



- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 75% 16% 9%





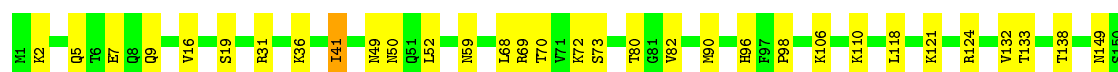
- Molecule 45: 60S ribosomal protein L8-A

Chain l8: 70% 20% 9%



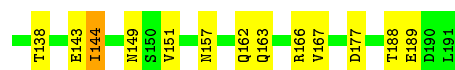
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 79% 19%



- Molecule 46: 60S ribosomal protein L9-A

Chain l9: 73% 26%



- Molecule 47: 60S ribosomal protein L10

Chain M0: 72% 22%



- Molecule 47: 60S ribosomal protein L10

Chain m0: 75% 21%





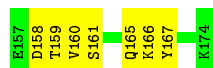
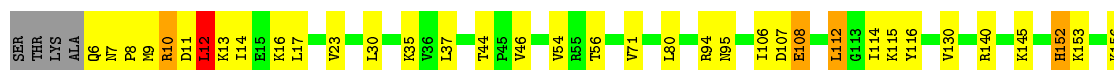
- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 77% 17% ..



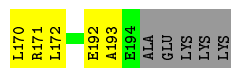
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 73% 22% ...



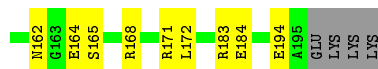
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 77% 19% ..



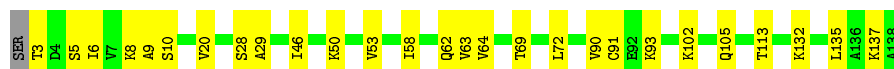
- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 75% 22% ..




- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 80% 20% .




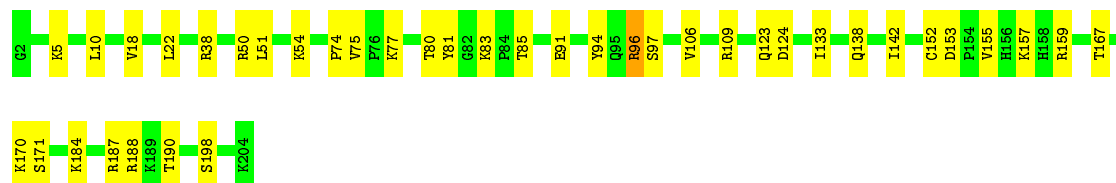
- Molecule 50: 60S ribosomal protein L14-A

Chain m4:  79% 20% .



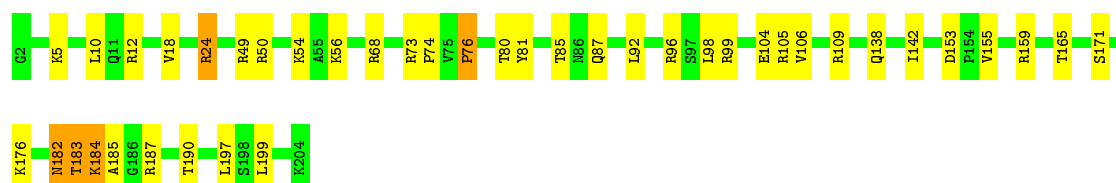
- Molecule 51: 60S ribosomal protein L15-A

Chain M5:  81% 19%



- Molecule 51: 60S ribosomal protein L15-A

Chain m5:  80% 18% .



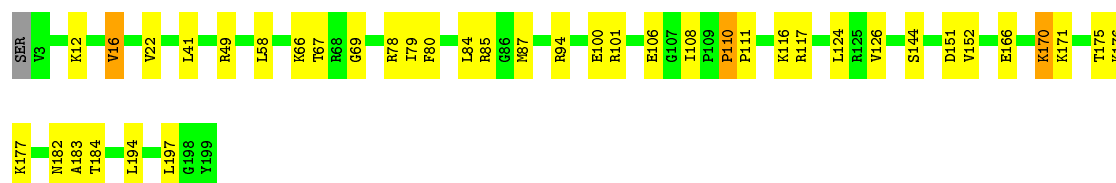
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:  86% 13% ..




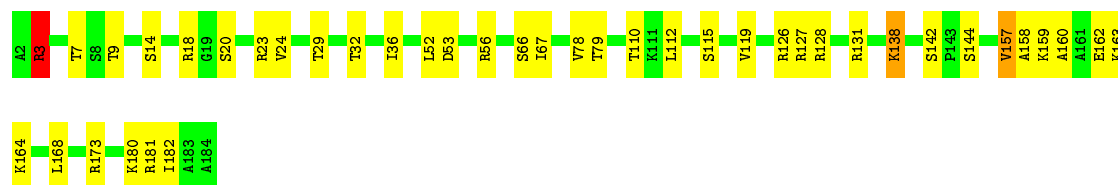
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:  79% 19% ..



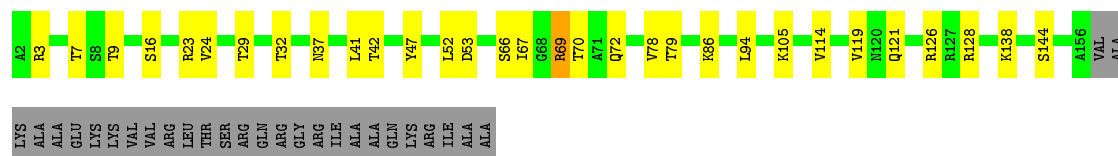
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:  78% 21% ..



- Molecule 53: 60S ribosomal protein L17-A

Chain m7: 68% 16% 15%



- Molecule 54: 60S ribosomal protein L18-A

Chain M8: 84% 16%



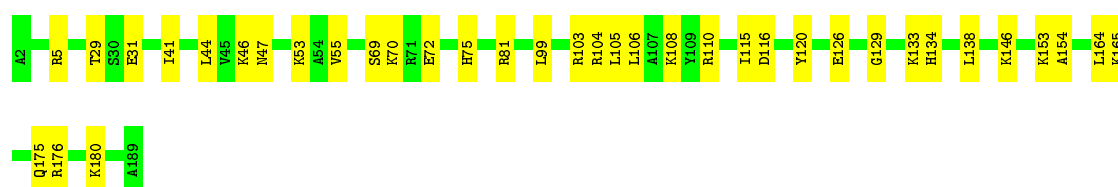
- Molecule 54: 60S ribosomal protein L18-A

Chain m8: 84% 15%



- Molecule 55: 60S ribosomal protein L19-A

Chain M9: 80% 20%



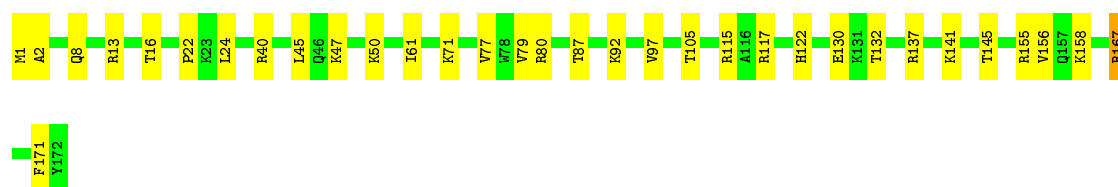
- Molecule 55: 60S ribosomal protein L19-A

Chain m9: 84% 15%



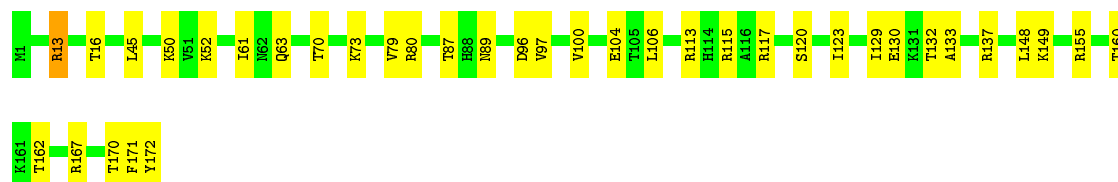
- Molecule 56: 60S ribosomal protein L20-A

Chain N0: 81% 19%



- Molecule 56: 60S ribosomal protein L20-A

Chain n0: 78% 21% .



- Molecule 57: 60S ribosomal protein L21-A

Chain N1: 80% 19% .



- Molecule 57: 60S ribosomal protein L21-A

Chain n1: 82% 16% .



- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 66% 18% 17%



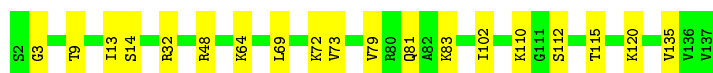
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 65% 16% 18%



- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 86% 14%



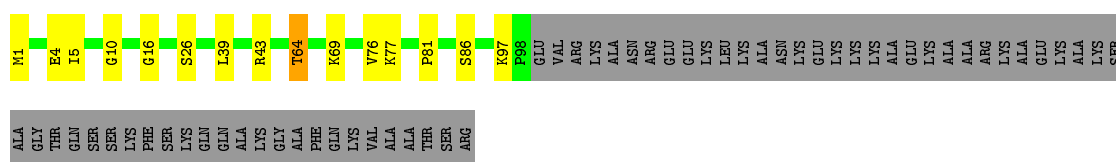
- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 85% 13%



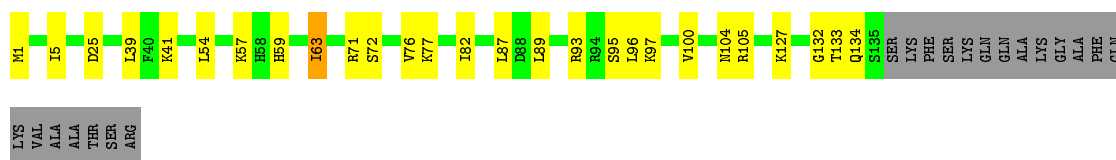
- Molecule 60: 60S ribosomal protein L24-A

Chain N4: 54% 9% 37%



- Molecule 60: 60S ribosomal protein L24-A

Chain n4: 70% 17% 13%



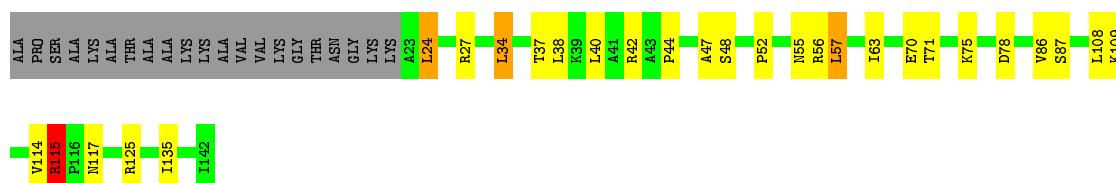
- Molecule 61: 60S ribosomal protein L25

Chain N5: 69% 15% 14%




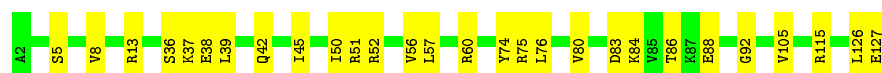
- Molecule 61: 60S ribosomal protein L25

Chain n5: 65% 17% 15%




- Molecule 62: 60S ribosomal protein L26-A

Chain N6:  78% 22%



- Molecule 62: 60S ribosomal protein L26-A

Chain n6:  78% 21%



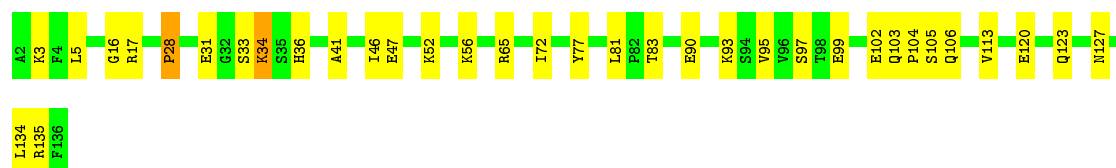
- Molecule 63: 60S ribosomal protein L27-A

Chain N7:  76% 21%




- Molecule 63: 60S ribosomal protein L27-A

Chain n7:  74% 24%




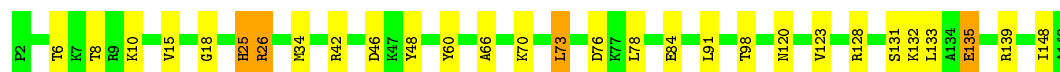
- Molecule 64: 60S ribosomal protein L28

Chain N8:  78% 20%



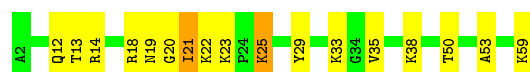
- Molecule 64: 60S ribosomal protein L28

Chain n8:  80% 17%



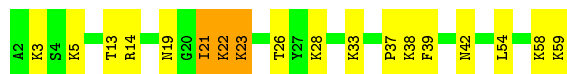
- Molecule 65: 60S ribosomal protein L29

Chain N9:  71% 26%




- Molecule 65: 60S ribosomal protein L29

Chain n9:  69% 26% 5%




- Molecule 66: 60S ribosomal protein L30

Chain O0:  76% 17% 7%




- Molecule 66: 60S ribosomal protein L30

Chain o0:  79% 17% 4%



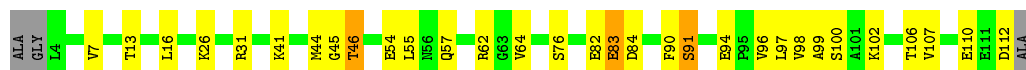
- Molecule 67: 60S ribosomal protein L31-A

Chain O1:  76% 20% 4% 2%




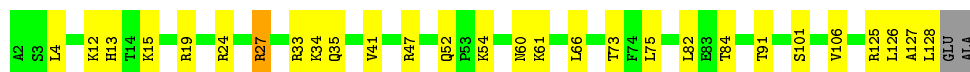
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:  70% 25% 5% 2%



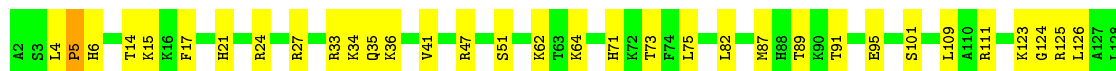
- Molecule 68: 60S ribosomal protein L32

Chain O2:  77% 21% 2% 2%




- Molecule 68: 60S ribosomal protein L32

Chain o2:  73% 25% 2% 2%




GLU
ALA

- Molecule 69: 60S ribosomal protein L33-A

Chain O3:  83% 16%




- Molecule 69: 60S ribosomal protein L33-A

Chain o3:  81% 18%



- Molecule 70: 60S ribosomal protein L34-A

Chain O4:  75% 18% 7%




- Molecule 70: 60S ribosomal protein L34-A

Chain o4:  77% 16% 7%




- Molecule 71: 60S ribosomal protein L35-A

Chain O5:  79% 20%



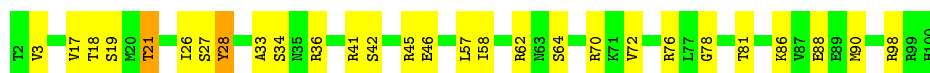
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:  77% 22%



- Molecule 72: 60S ribosomal protein L36-A

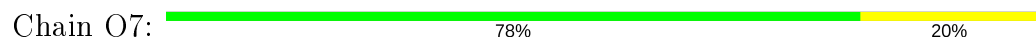
Chain O6:  72% 26%



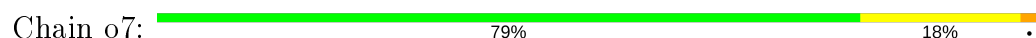
- Molecule 72: 60S ribosomal protein L36-A



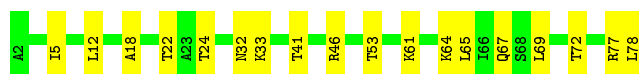
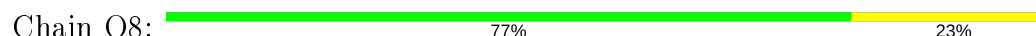
- Molecule 73: 60S ribosomal protein L37-A



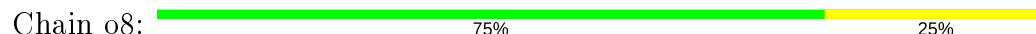
- Molecule 73: 60S ribosomal protein L37-A



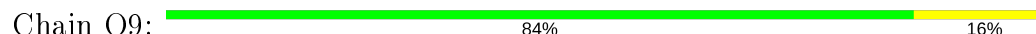
- Molecule 74: 60S ribosomal protein L38



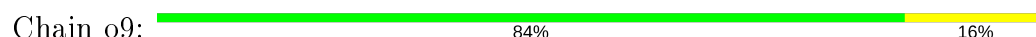
- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39

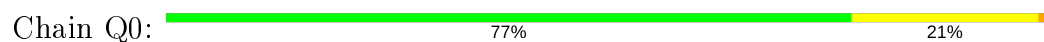


- Molecule 75: 60S ribosomal protein L39

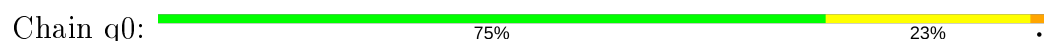




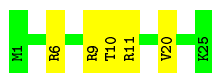
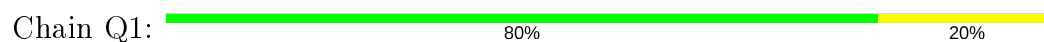
- Molecule 76: Ubiquitin-60S ribosomal protein L40



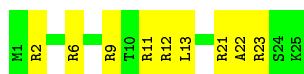
- Molecule 76: Ubiquitin-60S ribosomal protein L40



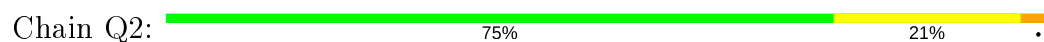
- Molecule 77: 60S ribosomal protein L41-A



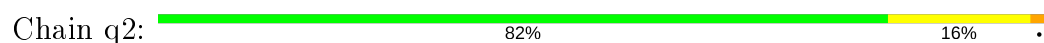
- Molecule 77: 60S ribosomal protein L41-A



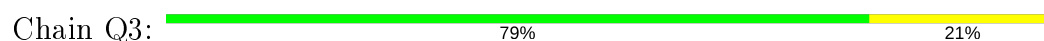
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 78: 60S ribosomal protein L42-A

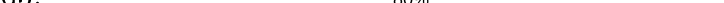


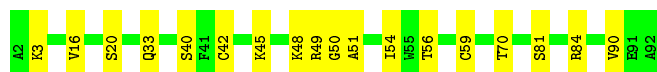
- Molecule 79: 60S ribosomal protein L43-A





- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  80% 20%

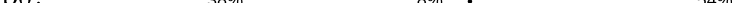


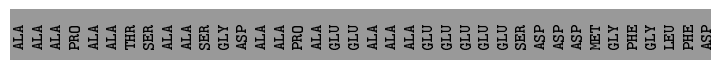
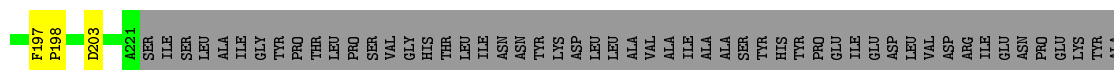
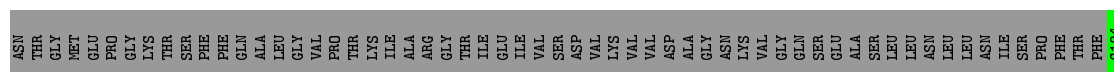
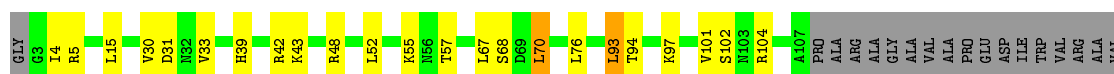
- Molecule 80: 40S ribosomal protein S30-A

Chain e0: 68% 29% .



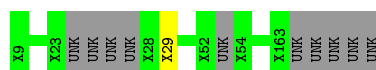
- Molecule 81: 60S acidic ribosomal protein P0

Chain p0:  38% 8% 54%



- Molecule 82: Unknown protein chain m2

Chain m2:  93% • 6%



- 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	435.15Å 287.07Å 303.24Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	99.87 – 3.20	Depositor
% Data completeness (in resolution range)	100.0 (99.87-3.20)	Depositor
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.194 , 0.246	Depositor
Wilson B-factor (Å ²)	88.0	Xtriage
Anisotropy	0.117	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	411206	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: MG, OHX, ZN, 3K8

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	0.79	5/41698 (0.0%)	1.34	378/64972 (0.6%)
1	6	0.90	17/42765 (0.0%)	1.39	452/66634 (0.7%)
2	S0	0.48	0/1617	0.67	0/2215
2	s0	0.47	0/1623	0.71	0/2222
3	S1	0.41	0/1735	0.68	2/2335 (0.1%)
3	s1	0.53	0/1748	0.70	0/2352
4	S2	0.52	0/1665	0.65	0/2263
4	s2	0.59	0/1665	0.74	0/2263
5	S3	0.50	0/1759	0.69	0/2368
5	s3	0.44	0/1759	0.59	0/2368
6	S4	0.51	0/2109	0.74	1/2839 (0.0%)
6	s4	0.55	0/2109	0.78	0/2839
7	S5	0.41	0/1629	0.62	0/2202
7	s5	0.46	0/1629	0.66	0/2202
8	S6	0.50	0/1823	0.67	0/2439
8	s6	0.59	0/1779	0.73	0/2379
9	S7	0.46	0/1506	0.69	0/2028
9	s7	0.47	0/1516	0.70	1/2043 (0.0%)
10	S8	0.59	0/1514	0.78	1/2021 (0.0%)
10	s8	0.64	0/1514	0.70	0/2021
11	S9	0.48	0/1519	0.69	0/2035
11	s9	0.57	0/1519	0.76	2/2035 (0.1%)
12	C0	0.44	0/790	0.67	1/1069 (0.1%)
12	c0	0.38	0/777	0.67	3/1049 (0.3%)
13	C1	0.62	0/1240	0.76	0/1675
13	c1	0.67	0/1194	0.77	0/1610
14	C2	0.37	0/900	0.64	0/1224
14	c2	0.29	0/900	0.56	0/1224
15	C3	0.51	0/1215	0.70	2/1638 (0.1%)
15	c3	0.61	0/1215	0.69	0/1638
16	C4	0.43	0/901	0.70	0/1217
16	c4	0.56	0/960	0.75	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.48	0/998	0.69	0/1341
17	c5	0.50	0/1060	0.69	0/1426
18	C6	0.46	0/1125	0.71	2/1510 (0.1%)
18	c6	0.49	0/1131	0.70	0/1518
19	C7	0.46	0/935	0.64	0/1254
19	c7	0.51	0/914	0.70	0/1224
20	C8	0.47	0/1211	0.65	1/1628 (0.1%)
20	c8	0.51	0/1211	0.73	2/1628 (0.1%)
21	C9	0.45	0/1130	0.66	0/1517
21	c9	0.52	0/1130	0.68	0/1517
22	D0	0.49	0/865	0.65	0/1169
22	d0	0.47	0/892	0.65	0/1205
23	D1	0.49	0/693	0.68	0/935
23	d1	0.52	0/693	0.69	0/935
24	D2	0.53	0/1038	0.74	2/1395 (0.1%)
24	d2	0.62	0/1038	0.78	1/1395 (0.1%)
25	D3	0.64	0/1139	0.80	2/1518 (0.1%)
25	d3	0.72	0/1139	0.85	2/1518 (0.1%)
26	D4	0.50	0/1087	0.64	0/1449
26	d4	0.54	0/1087	0.73	0/1449
27	D5	0.40	0/571	0.73	1/768 (0.1%)
27	d5	0.46	0/566	0.71	0/761
28	D6	0.51	0/782	0.69	0/1047
28	d6	0.56	0/782	0.69	0/1047
29	D7	0.47	0/620	0.66	0/838
29	d7	0.49	0/620	0.71	0/838
30	D8	0.37	0/499	0.58	0/670
30	d8	0.45	0/499	0.64	0/670
31	D9	0.56	0/452	0.73	1/600 (0.2%)
31	d9	0.51	0/452	0.68	0/600
32	E0	0.51	0/483	0.66	0/643
33	E1	0.47	0/577	0.81	0/770
33	e1	0.42	0/619	0.73	0/822
34	SR	0.41	0/2494	0.64	1/3393 (0.0%)
34	sR	0.38	0/2495	0.57	0/3395
35	SM	0.54	0/1113	0.75	2/1502 (0.1%)
35	sM	0.48	0/682	0.68	1/921 (0.1%)
36	1	1.25	247/75394 (0.3%)	1.73	2232/117545 (1.9%)
36	5	1.26	266/75414 (0.4%)	1.73	2109/117575 (1.8%)
37	3	1.02	0/2883	1.46	30/4491 (0.7%)
37	7	1.20	8/2883 (0.3%)	1.73	86/4491 (1.9%)
38	4	1.17	3/3746 (0.1%)	1.69	85/5832 (1.5%)
38	8	1.07	4/3746 (0.1%)	1.54	64/5832 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.81	0/1948	0.86	0/2617
39	l2	0.72	0/1946	0.88	3/2614 (0.1%)
40	L3	0.80	1/3146 (0.0%)	0.83	1/4228 (0.0%)
40	l3	0.90	1/3146 (0.0%)	0.89	2/4228 (0.0%)
41	L4	0.86	0/2800	0.94	7/3790 (0.2%)
41	l4	0.82	1/2800 (0.0%)	0.93	2/3790 (0.1%)
42	L5	0.58	0/2425	0.71	0/3271
42	l5	0.74	1/2408 (0.0%)	0.81	1/3248 (0.0%)
43	L6	0.82	0/1260	0.82	0/1694
43	l6	0.84	0/1269	0.88	1/1705 (0.1%)
44	L7	0.85	0/1821	0.92	3/2451 (0.1%)
44	l7	0.95	1/1828 (0.1%)	0.93	3/2461 (0.1%)
45	L8	0.60	0/1836	0.72	1/2481 (0.0%)
45	l8	0.54	0/1795	0.70	1/2429 (0.0%)
46	L9	0.73	0/1539	0.82	2/2073 (0.1%)
46	l9	0.84	0/1539	0.86	0/2073
47	M0	0.78	1/1741 (0.1%)	0.86	3/2335 (0.1%)
47	m0	0.80	1/1758 (0.1%)	0.88	0/2358
48	M1	0.53	0/1374	0.71	1/1842 (0.1%)
48	m1	0.69	0/1374	0.82	2/1842 (0.1%)
49	M3	0.81	0/1568	0.90	3/2106 (0.1%)
49	m3	0.73	0/1573	0.85	0/2113
50	M4	0.84	0/1068	0.86	0/1438
50	m4	0.92	0/1074	0.90	2/1446 (0.1%)
51	M5	0.83	1/1757 (0.1%)	0.89	2/2354 (0.1%)
51	m5	0.72	0/1757	0.86	4/2354 (0.2%)
52	M6	0.96	2/1585 (0.1%)	0.97	4/2128 (0.2%)
52	m6	1.04	2/1585 (0.1%)	0.96	4/2128 (0.2%)
53	M7	0.84	1/1443 (0.1%)	0.87	3/1944 (0.2%)
53	m7	0.97	1/1250 (0.1%)	0.93	1/1683 (0.1%)
54	M8	0.84	0/1465	0.88	0/1965
54	m8	0.78	0/1465	0.90	1/1965 (0.1%)
55	M9	0.61	0/1538	0.70	0/2050
55	m9	0.65	0/1538	0.71	0/2050
56	N0	0.86	0/1481	0.86	1/1990 (0.1%)
56	n0	0.93	0/1481	0.93	3/1990 (0.2%)
57	N1	0.84	0/1300	0.85	1/1743 (0.1%)
57	n1	0.93	3/1300 (0.2%)	0.85	1/1743 (0.1%)
58	N2	0.44	0/812	0.62	0/1099
58	n2	0.54	0/794	0.74	0/1076
59	N3	0.79	0/1018	0.87	0/1369
59	n3	0.90	0/1018	0.92	3/1369 (0.2%)
60	N4	0.64	0/712	0.74	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.69	0/1052	0.76	0/1398
61	N5	0.69	0/979	0.83	1/1321 (0.1%)
61	n5	0.68	0/974	0.79	2/1314 (0.2%)
62	N6	0.77	0/1004	0.89	1/1341 (0.1%)
62	n6	0.71	0/1004	0.89	1/1341 (0.1%)
63	N7	0.59	0/1118	0.71	0/1497
63	n7	0.53	0/1118	0.67	0/1497
64	N8	0.83	1/1204 (0.1%)	0.95	3/1612 (0.2%)
64	n8	0.78	0/1204	0.90	3/1612 (0.2%)
65	N9	0.74	0/473	0.88	1/629 (0.2%)
65	n9	0.85	0/473	1.01	1/629 (0.2%)
66	O0	0.55	0/751	0.68	0/1008
66	o0	0.53	0/775	0.69	0/1040
67	O1	0.70	0/890	0.78	1/1196 (0.1%)
67	o1	0.78	0/897	0.88	0/1205
68	O2	0.90	0/1041	0.91	3/1394 (0.2%)
68	o2	0.89	0/1041	0.94	2/1394 (0.1%)
69	O3	0.97	0/868	0.91	0/1168
69	o3	1.01	1/868 (0.1%)	0.94	2/1168 (0.2%)
70	O4	0.68	0/890	0.83	1/1189 (0.1%)
70	o4	0.63	0/890	0.78	0/1189
71	O5	0.78	0/978	0.85	0/1301
71	o5	0.61	0/974	0.75	0/1297
72	O6	0.67	0/778	0.86	0/1034
72	o6	0.63	0/777	0.77	0/1033
73	O7	0.90	0/696	1.01	3/923 (0.3%)
73	o7	0.75	0/696	0.86	2/923 (0.2%)
74	O8	0.59	0/618	0.70	0/826
74	o8	0.50	0/614	0.69	0/822
75	O9	0.81	0/443	0.93	0/588
75	o9	0.74	0/443	0.91	0/588
76	Q0	0.78	0/423	0.89	0/562
76	q0	0.93	1/423 (0.2%)	0.92	0/562
77	Q1	0.65	0/234	0.82	0/300
77	q1	0.81	0/234	1.10	1/300 (0.3%)
78	Q2	0.91	1/860 (0.1%)	0.84	0/1136
78	q2	0.89	2/860 (0.2%)	0.82	0/1136
79	Q3	0.80	0/701	0.83	0/934
79	q3	0.80	0/701	0.85	1/934 (0.1%)
80	e0	0.57	0/499	0.74	0/665
81	p0	0.46	0/1091	0.62	0/1472
All	All	0.96	573/430072 (0.1%)	1.35	5562/631360 (0.9%)

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
2	s0	0	1
7	S5	0	1
7	s5	0	2
9	S7	0	2
9	s7	0	1
10	S8	0	1
16	C4	0	3
16	c4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	1
24	d2	0	1
26	d4	0	1
27	D5	0	3
28	D6	0	1
39	L2	0	1
39	l2	0	4
44	l7	0	2
46	L9	0	1
48	M1	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	1
56	n0	0	1
57	N1	0	1
59	n3	0	1
64	N8	0	2
64	n8	0	3
65	N9	0	1
67	O1	0	1
80	e0	0	1
82	m2	0	1
All	All	0	46

All (573) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	14.54	2.06	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	14.44	2.06	1.82
36	5	1152	G	N9-C4	-12.25	1.28	1.38
36	5	2971	A	N9-C4	9.75	1.43	1.37
36	5	1152	G	N9-C8	9.62	1.44	1.37
36	1	2983	C	N3-C4	-8.85	1.27	1.33
36	1	3181	C	N3-C4	-8.65	1.27	1.33
36	1	2875	U	C2-N3	8.47	1.43	1.37
36	5	1152	G	C2-N3	-8.31	1.26	1.32
36	5	1152	G	N3-C4	-8.18	1.29	1.35
36	5	2726	C	N3-C4	-8.17	1.28	1.33
36	5	1152	G	C5-C6	-8.12	1.34	1.42
36	1	804	C	N1-C6	-8.07	1.32	1.37
36	1	2714	G	N9-C4	-8.00	1.31	1.38
36	5	2996	U	N1-C2	7.91	1.45	1.38
36	5	2138	A	N7-C5	-7.90	1.34	1.39
36	5	1592	G	C6-O6	7.89	1.31	1.24
36	5	1195	A	N9-C4	-7.83	1.33	1.37
36	5	1143	A	N9-C4	-7.78	1.33	1.37
36	1	1394	A	N9-C4	-7.75	1.33	1.37
36	1	2409	G	C5-C4	-7.73	1.32	1.38
36	5	2626	A	N9-C4	-7.59	1.33	1.37
36	1	2377	G	N3-C4	-7.58	1.30	1.35
36	1	931	C	N1-C6	-7.51	1.32	1.37
36	5	2138	A	N9-C4	-7.46	1.33	1.37
36	1	343	U	C2-N3	-7.46	1.32	1.37
36	5	2627	C	N1-C6	-7.44	1.32	1.37
36	5	3106	A	N7-C5	-7.42	1.34	1.39
36	5	2381	G	C5-C4	-7.38	1.33	1.38
36	5	706	A	N9-C4	-7.28	1.33	1.37
36	1	2419	A	N9-C4	-7.27	1.33	1.37
36	5	3362	A	N9-C4	-7.27	1.33	1.37
36	1	61	A	C6-N1	-7.23	1.30	1.35
36	1	1547	G	C5-C4	-7.17	1.33	1.38
36	5	1908	A	N3-C4	-7.11	1.30	1.34
36	1	2333	C	N1-C6	-7.10	1.32	1.37
36	5	3084	C	N1-C6	-7.10	1.32	1.37
36	5	2280	A	N9-C4	-7.10	1.33	1.37
36	1	2404	A	N3-C4	7.00	1.39	1.34
36	5	1188	U	C2-N3	-6.97	1.32	1.37
36	5	3245	A	C5-C6	-6.95	1.34	1.41
36	1	1335	C	N3-C4	-6.95	1.29	1.33
36	1	3306	U	N3-C4	-6.95	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	343	U	N3-C4	-6.94	1.32	1.38
36	5	882	A	N3-C4	-6.92	1.30	1.34
36	1	1154	A	N7-C5	-6.90	1.35	1.39
36	1	342	A	N9-C4	-6.86	1.33	1.37
1	6	1537	C	C2-N3	6.85	1.41	1.35
36	1	895	A	C5-C6	-6.84	1.34	1.41
36	1	925	A	N3-C4	-6.80	1.30	1.34
57	n1	104	GLU	CB-CG	6.78	1.65	1.52
36	1	1147	G	N9-C8	-6.76	1.33	1.37
36	1	1364	C	N1-C6	-6.75	1.33	1.37
36	1	3054	U	C4-O4	6.74	1.29	1.23
36	5	1189	C	N1-C6	-6.74	1.33	1.37
36	1	667	C	N3-C4	-6.72	1.29	1.33
36	1	2946	A	N7-C5	-6.71	1.35	1.39
36	5	924	G	C2-N3	-6.71	1.27	1.32
36	5	2138	A	N3-C4	-6.71	1.30	1.34
36	1	1367	G	N7-C5	-6.71	1.35	1.39
1	6	623	A	N9-C4	-6.66	1.33	1.37
36	5	1844	C	N3-C4	-6.66	1.29	1.33
36	1	884	A	N7-C5	-6.64	1.35	1.39
36	5	1189	C	N1-C2	-6.62	1.33	1.40
36	5	2243	A	N3-C4	-6.62	1.30	1.34
36	1	2645	G	N9-C8	-6.61	1.33	1.37
36	5	2917	G	N7-C5	-6.60	1.35	1.39
36	5	639	G	N9-C8	-6.58	1.33	1.37
36	1	638	C	N1-C6	-6.58	1.33	1.37
40	l3	251	CYS	CB-SG	-6.58	1.71	1.82
36	1	2138	A	N3-C4	-6.56	1.30	1.34
36	1	338	A	N7-C5	-6.56	1.35	1.39
36	1	2986	U	N1-C2	-6.54	1.32	1.38
36	5	1200	A	N3-C4	-6.54	1.30	1.34
36	1	1103	A	N7-C5	6.52	1.43	1.39
36	1	2169	G	C5-C6	6.52	1.48	1.42
36	1	92	G	N1-C2	-6.52	1.32	1.37
36	1	701	G	N3-C4	-6.51	1.30	1.35
36	1	423	A	N3-C4	-6.50	1.30	1.34
36	1	2404	A	N9-C4	6.49	1.41	1.37
36	1	1308	A	N3-C4	-6.48	1.30	1.34
36	1	1116	G	C5-C4	-6.47	1.33	1.38
36	1	1103	A	N9-C4	6.47	1.41	1.37
36	1	2977	G	C5-C4	-6.46	1.33	1.38
1	6	1800	A	N9-C4	6.45	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2970	C	N1-C6	-6.44	1.33	1.37
36	1	661	G	N1-C2	-6.42	1.32	1.37
36	1	34	A	N9-C4	-6.41	1.34	1.37
36	1	2619	G	C5-C4	-6.41	1.33	1.38
44	17	56	GLU	CG-CD	6.41	1.61	1.51
36	5	367	A	N9-C4	-6.40	1.34	1.37
47	m0	8	CYS	CB-SG	-6.39	1.71	1.82
36	5	883	A	C6-N1	-6.39	1.31	1.35
36	5	2875	U	C2-N3	6.39	1.42	1.37
36	1	919	U	C2-N3	-6.39	1.33	1.37
36	1	2396	G	N9-C8	-6.38	1.33	1.37
36	1	2138	A	N7-C5	-6.37	1.35	1.39
36	5	2954	U	N1-C2	6.37	1.44	1.38
36	1	2977	G	N1-C2	-6.37	1.32	1.37
36	5	2243	A	N9-C4	-6.37	1.34	1.37
36	5	523	A	N3-C4	-6.36	1.31	1.34
36	1	345	G	N9-C8	-6.35	1.33	1.37
36	5	804	C	N1-C6	-6.35	1.33	1.37
36	1	2326	A	N9-C4	-6.34	1.34	1.37
36	1	1371	G	C5-C4	-6.34	1.33	1.38
36	5	2704	A	N9-C4	-6.33	1.34	1.37
36	1	2357	A	N7-C5	-6.32	1.35	1.39
36	5	1331	U	C4-O4	-6.30	1.18	1.23
36	1	3273	A	N3-C4	-6.30	1.31	1.34
52	M6	100	GLU	CG-CD	6.29	1.61	1.51
36	1	2616	C	N1-C6	-6.29	1.33	1.37
41	14	94	CYS	CB-SG	-6.28	1.71	1.82
36	5	1159	A	N9-C4	-6.27	1.34	1.37
51	M5	152	CYS	CB-SG	-6.27	1.71	1.82
36	1	1369	A	N7-C5	-6.27	1.35	1.39
36	5	2881	C	C2-N3	-6.26	1.30	1.35
36	5	2943	G	N7-C5	-6.25	1.35	1.39
36	1	1116	G	N9-C8	-6.24	1.33	1.37
36	1	1142	G	C6-N1	-6.24	1.35	1.39
36	5	576	C	N1-C6	-6.24	1.33	1.37
36	1	716	A	N9-C4	-6.23	1.34	1.37
1	6	1744	A	N9-C4	-6.22	1.34	1.37
36	5	1061	A	N9-C4	-6.21	1.34	1.37
36	5	1177	G	C6-N1	-6.20	1.35	1.39
36	5	2872	A	N9-C4	-6.19	1.34	1.37
36	5	3218	A	C5-C6	-6.18	1.35	1.41
36	5	424	G	C5-C6	-6.16	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2855	U	C2-N3	-6.15	1.33	1.37
36	1	919	U	C4-O4	-6.15	1.18	1.23
36	1	1399	A	N9-C4	-6.15	1.34	1.37
36	1	716	A	C5-C6	-6.13	1.35	1.41
36	1	874	U	C2-N3	-6.13	1.33	1.37
36	1	1518	U	C4-O4	6.13	1.28	1.23
36	5	420	G	N9-C8	-6.12	1.33	1.37
36	1	3178	A	N7-C5	-6.12	1.35	1.39
36	1	653	A	C5-C6	-6.12	1.35	1.41
36	5	3107	U	C2-N3	-6.11	1.33	1.37
36	1	2893	C	N3-C4	-6.11	1.29	1.33
36	1	2640	A	C6-N6	-6.10	1.29	1.33
36	1	2333	C	N3-C4	-6.09	1.29	1.33
36	1	2939	G	N9-C8	-6.08	1.33	1.37
36	1	2986	U	C2-N3	-6.08	1.33	1.37
36	1	1405	U	N3-C4	-6.08	1.32	1.38
36	5	1904	C	N1-C6	-6.07	1.33	1.37
38	8	41	A	N7-C5	-6.06	1.35	1.39
36	1	646	A	C6-N1	-6.06	1.31	1.35
57	n1	104	GLU	CG-CD	6.06	1.61	1.51
36	1	35	A	C5-C6	-6.06	1.35	1.41
36	1	34	A	N3-C4	-6.05	1.31	1.34
36	1	656	A	N7-C5	-6.04	1.35	1.39
36	5	960	U	C4-O4	6.03	1.28	1.23
36	5	2334	U	C4-O4	-6.03	1.18	1.23
36	5	2620	G	C2-N3	-6.03	1.27	1.32
36	5	2986	U	N1-C6	-6.02	1.32	1.38
36	1	1114	U	C2-N3	-6.02	1.33	1.37
36	5	2943	G	N9-C8	-6.02	1.33	1.37
36	1	695	C	N1-C6	-6.01	1.33	1.37
36	5	1308	A	C6-N1	-6.00	1.31	1.35
36	5	2401	A	N3-C4	5.99	1.38	1.34
36	1	1103	A	N3-C4	5.98	1.38	1.34
36	5	2851	A	N3-C4	-5.97	1.31	1.34
36	5	1843	C	N1-C6	-5.96	1.33	1.37
36	1	1367	G	N9-C8	-5.96	1.33	1.37
36	1	2818	U	C2-N3	-5.96	1.33	1.37
36	1	2969	A	N7-C5	-5.95	1.35	1.39
36	5	793	C	N1-C6	-5.94	1.33	1.37
36	1	1417	G	N9-C4	-5.94	1.33	1.38
36	1	2357	A	C5-C6	-5.92	1.35	1.41
36	5	1148	G	N7-C5	-5.92	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	945	C	N3-C4	-5.92	1.29	1.33
36	1	636	C	C4-C5	-5.91	1.38	1.43
36	5	1858	A	N3-C4	-5.90	1.31	1.34
36	5	2987	A	N7-C5	-5.90	1.35	1.39
36	1	3142	A	N3-C4	-5.89	1.31	1.34
36	5	2394	G	N7-C5	-5.89	1.35	1.39
36	5	970	A	N9-C4	-5.88	1.34	1.37
36	5	1872	C	N3-C4	-5.87	1.29	1.33
36	1	2406	C	N1-C6	-5.86	1.33	1.37
36	5	2879	C	N1-C6	-5.86	1.33	1.37
1	6	17	C	N3-C4	-5.86	1.29	1.33
36	5	2855	U	N3-C4	-5.86	1.33	1.38
36	1	36	C	N1-C6	-5.85	1.33	1.37
36	5	2937	G	C5-C4	-5.85	1.34	1.38
36	5	1049	C	C4-C5	-5.84	1.38	1.43
36	5	2917	G	C5-C4	-5.84	1.34	1.38
36	5	895	A	N3-C4	-5.84	1.31	1.34
36	5	2358	A	N9-C4	-5.84	1.34	1.37
36	5	2818	U	C2-N3	-5.84	1.33	1.37
36	5	1874	A	N9-C4	-5.84	1.34	1.37
36	5	2910	A	N9-C4	-5.83	1.34	1.37
47	M0	8	CYS	CB-SG	-5.83	1.72	1.81
36	1	2939	G	C5-C4	-5.83	1.34	1.38
36	5	344	A	N7-C5	-5.83	1.35	1.39
36	1	2396	G	N3-C4	-5.83	1.31	1.35
36	5	1302	A	N7-C5	-5.83	1.35	1.39
36	5	1159	A	C5-C6	-5.82	1.35	1.41
36	5	2755	C	N3-C4	-5.82	1.29	1.33
36	5	2393	G	C5-C4	-5.81	1.34	1.38
36	1	886	C	N1-C6	-5.81	1.33	1.37
36	1	402	A	N3-C4	-5.80	1.31	1.34
36	5	523	A	N9-C4	-5.79	1.34	1.37
36	5	3374	U	C4-O4	-5.79	1.19	1.23
36	1	943	U	C2-N3	-5.79	1.33	1.37
36	1	3180	A	N7-C5	-5.79	1.35	1.39
36	5	1149	G	N9-C8	-5.78	1.33	1.37
36	5	2816	G	C5-C4	-5.78	1.34	1.38
36	1	2401	A	C5-C4	5.78	1.42	1.38
36	1	2620	G	N9-C4	-5.77	1.33	1.38
36	1	1153	A	N7-C5	-5.77	1.35	1.39
37	7	98	C	N1-C6	-5.77	1.33	1.37
36	5	653	A	C6-N6	-5.75	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	7	73	C	N1-C6	5.75	1.40	1.37
36	5	2876	C	N3-C4	-5.75	1.29	1.33
36	5	424	G	C5-C4	-5.75	1.34	1.38
36	1	92	G	C6-N1	-5.74	1.35	1.39
36	1	1371	G	N9-C8	-5.74	1.33	1.37
36	1	1891	A	N9-C4	-5.73	1.34	1.37
36	5	635	G	C5-C6	-5.73	1.36	1.42
36	5	2360	C	C4-C5	-5.73	1.38	1.43
36	5	2386	A	N7-C5	-5.73	1.35	1.39
1	2	1750	A	N7-C5	-5.73	1.35	1.39
36	1	1340	G	N9-C8	-5.73	1.33	1.37
36	1	2358	A	N3-C4	-5.73	1.31	1.34
36	1	2426	U	C2-N3	-5.73	1.33	1.37
36	1	1429	G	N9-C8	-5.72	1.33	1.37
36	5	3137	C	N3-C4	-5.72	1.29	1.33
36	5	957	C	N3-C4	-5.72	1.29	1.33
36	5	2375	G	C6-N1	-5.72	1.35	1.39
36	5	642	U	C2-N3	-5.71	1.33	1.37
36	1	1116	G	N3-C4	-5.71	1.31	1.35
36	5	2139	A	N3-C4	-5.71	1.31	1.34
36	5	3323	A	N9-C4	-5.71	1.34	1.37
1	6	317	C	N3-C4	-5.70	1.29	1.33
36	5	2819	A	N3-C4	-5.70	1.31	1.34
36	5	1432	C	N3-C4	-5.70	1.29	1.33
36	5	1137	C	N1-C6	-5.69	1.33	1.37
36	1	2869	U	N1-C2	-5.69	1.33	1.38
36	1	2138	A	N9-C4	-5.68	1.34	1.37
36	1	100	A	N3-C4	-5.68	1.31	1.34
36	1	2147	A	N9-C4	-5.67	1.34	1.37
36	1	2875	U	N3-C4	5.67	1.43	1.38
36	5	1307	G	P-O5'	-5.67	1.54	1.59
36	5	941	G	C6-N1	-5.67	1.35	1.39
36	5	943	U	C2-N3	-5.67	1.33	1.37
36	5	1902	G	N3-C4	-5.66	1.31	1.35
36	1	743	C	N1-C2	-5.66	1.34	1.40
36	1	1538	G	C6-N1	-5.65	1.35	1.39
36	5	1205	A	N7-C5	-5.65	1.35	1.39
36	1	1835	A	N9-C4	-5.65	1.34	1.37
36	5	3060	C	C4-C5	-5.64	1.38	1.43
36	1	635	G	C5-C4	-5.63	1.34	1.38
36	5	1146	C	N1-C6	-5.63	1.33	1.37
36	5	3207	U	C2-N3	5.63	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	1313	G	C5-C6	-5.63	1.36	1.42
36	5	2939	G	N9-C8	-5.63	1.33	1.37
36	1	1371	G	N7-C5	-5.62	1.35	1.39
36	5	577	C	N1-C6	-5.62	1.33	1.37
36	1	2130	G	C6-N1	-5.62	1.35	1.39
36	1	2396	G	C5-C4	-5.62	1.34	1.38
36	5	960	U	N1-C2	5.62	1.43	1.38
36	5	1199	C	N1-C6	-5.62	1.33	1.37
36	5	3218	A	N9-C4	-5.61	1.34	1.37
36	1	1373	A	C6-N1	-5.61	1.31	1.35
36	5	2363	A	N7-C5	-5.60	1.35	1.39
36	5	3047	U	N1-C6	-5.60	1.32	1.38
36	1	1429	G	C8-N7	-5.60	1.27	1.30
36	5	934	G	C5-C6	-5.60	1.36	1.42
1	6	1137	A	C5-C4	-5.60	1.34	1.38
36	1	940	G	C6-N1	-5.59	1.35	1.39
36	5	2401	A	N9-C4	5.59	1.41	1.37
36	1	2838	A	N9-C4	-5.59	1.34	1.37
36	5	967	A	C5-C4	-5.58	1.34	1.38
36	5	957	C	N1-C6	-5.58	1.33	1.37
36	5	793	C	C4-C5	-5.58	1.38	1.43
36	1	931	C	N3-C4	-5.57	1.30	1.33
36	1	2404	A	N7-C5	5.56	1.42	1.39
36	5	406	G	N1-C2	-5.56	1.33	1.37
52	M6	100	GLU	CD-OE2	5.56	1.31	1.25
36	1	1149	G	C6-O6	5.55	1.29	1.24
1	6	359	A	N9-C4	-5.55	1.34	1.37
36	5	820	A	N7-C5	-5.55	1.35	1.39
36	5	3206	C	N3-C4	-5.55	1.30	1.33
36	1	659	G	N3-C4	-5.55	1.31	1.35
36	5	2244	A	N9-C4	-5.54	1.34	1.37
36	1	1164	G	N7-C5	-5.54	1.35	1.39
36	5	3106	A	C5-C6	-5.54	1.36	1.41
36	5	2799	A	C6-N1	-5.53	1.31	1.35
36	1	919	U	N3-C4	-5.53	1.33	1.38
36	1	661	G	N7-C5	-5.52	1.35	1.39
36	5	3083	G	N1-C2	-5.52	1.33	1.37
1	6	1537	C	N1-C6	5.52	1.40	1.37
36	5	3183	A	C5-C6	-5.51	1.36	1.41
36	1	960	U	C2-N3	5.51	1.41	1.37
36	1	1886	A	N9-C4	-5.51	1.34	1.37
36	5	2814	G	C5-C4	-5.51	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2338	C	N1-C6	-5.50	1.33	1.37
36	5	2913	C	N1-C6	-5.50	1.33	1.37
1	6	1119	G	C6-N1	-5.50	1.35	1.39
36	5	903	U	C2-N3	-5.50	1.33	1.37
36	1	2281	A	N9-C4	-5.49	1.34	1.37
36	1	2169	G	N7-C5	5.49	1.42	1.39
36	5	2287	C	N3-C4	-5.49	1.30	1.33
36	5	659	G	C5-C4	-5.48	1.34	1.38
36	1	913	A	N7-C5	-5.48	1.35	1.39
76	q0	99	CYS	CB-SG	-5.48	1.72	1.81
36	5	650	C	N3-C4	-5.48	1.30	1.33
36	1	2396	G	N7-C5	-5.48	1.35	1.39
1	6	1765	A	N9-C4	-5.48	1.34	1.37
36	1	402	A	C5-C4	-5.47	1.34	1.38
36	5	2591	A	N9-C4	-5.47	1.34	1.37
53	M7	138	LYS	CD-CE	5.46	1.64	1.51
64	N8	48	TYR	CD1-CE1	-5.46	1.31	1.39
36	1	2409	G	N7-C5	-5.46	1.35	1.39
36	1	1116	G	N7-C5	-5.45	1.35	1.39
1	6	163	G	N9-C4	-5.45	1.33	1.38
36	1	938	C	C4-N4	-5.44	1.29	1.33
36	5	1178	G	N3-C4	-5.44	1.31	1.35
52	m6	16	VAL	CB-CG2	-5.44	1.41	1.52
36	1	1304	A	N9-C4	-5.44	1.34	1.37
38	4	138	A	N3-C4	-5.44	1.31	1.34
36	1	659	G	N9-C4	-5.44	1.33	1.38
36	5	1411	C	N1-C6	-5.44	1.33	1.37
36	1	2627	C	N1-C6	-5.44	1.33	1.37
36	5	924	G	N3-C4	-5.44	1.31	1.35
1	2	992	A	N9-C4	-5.43	1.34	1.37
36	5	1304	A	N7-C5	-5.43	1.35	1.39
36	1	206	G	C5-C4	-5.42	1.34	1.38
36	1	960	U	N3-C4	5.42	1.43	1.38
36	1	1593	A	N7-C5	-5.42	1.35	1.39
38	4	50	C	N1-C6	-5.42	1.33	1.37
36	5	2874	G	P-O5'	5.42	1.65	1.59
36	5	1061	A	N3-C4	-5.41	1.31	1.34
36	1	2714	G	N9-C8	5.40	1.41	1.37
36	5	1868	G	C5-C6	-5.40	1.36	1.42
36	1	1156	C	N3-C4	-5.39	1.30	1.33
36	1	2902	A	N3-C4	-5.39	1.31	1.34
36	1	1365	G	N7-C5	-5.39	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2640	A	C6-N1	-5.39	1.31	1.35
36	5	1295	G	N3-C4	-5.39	1.31	1.35
37	7	96	U	N1-C2	-5.39	1.33	1.38
36	1	1375	G	N7-C5	-5.39	1.36	1.39
36	5	1142	G	N3-C4	-5.38	1.31	1.35
36	5	1327	C	N1-C6	-5.38	1.33	1.37
36	5	3039	C	N1-C6	-5.38	1.33	1.37
36	1	2410	U	N1-C2	-5.38	1.33	1.38
36	1	3216	G	C5-C4	-5.38	1.34	1.38
36	5	2910	A	N3-C4	-5.38	1.31	1.34
36	1	609	G	C5-C4	-5.38	1.34	1.38
36	1	1369	A	C5-C4	-5.38	1.34	1.38
36	5	795	G	C5-C4	-5.38	1.34	1.38
36	1	282	G	N1-C2	-5.38	1.33	1.37
38	8	39	G	N7-C5	-5.37	1.36	1.39
36	5	1451	C	N1-C6	-5.37	1.33	1.37
36	1	668	G	C6-N1	-5.35	1.35	1.39
36	5	1195	A	N7-C5	-5.35	1.36	1.39
36	5	1348	U	N1-C2	5.35	1.43	1.38
36	5	2823	G	N7-C5	-5.35	1.36	1.39
1	2	1749	A	N9-C4	-5.35	1.34	1.37
36	5	2957	G	C8-N7	-5.35	1.27	1.30
36	1	1403	C	N1-C6	-5.34	1.33	1.37
36	1	3142	A	N9-C4	-5.34	1.34	1.37
36	5	2860	U	C2-O2	5.34	1.27	1.22
36	1	1395	G	C5-C4	-5.33	1.34	1.38
36	1	2276	G	N7-C5	-5.33	1.36	1.39
36	5	967	A	N3-C4	-5.33	1.31	1.34
36	5	1847	A	N9-C4	-5.33	1.34	1.37
36	5	3130	A	N3-C4	-5.33	1.31	1.34
36	5	3106	A	C5-C4	-5.33	1.35	1.38
37	7	73	C	N3-C4	5.33	1.37	1.33
38	8	96	A	N9-C4	-5.32	1.34	1.37
36	5	2400	G	N9-C4	-5.31	1.33	1.38
36	1	356	C	N1-C6	-5.31	1.33	1.37
36	5	2401	A	N7-C5	5.31	1.42	1.39
36	1	1116	G	N1-C2	-5.31	1.33	1.37
36	5	3120	C	N3-C4	-5.31	1.30	1.33
36	1	661	G	C6-N1	-5.30	1.35	1.39
36	1	1416	C	N3-C4	-5.30	1.30	1.33
36	5	1432	C	C4-C5	-5.30	1.38	1.43
36	5	424	G	N7-C5	-5.30	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1912	U	N1-C2	-5.30	1.33	1.38
36	1	3245	A	N9-C4	-5.30	1.34	1.37
36	1	854	G	N9-C8	-5.30	1.34	1.37
36	5	1320	C	N3-C4	-5.30	1.30	1.33
36	5	1843	C	C4-C5	-5.30	1.38	1.43
36	1	2380	U	C4-O4	-5.29	1.19	1.23
36	1	2818	U	C2-O2	-5.29	1.17	1.22
36	1	2373	A	N7-C5	-5.29	1.36	1.39
36	5	2627	C	N3-C4	-5.29	1.30	1.33
36	1	3000	A	N9-C4	-5.29	1.34	1.37
36	5	657	A	C5-C6	-5.29	1.36	1.41
36	1	908	G	N9-C8	-5.29	1.34	1.37
36	5	1366	A	N3-C4	-5.29	1.31	1.34
36	1	636	C	N1-C6	-5.28	1.33	1.37
36	5	1211	U	C4-O4	-5.28	1.19	1.23
78	q2	74	CYS	CB-SG	5.28	1.91	1.82
36	1	1143	A	N9-C4	-5.28	1.34	1.37
36	1	1148	G	N9-C8	-5.28	1.34	1.37
37	7	89	G	C5-C4	-5.28	1.34	1.38
36	5	646	A	C6-N1	-5.28	1.31	1.35
36	5	1174	G	C5-C4	-5.28	1.34	1.38
36	1	912	G	N9-C8	-5.27	1.34	1.37
36	1	2337	C	N3-C4	-5.27	1.30	1.33
36	1	3173	G	C8-N7	-5.27	1.27	1.30
36	1	1883	A	N9-C4	-5.27	1.34	1.37
36	1	2923	U	N1-C6	-5.27	1.33	1.38
36	5	653	A	C6-N1	-5.27	1.31	1.35
36	1	2910	A	N9-C4	-5.27	1.34	1.37
36	1	33	G	N7-C5	-5.26	1.36	1.39
36	5	3129	A	C5-C6	-5.26	1.36	1.41
36	5	2860	U	N1-C2	5.25	1.43	1.38
36	1	630	A	N7-C5	-5.25	1.36	1.39
1	6	1537	C	C5-C6	5.25	1.38	1.34
69	o3	81	VAL	CB-CG2	-5.25	1.41	1.52
36	5	2128	C	N1-C6	-5.25	1.33	1.37
36	1	591	G	N7-C5	-5.25	1.36	1.39
36	5	1327	C	N3-C4	-5.25	1.30	1.33
36	1	900	G	N9-C8	-5.24	1.34	1.37
36	5	2296	A	C6-N6	-5.24	1.29	1.33
36	1	719	U	N1-C2	5.24	1.43	1.38
36	1	1467	A	N3-C4	-5.24	1.31	1.34
36	1	658	G	C8-N7	-5.23	1.27	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2362	C	N3-C4	-5.23	1.30	1.33
36	5	2368	A	N7-C5	-5.23	1.36	1.39
36	5	658	G	C6-N1	-5.22	1.35	1.39
57	n1	101	CYS	CB-SG	5.22	1.91	1.82
36	5	425	G	N9-C8	-5.22	1.34	1.37
36	1	426	G	N1-C2	-5.22	1.33	1.37
37	7	84	A	C6-N1	-5.22	1.31	1.35
36	5	2375	G	N9-C8	-5.21	1.34	1.37
36	5	2404	A	C5-C6	5.21	1.45	1.41
36	1	653	A	N9-C4	-5.21	1.34	1.37
36	5	971	G	C5-C4	-5.21	1.34	1.38
36	5	2639	G	N7-C5	-5.21	1.36	1.39
36	1	2616	C	C2-N3	-5.21	1.31	1.35
36	1	107	A	C5-C6	-5.20	1.36	1.41
36	1	2762	A	N3-C4	-5.20	1.31	1.34
36	1	1369	A	N9-C4	-5.20	1.34	1.37
36	5	1174	G	N1-C2	-5.20	1.33	1.37
36	5	2893	C	N3-C4	-5.20	1.30	1.33
36	1	653	A	N7-C5	-5.20	1.36	1.39
36	1	2377	G	C5-C4	-5.20	1.34	1.38
36	1	2864	A	C5-C6	-5.20	1.36	1.41
36	5	955	U	C2-N3	-5.20	1.34	1.37
36	5	657	A	C5-C4	-5.20	1.35	1.38
36	5	1148	G	N9-C8	-5.20	1.34	1.37
36	5	2385	G	N9-C4	-5.19	1.33	1.38
36	5	2393	G	C5-C6	-5.19	1.37	1.42
1	6	384	G	N9-C8	-5.19	1.34	1.37
36	5	2167	A	N3-C4	-5.19	1.31	1.34
36	5	94	G	C6-N1	-5.18	1.35	1.39
36	5	2421	U	N3-C4	-5.18	1.33	1.38
36	1	1606	U	N1-C2	-5.18	1.33	1.38
36	5	1103	A	N9-C4	5.18	1.41	1.37
36	1	1379	G	C6-N1	-5.18	1.35	1.39
36	5	3183	A	N7-C5	-5.18	1.36	1.39
1	2	863	A	N9-C4	-5.17	1.34	1.37
36	5	2903	A	N9-C4	-5.17	1.34	1.37
36	1	1326	A	N9-C4	-5.17	1.34	1.37
36	5	2399	A	N9-C4	-5.17	1.34	1.37
36	5	2743	A	N7-C5	-5.17	1.36	1.39
36	1	2811	A	N9-C4	-5.17	1.34	1.37
1	6	397	A	N9-C4	-5.17	1.34	1.37
36	5	227	G	C6-O6	5.17	1.28	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	1402	C	N3-C4	-5.17	1.30	1.33
36	1	1192	C	N3-C4	5.16	1.37	1.33
36	5	645	A	C5-C6	5.16	1.45	1.41
36	5	2908	G	C5-C4	-5.16	1.34	1.38
36	5	428	A	N7-C5	-5.16	1.36	1.39
36	1	2923	U	C5-C6	-5.16	1.29	1.34
36	1	424	G	C5-C4	-5.15	1.34	1.38
36	5	1476	G	N3-C4	-5.15	1.31	1.35
36	5	2851	A	N9-C4	-5.15	1.34	1.37
36	5	636	C	N1-C6	-5.15	1.34	1.37
36	5	1328	C	N1-C6	-5.15	1.34	1.37
36	5	941	G	N1-C2	-5.15	1.33	1.37
36	5	2848	G	N3-C4	-5.15	1.31	1.35
36	5	2430	A	N7-C5	-5.15	1.36	1.39
36	1	1509	A	N9-C4	-5.14	1.34	1.37
36	5	924	G	N9-C4	-5.14	1.33	1.38
36	1	99	A	N7-C5	-5.14	1.36	1.39
36	1	665	A	C6-N1	-5.14	1.31	1.35
36	1	1394	A	N3-C4	-5.14	1.31	1.34
36	1	827	A	C6-N1	-5.14	1.31	1.35
36	5	2881	C	N3-C4	-5.14	1.30	1.33
36	5	636	C	C2-N3	-5.13	1.31	1.35
36	1	958	C	N3-C4	-5.13	1.30	1.33
38	4	23	U	C2-N3	5.13	1.41	1.37
36	1	1308	A	C6-N1	-5.12	1.31	1.35
36	1	790	U	C2-N3	-5.12	1.34	1.37
37	7	86	U	C2-N3	-5.12	1.34	1.37
36	5	416	A	N7-C5	-5.12	1.36	1.39
36	5	397	A	N3-C4	-5.12	1.31	1.34
36	5	2134	G	N1-C2	-5.12	1.33	1.37
36	5	3209	A	N3-C4	5.12	1.38	1.34
36	5	2911	A	C5-C6	-5.12	1.36	1.41
36	5	2950	G	C5-C6	-5.12	1.37	1.42
36	5	2290	C	N1-C6	-5.12	1.34	1.37
38	8	111	A	N7-C5	-5.12	1.36	1.39
36	1	1377	G	N9-C4	-5.11	1.33	1.38
36	5	367	A	C5-C4	-5.11	1.35	1.38
36	5	1889	G	N7-C5	-5.11	1.36	1.39
36	1	2931	C	N1-C6	-5.11	1.34	1.37
36	5	795	G	N3-C4	-5.11	1.31	1.35
36	5	2755	C	C4-C5	-5.11	1.38	1.43
36	1	636	C	N3-C4	-5.11	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	102	U	C2-N3	-5.11	1.34	1.37
36	5	2636	A	C6-N1	-5.10	1.31	1.35
36	5	922	U	C2-N3	-5.10	1.34	1.37
52	m6	80	PHE	CB-CG	-5.10	1.42	1.51
36	5	2379	U	C2-N3	-5.10	1.34	1.37
36	1	2657	A	N9-C4	-5.09	1.34	1.37
36	1	2313	A	N7-C5	-5.09	1.36	1.39
36	5	2389	C	N1-C6	-5.09	1.34	1.37
36	1	970	A	N3-C4	-5.09	1.31	1.34
1	6	317	C	N1-C6	-5.09	1.34	1.37
36	5	3040	A	N9-C4	-5.09	1.34	1.37
53	m7	126	ARG	CG-CD	5.09	1.64	1.51
36	1	21	G	N3-C4	-5.09	1.31	1.35
36	1	3139	A	P-O5'	-5.08	1.54	1.59
1	2	1762	A	N9-C4	-5.08	1.34	1.37
36	1	420	G	N9-C8	-5.08	1.34	1.37
36	5	981	U	N1-C2	5.08	1.43	1.38
36	5	2635	A	C6-N1	-5.08	1.31	1.35
36	5	2944	U	C2-N3	-5.08	1.34	1.37
36	1	933	A	C6-N1	-5.08	1.31	1.35
36	5	3005	A	N7-C5	-5.08	1.36	1.39
36	5	2954	U	C4-O4	5.07	1.27	1.23
36	5	884	A	N9-C4	-5.07	1.34	1.37
36	5	3138	U	C2-N3	-5.07	1.34	1.37
36	1	1119	C	N1-C6	-5.07	1.34	1.37
36	1	2358	A	C6-N1	-5.07	1.32	1.35
36	5	668	G	C6-N1	-5.07	1.36	1.39
36	5	2813	A	N7-C5	-5.07	1.36	1.39
36	5	2134	G	C6-N1	-5.06	1.36	1.39
36	5	2954	U	N3-C4	5.06	1.43	1.38
36	1	2401	A	C6-N1	5.05	1.39	1.35
36	5	3086	A	N3-C4	-5.05	1.31	1.34
36	1	2188	A	N9-C4	-5.05	1.34	1.37
36	1	2816	G	C5-C4	-5.05	1.34	1.38
36	1	884	A	N9-C4	-5.04	1.34	1.37
36	1	2986	U	C2-O2	-5.04	1.17	1.22
36	1	3147	G	C6-N1	-5.04	1.36	1.39
36	5	1311	G	C5-C4	-5.04	1.34	1.38
36	5	2860	U	C2-N3	5.04	1.41	1.37
36	1	826	G	C5-C4	-5.04	1.34	1.38
36	1	2797	C	N1-C6	-5.04	1.34	1.37
36	1	744	A	N9-C4	-5.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	930	U	C4-O4	-5.04	1.19	1.23
36	1	2355	G	N7-C5	-5.04	1.36	1.39
36	1	2968	G	N3-C4	-5.04	1.31	1.35
36	5	2409	G	C5-C4	-5.04	1.34	1.38
36	1	144	A	N9-C4	-5.03	1.34	1.37
36	1	651	G	N9-C4	5.03	1.42	1.38
36	5	1445	U	N1-C2	-5.03	1.34	1.38
36	5	967	A	C6-N1	-5.03	1.32	1.35
36	5	2792	A	N9-C4	5.03	1.40	1.37
36	5	2811	A	C6-N1	-5.03	1.32	1.35
36	5	2937	G	N9-C8	-5.03	1.34	1.37
36	5	1163	A	C6-N1	-5.03	1.32	1.35
36	5	3197	G	N9-C8	5.03	1.41	1.37
36	5	295	A	N9-C4	-5.02	1.34	1.37
36	1	206	G	N1-C2	-5.02	1.33	1.37
36	1	1660	C	C2-N3	-5.02	1.31	1.35
36	1	3209	A	C5-C4	5.02	1.42	1.38
36	5	2934	A	C6-N1	-5.02	1.32	1.35
37	7	11	A	C5-C6	-5.02	1.36	1.41
36	5	924	G	C5-C4	-5.01	1.34	1.38
36	5	2412	G	N7-C5	-5.01	1.36	1.39
36	1	2605	G	N9-C4	-5.01	1.33	1.38
36	1	805	G	N9-C8	-5.01	1.34	1.37
40	L3	200	GLU	CG-CD	5.01	1.59	1.51
36	5	2326	A	N3-C4	-5.01	1.31	1.34
42	15	257	GLU	CG-CD	5.01	1.59	1.51

All (5562) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	28.50	142.85	128.60
36	5	1152	G	N3-C4-N9	-25.34	110.80	126.00
36	5	1152	G	C2-N3-C4	-23.17	100.31	111.90
36	5	424	G	C5-C6-O6	-17.79	117.92	128.60
36	5	1152	G	C5-N7-C8	-14.52	97.04	104.30
36	1	1495	U	C5-C6-N1	-14.28	115.56	122.70
36	1	2714	G	N3-C4-C5	14.15	135.67	128.60
36	1	1149	G	N1-C6-O6	14.12	128.37	119.90
36	5	3183	A	N1-C6-N6	13.96	126.97	118.60
36	1	2714	G	N3-C4-N9	-13.57	117.86	126.00
36	1	3306	U	C5-C4-O4	13.38	133.93	125.90
36	5	1152	G	C4-C5-N7	13.26	116.11	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	922	U	N3-C2-O2	-13.25	112.92	122.20
36	5	1152	G	C8-N9-C1'	13.12	144.06	127.00
36	1	3306	U	N3-C4-O4	-13.08	110.25	119.40
36	5	3245	A	C2-N3-C4	-12.91	104.14	110.60
36	1	2617	U	N1-C2-N3	12.84	122.61	114.90
36	5	2199	G	N1-C6-O6	12.78	127.57	119.90
1	2	553	G	N1-C6-O6	12.67	127.50	119.90
36	5	2954	U	C2-N1-C1'	12.63	132.85	117.70
1	6	163	G	N3-C4-N9	-12.61	118.43	126.00
36	1	1849	C	O5'-P-OP1	-12.61	94.35	105.70
36	1	1367	G	N1-C6-O6	12.56	127.44	119.90
36	1	2355	G	N1-C6-O6	12.50	127.40	119.90
36	5	672	A	N1-C6-N6	12.49	126.10	118.60
36	5	776	U	C5-C6-N1	-12.38	116.51	122.70
36	1	282	G	O5'-P-OP1	-12.31	94.62	105.70
36	5	3245	A	C5-N7-C8	-12.22	97.79	103.90
1	6	1773	C	N3-C4-C5	-12.14	117.05	121.90
36	1	2884	C	N3-C4-C5	12.12	126.75	121.90
36	5	2364	G	C5-C6-O6	12.12	135.87	128.60
36	1	1149	G	N3-C2-N2	-11.92	111.55	119.90
36	5	861	C	C6-N1-C2	11.90	125.06	120.30
36	5	96	G	O5'-P-OP2	-11.87	95.01	105.70
36	5	3245	A	N1-C6-N6	11.86	125.72	118.60
36	1	3278	C	N1-C2-O2	11.84	126.00	118.90
1	6	1657	U	O5'-P-OP2	-11.80	95.08	105.70
36	5	1152	G	C4-N9-C1'	-11.80	111.16	126.50
36	5	3183	A	C5-C6-N6	-11.76	114.29	123.70
36	5	398	A	O5'-P-OP2	-11.76	95.12	105.70
37	7	93	C	O5'-P-OP2	-11.65	95.22	105.70
36	1	1846	C	O5'-P-OP1	-11.50	95.35	105.70
36	5	2400	G	C5-C6-O6	-11.46	121.72	128.60
36	5	424	G	N1-C6-O6	11.45	126.77	119.90
36	5	2726	C	C5-C4-N4	11.43	128.20	120.20
36	5	2400	G	N1-C6-O6	11.37	126.72	119.90
36	1	1001	G	N1-C6-O6	11.34	126.70	119.90
36	5	2899	C	C6-N1-C2	-11.34	115.77	120.30
36	5	2818	U	O5'-P-OP1	-11.33	95.50	105.70
36	5	3218	A	N1-C6-N6	11.26	125.36	118.60
36	5	216	G	N1-C6-O6	11.25	126.65	119.90
36	5	220	G	O5'-P-OP2	-11.13	95.68	105.70
36	1	1891	A	C8-N9-C4	11.13	110.25	105.80
36	5	2372	A	C8-N9-C4	-11.10	101.36	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	80	A	C8-N9-C4	-11.10	101.36	105.80
36	1	2846	U	N3-C2-O2	-11.09	114.43	122.20
36	5	1116	G	O5'-P-OP1	-11.08	95.73	105.70
36	1	888	A	N1-C6-N6	11.06	125.24	118.60
1	6	1473	U	N3-C2-O2	-11.04	114.47	122.20
36	1	1182	A	O5'-P-OP1	-11.03	95.78	105.70
36	1	716	A	N1-C6-N6	11.01	125.21	118.60
36	5	2700	G	C5-C6-O6	-11.01	121.99	128.60
36	5	877	C	N3-C4-C5	11.00	126.30	121.90
36	1	1838	G	N1-C6-O6	10.98	126.49	119.90
36	5	2726	C	C6-N1-C2	-10.86	115.96	120.30
37	3	94	C	N1-C2-O2	-10.85	112.39	118.90
36	1	1152	G	O5'-P-OP1	-10.82	95.96	105.70
36	5	2935	U	O5'-P-OP2	-10.81	95.97	105.70
1	2	1200	G	N1-C6-O6	10.78	126.37	119.90
36	5	3245	A	N7-C8-N9	10.78	119.19	113.80
36	1	2617	U	C4-C5-C6	10.72	126.13	119.70
1	2	137	U	O5'-P-OP1	-10.71	96.06	105.70
36	1	2870	C	C2-N1-C1'	-10.67	107.06	118.80
36	1	776	U	C4-C5-C6	10.67	126.10	119.70
36	1	639	G	N1-C6-O6	10.66	126.30	119.90
36	1	938	C	C5-C4-N4	-10.65	112.74	120.20
36	5	205	C	O5'-P-OP1	-10.64	96.12	105.70
36	5	2393	G	C5-C6-O6	-10.58	122.25	128.60
38	4	94	C	C6-N1-C2	10.55	124.52	120.30
36	1	1381	A	O5'-P-OP2	10.54	123.34	110.70
36	5	3245	A	C6-C5-N7	-10.53	124.93	132.30
36	5	2373	A	O5'-P-OP1	-10.51	96.24	105.70
36	5	1184	A	N1-C6-N6	-10.43	112.34	118.60
36	5	1117	G	O5'-P-OP1	-10.36	96.37	105.70
36	1	304	G	C4-C5-N7	-10.34	106.67	110.80
36	1	2714	G	C2-N3-C4	-10.34	106.73	111.90
36	1	1303	A	C8-N9-C4	10.33	109.93	105.80
36	1	1790	G	N1-C6-O6	10.32	126.09	119.90
36	1	939	U	O5'-P-OP2	-10.28	96.45	105.70
36	5	2971	A	C2-N3-C4	10.26	115.73	110.60
1	2	577	G	N1-C6-O6	10.24	126.05	119.90
36	1	2337	C	C6-N1-C2	-10.24	116.20	120.30
36	5	645	A	C6-N1-C2	-10.23	112.46	118.60
36	5	3141	A	O5'-P-OP1	-10.21	96.51	105.70
36	5	424	G	C4-C5-N7	10.20	114.88	110.80
36	5	2385	G	N3-C4-C5	10.20	133.70	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2624	G	C8-N9-C4	-10.19	102.32	106.40
36	5	2199	G	C6-C5-N7	-10.17	124.30	130.40
36	1	895	A	N1-C6-N6	10.16	124.70	118.60
36	1	957	C	N1-C2-O2	-10.16	112.80	118.90
36	1	1166	G	N1-C6-O6	10.09	125.95	119.90
36	5	1373	A	N1-C6-N6	10.08	124.65	118.60
36	5	1592	G	C5-C6-N1	-10.06	106.47	111.50
36	1	940	G	N1-C6-O6	-10.03	113.88	119.90
1	2	1039	A	O4'-C1'-N9	10.02	116.21	108.20
36	5	889	U	N3-C4-C5	9.97	120.58	114.60
36	5	3362	A	C2-N3-C4	-9.96	105.62	110.60
36	1	1433	A	C8-N9-C4	-9.96	101.82	105.80
36	5	2199	G	C5-C6-O6	-9.96	122.63	128.60
36	5	973	A	N1-C6-N6	9.94	124.57	118.60
36	5	1152	G	N3-C2-N2	-9.94	112.94	119.90
36	5	1912	U	N3-C2-O2	9.92	129.14	122.20
36	5	1897	G	N1-C6-O6	9.91	125.85	119.90
36	1	1495	U	C4-C5-C6	9.90	125.64	119.70
36	1	2983	C	C5-C6-N1	-9.90	116.05	121.00
1	2	577	G	C4-C5-N7	9.89	114.76	110.80
36	1	3181	C	C5-C4-N4	9.89	127.13	120.20
36	1	2760	C	N1-C2-O2	-9.89	112.97	118.90
36	1	1838	G	C5-C6-O6	-9.88	122.67	128.60
36	5	2136	C	C5-C6-N1	-9.88	116.06	121.00
36	5	630	A	C2-N3-C4	-9.87	105.66	110.60
36	1	2831	G	N1-C6-O6	9.87	125.82	119.90
36	1	2374	C	C6-N1-C2	-9.86	116.36	120.30
36	1	1329	U	C2-N1-C1'	9.86	129.53	117.70
36	1	406	G	O4'-C1'-N9	9.85	116.08	108.20
36	5	1416	C	N3-C4-C5	9.84	125.83	121.90
36	5	2857	C	N3-C4-C5	9.83	125.83	121.90
1	2	542	A	O4'-C1'-N9	9.81	116.05	108.20
36	5	948	C	C6-N1-C2	9.81	124.23	120.30
36	1	2693	C	C6-N1-C2	9.81	124.22	120.30
36	1	3344	A	N7-C8-N9	9.78	118.69	113.80
1	6	1773	C	N1-C2-O2	-9.78	113.03	118.90
36	1	2395	G	O5'-P-OP2	-9.77	96.91	105.70
36	5	1372	C	C6-N1-C2	9.77	124.21	120.30
36	5	2395	G	O5'-P-OP2	-9.76	96.91	105.70
36	1	1403	C	C6-N1-C2	9.75	124.20	120.30
36	5	1308	A	C8-N9-C4	-9.74	101.90	105.80
36	1	304	G	N9-C4-C5	9.73	109.29	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2405	C	C6-N1-C2	-9.73	116.41	120.30
36	5	1592	G	C8-N9-C4	-9.72	102.51	106.40
36	5	1149	G	N1-C6-O6	9.71	125.73	119.90
36	1	2121	G	N3-C2-N2	9.70	126.69	119.90
36	1	439	C	N1-C2-O2	9.68	124.70	118.90
36	1	635	G	C5-C6-O6	-9.67	122.80	128.60
36	5	938	C	N3-C4-C5	9.67	125.77	121.90
36	5	1592	G	C5-C6-O6	9.67	134.40	128.60
36	1	895	A	C2-N3-C4	-9.64	105.78	110.60
36	1	1367	G	C5-C6-O6	-9.64	122.82	128.60
36	5	3245	A	C4-C5-N7	9.64	115.52	110.70
36	5	1173	U	O5'-P-OP2	-9.62	97.04	105.70
1	6	163	G	N3-C4-C5	9.61	133.41	128.60
36	5	693	A	O5'-P-OP1	-9.61	97.06	105.70
36	5	957	C	N3-C2-O2	-9.60	115.18	121.90
36	1	2379	U	N1-C2-O2	-9.60	116.08	122.80
36	1	67	A	O5'-P-OP1	-9.59	97.07	105.70
36	1	1192	C	C2-N1-C1'	9.57	129.32	118.80
1	2	553	G	C5-C6-O6	-9.56	122.86	128.60
38	8	80	A	N7-C8-N9	9.56	118.58	113.80
36	5	1152	G	N1-C6-O6	9.54	125.62	119.90
36	5	2700	G	N1-C6-O6	9.53	125.62	119.90
36	5	2868	U	N1-C2-O2	9.52	129.47	122.80
36	1	1116	G	N3-C4-C5	-9.52	123.84	128.60
36	1	49	A	N1-C6-N6	9.52	124.31	118.60
36	1	3143	C	N3-C2-O2	9.51	128.55	121.90
36	1	2310	U	O5'-P-OP1	-9.49	97.16	105.70
36	1	2169	G	C4-C5-N7	-9.49	107.00	110.80
36	1	1949	G	O5'-P-OP1	-9.47	97.18	105.70
36	1	2987	A	N1-C6-N6	9.46	124.28	118.60
36	5	882	A	N1-C2-N3	9.46	134.03	129.30
36	5	835	G	N1-C6-O6	-9.45	114.23	119.90
36	5	2726	C	N3-C4-N4	-9.44	111.39	118.00
36	1	1454	A	O5'-P-OP1	-9.43	97.21	105.70
36	1	1556	C	N1-C2-O2	9.43	124.56	118.90
36	1	3181	C	N3-C4-N4	-9.41	111.41	118.00
36	5	2400	G	C4-C5-N7	9.40	114.56	110.80
36	1	2621	G	N3-C2-N2	-9.40	113.32	119.90
36	1	969	C	N1-C2-O2	-9.40	113.26	118.90
36	1	716	A	N9-C4-C5	-9.39	102.05	105.80
36	5	2899	C	N1-C2-N3	9.37	125.76	119.20
36	1	422	A	N1-C6-N6	-9.35	112.99	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	645	A	C6-N1-C2	-9.35	112.99	118.60
36	1	1556	C	C6-N1-C2	-9.35	116.56	120.30
38	4	38	U	N3-C2-O2	-9.35	115.66	122.20
36	1	895	A	O5'-P-OP1	-9.35	97.29	105.70
36	5	2726	C	N1-C2-N3	9.35	125.74	119.20
36	5	922	U	N1-C2-O2	9.34	129.34	122.80
36	1	933	A	O5'-P-OP2	-9.34	97.30	105.70
36	5	966	U	N3-C2-O2	-9.34	115.66	122.20
1	6	119	A	C2-N3-C4	-9.33	105.94	110.60
36	5	1316	C	N1-C2-O2	-9.33	113.30	118.90
36	1	1556	C	N3-C2-O2	-9.32	115.38	121.90
36	5	2278	C	C5-C6-N1	9.32	125.66	121.00
36	1	2873	U	C5-C4-O4	9.31	131.49	125.90
36	1	86	G	O5'-P-OP2	-9.30	97.33	105.70
36	1	3269	U	O5'-P-OP2	-9.30	97.33	105.70
36	1	1001	G	C5-C6-O6	-9.26	123.05	128.60
36	1	1116	G	O5'-P-OP1	-9.25	97.37	105.70
36	5	672	A	C6-C5-N7	-9.24	125.83	132.30
36	1	2298	U	N3-C4-O4	-9.23	112.94	119.40
36	5	1306	G	N1-C6-O6	9.23	125.44	119.90
36	1	1306	G	C5-C6-O6	-9.22	123.07	128.60
36	1	2121	G	N1-C6-O6	-9.21	114.37	119.90
36	1	49	A	C8-N9-C4	9.21	109.48	105.80
36	1	2827	U	N3-C2-O2	-9.20	115.76	122.20
36	5	1116	G	N3-C4-C5	-9.20	124.00	128.60
36	1	2343	C	N3-C4-C5	9.19	125.58	121.90
36	5	3197	G	N3-C2-N2	-9.18	113.47	119.90
36	5	437	G	N3-C2-N2	-9.18	113.48	119.90
1	6	1537	C	C6-N1-C2	-9.17	116.63	120.30
37	7	11	A	N1-C6-N6	9.17	124.10	118.60
36	1	639	G	C5-C6-O6	-9.16	123.10	128.60
36	5	2917	G	C5-C6-O6	-9.16	123.11	128.60
36	1	808	A	N1-C2-N3	9.15	133.88	129.30
36	1	933	A	N1-C2-N3	9.15	133.88	129.30
36	1	2833	A	O5'-P-OP2	-9.15	97.46	105.70
36	1	610	G	O5'-P-OP2	-9.14	97.47	105.70
36	1	949	C	C4-C5-C6	9.13	121.97	117.40
36	5	2117	A	N1-C6-N6	-9.13	113.12	118.60
36	1	2870	C	C6-N1-C1'	9.12	131.74	120.80
36	5	2849	C	N3-C2-O2	9.11	128.28	121.90
1	2	453	U	N3-C2-O2	-9.10	115.83	122.20
36	1	304	G	N1-C6-O6	-9.10	114.44	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3344	A	C8-N9-C4	-9.10	102.16	105.80
36	5	1891	A	O5'-P-OP2	-9.09	97.52	105.70
36	5	2893	C	C4-C5-C6	9.09	121.95	117.40
36	5	2364	G	N1-C6-O6	-9.08	114.45	119.90
36	5	2403	G	O5'-P-OP2	-9.08	97.53	105.70
36	1	1846	C	N1-C2-O2	-9.08	113.45	118.90
1	6	453	U	N3-C2-O2	-9.08	115.84	122.20
36	5	938	C	C5-C4-N4	-9.07	113.85	120.20
36	1	895	A	C4-C5-N7	9.07	115.24	110.70
36	1	1901	A	N1-C6-N6	-9.07	113.16	118.60
36	1	397	A	N1-C6-N6	-9.06	113.16	118.60
36	1	2412	G	C5-C6-O6	-9.06	123.17	128.60
36	1	2617	U	N3-C2-O2	-9.05	115.86	122.20
36	5	585	A	O5'-P-OP2	-9.06	97.55	105.70
36	1	3107	U	O5'-P-OP2	-9.05	97.56	105.70
36	5	1161	G	C5-C6-O6	-9.04	123.17	128.60
36	1	2831	G	C5-C6-O6	-9.04	123.18	128.60
36	5	63	A	N1-C6-N6	9.04	124.02	118.60
1	6	957	G	N1-C6-O6	9.03	125.32	119.90
36	1	1329	U	N3-C2-O2	-9.02	115.89	122.20
1	6	1634	C	C2-N1-C1'	9.02	128.72	118.80
36	1	3278	C	N3-C2-O2	-9.02	115.59	121.90
36	1	3122	A	O5'-P-OP1	-9.01	97.59	105.70
36	1	1838	G	C6-C5-N7	-8.99	125.00	130.40
36	5	227	G	O5'-P-OP2	-8.99	97.61	105.70
36	5	1149	G	C5-C6-O6	-8.99	123.20	128.60
36	1	1308	A	C8-N9-C4	-8.99	102.20	105.80
36	1	958	C	N3-C4-C5	8.98	125.49	121.90
36	1	1556	C	C2-N1-C1'	8.98	128.68	118.80
36	1	2148	U	N3-C2-O2	8.97	128.48	122.20
36	1	2624	G	N7-C8-N9	8.97	117.58	113.10
36	5	41	G	C4-C5-N7	8.96	114.38	110.80
36	5	3084	C	O5'-P-OP1	-8.96	97.64	105.70
36	5	1335	C	N1-C2-O2	-8.96	113.53	118.90
36	1	3209	A	N1-C6-N6	8.95	123.97	118.60
36	5	2954	U	C6-N1-C1'	-8.94	108.69	121.20
48	m1	112	LEU	CA-CB-CG	8.93	135.84	115.30
36	5	3218	A	C4-C5-N7	8.92	115.16	110.70
36	1	2983	C	N3-C4-N4	-8.92	111.76	118.00
36	5	2234	G	C5-C6-O6	-8.90	123.26	128.60
36	1	1495	U	C2-N1-C1'	-8.90	107.03	117.70
36	5	2345	A	N1-C6-N6	8.90	123.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	653	A	O5'-P-OP1	-8.89	97.69	105.70
36	5	1373	A	C5-C6-N6	-8.89	116.59	123.70
36	5	1476	G	O5'-P-OP2	-8.89	97.70	105.70
36	1	901	G	N1-C6-O6	8.88	125.23	119.90
36	5	1556	C	C6-N1-C2	-8.88	116.75	120.30
36	5	3137	C	N3-C4-N4	-8.88	111.79	118.00
36	1	895	A	C6-C5-N7	-8.87	126.09	132.30
36	5	1208	U	C5-C4-O4	8.87	131.22	125.90
36	1	1362	G	C8-N9-C4	8.86	109.94	106.40
1	6	163	G	C2-N3-C4	-8.86	107.47	111.90
36	5	337	G	N3-C4-C5	-8.86	124.17	128.60
36	5	1110	U	N1-C2-O2	8.86	129.00	122.80
36	5	1473	G	C8-N9-C4	8.86	109.94	106.40
36	1	2169	G	N1-C6-O6	-8.85	114.59	119.90
36	5	895	A	N1-C2-N3	8.85	133.72	129.30
36	5	3197	G	N3-C4-N9	-8.83	120.70	126.00
36	5	56	G	O5'-P-OP2	-8.82	97.76	105.70
36	5	1142	G	C8-N9-C4	-8.82	102.87	106.40
36	5	963	G	O5'-P-OP2	-8.81	97.77	105.70
36	5	3374	U	N3-C4-O4	-8.80	113.24	119.40
36	1	2816	G	C8-N9-C4	8.80	109.92	106.40
36	5	2400	G	N9-C4-C5	-8.80	101.88	105.40
1	2	334	G	C2-N3-C4	-8.80	107.50	111.90
36	1	608	A	N1-C6-N6	8.79	123.88	118.60
1	2	639	U	N3-C2-O2	-8.79	116.05	122.20
36	5	2400	G	C8-N9-C4	8.79	109.91	106.40
36	5	3209	A	O4'-C1'-N9	8.78	115.23	108.20
36	5	2234	G	C8-N9-C4	8.78	109.91	106.40
36	1	1060	U	C5-C6-N1	-8.77	118.31	122.70
36	5	630	A	C8-N9-C4	8.77	109.31	105.80
36	1	699	A	O5'-P-OP2	-8.76	97.82	105.70
36	5	1879	A	N1-C6-N6	8.76	123.86	118.60
36	5	2205	U	O4'-C1'-N1	8.75	115.20	108.20
36	1	1190	A	N1-C6-N6	8.74	123.84	118.60
36	1	1520	G	N7-C8-N9	-8.74	108.73	113.10
36	1	2996	U	C2-N1-C1'	8.74	128.19	117.70
36	5	2392	C	N3-C4-C5	8.74	125.39	121.90
36	1	1883	A	C8-N9-C4	8.73	109.29	105.80
36	1	2726	C	N3-C4-N4	-8.73	111.89	118.00
36	1	1495	U	N1-C2-N3	8.72	120.14	114.90
36	5	2280	A	C2-N3-C4	-8.72	106.24	110.60
36	1	912	G	C6-N1-C2	-8.71	119.87	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1520	G	C5-N7-C8	8.71	108.66	104.30
36	1	2357	A	N1-C6-N6	8.71	123.83	118.60
36	1	2620	G	N1-C6-O6	8.71	125.12	119.90
36	5	2272	G	O4'-C1'-N9	8.70	115.16	108.20
36	5	3184	A	N1-C6-N6	8.70	123.82	118.60
1	6	435	C	N1-C2-O2	8.69	124.12	118.90
36	5	1879	A	C4-C5-N7	8.69	115.05	110.70
36	5	1208	U	N3-C2-O2	-8.69	116.12	122.20
36	1	3264	G	C8-N9-C4	8.68	109.87	106.40
36	1	2923	U	O5'-P-OP1	-8.66	97.90	105.70
36	5	672	A	C5-C6-N6	-8.66	116.77	123.70
36	1	648	C	O5'-P-OP1	-8.66	97.91	105.70
36	1	2873	U	N3-C2-O2	-8.66	116.14	122.20
36	1	716	A	C4-C5-N7	8.65	115.03	110.70
38	4	47	C	C5-C6-N1	-8.65	116.67	121.00
36	1	2617	U	C5-C6-N1	-8.65	118.38	122.70
36	1	2868	U	N3-C2-O2	-8.64	116.15	122.20
36	1	3057	U	N3-C4-O4	-8.64	113.35	119.40
1	6	1767	G	C8-N9-C4	8.64	109.86	106.40
36	5	3184	A	C8-N9-C4	8.64	109.25	105.80
36	1	716	A	C2-N3-C4	-8.63	106.28	110.60
36	5	1889	G	C5-C6-O6	-8.63	123.42	128.60
36	1	2344	U	O5'-P-OP2	-8.61	97.95	105.70
36	5	1908	A	N9-C4-C5	8.61	109.25	105.80
36	1	1001	G	C6-C5-N7	-8.61	125.24	130.40
1	6	308	C	C5-C6-N1	-8.61	116.70	121.00
36	1	611	A	O5'-P-OP2	-8.60	97.96	105.70
36	1	1313	G	N1-C6-O6	8.60	125.06	119.90
36	1	2937	G	C8-N9-C4	8.60	109.84	106.40
1	2	1096	C	N1-C2-O2	8.59	124.05	118.90
36	5	2315	G	O5'-P-OP1	-8.58	97.98	105.70
36	5	2939	G	C8-N9-C4	8.57	109.83	106.40
36	1	229	G	N3-C2-N2	-8.57	113.90	119.90
36	1	979	U	C6-N1-C2	-8.57	115.86	121.00
1	6	421	A	C8-N9-C4	8.57	109.23	105.80
36	5	3308	C	N1-C2-O2	-8.57	113.76	118.90
1	2	1600	A	C2-N3-C4	-8.57	106.32	110.60
36	1	2606	G	C6-C5-N7	-8.55	125.27	130.40
1	6	1473	U	N1-C2-O2	8.55	128.79	122.80
36	1	972	A	C8-N9-C4	8.55	109.22	105.80
36	1	1326	A	O5'-P-OP1	8.54	120.95	110.70
36	1	897	U	O5'-P-OP1	-8.54	98.01	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1481	A	C8-N9-C4	-8.54	102.38	105.80
36	1	2868	U	N1-C2-O2	8.54	128.78	122.80
73	O7	65	ARG	NE-CZ-NH1	8.54	124.57	120.30
36	5	1910	A	O5'-P-OP1	-8.54	98.02	105.70
36	5	929	A	O5'-P-OP2	-8.53	98.02	105.70
36	1	85	A	O5'-P-OP2	-8.53	98.02	105.70
36	1	2867	C	C2-N3-C4	-8.53	115.64	119.90
36	1	1389	G	C4-C5-N7	8.52	114.21	110.80
36	1	950	G	C4-C5-N7	8.52	114.21	110.80
36	1	2209	U	C5-C6-N1	8.52	126.96	122.70
36	1	143	G	N1-C6-O6	-8.51	114.79	119.90
36	5	358	G	N1-C6-O6	8.50	125.00	119.90
1	2	73	U	O4'-C1'-N1	8.50	115.00	108.20
37	7	101	G	N1-C6-O6	8.50	125.00	119.90
36	5	2953	U	N3-C4-O4	8.49	125.34	119.40
36	1	2808	A	O4'-C1'-N9	-8.47	101.42	108.20
36	5	1156	C	C6-N1-C2	-8.47	116.91	120.30
36	1	1365	G	N3-C4-C5	-8.47	124.37	128.60
36	1	1477	A	O5'-P-OP1	-8.47	98.08	105.70
36	5	934	G	C5-C6-O6	-8.46	123.52	128.60
36	5	2873	U	C5-C6-N1	-8.46	118.47	122.70
36	5	2968	G	C8-N9-C4	8.46	109.78	106.40
36	5	1482	A	O5'-P-OP2	-8.46	98.08	105.70
1	6	1473	U	C5-C4-O4	8.46	130.97	125.90
36	5	216	G	C5-C6-O6	-8.46	123.53	128.60
36	5	706	A	C8-N9-C4	8.46	109.18	105.80
36	5	1851	G	N1-C6-O6	8.45	124.97	119.90
36	1	925	A	N1-C2-N3	8.44	133.52	129.30
36	1	776	U	N1-C2-N3	8.43	119.96	114.90
1	2	453	U	C2-N1-C1'	8.43	127.81	117.70
36	1	2121	G	N1-C2-N2	-8.43	108.62	116.20
36	1	646	A	O5'-P-OP2	-8.42	98.12	105.70
36	5	1710	C	C6-N1-C2	8.42	123.67	120.30
36	5	1143	A	C2-N3-C4	-8.41	106.39	110.60
36	5	1848	G	C5-C6-N1	8.41	115.71	111.50
36	1	1377	G	C4-C5-N7	8.41	114.16	110.80
1	2	447	U	C6-N1-C2	-8.41	115.96	121.00
1	2	1600	A	N1-C6-N6	8.40	123.64	118.60
36	1	3079	U	C2-N1-C1'	-8.40	107.62	117.70
36	5	2796	G	O5'-P-OP2	-8.39	98.14	105.70
36	1	672	A	N1-C6-N6	8.39	123.64	118.60
36	5	518	G	N1-C6-O6	-8.39	114.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1192	C	N3-C2-O2	-8.39	116.03	121.90
36	1	1313	G	C5-C6-O6	-8.38	123.57	128.60
1	6	17	C	N1-C2-O2	8.38	123.93	118.90
36	1	1480	G	C4-C5-N7	8.37	114.15	110.80
36	5	2412	G	N3-C4-C5	-8.36	124.42	128.60
36	5	2145	A	C6-N1-C2	-8.36	113.58	118.60
36	5	960	U	N1-C2-O2	8.35	128.65	122.80
36	5	2234	G	N9-C4-C5	-8.35	102.06	105.40
1	2	577	G	C5-C6-O6	-8.34	123.59	128.60
36	1	1177	G	O5'-P-OP2	-8.33	98.20	105.70
36	1	1405	U	N3-C4-O4	-8.33	113.57	119.40
36	5	939	U	C5-C4-O4	-8.32	120.91	125.90
37	7	120	C	C6-N1-C2	8.32	123.63	120.30
36	1	206	G	N1-C6-O6	-8.31	114.91	119.90
36	1	1306	G	N1-C6-O6	8.31	124.89	119.90
36	1	917	A	N1-C6-N6	-8.31	113.62	118.60
36	1	2169	G	C6-C5-N7	8.31	135.38	130.40
36	5	2954	U	O4'-C1'-N1	8.31	114.84	108.20
36	1	2893	C	N3-C4-N4	-8.30	112.19	118.00
38	4	32	C	N3-C4-C5	8.30	125.22	121.90
1	6	542	A	O5'-P-OP1	-8.30	98.23	105.70
36	5	2996	U	N1-C2-O2	8.30	128.61	122.80
36	1	358	G	N1-C6-O6	8.29	124.87	119.90
36	1	1433	A	N9-C4-C5	8.29	109.11	105.80
36	1	2920	U	C5-C6-N1	-8.28	118.56	122.70
36	1	1001	G	C4-C5-N7	8.28	114.11	110.80
36	1	1187	C	C6-N1-C2	8.28	123.61	120.30
36	1	2625	C	N1-C2-O2	-8.28	113.93	118.90
36	1	811	U	N3-C2-O2	-8.28	116.41	122.20
36	5	2849	C	N1-C2-O2	-8.28	113.93	118.90
36	1	640	U	C5-C4-O4	-8.27	120.94	125.90
36	1	2379	U	C5-C4-O4	-8.27	120.94	125.90
36	1	1797	A	O5'-P-OP1	-8.27	98.26	105.70
36	5	2944	U	N1-C2-O2	8.27	128.59	122.80
36	1	2373	A	O5'-P-OP1	-8.26	98.27	105.70
37	7	90	U	C5-C6-N1	-8.26	118.57	122.70
36	1	2418	G	N3-C4-C5	-8.25	124.47	128.60
1	2	992	A	C2-N3-C4	-8.25	106.47	110.60
36	5	1292	C	C6-N1-C2	8.25	123.60	120.30
36	1	1151	U	C6-N1-C2	-8.24	116.05	121.00
36	5	1481	A	O4'-C1'-N9	8.24	114.80	108.20
36	1	880	G	N1-C6-O6	-8.24	114.96	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2197	C	C6-N1-C2	8.24	123.60	120.30
36	1	2379	U	N3-C4-O4	8.24	125.17	119.40
36	1	2308	C	N1-C2-O2	-8.24	113.96	118.90
36	1	2987	A	C4-C5-C6	8.24	121.12	117.00
36	5	960	U	N3-C2-O2	-8.24	116.43	122.20
36	1	2964	G	O5'-P-OP2	-8.23	98.29	105.70
36	5	776	U	C4-C5-C6	8.23	124.64	119.70
36	5	1154	A	C2-N3-C4	8.23	114.72	110.60
1	2	1761	U	C6-N1-C2	-8.23	116.06	121.00
36	1	2351	U	O5'-P-OP2	8.23	120.57	110.70
36	5	2372	A	N7-C8-N9	8.23	117.91	113.80
36	1	645	A	C5-C6-N1	8.22	121.81	117.70
36	5	3183	A	C6-C5-N7	-8.22	126.55	132.30
36	5	2385	G	C2-N3-C4	-8.21	107.79	111.90
36	5	522	A	O5'-P-OP1	-8.21	98.31	105.70
1	6	453	U	C2-N1-C1'	8.21	127.55	117.70
36	5	2283	G	O5'-P-OP2	-8.21	98.31	105.70
36	5	216	G	C4-C5-N7	8.20	114.08	110.80
36	1	2400	G	C6-C5-N7	-8.20	125.48	130.40
36	1	1313	G	C4-C5-N7	8.20	114.08	110.80
36	5	424	G	N9-C4-C5	-8.19	102.12	105.40
36	1	358	G	C5-C6-O6	-8.19	123.69	128.60
36	5	1592	G	N9-C4-C5	8.18	108.67	105.40
36	1	1367	G	C6-C5-N7	-8.18	125.49	130.40
36	1	3217	C	C2-N1-C1'	8.18	127.80	118.80
1	2	404	G	C8-N9-C4	8.17	109.67	106.40
36	5	1552	G	C5-C6-O6	-8.17	123.70	128.60
36	5	2875	U	N3-C4-O4	8.17	125.12	119.40
36	1	709	A	C8-N9-C4	8.16	109.07	105.80
36	1	2818	U	O5'-P-OP1	-8.16	98.36	105.70
36	1	1175	C	C2-N3-C4	-8.15	115.82	119.90
36	1	2286	U	O5'-P-OP2	-8.14	98.37	105.70
36	5	2572	C	N1-C2-O2	8.14	123.78	118.90
1	2	1274	C	C2-N1-C1'	8.14	127.75	118.80
1	6	1773	C	N3-C4-N4	8.13	123.69	118.00
36	1	339	C	N3-C4-N4	-8.13	112.31	118.00
36	5	2930	A	C5-C6-N1	8.12	121.76	117.70
36	1	2983	C	C5-C4-N4	8.12	125.89	120.20
36	5	2709	C	C6-N1-C2	8.11	123.55	120.30
36	1	1518	U	C4-C5-C6	8.11	124.57	119.70
36	5	800	G	N3-C2-N2	-8.11	114.22	119.90
36	5	1300	G	C5-C6-O6	-8.11	123.73	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	701	G	N1-C6-O6	8.11	124.76	119.90
36	1	2865	U	N3-C4-C5	8.11	119.46	114.60
36	1	1552	G	C5-C6-O6	-8.10	123.74	128.60
36	5	2412	G	N3-C4-N9	8.10	130.86	126.00
36	1	651	G	N3-C4-C5	-8.09	124.55	128.60
36	1	327	A	C8-N9-C4	8.09	109.03	105.80
36	5	2619	G	C5-C6-O6	-8.09	123.75	128.60
36	1	933	A	O5'-P-OP1	-8.09	98.42	105.70
40	l3	26	ARG	NE-CZ-NH1	-8.09	116.26	120.30
36	1	2418	G	N3-C4-N9	8.08	130.85	126.00
36	5	804	C	C4-C5-C6	8.08	121.44	117.40
36	5	1316	C	N3-C4-N4	8.08	123.66	118.00
36	1	721	G	C8-N9-C4	-8.07	103.17	106.40
56	n0	13	ARG	NE-CZ-NH1	8.07	124.34	120.30
36	5	1389	G	C5-C6-O6	-8.07	123.76	128.60
36	5	3183	A	N9-C4-C5	-8.07	102.57	105.80
1	6	1634	C	N1-C2-O2	8.07	123.74	118.90
1	2	1773	C	N3-C4-N4	8.06	123.64	118.00
36	5	1513	G	C8-N9-C4	-8.06	103.18	106.40
36	5	642	U	O5'-P-OP2	-8.06	98.45	105.70
36	5	2700	G	N9-C4-C5	-8.05	102.18	105.40
1	6	863	A	C8-N9-C4	8.05	109.02	105.80
38	4	12	A	O5'-P-OP2	-8.04	98.46	105.70
36	1	1114	U	C4-C5-C6	-8.04	114.88	119.70
36	1	2355	G	C5-C6-N1	-8.04	107.48	111.50
1	6	317	C	C2-N3-C4	-8.03	115.88	119.90
36	1	1896	A	O5'-P-OP1	-8.03	98.47	105.70
36	1	3362	A	N7-C8-N9	8.03	117.82	113.80
36	5	2211	U	N3-C2-O2	-8.03	116.58	122.20
36	1	2142	A	C6-N1-C2	-8.02	113.79	118.60
38	8	96	A	C8-N9-C4	8.02	109.01	105.80
1	2	1114	G	C5-C6-O6	-8.02	123.79	128.60
36	1	2893	C	N3-C4-C5	8.01	125.11	121.90
36	1	2130	G	N1-C2-N2	-8.01	108.99	116.20
36	1	2643	A	N1-C6-N6	8.01	123.41	118.60
36	5	708	G	C8-N9-C4	-8.01	103.20	106.40
36	5	2978	U	C5-C6-N1	-8.01	118.70	122.70
36	5	3099	C	N1-C2-O2	-8.01	114.10	118.90
36	1	1149	G	C5-C6-N1	-8.00	107.50	111.50
36	1	3048	A	O5'-P-OP2	-8.00	98.50	105.70
36	5	2323	G	O5'-P-OP2	8.00	120.30	110.70
36	1	1313	G	C6-C5-N7	-8.00	125.60	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	874	U	O5'-P-OP1	-8.00	98.50	105.70
1	2	1114	G	N1-C6-O6	8.00	124.70	119.90
36	1	1365	G	N3-C4-N9	8.00	130.80	126.00
36	1	3181	C	N3-C2-O2	-8.00	116.30	121.90
36	1	3057	U	C5-C4-O4	7.99	130.69	125.90
36	5	973	A	C6-C5-N7	-7.99	126.71	132.30
36	5	1869	C	C6-N1-C2	7.99	123.50	120.30
36	1	2846	U	C5-C4-O4	7.99	130.69	125.90
36	5	2758	A	N9-C4-C5	7.98	108.99	105.80
36	5	2726	C	N3-C2-O2	-7.98	116.32	121.90
36	5	636	C	C6-N1-C2	7.98	123.49	120.30
36	1	2608	G	N1-C6-O6	7.97	124.68	119.90
36	1	2422	C	N3-C4-N4	-7.97	112.42	118.00
36	1	1343	A	N1-C6-N6	7.96	123.38	118.60
38	4	100	U	O5'-P-OP2	-7.96	98.54	105.70
1	2	576	G	C5-C6-O6	-7.96	123.83	128.60
36	1	859	G	N9-C4-C5	-7.96	102.22	105.40
1	2	75	U	N1-C2-O2	7.95	128.37	122.80
36	1	2417	U	N1-C2-O2	-7.95	117.23	122.80
36	1	635	G	C6-N1-C2	-7.95	120.33	125.10
36	5	2306	C	N1-C2-O2	7.95	123.67	118.90
36	5	939	U	N3-C2-O2	7.94	127.76	122.20
36	5	2356	A	C5-C6-N1	-7.94	113.73	117.70
36	1	609	G	C2-N3-C4	7.94	115.87	111.90
36	1	2693	C	N3-C4-C5	7.93	125.07	121.90
36	5	3374	U	C5-C6-N1	-7.93	118.73	122.70
36	1	2945	G	O5'-P-OP1	-7.93	98.56	105.70
36	1	1192	C	C5-C6-N1	7.93	124.96	121.00
36	1	2714	G	C5-N7-C8	-7.93	100.34	104.30
36	1	955	U	C5-C6-N1	-7.92	118.74	122.70
36	1	2726	C	N3-C2-O2	-7.92	116.36	121.90
36	5	1152	G	C5-C6-N1	-7.92	107.54	111.50
36	1	668	G	N1-C6-O6	-7.91	115.15	119.90
36	1	2177	G	C5-C6-N1	7.90	115.45	111.50
36	5	651	G	N3-C4-C5	-7.90	124.65	128.60
36	5	1306	G	C6-C5-N7	-7.90	125.66	130.40
36	1	328	U	N3-C2-O2	-7.90	116.67	122.20
36	5	1306	G	C5-C6-O6	-7.90	123.86	128.60
1	6	609	U	N3-C2-O2	-7.90	116.67	122.20
36	5	636	C	N3-C4-C5	7.89	125.06	121.90
36	1	1586	G	O5'-P-OP2	-7.89	98.60	105.70
36	5	337	G	N1-C6-O6	-7.88	115.17	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	S8	29	LEU	CA-CB-CG	7.88	133.42	115.30
36	5	3144	G	C8-N9-C4	-7.88	103.25	106.40
36	1	1435	A	O5'-P-OP2	7.88	120.15	110.70
36	1	1495	U	N1-C2-O2	-7.88	117.29	122.80
36	5	3092	C	N1-C2-O2	7.88	123.62	118.90
36	1	2550	U	N3-C2-O2	-7.87	116.69	122.20
36	1	651	G	N3-C4-N9	7.86	130.72	126.00
1	2	348	U	O5'-P-OP2	-7.86	98.63	105.70
37	7	110	G	O5'-P-OP2	-7.86	98.63	105.70
36	1	1432	C	C6-N1-C2	-7.86	117.16	120.30
36	5	1160	C	N1-C2-O2	-7.86	114.19	118.90
36	5	3331	U	C5-C6-N1	-7.86	118.77	122.70
36	1	2345	A	N1-C6-N6	7.85	123.31	118.60
36	5	105	C	C6-N1-C2	7.85	123.44	120.30
37	7	101	G	N9-C4-C5	-7.85	102.26	105.40
36	5	1868	G	C6-C5-N7	-7.85	125.69	130.40
36	1	2618	G	N1-C6-O6	-7.84	115.19	119.90
36	1	2946	A	N1-C6-N6	7.84	123.31	118.60
36	1	2871	G	O5'-P-OP2	-7.84	98.64	105.70
38	4	109	A	C5-C6-N6	-7.84	117.43	123.70
36	5	1307	G	P-O3'-C3'	7.84	129.10	119.70
36	5	1912	U	C6-N1-C2	7.83	125.70	121.00
36	5	2816	G	C5-C6-O6	-7.83	123.90	128.60
1	2	553	G	C6-C5-N7	-7.83	125.70	130.40
36	5	3035	A	C8-N9-C4	7.83	108.93	105.80
36	1	940	G	O5'-P-OP1	-7.82	98.66	105.70
36	1	2245	C	N3-C4-C5	-7.82	118.77	121.90
36	5	1187	C	C6-N1-C2	7.82	123.43	120.30
36	5	2317	A	O5'-P-OP2	-7.81	98.67	105.70
36	1	1442	U	N3-C2-O2	7.81	127.67	122.20
36	1	2302	G	C5-C6-O6	7.81	133.29	128.60
1	6	1001	A	N1-C6-N6	7.81	123.29	118.60
36	1	2884	C	C6-N1-C2	7.81	123.42	120.30
36	1	1417	G	N3-C4-C5	7.81	132.50	128.60
36	5	1110	U	N3-C2-O2	-7.80	116.74	122.20
36	5	2924	U	O5'-P-OP1	-7.80	98.68	105.70
36	1	895	A	C5-N7-C8	-7.80	100.00	103.90
36	1	107	A	N1-C6-N6	7.79	123.28	118.60
36	1	1001	G	N9-C4-C5	-7.79	102.28	105.40
36	5	957	C	N1-C2-N3	7.79	124.66	119.20
36	1	1723	A	C2-N3-C4	7.79	114.49	110.60
38	4	94	C	N3-C4-C5	7.79	125.01	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1305	U	O5'-P-OP1	-7.79	98.69	105.70
36	5	1308	A	OP1-P-OP2	-7.79	107.92	119.60
36	5	395	A	O5'-P-OP2	-7.78	98.70	105.70
11	s9	3	ARG	NE-CZ-NH2	7.77	124.19	120.30
36	5	3026	G	C5-C6-O6	-7.77	123.94	128.60
36	1	1741	A	C2-N3-C4	-7.77	106.71	110.60
1	2	647	G	N3-C4-N9	-7.77	121.34	126.00
36	1	2936	A	O5'-P-OP1	-7.77	98.71	105.70
36	1	3103	A	O5'-P-OP2	-7.77	98.71	105.70
36	5	641	C	O5'-P-OP1	-7.76	98.71	105.70
36	5	3084	C	C6-N1-C2	7.76	123.41	120.30
36	1	2371	G	C4-C5-N7	7.76	113.91	110.80
36	1	1405	U	C2-N1-C1'	-7.76	108.39	117.70
36	1	1137	C	O5'-P-OP2	-7.76	98.72	105.70
36	5	1592	G	C4-C5-C6	7.76	123.45	118.80
3	S1	218	LEU	CA-CB-CG	7.76	133.14	115.30
36	1	2643	A	N9-C4-C5	-7.76	102.70	105.80
36	5	2727	A	O5'-P-OP2	-7.76	98.72	105.70
36	1	979	U	N1-C2-N3	7.75	119.55	114.90
36	1	1296	C	N3-C4-C5	-7.75	118.80	121.90
36	5	1127	G	O5'-P-OP2	-7.74	98.73	105.70
36	5	361	A	N1-C6-N6	-7.74	113.95	118.60
36	5	437	G	N3-C4-N9	-7.74	121.36	126.00
36	1	2617	U	C5-C4-O4	7.74	130.54	125.90
38	4	23	U	O5'-P-OP1	-7.74	98.74	105.70
36	1	3362	A	O4'-C1'-N9	7.73	114.38	108.20
36	5	706	A	C2-N3-C4	-7.73	106.73	110.60
36	5	2848	G	N1-C6-O6	7.73	124.54	119.90
36	1	2316	G	N1-C6-O6	7.72	124.53	119.90
36	5	576	C	O5'-P-OP2	-7.72	98.75	105.70
36	5	3154	C	N1-C2-O2	7.72	123.53	118.90
36	1	2410	U	N3-C2-O2	7.72	127.60	122.20
36	5	2376	G	C5-C6-O6	-7.72	123.97	128.60
1	6	901	G	C4-C5-N7	7.72	113.89	110.80
36	1	776	U	C5-C6-N1	-7.71	118.84	122.70
36	5	776	U	N1-C2-N3	7.71	119.53	114.90
36	1	2867	C	C5-C6-N1	-7.71	117.14	121.00
36	5	2186	U	O5'-P-OP2	-7.71	98.76	105.70
36	1	1429	G	N3-C4-N9	7.71	130.63	126.00
36	5	1912	U	N1-C2-O2	-7.71	117.40	122.80
36	5	1194	G	C5-C6-N1	7.71	115.35	111.50
62	n6	76	LEU	CA-CB-CG	7.70	133.02	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3306	U	N3-C2-O2	-7.70	116.81	122.20
36	5	1300	G	N1-C6-O6	7.70	124.52	119.90
36	5	1429	G	N1-C6-O6	-7.70	115.28	119.90
36	5	2364	G	N9-C4-C5	7.70	108.48	105.40
36	1	2818	U	N3-C2-O2	-7.70	116.81	122.20
36	5	1308	A	N9-C4-C5	7.70	108.88	105.80
36	5	2643	A	C8-N9-C4	7.69	108.88	105.80
36	5	2848	G	C6-C5-N7	-7.69	125.78	130.40
36	5	834	U	N3-C4-C5	7.69	119.21	114.60
36	1	639	G	C8-N9-C4	7.68	109.47	106.40
36	1	2142	A	C5-C6-N1	7.68	121.54	117.70
36	5	2849	C	N3-C4-N4	7.68	123.38	118.00
36	1	2148	U	C6-N1-C2	7.68	125.61	121.00
1	6	448	C	C6-N1-C2	-7.68	117.23	120.30
36	5	1128	U	C5-C6-N1	-7.68	118.86	122.70
36	5	2700	G	C4-C5-N7	7.68	113.87	110.80
36	5	3245	A	C5-C6-N1	-7.68	113.86	117.70
1	6	1653	C	C6-N1-C2	-7.67	117.23	120.30
36	5	2994	A	N1-C2-N3	7.67	133.14	129.30
36	1	2634	U	C2-N3-C4	-7.67	122.40	127.00
36	1	3178	A	C5-C6-N1	-7.67	113.86	117.70
36	5	3142	A	O5'-P-OP1	-7.67	98.80	105.70
36	1	1043	C	N3-C4-C5	7.67	124.97	121.90
25	d3	33	LEU	CA-CB-CG	-7.66	97.67	115.30
1	2	1274	C	N3-C2-O2	-7.66	116.54	121.90
36	1	3344	A	C5-N7-C8	-7.66	100.07	103.90
36	5	719	U	N1-C2-O2	7.66	128.16	122.80
36	5	776	U	C2-N3-C4	-7.66	122.41	127.00
36	1	2278	C	N3-C4-C5	7.65	124.96	121.90
36	1	92	G	C5-C6-N1	7.64	115.32	111.50
36	1	1335	C	N3-C4-N4	-7.64	112.65	118.00
36	1	859	G	C6-C5-N7	-7.64	125.82	130.40
36	1	859	G	C8-N9-C1'	-7.63	117.08	127.00
36	5	959	C	O5'-P-OP2	-7.63	98.83	105.70
36	1	2773	C	O5'-P-OP2	-7.63	98.83	105.70
36	5	1897	G	C4-C5-N7	7.63	113.85	110.80
1	2	1658	G	C4-C5-N7	7.63	113.85	110.80
36	1	2368	A	N1-C6-N6	-7.62	114.03	118.60
36	1	919	U	O5'-P-OP1	7.62	119.85	110.70
36	1	1484	U	P-O3'-C3'	7.62	128.85	119.70
36	1	2764	C	N3-C4-C5	-7.62	118.85	121.90
36	1	2695	A	O5'-P-OP1	-7.62	98.84	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2857	C	C6-N1-C2	7.62	123.35	120.30
36	1	636	C	C5-C4-N4	-7.62	114.87	120.20
1	6	29	U	C5-C4-O4	7.62	130.47	125.90
36	1	770	G	O4'-C1'-N9	7.61	114.29	108.20
36	1	1119	C	C6-N1-C2	7.61	123.34	120.30
36	1	1116	G	C2-N3-C4	7.61	115.71	111.90
36	1	2410	U	N1-C2-O2	-7.61	117.47	122.80
36	5	2183	A	N1-C6-N6	7.61	123.17	118.60
36	1	2355	G	C6-C5-N7	-7.61	125.83	130.40
1	6	1537	C	N3-C4-C5	-7.61	118.86	121.90
36	1	652	G	N1-C2-N2	-7.61	109.36	116.20
1	2	1212	G	C5-C6-O6	-7.60	124.04	128.60
36	1	1310	G	C5-C6-O6	7.60	133.16	128.60
53	M7	138	LYS	CD-CE-NZ	7.60	129.18	111.70
36	5	424	G	C5-C6-N1	7.60	115.30	111.50
36	5	2889	C	N3-C2-O2	-7.60	116.58	121.90
36	1	1190	A	C6-C5-N7	-7.60	126.98	132.30
36	1	2308	C	C2-N3-C4	-7.60	116.10	119.90
36	1	2405	C	N3-C4-C5	-7.60	118.86	121.90
36	1	1414	G	N1-C6-O6	7.59	124.46	119.90
36	1	1530	U	C6-N1-C2	7.59	125.56	121.00
36	1	2724	U	N1-C2-O2	-7.59	117.49	122.80
36	5	3136	G	C2-N3-C4	-7.59	108.10	111.90
36	5	3218	A	C5-N7-C8	-7.59	100.11	103.90
36	1	85	A	C2-N3-C4	-7.59	106.81	110.60
36	5	424	G	C6-C5-N7	-7.58	125.85	130.40
36	5	3184	A	N9-C4-C5	-7.58	102.77	105.80
38	4	54	A	N1-C6-N6	7.58	123.15	118.60
36	5	2421	U	N1-C2-N3	7.58	119.45	114.90
1	2	145	A	C8-N9-C4	-7.58	102.77	105.80
36	5	889	U	C6-N1-C2	7.58	125.55	121.00
36	5	1163	A	N1-C6-N6	-7.58	114.06	118.60
37	7	92	A	C8-N9-C4	7.57	108.83	105.80
36	5	287	G	O5'-P-OP1	-7.57	98.89	105.70
36	1	282	G	C8-N9-C4	-7.57	103.37	106.40
1	6	1600	A	O4'-C1'-N9	7.57	114.26	108.20
1	2	499	U	C2-N1-C1'	7.57	126.78	117.70
36	5	607	A	N1-C6-N6	-7.56	114.06	118.60
36	5	2794	G	C5-C6-O6	-7.56	124.06	128.60
36	1	999	G	O5'-P-OP1	-7.56	98.90	105.70
36	5	1803	C	N3-C4-C5	7.56	124.92	121.90
1	6	1634	C	C6-N1-C2	-7.56	117.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2191	U	N1-C2-O2	7.55	128.09	122.80
36	5	2306	C	N3-C2-O2	-7.54	116.62	121.90
36	1	949	C	C6-N1-C2	-7.54	117.28	120.30
36	1	1148	G	N1-C6-O6	7.54	124.43	119.90
36	5	835	G	C5-C6-O6	7.54	133.13	128.60
36	1	339	C	OP1-P-OP2	-7.54	108.29	119.60
36	5	437	G	N9-C4-C5	7.54	108.42	105.40
1	2	554	C	N1-C2-O2	7.53	123.42	118.90
36	1	2658	G	O5'-P-OP2	-7.53	98.92	105.70
36	5	2434	U	O5'-P-OP2	-7.53	98.92	105.70
36	5	948	C	C5-C4-N4	-7.53	114.93	120.20
36	5	2192	C	O5'-P-OP2	-7.53	98.92	105.70
36	1	1507	G	N3-C4-N9	7.53	130.52	126.00
36	5	3183	A	C4-C5-N7	7.53	114.46	110.70
36	1	33	G	O5'-P-OP1	-7.52	98.93	105.70
36	5	1710	C	N3-C4-C5	7.52	124.91	121.90
36	1	1153	A	O5'-P-OP1	-7.52	98.93	105.70
1	6	639	U	N3-C2-O2	-7.52	116.94	122.20
36	5	2385	G	N1-C6-O6	7.52	124.41	119.90
36	1	907	G	O5'-P-OP2	-7.52	98.93	105.70
37	7	98	C	C6-N1-C2	7.52	123.31	120.30
36	1	1820	U	N3-C2-O2	-7.52	116.94	122.20
36	1	1315	U	C5-C6-N1	-7.51	118.94	122.70
44	17	229	PHE	CB-CG-CD1	7.51	126.06	120.80
36	1	1334	U	N3-C4-C5	-7.51	110.09	114.60
36	5	1592	G	C4-C5-N7	-7.51	107.80	110.80
1	2	1600	A	C5-C6-N1	-7.51	113.95	117.70
36	5	2326	A	C8-N9-C4	7.51	108.80	105.80
36	1	1303	A	N7-C8-N9	-7.51	110.05	113.80
36	1	1489	A	N1-C6-N6	7.50	123.10	118.60
36	1	2333	C	C5-C6-N1	-7.50	117.25	121.00
36	5	632	G	C5-C6-N1	7.50	115.25	111.50
36	1	1419	A	N1-C6-N6	7.50	123.10	118.60
36	1	3057	U	N3-C2-O2	-7.50	116.95	122.20
36	5	2134	G	C5-C6-O6	7.50	133.10	128.60
36	1	662	U	O5'-P-OP2	-7.49	98.96	105.70
36	5	2811	A	N1-C6-N6	-7.49	114.10	118.60
1	2	190	C	O4'-C1'-N1	7.49	114.19	108.20
36	5	2572	C	C2-N1-C1'	7.49	127.04	118.80
12	C0	88	PRO	N-CA-CB	7.49	112.28	103.30
36	5	2327	U	C5-C6-N1	-7.49	118.96	122.70
36	1	896	A	C8-N9-C4	-7.49	102.81	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2142	A	C2-N3-C4	7.49	114.34	110.60
36	1	2191	U	N3-C2-O2	-7.48	116.96	122.20
36	1	2983	C	C4-C5-C6	7.48	121.14	117.40
36	1	950	G	N9-C4-C5	-7.48	102.41	105.40
36	5	1128	U	C2-N3-C4	-7.48	122.51	127.00
36	1	912	G	N1-C2-N3	7.48	128.38	123.90
36	5	337	G	C8-N9-C4	-7.48	103.41	106.40
36	5	2158	A	N1-C6-N6	-7.48	114.11	118.60
36	1	1149	G	C5-C6-O6	-7.47	124.11	128.60
70	O4	51	LEU	CA-CB-CG	7.47	132.49	115.30
36	5	1348	U	C6-N1-C2	-7.47	116.52	121.00
36	1	924	G	N3-C2-N2	7.47	125.13	119.90
1	6	1700	C	C2-N1-C1'	7.47	127.02	118.80
36	1	1156	C	N3-C2-O2	-7.47	116.67	121.90
36	1	2726	C	C6-N1-C2	-7.47	117.31	120.30
24	d2	93	LEU	CA-CB-CG	7.47	132.48	115.30
36	5	668	G	N1-C6-O6	-7.47	115.42	119.90
36	5	1124	U	N3-C4-C5	7.47	119.08	114.60
36	1	398	A	C8-N9-C4	7.47	108.79	105.80
36	1	703	G	N3-C4-N9	-7.47	121.52	126.00
36	1	2795	U	O5'-P-OP1	-7.47	98.98	105.70
36	1	2884	C	C4-C5-C6	-7.46	113.67	117.40
1	6	1643	U	C2-N3-C4	-7.46	122.52	127.00
36	5	2954	U	N1-C2-O2	7.46	128.02	122.80
1	6	1100	G	N3-C4-C5	-7.46	124.87	128.60
1	2	1340	U	N3-C2-O2	-7.45	116.98	122.20
36	5	3245	A	C8-N9-C4	-7.45	102.82	105.80
36	5	1004	U	C6-N1-C2	-7.45	116.53	121.00
36	5	2933	A	N1-C6-N6	7.45	123.07	118.60
36	5	3218	A	N9-C4-C5	-7.45	102.82	105.80
1	6	1582	U	C5-C6-N1	-7.45	118.98	122.70
36	5	2323	G	OP1-P-OP2	-7.45	108.43	119.60
36	5	3303	G	N1-C6-O6	-7.45	115.43	119.90
1	6	144	U	N3-C2-O2	-7.44	116.99	122.20
1	6	1000	C	C2-N1-C1'	7.44	126.99	118.80
36	1	1165	A	C8-N9-C4	7.44	108.78	105.80
36	1	282	G	O5'-P-OP2	7.44	119.63	110.70
1	6	1022	C	N1-C2-O2	-7.44	114.44	118.90
36	1	304	G	C6-C5-N7	7.44	134.86	130.40
36	1	968	G	N3-C4-C5	-7.44	124.88	128.60
36	5	227	G	N1-C6-O6	7.44	124.36	119.90
36	1	929	A	N1-C6-N6	7.43	123.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3243	A	N1-C6-N6	7.43	123.06	118.60
36	5	2951	G	N3-C4-N9	7.43	130.46	126.00
36	5	1129	A	O5'-P-OP2	-7.43	99.01	105.70
36	1	2646	C	C6-N1-C2	7.43	123.27	120.30
36	1	967	A	OP2-P-O3'	7.43	121.54	105.20
36	5	1329	U	N1-C1'-C2'	-7.43	103.83	112.00
36	5	3154	C	C2-N1-C1'	7.43	126.97	118.80
36	1	3362	A	C6-C5-N7	-7.42	127.10	132.30
36	5	2231	C	C2-N1-C1'	7.42	126.97	118.80
1	2	359	A	C4-C5-C6	-7.42	113.29	117.00
36	1	2634	U	C5-C6-N1	-7.42	118.99	122.70
36	5	1366	A	N9-C4-C5	7.42	108.77	105.80
36	5	1302	A	OP2-P-O3'	7.42	121.52	105.20
36	1	496	C	O5'-P-OP2	7.42	119.60	110.70
36	5	2211	U	C5-C4-O4	7.42	130.35	125.90
36	5	776	U	N3-C2-O2	-7.41	117.01	122.20
36	5	3093	C	C2-N3-C4	-7.41	116.19	119.90
36	1	3326	G	C8-N9-C4	7.41	109.36	106.40
36	5	1879	A	C6-C5-N7	-7.41	127.11	132.30
36	5	2875	U	C5-C4-O4	-7.41	121.45	125.90
36	5	2954	U	N3-C4-O4	7.41	124.58	119.40
36	5	3047	U	C4-C5-C6	7.41	124.14	119.70
36	1	2617	U	C2-N3-C4	-7.41	122.56	127.00
37	3	75	G	O5'-P-OP1	-7.40	99.04	105.70
36	5	1516	C	N3-C4-C5	7.40	124.86	121.90
36	5	2616	C	O5'-P-OP1	-7.40	99.04	105.70
36	5	2142	A	C5-C6-N1	7.40	121.40	117.70
36	5	2290	C	C6-N1-C2	7.40	123.26	120.30
36	1	2162	U	O5'-P-OP2	-7.39	99.05	105.70
36	1	346	C	C5-C6-N1	-7.39	117.31	121.00
36	1	1581	C	N1-C2-O2	7.38	123.33	118.90
36	1	2633	U	N1-C2-N3	7.38	119.33	114.90
36	5	38	U	C6-N1-C2	7.38	125.43	121.00
38	4	57	C	C6-N1-C2	7.38	123.25	120.30
38	4	114	G	O5'-P-OP1	-7.38	99.06	105.70
36	5	3143	C	N3-C4-N4	7.38	123.16	118.00
36	1	1192	C	N1-C2-O2	7.37	123.32	118.90
1	6	438	A	O5'-P-OP1	-7.37	99.06	105.70
1	2	507	U	N3-C2-O2	-7.37	117.04	122.20
1	2	1114	G	C4-C5-N7	7.37	113.75	110.80
36	1	3016	A	N1-C6-N6	7.37	123.02	118.60
36	1	3217	C	N3-C2-O2	-7.37	116.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	830	U	N3-C2-O2	-7.37	117.04	122.20
36	1	2688	U	N1-C2-N3	-7.37	110.48	114.90
36	5	216	G	C6-C5-N7	-7.37	125.98	130.40
36	5	2761	G	C5-C6-O6	-7.36	124.18	128.60
36	5	2400	G	N3-C4-C5	7.36	132.28	128.60
36	5	2870	C	C2-N1-C1'	-7.36	110.71	118.80
36	1	888	A	C5-C6-N6	-7.35	117.82	123.70
36	1	2352	A	O5'-P-OP2	-7.35	99.08	105.70
35	SM	167	PRO	N-CA-CB	7.35	112.12	103.30
36	1	2183	A	C2-N3-C4	-7.35	106.93	110.60
36	1	2823	G	N3-C2-N2	-7.35	114.76	119.90
36	5	878	G	C8-N9-C4	-7.35	103.46	106.40
38	4	61	A	C5-C6-N1	7.35	121.37	117.70
36	1	2647	A	C6-N1-C2	-7.34	114.19	118.60
1	6	1137	A	N7-C8-N9	-7.34	110.13	113.80
36	1	1114	U	N1-C2-O2	7.34	127.94	122.80
1	6	337	G	N3-C2-N2	7.34	125.04	119.90
37	7	11	A	C6-C5-N7	-7.34	127.16	132.30
36	5	2363	A	C5-C6-N6	-7.34	117.83	123.70
1	2	1560	U	C5-C4-O4	7.34	130.30	125.90
36	5	2757	U	N1-C2-N3	7.34	119.30	114.90
36	1	1417	G	C8-N9-C4	7.33	109.33	106.40
1	6	44	U	N1-C2-O2	-7.33	117.67	122.80
36	5	1181	U	N1-C2-N3	7.33	119.30	114.90
36	1	1509	A	C2-N3-C4	-7.33	106.94	110.60
36	5	437	G	C8-N9-C4	-7.33	103.47	106.40
36	1	859	G	N3-C4-N9	7.32	130.39	126.00
1	6	416	A	C2-N3-C4	-7.32	106.94	110.60
36	5	1657	C	N1-C2-O2	7.32	123.29	118.90
1	2	334	G	N3-C4-C5	7.32	132.26	128.60
36	1	2627	C	N1-C2-O2	-7.31	114.51	118.90
36	1	47	C	C6-N1-C2	7.31	123.22	120.30
36	5	52	A	C5-C6-N1	-7.31	114.04	117.70
36	1	1858	A	C8-N9-C4	-7.31	102.88	105.80
36	5	776	U	C5-C4-O4	7.31	130.28	125.90
38	8	79	A	C8-N9-C4	-7.31	102.88	105.80
36	5	3374	U	N3-C4-C5	7.30	118.98	114.60
36	5	393	U	C6-N1-C2	-7.30	116.62	121.00
36	1	2624	G	N1-C6-O6	7.30	124.28	119.90
36	5	2136	C	C2-N3-C4	-7.30	116.25	119.90
36	5	3040	A	C8-N9-C4	7.30	108.72	105.80
36	5	1908	A	N1-C6-N6	-7.30	114.22	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3092	C	N3-C2-O2	-7.30	116.79	121.90
36	1	767	U	O4'-C1'-N1	7.29	114.03	108.20
36	1	25	U	N3-C4-O4	7.29	124.50	119.40
36	1	1433	A	N1-C6-N6	-7.28	114.23	118.60
52	M6	78	ARG	NE-CZ-NH2	-7.28	116.66	120.30
36	5	2310	U	C5-C4-O4	7.28	130.27	125.90
36	1	87	U	C2-N1-C1'	7.28	126.44	117.70
36	5	922	U	N3-C4-O4	-7.28	114.31	119.40
36	1	1364	C	OP2-P-O3'	7.28	121.20	105.20
36	5	586	C	N3-C4-C5	7.28	124.81	121.90
36	5	2697	A	N1-C6-N6	7.28	122.97	118.60
36	5	2278	C	C6-N1-C2	-7.27	117.39	120.30
36	1	2816	G	N7-C8-N9	-7.27	109.46	113.10
36	1	979	U	O4'-C1'-N1	7.27	114.02	108.20
1	2	507	U	N1-C2-O2	7.27	127.89	122.80
36	1	102	C	N1-C2-O2	-7.27	114.54	118.90
36	1	2624	G	C4-C5-N7	7.27	113.71	110.80
36	1	2918	G	N1-C6-O6	7.27	124.26	119.90
36	5	1194	G	N1-C6-O6	-7.27	115.54	119.90
36	5	822	G	O5'-P-OP1	-7.26	99.16	105.70
36	1	211	A	O5'-P-OP1	-7.26	99.17	105.70
36	1	1445	U	N1-C2-O2	-7.25	117.72	122.80
36	5	437	G	N1-C2-N2	7.25	122.73	116.20
36	5	2821	C	N1-C2-O2	-7.25	114.55	118.90
36	5	1897	G	C6-C5-N7	-7.25	126.05	130.40
36	5	3374	U	C6-N1-C2	7.25	125.35	121.00
36	5	2140	U	N1-C2-N3	7.25	119.25	114.90
1	2	1560	U	N3-C2-O2	-7.25	117.13	122.20
36	5	969	C	C5-C6-N1	-7.25	117.38	121.00
36	5	2393	G	C5-C6-N1	7.25	115.12	111.50
36	1	2606	G	N3-C4-N9	7.25	130.35	126.00
38	4	109	A	N1-C6-N6	7.25	122.95	118.60
36	1	1314	C	C6-N1-C2	-7.25	117.40	120.30
36	1	2358	A	C2-N3-C4	-7.25	106.98	110.60
36	1	1329	U	C6-N1-C2	-7.24	116.65	121.00
36	5	2283	G	C5-C6-O6	-7.24	124.25	128.60
36	1	1373	A	C6-N1-C2	-7.24	114.25	118.60
1	2	48	G	O5'-P-OP2	-7.24	99.18	105.70
36	1	116	A	O4'-C1'-N9	7.24	113.99	108.20
36	1	1151	U	N3-C4-O4	7.24	124.47	119.40
36	5	38	U	C5-C6-N1	-7.24	119.08	122.70
1	2	1114	G	N9-C4-C5	-7.24	102.51	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	410	U	N1-C2-O2	-7.24	117.73	122.80
36	5	3220	G	N1-C6-O6	-7.24	115.56	119.90
36	1	1525	G	O5'-P-OP2	-7.23	99.19	105.70
38	8	4	C	N3-C2-O2	-7.23	116.84	121.90
36	1	1367	G	N9-C4-C5	-7.23	102.51	105.40
36	1	1897	G	C5-C6-O6	-7.23	124.26	128.60
1	6	1535	U	N3-C2-O2	-7.23	117.14	122.20
65	n9	23	LYS	C-N-CD	7.23	143.59	128.40
36	1	1475	A	C8-N9-C4	7.23	108.69	105.80
36	5	2983	C	C4-C5-C6	7.23	121.01	117.40
36	1	1897	G	C6-C5-N7	-7.22	126.07	130.40
36	1	972	A	N7-C8-N9	-7.22	110.19	113.80
36	1	2610	G	N1-C6-O6	7.22	124.23	119.90
36	5	2186	U	C5-C4-O4	7.22	130.23	125.90
36	1	1381	A	O5'-P-OP1	-7.22	99.20	105.70
36	5	426	G	O5'-P-OP2	-7.22	99.20	105.70
36	5	942	U	N3-C4-O4	7.22	124.45	119.40
36	1	496	C	O5'-P-OP1	-7.22	99.20	105.70
38	4	32	C	O5'-P-OP2	-7.22	99.20	105.70
36	1	3221	C	O5'-P-OP1	-7.21	99.21	105.70
36	5	645	A	N1-C2-N3	7.21	132.91	129.30
36	5	805	G	C8-N9-C4	7.21	109.28	106.40
36	5	2341	A	C8-N9-C4	7.21	108.69	105.80
36	1	2978	U	O4'-C1'-N1	7.21	113.97	108.20
36	5	2921	U	N1-C2-O2	-7.21	117.75	122.80
36	5	635	G	C6-C5-N7	-7.21	126.08	130.40
36	1	993	G	C5-C6-N1	7.20	115.10	111.50
36	5	1373	A	C6-C5-N7	-7.20	127.26	132.30
36	5	2359	C	C6-N1-C2	7.20	123.18	120.30
1	2	973	A	N1-C2-N3	7.20	132.90	129.30
36	1	588	G	C4-C5-N7	-7.20	107.92	110.80
36	5	1142	G	N9-C4-C5	7.20	108.28	105.40
36	5	2287	C	C6-N1-C2	-7.20	117.42	120.30
36	1	959	C	N3-C4-C5	7.19	124.78	121.90
36	1	430	U	N3-C2-O2	-7.19	117.17	122.20
36	5	1429	G	N3-C2-N2	7.19	124.93	119.90
1	6	1642	G	C5-C6-O6	-7.19	124.29	128.60
1	2	1600	A	N9-C4-C5	-7.18	102.93	105.80
36	1	910	G	C8-N9-C4	-7.18	103.53	106.40
36	5	1307	G	C2'-C3'-O3'	7.18	125.30	109.50
37	7	101	G	C6-C5-N7	-7.18	126.09	130.40
36	1	1520	G	C8-N9-C4	7.18	109.27	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2426	U	C5-C4-O4	7.18	130.21	125.90
36	5	1064	A	P-O3'-C3'	7.18	128.31	119.70
36	5	1834	U	N3-C4-C5	-7.18	110.30	114.60
36	1	2402	A	O5'-P-OP2	-7.17	99.24	105.70
36	1	2726	C	C5-C4-N4	7.17	125.22	120.20
36	1	2944	U	N3-C4-C5	7.17	118.91	114.60
36	1	86	G	O4'-C1'-N9	7.17	113.94	108.20
36	1	788	C	C2-N1-C1'	-7.17	110.91	118.80
36	1	1196	C	C6-N1-C2	7.17	123.17	120.30
36	1	765	C	N1-C2-O2	7.17	123.20	118.90
36	1	1148	G	C5-C6-O6	-7.17	124.30	128.60
36	5	727	G	O5'-P-OP1	-7.17	99.25	105.70
36	1	938	C	N3-C4-C5	7.17	124.77	121.90
36	5	1592	G	N3-C4-C5	-7.17	125.02	128.60
36	1	2996	U	C6-N1-C1'	-7.16	111.17	121.20
36	1	706	A	C8-N9-C4	7.16	108.66	105.80
36	1	2987	A	C6-C5-N7	-7.16	127.29	132.30
1	6	1288	G	O5'-P-OP2	-7.16	99.25	105.70
36	5	676	G	C8-N9-C4	-7.16	103.54	106.40
36	5	3308	C	C2-N3-C4	-7.16	116.32	119.90
36	1	701	G	N3-C2-N2	-7.16	114.89	119.90
36	1	2130	G	N1-C2-N3	7.16	128.19	123.90
36	5	796	U	N1-C2-N3	7.16	119.19	114.90
36	5	1184	A	N9-C4-C5	7.15	108.66	105.80
1	2	1291	G	N1-C2-N3	7.15	128.19	123.90
36	1	2915	U	N1-C2-O2	-7.15	117.79	122.80
1	6	13	C	N3-C4-C5	-7.15	119.04	121.90
36	5	1825	G	O5'-P-OP2	-7.15	99.26	105.70
36	1	2238	G	N1-C6-O6	7.15	124.19	119.90
1	6	1536	G	O5'-P-OP1	-7.15	99.27	105.70
1	6	13	C	C6-N1-C2	-7.14	117.44	120.30
36	5	2278	C	N1-C2-O2	7.14	123.19	118.90
36	5	2626	A	C2-N3-C4	-7.14	107.03	110.60
36	1	2836	C	C5-C4-N4	7.14	125.20	120.20
36	1	2875	U	N3-C4-O4	7.14	124.40	119.40
36	5	339	C	O5'-P-OP1	-7.14	99.28	105.70
36	5	957	C	C6-N1-C2	-7.14	117.44	120.30
36	5	1153	A	N1-C6-N6	7.13	122.88	118.60
36	5	2758	A	C8-N9-C4	-7.13	102.95	105.80
36	5	227	G	N9-C4-C5	-7.13	102.55	105.40
36	5	2358	A	C8-N9-C4	7.13	108.65	105.80
36	1	1820	U	P-O3'-C3'	7.13	128.26	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2642	A	C6-N1-C2	7.13	122.88	118.60
36	5	1368	U	C5-C4-O4	-7.13	121.62	125.90
1	6	1634	C	N3-C2-O2	-7.13	116.91	121.90
36	1	950	G	N3-C2-N2	7.13	124.89	119.90
36	5	1412	G	C8-N9-C4	-7.13	103.55	106.40
36	1	2184	U	C5-C6-N1	7.12	126.26	122.70
36	5	2887	A	N1-C6-N6	7.12	122.87	118.60
36	1	1425	U	N1-C2-N3	7.12	119.17	114.90
38	8	3	A	C5-C6-N1	7.12	121.26	117.70
36	1	919	U	O5'-P-OP2	-7.12	99.29	105.70
36	1	1190	A	C4-C5-N7	7.12	114.26	110.70
36	1	2836	C	N3-C2-O2	-7.12	116.92	121.90
36	1	1190	A	C5-N7-C8	-7.11	100.34	103.90
36	5	1187	C	O5'-P-OP2	-7.11	99.30	105.70
36	1	2946	A	C5-C6-N1	-7.11	114.14	117.70
1	6	402	C	O5'-P-OP2	-7.11	99.30	105.70
36	5	2353	G	C5-C6-O6	-7.11	124.33	128.60
36	5	1452	A	N1-C6-N6	7.11	122.86	118.60
36	5	2136	C	C4-C5-C6	7.11	120.95	117.40
1	2	1642	G	N1-C6-O6	7.10	124.16	119.90
36	5	973	A	C5-C6-N6	-7.10	118.02	123.70
38	4	113	U	C5-C6-N1	-7.09	119.15	122.70
36	5	3200	G	N1-C6-O6	7.09	124.16	119.90
36	1	1375	G	C5-C6-N1	-7.09	107.95	111.50
36	1	2731	U	N3-C4-O4	7.09	124.36	119.40
36	1	2912	G	C5-C6-N1	7.09	115.05	111.50
36	5	3014	U	C5-C6-N1	-7.09	119.16	122.70
36	1	2142	A	N3-C4-C5	-7.09	121.84	126.80
36	5	974	G	C8-N9-C4	-7.09	103.56	106.40
36	5	1307	G	C5-C6-N1	7.09	115.04	111.50
36	5	630	A	C5-C6-N1	-7.08	114.16	117.70
36	5	718	G	O4'-C1'-N9	7.08	113.87	108.20
36	1	2827	U	N1-C2-N3	7.08	119.15	114.90
36	5	2825	C	C5-C4-N4	-7.08	115.24	120.20
1	6	92	A	N1-C6-N6	7.08	122.85	118.60
36	5	668	G	N3-C4-C5	-7.08	125.06	128.60
36	5	693	A	O5'-P-OP2	7.08	119.20	110.70
36	5	1483	G	O4'-C1'-N9	7.08	113.86	108.20
1	2	416	A	C8-N9-C4	7.08	108.63	105.80
36	1	810	A	C6-N1-C2	-7.08	114.36	118.60
36	1	938	C	N1-C2-O2	-7.08	114.65	118.90
36	1	2827	U	C5-C4-O4	7.08	130.15	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	699	A	C2-N3-C4	-7.08	107.06	110.60
36	5	882	A	C6-N1-C2	-7.08	114.36	118.60
36	5	1897	G	C5-N7-C8	-7.08	100.76	104.30
36	1	2700	G	C5-C6-O6	-7.07	124.36	128.60
36	1	2643	A	C8-N9-C4	7.07	108.63	105.80
36	5	2356	A	C2-N3-C4	-7.07	107.06	110.60
36	5	3144	G	N7-C8-N9	7.07	116.64	113.10
1	2	639	U	N1-C2-O2	7.07	127.75	122.80
36	1	343	U	N1-C2-N3	7.07	119.14	114.90
36	1	717	C	N1-C2-O2	-7.07	114.66	118.90
44	L7	83	LEU	CA-CB-CG	7.07	131.56	115.30
36	5	927	C	N1-C2-O2	-7.07	114.66	118.90
1	2	1745	G	C5-C6-O6	-7.06	124.36	128.60
36	5	3137	C	C5-C6-N1	-7.06	117.47	121.00
36	5	1149	G	C6-C5-N7	-7.06	126.16	130.40
36	5	2185	G	C5-C6-N1	-7.06	107.97	111.50
36	1	59	G	N1-C6-O6	7.06	124.14	119.90
36	1	2572	C	N1-C2-O2	7.06	123.13	118.90
36	5	41	G	N9-C4-C5	-7.06	102.58	105.40
36	5	3216	G	C5-C6-O6	-7.06	124.37	128.60
36	5	1200	A	C4-C5-C6	7.06	120.53	117.00
36	1	961	C	C6-N1-C2	7.05	123.12	120.30
36	5	2857	C	N1-C2-O2	7.05	123.13	118.90
36	5	2983	C	O5'-P-OP1	-7.05	99.35	105.70
45	18	69	LEU	CA-CB-CG	7.05	131.53	115.30
36	1	646	A	C8-N9-C4	-7.05	102.98	105.80
36	1	919	U	N3-C4-O4	-7.05	114.46	119.40
36	5	2186	U	N3-C2-O2	-7.05	117.26	122.20
36	1	778	U	C5-C4-O4	7.05	130.13	125.90
36	1	2130	G	C2-N3-C4	-7.05	108.38	111.90
36	1	347	G	C4-C5-N7	7.05	113.62	110.80
36	1	2912	G	N1-C6-O6	-7.05	115.67	119.90
38	4	25	G	C4-C5-N7	-7.05	107.98	110.80
36	1	2811	A	C6-N1-C2	-7.04	114.38	118.60
36	5	646	A	C5-C6-N6	7.04	129.33	123.70
36	5	1174	G	C5-C6-N1	7.04	115.02	111.50
36	1	637	C	P-O3'-C3'	7.04	128.15	119.70
36	5	523	A	N1-C6-N6	-7.04	114.38	118.60
36	1	1655	G	N3-C4-N9	7.04	130.22	126.00
36	1	2177	G	N3-C4-N9	7.04	130.22	126.00
36	5	1189	C	N1-C2-O2	-7.04	114.68	118.90
36	5	1148	G	C5-C6-O6	-7.04	124.38	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2353	G	N1-C6-O6	7.04	124.12	119.90
36	1	2406	C	C5-C4-N4	-7.03	115.28	120.20
36	1	3270	U	C2-N1-C1'	-7.03	109.26	117.70
36	5	1366	A	C8-N9-C4	-7.03	102.99	105.80
36	5	2364	G	C4-C5-N7	-7.03	107.99	110.80
38	8	95	G	C4-N9-C1'	-7.03	117.36	126.50
36	5	1208	U	N3-C4-O4	-7.03	114.48	119.40
36	5	2290	C	C5-C6-N1	-7.03	117.48	121.00
36	1	2700	G	C6-C5-N7	-7.03	126.18	130.40
36	5	2940	A	C5-C6-N1	7.03	121.22	117.70
36	1	2983	C	N3-C2-O2	-7.03	116.98	121.90
1	6	85	A	C8-N9-C4	-7.03	102.99	105.80
36	5	410	U	N1-C2-O2	-7.03	117.88	122.80
36	5	2796	G	C5-C6-O6	7.03	132.82	128.60
36	1	589	A	O5'-P-OP1	-7.03	99.38	105.70
36	1	608	A	C4-C5-C6	7.02	120.51	117.00
36	5	229	G	N3-C2-N2	-7.02	114.98	119.90
36	1	2376	G	C8-N9-C4	-7.02	103.59	106.40
36	5	817	A	O5'-P-OP1	-7.02	99.38	105.70
36	1	2986	U	N1-C2-N3	7.02	119.11	114.90
36	1	1279	C	C6-N1-C2	-7.02	117.49	120.30
36	5	2996	U	O5'-P-OP2	-7.02	99.39	105.70
36	5	1367	G	C5-C6-N1	-7.01	107.99	111.50
37	7	49	G	N1-C6-O6	7.01	124.11	119.90
50	m4	72	LEU	CA-CB-CG	7.01	131.42	115.30
36	5	939	U	O5'-P-OP2	-7.01	99.39	105.70
1	2	1241	G	O4'-C1'-N9	7.00	113.80	108.20
36	1	806	A	C8-N9-C4	7.00	108.60	105.80
1	6	647	G	N3-C4-N9	-7.00	121.80	126.00
36	1	1369	A	O5'-P-OP1	-7.00	99.40	105.70
1	6	609	U	C5-C4-O4	7.00	130.10	125.90
36	5	1311	G	O5'-P-OP2	-7.00	99.40	105.70
36	1	943	U	N1-C2-N3	7.00	119.10	114.90
36	5	1388	U	O5'-P-OP2	-7.00	99.40	105.70
36	1	2973	G	N1-C6-O6	7.00	124.10	119.90
36	5	2608	G	OP2-P-O3'	7.00	120.59	105.20
36	1	1151	U	C5-C6-N1	6.99	126.20	122.70
36	5	2857	C	C6-N1-C1'	-6.99	112.41	120.80
36	5	1169	A	O5'-P-OP2	-6.99	99.41	105.70
36	1	3041	U	N1-C2-O2	-6.99	117.91	122.80
36	1	2876	C	C6-N1-C2	-6.99	117.50	120.30
36	5	964	G	C8-N9-C4	-6.99	103.61	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3105	U	N1-C2-N3	6.99	119.09	114.90
36	1	53	G	N1-C6-O6	-6.98	115.71	119.90
36	5	2327	U	C6-N1-C2	6.98	125.19	121.00
36	5	82	C	C4-C5-C6	6.98	120.89	117.40
36	5	2920	U	C5-C4-O4	-6.98	121.71	125.90
36	1	2365	C	C6-N1-C2	6.98	123.09	120.30
36	1	2640	A	C5-C6-N1	6.98	121.19	117.70
36	5	350	C	N3-C2-O2	-6.97	117.02	121.90
36	5	1192	C	N1-C2-O2	6.97	123.08	118.90
36	5	1300	G	C4-C5-N7	6.97	113.59	110.80
36	1	2846	U	N3-C4-O4	-6.97	114.52	119.40
36	5	2961	G	C8-N9-C4	-6.97	103.61	106.40
1	2	1761	U	P-O3'-C3'	6.97	128.06	119.70
36	1	2121	G	C5-C6-O6	6.97	132.78	128.60
36	5	61	A	C5-C6-N6	6.96	129.27	123.70
36	1	2176	U	N3-C2-O2	-6.96	117.33	122.20
36	1	1495	U	C2-N3-C4	-6.96	122.82	127.00
36	1	2374	C	N3-C2-O2	-6.96	117.03	121.90
36	1	3266	G	N9-C4-C5	6.96	108.18	105.40
36	1	1365	G	C6-C5-N7	-6.96	126.23	130.40
36	1	1411	C	C2-N3-C4	-6.95	116.42	119.90
36	5	1198	C	C6-N1-C2	-6.95	117.52	120.30
1	6	1700	C	N1-C2-O2	6.95	123.07	118.90
36	5	1149	G	C4-C5-C6	6.95	122.97	118.80
36	5	2278	C	C4-C5-C6	-6.95	113.92	117.40
51	m5	187	ARG	NE-CZ-NH1	-6.95	116.83	120.30
1	2	404	G	O5'-P-OP2	-6.95	99.45	105.70
36	1	423	A	C4-C5-C6	6.95	120.47	117.00
36	1	919	U	N3-C4-C5	6.95	118.77	114.60
36	5	877	C	C4-C5-C6	-6.95	113.93	117.40
1	6	75	U	N1-C2-O2	6.95	127.66	122.80
36	5	562	C	N3-C4-C5	6.95	124.68	121.90
36	5	2255	A	O5'-P-OP1	-6.95	99.45	105.70
36	5	3123	A	C8-N9-C4	6.95	108.58	105.80
38	4	32	C	C2-N1-C1'	-6.94	111.16	118.80
36	1	1329	U	C5-C6-N1	6.94	126.17	122.70
36	1	2124	G	C5-C6-O6	-6.94	124.44	128.60
36	5	2295	A	C5-C6-N6	-6.94	118.15	123.70
36	5	2399	A	C2-N3-C4	-6.94	107.13	110.60
36	5	1879	A	N9-C4-C5	-6.94	103.03	105.80
36	5	2682	C	C6-N1-C2	6.94	123.08	120.30
36	5	3351	U	N3-C2-O2	-6.94	117.34	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	122	A	OP1-P-OP2	-6.93	109.20	119.60
36	1	1113	G	N1-C6-O6	6.93	124.06	119.90
36	1	1433	A	O5'-P-OP1	-6.93	99.46	105.70
1	6	17	C	N3-C2-O2	-6.93	117.05	121.90
36	5	1897	G	C5-C6-O6	-6.93	124.44	128.60
36	5	2954	U	C5-C6-N1	6.93	126.16	122.70
36	1	2878	G	C8-N9-C4	6.93	109.17	106.40
36	1	2379	U	N3-C2-O2	6.92	127.05	122.20
36	1	2859	U	C5-C6-N1	-6.92	119.24	122.70
36	5	706	A	N3-C4-C5	6.92	131.65	126.80
36	1	3316	A	C2-N3-C4	-6.92	107.14	110.60
36	1	1133	A	N1-C6-N6	6.92	122.75	118.60
36	1	2700	G	N1-C6-O6	6.92	124.05	119.90
36	5	2411	U	N3-C4-C5	6.92	118.75	114.60
36	5	3218	A	C6-C5-N7	-6.92	127.45	132.30
1	2	1100	G	C6-C5-N7	-6.92	126.25	130.40
36	5	3050	U	C5-C4-O4	6.92	130.05	125.90
36	1	105	C	C5-C4-N4	-6.92	115.36	120.20
1	2	1200	G	C6-C5-N7	-6.91	126.25	130.40
1	6	696	C	O4'-C1'-N1	6.91	113.73	108.20
1	2	1671	A	O5'-P-OP1	-6.91	99.48	105.70
36	1	2756	C	C6-N1-C2	-6.91	117.54	120.30
1	6	1028	C	N1-C2-O2	6.91	123.05	118.90
36	1	93	C	C6-N1-C2	-6.91	117.54	120.30
36	5	2249	G	C8-N9-C4	-6.91	103.64	106.40
37	7	74	C	N3-C2-O2	6.91	126.73	121.90
36	1	1216	C	O5'-P-OP2	-6.91	99.48	105.70
36	1	1792	C	N1-C2-O2	-6.91	114.76	118.90
36	1	3362	A	C5-N7-C8	-6.91	100.45	103.90
36	1	2949	U	N1-C2-N3	-6.90	110.76	114.90
36	1	343	U	O5'-P-OP2	-6.90	99.49	105.70
36	1	818	C	N3-C4-C5	-6.90	119.14	121.90
41	L4	98	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	2	448	C	C6-N1-C2	-6.90	117.54	120.30
36	1	1139	G	C2-N3-C4	-6.90	108.45	111.90
1	6	163	G	N9-C4-C5	6.89	108.16	105.40
36	1	1182	A	C8-N9-C4	6.89	108.56	105.80
36	1	2639	G	C6-C5-N7	-6.89	126.27	130.40
36	5	834	U	C6-N1-C2	6.89	125.13	121.00
36	1	1510	G	C4-C5-N7	6.88	113.55	110.80
36	1	1518	U	N1-C2-N3	6.88	119.03	114.90
36	1	2298	U	C5-C4-O4	6.88	130.03	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3212	C	C6-N1-C2	6.88	123.05	120.30
1	2	1033	C	N3-C2-O2	-6.88	117.08	121.90
36	1	2988	C	N1-C2-O2	-6.88	114.77	118.90
1	2	577	G	C6-C5-N7	-6.88	126.27	130.40
1	6	777	C	C5-C6-N1	6.88	124.44	121.00
36	1	676	G	C8-N9-C4	-6.88	103.65	106.40
1	6	65	A	C2-N3-C4	-6.87	107.16	110.60
36	5	2618	G	N3-C4-C5	-6.87	125.16	128.60
36	5	2816	G	C8-N9-C4	6.87	109.15	106.40
36	5	2925	C	C6-N1-C2	-6.87	117.55	120.30
38	8	40	A	C8-N9-C4	-6.87	103.05	105.80
36	1	3248	C	C6-N1-C2	-6.87	117.55	120.30
36	5	998	A	OP2-P-O3'	6.87	120.30	105.20
36	5	952	A	N1-C6-N6	6.86	122.72	118.60
38	8	3	A	C2-N3-C4	6.86	114.03	110.60
36	1	743	C	N1-C2-O2	-6.86	114.78	118.90
36	1	2397	A	O5'-P-OP2	-6.86	99.53	105.70
36	1	2406	C	C6-N1-C2	6.86	123.04	120.30
1	6	1137	A	C8-N9-C4	6.86	108.54	105.80
37	7	37	G	C5-C6-O6	-6.86	124.49	128.60
73	o7	65	ARG	NE-CZ-NH1	6.86	123.73	120.30
36	5	645	A	N3-C4-C5	-6.86	122.00	126.80
36	5	2345	A	C5-C6-N6	-6.86	118.22	123.70
36	5	2700	G	C6-C5-N7	-6.86	126.29	130.40
36	5	2856	G	OP1-P-OP2	6.86	129.88	119.60
36	5	2339	C	OP1-P-OP2	6.85	129.88	119.60
36	5	2400	G	C2-N3-C4	-6.85	108.47	111.90
36	5	2993	G	C4-C5-N7	6.85	113.54	110.80
36	5	3362	A	N3-C4-C5	6.85	131.60	126.80
36	1	2357	A	C6-C5-N7	-6.85	127.51	132.30
38	8	95	G	N3-C4-C5	6.85	132.02	128.60
36	1	229	G	N1-C6-O6	6.85	124.01	119.90
36	1	1148	G	C8-N9-C4	6.85	109.14	106.40
36	5	939	U	N1-C2-O2	-6.85	118.01	122.80
36	5	1909	A	O5'-P-OP2	-6.85	99.54	105.70
36	5	2661	G	N3-C4-N9	6.85	130.11	126.00
1	2	1274	C	C6-N1-C2	-6.84	117.56	120.30
36	1	667	C	N3-C4-N4	-6.84	113.21	118.00
36	1	1838	G	N9-C4-C5	-6.84	102.66	105.40
37	3	82	G	N1-C2-N2	-6.84	110.04	116.20
1	2	42	G	N1-C6-O6	-6.84	115.79	119.90
36	1	1475	A	N7-C8-N9	-6.84	110.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	908	G	C8-N9-C1'	-6.84	118.11	127.00
1	6	1614	A	C2-N3-C4	-6.84	107.18	110.60
36	5	1628	C	C6-N1-C2	-6.84	117.56	120.30
36	1	2698	G	O5'-P-OP1	-6.83	99.55	105.70
36	5	925	A	C8-N9-C4	6.83	108.53	105.80
36	5	2957	G	O5'-P-OP1	-6.83	99.55	105.70
36	5	1116	G	C4-C5-C6	6.83	122.90	118.80
36	5	2980	U	N3-C2-O2	-6.83	117.42	122.20
36	1	3361	G	N3-C4-N9	6.83	130.10	126.00
36	5	3214	U	N3-C2-O2	-6.83	117.42	122.20
1	2	728	U	C2-N1-C1'	6.82	125.89	117.70
36	5	1151	U	N3-C4-O4	6.82	124.18	119.40
36	1	880	G	C5-C6-O6	6.82	132.69	128.60
1	6	1773	C	C4-C5-C6	6.82	120.81	117.40
36	1	2633	U	N3-C2-O2	-6.82	117.43	122.20
1	6	432	G	C5-C6-O6	-6.82	124.51	128.60
36	5	2121	G	N9-C4-C5	-6.82	102.67	105.40
1	2	75	U	C2-N1-C1'	6.81	125.87	117.70
69	o3	99	ARG	NE-CZ-NH1	-6.81	116.89	120.30
36	5	2758	A	N1-C6-N6	-6.81	114.51	118.60
36	1	1160	C	C6-N1-C2	6.81	123.02	120.30
36	1	2899	C	C4-C5-C6	6.81	120.80	117.40
36	5	3154	C	C6-N1-C2	-6.81	117.58	120.30
36	5	1452	A	C5-C6-N6	-6.81	118.25	123.70
36	5	1879	A	C5-N7-C8	-6.81	100.50	103.90
36	5	2917	G	C6-C5-N7	-6.81	126.32	130.40
36	5	971	G	N7-C8-N9	-6.81	109.70	113.10
36	5	2635	A	C8-N9-C4	-6.80	103.08	105.80
36	5	894	G	C8-N9-C4	6.80	109.12	106.40
36	1	2620	G	C2-N3-C4	-6.80	108.50	111.90
1	6	163	G	C8-N9-C1'	6.80	135.84	127.00
36	1	397	A	C5-C6-N1	6.80	121.10	117.70
36	5	2375	G	C5-C6-O6	6.80	132.68	128.60
36	1	35	A	C4-C5-N7	6.79	114.10	110.70
1	2	831	U	C5-C6-N1	6.79	126.10	122.70
36	1	1300	G	C5-C6-O6	-6.79	124.52	128.60
36	1	1349	G	N3-C4-C5	-6.79	125.20	128.60
36	1	2645	G	C8-N9-C4	6.79	109.12	106.40
36	5	577	C	C5-C4-N4	-6.79	115.45	120.20
36	1	100	A	C4-C5-C6	6.79	120.39	117.00
36	1	201	A	C2-N3-C4	-6.79	107.21	110.60
36	1	2687	G	N1-C6-O6	-6.79	115.83	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	11	A	C5-N7-C8	-6.79	100.51	103.90
1	2	966	A	N1-C6-N6	6.78	122.67	118.60
36	5	2296	A	O5'-P-OP2	6.78	118.84	110.70
36	5	3067	C	C6-N1-C2	6.78	123.01	120.30
36	1	639	G	N9-C4-C5	-6.78	102.69	105.40
47	M0	10	ARG	NE-CZ-NH1	-6.78	116.91	120.30
36	5	1496	C	C2-N1-C1'	6.78	126.25	118.80
36	1	347	G	N9-C4-C5	-6.78	102.69	105.40
1	6	308	C	C2-N1-C1'	-6.78	111.35	118.80
36	5	645	A	N9-C4-C5	6.78	108.51	105.80
36	5	3097	C	O5'-P-OP1	6.78	118.83	110.70
36	1	1435	A	N1-C2-N3	-6.77	125.91	129.30
36	1	2249	G	N3-C4-N9	6.77	130.06	126.00
36	1	2619	G	O5'-P-OP1	-6.77	99.61	105.70
37	3	13	A	O5'-P-OP1	-6.77	99.61	105.70
38	8	79	A	N7-C8-N9	6.77	117.19	113.80
36	5	1524	A	C8-N9-C4	6.77	108.51	105.80
1	2	1426	C	C4-C5-C6	-6.76	114.02	117.40
36	1	402	A	C8-N9-C4	6.76	108.50	105.80
36	5	1906	G	O5'-P-OP1	-6.76	99.61	105.70
1	2	360	A	C8-N9-C4	6.76	108.50	105.80
36	1	900	G	C8-N9-C4	6.76	109.10	106.40
36	5	1868	G	C4-C5-N7	6.76	113.50	110.80
36	5	3153	U	N1-C2-O2	6.76	127.53	122.80
36	1	3057	U	N1-C2-N3	6.76	118.95	114.90
61	N5	34	LEU	CA-CB-CG	6.76	130.84	115.30
36	5	297	G	C4-N9-C1'	6.76	135.28	126.50
36	5	2704	A	O5'-P-OP1	-6.76	99.62	105.70
37	3	82	G	N1-C2-N3	6.75	127.95	123.90
36	1	1136	A	C6-N1-C2	-6.75	114.55	118.60
36	1	2177	G	N3-C4-C5	-6.75	125.22	128.60
36	5	640	U	N1-C2-O2	-6.75	118.07	122.80
36	5	776	U	N3-C4-O4	-6.75	114.67	119.40
36	1	3243	A	C5-C6-N6	-6.75	118.30	123.70
36	5	2231	C	O4'-C1'-N1	6.75	113.60	108.20
36	5	2951	G	O5'-P-OP1	-6.75	99.62	105.70
36	1	2301	U	O5'-P-OP2	-6.75	99.62	105.70
36	1	1377	G	C5-N7-C8	-6.75	100.93	104.30
37	3	35	C	N1-C2-O2	6.75	122.95	118.90
36	5	1203	A	N1-C6-N6	6.75	122.65	118.60
36	5	1886	A	N1-C2-N3	-6.75	125.92	129.30
36	1	2243	A	O5'-P-OP2	-6.75	99.63	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1349	G	N3-C4-N9	6.75	130.05	126.00
36	5	3137	C	C2-N1-C1'	-6.75	111.38	118.80
36	1	1303	A	N9-C4-C5	-6.74	103.10	105.80
36	1	2869	U	O5'-P-OP1	-6.74	99.63	105.70
36	1	2403	G	OP1-P-O3'	6.74	120.03	105.20
36	1	3214	U	N3-C2-O2	-6.74	117.48	122.20
36	1	1431	G	N1-C6-O6	-6.74	115.86	119.90
36	5	880	G	C8-N9-C4	6.74	109.10	106.40
38	8	54	A	C2-N3-C4	-6.74	107.23	110.60
36	1	2378	C	C5-C4-N4	-6.74	115.48	120.20
36	5	43	A	C5-N7-C8	-6.74	100.53	103.90
36	5	1506	A	N1-C6-N6	-6.73	114.56	118.60
36	5	2376	G	N1-C6-O6	6.73	123.94	119.90
36	5	3382	U	N3-C2-O2	-6.73	117.49	122.20
36	5	3382	U	C2-N1-C1'	6.73	125.78	117.70
36	1	498	A	O5'-P-OP2	-6.73	99.64	105.70
36	5	2323	G	C8-N9-C4	-6.73	103.71	106.40
40	l3	275	ARG	NE-CZ-NH1	-6.73	116.94	120.30
59	n3	89	ASP	CB-CG-OD1	-6.73	112.24	118.30
36	1	586	C	C6-N1-C2	6.73	122.99	120.30
36	1	2937	G	N7-C8-N9	-6.73	109.73	113.10
36	5	2972	G	C5-C6-O6	6.73	132.64	128.60
36	5	3060	C	C5-C6-N1	6.73	124.36	121.00
36	5	3317	U	C5-C4-O4	6.72	129.93	125.90
36	1	2624	G	C5-N7-C8	-6.72	100.94	104.30
36	1	1148	G	N9-C4-C5	-6.72	102.71	105.40
37	3	82	G	N3-C4-N9	6.72	130.03	126.00
36	5	646	A	N1-C6-N6	-6.72	114.57	118.60
36	5	2400	G	C6-C5-N7	-6.72	126.37	130.40
37	7	73	C	C5-C6-N1	6.72	124.36	121.00
36	1	931	C	C6-N1-C2	6.71	122.99	120.30
1	2	1258	U	N3-C2-O2	-6.71	117.50	122.20
36	1	372	A	O5'-P-OP2	-6.71	99.66	105.70
36	1	895	A	C5-C6-N6	-6.71	118.33	123.70
36	1	3382	U	N1-C2-O2	6.71	127.50	122.80
36	5	3128	G	C4-C5-N7	6.71	113.48	110.80
1	6	1747	G	C8-N9-C4	6.71	109.08	106.40
36	5	2635	A	N9-C4-C5	6.71	108.48	105.80
36	5	2885	C	N3-C4-N4	6.71	122.70	118.00
36	1	2797	C	O5'-P-OP1	-6.71	99.66	105.70
36	5	1941	C	N1-C2-O2	-6.71	114.88	118.90
36	5	337	G	N9-C4-C5	6.71	108.08	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1160	C	C2-N1-C1'	-6.71	111.42	118.80
36	1	808	A	C6-N1-C2	-6.70	114.58	118.60
36	1	2408	U	O5'-P-OP1	-6.70	99.67	105.70
36	1	936	A	O5'-P-OP2	-6.70	99.67	105.70
36	1	2819	A	O5'-P-OP2	-6.70	99.67	105.70
36	5	869	G	C5-C6-N1	6.70	114.85	111.50
36	5	3313	U	O5'-P-OP2	-6.70	99.67	105.70
36	1	716	A	C6-C5-N7	-6.70	127.61	132.30
36	5	2944	U	N3-C2-O2	-6.70	117.51	122.20
1	2	465	G	O5'-P-OP1	-6.70	99.67	105.70
1	2	1740	A	N1-C6-N6	6.70	122.62	118.60
36	1	884	A	N1-C6-N6	6.70	122.62	118.60
36	5	3197	G	N3-C4-C5	6.69	131.95	128.60
36	1	2358	A	C8-N9-C4	6.69	108.48	105.80
53	M7	3	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	6	1600	A	N9-C1'-C2'	6.69	122.70	114.00
36	5	518	G	C5-C6-O6	6.69	132.62	128.60
36	5	2385	G	O5'-P-OP1	-6.69	99.68	105.70
36	1	968	G	C5-C6-O6	-6.69	124.58	128.60
36	1	2356	A	N1-C6-N6	6.69	122.61	118.60
36	1	2422	C	N3-C4-C5	6.69	124.58	121.90
36	5	957	C	C4-C5-C6	6.69	120.75	117.40
36	5	1433	A	N9-C4-C5	6.69	108.48	105.80
36	5	2383	C	N3-C4-N4	6.69	122.68	118.00
1	2	577	G	N9-C4-C5	-6.69	102.72	105.40
1	6	29	U	N3-C2-O2	-6.69	117.52	122.20
37	7	101	G	C8-N9-C4	6.69	109.08	106.40
36	5	1912	U	C5-C4-O4	-6.69	121.89	125.90
36	1	802	C	O5'-P-OP2	6.68	118.72	110.70
36	1	2168	A	N1-C6-N6	-6.68	114.59	118.60
36	5	1878	G	C4-N9-C1'	6.68	135.19	126.50
36	1	1379	G	N1-C2-N3	6.68	127.91	123.90
36	1	2811	A	N1-C6-N6	-6.68	114.59	118.60
36	5	3382	U	N1-C2-O2	6.68	127.47	122.80
36	5	1116	G	N9-C4-C5	6.67	108.07	105.40
77	q1	12	ARG	NE-CZ-NH1	-6.67	116.97	120.30
64	N8	4	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	6	432	G	N1-C6-O6	6.67	123.90	119.90
36	1	1149	G	C4-C5-C6	6.67	122.80	118.80
36	1	2247	G	N1-C6-O6	6.67	123.90	119.90
36	1	2731	U	N1-C2-O2	-6.67	118.13	122.80
36	5	587	U	N3-C2-O2	6.67	126.87	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2371	G	C5-N7-C8	-6.66	100.97	104.30
36	5	2870	C	C6-N1-C1'	6.66	128.80	120.80
1	2	1096	C	C2-N1-C1'	6.66	126.13	118.80
36	1	1116	G	OP2-P-O3'	6.66	119.85	105.20
36	5	200	C	N3-C4-N4	6.66	122.66	118.00
36	1	54	C	C2-N3-C4	-6.66	116.57	119.90
37	7	104	A	C8-N9-C4	6.66	108.46	105.80
53	m7	69	ARG	NE-CZ-NH2	-6.66	116.97	120.30
36	1	2879	C	N1-C2-O2	-6.66	114.91	118.90
38	8	32	C	C6-N1-C2	6.66	122.96	120.30
51	m5	197	LEU	CA-CB-CG	-6.66	99.99	115.30
36	1	585	A	N7-C8-N9	-6.65	110.47	113.80
36	1	934	G	C4-N9-C1'	6.65	135.15	126.50
36	1	1472	U	C6-N1-C2	6.65	124.99	121.00
36	1	1190	A	N7-C8-N9	6.65	117.12	113.80
36	5	2371	G	C4-C5-N7	6.65	113.46	110.80
36	5	2860	U	O5'-P-OP1	-6.65	99.72	105.70
37	7	11	A	C4-C5-N7	6.65	114.03	110.70
36	1	3266	G	N3-C4-N9	-6.65	122.01	126.00
36	1	2897	A	C8-N9-C4	6.65	108.46	105.80
36	5	2211	U	N1-C2-N3	6.65	118.89	114.90
36	1	1520	G	C4-C5-N7	-6.65	108.14	110.80
36	1	86	G	O5'-P-OP1	6.64	118.67	110.70
36	1	1136	A	C5-C6-N1	6.64	121.02	117.70
36	1	2309	A	N1-C6-N6	6.64	122.59	118.60
36	1	969	C	C2-N3-C4	-6.64	116.58	119.90
1	6	317	C	C5-C6-N1	-6.64	117.68	121.00
36	1	908	G	C4-N9-C1'	6.64	135.13	126.50
36	1	3378	C	C6-N1-C2	6.64	122.96	120.30
36	5	2338	C	N1-C2-O2	-6.64	114.92	118.90
36	1	1901	A	C5-C6-N1	6.64	121.02	117.70
36	5	924	G	N3-C4-C5	6.64	131.92	128.60
36	1	1269	U	C2-N1-C1'	6.64	125.67	117.70
36	5	1390	A	C8-N9-C4	-6.64	103.14	105.80
1	2	779	U	O4'-C1'-N1	6.64	113.51	108.20
36	1	2987	A	C5-C6-N6	-6.64	118.39	123.70
36	5	1300	G	C6-C5-N7	-6.64	126.42	130.40
36	5	656	A	C8-N9-C4	6.63	108.45	105.80
36	1	2961	G	C6-C5-N7	-6.63	126.42	130.40
37	3	98	C	N1-C2-O2	-6.63	114.92	118.90
36	1	1429	G	C8-N9-C1'	-6.63	118.38	127.00
36	1	2130	G	C5-C6-O6	6.63	132.58	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	11	C	OP2-P-O3'	6.63	119.79	105.20
36	5	2953	U	N3-C2-O2	6.63	126.84	122.20
36	5	840	C	O5'-P-OP2	-6.63	99.73	105.70
36	1	1396	C	C6-N1-C2	6.63	122.95	120.30
36	5	2815	G	C5-C6-O6	-6.63	124.62	128.60
1	2	158	U	C2-N1-C1'	6.63	125.65	117.70
1	6	1568	C	P-O3'-C3'	6.63	127.65	119.70
36	5	1115	G	C4-N9-C1'	6.63	135.11	126.50
36	1	2906	C	C2-N3-C4	-6.62	116.59	119.90
36	5	2354	C	N3-C2-O2	6.62	126.54	121.90
36	1	2886	U	C5-C4-O4	-6.62	121.93	125.90
36	5	948	C	N3-C2-O2	6.62	126.53	121.90
36	1	1192	C	C6-N1-C1'	-6.62	112.86	120.80
36	1	2550	U	C5-C4-O4	6.62	129.87	125.90
1	6	1000	C	N3-C2-O2	-6.62	117.27	121.90
36	5	1908	A	C5-C6-N6	6.62	128.99	123.70
36	5	2402	A	O4'-C1'-N9	6.62	113.49	108.20
36	5	2832	C	C6-N1-C2	6.62	122.95	120.30
36	1	983	A	N1-C2-N3	6.61	132.61	129.30
36	5	2836	C	C4-C5-C6	6.61	120.71	117.40
36	5	895	A	C4-C5-C6	6.61	120.31	117.00
36	5	1868	G	N1-C6-O6	6.61	123.87	119.90
1	2	4	C	N1-C2-O2	-6.61	114.93	118.90
36	5	1889	G	C4-C5-N7	6.61	113.44	110.80
36	1	2194	G	C6-C5-N7	-6.61	126.44	130.40
36	1	2620	G	N3-C4-C5	6.61	131.90	128.60
36	1	2979	U	C5-C6-N1	-6.61	119.40	122.70
36	5	1152	G	C4-C5-C6	-6.61	114.83	118.80
36	5	2709	C	N3-C4-C5	6.61	124.54	121.90
1	2	1749	A	C8-N9-C4	6.61	108.44	105.80
36	1	2238	G	C4-C5-N7	6.61	113.44	110.80
36	1	1094	U	C5-C6-N1	6.60	126.00	122.70
36	1	1307	G	P-O3'-C3'	6.60	127.62	119.70
36	1	2920	U	C2-N3-C4	-6.60	123.04	127.00
36	5	43	A	N1-C6-N6	6.60	122.56	118.60
36	5	2403	G	O5'-P-OP1	6.60	118.62	110.70
36	5	3128	G	N9-C4-C5	-6.60	102.76	105.40
36	1	1790	G	C5-C6-N1	-6.60	108.20	111.50
36	1	2975	U	N1-C2-O2	6.60	127.42	122.80
38	4	24	G	C4-C5-N7	6.60	113.44	110.80
36	5	2147	A	N1-C6-N6	6.60	122.56	118.60
36	5	2635	A	N1-C6-N6	-6.60	114.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2283	G	C8-N9-C4	6.60	109.04	106.40
36	5	2643	A	N9-C4-C5	-6.59	103.16	105.80
36	5	3050	U	N3-C2-O2	-6.59	117.58	122.20
36	5	3184	A	C5-C6-N6	-6.59	118.42	123.70
36	1	967	A	C2-N3-C4	-6.59	107.31	110.60
36	5	672	A	C4-C5-N7	6.59	114.00	110.70
36	5	2870	C	C2-N3-C4	-6.59	116.61	119.90
36	1	1175	C	N3-C4-C5	6.59	124.54	121.90
36	1	3361	G	N3-C4-C5	-6.59	125.31	128.60
36	1	810	A	C5-C6-N1	6.59	120.99	117.70
36	5	2849	C	C5-C6-N1	6.59	124.29	121.00
36	5	610	G	C8-N9-C4	-6.58	103.77	106.40
36	5	2816	G	N7-C8-N9	-6.58	109.81	113.10
36	1	2627	C	C6-N1-C2	6.58	122.93	120.30
36	1	2836	C	C6-N1-C2	-6.58	117.67	120.30
1	6	901	G	C5-C6-O6	-6.58	124.65	128.60
36	5	2879	C	O5'-P-OP2	-6.58	99.78	105.70
36	5	3041	U	O5'-P-OP2	-6.58	99.78	105.70
36	1	1897	G	C4-C5-N7	6.58	113.43	110.80
36	5	3218	A	C5-C6-N6	-6.58	118.44	123.70
36	1	54	C	N3-C4-C5	6.58	124.53	121.90
1	6	523	G	C8-N9-C4	6.58	109.03	106.40
36	5	1213	G	C5-C6-N1	6.58	114.79	111.50
1	6	453	U	C6-N1-C2	-6.58	117.05	121.00
36	5	3362	A	C5-N7-C8	-6.58	100.61	103.90
36	1	1153	A	N1-C6-N6	6.58	122.55	118.60
36	1	1405	U	C5-C6-N1	-6.58	119.41	122.70
36	1	3183	A	N1-C6-N6	6.58	122.55	118.60
36	5	1433	A	C8-N9-C4	-6.58	103.17	105.80
36	5	2699	G	C5-C6-O6	-6.58	124.65	128.60
36	5	1124	U	N3-C4-O4	-6.57	114.80	119.40
36	1	1151	U	N3-C4-C5	-6.57	110.66	114.60
1	2	1773	C	N3-C4-C5	-6.57	119.27	121.90
36	1	292	U	N1-C2-N3	6.57	118.84	114.90
36	1	589	A	N7-C8-N9	-6.57	110.52	113.80
36	1	974	G	N3-C4-C5	-6.57	125.31	128.60
36	1	2624	G	C5-C6-O6	-6.57	124.66	128.60
36	1	3092	C	C6-N1-C2	6.57	122.93	120.30
36	5	2661	G	C6-N1-C2	-6.57	121.16	125.10
38	8	33	A	C8-N9-C4	6.57	108.43	105.80
36	5	1892	G	O5'-P-OP2	-6.57	99.79	105.70
1	2	1762	A	O5'-P-OP1	-6.57	99.79	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	797	U	OP2-P-O3'	6.57	119.64	105.20
36	1	2615	G	C5-C6-O6	-6.57	124.66	128.60
36	1	2627	C	C5-C6-N1	-6.57	117.72	121.00
36	1	1904	C	N3-C4-N4	6.56	122.59	118.00
36	1	3275	U	C5-C6-N1	6.56	125.98	122.70
36	5	1060	U	N3-C4-O4	-6.56	114.81	119.40
36	5	1190	A	C8-N9-C4	-6.56	103.17	105.80
36	5	2994	A	C6-N1-C2	-6.56	114.66	118.60
1	6	863	A	N1-C6-N6	6.56	122.54	118.60
36	5	297	G	N3-C4-N9	6.56	129.94	126.00
36	1	3362	A	C8-N9-C4	-6.56	103.18	105.80
36	5	2685	C	C2-N3-C4	-6.56	116.62	119.90
36	5	2830	G	C4-C5-N7	-6.56	108.18	110.80
36	1	3209	A	C5-N7-C8	-6.56	100.62	103.90
36	5	2211	U	C4-C5-C6	6.56	123.64	119.70
36	1	3079	U	N1-C2-O2	-6.56	118.21	122.80
1	6	558	U	N1-C2-O2	6.55	127.39	122.80
36	5	645	A	C8-N9-C4	-6.55	103.18	105.80
36	5	2349	U	OP1-P-O3'	6.55	119.62	105.20
36	5	2366	C	N3-C4-N4	6.55	122.59	118.00
36	5	3294	A	C8-N9-C4	-6.55	103.18	105.80
36	5	1329	U	C5-C4-O4	-6.55	121.97	125.90
36	5	2661	G	N3-C4-C5	-6.55	125.32	128.60
1	2	499	U	C6-N1-C1'	-6.55	112.03	121.20
36	1	99	A	O4'-C1'-N9	6.55	113.44	108.20
36	5	640	U	C5-C4-O4	-6.55	121.97	125.90
37	7	37	G	C6-C5-N7	-6.54	126.47	130.40
36	5	3245	A	N1-C2-N3	6.54	132.57	129.30
36	1	697	A	C8-N9-C4	6.54	108.42	105.80
36	1	1373	A	N1-C2-N3	6.54	132.57	129.30
36	1	2378	C	N3-C4-C5	6.54	124.52	121.90
1	6	1776	A	N1-C6-N6	6.54	122.52	118.60
36	5	1420	C	N1-C2-O2	-6.53	114.98	118.90
36	5	2405	C	N1-C2-N3	6.53	123.77	119.20
36	1	369	A	C8-N9-C4	-6.53	103.19	105.80
36	1	54	C	C6-N1-C2	6.53	122.91	120.30
36	1	1324	U	O5'-P-OP2	-6.53	99.83	105.70
36	1	1484	U	OP2-P-O3'	6.53	119.56	105.20
36	5	1581	C	C2-N3-C4	6.53	123.16	119.90
36	5	2600	C	C6-N1-C2	-6.53	117.69	120.30
36	1	716	A	C5-C6-N6	-6.53	118.48	123.70
36	1	3344	A	O4'-C1'-N9	6.53	113.42	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	378	A	N1-C6-N6	6.53	122.52	118.60
36	5	1424	C	N3-C2-O2	6.53	126.47	121.90
36	1	847	A	N1-C6-N6	6.52	122.51	118.60
1	2	359	A	C6-C5-N7	6.52	136.87	132.30
36	5	414	U	N3-C4-O4	6.52	123.97	119.40
36	5	2759	U	N1-C2-O2	-6.52	118.23	122.80
47	M0	24	ARG	NE-CZ-NH1	6.52	123.56	120.30
36	5	1153	A	C5-C6-N6	-6.52	118.48	123.70
36	5	2351	U	C6-N1-C2	-6.52	117.09	121.00
36	5	2403	G	C2-N3-C4	6.52	115.16	111.90
36	1	589	A	C8-N9-C4	6.52	108.41	105.80
36	1	608	A	C6-C5-N7	-6.52	127.74	132.30
36	1	787	G	N3-C4-N9	6.52	129.91	126.00
1	2	380	U	N1-C2-O2	6.52	127.36	122.80
36	1	934	G	C8-N9-C1'	-6.52	118.53	127.00
36	5	706	A	N1-C6-N6	6.52	122.51	118.60
36	5	2299	A	C5-C6-N1	-6.52	114.44	117.70
36	5	2395	G	C8-N9-C4	6.52	109.01	106.40
1	2	1462	G	N1-C6-O6	6.51	123.81	119.90
36	1	3081	C	C5-C6-N1	-6.51	117.74	121.00
36	5	1286	A	C8-N9-C4	6.51	108.41	105.80
36	5	3014	U	C2-N3-C4	-6.51	123.09	127.00
1	6	1472	C	N1-C2-O2	-6.51	115.00	118.90
36	5	2988	C	C2-N3-C4	-6.51	116.64	119.90
36	5	882	A	C4-C5-C6	6.51	120.25	117.00
36	1	949	C	N1-C2-N3	6.50	123.75	119.20
36	1	968	G	C6-N1-C2	-6.50	121.20	125.10
1	6	1058	U	OP1-P-O3'	6.50	119.51	105.20
1	6	1614	A	O4'-C1'-N9	6.50	113.40	108.20
36	5	1882	G	C8-N9-C4	6.50	109.00	106.40
36	5	2117	A	C5-C6-N6	6.50	128.90	123.70
36	1	1907	C	N3-C4-C5	-6.50	119.30	121.90
36	1	2932	U	C5-C6-N1	-6.50	119.45	122.70
36	5	577	C	N3-C4-N4	6.50	122.55	118.00
36	5	3243	A	O4'-C1'-N9	-6.50	103.00	108.20
36	1	689	U	N1-C2-N3	6.50	118.80	114.90
36	5	61	A	N1-C6-N6	-6.50	114.70	118.60
36	5	2388	U	OP2-P-O3'	6.50	119.49	105.20
1	2	287	G	O4'-C1'-N9	6.49	113.39	108.20
36	1	645	A	O5'-P-OP1	-6.49	99.86	105.70
36	1	3178	A	C4-C5-C6	6.49	120.25	117.00
37	7	100	C	C6-N1-C2	6.49	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	659	G	C5-N7-C8	-6.49	101.05	104.30
36	1	2852	C	C6-N1-C2	6.49	122.90	120.30
36	1	188	U	N1-C2-O2	-6.49	118.26	122.80
36	1	2305	G	C6-C5-N7	-6.49	126.51	130.40
36	1	2333	C	C4-C5-C6	6.49	120.64	117.40
36	1	1385	C	N3-C2-O2	6.49	126.44	121.90
36	1	2132	C	O5'-P-OP2	-6.49	99.86	105.70
36	5	1041	U	O5'-P-OP2	-6.49	99.86	105.70
36	5	1187	C	C5-C6-N1	-6.49	117.76	121.00
15	C3	22	ALA	C-N-CD	-6.48	106.33	120.60
36	1	101	G	N3-C2-N2	-6.48	115.36	119.90
36	5	666	A	C6-N1-C2	-6.48	114.71	118.60
36	5	2825	C	N3-C2-O2	6.48	126.44	121.90
1	2	1746	A	O5'-P-OP1	-6.48	99.87	105.70
36	1	2794	G	N3-C4-C5	-6.48	125.36	128.60
36	1	3079	U	C6-N1-C1'	6.48	130.27	121.20
36	5	2917	G	O5'-P-OP2	-6.48	99.87	105.70
1	2	453	U	N1-C2-O2	6.48	127.33	122.80
36	1	979	U	N3-C2-O2	-6.48	117.67	122.20
1	6	1791	A	N1-C6-N6	6.48	122.49	118.60
36	5	3154	C	C5-C6-N1	6.48	124.24	121.00
37	7	92	A	N9-C4-C5	-6.48	103.21	105.80
36	1	35	A	N1-C6-N6	6.47	122.48	118.60
36	5	2156	C	C6-N1-C2	6.47	122.89	120.30
36	1	2293	C	N1-C2-O2	6.47	122.78	118.90
36	5	2942	C	C5-C4-N4	-6.47	115.67	120.20
1	2	1745	G	N3-C4-N9	6.47	129.88	126.00
36	5	2899	C	C4-C5-C6	6.47	120.63	117.40
36	1	3266	G	C8-N9-C4	-6.47	103.81	106.40
36	5	1474	A	C8-N9-C4	6.47	108.39	105.80
36	5	2354	C	N1-C2-O2	-6.47	115.02	118.90
36	1	1128	U	N3-C4-C5	6.46	118.48	114.60
1	6	630	A	C2-N3-C4	-6.46	107.37	110.60
36	1	644	G	C8-N9-C4	-6.46	103.81	106.40
36	1	1124	U	C5-C6-N1	6.46	125.93	122.70
36	1	2954	U	OP1-P-O3'	6.46	119.41	105.20
36	5	2851	A	N1-C2-N3	6.46	132.53	129.30
37	7	37	G	N9-C4-C5	-6.46	102.81	105.40
36	1	394	G	N3-C4-N9	-6.46	122.12	126.00
36	1	2621	G	N1-C2-N2	6.46	122.01	116.20
36	5	1885	U	C2-N1-C1'	-6.46	109.95	117.70
37	7	48	U	N3-C4-O4	6.46	123.92	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1761	U	C5-C4-O4	6.46	129.77	125.90
36	5	793	C	N3-C4-N4	6.46	122.52	118.00
36	1	206	G	C2-N3-C4	6.46	115.13	111.90
1	2	404	G	N9-C4-C5	-6.45	102.82	105.40
36	1	914	A	N1-C6-N6	-6.45	114.73	118.60
36	1	1518	U	N3-C4-O4	6.45	123.92	119.40
36	1	2996	U	N1-C2-O2	6.45	127.32	122.80
36	1	286	U	N3-C2-O2	-6.45	117.68	122.20
36	5	1006	A	O5'-P-OP2	-6.45	99.89	105.70
36	5	2350	C	O5'-P-OP1	6.45	118.44	110.70
36	5	895	A	C6-N1-C2	-6.45	114.73	118.60
36	5	2895	G	C4-C5-C6	6.45	122.67	118.80
1	2	1198	G	C8-N9-C4	-6.45	103.82	106.40
36	5	2140	U	N1-C2-O2	-6.45	118.29	122.80
36	5	3380	U	C5-C4-O4	6.45	129.77	125.90
36	1	37	U	C4-C5-C6	6.44	123.57	119.70
36	1	1450	G	C8-N9-C4	6.44	108.98	106.40
36	1	1385	C	N1-C2-O2	-6.44	115.03	118.90
1	6	1112	G	N3-C4-N9	6.44	129.87	126.00
36	5	1299	U	C5-C4-O4	-6.44	122.03	125.90
36	5	1367	G	C8-N9-C1'	-6.44	118.62	127.00
36	5	2874	G	C8-N9-C4	-6.44	103.82	106.40
36	1	948	C	N1-C2-O2	-6.44	115.04	118.90
1	6	1481	C	C6-N1-C2	-6.44	117.72	120.30
36	1	1405	U	N3-C4-C5	6.44	118.46	114.60
36	1	3201	C	C6-N1-C2	-6.44	117.72	120.30
1	6	371	G	C4-N9-C1'	6.44	134.87	126.50
1	2	1057	U	C2-N1-C1'	6.44	125.42	117.70
36	1	952	A	N1-C6-N6	6.44	122.46	118.60
36	1	1104	G	O5'-P-OP1	-6.44	99.91	105.70
1	6	609	U	N1-C2-N3	6.43	118.76	114.90
36	1	62	A	O5'-P-OP2	-6.43	99.91	105.70
36	1	155	G	N3-C4-N9	6.43	129.86	126.00
36	1	439	C	C2-N1-C1'	6.43	125.88	118.80
36	1	1822	C	C6-N1-C2	-6.43	117.73	120.30
36	1	2283	G	N1-C6-O6	6.43	123.76	119.90
36	1	954	U	C5-C6-N1	6.43	125.91	122.70
36	1	2400	G	N9-C4-C5	-6.43	102.83	105.40
36	1	2924	U	C5-C6-N1	-6.43	119.49	122.70
36	5	1124	U	C4-C5-C6	-6.43	115.84	119.70
36	5	2402	A	N9-C4-C5	6.43	108.37	105.80
1	2	394	C	N1-C2-O2	6.42	122.75	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3277	U	N3-C2-O2	-6.42	117.70	122.20
36	5	3119	U	O5'-P-OP1	-6.42	99.92	105.70
1	2	1633	A	N1-C6-N6	-6.42	114.75	118.60
1	2	1462	G	N9-C4-C5	-6.42	102.83	105.40
36	1	2869	U	N1-C2-O2	-6.42	118.31	122.80
36	1	2906	C	N3-C2-O2	-6.42	117.41	121.90
1	6	965	U	C2-N1-C1'	6.42	125.40	117.70
36	1	1411	C	O5'-P-OP2	-6.42	99.92	105.70
36	1	2334	U	O5'-P-OP2	-6.42	99.92	105.70
36	1	2975	U	N3-C2-O2	-6.42	117.71	122.20
1	2	1280	C	N3-C4-C5	-6.42	119.33	121.90
36	1	2642	A	C5-C6-N1	-6.42	114.49	117.70
36	5	2135	U	C5-C4-O4	-6.42	122.05	125.90
1	2	1082	C	N3-C2-O2	-6.41	117.41	121.90
36	1	938	C	N3-C4-N4	6.41	122.49	118.00
36	1	1307	G	C2'-C3'-O3'	6.41	123.96	113.70
38	4	48	A	C5-C6-N6	-6.41	118.57	123.70
36	1	788	C	C5-C6-N1	-6.41	117.79	121.00
1	6	936	G	C5-C6-O6	-6.41	124.75	128.60
1	6	1113	A	C2-N3-C4	-6.41	107.40	110.60
36	5	1716	U	P-O3'-C3'	6.41	127.39	119.70
37	7	87	G	N3-C2-N2	-6.41	115.42	119.90
36	1	3143	C	C6-N1-C2	6.41	122.86	120.30
36	5	1126	G	C8-N9-C4	-6.41	103.84	106.40
36	1	28	C	N3-C4-C5	6.40	124.46	121.90
36	1	47	C	C5-C6-N1	-6.40	117.80	121.00
36	1	716	A	C5-N7-C8	-6.40	100.70	103.90
36	1	1155	C	C6-N1-C2	-6.40	117.74	120.30
36	1	2283	G	C5-C6-O6	-6.40	124.76	128.60
36	1	609	G	O5'-P-OP2	-6.40	99.94	105.70
36	1	915	A	N1-C6-N6	-6.40	114.76	118.60
36	1	2620	G	C5-C6-O6	-6.40	124.76	128.60
1	6	795	U	N3-C2-O2	-6.40	117.72	122.20
52	m6	69	GLY	N-CA-C	-6.40	97.09	113.10
36	1	1505	C	N3-C4-C5	6.40	124.46	121.90
1	6	85	A	N9-C4-C5	6.40	108.36	105.80
1	6	1662	G	N1-C6-O6	-6.40	116.06	119.90
36	5	2904	U	N1-C2-N3	6.40	118.74	114.90
36	1	2885	C	C6-N1-C2	6.40	122.86	120.30
1	6	577	G	C8-N9-C4	-6.40	103.84	106.40
36	5	2864	A	C5-C6-N6	-6.40	118.58	123.70
37	7	81	U	N3-C4-C5	6.40	118.44	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1782	A	C8-N9-C4	-6.40	103.24	105.80
37	3	89	G	N3-C4-N9	6.39	129.84	126.00
36	5	1307	G	OP1-P-O3'	6.39	119.27	105.20
36	5	2134	G	C8-N9-C4	6.39	108.96	106.40
36	5	2338	C	N3-C4-C5	-6.39	119.34	121.90
36	5	2396	G	OP1-P-OP2	-6.39	110.01	119.60
36	5	2796	G	OP2-P-O3'	6.39	119.27	105.20
36	1	2830	G	O5'-P-OP1	6.39	118.37	110.70
1	6	1748	G	N9-C4-C5	-6.39	102.84	105.40
36	5	2873	U	C6-N1-C2	6.39	124.83	121.00
1	2	1370	U	P-O3'-C3'	6.39	127.37	119.70
36	1	1838	G	N3-C4-N9	6.39	129.83	126.00
36	1	2406	C	N3-C2-O2	6.39	126.37	121.90
1	6	1666	U	C5-C6-N1	-6.39	119.50	122.70
36	5	645	A	C4-C5-N7	-6.39	107.50	110.70
36	5	1160	C	C6-N1-C1'	6.39	128.47	120.80
36	5	2531	C	C2-N1-C1'	6.39	125.83	118.80
38	8	4	C	N1-C2-O2	6.39	122.73	118.90
1	6	21	U	N3-C4-O4	6.39	123.87	119.40
36	5	1308	A	N1-C6-N6	-6.39	114.77	118.60
1	2	316	A	C8-N9-C4	6.39	108.36	105.80
36	1	2231	C	N3-C2-O2	6.39	126.37	121.90
36	5	1149	G	N3-C4-N9	6.39	129.83	126.00
36	5	1181	U	C4-C5-C6	6.39	123.53	119.70
36	5	3136	G	N1-C2-N2	-6.39	110.45	116.20
1	6	542	A	O4'-C1'-N9	6.38	113.31	108.20
1	6	597	G	O5'-P-OP2	-6.38	99.95	105.70
36	5	2759	U	N1-C2-N3	6.38	118.73	114.90
36	1	69	C	C4-C5-C6	6.38	120.59	117.40
36	5	3319	U	C5-C6-N1	6.38	125.89	122.70
36	1	779	G	O5'-P-OP2	-6.38	99.96	105.70
1	6	1634	C	C5-C6-N1	6.38	124.19	121.00
36	5	3092	C	N3-C4-N4	-6.38	113.53	118.00
37	7	37	G	N3-C4-N9	6.38	129.83	126.00
36	1	2620	G	N3-C2-N2	-6.38	115.44	119.90
36	5	820	A	N1-C6-N6	6.38	122.43	118.60
36	5	1189	C	OP1-P-OP2	-6.38	110.03	119.60
36	5	2727	A	C5-C6-N1	6.38	120.89	117.70
36	5	3179	U	O5'-P-OP1	-6.38	99.96	105.70
36	1	2809	C	N3-C2-O2	-6.38	117.44	121.90
1	6	426	G	N1-C6-O6	-6.38	116.07	119.90
36	1	869	G	C5-C6-O6	-6.38	124.78	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	668	G	N3-C4-N9	6.38	129.82	126.00
36	1	59	G	C6-C5-N7	-6.37	126.58	130.40
36	1	350	C	N1-C2-O2	6.37	122.72	118.90
36	5	2134	G	N7-C8-N9	-6.37	109.91	113.10
37	7	112	G	C8-N9-C4	-6.37	103.85	106.40
36	1	406	G	O5'-P-OP2	-6.37	99.97	105.70
36	1	3135	U	C5-C6-N1	-6.37	119.52	122.70
52	M6	78	ARG	NE-CZ-NH1	6.37	123.48	120.30
36	5	2186	U	N1-C2-O2	6.37	127.26	122.80
1	6	272	U	P-O3'-C3'	6.37	127.34	119.70
36	5	2134	G	N1-C6-O6	-6.36	116.08	119.90
36	5	2183	A	C5-C6-N6	-6.36	118.61	123.70
36	5	2385	G	C8-N9-C4	6.36	108.94	106.40
36	1	63	A	C8-N9-C4	-6.36	103.25	105.80
36	1	1351	U	N1-C2-O2	6.36	127.25	122.80
36	1	1000	C	C6-N1-C2	6.36	122.84	120.30
36	1	2965	U	C2-N3-C4	-6.36	123.19	127.00
1	2	359	A	C8-N9-C4	6.36	108.34	105.80
36	5	3103	A	C5-C6-N1	6.36	120.88	117.70
36	1	424	G	N3-C4-N9	6.36	129.81	126.00
36	1	860	G	N1-C6-O6	6.36	123.71	119.90
36	1	1804	A	C8-N9-C4	6.35	108.34	105.80
36	1	805	G	C8-N9-C4	6.35	108.94	106.40
36	1	2916	U	C5-C4-O4	-6.35	122.09	125.90
36	1	2917	G	C2-N3-C4	6.35	115.08	111.90
36	5	2950	G	O4'-C1'-N9	6.35	113.28	108.20
36	5	3218	A	C2-N3-C4	-6.35	107.42	110.60
36	5	424	G	N3-C4-N9	6.35	129.81	126.00
36	1	1102	A	OP1-P-O3'	6.35	119.17	105.20
38	4	48	A	N1-C6-N6	6.35	122.41	118.60
1	2	158	U	N3-C2-O2	-6.35	117.76	122.20
1	2	577	G	C5-N7-C8	-6.35	101.13	104.30
36	1	2816	G	O4'-C1'-N9	6.35	113.28	108.20
36	5	2950	G	C4-C5-N7	6.35	113.34	110.80
36	1	676	G	C6-C5-N7	-6.35	126.59	130.40
36	1	885	U	O5'-P-OP1	-6.34	99.99	105.70
36	1	2987	A	N3-C4-N9	6.34	132.48	127.40
36	5	2865	U	N1-C2-O2	6.34	127.24	122.80
36	1	51	A	O5'-P-OP2	-6.34	99.99	105.70
36	1	2942	C	N3-C4-C5	6.34	124.44	121.90
1	2	321	C	N1-C2-O2	6.34	122.70	118.90
36	1	2357	A	C5-C6-N6	-6.34	118.63	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2572	C	C2-N1-C1'	6.34	125.78	118.80
36	5	1193	A	C2-N3-C4	-6.34	107.43	110.60
68	o2	47	ARG	NE-CZ-NH2	-6.34	117.13	120.30
36	1	3184	A	C8-N9-C4	6.34	108.34	105.80
36	1	3209	A	C4-C5-N7	6.34	113.87	110.70
36	5	726	G	N1-C6-O6	6.34	123.70	119.90
36	5	2792	A	N3-C4-C5	-6.34	122.36	126.80
36	5	2965	U	N3-C4-O4	6.34	123.84	119.40
36	1	2899	C	N3-C2-O2	-6.34	117.46	121.90
36	5	1851	G	C4-C5-N7	6.34	113.33	110.80
1	2	1212	G	N1-C6-O6	6.33	123.70	119.90
36	1	1303	A	C5-C6-N6	-6.33	118.63	123.70
36	5	2978	U	C4-C5-C6	6.33	123.50	119.70
36	1	1365	G	C8-N9-C4	-6.33	103.87	106.40
36	1	2425	G	C4-C5-N7	6.33	113.33	110.80
37	3	90	U	C2-N3-C4	-6.33	123.20	127.00
36	5	672	A	C4-C5-C6	6.33	120.17	117.00
36	1	143	G	C5-C6-O6	6.33	132.40	128.60
36	1	1503	A	C2-N3-C4	-6.33	107.44	110.60
1	6	305	C	N1-C2-O2	-6.33	115.10	118.90
1	2	973	A	C2-N3-C4	-6.33	107.44	110.60
36	1	2417	U	N1-C2-N3	6.33	118.70	114.90
1	6	1119	G	C5-C6-O6	6.33	132.40	128.60
36	5	568	G	C5-C6-O6	-6.33	124.80	128.60
36	5	650	C	N3-C4-C5	6.33	124.43	121.90
36	5	951	A	C6-N1-C2	6.33	122.40	118.60
36	1	217	U	OP1-P-O3'	6.33	119.12	105.20
36	1	3201	C	N3-C4-C5	-6.33	119.37	121.90
36	1	3228	C	N3-C2-O2	-6.33	117.47	121.90
1	6	1776	A	C5-C6-N6	-6.33	118.64	123.70
36	1	36	C	N3-C4-N4	6.32	122.43	118.00
36	1	499	G	N3-C2-N2	-6.32	115.47	119.90
36	1	3178	A	C2-N3-C4	-6.32	107.44	110.60
36	5	975	C	C6-N1-C2	-6.32	117.77	120.30
36	5	1107	C	N1-C2-O2	-6.32	115.11	118.90
36	5	1170	A	OP1-P-OP2	6.32	129.08	119.60
36	5	2145	A	N1-C2-N3	6.32	132.46	129.30
36	1	1308	A	C4-C5-C6	6.32	120.16	117.00
36	5	2113	A	O4'-C1'-N9	-6.32	103.14	108.20
1	6	1150	G	C2-N3-C4	-6.32	108.74	111.90
36	1	107	A	C5-C6-N6	-6.32	118.64	123.70
36	1	960	U	O5'-P-OP2	-6.32	100.01	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	45	C	O5'-P-OP2	-6.32	100.01	105.70
36	5	1858	A	N1-C2-N3	6.32	132.46	129.30
36	5	561	C	C5-C6-N1	6.32	124.16	121.00
36	5	806	A	C2-N3-C4	-6.32	107.44	110.60
37	7	87	G	N1-C6-O6	6.32	123.69	119.90
36	1	281	G	C6-N1-C2	-6.32	121.31	125.10
36	5	1837	U	O5'-P-OP1	-6.32	100.02	105.70
36	5	1843	C	C5-C4-N4	-6.32	115.78	120.20
41	14	300	ARG	NE-CZ-NH1	6.31	123.46	120.30
37	7	11	A	C5-C6-N6	-6.31	118.65	123.70
36	1	3143	C	N1-C2-O2	-6.31	115.11	118.90
36	5	3212	C	C5-C6-N1	-6.31	117.84	121.00
1	2	1300	A	N1-C6-N6	-6.31	114.81	118.60
1	2	1654	G	N3-C4-N9	6.31	129.79	126.00
36	1	1943	C	C6-N1-C2	-6.31	117.78	120.30
36	1	2827	U	C5-C6-N1	-6.31	119.55	122.70
1	2	1761	U	N1-C2-N3	6.31	118.68	114.90
36	1	1513	G	N3-C4-C5	-6.31	125.45	128.60
36	5	1426	C	N3-C4-C5	6.31	124.42	121.90
36	5	111	C	O5'-P-OP2	-6.31	100.03	105.70
36	1	1113	G	C8-N9-C4	-6.30	103.88	106.40
36	1	1437	C	C6-N1-C2	-6.30	117.78	120.30
35	sM	167	PRO	N-CA-CB	6.30	110.86	103.30
36	5	957	C	C2-N3-C4	-6.30	116.75	119.90
36	5	2917	G	N3-C4-N9	6.30	129.78	126.00
36	1	1049	C	O5'-P-OP2	-6.30	100.03	105.70
36	5	297	G	N3-C4-C5	-6.30	125.45	128.60
36	1	650	C	OP2-P-O3'	6.30	119.06	105.20
1	6	1031	U	C6-N1-C2	6.30	124.78	121.00
36	5	2403	G	N3-C4-C5	-6.30	125.45	128.60
36	5	3143	C	N1-C2-O2	-6.30	115.12	118.90
1	2	1762	A	C2-N3-C4	-6.30	107.45	110.60
36	5	719	U	N3-C2-O2	-6.30	117.79	122.20
36	1	295	A	O5'-P-OP1	-6.30	100.03	105.70
36	1	585	A	C8-N9-C4	6.30	108.32	105.80
36	1	2764	C	N3-C4-N4	6.30	122.41	118.00
36	1	1154	A	C6-C5-N7	-6.30	127.89	132.30
36	1	1407	A	C8-N9-C4	6.30	108.32	105.80
36	1	2760	C	N3-C2-O2	6.30	126.31	121.90
37	7	20	A	C8-N9-C4	6.30	108.32	105.80
36	1	718	G	N7-C8-N9	6.29	116.25	113.10
36	1	1405	U	OP1-P-OP2	6.29	129.04	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	74	U	N1-C2-O2	-6.29	118.39	122.80
20	c8	15	LEU	CA-CB-CG	6.29	129.78	115.30
36	5	587	U	C6-N1-C2	6.29	124.78	121.00
36	1	2356	A	C5-N7-C8	-6.29	100.75	103.90
36	1	3228	C	N1-C2-O2	6.29	122.67	118.90
36	5	394	G	C4-C5-N7	-6.29	108.28	110.80
36	5	2959	C	OP2-P-O3'	6.29	119.04	105.20
36	1	1166	G	C5-C6-O6	-6.29	124.83	128.60
36	5	2965	U	C5-C4-O4	-6.29	122.13	125.90
1	2	1426	C	C5-C6-N1	6.29	124.14	121.00
36	1	1000	C	C5-C4-N4	-6.29	115.80	120.20
36	1	1617	G	N3-C4-C5	6.29	131.74	128.60
36	1	681	U	C2-N3-C4	-6.29	123.23	127.00
36	1	808	A	N9-C4-C5	6.29	108.31	105.80
36	5	2406	C	N1-C2-O2	-6.29	115.13	118.90
36	1	2870	C	N3-C4-N4	-6.28	113.60	118.00
65	N9	20	GLY	N-CA-C	6.28	128.81	113.10
36	5	2709	C	C2-N3-C4	-6.28	116.76	119.90
36	5	3075	G	N1-C6-O6	6.28	123.67	119.90
1	2	169	A	N1-C6-N6	6.28	122.37	118.60
1	6	1123	C	O5'-P-OP1	-6.28	100.05	105.70
36	1	2137	U	C2-N1-C1'	6.28	125.24	117.70
36	1	2815	G	C8-N9-C4	6.28	108.91	106.40
36	5	710	A	C8-N9-C4	-6.28	103.29	105.80
36	1	968	G	N3-C4-N9	6.28	129.77	126.00
36	1	1386	A	C6-N1-C2	-6.28	114.83	118.60
36	1	1520	G	C2-N3-C4	6.28	115.04	111.90
1	6	606	A	N9-C4-C5	-6.28	103.29	105.80
36	1	1192	C	C6-N1-C2	-6.28	117.79	120.30
36	1	2859	U	C4-C5-C6	6.28	123.47	119.70
36	5	1206	G	N1-C6-O6	-6.28	116.14	119.90
36	1	859	G	C4-N9-C1'	6.27	134.66	126.50
36	1	2148	U	C5-C4-O4	-6.27	122.14	125.90
1	2	144	U	N3-C2-O2	-6.27	117.81	122.20
36	1	1308	A	O5'-P-OP2	-6.27	100.06	105.70
36	1	1377	G	C5-C6-O6	-6.27	124.84	128.60
36	5	1858	A	C8-N9-C4	-6.27	103.29	105.80
1	2	1100	G	N1-C6-O6	6.27	123.66	119.90
1	6	1796	C	N3-C4-N4	-6.27	113.61	118.00
36	5	1239	C	C2-N1-C1'	6.27	125.70	118.80
36	1	2817	A	C5-C6-N1	6.27	120.83	117.70
36	5	302	U	N3-C4-O4	-6.27	115.01	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	29	C	C6-N1-C2	6.27	122.81	120.30
36	5	3128	G	C5-C6-O6	-6.27	124.84	128.60
36	1	935	U	N1-C2-N3	6.27	118.66	114.90
1	6	351	C	C5-C4-N4	-6.27	115.81	120.20
36	5	2351	U	N1-C2-N3	6.27	118.66	114.90
36	1	2846	U	N1-C2-N3	6.26	118.66	114.90
36	1	2231	C	N1-C2-O2	-6.26	115.14	118.90
36	1	2761	G	N1-C6-O6	6.26	123.66	119.90
36	1	2967	A	C8-N9-C4	6.26	108.30	105.80
36	1	3248	C	C5-C6-N1	6.26	124.13	121.00
38	4	109	A	C4-C5-N7	6.26	113.83	110.70
37	3	88	G	N3-C4-C5	-6.26	125.47	128.60
1	6	1629	G	OP2-P-O3'	6.26	118.97	105.20
1	2	864	U	N3-C2-O2	-6.26	117.82	122.20
36	1	1367	G	C4-C5-N7	6.26	113.30	110.80
1	6	1539	G	N3-C4-N9	-6.26	122.25	126.00
1	6	1744	A	N1-C6-N6	6.26	122.35	118.60
36	5	1178	G	C6-C5-N7	-6.26	126.65	130.40
36	5	973	A	C4-C5-C6	6.25	120.13	117.00
1	2	1273	G	N1-C6-O6	-6.25	116.15	119.90
36	1	49	A	N9-C4-C5	-6.25	103.30	105.80
36	1	386	A	N1-C6-N6	6.25	122.35	118.60
36	1	2781	U	N1-C2-O2	-6.25	118.42	122.80
38	4	49	G	C5-C6-O6	-6.25	124.85	128.60
36	5	334	A	C8-N9-C4	6.25	108.30	105.80
36	5	337	G	C2-N3-C4	6.25	115.03	111.90
1	2	402	C	O5'-P-OP1	-6.25	100.07	105.70
36	1	1374	G	N3-C2-N2	6.25	124.28	119.90
12	c0	97	PRO	N-CA-CB	6.25	110.80	103.30
36	5	1908	A	C8-N9-C4	-6.25	103.30	105.80
36	5	3128	G	C8-N9-C4	6.25	108.90	106.40
36	1	2609	A	O5'-P-OP1	6.25	118.20	110.70
36	1	2961	G	C4-C5-N7	6.25	113.30	110.80
36	5	787	G	C2-N3-C4	-6.25	108.78	111.90
36	1	1351	U	C2-N1-C1'	6.25	125.20	117.70
38	4	29	U	C5-C4-O4	-6.25	122.15	125.90
1	6	1662	G	O5'-P-OP2	-6.25	100.08	105.70
36	5	1116	G	N1-C2-N3	6.25	127.65	123.90
1	2	294	C	C6-N1-C2	6.25	122.80	120.30
36	1	836	A	C6-N1-C2	-6.25	114.85	118.60
36	1	2585	G	N3-C4-C5	-6.25	125.48	128.60
36	1	801	A	N1-C6-N6	6.25	122.35	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	681	U	C5-C4-O4	-6.24	122.15	125.90
36	1	2356	A	C4-C5-N7	6.24	113.82	110.70
36	1	2979	U	C5-C4-O4	-6.24	122.15	125.90
36	5	2913	C	O5'-P-OP1	-6.24	100.08	105.70
36	1	1310	G	N1-C2-N2	-6.24	110.58	116.20
1	6	308	C	N3-C4-N4	-6.24	113.63	118.00
36	1	973	A	C6-N1-C2	-6.24	114.86	118.60
36	1	2794	G	O5'-P-OP2	-6.24	100.08	105.70
36	1	2932	U	C2-N3-C4	-6.24	123.26	127.00
36	1	3054	U	N3-C4-C5	-6.24	110.86	114.60
1	6	1513	G	C8-N9-C4	-6.24	103.91	106.40
36	5	1308	A	C5-C6-N6	6.24	128.69	123.70
36	5	1790	G	C5-C6-N1	-6.24	108.38	111.50
36	1	158	G	N1-C6-O6	6.24	123.64	119.90
1	6	1180	C	C6-N1-C2	-6.24	117.81	120.30
1	2	400	A	N1-C6-N6	6.24	122.34	118.60
36	1	1399	A	C2-N3-C4	-6.24	107.48	110.60
36	1	3000	A	C8-N9-C4	6.24	108.30	105.80
38	4	109	A	N9-C4-C5	-6.24	103.31	105.80
36	5	3107	U	C2-N3-C4	-6.24	123.26	127.00
36	5	804	C	N3-C4-C5	-6.23	119.41	121.90
36	5	1850	A	O5'-P-OP1	-6.23	100.09	105.70
36	1	908	G	O4'-C1'-N9	-6.23	103.22	108.20
1	6	863	A	N9-C4-C5	-6.23	103.31	105.80
1	6	1026	A	O5'-P-OP1	-6.23	100.09	105.70
1	6	1745	G	C5-C6-O6	-6.23	124.86	128.60
36	5	720	A	N1-C6-N6	6.23	122.34	118.60
36	5	2120	A	N1-C6-N6	-6.23	114.86	118.60
36	1	304	G	C5-C6-O6	6.23	132.34	128.60
1	6	1639	C	N3-C4-C5	6.23	124.39	121.90
36	5	104	G	N1-C6-O6	6.23	123.64	119.90
36	5	1335	C	N3-C2-O2	6.23	126.26	121.90
36	1	1408	G	C5-C6-O6	-6.23	124.86	128.60
36	1	3104	U	N3-C2-O2	-6.23	117.84	122.20
36	5	2913	C	N3-C4-C5	-6.23	119.41	121.90
36	1	2417	U	C2-N3-C4	-6.22	123.27	127.00
36	1	2647	A	N1-C2-N3	6.22	132.41	129.30
36	1	34	A	C5-N7-C8	-6.22	100.79	103.90
36	5	1480	G	O4'-C1'-N9	6.22	113.18	108.20
36	1	82	C	N1-C2-O2	-6.22	115.17	118.90
36	1	131	C	C6-N1-C2	-6.22	117.81	120.30
36	1	1303	A	O5'-P-OP1	-6.22	100.10	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	632	G	N1-C6-O6	-6.22	116.17	119.90
36	5	890	C	C5-C4-N4	-6.22	115.85	120.20
36	5	2801	A	N7-C8-N9	-6.22	110.69	113.80
1	2	992	A	C5-N7-C8	-6.22	100.79	103.90
36	1	1332	A	O5'-P-OP2	6.22	118.16	110.70
36	5	650	C	N3-C4-N4	-6.22	113.65	118.00
36	5	1367	G	C4-N9-C1'	6.22	134.58	126.50
36	5	2383	C	C6-N1-C2	-6.22	117.81	120.30
36	1	1329	U	C6-N1-C1'	-6.22	112.50	121.20
36	1	2345	A	C5-C6-N6	-6.22	118.73	123.70
36	1	2813	A	N1-C2-N3	6.22	132.41	129.30
36	5	3105	U	N1-C2-O2	-6.22	118.45	122.80
1	2	758	U	N3-C2-O2	-6.21	117.85	122.20
1	6	416	A	N1-C6-N6	6.21	122.33	118.60
36	5	1329	U	C2-N3-C4	-6.21	123.27	127.00
36	1	2875	U	C5-C4-O4	-6.21	122.17	125.90
36	1	683	U	C5-C6-N1	-6.21	119.59	122.70
36	1	2414	G	N1-C2-N3	6.21	127.63	123.90
36	1	3178	A	N1-C6-N6	6.21	122.33	118.60
1	6	874	C	C2-N1-C1'	6.21	125.63	118.80
25	D3	33	LEU	CA-CB-CG	-6.21	101.02	115.30
36	1	1331	U	C5-C6-N1	-6.21	119.60	122.70
36	1	1474	A	O5'-P-OP2	6.21	118.15	110.70
36	1	1495	U	C5-C4-O4	6.21	129.62	125.90
1	6	1046	G	C8-N9-C4	6.21	108.88	106.40
37	7	26	C	C4-C5-C6	6.21	120.50	117.40
36	1	105	C	N3-C2-O2	6.20	126.24	121.90
36	1	2605	G	C5-C6-O6	-6.20	124.88	128.60
36	5	640	U	N3-C4-O4	6.20	123.74	119.40
36	5	646	A	C4-C5-N7	-6.20	107.60	110.70
36	5	2280	A	C5-C6-N1	-6.20	114.60	117.70
36	5	2798	C	N3-C4-N4	-6.20	113.66	118.00
37	7	66	A	C8-N9-C4	6.20	108.28	105.80
37	7	105	C	C6-N1-C2	-6.20	117.82	120.30
1	2	321	C	N3-C2-O2	-6.20	117.56	121.90
36	1	627	U	N3-C2-O2	6.20	126.54	122.20
36	1	2344	U	C5-C6-N1	-6.20	119.60	122.70
1	6	541	A	P-O3'-C3'	-6.20	112.26	119.70
36	1	958	C	N3-C4-N4	-6.20	113.66	118.00
36	1	1124	U	N1-C2-O2	6.20	127.14	122.80
36	1	2434	U	N3-C2-O2	-6.20	117.86	122.20
36	5	2885	C	C5-C4-N4	-6.20	115.86	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	69	C	C6-N1-C2	6.20	122.78	120.30
1	2	1606	C	O5'-P-OP2	-6.20	100.12	105.70
36	1	721	G	N7-C8-N9	6.20	116.20	113.10
36	1	905	U	N1-C2-N3	6.20	118.62	114.90
36	1	1507	G	C6-C5-N7	-6.20	126.68	130.40
36	5	590	G	C5-C6-O6	-6.20	124.88	128.60
36	5	1366	A	N1-C6-N6	-6.20	114.88	118.60
36	5	1374	G	N3-C2-N2	6.20	124.24	119.90
36	1	612	U	C2-N3-C4	-6.20	123.28	127.00
38	4	47	C	C2-N3-C4	-6.20	116.80	119.90
36	5	2895	G	C6-C5-N7	-6.20	126.68	130.40
36	1	284	A	O4'-C1'-N9	6.20	113.16	108.20
36	1	640	U	N3-C4-O4	6.20	123.74	119.40
36	1	1494	U	C5-C4-O4	6.20	129.62	125.90
1	6	350	U	N1-C2-N3	6.20	118.62	114.90
36	5	1431	G	C4-C5-N7	-6.20	108.32	110.80
36	1	3183	A	OP2-P-O3'	6.19	118.83	105.20
36	1	804	C	N3-C4-C5	-6.19	119.42	121.90
36	1	1560	G	C4-N9-C1'	-6.19	118.45	126.50
36	1	3362	A	N1-C6-N6	6.19	122.31	118.60
37	3	86	U	N3-C4-C5	6.19	118.31	114.60
1	6	362	G	N3-C4-N9	6.19	129.72	126.00
36	5	2763	U	C5-C4-O4	-6.19	122.19	125.90
36	1	858	A	C8-N9-C4	-6.19	103.32	105.80
36	1	2374	C	N1-C2-N3	6.19	123.53	119.20
1	2	1658	G	C6-C5-N7	-6.19	126.69	130.40
36	1	1733	G	N3-C4-C5	-6.19	125.51	128.60
36	1	2404	A	C2-N3-C4	6.19	113.69	110.60
1	6	259	U	N1-C2-O2	-6.19	118.47	122.80
1	6	1614	A	N1-C6-N6	6.19	122.31	118.60
36	1	339	C	C2-N3-C4	-6.18	116.81	119.90
36	5	2874	G	C5-C6-O6	6.18	132.31	128.60
36	5	1513	G	N7-C8-N9	6.18	116.19	113.10
36	5	873	C	OP2-P-O3'	6.18	118.80	105.20
36	5	3115	C	C6-N1-C2	-6.18	117.83	120.30
1	2	1142	A	O5'-P-OP2	-6.18	100.14	105.70
36	5	1324	U	O5'-P-OP2	-6.18	100.14	105.70
36	5	2909	U	N1-C2-N3	6.18	118.61	114.90
38	8	95	G	C8-N9-C1'	6.18	135.03	127.00
36	1	2646	C	C5-C6-N1	-6.18	117.91	121.00
36	1	105	C	N1-C2-O2	-6.18	115.19	118.90
1	6	1013	A	C5-C6-N6	-6.18	118.76	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2821	C	N3-C2-O2	6.18	126.22	121.90
1	6	75	U	C2-N1-C1'	6.17	125.11	117.70
36	5	2132	C	C6-N1-C2	-6.17	117.83	120.30
73	o7	5	THR	C-N-CD	6.17	141.37	128.40
1	6	1000	C	C2-N3-C4	-6.17	116.81	119.90
1	2	736	C	C5-C6-N1	6.17	124.09	121.00
36	1	515	C	C2-N3-C4	6.17	122.98	119.90
36	1	1160	C	N1-C2-N3	-6.17	114.88	119.20
36	5	1137	C	C4-C5-C6	6.17	120.48	117.40
36	5	1303	A	C5-C6-N6	-6.17	118.76	123.70
36	5	2913	C	N1-C2-O2	-6.17	115.20	118.90
36	5	2988	C	C5-C6-N1	-6.17	117.91	121.00
36	5	3137	C	C5-C4-N4	6.17	124.52	120.20
36	1	1421	G	OP2-P-O3'	6.17	118.77	105.20
1	6	543	C	C5-C6-N1	6.17	124.08	121.00
36	5	635	G	C5-C6-N1	-6.17	108.42	111.50
36	1	2643	A	C5-C6-N6	-6.17	118.77	123.70
36	5	1833	G	C2-N3-C4	6.17	114.98	111.90
36	5	3225	C	N3-C2-O2	-6.17	117.58	121.90
36	1	1187	C	N3-C4-C5	6.16	124.36	121.90
36	1	1402	C	N3-C2-O2	-6.16	117.59	121.90
1	6	1657	U	O5'-P-OP1	6.16	118.10	110.70
36	5	2149	A	N1-C6-N6	6.16	122.30	118.60
36	1	274	G	C5-C6-N1	-6.16	108.42	111.50
36	1	994	G	N1-C6-O6	-6.16	116.20	119.90
36	1	1518	U	C5-C6-N1	-6.16	119.62	122.70
36	1	2627	C	C2-N3-C4	-6.16	116.82	119.90
36	1	877	C	N1-C2-O2	-6.16	115.20	118.90
38	8	68	G	C6-C5-N7	-6.16	126.70	130.40
36	1	639	G	C6-C5-N7	-6.16	126.71	130.40
36	1	2124	G	N1-C6-O6	6.16	123.59	119.90
36	1	3221	C	O5'-P-OP2	6.16	118.09	110.70
36	5	2199	G	C4-C5-C6	6.16	122.49	118.80
36	1	1296	C	C4-C5-C6	6.16	120.48	117.40
36	1	1437	C	N3-C2-O2	-6.16	117.59	121.90
36	1	281	G	C5-C6-O6	-6.15	124.91	128.60
36	1	1296	C	C6-N1-C2	-6.15	117.84	120.30
1	6	1112	G	C5-C6-N1	6.15	114.58	111.50
36	5	2965	U	N1-C2-O2	-6.15	118.49	122.80
1	2	1291	G	C2-N3-C4	-6.15	108.82	111.90
1	2	1782	A	C5-C6-N6	6.15	128.62	123.70
36	1	1343	A	C5-C6-N6	-6.15	118.78	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	686	G	OP1-P-OP2	-6.15	110.37	119.60
36	5	2972	G	N1-C6-O6	-6.15	116.21	119.90
36	1	614	C	C6-N1-C2	6.15	122.76	120.30
36	1	2416	U	C6-N1-C2	-6.15	117.31	121.00
18	C6	40	GLU	C-N-CD	-6.15	107.07	120.60
36	1	2979	U	C2-N3-C4	-6.15	123.31	127.00
36	5	2371	G	N3-C2-N2	6.15	124.20	119.90
36	1	25	U	N1-C2-O2	-6.15	118.50	122.80
36	1	366	A	O5'-P-OP2	-6.15	100.17	105.70
1	6	967	A	C2-N3-C4	6.15	113.67	110.60
36	5	2917	G	N1-C6-O6	6.15	123.59	119.90
36	1	718	G	C5-N7-C8	-6.15	101.23	104.30
36	5	1367	G	C6-C5-N7	-6.15	126.71	130.40
38	4	113	U	C4-C5-C6	6.14	123.39	119.70
1	2	1194	A	N1-C6-N6	6.14	122.29	118.60
1	6	398	G	C5-C6-O6	6.14	132.29	128.60
36	5	589	A	O4'-C1'-N9	-6.14	103.29	108.20
36	5	938	C	C4-C5-C6	-6.14	114.33	117.40
36	5	1429	G	N1-C2-N2	-6.14	110.67	116.20
36	1	1421	G	O5'-P-OP2	-6.14	100.17	105.70
36	1	2373	A	C8-N9-C4	-6.14	103.34	105.80
36	5	796	U	C4-C5-C6	6.14	123.38	119.70
36	1	1898	G	N1-C6-O6	6.14	123.58	119.90
36	1	87	U	N3-C4-C5	-6.14	110.92	114.60
36	5	3	U	N3-C2-O2	-6.14	117.90	122.20
36	5	152	U	N1-C2-N3	6.14	118.58	114.90
1	2	1241	G	C4-C5-N7	6.13	113.25	110.80
36	1	1141	C	C4-C5-C6	6.13	120.47	117.40
36	1	1176	C	N3-C2-O2	6.13	126.19	121.90
36	1	1351	U	N3-C2-O2	-6.13	117.91	122.20
36	1	2777	G	C5-C6-O6	6.13	132.28	128.60
36	1	3081	C	C2-N3-C4	-6.13	116.83	119.90
1	6	371	G	C6-C5-N7	-6.13	126.72	130.40
36	5	41	G	OP2-P-O3'	6.13	118.70	105.20
34	SR	161	LYS	N-CA-C	6.13	127.56	111.00
36	1	1507	G	C8-N9-C1'	-6.13	119.03	127.00
36	1	2966	G	C6-C5-N7	-6.13	126.72	130.40
1	6	1775	U	C5-C6-N1	-6.13	119.63	122.70
36	5	515	C	N3-C4-N4	6.13	122.29	118.00
36	1	1917	C	C6-N1-C2	6.13	122.75	120.30
36	5	410	U	N3-C4-C5	-6.13	110.92	114.60
1	2	1145	U	N3-C4-O4	6.13	123.69	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1600	A	C6-C5-N7	-6.13	128.01	132.30
36	1	143	G	C4-C5-N7	-6.13	108.35	110.80
1	6	1640	C	C5-C4-N4	-6.13	115.91	120.20
36	5	1054	A	C8-N9-C4	6.13	108.25	105.80
36	5	1154	A	N1-C6-N6	-6.13	114.92	118.60
36	5	1300	G	N9-C4-C5	-6.13	102.95	105.40
36	5	3177	G	C2-N3-C4	-6.13	108.84	111.90
1	2	458	G	C5-C6-N1	-6.13	108.44	111.50
36	1	611	A	O5'-P-OP1	6.13	118.05	110.70
36	1	1897	G	N1-C6-O6	6.13	123.58	119.90
36	5	36	C	N1-C2-O2	-6.13	115.22	118.90
36	5	803	C	C6-N1-C2	-6.13	117.85	120.30
36	1	2723	U	C6-N1-C2	6.12	124.67	121.00
36	5	1322	U	O5'-P-OP2	-6.12	100.19	105.70
36	5	2234	G	N1-C6-O6	6.12	123.58	119.90
36	5	3026	G	N1-C6-O6	6.12	123.58	119.90
36	1	339	C	N3-C4-C5	6.12	124.35	121.90
36	1	804	C	N3-C2-O2	-6.12	117.61	121.90
36	1	2138	A	C8-N9-C4	-6.12	103.35	105.80
1	6	603	U	N1-C2-O2	-6.12	118.51	122.80
36	5	631	U	C6-N1-C2	6.12	124.67	121.00
36	5	2919	A	N1-C6-N6	-6.12	114.93	118.60
36	5	3204	C	C5-C6-N1	-6.12	117.94	121.00
36	5	3331	U	C6-N1-C2	6.12	124.67	121.00
36	1	940	G	C5-C6-N1	6.12	114.56	111.50
36	1	2144	A	C6-N1-C2	-6.12	114.93	118.60
36	1	2329	C	N3-C2-O2	6.12	126.18	121.90
36	1	2418	G	C4-N9-C1'	6.12	134.45	126.50
1	6	957	G	C5-C6-N1	-6.12	108.44	111.50
36	1	1167	U	C5-C6-N1	-6.12	119.64	122.70
36	5	3143	C	N3-C2-O2	6.12	126.18	121.90
1	6	1129	U	N3-C4-O4	-6.12	115.12	119.40
36	5	2246	G	N3-C4-C5	-6.12	125.54	128.60
1	6	1112	G	N3-C4-C5	-6.11	125.54	128.60
36	5	2996	U	N3-C2-O2	-6.11	117.92	122.20
38	8	56	G	N1-C6-O6	6.11	123.57	119.90
36	1	496	C	C6-N1-C2	-6.11	117.86	120.30
36	1	801	A	N9-C4-C5	-6.11	103.36	105.80
36	1	2889	C	N3-C2-O2	-6.11	117.62	121.90
36	5	2792	A	C8-N9-C4	-6.11	103.36	105.80
36	1	1547	G	N7-C8-N9	-6.11	110.05	113.10
36	1	3050	U	N1-C2-O2	6.11	127.08	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	218	G	N3-C2-N2	6.11	124.18	119.90
36	5	1879	A	O5'-P-OP1	6.11	118.03	110.70
1	2	1749	A	C2-N3-C4	-6.11	107.55	110.60
36	1	656	A	C8-N9-C4	-6.11	103.36	105.80
36	1	2281	A	C2-N3-C4	-6.11	107.55	110.60
36	5	861	C	C5-C6-N1	-6.11	117.95	121.00
36	5	2309	A	N1-C6-N6	-6.11	114.94	118.60
1	6	1026	A	C8-N9-C4	6.11	108.24	105.80
36	5	788	C	OP2-P-O3'	6.11	118.63	105.20
36	5	2941	A	N1-C2-N3	6.11	132.35	129.30
38	8	111	A	C2-N3-C4	-6.11	107.55	110.60
36	5	95	A	C8-N9-C4	6.10	108.24	105.80
1	2	1486	G	C5-N7-C8	-6.10	101.25	104.30
1	2	1773	C	N1-C2-O2	-6.10	115.24	118.90
36	1	1837	U	N1-C2-O2	-6.10	118.53	122.80
36	5	2834	G	O5'-P-OP2	-6.10	100.21	105.70
36	1	1114	U	N1-C2-N3	-6.10	111.24	114.90
1	2	1082	C	C6-N1-C2	-6.10	117.86	120.30
38	4	59	A	C2-N3-C4	6.10	113.65	110.60
36	5	636	C	N3-C4-N4	-6.10	113.73	118.00
36	1	719	U	N1-C2-O2	6.10	127.07	122.80
36	1	797	U	N3-C4-O4	6.10	123.67	119.40
36	1	1386	A	C5-C6-N6	-6.10	118.82	123.70
1	6	352	A	OP2-P-O3'	6.10	118.62	105.20
36	5	2404	A	O5'-P-OP1	6.10	118.02	110.70
36	1	1428	A	N1-C6-N6	6.10	122.26	118.60
36	1	3212	C	C6-N1-C2	6.10	122.74	120.30
36	5	1317	A	N1-C2-N3	-6.10	126.25	129.30
36	1	2118	C	C5-C6-N1	6.09	124.05	121.00
36	5	708	G	N7-C8-N9	6.09	116.15	113.10
36	5	1550	C	O5'-P-OP1	-6.09	100.22	105.70
36	5	2993	G	C5-C6-O6	-6.09	124.94	128.60
36	5	3039	C	O5'-P-OP2	-6.09	100.21	105.70
36	5	2318	U	N1-C2-O2	6.09	127.06	122.80
36	5	1196	C	N1-C2-O2	6.09	122.55	118.90
36	5	2353	G	C6-C5-N7	-6.09	126.75	130.40
36	5	2388	U	N3-C4-C5	-6.09	110.94	114.60
36	5	41	G	C5-C6-O6	-6.09	124.95	128.60
36	5	1445	U	N1-C2-O2	-6.09	118.54	122.80
36	5	1487	G	N3-C4-C5	-6.09	125.56	128.60
36	5	3147	G	C2-N3-C4	-6.09	108.86	111.90
36	1	75	G	C4-C5-N7	6.09	113.23	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1581	C	C5-C6-N1	6.09	124.04	121.00
36	1	922	U	C2-N1-C1'	6.09	125.00	117.70
36	1	1510	G	C6-C5-N7	-6.09	126.75	130.40
36	1	1835	A	C5-C6-N6	6.09	128.57	123.70
1	6	619	A	N1-C6-N6	-6.09	114.95	118.60
1	6	1767	G	O5'-P-OP1	-6.09	100.22	105.70
36	1	2222	A	N9-C4-C5	6.08	108.23	105.80
36	5	924	G	C5-C6-N1	-6.08	108.46	111.50
36	5	2363	A	N1-C6-N6	6.08	122.25	118.60
36	5	2620	G	O5'-P-OP1	6.08	118.00	110.70
36	1	88	A	N1-C6-N6	6.08	122.25	118.60
36	1	214	G	N1-C6-O6	6.08	123.55	119.90
36	1	709	A	N7-C8-N9	-6.08	110.76	113.80
1	6	85	A	N1-C6-N6	-6.08	114.95	118.60
36	1	1495	U	C6-N1-C1'	6.08	129.71	121.20
36	5	1317	A	C8-N9-C4	6.08	108.23	105.80
37	7	101	G	C4-C5-N7	6.08	113.23	110.80
36	1	3307	A	C5-N7-C8	-6.08	100.86	103.90
36	5	2631	U	C5-C4-O4	-6.08	122.25	125.90
1	2	1274	C	N1-C2-O2	6.08	122.55	118.90
36	1	585	A	O5'-P-OP2	-6.08	100.23	105.70
1	6	767	U	N3-C2-O2	-6.08	117.95	122.20
36	5	1172	G	O5'-P-OP1	-6.08	100.23	105.70
36	1	2146	C	OP1-P-OP2	-6.07	110.49	119.60
36	5	2134	G	C5-N7-C8	6.07	107.34	104.30
36	5	786	A	O5'-P-OP2	-6.07	100.23	105.70
36	5	3107	U	N3-C4-C5	6.07	118.24	114.60
36	5	3380	U	N3-C4-O4	-6.07	115.15	119.40
36	5	98	G	C2-N3-C4	-6.07	108.86	111.90
36	5	1052	U	O5'-P-OP2	-6.07	100.24	105.70
37	7	77	G	C5-C6-O6	-6.07	124.96	128.60
36	1	1901	A	C2-N3-C4	6.07	113.63	110.60
38	4	146	U	C5-C6-N1	-6.07	119.67	122.70
36	5	803	C	N3-C4-N4	6.07	122.25	118.00
1	2	610	G	C4-N9-C1'	6.07	134.38	126.50
36	1	1903	U	C5-C6-N1	6.07	125.73	122.70
36	5	1820	U	O4'-C1'-N1	6.07	113.05	108.20
1	6	577	G	N7-C8-N9	6.06	116.13	113.10
36	5	922	U	C5-C6-N1	-6.06	119.67	122.70
36	5	3180	A	N7-C8-N9	-6.06	110.77	113.80
36	1	143	G	N9-C4-C5	6.06	107.83	105.40
36	1	2354	C	O5'-P-OP2	-6.06	100.24	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	3	U	C6-N1-C2	6.06	124.64	121.00
36	5	668	G	N3-C2-N2	6.06	124.14	119.90
36	5	2982	A	C2-N3-C4	6.06	113.63	110.60
1	2	576	G	N1-C6-O6	6.06	123.54	119.90
36	1	3278	C	C2-N1-C1'	6.06	125.47	118.80
1	2	1241	G	C6-C5-N7	-6.06	126.77	130.40
1	6	48	G	O5'-P-OP2	-6.06	100.25	105.70
36	1	399	A	O5'-P-OP1	-6.06	100.25	105.70
36	1	757	C	N1-C2-O2	-6.06	115.27	118.90
36	5	35	A	C2-N3-C4	-6.06	107.57	110.60
36	5	960	U	C2-N1-C1'	6.06	124.97	117.70
36	5	2323	G	N9-C4-C5	6.06	107.82	105.40
1	6	337	G	C4-N9-C1'	6.06	134.37	126.50
36	5	1847	A	C2-N3-C4	-6.06	107.57	110.60
36	5	2694	A	C2-N3-C4	6.06	113.63	110.60
36	1	1290	A	C8-N9-C4	6.05	108.22	105.80
36	1	3016	A	C4-C5-C6	6.05	120.03	117.00
36	1	3181	C	C6-N1-C2	-6.05	117.88	120.30
36	5	2872	A	N3-C4-C5	6.05	131.04	126.80
36	5	2618	G	C6-N1-C2	-6.05	121.47	125.10
1	2	694	U	C2-N1-C1'	6.05	124.96	117.70
36	1	2723	U	C5-C6-N1	-6.05	119.67	122.70
36	5	411	U	N1-C2-O2	-6.05	118.56	122.80
36	5	2619	G	N1-C6-O6	6.05	123.53	119.90
1	2	610	G	C8-N9-C1'	-6.05	119.14	127.00
36	1	1126	G	C6-C5-N7	-6.05	126.77	130.40
1	6	455	C	N3-C4-N4	6.05	122.23	118.00
36	5	2362	C	N3-C4-N4	-6.05	113.77	118.00
1	2	1462	G	C5-C6-O6	-6.05	124.97	128.60
36	5	1481	A	OP1-P-OP2	6.05	128.67	119.60
1	6	390	G	O5'-P-OP2	-6.04	100.26	105.70
1	2	499	U	C5-C6-N1	6.04	125.72	122.70
36	1	2808	A	N1-C6-N6	6.04	122.23	118.60
1	6	1748	G	C8-N9-C4	6.04	108.82	106.40
36	5	656	A	N1-C6-N6	6.04	122.23	118.60
36	5	1433	A	N1-C6-N6	-6.04	114.97	118.60
36	1	395	A	C8-N9-C4	-6.04	103.38	105.80
36	5	1851	G	C6-C5-N7	-6.04	126.78	130.40
38	8	51	G	N1-C6-O6	6.04	123.52	119.90
36	5	888	A	N1-C6-N6	6.04	122.22	118.60
36	5	2342	U	O5'-P-OP2	-6.04	100.26	105.70
36	1	2406	C	N3-C4-N4	6.04	122.23	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	92	A	N1-C6-N6	6.04	122.22	118.60
36	1	2144	A	C5-C6-N1	6.04	120.72	117.70
36	5	2141	U	OP1-P-OP2	-6.04	110.54	119.60
36	5	3145	C	C5-C6-N1	-6.04	117.98	121.00
1	2	600	U	C5-C4-O4	6.04	129.52	125.90
36	1	898	U	N1-C2-O2	6.04	127.03	122.80
38	4	13	A	N1-C6-N6	6.04	122.22	118.60
1	6	515	A	C8-N9-C4	-6.04	103.39	105.80
36	5	841	A	C8-N9-C4	6.04	108.21	105.80
36	5	1198	C	C2-N3-C4	-6.04	116.88	119.90
1	2	320	U	C5-C4-O4	-6.03	122.28	125.90
36	1	1917	C	C5-C6-N1	-6.03	117.98	121.00
36	5	1419	A	O5'-P-OP2	-6.03	100.27	105.70
36	5	2820	A	N7-C8-N9	6.03	116.82	113.80
52	m6	151	ASP	CB-CG-OD1	-6.03	112.87	118.30
36	5	3322	A	O5'-P-OP2	-6.03	100.27	105.70
36	1	2899	C	C2-N3-C4	-6.03	116.88	119.90
36	5	1065	A	C8-N9-C4	6.03	108.21	105.80
1	2	1657	U	O4'-C1'-N1	6.03	113.02	108.20
36	1	107	A	C6-C5-N7	-6.03	128.08	132.30
1	6	901	G	C5-N7-C8	-6.03	101.29	104.30
36	1	1389	G	N9-C4-C5	-6.03	102.99	105.40
36	1	2351	U	N3-C2-O2	-6.03	117.98	122.20
36	5	859	G	O5'-P-OP1	-6.03	100.28	105.70
36	1	703	G	C5-C6-O6	6.02	132.21	128.60
1	6	1796	C	C5-C6-N1	-6.02	117.99	121.00
36	5	3101	G	N1-C6-O6	-6.02	116.29	119.90
36	1	827	A	C8-N9-C4	6.02	108.21	105.80
36	1	1124	U	N3-C2-O2	-6.02	117.99	122.20
36	1	2202	C	C5-C4-N4	-6.02	115.98	120.20
36	5	2631	U	OP1-P-O3'	6.02	118.44	105.20
36	1	805	G	C4-C5-N7	-6.02	108.39	110.80
36	1	2412	G	C2-N3-C4	6.02	114.91	111.90
36	5	2775	U	N3-C4-O4	-6.02	115.19	119.40
36	1	49	A	N7-C8-N9	-6.02	110.79	113.80
36	1	644	G	O5'-P-OP1	-6.02	100.28	105.70
36	5	1367	G	C4-C5-C6	6.02	122.41	118.80
37	7	101	G	C5-C6-O6	-6.02	124.99	128.60
36	5	587	U	C5-C4-O4	-6.02	122.29	125.90
36	1	1408	G	N1-C6-O6	6.01	123.51	119.90
36	1	2888	U	C2-N3-C4	-6.01	123.39	127.00
1	6	426	G	N3-C4-C5	-6.01	125.59	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	963	G	O5'-P-OP1	6.01	117.92	110.70
36	5	974	G	N3-C4-C5	-6.01	125.59	128.60
36	1	1008	U	C5-C6-N1	-6.01	119.69	122.70
36	5	820	A	C6-C5-N7	-6.01	128.09	132.30
1	2	1642	G	C5-C6-O6	-6.01	124.99	128.60
36	1	3016	A	C6-C5-N7	-6.01	128.09	132.30
1	6	1698	G	P-O3'-C3'	6.01	126.91	119.70
36	5	49	A	C8-N9-C4	6.01	108.20	105.80
36	5	1838	G	O5'-P-OP2	-6.01	100.29	105.70
36	5	2288	G	C5-C6-O6	-6.01	124.99	128.60
1	2	499	U	P-O3'-C3'	6.01	126.91	119.70
36	1	2636	A	C8-N9-C4	-6.01	103.40	105.80
36	1	2901	G	N1-C6-O6	6.01	123.51	119.90
1	6	542	A	C6-C5-N7	-6.01	128.09	132.30
36	5	2199	G	C4-C5-N7	6.01	113.20	110.80
37	7	98	C	O5'-P-OP2	-6.01	100.29	105.70
1	2	704	C	N1-C2-O2	6.01	122.50	118.90
36	5	2142	A	OP1-P-OP2	-6.01	110.59	119.60
36	1	64	G	C5-C6-O6	6.01	132.20	128.60
36	1	1157	G	N1-C2-N3	6.01	127.50	123.90
1	6	119	A	C5-C6-N1	-6.01	114.70	117.70
36	5	1545	A	N1-C6-N6	6.01	122.20	118.60
36	1	1188	U	O5'-P-OP2	-6.00	100.30	105.70
36	5	3362	A	O4'-C1'-N9	6.00	113.00	108.20
36	1	2808	A	C6-C5-N7	-6.00	128.10	132.30
36	1	2812	C	O5'-P-OP2	6.00	117.90	110.70
38	4	61	A	O5'-P-OP1	-6.00	100.30	105.70
36	5	3362	A	N3-C4-N9	-6.00	122.60	127.40
37	7	103	A	C2-N3-C4	6.00	113.60	110.60
1	2	581	U	C2-N1-C1'	6.00	124.90	117.70
36	1	2222	A	C8-N9-C4	-6.00	103.40	105.80
38	4	140	G	C8-N9-C4	-6.00	104.00	106.40
36	5	395	A	C5-C6-N1	6.00	120.70	117.70
37	7	78	U	O5'-P-OP2	-6.00	100.30	105.70
38	8	77	A	C8-N9-C4	6.00	108.20	105.80
36	1	105	C	C6-N1-C2	6.00	122.70	120.30
36	1	961	C	C2-N3-C4	-6.00	116.90	119.90
38	4	20	U	C5-C6-N1	-6.00	119.70	122.70
36	5	1082	U	C6-N1-C2	-6.00	117.40	121.00
36	5	1239	C	C5-C6-N1	6.00	124.00	121.00
36	5	2996	U	C2-N1-C1'	6.00	124.90	117.70
1	2	1399	C	C5-C6-N1	6.00	124.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2308	C	C5-C6-N1	-6.00	118.00	121.00
1	6	371	G	N3-C4-N9	6.00	129.60	126.00
36	5	2893	C	N3-C4-C5	-6.00	119.50	121.90
36	5	3123	A	O5'-P-OP1	-6.00	100.30	105.70
36	1	925	A	C6-N1-C2	-5.99	115.00	118.60
1	6	364	G	C8-N9-C4	5.99	108.80	106.40
36	5	348	A	C8-N9-C4	5.99	108.20	105.80
1	2	799	A	N1-C6-N6	5.99	122.19	118.60
36	1	41	G	OP2-P-O3'	5.99	118.38	105.20
36	5	969	C	C2-N1-C1'	-5.99	112.21	118.80
1	2	1202	A	C2-N3-C4	5.99	113.59	110.60
36	1	2612	U	C5-C6-N1	-5.99	119.70	122.70
38	4	12	A	C8-N9-C4	5.99	108.20	105.80
1	6	382	C	N3-C4-C5	5.99	124.30	121.90
36	5	297	G	N1-C2-N2	-5.99	110.81	116.20
36	5	656	A	C4-C5-C6	5.99	120.00	117.00
36	5	1131	G	OP2-P-O3'	5.99	118.38	105.20
36	1	53	G	C6-N1-C2	-5.99	121.51	125.10
36	1	345	G	N3-C4-C5	-5.99	125.61	128.60
1	6	371	G	C8-N9-C1'	-5.99	119.22	127.00
1	6	414	C	N1-C2-O2	5.99	122.49	118.90
36	5	865	U	N1-C2-O2	-5.99	118.61	122.80
1	2	1280	C	N3-C4-N4	5.99	122.19	118.00
36	1	1121	U	N1-C2-O2	-5.99	118.61	122.80
36	1	2766	U	N3-C2-O2	-5.99	118.01	122.20
1	2	765	G	O4'-C1'-N9	-5.98	103.41	108.20
1	2	831	U	C6-N1-C2	-5.98	117.41	121.00
36	1	621	A	N7-C8-N9	5.98	116.79	113.80
36	1	1103	A	O5'-P-OP2	5.98	117.88	110.70
36	1	1149	G	N1-C2-N2	5.98	121.58	116.20
36	1	3310	A	C8-N9-C4	5.98	108.19	105.80
49	M3	85	LEU	CA-CB-CG	5.98	129.06	115.30
36	5	966	U	N1-C2-O2	5.98	126.99	122.80
36	1	1883	A	N7-C8-N9	-5.98	110.81	113.80
37	3	94	C	N3-C2-O2	5.98	126.09	121.90
38	4	44	A	N1-C6-N6	5.98	122.19	118.60
1	6	610	G	C8-N9-C1'	-5.98	119.23	127.00
1	6	804	A	N1-C6-N6	5.98	122.19	118.60
1	6	1748	G	N1-C6-O6	5.98	123.49	119.90
36	5	58	G	N1-C6-O6	5.98	123.49	119.90
36	5	1376	C	OP1-P-OP2	5.98	128.57	119.60
36	1	679	U	O5'-P-OP2	-5.98	100.32	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	98	G	C5-C6-O6	5.98	132.19	128.60
36	5	227	G	C8-N9-C4	5.98	108.79	106.40
36	5	350	C	C6-N1-C2	-5.98	117.91	120.30
36	1	424	G	N9-C4-C5	-5.98	103.01	105.40
36	1	2368	A	N9-C4-C5	5.98	108.19	105.80
36	1	2405	C	C4-C5-C6	5.98	120.39	117.40
36	1	2946	A	C6-C5-N7	-5.98	128.12	132.30
36	5	216	G	C5-N7-C8	-5.98	101.31	104.30
36	5	706	A	N9-C4-C5	-5.98	103.41	105.80
36	5	1885	U	N1-C2-O2	-5.98	118.62	122.80
1	6	1570	A	O5'-P-OP1	-5.97	100.32	105.70
36	1	1097	G	C8-N9-C4	-5.97	104.01	106.40
36	1	2192	C	C4-C5-C6	5.97	120.39	117.40
1	6	606	A	C8-N9-C4	5.97	108.19	105.80
38	8	95	G	N3-C4-N9	-5.97	122.42	126.00
36	5	2944	U	C5-C6-N1	5.97	125.69	122.70
37	7	50	U	N1-C2-O2	-5.97	118.62	122.80
1	6	609	U	N3-C4-O4	-5.97	115.22	119.40
36	5	1384	U	C2-N3-C4	5.97	130.58	127.00
36	5	2155	G	C8-N9-C4	5.97	108.79	106.40
36	5	2862	U	C5-C6-N1	-5.97	119.72	122.70
36	1	1496	C	C2-N1-C1'	5.97	125.36	118.80
36	5	635	G	C4-C5-N7	5.97	113.19	110.80
36	5	1348	U	N3-C2-O2	-5.97	118.02	122.20
36	5	1889	G	N9-C4-C5	-5.97	103.01	105.40
36	1	934	G	N3-C2-N2	5.96	124.08	119.90
36	1	1322	U	N1-C2-O2	-5.96	118.62	122.80
36	1	1379	G	N1-C2-N2	-5.96	110.83	116.20
36	1	2422	C	N1-C2-O2	5.96	122.48	118.90
36	5	2759	U	C4-C5-C6	5.96	123.28	119.70
36	1	2942	C	C4-C5-C6	-5.96	114.42	117.40
36	1	3344	A	C6-C5-N7	-5.96	128.13	132.30
36	5	1340	G	C8-N9-C4	5.96	108.78	106.40
36	5	3181	C	O5'-P-OP1	5.96	117.85	110.70
24	D2	93	LEU	CA-CB-CG	5.96	129.01	115.30
38	4	25	G	C5-N7-C8	5.96	107.28	104.30
36	5	2284	C	C6-N1-C1'	-5.96	113.65	120.80
36	5	2375	G	N1-C6-O6	-5.96	116.32	119.90
36	5	636	C	OP1-P-O3'	5.96	118.31	105.20
1	2	1189	A	C8-N9-C4	5.96	108.18	105.80
36	1	2411	U	N3-C4-C5	5.96	118.17	114.60
1	6	687	G	N3-C4-N9	-5.96	122.43	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1280	C	N1-C2-O2	-5.96	115.33	118.90
36	1	3106	A	N1-C2-N3	-5.96	126.32	129.30
36	1	1308	A	N9-C4-C5	5.95	108.18	105.80
36	5	3147	G	N1-C2-N3	5.95	127.47	123.90
31	D9	36	LEU	CA-CB-CG	5.95	128.99	115.30
36	5	577	C	N3-C2-O2	5.95	126.07	121.90
1	2	1200	G	C5-C6-N1	-5.95	108.53	111.50
36	1	98	G	OP2-P-O3'	5.95	118.29	105.20
44	L7	163	LEU	CA-CB-CG	-5.95	101.61	115.30
1	6	19	A	N1-C6-N6	5.95	122.17	118.60
36	5	2610	G	C8-N9-C4	-5.95	104.02	106.40
36	1	394	G	C6-C5-N7	5.95	133.97	130.40
36	1	2412	G	C5-C6-N1	5.95	114.47	111.50
36	5	1124	U	OP2-P-O3'	5.95	118.29	105.20
36	5	3188	G	N1-C6-O6	-5.95	116.33	119.90
36	1	938	C	C2-N1-C1'	5.95	125.34	118.80
36	1	3214	U	C5-C4-O4	5.95	129.47	125.90
1	6	1196	A	C8-N9-C4	5.95	108.18	105.80
36	5	43	A	O4'-C1'-N9	5.95	112.96	108.20
36	5	297	G	C8-N9-C1'	-5.95	119.27	127.00
36	5	3120	C	C6-N1-C2	-5.95	117.92	120.30
36	1	2827	U	C4-C5-C6	5.94	123.27	119.70
36	1	3205	G	N1-C2-N3	5.94	127.47	123.90
38	4	44	A	C8-N9-C4	5.94	108.18	105.80
36	5	1876	U	C5-C6-N1	-5.94	119.73	122.70
36	1	2238	G	C5-C6-O6	-5.94	125.03	128.60
36	1	2624	G	C6-C5-N7	-5.94	126.83	130.40
37	7	37	G	C4-C5-N7	5.94	113.18	110.80
57	n1	88	ARG	NE-CZ-NH1	-5.94	117.33	120.30
36	1	3173	G	O5'-P-OP1	-5.94	100.35	105.70
25	d3	16	ARG	NE-CZ-NH2	-5.94	117.33	120.30
36	5	1373	A	C4-C5-N7	5.94	113.67	110.70
36	5	2735	U	C5-C6-N1	5.94	125.67	122.70
36	5	3307	A	N1-C6-N6	5.94	122.16	118.60
1	2	1212	G	C6-C5-N7	-5.94	126.84	130.40
36	5	2848	G	C4-C5-N7	5.94	113.17	110.80
1	2	570	A	N1-C6-N6	5.94	122.16	118.60
36	1	1182	A	OP1-P-OP2	5.94	128.50	119.60
36	5	1853	U	N1-C2-N3	5.94	118.46	114.90
1	2	169	A	N9-C4-C5	-5.93	103.43	105.80
36	1	652	G	N1-C2-N3	5.93	127.46	123.90
36	1	972	A	N1-C2-N3	-5.93	126.33	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1447	G	C5-C6-N1	5.93	114.47	111.50
36	1	1904	C	C5-C4-N4	-5.93	116.05	120.20
36	5	2801	A	C5-C6-N1	5.93	120.67	117.70
36	1	701	G	C5-C6-N1	-5.93	108.53	111.50
36	1	1408	G	C6-C5-N7	-5.93	126.84	130.40
36	1	1437	C	C4-C5-C6	5.93	120.37	117.40
36	5	3130	A	O5'-P-OP1	-5.93	100.36	105.70
36	1	907	G	N3-C4-N9	5.93	129.56	126.00
36	1	2305	G	N1-C6-O6	5.93	123.46	119.90
36	5	1180	A	C8-N9-C4	-5.93	103.43	105.80
36	5	1657	C	C2-N1-C1'	5.93	125.33	118.80
1	2	1340	U	C5-C4-O4	5.93	129.46	125.90
36	1	34	A	C2-N3-C4	-5.93	107.64	110.60
36	1	864	G	N9-C4-C5	5.93	107.77	105.40
48	M1	112	LEU	CA-CB-CG	5.93	128.94	115.30
1	6	1001	A	C5-C6-N6	-5.93	118.96	123.70
36	5	2909	U	C2-N3-C4	-5.93	123.44	127.00
36	1	1397	C	C2-N3-C4	-5.93	116.94	119.90
36	1	1604	G	N3-C4-C5	-5.93	125.64	128.60
38	4	20	U	C2-N3-C4	-5.93	123.44	127.00
36	5	74	G	C8-N9-C4	-5.93	104.03	106.40
51	m5	24	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	2	507	U	C2-N1-C1'	5.92	124.81	117.70
36	5	3206	C	OP1-P-OP2	5.92	128.49	119.60
1	2	1658	G	N9-C4-C5	-5.92	103.03	105.40
36	1	2216	G	C4-C5-N7	-5.92	108.43	110.80
36	1	2915	U	N3-C2-O2	5.92	126.35	122.20
36	5	439	C	C6-N1-C2	-5.92	117.93	120.30
36	5	1833	G	C6-C5-N7	5.92	133.95	130.40
36	1	418	A	OP2-P-O3'	5.92	118.22	105.20
36	5	2298	U	C5-C6-N1	-5.92	119.74	122.70
36	1	355	A	C2-N3-C4	-5.92	107.64	110.60
36	5	2531	C	O4'-C1'-N1	5.92	112.93	108.20
36	5	3368	U	C2-N1-C1'	-5.92	110.60	117.70
36	1	2779	A	C2-N3-C4	-5.92	107.64	110.60
36	5	3129	A	N1-C6-N6	5.92	122.15	118.60
38	8	32	C	C5-C6-N1	-5.92	118.04	121.00
36	1	92	G	N1-C6-O6	-5.92	116.35	119.90
41	L4	31	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	6	1772	C	C5-C6-N1	-5.92	118.04	121.00
36	5	659	G	C5-C6-N1	5.92	114.46	111.50
36	1	1171	G	C8-N9-C4	-5.91	104.03	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1838	G	C8-N9-C1'	-5.91	119.31	127.00
36	1	2093	A	C2-N3-C4	5.91	113.56	110.60
36	5	35	A	N1-C2-N3	5.91	132.26	129.30
36	5	1885	U	N3-C2-O2	5.91	126.34	122.20
36	1	1552	G	N1-C6-O6	5.91	123.45	119.90
36	1	716	A	C8-N9-C4	5.91	108.16	105.80
36	1	3368	U	C2-N1-C1'	-5.91	110.61	117.70
36	1	843	A	N1-C6-N6	5.91	122.14	118.60
36	1	1655	G	N9-C4-C5	-5.91	103.04	105.40
36	5	712	G	O5'-P-OP2	-5.91	100.38	105.70
36	5	2613	U	C5-C4-O4	5.91	129.44	125.90
1	6	542	A	N1-C6-N6	5.91	122.14	118.60
36	5	37	U	N1-C2-N3	5.91	118.44	114.90
36	5	705	A	O5'-P-OP2	-5.91	100.38	105.70
36	5	2754	G	N1-C6-O6	-5.91	116.36	119.90
1	2	1273	G	O4'-C1'-N9	5.91	112.92	108.20
1	2	1314	U	N1-C2-N3	5.91	118.44	114.90
36	1	1387	G	C5-C6-O6	5.91	132.14	128.60
36	1	2418	G	OP1-P-O3'	5.91	118.19	105.20
1	6	1743	U	OP2-P-O3'	5.91	118.19	105.20
36	5	2191	U	N3-C4-O4	-5.91	115.27	119.40
36	5	2611	U	C4-C5-C6	5.91	123.24	119.70
36	5	1829	G	C4-C5-N7	-5.90	108.44	110.80
1	2	734	A	OP1-P-O3'	5.90	118.19	105.20
36	1	1604	G	C4-N9-C1'	5.90	134.17	126.50
36	1	1854	C	N3-C4-C5	5.90	124.26	121.90
36	5	807	A	C5-C6-N1	5.90	120.65	117.70
36	5	923	C	N3-C4-N4	5.90	122.13	118.00
1	2	542	A	N7-C8-N9	5.90	116.75	113.80
36	1	1332	A	O5'-P-OP1	-5.90	100.39	105.70
1	6	1361	U	C2-N1-C1'	5.90	124.78	117.70
36	5	1466	G	OP1-P-OP2	-5.90	110.75	119.60
36	5	2877	G	C4-C5-N7	-5.90	108.44	110.80
1	2	564	G	C6-C5-N7	5.90	133.94	130.40
36	5	1152	G	O5'-P-OP1	-5.90	100.39	105.70
36	5	1914	G	C4-N9-C1'	5.90	134.17	126.50
36	5	2854	U	O5'-P-OP1	-5.90	100.39	105.70
36	1	171	G	N3-C4-C5	5.89	131.55	128.60
36	1	1437	C	C2-N1-C1'	5.89	125.28	118.80
36	5	2199	G	C4-N9-C1'	5.89	134.16	126.50
36	1	339	C	O5'-P-OP2	5.89	117.77	110.70
36	1	955	U	C6-N1-C2	5.89	124.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1159	A	OP1-P-O3'	5.89	118.17	105.20
36	1	2163	C	C5-C4-N4	5.89	124.33	120.20
36	1	2376	G	N7-C8-N9	5.89	116.05	113.10
36	5	1296	C	N1-C2-O2	-5.89	115.36	118.90
36	5	1803	C	C6-N1-C2	5.89	122.66	120.30
36	5	2805	G	C5-C6-O6	-5.89	125.06	128.60
36	1	948	C	C2-N3-C4	-5.89	116.95	119.90
38	4	38	U	N1-C2-O2	5.89	126.92	122.80
36	5	948	C	N3-C4-C5	5.89	124.26	121.90
36	1	866	A	C8-N9-C4	5.89	108.16	105.80
36	5	942	U	N1-C2-O2	-5.89	118.68	122.80
1	2	1600	A	C4-C5-N7	5.89	113.64	110.70
36	1	2168	A	C2-N3-C4	5.89	113.54	110.60
36	1	2278	C	N1-C2-O2	5.89	122.43	118.90
36	1	2966	G	N3-C4-N9	5.89	129.53	126.00
36	5	1701	C	N3-C4-C5	-5.89	119.55	121.90
36	1	2137	U	C6-N1-C1'	-5.88	112.96	121.20
38	4	9	A	N1-C6-N6	-5.88	115.07	118.60
36	5	606	C	C6-N1-C2	5.88	122.65	120.30
36	5	2371	G	O5'-P-OP2	-5.88	100.40	105.70
36	5	76	G	C2-N3-C4	-5.88	108.96	111.90
79	q3	50	GLY	N-CA-C	-5.88	98.39	113.10
1	2	1422	A	C8-N9-C4	5.88	108.15	105.80
36	1	891	G	N1-C6-O6	-5.88	116.37	119.90
36	1	1153	A	C6-C5-N7	-5.88	128.18	132.30
36	1	1340	G	N3-C4-N9	5.88	129.53	126.00
36	1	1548	C	N1-C2-O2	-5.88	115.37	118.90
36	5	1372	C	N3-C4-C5	5.88	124.25	121.90
36	5	2728	G	O5'-P-OP2	-5.88	100.41	105.70
36	1	1606	U	N1-C2-O2	-5.88	118.68	122.80
36	1	2679	A	O4'-C1'-N9	5.88	112.90	108.20
36	5	1055	A	O5'-P-OP2	-5.88	100.41	105.70
36	5	1745	C	O5'-P-OP2	-5.88	100.41	105.70
36	1	327	A	N7-C8-N9	-5.88	110.86	113.80
36	1	2169	G	C5-C6-O6	5.88	132.13	128.60
36	1	2610	G	C5-C6-O6	-5.88	125.07	128.60
36	5	61	A	N9-C4-C5	5.88	108.15	105.80
1	2	1164	G	N1-C6-O6	5.88	123.43	119.90
36	1	28	C	C6-N1-C2	5.88	122.65	120.30
36	1	432	G	C5-C6-N1	-5.88	108.56	111.50
36	5	342	A	O5'-P-OP2	-5.88	100.41	105.70
36	5	966	U	C2-N1-C1'	5.88	124.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1548	C	N1-C2-O2	-5.88	115.38	118.90
36	5	2376	G	C6-C5-N7	-5.88	126.87	130.40
1	2	89	G	C8-N9-C4	5.88	108.75	106.40
36	1	2168	A	O5'-P-OP2	-5.88	100.41	105.70
1	6	1700	C	C6-N1-C1'	-5.88	113.75	120.80
36	5	800	G	C6-N1-C2	-5.88	121.58	125.10
36	5	1137	C	C5-C6-N1	-5.88	118.06	121.00
36	1	1000	C	N1-C2-N3	-5.87	115.09	119.20
36	1	1154	A	C4-C5-C6	5.87	119.94	117.00
36	1	2146	C	O5'-P-OP1	5.87	117.75	110.70
36	1	2343	C	C5-C4-N4	-5.87	116.09	120.20
36	1	2872	A	OP2-P-O3'	5.87	118.12	105.20
1	6	1112	G	C6-N1-C2	-5.87	121.58	125.10
36	5	63	A	C5-C6-N6	-5.87	119.00	123.70
36	5	2117	A	N9-C4-C5	5.87	108.15	105.80
36	1	636	C	C5-C6-N1	-5.87	118.06	121.00
38	8	85	G	N7-C8-N9	5.87	116.04	113.10
1	2	370	A	N1-C6-N6	-5.87	115.08	118.60
1	2	734	A	P-O3'-C3'	5.87	126.74	119.70
1	2	1145	U	N1-C2-O2	-5.87	118.69	122.80
36	1	1116	G	N9-C4-C5	5.87	107.75	105.40
36	1	2355	G	C4-C5-C6	5.87	122.32	118.80
36	5	2402	A	C8-N9-C4	-5.87	103.45	105.80
37	7	90	U	C6-N1-C2	5.87	124.52	121.00
36	1	2619	G	N7-C8-N9	-5.87	110.17	113.10
36	1	2846	U	N1-C2-O2	5.87	126.91	122.80
1	2	142	G	N3-C2-N2	-5.87	115.80	119.90
1	2	1340	U	N1-C2-O2	5.87	126.91	122.80
36	5	815	G	N3-C4-C5	-5.87	125.67	128.60
36	5	1149	G	O5'-P-OP2	-5.87	100.42	105.70
36	5	1384	U	C5-C6-N1	5.87	125.63	122.70
36	1	89	A	N3-C4-C5	-5.86	122.70	126.80
36	1	132	C	N1-C2-O2	-5.86	115.38	118.90
36	1	2869	U	OP2-P-O3'	5.86	118.10	105.20
37	7	88	G	N1-C2-N2	-5.86	110.92	116.20
36	1	2345	A	N9-C4-C5	-5.86	103.45	105.80
36	5	1592	G	C4-N9-C1'	5.86	134.12	126.50
36	1	1384	U	N3-C2-O2	5.86	126.30	122.20
36	1	2761	G	C5-C6-O6	-5.86	125.08	128.60
1	6	543	C	C6-N1-C2	-5.86	117.96	120.30
1	6	1535	U	N1-C2-O2	5.86	126.90	122.80
36	5	2661	G	C5-C6-O6	-5.86	125.08	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1389	G	N1-C6-O6	5.86	123.42	119.90
36	5	2825	C	N1-C2-O2	-5.86	115.38	118.90
37	7	81	U	C4-C5-C6	-5.86	116.19	119.70
1	2	1212	G	C4-C5-N7	5.86	113.14	110.80
36	1	1365	G	C4-N9-C1'	5.86	134.11	126.50
36	1	1419	A	O5'-P-OP2	-5.86	100.43	105.70
36	1	2621	G	N1-C6-O6	5.86	123.41	119.90
36	1	2942	C	C6-N1-C2	5.86	122.64	120.30
36	1	1466	G	N9-C4-C5	-5.86	103.06	105.40
36	1	2608	G	C5-C6-O6	-5.86	125.09	128.60
36	5	653	A	C2-N3-C4	-5.86	107.67	110.60
36	5	870	G	N1-C2-N2	-5.86	110.93	116.20
36	5	1122	U	C5-C4-O4	5.86	129.41	125.90
36	5	2813	A	C4-C5-C6	5.86	119.93	117.00
38	8	30	C	N1-C2-O2	-5.86	115.39	118.90
36	1	816	A	N1-C6-N6	-5.85	115.09	118.60
36	1	2924	U	C2-N3-C4	-5.85	123.49	127.00
36	5	925	A	N7-C8-N9	-5.85	110.87	113.80
36	5	2394	G	N1-C6-O6	5.85	123.41	119.90
38	8	106	C	C6-N1-C2	5.85	122.64	120.30
1	2	1119	G	C8-N9-C4	-5.85	104.06	106.40
36	1	56	G	C5-C6-N1	5.85	114.43	111.50
1	6	453	U	N1-C2-O2	5.85	126.90	122.80
1	6	1658	G	N1-C6-O6	-5.85	116.39	119.90
36	5	1853	U	N1-C2-O2	-5.85	118.70	122.80
36	5	2626	A	C5-C6-N1	-5.85	114.77	117.70
36	1	357	A	C5-C6-N6	-5.85	119.02	123.70
36	1	878	G	N1-C2-N3	5.85	127.41	123.90
36	1	1419	A	C5'-C4'-O4'	5.85	116.12	109.10
36	5	2396	G	C5-N7-C8	-5.85	101.38	104.30
36	1	1154	A	N1-C6-N6	5.85	122.11	118.60
38	4	64	U	N3-C2-O2	-5.85	118.11	122.20
1	6	173	A	N1-C6-N6	5.85	122.11	118.60
36	5	192	C	N3-C2-O2	-5.85	117.81	121.90
36	5	1481	A	N7-C8-N9	5.85	116.72	113.80
36	5	2648	G	C5-C6-N1	5.85	114.42	111.50
36	5	2727	A	C2-N3-C4	5.85	113.53	110.60
1	6	426	G	O5'-P-OP2	-5.85	100.44	105.70
1	6	795	U	N1-C2-O2	5.85	126.89	122.80
36	5	2827	U	OP1-P-O3'	5.85	118.06	105.20
1	2	1114	G	C6-C5-N7	-5.84	126.89	130.40
36	1	992	A	OP1-P-OP2	5.84	128.37	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2916	U	OP1-P-O3'	5.84	118.06	105.20
36	5	1306	G	C4-C5-N7	5.84	113.14	110.80
36	5	2825	C	N3-C4-N4	5.84	122.09	118.00
36	5	2954	U	N3-C2-O2	-5.84	118.11	122.20
36	1	1137	C	OP1-P-OP2	5.84	128.37	119.60
1	6	422	G	C8-N9-C4	-5.84	104.06	106.40
1	2	136	C	OP1-P-O3'	5.84	118.05	105.20
36	1	2295	A	C5-N7-C8	-5.84	100.98	103.90
36	1	2794	G	C2-N3-C4	5.84	114.82	111.90
38	4	17	A	N1-C2-N3	5.84	132.22	129.30
36	5	2836	C	C5-C6-N1	-5.84	118.08	121.00
36	5	2914	G	N3-C4-C5	-5.84	125.68	128.60
36	1	888	A	C4-C5-N7	5.84	113.62	110.70
1	6	158	U	P-O3'-C3'	5.84	126.71	119.70
1	6	1119	G	N1-C2-N2	-5.84	110.94	116.20
36	5	632	G	N3-C4-N9	5.84	129.50	126.00
36	5	2953	U	C5-C4-O4	-5.84	122.40	125.90
36	5	3396	U	O4'-C1'-N1	5.84	112.87	108.20
36	1	2212	C	C6-N1-C2	5.84	122.64	120.30
36	1	2606	G	C8-N9-C1'	-5.84	119.41	127.00
36	5	339	C	N1-C2-O2	-5.84	115.40	118.90
36	5	820	A	C5-C6-N6	-5.84	119.03	123.70
36	5	1889	G	N3-C4-N9	5.84	129.50	126.00
36	1	2550	U	N1-C2-N3	5.83	118.40	114.90
1	6	382	C	C2-N3-C4	-5.83	116.98	119.90
1	6	1602	C	N1-C2-O2	5.83	122.40	118.90
36	1	2918	G	C6-C5-N7	-5.83	126.90	130.40
36	1	2944	U	N1-C2-O2	5.83	126.88	122.80
36	1	660	A	C2-N3-C4	5.83	113.52	110.60
36	1	999	G	C5-C6-O6	-5.83	125.10	128.60
36	1	1136	A	C8-N9-C4	-5.83	103.47	105.80
36	5	656	A	C5-C6-N1	-5.83	114.78	117.70
36	5	2364	G	O4'-C1'-N9	5.83	112.86	108.20
36	5	2819	A	O5'-P-OP2	-5.83	100.45	105.70
36	5	229	G	N1-C2-N2	5.83	121.45	116.20
36	5	1522	U	C5-C6-N1	-5.83	119.78	122.70
36	1	326	U	N3-C4-O4	5.83	123.48	119.40
36	1	694	C	N3-C4-C5	5.83	124.23	121.90
36	1	2434	U	C5-C6-N1	-5.83	119.79	122.70
1	6	1736	G	N1-C6-O6	5.83	123.40	119.90
36	5	2140	U	C6-N1-C2	-5.83	117.50	121.00
36	5	2646	C	N3-C4-N4	-5.83	113.92	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2366	C	C5-C6-N1	5.83	123.91	121.00
36	5	1200	A	N1-C2-N3	5.83	132.21	129.30
36	5	2234	G	C4-C5-N7	5.83	113.13	110.80
1	2	75	U	N3-C2-O2	-5.83	118.12	122.20
36	1	2836	C	C4-C5-C6	5.83	120.31	117.40
12	c0	88	PRO	N-CA-CB	5.83	110.29	103.30
36	5	153	U	N1-C2-O2	-5.83	118.72	122.80
36	5	3129	A	C4-C5-N7	5.83	113.61	110.70
38	8	40	A	N7-C8-N9	5.83	116.71	113.80
1	2	1200	G	C5-C6-O6	-5.82	125.11	128.60
1	2	1200	G	C4-C5-C6	5.82	122.30	118.80
36	1	2395	G	C5-C6-O6	-5.82	125.11	128.60
38	4	32	C	C6-N1-C1'	5.82	127.79	120.80
36	5	2849	C	C5-C4-N4	-5.82	116.12	120.20
36	5	2971	A	N3-C4-N9	5.82	132.06	127.40
1	6	440	U	N1-C2-N3	5.82	118.39	114.90
36	1	1190	A	C5-C6-N6	-5.82	119.04	123.70
36	1	1820	U	C5-C4-O4	5.82	129.39	125.90
37	7	37	G	N1-C6-O6	5.82	123.39	119.90
36	1	1555	U	C2-N1-C1'	-5.82	110.72	117.70
1	6	1127	G	N1-C2-N3	5.82	127.39	123.90
36	1	1820	U	C6-N1-C2	-5.82	117.51	121.00
1	6	542	A	N7-C8-N9	5.82	116.71	113.80
36	5	63	A	C6-C5-N7	-5.82	128.23	132.30
36	5	2261	G	C8-N9-C4	5.82	108.73	106.40
24	D2	76	SER	C-N-CD	5.82	140.61	128.40
36	1	232	G	N3-C4-C5	-5.82	125.69	128.60
36	5	835	G	O4'-C1'-N9	5.82	112.85	108.20
36	5	1931	U	C2-N1-C1'	-5.82	110.72	117.70
36	5	2727	A	C8-N9-C4	-5.82	103.47	105.80
36	1	1425	U	N3-C2-O2	-5.81	118.13	122.20
45	L8	189	LEU	CA-CB-CG	5.81	128.67	115.30
36	5	644	G	C8-N9-C4	-5.81	104.08	106.40
36	1	778	U	N3-C4-O4	-5.81	115.33	119.40
36	1	2905	U	N1-C2-O2	-5.81	118.73	122.80
38	4	100	U	O5'-P-OP1	5.81	117.67	110.70
36	1	695	C	C6-N1-C2	5.81	122.62	120.30
36	1	933	A	C4-C5-C6	5.81	119.91	117.00
36	1	941	G	C5-C6-N1	5.81	114.41	111.50
36	1	2942	C	N3-C2-O2	5.81	125.97	121.90
36	1	2177	G	N3-C2-N2	5.81	123.97	119.90
38	4	57	C	N3-C4-C5	5.81	124.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1523	G	N1-C6-O6	-5.81	116.41	119.90
36	5	2215	A	C8-N9-C4	5.81	108.12	105.80
36	1	200	C	C2-N3-C4	-5.81	117.00	119.90
36	1	292	U	C5-C6-N1	-5.81	119.80	122.70
36	1	2606	G	C4-N9-C1'	5.81	134.05	126.50
36	5	915	A	O5'-P-OP1	-5.81	100.47	105.70
36	5	1398	U	C5-C4-O4	5.81	129.38	125.90
36	5	2120	A	C5-C6-N6	5.81	128.35	123.70
36	5	2820	A	C5-C6-N6	-5.81	119.05	123.70
37	7	82	G	C6-C5-N7	-5.81	126.92	130.40
36	1	2355	G	C5-C6-O6	-5.81	125.12	128.60
36	5	807	A	C8-N9-C4	-5.81	103.48	105.80
36	1	432	G	C6-C5-N7	-5.80	126.92	130.40
36	5	1609	C	N3-C4-N4	5.80	122.06	118.00
36	5	2190	U	N1-C2-N3	5.80	118.38	114.90
36	5	2630	C	N3-C4-C5	5.80	124.22	121.90
36	1	1432	C	C5-C6-N1	5.80	123.90	121.00
36	5	1595	U	C2-N1-C1'	-5.80	110.74	117.70
36	5	2112	U	O5'-P-OP1	-5.80	100.48	105.70
36	5	2816	G	C4-N9-C1'	-5.80	118.96	126.50
1	2	1386	G	C8-N9-C4	5.80	108.72	106.40
36	1	2201	G	O5'-P-OP2	-5.80	100.48	105.70
1	6	75	U	N3-C2-O2	-5.80	118.14	122.20
36	5	567	G	N1-C6-O6	5.80	123.38	119.90
36	5	2509	U	N1-C2-O2	5.80	126.86	122.80
36	1	422	A	N9-C4-C5	5.80	108.12	105.80
36	1	1107	C	C6-N1-C2	5.80	122.62	120.30
36	5	931	C	C6-N1-C2	5.80	122.62	120.30
36	5	1101	G	N3-C2-N2	5.80	123.96	119.90
36	5	2112	U	C6-N1-C2	-5.80	117.52	121.00
36	5	2831	G	C5-C6-O6	-5.80	125.12	128.60
36	5	3211	C	C6-N1-C2	5.80	122.62	120.30
36	1	587	U	N3-C4-C5	5.79	118.08	114.60
36	1	282	G	C2'-C3'-O3'	5.79	122.97	113.70
36	1	895	A	N1-C2-N3	5.79	132.20	129.30
36	1	1366	A	C5-N7-C8	-5.79	101.00	103.90
36	1	2923	U	C5-C4-O4	-5.79	122.42	125.90
1	6	886	U	O4'-C1'-N1	5.79	112.83	108.20
36	5	811	U	C2-N3-C4	-5.79	123.52	127.00
36	5	1730	G	C8-N9-C4	5.79	108.72	106.40
1	2	1782	A	C5-C6-N1	-5.79	114.80	117.70
36	1	3361	G	N3-C2-N2	5.79	123.95	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	57	G	N3-C4-C5	-5.79	125.70	128.60
36	5	2865	U	C5-C6-N1	5.79	125.60	122.70
36	5	3216	G	N1-C6-O6	5.79	123.38	119.90
38	8	119	C	C6-N1-C2	5.79	122.62	120.30
36	1	917	A	C6-C5-N7	5.79	136.35	132.30
36	1	2372	A	C8-N9-C4	-5.79	103.48	105.80
1	6	1674	C	N1-C2-O2	-5.79	115.43	118.90
36	5	349	A	O5'-P-OP2	-5.79	100.49	105.70
36	5	1304	A	O5'-P-OP1	-5.79	100.49	105.70
37	7	90	U	C2-N3-C4	-5.79	123.53	127.00
1	2	1218	G	N1-C6-O6	5.79	123.37	119.90
36	1	1466	G	C4-C5-N7	5.79	113.11	110.80
36	5	417	A	C5-C6-N1	5.79	120.59	117.70
36	5	1183	C	C2-N3-C4	-5.79	117.01	119.90
36	1	24	G	N1-C2-N3	5.79	127.37	123.90
36	1	1334	U	N1-C2-O2	-5.79	118.75	122.80
36	1	2968	G	C2-N3-C4	-5.79	109.01	111.90
1	6	352	A	C8-N9-C4	5.79	108.11	105.80
36	5	2754	G	C8-N9-C4	5.79	108.71	106.40
36	1	35	A	C5-N7-C8	-5.78	101.01	103.90
36	1	101	G	O4'-C1'-N9	5.78	112.83	108.20
36	1	435	C	C6-N1-C2	5.78	122.61	120.30
1	6	163	G	N3-C2-N2	-5.78	115.85	119.90
36	5	422	A	O5'-P-OP1	-5.78	100.49	105.70
36	5	1942	U	N1-C2-N3	5.78	118.37	114.90
36	5	2372	A	O4'-C1'-N9	-5.78	103.57	108.20
36	5	2823	G	C5-C6-O6	-5.78	125.13	128.60
36	1	2419	A	C5-N7-C8	-5.78	101.01	103.90
36	5	2917	G	C6-N1-C2	-5.78	121.63	125.10
36	5	2930	A	O4'-C1'-N9	5.78	112.83	108.20
36	1	3368	U	C6-N1-C1'	5.78	129.29	121.20
1	2	765	G	C2-N3-C4	5.78	114.79	111.90
1	2	857	U	N1-C2-O2	5.78	126.84	122.80
1	6	892	A	C8-N9-C4	-5.78	103.49	105.80
36	5	974	G	C6-N1-C2	-5.78	121.63	125.10
36	5	1085	A	C2-N3-C4	-5.78	107.71	110.60
36	5	2165	G	N3-C4-N9	5.78	129.47	126.00
36	1	1269	U	N1-C2-O2	5.78	126.84	122.80
36	1	2952	G	N1-C6-O6	5.78	123.36	119.90
36	5	2421	U	C4-C5-C6	5.77	123.17	119.70
36	1	2917	G	C5-C6-O6	-5.77	125.14	128.60
36	5	660	A	O5'-P-OP2	-5.77	100.50	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2871	G	O5'-P-OP2	-5.77	100.50	105.70
36	5	3204	C	C2-N3-C4	-5.77	117.01	119.90
36	1	635	G	C5-C6-N1	5.77	114.39	111.50
1	2	1432	U	C6-N1-C2	5.77	124.46	121.00
36	1	1344	G	OP2-P-O3'	5.77	117.89	105.20
36	1	3382	U	N3-C2-O2	-5.77	118.16	122.20
36	5	1001	G	O5'-P-OP1	-5.77	100.51	105.70
1	2	1116	A	N1-C6-N6	5.77	122.06	118.60
1	6	50	C	C4-C5-C6	5.77	120.28	117.40
1	6	1582	U	C5-C4-O4	5.77	129.36	125.90
36	5	2609	A	O5'-P-OP2	-5.77	100.51	105.70
36	5	2616	C	N3-C2-O2	5.77	125.94	121.90
36	1	76	G	N3-C4-C5	-5.76	125.72	128.60
36	1	1931	U	C5-C4-O4	5.76	129.36	125.90
36	1	2169	G	C5-N7-C8	5.76	107.18	104.30
36	1	2923	U	O5'-P-OP2	5.76	117.62	110.70
36	1	3229	G	N9-C4-C5	-5.76	103.09	105.40
1	6	1000	C	C6-N1-C1'	-5.76	113.88	120.80
36	5	3195	U	P-O3'-C3'	5.76	126.62	119.70
38	8	42	G	N3-C4-N9	-5.76	122.54	126.00
36	5	1420	C	OP2-P-O3'	5.76	117.88	105.20
36	1	350	C	C2-N1-C1'	5.76	125.14	118.80
36	1	639	G	O5'-P-OP1	5.76	117.61	110.70
36	1	2241	U	C5-C4-O4	5.76	129.36	125.90
36	1	2864	A	O5'-P-OP1	-5.76	100.51	105.70
36	5	1194	G	C2-N3-C4	5.76	114.78	111.90
36	5	2341	A	N7-C8-N9	-5.76	110.92	113.80
36	5	3214	U	C5-C4-O4	5.76	129.36	125.90
36	1	286	U	N1-C2-O2	5.76	126.83	122.80
36	1	1696	A	C8-N9-C4	-5.76	103.50	105.80
36	1	2769	A	O5'-P-OP2	-5.76	100.52	105.70
49	M3	7	LEU	CA-CB-CG	-5.76	102.06	115.30
1	6	583	C	C2-N1-C1'	5.76	125.14	118.80
1	6	1300	A	N1-C6-N6	-5.76	115.14	118.60
36	5	2759	U	N3-C4-O4	5.76	123.43	119.40
36	1	808	A	N1-C6-N6	-5.76	115.14	118.60
36	1	1891	A	N9-C4-C5	-5.76	103.50	105.80
36	5	1381	A	N1-C6-N6	-5.76	115.14	118.60
36	5	1847	A	N3-C4-C5	5.76	130.83	126.80
36	5	2951	G	C8-N9-C4	5.76	108.70	106.40
36	5	3200	G	C6-C5-N7	-5.76	126.94	130.40
1	2	1176	G	C6-C5-N7	-5.76	126.95	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	606	C	C6-N1-C2	5.76	122.60	120.30
36	1	1431	G	C5-C6-O6	5.76	132.05	128.60
1	6	941	A	N1-C6-N6	-5.76	115.15	118.60
1	6	1097	U	C5-C4-O4	5.76	129.35	125.90
1	6	1129	U	C5-C4-O4	5.76	129.35	125.90
1	6	1200	G	N3-C4-C5	5.76	131.48	128.60
36	5	632	G	O5'-P-OP1	5.76	117.61	110.70
36	5	1522	U	C2-N3-C4	-5.76	123.55	127.00
36	5	567	G	C6-C5-N7	-5.75	126.95	130.40
36	5	1164	G	C8-N9-C4	5.75	108.70	106.40
36	1	1548	C	N3-C2-O2	5.75	125.93	121.90
36	1	1842	A	N1-C6-N6	-5.75	115.15	118.60
36	5	308	A	O5'-P-OP1	5.75	117.60	110.70
36	5	1593	A	N1-C6-N6	5.75	122.05	118.60
36	1	1845	G	OP2-P-O3'	5.75	117.85	105.20
36	1	2808	A	C8-N9-C1'	-5.75	117.35	127.70
1	6	1285	U	C5-C4-O4	5.75	129.35	125.90
36	5	343	U	C5-C4-O4	5.75	129.35	125.90
36	5	1851	G	C5-C6-O6	-5.75	125.15	128.60
36	1	53	G	C5-C6-N1	5.75	114.38	111.50
36	1	426	G	N3-C4-N9	5.75	129.45	126.00
36	1	959	C	C6-N1-C2	5.75	122.60	120.30
36	1	1204	A	C8-N9-C4	5.75	108.10	105.80
36	1	1931	U	C2-N1-C1'	-5.75	110.80	117.70
1	6	1503	A	N7-C8-N9	5.75	116.67	113.80
36	5	1869	C	C2-N1-C1'	-5.75	112.48	118.80
36	5	3101	G	N3-C4-C5	-5.75	125.73	128.60
36	5	3186	A	N1-C6-N6	-5.75	115.15	118.60
36	1	320	G	C5-C6-O6	-5.75	125.15	128.60
36	5	2246	G	C8-N9-C4	-5.75	104.10	106.40
36	5	2772	C	P-O3'-C3'	5.75	126.59	119.70
36	5	2820	A	C5-N7-C8	-5.75	101.03	103.90
36	1	937	G	N1-C6-O6	5.75	123.35	119.90
64	N8	32	ARG	NE-CZ-NH1	-5.75	117.43	120.30
36	5	923	C	C5-C4-N4	-5.75	116.18	120.20
36	5	1522	U	C5-C4-O4	-5.75	122.45	125.90
36	1	931	C	C5-C6-N1	-5.74	118.13	121.00
36	1	1189	C	N1-C2-O2	-5.74	115.45	118.90
36	1	1468	A	C2-N3-C4	-5.74	107.73	110.60
36	1	1498	A	C6-N1-C2	-5.74	115.15	118.60
36	1	2406	C	N1-C2-O2	-5.74	115.45	118.90
36	1	2818	U	N1-C2-N3	5.74	118.35	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2912	G	C6-C5-N7	5.74	133.85	130.40
36	5	1367	G	N1-C6-O6	5.74	123.35	119.90
36	5	2651	G	C5-C6-N1	-5.74	108.63	111.50
36	1	2861	U	N3-C2-O2	-5.74	118.18	122.20
1	6	337	G	C8-N9-C1'	-5.74	119.53	127.00
36	1	1176	C	C5-C4-N4	-5.74	116.18	120.20
36	1	1534	A	N1-C6-N6	5.74	122.04	118.60
1	6	777	C	C6-N1-C2	-5.74	118.00	120.30
36	5	3047	U	N3-C4-C5	-5.74	111.16	114.60
1	2	1782	A	O5'-P-OP1	-5.74	100.53	105.70
36	1	281	G	OP1-P-OP2	-5.74	110.99	119.60
36	5	1833	G	N1-C6-O6	-5.74	116.46	119.90
37	7	105	C	C2-N1-C1'	5.74	125.11	118.80
36	5	2950	G	OP1-P-O3'	5.74	117.82	105.20
36	1	805	G	C5-N7-C8	5.74	107.17	104.30
36	5	1556	C	C5-C6-N1	5.74	123.87	121.00
36	5	3055	U	C5-C4-O4	-5.74	122.46	125.90
36	1	2836	C	N1-C2-N3	5.73	123.21	119.20
1	6	765	G	C8-N9-C4	5.73	108.69	106.40
36	1	92	G	N3-C2-N2	5.73	123.91	119.90
36	1	650	C	N1-C2-O2	-5.73	115.46	118.90
36	1	1916	U	C5-C6-N1	-5.73	119.83	122.70
36	1	2923	U	N3-C4-O4	5.73	123.41	119.40
36	1	2953	U	N3-C2-O2	5.73	126.21	122.20
1	6	1027	A	C5-N7-C8	-5.73	101.03	103.90
36	5	2393	G	N3-C4-C5	-5.73	125.73	128.60
20	C8	3	LEU	CA-CB-CG	5.73	128.48	115.30
1	6	639	U	N1-C2-O2	5.73	126.81	122.80
1	6	996	U	C5-C4-O4	5.73	129.34	125.90
1	6	1751	C	C6-N1-C2	5.73	122.59	120.30
36	5	13	A	N1-C6-N6	-5.73	115.16	118.60
36	5	898	U	O5'-P-OP2	5.73	117.58	110.70
36	5	1110	U	N3-C4-O4	-5.73	115.39	119.40
36	5	2961	G	N7-C8-N9	5.73	115.97	113.10
37	7	84	A	OP1-P-O3'	5.73	117.80	105.20
36	5	1372	C	C5-C6-N1	-5.73	118.14	121.00
36	5	2309	A	N9-C4-C5	5.73	108.09	105.80
36	1	328	U	N1-C2-O2	5.72	126.81	122.80
36	1	1133	A	C5-C6-N6	-5.72	119.12	123.70
36	1	1389	G	C6-C5-N7	-5.72	126.97	130.40
1	6	308	C	C2-N3-C4	-5.72	117.04	119.90
1	6	337	G	N3-C4-N9	5.72	129.44	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	636	C	C2-N3-C4	-5.72	117.04	119.90
36	1	1425	U	C5-C4-O4	5.72	129.33	125.90
36	1	3217	C	N1-C2-O2	5.72	122.33	118.90
36	5	1103	A	C8-N9-C4	-5.72	103.51	105.80
36	5	1879	A	C2-N3-C4	-5.72	107.74	110.60
37	7	84	A	C8-N9-C4	-5.72	103.51	105.80
36	1	808	A	C4-C5-N7	-5.72	107.84	110.70
36	1	2356	A	C5-C6-N6	-5.72	119.12	123.70
36	1	2973	G	C8-N9-C4	5.72	108.69	106.40
36	1	790	U	N3-C2-O2	-5.72	118.20	122.20
36	1	927	C	C2-N3-C4	-5.72	117.04	119.90
36	1	1581	C	N3-C2-O2	-5.72	117.90	121.90
36	1	3209	A	N9-C4-C5	-5.72	103.51	105.80
38	4	13	A	C6-C5-N7	-5.72	128.30	132.30
36	5	304	G	C5-C6-O6	5.72	132.03	128.60
36	5	589	A	N1-C6-N6	5.72	122.03	118.60
36	5	1312	C	N1-C2-O2	-5.72	115.47	118.90
36	5	3105	U	C2-N3-C4	-5.72	123.57	127.00
36	1	648	C	OP1-P-O3'	5.72	117.78	105.20
36	1	915	A	O5'-P-OP2	-5.72	100.55	105.70
36	5	334	A	N7-C8-N9	-5.72	110.94	113.80
36	1	869	G	N1-C6-O6	5.72	123.33	119.90
36	1	1835	A	N1-C6-N6	-5.72	115.17	118.60
36	1	2302	G	N1-C6-O6	-5.72	116.47	119.90
36	1	2899	C	N1-C2-N3	5.72	123.20	119.20
37	3	14	U	C6-N1-C2	5.72	124.43	121.00
36	1	567	G	C8-N9-C4	-5.71	104.11	106.40
36	1	940	G	N3-C4-C5	-5.71	125.74	128.60
36	1	1059	G	C5-C6-O6	5.71	132.03	128.60
36	1	2602	G	C5-C6-O6	5.71	132.03	128.60
36	1	410	U	N1-C2-N3	5.71	118.33	114.90
36	5	2600	C	C5-C6-N1	5.71	123.86	121.00
36	5	3145	C	C6-N1-C2	5.71	122.58	120.30
1	2	1592	A	C8-N9-C4	-5.71	103.52	105.80
36	5	81	C	C6-N1-C2	5.71	122.58	120.30
37	7	95	A	OP1-P-OP2	-5.71	111.03	119.60
36	1	279	U	C5-C6-N1	-5.71	119.85	122.70
36	5	50	U	C5-C6-N1	5.71	125.55	122.70
36	5	835	G	N3-C2-N2	5.71	123.90	119.90
36	5	1014	U	C2-N1-C1'	5.71	124.55	117.70
36	5	2306	C	C2-N1-C1'	5.71	125.08	118.80
36	5	2965	U	N3-C2-O2	5.71	126.20	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1619	A	C8-N9-C4	5.71	108.08	105.80
36	1	2142	A	N1-C6-N6	-5.71	115.18	118.60
36	1	2865	U	C6-N1-C2	5.71	124.42	121.00
38	8	103	G	N3-C4-N9	5.71	129.42	126.00
36	1	65	A	OP1-P-O3'	5.71	117.75	105.20
36	1	1602	A	N1-C6-N6	5.71	122.02	118.60
36	1	2174	G	C8-N9-C4	-5.70	104.12	106.40
36	1	2871	G	C5-C6-O6	-5.70	125.18	128.60
36	5	804	C	OP1-P-O3'	5.70	117.75	105.20
36	5	869	G	N1-C6-O6	-5.70	116.48	119.90
36	5	3136	G	N1-C2-N3	5.70	127.32	123.90
44	17	232	ARG	NE-CZ-NH1	-5.70	117.45	120.30
36	5	770	G	O4'-C1'-N9	5.70	112.76	108.20
36	1	983	A	C6-N1-C2	-5.70	115.18	118.60
1	6	1046	G	N7-C8-N9	-5.70	110.25	113.10
36	5	225	C	C2-N3-C4	-5.70	117.05	119.90
36	1	919	U	N1-C2-O2	5.70	126.79	122.80
36	1	1154	A	C5-C6-N6	-5.70	119.14	123.70
36	5	3184	A	C4-C5-N7	5.70	113.55	110.70
36	1	804	C	C4-C5-C6	5.70	120.25	117.40
36	5	43	A	C4-C5-N7	5.70	113.55	110.70
36	5	417	A	OP2-P-O3'	5.69	117.73	105.20
36	1	895	A	N9-C4-C5	-5.69	103.52	105.80
36	1	3270	U	O5'-P-OP1	-5.69	100.58	105.70
1	6	66	U	P-O3'-C3'	5.69	126.53	119.70
36	5	637	C	N1-C2-O2	-5.69	115.48	118.90
36	5	1116	G	C4-C5-N7	-5.69	108.52	110.80
36	1	1340	G	C8-N9-C4	5.69	108.68	106.40
1	6	544	A	C8-N9-C4	5.69	108.08	105.80
36	5	1114	U	OP1-P-O3'	5.69	117.72	105.20
36	5	2943	G	C6-C5-N7	-5.69	126.98	130.40
38	8	10	A	N1-C6-N6	5.69	122.01	118.60
36	1	498	A	C8-N9-C4	-5.69	103.52	105.80
36	1	1891	A	N7-C8-N9	-5.69	110.96	113.80
36	5	1161	G	N3-C4-N9	5.69	129.41	126.00
38	8	54	A	C5-C6-N1	-5.69	114.86	117.70
36	1	2729	U	N3-C2-O2	-5.69	118.22	122.20
36	5	2164	A	C4-C5-C6	5.69	119.84	117.00
36	5	2759	U	N3-C4-C5	-5.69	111.19	114.60
36	5	1911	A	C2-N3-C4	-5.69	107.76	110.60
1	2	857	U	N3-C2-O2	-5.68	118.22	122.20
36	1	1796	G	C8-N9-C4	-5.68	104.13	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1865	A	OP1-P-O3'	5.68	117.70	105.20
36	1	2159	U	C6-N1-C2	5.68	124.41	121.00
36	5	890	C	N3-C4-N4	5.68	121.98	118.00
36	5	2128	C	C6-N1-C2	-5.68	118.03	120.30
36	5	2814	G	N3-C2-N2	5.68	123.88	119.90
38	8	54	A	N1-C6-N6	5.68	122.01	118.60
36	1	3029	A	C8-N9-C4	-5.68	103.53	105.80
36	5	1872	C	N3-C2-O2	-5.68	117.92	121.90
36	5	3083	G	N1-C6-O6	-5.68	116.49	119.90
1	2	186	C	C6-N1-C2	-5.68	118.03	120.30
36	5	1198	C	N1-C2-N3	5.68	123.18	119.20
36	5	2691	A	C8-N9-C4	-5.68	103.53	105.80
36	1	1404	G	C5-C6-O6	5.68	132.01	128.60
36	1	2613	U	C5-C4-O4	5.68	129.31	125.90
36	5	209	A	C5-C6-N6	-5.68	119.16	123.70
36	5	622	A	O5'-P-OP1	-5.68	100.59	105.70
36	5	1119	C	C2-N3-C4	-5.68	117.06	119.90
36	5	1546	A	N1-C6-N6	5.68	122.01	118.60
36	1	300	G	N1-C6-O6	-5.68	116.49	119.90
36	1	954	U	O5'-P-OP2	-5.68	100.59	105.70
36	1	1051	U	C2-N1-C1'	-5.68	110.89	117.70
36	1	1105	A	C8-N9-C4	5.68	108.07	105.80
36	1	1389	G	C5-C6-O6	-5.68	125.19	128.60
36	1	394	G	C4-N9-C1'	-5.68	119.12	126.50
36	1	2418	G	C2-N3-C4	5.68	114.74	111.90
36	1	2954	U	C5-C6-N1	-5.68	119.86	122.70
36	5	288	C	N1-C2-O2	-5.68	115.49	118.90
36	5	2345	A	N9-C4-C5	-5.68	103.53	105.80
36	5	2524	A	N7-C8-N9	5.68	116.64	113.80
36	5	2572	C	N3-C2-O2	-5.68	117.93	121.90
36	5	2939	G	N7-C8-N9	-5.68	110.26	113.10
36	1	501	A	C8-N9-C4	5.67	108.07	105.80
36	1	957	C	O5'-P-OP2	-5.67	100.59	105.70
36	5	1210	U	C5-C6-N1	-5.67	119.86	122.70
36	1	1379	G	C2-N3-C4	-5.67	109.06	111.90
36	5	610	G	N9-C4-C5	5.67	107.67	105.40
36	1	697	A	N9-C4-C5	-5.67	103.53	105.80
36	1	2808	A	C2-N3-C4	-5.67	107.77	110.60
38	4	107	G	C6-C5-N7	5.67	133.80	130.40
1	6	33	U	C2-N1-C1'	-5.67	110.89	117.70
1	6	1634	C	C6-N1-C1'	-5.67	114.00	120.80
36	5	1313	G	O5'-P-OP2	-5.67	100.59	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2885	C	N1-C2-O2	-5.67	115.50	118.90
36	1	1930	A	C4-C5-C6	5.67	119.83	117.00
36	1	3044	G	C5-C6-O6	5.67	132.00	128.60
1	6	434	G	C5-C6-O6	-5.67	125.20	128.60
36	1	920	A	N1-C6-N6	-5.67	115.20	118.60
36	1	3094	A	O5'-P-OP1	-5.67	100.60	105.70
1	6	362	G	C8-N9-C1'	-5.67	119.63	127.00
36	5	941	G	N1-C6-O6	-5.67	116.50	119.90
36	5	1598	G	N1-C6-O6	-5.67	116.50	119.90
36	5	1599	G	C8-N9-C4	5.67	108.67	106.40
36	5	2147	A	C5-C6-N6	-5.67	119.17	123.70
36	5	2361	A	N1-C2-N3	5.67	132.13	129.30
36	5	2623	G	N1-C6-O6	5.67	123.30	119.90
1	2	720	G	P-O3'-C3'	5.67	126.50	119.70
36	5	371	G	C5-C6-O6	-5.67	125.20	128.60
36	1	364	G	N3-C4-C5	5.66	131.43	128.60
36	1	1123	U	N3-C4-O4	5.66	123.36	119.40
36	1	1152	G	O4'-C1'-N9	5.66	112.73	108.20
36	1	1932	A	N1-C6-N6	5.66	122.00	118.60
36	1	2335	G	N1-C6-O6	-5.66	116.50	119.90
36	5	41	G	C5-N7-C8	-5.66	101.47	104.30
36	5	2168	A	O5'-P-OP2	-5.66	100.60	105.70
36	5	2811	A	O5'-P-OP2	-5.66	100.60	105.70
36	5	2941	A	N9-C4-C5	5.66	108.07	105.80
36	5	3054	U	C6-N1-C2	-5.66	117.60	121.00
1	2	1057	U	C5-C6-N1	5.66	125.53	122.70
1	2	1426	C	N3-C2-O2	5.66	125.86	121.90
27	D5	95	HIS	N-CA-C	5.66	126.28	111.00
36	1	1210	U	C6-N1-C2	5.66	124.40	121.00
36	1	2874	G	C8-N9-C4	-5.66	104.14	106.40
1	6	16	G	N1-C6-O6	-5.66	116.50	119.90
1	6	1582	U	N3-C4-O4	-5.66	115.44	119.40
36	1	234	G	N1-C6-O6	5.66	123.30	119.90
36	1	1807	G	N3-C4-N9	5.66	129.40	126.00
1	6	1583	A	C8-N9-C4	5.66	108.06	105.80
36	5	1187	C	N3-C4-C5	5.66	124.16	121.90
36	5	2953	U	N1-C2-O2	-5.66	118.84	122.80
36	1	716	A	N3-C4-C5	5.66	130.76	126.80
36	1	1373	A	C5-C6-N1	5.66	120.53	117.70
36	1	2178	A	N1-C6-N6	-5.66	115.21	118.60
36	5	1766	G	N7-C8-N9	5.66	115.93	113.10
1	2	720	G	OP1-P-O3'	5.66	117.64	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	687	U	N3-C4-O4	5.66	123.36	119.40
36	1	997	A	C4-C5-C6	5.66	119.83	117.00
36	1	2425	G	C5-N7-C8	-5.66	101.47	104.30
36	5	2276	G	C5-C6-N1	5.66	114.33	111.50
36	5	3049	A	C8-N9-C4	5.65	108.06	105.80
1	6	558	U	C2-N1-C1'	5.65	124.48	117.70
36	5	74	G	N7-C8-N9	5.65	115.93	113.10
36	5	654	C	O5'-P-OP1	-5.65	100.61	105.70
36	5	922	U	C2-N3-C4	-5.65	123.61	127.00
36	5	1509	A	N9-C4-C5	-5.65	103.54	105.80
36	1	879	U	N3-C4-O4	-5.65	115.44	119.40
36	1	2766	U	C2-N1-C1'	5.65	124.48	117.70
1	6	939	A	C8-N9-C4	-5.65	103.54	105.80
36	5	2869	U	N1-C2-N3	5.65	118.29	114.90
69	o3	18	ARG	NE-CZ-NH1	-5.65	117.47	120.30
36	1	2343	C	OP2-P-O3'	5.65	117.63	105.20
36	5	2354	C	N3-C4-C5	-5.65	119.64	121.90
38	8	8	C	N1-C2-O2	-5.65	115.51	118.90
1	2	942	G	N1-C6-O6	-5.65	116.51	119.90
36	1	22	G	C6-C5-N7	-5.65	127.01	130.40
36	1	1918	C	C6-N1-C2	-5.65	118.04	120.30
38	4	153	U	C6-N1-C2	5.65	124.39	121.00
1	6	111	U	C6-N1-C2	-5.65	117.61	121.00
36	5	2899	C	N3-C2-O2	-5.65	117.95	121.90
37	7	74	C	N1-C2-O2	-5.65	115.51	118.90
36	1	375	A	OP1-P-O3'	5.65	117.62	105.20
53	M7	131	ARG	NE-CZ-NH1	-5.65	117.48	120.30
36	5	907	G	N9-C4-C5	-5.65	103.14	105.40
36	1	402	A	N7-C8-N9	-5.64	110.98	113.80
36	1	801	A	C4-C5-N7	5.64	113.52	110.70
36	1	1202	A	C2-N3-C4	-5.64	107.78	110.60
36	1	1362	G	N7-C8-N9	-5.64	110.28	113.10
36	1	2910	A	C2-N3-C4	-5.64	107.78	110.60
36	5	343	U	OP1-P-O3'	5.64	117.62	105.20
36	5	2158	A	C5-C6-N1	5.64	120.52	117.70
1	2	16	G	N3-C4-N9	5.64	129.39	126.00
36	1	1056	U	C5-C6-N1	5.64	125.52	122.70
36	1	1181	U	C5-C4-O4	5.64	129.29	125.90
36	1	2373	A	N9-C4-C5	5.64	108.06	105.80
36	1	2647	A	C4-C5-C6	5.64	119.82	117.00
36	5	414	U	C5-C4-O4	-5.64	122.52	125.90
36	1	945	C	N3-C4-N4	-5.64	114.05	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1116	G	C4-C5-C6	5.64	122.18	118.80
36	1	1124	U	N3-C4-C5	5.64	117.98	114.60
36	1	1309	U	OP1-P-OP2	5.64	128.06	119.60
36	1	2554	A	C8-N9-C4	5.64	108.06	105.80
1	6	1773	C	C6-N1-C2	-5.64	118.04	120.30
36	5	227	G	C5-C6-O6	-5.64	125.22	128.60
36	5	567	G	C4-C5-N7	5.64	113.06	110.80
36	5	967	A	OP2-P-O3'	5.64	117.61	105.20
36	5	794	U	O5'-P-OP2	-5.64	100.63	105.70
36	5	2379	U	C5-C6-N1	-5.64	119.88	122.70
36	1	776	U	N3-C4-C5	-5.64	111.22	114.60
36	1	1929	G	N9-C4-C5	-5.64	103.15	105.40
36	5	368	G	C8-N9-C4	-5.64	104.14	106.40
36	5	1208	U	N1-C2-O2	5.64	126.75	122.80
36	5	1919	G	C8-N9-C4	-5.64	104.14	106.40
36	5	2142	A	C6-N1-C2	-5.64	115.22	118.60
1	2	323	A	C8-N9-C4	-5.63	103.55	105.80
36	1	936	A	P-O3'-C3'	5.63	126.46	119.70
36	1	2296	A	C2-N3-C4	-5.63	107.78	110.60
36	5	646	A	N1-C2-N3	5.63	132.12	129.30
36	5	2242	A	C6-N1-C2	-5.63	115.22	118.60
36	5	3080	G	C5-C6-O6	-5.63	125.22	128.60
1	6	452	A	N1-C6-N6	5.63	121.98	118.60
36	5	1546	A	C5-C6-N6	-5.63	119.19	123.70
38	8	29	U	N3-C2-O2	-5.63	118.26	122.20
1	2	1614	A	N1-C6-N6	5.63	121.98	118.60
36	1	1450	G	O5'-P-OP1	-5.63	100.63	105.70
36	1	1486	G	N1-C6-O6	5.63	123.28	119.90
36	1	2527	G	N3-C4-N9	-5.63	122.62	126.00
38	4	61	A	N1-C2-N3	-5.63	126.48	129.30
12	c0	83	PRO	N-CA-CB	5.63	110.06	103.30
36	5	1152	G	N7-C8-N9	5.63	115.92	113.10
36	5	1177	G	C6-N1-C2	-5.63	121.72	125.10
36	1	96	G	N3-C4-C5	5.63	131.41	128.60
36	1	1663	C	C6-N1-C2	5.63	122.55	120.30
1	6	151	G	N3-C2-N2	-5.63	115.96	119.90
36	5	218	G	N3-C4-C5	-5.63	125.78	128.60
36	5	3336	A	C8-N9-C4	5.63	108.05	105.80
61	n5	115	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	2	192	U	C2-N1-C1'	5.63	124.45	117.70
36	1	1004	U	C5-C6-N1	5.63	125.51	122.70
36	1	1557	A	O5'-P-OP2	-5.63	100.64	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3154	C	C2-N1-C1'	5.63	124.99	118.80
1	6	577	G	C5-N7-C8	-5.63	101.49	104.30
36	5	1499	C	N1-C2-O2	-5.63	115.52	118.90
36	5	2894	C	O5'-P-OP1	-5.63	100.64	105.70
1	2	647	G	N9-C4-C5	5.63	107.65	105.40
36	1	1656	A	C8-N9-C4	5.63	108.05	105.80
36	5	1185	C	N1-C2-O2	-5.63	115.52	118.90
36	5	2231	C	C6-N1-C1'	-5.63	114.05	120.80
36	5	2684	C	O5'-P-OP2	-5.63	100.64	105.70
36	1	198	A	N1-C6-N6	5.62	121.97	118.60
36	1	1507	G	N9-C4-C5	-5.62	103.15	105.40
36	1	2192	C	N1-C2-O2	-5.62	115.53	118.90
1	6	936	G	C4-C5-N7	5.62	113.05	110.80
1	6	1758	U	N1-C2-O2	5.62	126.74	122.80
36	5	369	A	C8-N9-C4	-5.62	103.55	105.80
36	5	651	G	N3-C4-N9	5.62	129.37	126.00
36	1	435	C	N1-C2-O2	-5.62	115.53	118.90
36	1	663	C	N1-C2-O2	-5.62	115.53	118.90
36	1	1155	C	C5-C6-N1	5.62	123.81	121.00
36	1	1303	A	N1-C6-N6	5.62	121.97	118.60
36	1	2918	G	OP2-P-O3'	5.62	117.56	105.20
1	6	639	U	C5-C4-O4	5.62	129.27	125.90
36	1	2400	G	C4-C5-N7	5.62	113.05	110.80
1	6	942	G	O5'-P-OP2	-5.62	100.64	105.70
36	5	1189	C	N3-C2-O2	5.62	125.83	121.90
36	5	1846	C	C5-C6-N1	-5.62	118.19	121.00
36	1	32	U	O5'-P-OP2	-5.62	100.64	105.70
36	1	59	G	C4-C5-N7	5.62	113.05	110.80
36	1	1663	C	N3-C4-C5	5.62	124.15	121.90
36	1	2257	C	C2-N1-C1'	5.62	124.98	118.80
36	1	2395	G	OP2-P-O3'	5.62	117.56	105.20
36	1	2918	G	C4-C5-C6	5.62	122.17	118.80
36	5	1545	A	C5-C6-N6	-5.62	119.21	123.70
36	5	2244	A	O5'-P-OP1	5.62	117.44	110.70
36	5	2821	C	C6-N1-C2	5.62	122.55	120.30
36	5	3098	G	C2-N3-C4	5.62	114.71	111.90
38	4	59	A	C5-C6-N1	5.62	120.51	117.70
36	5	1561	G	O4'-C1'-N9	5.62	112.69	108.20
1	2	1745	G	N9-C4-C5	-5.62	103.15	105.40
36	1	108	A	OP2-P-O3'	5.62	117.56	105.20
36	1	1513	G	N3-C4-N9	5.62	129.37	126.00
36	1	2688	U	C6-N1-C2	5.62	124.37	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3184	A	N7-C8-N9	-5.62	110.99	113.80
36	5	2906	C	C5-C6-N1	-5.62	118.19	121.00
36	5	3093	C	N1-C2-O2	-5.62	115.53	118.90
1	2	380	U	N3-C2-O2	-5.61	118.27	122.20
36	1	958	C	C2-N3-C4	-5.61	117.09	119.90
1	6	66	U	OP1-P-O3'	5.61	117.55	105.20
36	5	1331	U	O4'-C1'-N1	-5.61	103.71	108.20
37	7	76	A	C8-N9-C4	5.61	108.05	105.80
36	5	2704	A	OP1-P-OP2	5.61	128.02	119.60
1	2	1486	G	N1-C6-O6	5.61	123.27	119.90
1	2	1782	A	N7-C8-N9	5.61	116.61	113.80
1	6	1210	C	C6-N1-C2	-5.61	118.06	120.30
36	5	650	C	OP2-P-O3'	5.61	117.54	105.20
36	5	1412	G	O5'-P-OP2	-5.61	100.65	105.70
36	1	2153	U	N3-C2-O2	-5.61	118.27	122.20
36	5	2242	A	OP1-P-O3'	5.61	117.54	105.20
36	1	2836	C	N3-C4-N4	-5.61	114.08	118.00
1	6	102	U	O5'-P-OP1	-5.61	100.65	105.70
1	6	863	A	C5-C6-N6	-5.61	119.21	123.70
36	5	394	G	C5-N7-C8	5.61	107.10	104.30
36	5	968	G	N1-C6-O6	5.61	123.27	119.90
36	5	1873	U	N3-C4-O4	5.61	123.33	119.40
36	5	2199	G	C8-N9-C1'	-5.61	119.71	127.00
36	5	2350	C	OP1-P-OP2	-5.61	111.19	119.60
1	2	1486	G	C4-C5-N7	5.61	113.04	110.80
36	1	1421	G	C8-N9-C4	5.61	108.64	106.40
37	3	42	A	C5-C6-N1	-5.61	114.90	117.70
36	5	3272	C	O5'-P-OP1	-5.61	100.66	105.70
1	2	422	G	C4-C5-N7	5.60	113.04	110.80
36	1	653	A	C5-N7-C8	-5.60	101.10	103.90
36	1	2364	G	O4'-C1'-N9	5.60	112.68	108.20
1	2	934	C	C2-N1-C1'	5.60	124.96	118.80
36	1	665	A	N1-C6-N6	-5.60	115.24	118.60
1	6	1288	G	O5'-P-OP1	5.60	117.42	110.70
37	7	105	C	N3-C4-C5	-5.60	119.66	121.90
1	2	158	U	N1-C2-O2	5.60	126.72	122.80
1	2	402	C	C6-N1-C2	5.60	122.54	120.30
1	2	1654	G	N3-C4-C5	-5.60	125.80	128.60
36	1	882	A	N1-C2-N3	5.60	132.10	129.30
36	1	3072	C	C2-N1-C1'	-5.60	112.64	118.80
1	2	830	U	N1-C2-O2	5.60	126.72	122.80
36	1	232	G	N3-C4-N9	5.60	129.36	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	649	A	C6-N1-C2	-5.60	115.24	118.60
36	5	2870	C	N3-C4-C5	5.60	124.14	121.90
36	5	1380	G	O5'-P-OP1	5.60	117.42	110.70
36	1	1292	C	C6-N1-C2	5.59	122.54	120.30
36	1	2231	C	C6-N1-C2	5.59	122.54	120.30
1	6	1537	C	C6-N1-C1'	5.59	127.51	120.80
36	5	1001	G	N1-C6-O6	-5.59	116.54	119.90
36	5	3093	C	C5-C6-N1	-5.59	118.20	121.00
36	1	652	G	N3-C4-N9	5.59	129.36	126.00
36	1	963	G	O5'-P-OP2	-5.59	100.67	105.70
36	1	2375	G	C5-C6-N1	5.59	114.30	111.50
36	5	1882	G	N9-C4-C5	-5.59	103.16	105.40
36	1	1112	A	C8-N9-C4	5.59	108.04	105.80
36	1	1560	G	N3-C4-C5	5.59	131.40	128.60
36	1	3214	U	N1-C2-O2	5.59	126.71	122.80
36	5	927	C	C2-N3-C4	-5.59	117.10	119.90
36	1	2333	C	OP2-P-O3'	5.59	117.50	105.20
36	1	2861	U	N1-C2-O2	5.59	126.71	122.80
36	1	2865	U	N3-C4-O4	-5.59	115.49	119.40
36	5	112	U	O4'-C1'-N1	5.59	112.67	108.20
36	5	966	U	C6-N1-C2	-5.59	117.65	121.00
37	7	96	U	C5-C4-O4	5.59	129.25	125.90
36	1	915	A	OP1-P-OP2	5.59	127.98	119.60
36	5	1348	U	C4-C5-C6	5.59	123.05	119.70
36	1	546	C	C6-N1-C2	-5.59	118.06	120.30
1	6	272	U	C2-N1-C1'	5.59	124.40	117.70
36	5	2800	G	O5'-P-OP1	5.59	117.40	110.70
36	1	24	G	N1-C2-N2	-5.58	111.17	116.20
36	1	93	C	C5-C6-N1	5.58	123.79	121.00
38	4	55	U	C5-C4-O4	-5.58	122.55	125.90
36	5	152	U	C4-C5-C6	5.58	123.05	119.70
36	5	796	U	N3-C2-O2	-5.58	118.29	122.20
37	7	81	U	C6-N1-C2	5.58	124.35	121.00
38	8	33	A	N9-C4-C5	-5.58	103.57	105.80
36	1	514	G	C8-N9-C4	5.58	108.63	106.40
36	1	910	G	C5-C6-N1	-5.58	108.71	111.50
36	1	936	A	C5-C6-N1	-5.58	114.91	117.70
36	1	2619	G	C2-N3-C4	5.58	114.69	111.90
36	5	2314	U	C6-N1-C2	-5.58	117.65	121.00
36	5	2868	U	N3-C2-O2	-5.58	118.29	122.20
1	2	428	A	O5'-P-OP2	-5.58	100.68	105.70
36	1	2633	U	C4-C5-C6	5.58	123.05	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	936	A	C6-N1-C2	5.58	121.95	118.60
36	1	2250	G	N7-C8-N9	-5.58	110.31	113.10
36	1	2777	G	C4-C5-N7	-5.58	108.57	110.80
36	1	3084	C	N1-C2-O2	-5.58	115.55	118.90
36	5	1303	A	C8-N9-C4	5.58	108.03	105.80
36	5	1431	G	N1-C6-O6	-5.58	116.55	119.90
36	5	2191	U	N1-C2-O2	5.58	126.70	122.80
36	5	2830	G	N1-C2-N3	5.58	127.25	123.90
36	1	753	C	N3-C4-C5	5.58	124.13	121.90
1	6	374	U	O5'-P-OP2	-5.58	100.68	105.70
36	5	2692	A	N1-C6-N6	-5.58	115.25	118.60
1	2	543	C	N3-C2-O2	-5.58	118.00	121.90
1	2	553	G	C4-C5-N7	5.58	113.03	110.80
36	1	798	G	C8-N9-C4	-5.58	104.17	106.40
36	1	1513	G	C6-N1-C2	-5.58	121.75	125.10
36	1	2392	C	N3-C4-C5	5.58	124.13	121.90
36	1	2610	G	C6-C5-N7	-5.58	127.06	130.40
36	1	3217	C	C6-N1-C1'	-5.58	114.11	120.80
36	1	3229	G	N1-C6-O6	5.58	123.25	119.90
36	5	218	G	N3-C4-N9	5.58	129.35	126.00
36	5	2334	U	N1-C2-N3	5.58	118.25	114.90
1	2	412	A	N1-C6-N6	5.57	121.94	118.60
36	1	365	A	N1-C6-N6	5.57	121.94	118.60
36	1	711	A	C8-N9-C4	5.57	108.03	105.80
36	1	892	U	C5-C4-O4	5.57	129.25	125.90
36	1	1176	C	O5'-P-OP2	5.57	117.39	110.70
38	4	58	G	O5'-P-OP2	-5.57	100.68	105.70
36	5	758	C	C2-N1-C1'	-5.57	112.67	118.80
36	5	1905	G	C5-C6-O6	-5.57	125.26	128.60
36	1	338	A	OP2-P-O3'	5.57	117.45	105.20
36	1	3207	U	C2-N1-C1'	-5.57	111.02	117.70
36	1	3217	C	C6-N1-C2	-5.57	118.07	120.30
1	6	1047	G	N1-C6-O6	5.57	123.24	119.90
36	5	222	A	O5'-P-OP2	-5.57	100.69	105.70
36	5	720	A	C5-C6-N6	-5.57	119.24	123.70
36	5	869	G	C8-N9-C4	5.57	108.63	106.40
36	5	1296	C	C6-N1-C2	-5.57	118.07	120.30
36	5	1534	A	C4-C5-C6	5.57	119.78	117.00
36	5	2136	C	C6-N1-C2	5.57	122.53	120.30
1	2	1560	U	N3-C4-O4	-5.57	115.50	119.40
36	1	432	G	C2-N3-C4	-5.57	109.11	111.90
36	1	2606	G	N3-C4-C5	-5.57	125.81	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1500	G	C8-N9-C4	5.57	108.63	106.40
36	5	2393	G	C2-N3-C4	5.57	114.69	111.90
36	5	2599	U	C5-C6-N1	-5.57	119.92	122.70
36	1	424	G	C5-C6-O6	-5.57	125.26	128.60
36	1	3215	A	N1-C6-N6	5.57	121.94	118.60
36	1	3362	A	C2-N3-C4	-5.57	107.82	110.60
36	5	52	A	C2-N3-C4	-5.57	107.82	110.60
36	5	346	C	C5-C4-N4	-5.57	116.30	120.20
36	5	1115	G	N7-C8-N9	5.57	115.88	113.10
36	1	1185	C	C6-N1-C2	5.57	122.53	120.30
1	6	343	C	N1-C2-O2	-5.57	115.56	118.90
36	5	2380	U	C5-C4-O4	-5.57	122.56	125.90
36	5	2699	G	C8-N9-C4	5.57	108.63	106.40
36	5	2797	C	N3-C4-C5	-5.57	119.67	121.90
36	5	2827	U	O4'-C1'-N1	5.57	112.65	108.20
36	5	2947	G	OP1-P-O3'	5.57	117.45	105.20
36	5	3164	C	O4'-C1'-N1	5.57	112.65	108.20
1	6	432	G	C4-C5-N7	5.56	113.03	110.80
36	5	2857	C	C5-C4-N4	-5.56	116.31	120.20
1	2	1473	U	N3-C2-O2	-5.56	118.31	122.20
36	1	28	C	C5-C4-N4	-5.56	116.31	120.20
36	1	2367	A	C6-N1-C2	-5.56	115.26	118.60
36	1	2395	G	O5'-P-OP1	5.56	117.38	110.70
36	1	2572	C	C6-N1-C2	-5.56	118.08	120.30
36	1	2748	A	N1-C6-N6	5.56	121.94	118.60
36	5	960	U	OP2-P-O3'	5.56	117.44	105.20
36	1	1480	G	C5-N7-C8	-5.56	101.52	104.30
36	5	1226	G	N9-C4-C5	-5.56	103.18	105.40
36	5	2410	U	O5'-P-OP1	-5.56	100.69	105.70
36	1	1097	G	P-O3'-C3'	5.56	126.37	119.70
1	6	1274	C	C6-N1-C2	-5.56	118.08	120.30
36	5	1499	C	OP2-P-O3'	5.56	117.43	105.20
36	5	2661	G	OP1-P-O3'	5.56	117.43	105.20
36	5	3386	G	O5'-P-OP2	-5.56	100.70	105.70
36	1	1807	G	C6-C5-N7	-5.56	127.06	130.40
36	1	1932	A	C5-C6-N6	-5.56	119.25	123.70
36	5	417	A	N1-C6-N6	-5.56	115.27	118.60
36	5	1793	C	O5'-P-OP1	-5.56	100.70	105.70
36	5	1917	C	N1-C2-O2	-5.56	115.57	118.90
36	1	1518	U	N3-C4-C5	-5.55	111.27	114.60
36	5	1496	C	O5'-P-OP1	5.55	117.36	110.70
36	5	2290	C	C2-N3-C4	-5.55	117.12	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2765	C	C6-N1-C2	-5.55	118.08	120.30
36	1	3377	G	N3-C4-N9	5.55	129.33	126.00
1	6	426	G	C8-N9-C4	-5.55	104.18	106.40
3	S1	96	LEU	CA-CB-CG	5.55	128.07	115.30
36	1	99	A	C5'-C4'-O4'	5.55	115.76	109.10
36	1	615	U	C5-C4-O4	5.55	129.23	125.90
36	1	3045	G	N3-C4-N9	5.55	129.33	126.00
36	1	3120	C	O5'-P-OP2	-5.55	100.70	105.70
1	6	1026	A	N7-C8-N9	-5.55	111.03	113.80
36	1	22	G	N3-C4-N9	5.55	129.33	126.00
38	4	17	A	C2-N3-C4	-5.55	107.83	110.60
36	5	1374	G	C8-N9-C4	5.55	108.62	106.40
36	5	2524	A	N9-C1'-C2'	5.55	121.21	114.00
36	5	3176	G	N3-C4-C5	-5.55	125.83	128.60
36	1	224	C	C6-N1-C2	-5.55	118.08	120.30
36	1	277	G	O5'-P-OP1	-5.55	100.71	105.70
36	1	644	G	N7-C8-N9	5.55	115.87	113.10
36	1	888	A	N9-C4-C5	-5.55	103.58	105.80
36	1	1306	G	C6-C5-N7	-5.55	127.07	130.40
1	6	1058	U	P-O3'-C3'	5.55	126.36	119.70
36	5	753	C	C5-C6-N1	-5.55	118.23	121.00
36	5	779	G	O5'-P-OP2	-5.55	100.71	105.70
36	1	2965	U	C5-C6-N1	-5.54	119.93	122.70
1	6	1297	G	O5'-P-OP2	-5.54	100.71	105.70
1	2	1200	G	N3-C2-N2	-5.54	116.02	119.90
36	1	2177	G	C6-N1-C2	-5.54	121.77	125.10
36	1	2357	A	C4-C5-N7	5.54	113.47	110.70
38	4	59	A	C5-C6-N6	-5.54	119.27	123.70
1	6	1697	G	N3-C4-C5	-5.54	125.83	128.60
36	5	197	G	N3-C4-N9	5.54	129.33	126.00
36	1	304	G	C2-N3-C4	5.54	114.67	111.90
36	1	896	A	N9-C4-C5	5.54	108.02	105.80
36	5	689	U	N3-C2-O2	-5.54	118.32	122.20
36	5	229	G	N3-C4-N9	-5.54	122.68	126.00
36	1	334	A	C8-N9-C4	-5.54	103.58	105.80
36	1	803	C	O5'-P-OP1	5.54	117.35	110.70
36	5	1348	U	O4'-C1'-N1	5.54	112.63	108.20
36	5	2879	C	C5-C4-N4	-5.54	116.32	120.20
1	6	317	C	N1-C2-N3	5.54	123.08	119.20
1	6	1031	U	C5-C6-N1	-5.54	119.93	122.70
36	5	520	U	N1-C2-O2	-5.54	118.92	122.80
36	5	1153	A	C6-C5-N7	-5.54	128.43	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1161	G	C5-C6-N1	5.54	114.27	111.50
36	5	2383	C	N1-C2-O2	-5.54	115.58	118.90
36	5	2735	U	C6-N1-C2	-5.54	117.68	121.00
37	7	82	G	OP2-P-O3'	5.54	117.38	105.20
36	1	1854	C	N3-C4-N4	-5.53	114.13	118.00
36	5	348	A	C2-N3-C4	-5.53	107.83	110.60
36	5	1148	G	N1-C6-O6	5.53	123.22	119.90
36	5	2186	U	N3-C4-O4	-5.53	115.53	119.40
36	5	2700	G	N3-C4-N9	5.53	129.32	126.00
36	1	1316	C	N3-C4-N4	5.53	121.87	118.00
36	1	1324	U	O5'-P-OP1	5.53	117.33	110.70
36	1	2623	G	N1-C2-N2	-5.53	111.22	116.20
36	1	2802	A	O4'-C1'-N9	5.53	112.62	108.20
1	6	309	C	O5'-P-OP1	-5.53	100.72	105.70
36	5	515	C	O5'-P-OP2	-5.53	100.72	105.70
64	n8	73	LEU	CA-CB-CG	5.53	128.02	115.30
36	1	1124	U	C4-C5-C6	-5.53	116.38	119.70
36	1	2148	U	N1-C2-O2	-5.53	118.93	122.80
36	5	659	G	C2-N3-C4	5.53	114.66	111.90
36	1	2150	G	C4-C5-C6	5.53	122.12	118.80
36	1	2326	A	C5-N7-C8	-5.53	101.14	103.90
36	1	3140	G	N1-C6-O6	5.53	123.22	119.90
36	1	3261	C	N3-C4-N4	5.53	121.87	118.00
36	5	639	G	C8-N9-C4	5.53	108.61	106.40
36	5	673	U	C5-C6-N1	-5.53	119.94	122.70
36	5	1884	A	OP2-P-O3'	5.53	117.36	105.20
36	5	2397	A	C8-N9-C4	5.53	108.01	105.80
1	2	95	G	C5-C6-O6	5.53	131.92	128.60
36	1	350	C	N3-C2-O2	-5.53	118.03	121.90
36	1	425	G	O5'-P-OP1	5.53	117.33	110.70
36	1	1481	A	C5-N7-C8	-5.53	101.14	103.90
36	1	2355	G	C2-N3-C4	-5.53	109.14	111.90
36	1	2396	G	C5-C6-N1	-5.53	108.74	111.50
36	1	3154	C	C6-N1-C2	-5.53	118.09	120.30
36	5	41	G	N1-C6-O6	5.53	123.22	119.90
36	5	2121	G	O5'-P-OP2	-5.53	100.73	105.70
36	5	2315	G	N1-C6-O6	5.53	123.22	119.90
1	2	925	G	C5-C6-O6	-5.52	125.28	128.60
36	5	1846	C	C6-N1-C2	5.52	122.51	120.30
1	2	1268	G	O5'-P-OP2	-5.52	100.73	105.70
36	1	1305	U	N1-C2-O2	5.52	126.67	122.80
36	1	2679	A	C2-N3-C4	-5.52	107.84	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	440	U	N1-C2-O2	-5.52	118.93	122.80
36	5	330	G	C8-N9-C4	5.52	108.61	106.40
36	5	2887	A	C6-C5-N7	-5.52	128.43	132.30
1	2	315	A	N1-C6-N6	5.52	121.91	118.60
36	5	609	G	O5'-P-OP2	-5.52	100.73	105.70
36	5	2381	G	C5-C6-O6	-5.52	125.29	128.60
1	2	73	U	OP1-P-O3'	5.52	117.34	105.20
36	1	211	A	C2-N3-C4	-5.52	107.84	110.60
36	1	869	G	C6-C5-N7	-5.52	127.09	130.40
36	1	1677	G	C8-N9-C4	-5.52	104.19	106.40
36	5	877	C	N3-C4-N4	-5.52	114.14	118.00
36	5	1488	G	OP1-P-O3'	5.52	117.34	105.20
1	2	254	A	C8-N9-C4	5.52	108.01	105.80
1	2	308	C	C2-N3-C4	-5.52	117.14	119.90
36	1	906	A	C6-N1-C2	-5.52	115.29	118.60
36	1	1432	C	N3-C4-C5	-5.52	119.69	121.90
36	1	2145	A	C6-C5-N7	-5.52	128.44	132.30
36	1	2940	A	C2-N3-C4	5.52	113.36	110.60
36	5	2724	U	N1-C2-N3	5.52	118.21	114.90
52	m6	151	ASP	CB-CG-OD2	5.52	123.27	118.30
36	1	720	A	N1-C6-N6	5.52	121.91	118.60
36	5	686	G	C8-N9-C4	5.52	108.61	106.40
36	5	2311	G	C8-N9-C4	5.52	108.61	106.40
36	1	1047	A	C2-N3-C4	-5.51	107.84	110.60
36	1	1059	G	N1-C6-O6	-5.51	116.59	119.90
36	1	2808	A	C4-N9-C1'	5.51	136.23	126.30
36	5	1302	A	N9-C4-C5	5.51	108.01	105.80
36	5	1848	G	C5-C6-O6	-5.51	125.29	128.60
36	1	1741	A	N1-C2-N3	5.51	132.06	129.30
36	5	21	G	C8-N9-C4	5.51	108.61	106.40
36	1	33	G	C4-C5-C6	5.51	122.11	118.80
36	1	226	C	N3-C4-C5	-5.51	119.69	121.90
36	1	900	G	N7-C8-N9	-5.51	110.34	113.10
1	6	298	C	N1-C2-O2	-5.51	115.59	118.90
36	5	687	U	O5'-P-OP2	-5.51	100.74	105.70
36	5	2572	C	C6-N1-C1'	-5.51	114.19	120.80
36	5	2697	A	C5-C6-N6	-5.51	119.29	123.70
36	5	2821	C	C2-N1-C1'	-5.51	112.74	118.80
36	5	3287	U	N3-C2-O2	-5.51	118.34	122.20
36	5	3309	G	C4-N9-C1'	5.51	133.67	126.50
36	1	776	U	C5-C4-O4	5.51	129.21	125.90
1	6	1150	G	N3-C4-C5	5.51	131.35	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1434	G	N9-C4-C5	5.51	107.60	105.40
36	5	3196	U	O5'-P-OP1	-5.51	100.74	105.70
36	1	3208	G	N3-C4-C5	-5.51	125.85	128.60
38	4	17	A	C4-C5-C6	5.51	119.75	117.00
36	5	2765	C	C5-C6-N1	5.51	123.75	121.00
1	2	354	C	N3-C4-C5	-5.51	119.70	121.90
36	1	803	C	N1-C2-O2	-5.51	115.60	118.90
36	1	1447	G	C2-N3-C4	5.51	114.65	111.90
36	1	2714	G	C8-N9-C1'	5.51	134.16	127.00
38	4	44	A	N9-C4-C5	-5.51	103.60	105.80
36	5	216	G	N9-C4-C5	-5.51	103.20	105.40
36	1	1790	G	C6-C5-N7	-5.50	127.10	130.40
36	1	3265	C	C6-N1-C2	5.50	122.50	120.30
36	5	904	A	C5-C6-N1	5.50	120.45	117.70
36	5	1045	C	C6-N1-C2	-5.50	118.10	120.30
36	1	1180	A	O4'-C1'-N9	-5.50	103.80	108.20
36	1	1849	C	N3-C4-C5	5.50	124.10	121.90
40	L3	4	ARG	NE-CZ-NH2	-5.50	117.55	120.30
36	5	610	G	N3-C4-C5	-5.50	125.85	128.60
36	5	2297	U	O5'-P-OP2	-5.50	100.75	105.70
36	5	2401	A	OP1-P-OP2	5.50	127.86	119.60
36	5	2930	A	C6-N1-C2	-5.50	115.30	118.60
1	2	988	A	C2-N3-C4	-5.50	107.85	110.60
36	1	591	G	C6-C5-N7	-5.50	127.10	130.40
36	1	3344	A	C4-C5-N7	5.50	113.45	110.70
36	5	1390	A	C2-N3-C4	5.50	113.35	110.60
36	5	3378	C	N3-C4-C5	5.50	124.10	121.90
1	2	1458	G	C4-N9-C1'	5.50	133.65	126.50
1	2	968	U	C5-C6-N1	-5.50	119.95	122.70
1	2	1202	A	C8-N9-C4	-5.50	103.60	105.80
36	1	352	A	O4'-C1'-N9	5.50	112.60	108.20
36	1	880	G	C6-C5-N7	5.50	133.70	130.40
36	1	3194	C	N3-C4-C5	-5.50	119.70	121.90
1	6	638	U	N3-C2-O2	-5.50	118.35	122.20
36	1	1326	A	O5'-P-OP2	-5.50	100.75	105.70
36	1	1849	C	N3-C2-O2	5.50	125.75	121.90
36	1	1934	G	N1-C6-O6	5.50	123.20	119.90
36	1	2162	U	N3-C4-C5	5.50	117.90	114.60
1	6	60	U	N1-C2-O2	5.50	126.65	122.80
36	5	2630	C	N3-C2-O2	5.50	125.75	121.90
1	2	857	U	C2-N1-C1'	5.50	124.29	117.70
1	2	1657	U	C5-C4-O4	5.50	129.20	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1380	G	C8-N9-C4	5.50	108.60	106.40
36	5	1846	C	OP2-P-O3'	5.50	117.29	105.20
36	5	2197	C	C6-N1-C2	5.50	122.50	120.30
36	1	1199	C	N1-C2-O2	5.49	122.20	118.90
36	1	2278	C	C4-C5-C6	-5.49	114.65	117.40
36	1	2329	C	N1-C2-O2	-5.49	115.60	118.90
36	1	2610	G	O5'-P-OP1	5.49	117.29	110.70
1	6	21	U	C5-C4-O4	-5.49	122.60	125.90
36	5	869	G	C6-N1-C2	-5.49	121.80	125.10
36	5	971	G	C8-N9-C4	5.49	108.60	106.40
36	5	2165	G	N3-C4-C5	-5.49	125.85	128.60
36	5	2385	G	N3-C4-N9	-5.49	122.70	126.00
36	5	2813	A	C8-N9-C4	-5.49	103.60	105.80
36	5	2893	C	N1-C2-O2	-5.49	115.60	118.90
36	5	3373	U	N3-C2-O2	-5.49	118.36	122.20
36	1	1365	G	N7-C8-N9	5.49	115.85	113.10
1	6	609	U	O5'-P-OP2	-5.49	100.76	105.70
36	5	689	U	N1-C2-O2	5.49	126.64	122.80
36	5	2245	C	N3-C4-C5	-5.49	119.70	121.90
36	5	2891	U	N3-C4-C5	5.49	117.89	114.60
36	5	2971	A	N1-C2-N3	-5.49	126.55	129.30
36	1	2395	G	C6-C5-N7	-5.49	127.11	130.40
36	1	2419	A	OP1-P-OP2	-5.49	111.36	119.60
1	6	1280	C	N3-C4-C5	-5.49	119.70	121.90
36	5	518	G	N9-C4-C5	5.49	107.60	105.40
36	5	1547	G	C8-N9-C4	5.49	108.60	106.40
36	5	2285	C	C6-N1-C2	-5.49	118.10	120.30
36	5	3190	C	N3-C4-C5	-5.49	119.70	121.90
1	2	829	A	P-O3'-C3'	5.49	126.29	119.70
36	1	864	G	C4-C5-N7	-5.49	108.61	110.80
36	1	917	A	O5'-P-OP2	-5.49	100.76	105.70
36	1	2688	U	C6-N1-C1'	-5.49	113.52	121.20
36	1	2714	G	C4-C5-N7	5.49	113.00	110.80
36	5	46	U	N3-C2-O2	5.49	126.04	122.20
36	5	1331	U	N3-C4-C5	5.49	117.89	114.60
36	5	2134	G	N1-C2-N2	-5.49	111.26	116.20
36	5	2916	U	C4-C5-C6	5.49	122.99	119.70
36	5	3190	C	C6-N1-C2	-5.49	118.11	120.30
18	C6	53	LEU	CA-CB-CG	-5.49	102.68	115.30
1	6	363	G	C5-C6-O6	-5.49	125.31	128.60
36	5	2811	A	C8-N9-C4	5.49	108.00	105.80
38	8	8	C	C6-N1-C2	-5.49	118.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	12	179	LEU	CA-CB-CG	5.49	127.92	115.30
36	5	43	A	C2-N3-C4	-5.49	107.86	110.60
36	5	672	A	N7-C8-N9	5.49	116.54	113.80
36	5	1922	A	C2-N3-C4	-5.49	107.86	110.60
36	1	888	A	C6-C5-N7	-5.48	128.46	132.30
36	1	981	U	C6-N1-C2	-5.48	117.71	121.00
36	1	2572	C	N3-C2-O2	-5.48	118.06	121.90
36	5	1133	A	C5-C6-N1	5.48	120.44	117.70
36	5	1552	G	N9-C4-C5	-5.48	103.21	105.40
36	1	1121	U	N1-C2-N3	5.48	118.19	114.90
36	1	1846	C	N1-C2-N3	5.48	123.04	119.20
36	1	2878	G	N9-C4-C5	-5.48	103.21	105.40
36	1	3177	G	N1-C6-O6	5.48	123.19	119.90
36	1	3228	C	C2-N1-C1'	5.48	124.83	118.80
1	6	782	U	N3-C2-O2	-5.48	118.36	122.20
36	5	708	G	O5'-P-OP1	-5.48	100.77	105.70
36	5	1846	C	C2-N3-C4	-5.48	117.16	119.90
37	7	68	C	N3-C2-O2	-5.48	118.06	121.90
64	n8	25	HIS	N-CA-C	-5.48	96.20	111.00
36	1	2958	A	C5-C6-N1	5.48	120.44	117.70
36	5	715	A	O4'-C1'-N9	5.48	112.58	108.20
36	5	1115	G	C8-N9-C4	-5.48	104.21	106.40
36	1	88	A	N9-C4-C5	-5.48	103.61	105.80
36	1	159	A	C8-N9-C4	5.48	107.99	105.80
36	1	690	A	N1-C6-N6	-5.48	115.31	118.60
36	5	349	A	C5-C6-N1	5.48	120.44	117.70
36	5	3083	G	N1-C2-N2	-5.48	111.27	116.20
1	2	579	A	N1-C2-N3	5.48	132.04	129.30
36	1	36	C	C5-C4-N4	-5.48	116.37	120.20
36	1	304	G	N3-C2-N2	-5.48	116.07	119.90
36	5	2377	G	C8-N9-C4	5.48	108.59	106.40
36	1	1203	A	C5-N7-C8	-5.47	101.16	103.90
36	5	1854	C	C6-N1-C2	-5.47	118.11	120.30
43	16	173	MET	CB-CG-SD	-5.47	95.98	112.40
36	1	880	G	C4-N9-C1'	-5.47	119.39	126.50
36	1	1619	A	N9-C4-C5	-5.47	103.61	105.80
36	1	2966	G	C4-C5-N7	5.47	112.99	110.80
37	3	92	A	C2-N3-C4	-5.47	107.86	110.60
1	6	454	U	C6-N1-C2	5.47	124.28	121.00
1	6	634	G	O4'-C1'-N9	5.47	112.58	108.20
36	5	915	A	OP1-P-OP2	5.47	127.81	119.60
1	2	1241	G	C4-N9-C1'	5.47	133.61	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	395	A	C6-N1-C2	-5.47	115.32	118.60
36	5	514	G	N1-C6-O6	5.47	123.18	119.90
36	1	220	G	C5-C6-O6	-5.47	125.32	128.60
36	1	2309	A	C5-C6-N6	-5.47	119.32	123.70
36	1	2400	G	N3-C4-N9	5.47	129.28	126.00
36	1	2426	U	N3-C2-O2	-5.47	118.37	122.20
36	1	2813	A	C4-C5-C6	5.47	119.73	117.00
36	5	969	C	C2-N3-C4	-5.47	117.17	119.90
36	5	1881	A	N1-C6-N6	5.47	121.88	118.60
36	5	364	G	OP2-P-O3'	5.47	117.23	105.20
36	5	2805	G	N1-C6-O6	5.47	123.18	119.90
36	1	888	A	C5-N7-C8	-5.47	101.17	103.90
36	1	1837	U	N3-C2-O2	5.47	126.03	122.20
38	4	47	C	C4-C5-C6	5.47	120.13	117.40
37	7	100	C	C5-C6-N1	-5.47	118.27	121.00
36	1	2698	G	N3-C4-C5	-5.46	125.87	128.60
1	6	215	A	C8-N9-C4	-5.46	103.61	105.80
1	6	541	A	C8-N9-C4	-5.46	103.61	105.80
36	5	951	A	N1-C2-N3	-5.46	126.57	129.30
36	5	1286	A	N7-C8-N9	-5.46	111.07	113.80
36	5	2273	G	C8-N9-C1'	5.46	134.10	127.00
1	2	448	C	N3-C2-O2	-5.46	118.08	121.90
36	1	970	A	C6-N1-C2	-5.46	115.32	118.60
36	1	1005	G	C5-C6-O6	5.46	131.88	128.60
36	1	2179	C	OP2-P-O3'	5.46	117.22	105.20
1	6	782	U	C2-N1-C1'	5.46	124.25	117.70
36	5	1150	A	O5'-P-OP2	-5.46	100.78	105.70
36	1	99	A	C8-N9-C4	-5.46	103.61	105.80
36	1	2915	U	C5-C4-O4	-5.46	122.62	125.90
36	5	374	A	N9-C4-C5	5.46	107.98	105.80
36	5	1490	A	C5-C6-N1	5.46	120.43	117.70
36	5	2355	G	OP2-P-O3'	5.46	117.22	105.20
1	2	1096	C	C6-N1-C1'	-5.46	114.25	120.80
36	1	3326	G	N9-C4-C5	-5.46	103.22	105.40
36	5	2685	C	C5-C6-N1	-5.46	118.27	121.00
36	1	710	A	C5-C6-N6	-5.46	119.33	123.70
36	1	2522	G	C4-N9-C1'	5.46	133.60	126.50
36	1	2866	U	N3-C2-O2	-5.46	118.38	122.20
1	6	634	G	O5'-P-OP2	-5.46	100.79	105.70
36	5	2738	A	O5'-P-OP2	-5.46	100.79	105.70
36	5	2899	C	N3-C4-C5	-5.46	119.72	121.90
36	5	2991	A	OP2-P-O3'	5.46	117.21	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1100	G	C4-N9-C1'	5.46	133.59	126.50
36	5	2379	U	O5'-P-OP1	5.46	117.25	110.70
36	1	423	A	C5-C6-N1	-5.46	114.97	117.70
67	O1	62	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	6	421	A	N9-C4-C5	-5.46	103.62	105.80
1	2	142	G	N3-C4-N9	-5.45	122.73	126.00
36	1	2380	U	C2-N3-C4	-5.45	123.73	127.00
1	6	1266	U	C5-C6-N1	5.45	125.43	122.70
36	5	921	A	OP2-P-O3'	5.45	117.20	105.20
36	5	1103	A	N7-C8-N9	5.45	116.53	113.80
36	5	1129	A	O5'-P-OP1	5.45	117.24	110.70
36	1	787	G	N3-C4-C5	-5.45	125.87	128.60
36	1	984	G	C8-N9-C4	-5.45	104.22	106.40
36	1	2402	A	N1-C6-N6	5.45	121.87	118.60
1	6	1399	C	C6-N1-C2	-5.45	118.12	120.30
36	5	2400	G	C5-N7-C8	-5.45	101.57	104.30
36	1	1158	A	C5-C6-N6	-5.45	119.34	123.70
36	1	2372	A	OP1-P-O3'	5.45	117.19	105.20
36	1	2838	A	N1-C2-N3	5.45	132.03	129.30
1	6	1025	A	C2-N3-C4	-5.45	107.88	110.60
1	6	1581	C	C6-N1-C2	5.45	122.48	120.30
36	5	348	A	O5'-P-OP1	-5.45	100.80	105.70
36	5	1294	A	C5-C6-N1	5.45	120.43	117.70
36	5	2584	G	OP2-P-O3'	5.45	117.19	105.20
36	5	2872	A	C2-N3-C4	-5.45	107.88	110.60
36	5	2898	G	O4'-C1'-N9	-5.45	103.84	108.20
1	2	359	A	C4-N9-C1'	-5.45	116.49	126.30
36	1	318	A	O5'-P-OP1	-5.45	100.80	105.70
36	1	2944	U	C4-C5-C6	-5.45	116.43	119.70
36	1	2953	U	N1-C2-O2	-5.45	118.99	122.80
36	5	1452	A	C4-C5-N7	5.45	113.42	110.70
36	5	3204	C	C6-N1-C2	5.45	122.48	120.30
36	1	2145	A	N1-C6-N6	5.45	121.87	118.60
36	1	2622	C	N1-C2-O2	-5.45	115.63	118.90
36	1	798	G	C5-C6-N1	-5.45	108.78	111.50
36	1	3099	C	O4'-C1'-N1	5.45	112.56	108.20
36	5	1099	A	N1-C6-N6	5.45	121.87	118.60
36	1	394	G	C5-C6-O6	5.44	131.87	128.60
1	2	1082	C	C2-N1-C1'	5.44	124.79	118.80
36	1	1166	G	C4-C5-N7	5.44	112.98	110.80
36	1	2973	G	C5-C6-N1	-5.44	108.78	111.50
36	5	617	G	N9-C4-C5	-5.44	103.22	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2843	U	N3-C2-O2	-5.44	118.39	122.20
36	5	2951	G	N9-C4-C5	-5.44	103.22	105.40
36	5	3043	C	N3-C4-N4	-5.44	114.19	118.00
1	2	48	G	OP2-P-O3'	5.44	117.17	105.20
1	2	1100	G	C5-C6-O6	-5.44	125.34	128.60
36	5	2837	A	O5'-P-OP1	-5.44	100.80	105.70
36	5	915	A	OP1-P-O3'	5.44	117.17	105.20
36	5	2356	A	C6-N1-C2	5.44	121.86	118.60
1	2	1535	U	N1-C2-O2	5.44	126.61	122.80
36	1	1158	A	N1-C6-N6	5.44	121.86	118.60
36	1	3229	G	C5-C6-O6	-5.44	125.34	128.60
36	5	504	A	C8-N9-C4	5.44	107.97	105.80
36	5	3096	C	N1-C2-O2	-5.44	115.64	118.90
38	8	85	G	C8-N9-C4	-5.44	104.22	106.40
36	1	3180	A	C2-N3-C4	-5.44	107.88	110.60
36	5	1079	A	C5-C6-N1	5.44	120.42	117.70
1	2	316	A	N7-C8-N9	-5.43	111.08	113.80
36	1	580	C	N1-C2-O2	-5.43	115.64	118.90
36	1	1445	U	N3-C2-O2	5.43	126.00	122.20
36	1	3368	U	N1-C2-O2	-5.43	119.00	122.80
36	5	2165	G	C8-N9-C1'	-5.43	119.93	127.00
36	5	3368	U	C6-N1-C1'	5.43	128.81	121.20
36	1	1153	A	C4-C5-C6	5.43	119.72	117.00
36	1	2817	A	OP2-P-O3'	5.43	117.15	105.20
36	1	3319	U	P-O3'-C3'	5.43	126.22	119.70
1	6	1001	A	C6-C5-N7	-5.43	128.50	132.30
36	5	2204	C	OP1-P-O3'	5.43	117.15	105.20
36	5	2899	C	C2-N1-C1'	5.43	124.78	118.80
36	5	3277	U	N1-C2-O2	5.43	126.60	122.80
36	5	3288	G	C5-C6-N1	5.43	114.22	111.50
36	5	361	A	C2-N3-C4	5.43	113.31	110.60
36	5	679	U	C5-C4-O4	5.43	129.16	125.90
38	4	119	C	O5'-P-OP2	-5.43	100.81	105.70
1	6	65	A	N3-C4-C5	5.43	130.60	126.80
1	6	1539	G	N3-C4-C5	5.43	131.31	128.60
1	2	142	G	N3-C4-C5	5.43	131.31	128.60
1	2	1733	C	N3-C4-N4	5.43	121.80	118.00
36	1	356	C	O5'-P-OP2	-5.43	100.82	105.70
36	1	690	A	C5-C6-N6	5.43	128.04	123.70
36	1	1422	G	C8-N9-C4	5.43	108.57	106.40
36	1	1521	G	C2-N3-C4	-5.43	109.19	111.90
36	1	1897	G	C5-N7-C8	-5.43	101.59	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	387	A	O5'-P-OP2	-5.43	100.82	105.70
36	5	56	G	O5'-P-OP1	5.43	117.21	110.70
36	5	1180	A	N9-C4-C5	5.43	107.97	105.80
36	5	2326	A	OP2-P-O3'	5.43	117.14	105.20
36	5	2412	G	C5-C6-N1	5.43	114.21	111.50
36	5	2756	C	C6-N1-C2	5.43	122.47	120.30
37	7	26	C	N3-C4-C5	-5.43	119.73	121.90
36	1	2818	U	O4'-C1'-N1	-5.42	103.86	108.20
1	6	51	A	N1-C6-N6	-5.42	115.34	118.60
36	5	3	U	N1-C2-O2	5.42	126.60	122.80
36	5	621	A	C5-C6-N1	5.42	120.41	117.70
1	2	581	U	C5-C6-N1	5.42	125.41	122.70
36	1	383	G	C5-C6-O6	-5.42	125.35	128.60
36	1	577	C	C4-C5-C6	5.42	120.11	117.40
36	1	645	A	N1-C2-N3	5.42	132.01	129.30
36	1	1307	G	N9-C4-C5	5.42	107.57	105.40
1	6	455	C	C5-C4-N4	-5.42	116.40	120.20
1	6	901	G	N1-C6-O6	5.42	123.15	119.90
36	1	45	A	N1-C6-N6	-5.42	115.35	118.60
36	1	1389	G	C5-N7-C8	-5.42	101.59	104.30
1	6	25	C	P-O3'-C3'	5.42	126.21	119.70
1	6	747	C	C6-N1-C2	-5.42	118.13	120.30
36	5	1868	G	N9-C4-C5	-5.42	103.23	105.40
36	5	2556	C	N3-C2-O2	-5.42	118.11	121.90
38	4	40	A	C5-C6-N6	-5.42	119.36	123.70
36	5	1012	G	N3-C4-C5	5.42	131.31	128.60
36	5	1303	A	N1-C6-N6	5.42	121.85	118.60
36	5	1339	C	N3-C4-N4	5.42	121.79	118.00
1	2	1131	A	C8-N9-C4	5.42	107.97	105.80
1	2	1311	U	C5-C6-N1	-5.42	119.99	122.70
1	6	359	A	N3-C4-C5	5.42	130.59	126.80
36	5	2295	A	C5-C6-N1	5.42	120.41	117.70
36	1	58	G	C5-C6-O6	-5.42	125.35	128.60
36	1	1741	A	N1-C6-N6	5.42	121.85	118.60
36	1	1745	C	O5'-P-OP2	-5.42	100.83	105.70
36	5	2763	U	C2-N3-C4	-5.42	123.75	127.00
36	5	3032	A	OP1-P-O3'	5.42	117.11	105.20
36	1	1520	G	C6-C5-N7	5.42	133.65	130.40
36	1	1874	A	O5'-P-OP1	-5.42	100.83	105.70
36	5	1435	A	O5'-P-OP2	5.42	117.20	110.70
36	1	1156	C	C5-C6-N1	-5.41	118.29	121.00
36	1	1429	G	N3-C4-C5	-5.41	125.89	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3177	G	C5-C6-O6	-5.41	125.35	128.60
36	5	1533	U	N3-C2-O2	-5.41	118.41	122.20
36	5	1856	C	C5-C6-N1	5.41	123.71	121.00
36	5	2236	G	O5'-P-OP1	-5.41	100.83	105.70
36	1	430	U	N1-C2-N3	5.41	118.15	114.90
36	1	1723	A	N1-C2-N3	-5.41	126.59	129.30
36	1	1891	A	C2-N3-C4	-5.41	107.89	110.60
1	6	308	C	C5-C4-N4	5.41	123.99	120.20
36	5	3084	C	C5-C6-N1	-5.41	118.30	121.00
1	2	16	G	N3-C4-C5	-5.41	125.89	128.60
36	1	1444	G	C5-C6-O6	-5.41	125.36	128.60
36	1	1589	A	O4'-C1'-N9	-5.41	103.87	108.20
38	4	97	A	C8-N9-C4	-5.41	103.64	105.80
36	5	758	C	C5-C6-N1	-5.41	118.30	121.00
1	2	794	U	P-O3'-C3'	5.41	126.19	119.70
36	1	805	G	N7-C8-N9	-5.41	110.40	113.10
36	5	836	A	N1-C2-N3	5.41	132.00	129.30
36	5	2664	C	C5-C4-N4	-5.41	116.42	120.20
36	5	2909	U	N1-C2-O2	-5.41	119.02	122.80
1	2	1568	C	P-O3'-C3'	5.41	126.19	119.70
36	1	69	C	N3-C4-C5	-5.41	119.74	121.90
36	1	3362	A	N1-C2-N3	5.41	132.00	129.30
1	6	541	A	OP1-P-O3'	5.41	117.09	105.20
36	5	2310	U	C6-N1-C2	-5.41	117.76	121.00
36	5	2381	G	OP1-P-O3'	5.41	117.09	105.20
36	5	2531	C	C6-N1-C1'	-5.41	114.31	120.80
36	5	2978	U	O4'-C1'-N1	5.41	112.52	108.20
36	1	1838	G	C4-C5-C6	5.40	122.04	118.80
1	6	194	U	C2-N1-C1'	5.40	124.19	117.70
1	6	340	U	N1-C2-N3	5.40	118.14	114.90
36	5	2618	G	N3-C4-N9	5.40	129.24	126.00
36	5	3044	G	C8-N9-C4	-5.40	104.24	106.40
36	1	346	C	C6-N1-C2	5.40	122.46	120.30
36	1	424	G	C8-N9-C4	5.40	108.56	106.40
36	1	1164	G	O5'-P-OP1	5.40	117.18	110.70
36	1	1320	C	N3-C4-C5	-5.40	119.74	121.90
36	1	1445	U	C2-N3-C4	-5.40	123.76	127.00
1	6	454	U	C5-C6-N1	-5.40	120.00	122.70
36	5	3021	A	C2-N3-C4	5.40	113.30	110.60
36	1	1329	U	N1-C2-O2	5.40	126.58	122.80
36	1	2226	U	O5'-P-OP1	-5.40	100.84	105.70
1	6	369	A	N1-C6-N6	5.40	121.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	882	U	O5'-P-OP1	-5.40	100.84	105.70
1	6	1766	A	OP1-P-O3'	5.40	117.08	105.20
36	5	3368	U	C4-C5-C6	5.40	122.94	119.70
25	D3	133	LEU	CA-CB-CG	5.40	127.72	115.30
36	1	588	G	C5-N7-C8	5.40	107.00	104.30
36	5	1528	G	C4-N9-C1'	5.40	133.52	126.50
36	5	1724	U	N1-C2-N3	5.40	118.14	114.90
36	5	2397	A	C6-N1-C2	-5.40	115.36	118.60
36	5	3043	C	N3-C4-C5	5.40	124.06	121.90
37	7	68	C	N1-C2-O2	5.40	122.14	118.90
36	5	85	A	C8-N9-C4	5.40	107.96	105.80
1	2	1503	A	N1-C6-N6	5.39	121.84	118.60
36	1	912	G	N3-C2-N2	-5.39	116.12	119.90
36	1	1300	G	N3-C4-N9	5.39	129.24	126.00
36	1	1375	G	N1-C6-O6	5.39	123.14	119.90
36	1	1425	U	C4-C5-C6	5.39	122.94	119.70
52	M6	84	LEU	CA-CB-CG	5.39	127.70	115.30
36	5	407	A	C8-N9-C1'	-5.39	117.99	127.70
36	5	3309	G	N3-C4-C5	-5.39	125.90	128.60
54	m8	3	ILE	CB-CA-C	-5.39	100.81	111.60
36	1	821	U	N3-C4-O4	-5.39	115.62	119.40
36	1	1166	G	C8-N9-C4	5.39	108.56	106.40
36	1	2527	G	N3-C2-N2	-5.39	116.13	119.90
36	1	2712	U	N1-C2-N3	5.39	118.14	114.90
1	6	1200	G	N1-C6-O6	5.39	123.14	119.90
1	6	1726	G	OP2-P-O3'	5.39	117.06	105.20
36	5	217	U	OP1-P-O3'	5.39	117.06	105.20
36	5	676	G	N7-C8-N9	5.39	115.80	113.10
36	5	1497	C	O5'-P-OP1	-5.39	100.85	105.70
36	5	1514	G	N1-C6-O6	5.39	123.14	119.90
36	5	2377	G	N1-C6-O6	-5.39	116.66	119.90
36	5	2727	A	N1-C6-N6	-5.39	115.36	118.60
1	2	942	G	C8-N9-C4	-5.39	104.24	106.40
36	1	2295	A	N1-C6-N6	5.39	121.83	118.60
36	1	1044	U	N1-C2-N3	-5.39	111.67	114.90
36	1	1407	A	N7-C8-N9	-5.39	111.11	113.80
36	1	1443	G	C5-C6-N1	-5.39	108.81	111.50
36	1	2609	A	C8-N9-C4	5.39	107.96	105.80
38	4	54	A	C6-C5-N7	-5.39	128.53	132.30
1	6	630	A	C8-N9-C4	5.39	107.96	105.80
36	5	2931	C	N1-C2-O2	-5.39	115.67	118.90
39	12	242	ARG	NE-CZ-NH2	-5.39	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	45	A	C6-N1-C2	-5.39	115.37	118.60
36	5	767	U	O4'-C1'-N1	5.39	112.51	108.20
36	5	2157	G	O5'-P-OP1	-5.39	100.85	105.70
36	5	2264	U	O5'-P-OP2	-5.39	100.85	105.70
36	5	2889	C	N1-C2-N3	5.39	122.97	119.20
1	2	794	U	OP1-P-O3'	5.39	117.05	105.20
1	2	1600	A	P-O3'-C3'	5.39	126.16	119.70
36	1	711	A	N7-C8-N9	-5.39	111.11	113.80
36	1	861	C	N3-C4-C5	5.39	124.05	121.90
36	1	2796	G	C8-N9-C4	-5.39	104.25	106.40
36	1	2881	C	O4'-C1'-N1	5.39	112.51	108.20
36	5	838	G	C5-C6-O6	5.39	131.83	128.60
36	5	3093	C	C6-N1-C2	5.39	122.45	120.30
1	2	577	G	N3-C4-C5	5.38	131.29	128.60
1	2	1798	U	C2-N1-C1'	5.38	124.16	117.70
36	1	404	G	C5-C6-N1	-5.38	108.81	111.50
36	1	2876	C	N3-C4-C5	-5.38	119.75	121.90
36	1	2883	U	N1-C2-N3	-5.38	111.67	114.90
36	1	3269	U	C5-C4-O4	5.38	129.13	125.90
36	5	2355	G	C5-C6-O6	-5.38	125.37	128.60
37	7	26	C	O5'-P-OP2	-5.38	100.85	105.70
36	1	3081	C	C4-C5-C6	5.38	120.09	117.40
36	1	82	C	N3-C4-C5	-5.38	119.75	121.90
36	1	867	G	N3-C2-N2	-5.38	116.13	119.90
36	1	939	U	O5'-P-OP1	5.38	117.16	110.70
36	1	1172	G	O5'-P-OP1	-5.38	100.86	105.70
36	1	1838	G	C4-C5-N7	5.38	112.95	110.80
36	1	2731	U	C5-C4-O4	-5.38	122.67	125.90
36	5	1884	A	C8-N9-C4	-5.38	103.65	105.80
36	5	2651	G	OP2-P-O3'	5.38	117.04	105.20
36	5	63	A	N9-C4-C5	-5.38	103.65	105.80
36	5	327	A	C8-N9-C4	5.38	107.95	105.80
36	1	765	C	C2-N1-C1'	5.38	124.72	118.80
36	1	1414	G	C4-C5-N7	5.38	112.95	110.80
36	1	1531	C	C2-N1-C1'	5.38	124.72	118.80
36	5	691	A	N1-C6-N6	-5.38	115.37	118.60
36	5	1174	G	N3-C4-N9	5.38	129.23	126.00
36	5	2300	G	O5'-P-OP1	-5.38	100.86	105.70
41	14	230	VAL	CB-CA-C	-5.38	101.18	111.40
36	1	2137	U	N1-C2-O2	5.38	126.56	122.80
36	1	2385	G	N3-C4-C5	5.38	131.29	128.60
36	1	3044	G	N1-C6-O6	-5.38	116.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	525	C	N1-C2-O2	-5.38	115.67	118.90
36	5	3047	U	C5-C4-O4	5.38	129.13	125.90
36	5	3133	C	C6-N1-C2	-5.38	118.15	120.30
36	1	394	G	N7-C8-N9	-5.38	110.41	113.10
36	1	2714	G	O5'-P-OP1	-5.38	100.86	105.70
36	5	2253	G	O5'-P-OP2	-5.38	100.86	105.70
36	5	2798	C	C5-C4-N4	5.38	123.96	120.20
36	5	2818	U	C5'-C4'-O4'	-5.38	102.65	109.10
36	5	2889	C	C2-N3-C4	-5.38	117.21	119.90
36	1	1403	C	C5-C6-N1	-5.37	118.31	121.00
36	1	2724	U	N1-C2-N3	5.37	118.12	114.90
36	5	970	A	C8-N9-C4	5.37	107.95	105.80
36	5	1695	U	N3-C2-O2	-5.37	118.44	122.20
36	5	1876	U	C2-N3-C4	-5.37	123.78	127.00
36	1	439	C	C6-N1-C1'	-5.37	114.35	120.80
36	1	801	A	O4'-C1'-N9	-5.37	103.90	108.20
36	1	1743	G	C8-N9-C4	5.37	108.55	106.40
1	6	92	A	C2-N3-C4	-5.37	107.92	110.60
36	5	1482	A	O5'-P-OP1	5.37	117.15	110.70
36	5	2361	A	C2-N3-C4	-5.37	107.91	110.60
36	1	3382	U	C2-N1-C1'	5.37	124.14	117.70
36	5	753	C	C6-N1-C2	5.37	122.45	120.30
1	2	2	A	O4'-C1'-N9	-5.37	103.91	108.20
36	1	229	G	C5-C6-O6	-5.37	125.38	128.60
36	1	645	A	N3-C4-C5	-5.37	123.04	126.80
36	1	714	G	N1-C6-O6	5.37	123.12	119.90
36	1	2418	G	C8-N9-C1'	-5.37	120.02	127.00
1	6	44	U	N3-C2-O2	5.37	125.96	122.20
39	12	216	HIS	N-CA-C	-5.37	96.51	111.00
1	2	16	G	N3-C2-N2	5.37	123.66	119.90
36	1	658	G	N1-C6-O6	5.37	123.12	119.90
36	1	1475	A	C5-N7-C8	5.37	106.58	103.90
36	1	1733	G	C8-N9-C4	-5.37	104.25	106.40
6	S4	12	LEU	CA-CB-CG	5.37	127.64	115.30
36	1	523	A	C8-N9-C4	5.37	107.95	105.80
36	1	715	A	O5'-P-OP2	-5.37	100.87	105.70
36	1	922	U	N1-C2-O2	5.37	126.56	122.80
36	1	1800	A	C2-N3-C4	5.37	113.28	110.60
1	6	804	A	N9-C4-C5	-5.37	103.65	105.80
36	5	1203	A	C4-C5-N7	5.37	113.38	110.70
36	5	2894	C	N3-C4-C5	5.37	124.05	121.90
36	5	2933	A	C5-C6-N6	-5.37	119.41	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2991	A	C2-N3-C4	5.37	113.28	110.60
36	5	3262	U	C6-N1-C2	-5.37	117.78	121.00
38	8	45	C	C6-N1-C2	-5.37	118.15	120.30
36	1	201	A	N1-C2-N3	5.36	131.98	129.30
36	1	2883	U	C4-C5-C6	-5.36	116.48	119.70
36	5	1878	G	C8-N9-C1'	-5.36	120.03	127.00
36	5	2606	G	C5-C6-O6	5.36	131.82	128.60
1	6	101	U	N3-C2-O2	-5.36	118.45	122.20
36	5	911	C	N1-C2-O2	-5.36	115.68	118.90
36	5	2190	U	C4-C5-C6	5.36	122.92	119.70
37	7	100	C	O5'-P-OP2	-5.36	100.87	105.70
38	8	84	C	C6-N1-C2	-5.36	118.16	120.30
1	2	313	U	N1-C2-N3	5.36	118.12	114.90
1	2	499	U	C5-C4-O4	-5.36	122.68	125.90
36	1	1103	A	C4-C5-C6	-5.36	114.32	117.00
1	6	351	C	N3-C4-N4	5.36	121.75	118.00
36	5	82	C	N3-C4-C5	-5.36	119.76	121.90
36	5	1485	G	N3-C4-C5	-5.36	125.92	128.60
37	7	93	C	O5'-P-OP1	5.36	117.13	110.70
36	1	1856	C	C5-C4-N4	-5.36	116.45	120.20
36	1	2914	G	C8-N9-C4	5.36	108.54	106.40
36	1	3173	G	C5-C6-O6	-5.36	125.39	128.60
36	5	1921	A	O5'-P-OP2	-5.36	100.88	105.70
1	2	1657	U	P-O3'-C3'	5.36	126.13	119.70
1	2	1761	U	N3-C2-O2	-5.36	118.45	122.20
36	1	124	U	N1-C2-O2	5.36	126.55	122.80
36	1	398	A	C5-C6-N6	-5.36	119.41	123.70
36	1	945	C	C5-C6-N1	-5.36	118.32	121.00
36	1	2191	U	C5-C4-O4	5.36	129.11	125.90
36	1	2527	G	N3-C4-C5	5.36	131.28	128.60
36	5	2353	G	OP2-P-O3'	5.36	116.99	105.20
51	m5	99	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	2	1100	G	C4-N9-C1'	5.36	133.46	126.50
36	1	24	G	C2-N3-C4	-5.36	109.22	111.90
36	1	589	A	C5-N7-C8	5.36	106.58	103.90
36	1	2603	G	N3-C2-N2	5.36	123.65	119.90
1	6	15	U	C5-C4-O4	5.36	129.11	125.90
36	5	1319	G	C4-C5-N7	-5.36	108.66	110.80
36	5	2396	G	C5-C6-O6	-5.36	125.39	128.60
36	5	2871	G	N3-C4-C5	-5.36	125.92	128.60
36	1	1152	G	OP1-P-OP2	5.35	127.63	119.60
1	6	92	A	N9-C4-C5	-5.35	103.66	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1614	A	C6-C5-N7	-5.35	128.55	132.30
36	5	2700	G	C8-N9-C1'	-5.35	120.04	127.00
36	1	614	C	N3-C4-C5	5.35	124.04	121.90
36	1	1118	C	C6-N1-C2	-5.35	118.16	120.30
36	1	1419	A	C5-C6-N6	-5.35	119.42	123.70
36	1	2712	U	C5-C4-O4	5.35	129.11	125.90
36	5	2864	A	N1-C6-N6	5.35	121.81	118.60
36	1	1004	U	C2-N1-C1'	5.35	124.12	117.70
36	1	2874	G	C5-C6-N1	-5.35	108.82	111.50
36	5	716	A	C8-N9-C4	5.35	107.94	105.80
36	1	22	G	N3-C4-C5	-5.35	125.93	128.60
36	1	2968	G	C6-C5-N7	-5.35	127.19	130.40
36	1	3178	A	C6-C5-N7	-5.35	128.56	132.30
36	5	2173	U	C5-C4-O4	5.35	129.11	125.90
36	5	3049	A	C2-N3-C4	-5.35	107.93	110.60
1	2	1082	C	N1-C2-O2	5.35	122.11	118.90
1	2	1124	A	C2-N3-C4	-5.35	107.93	110.60
36	1	92	G	N1-C2-N2	-5.35	111.39	116.20
36	1	689	U	N1-C2-O2	-5.35	119.06	122.80
36	1	1113	G	N3-C2-N2	-5.35	116.16	119.90
36	1	1366	A	C4-C5-N7	5.35	113.37	110.70
1	6	119	A	N3-C4-C5	5.35	130.54	126.80
36	5	805	G	N7-C8-N9	-5.35	110.43	113.10
36	5	907	G	N3-C4-N9	5.35	129.21	126.00
36	5	2345	A	C6-C5-N7	-5.35	128.56	132.30
37	7	7	G	N1-C6-O6	-5.35	116.69	119.90
36	1	1604	G	C8-N9-C4	-5.35	104.26	106.40
36	5	2951	G	C8-N9-C1'	-5.35	120.05	127.00
36	5	3154	C	N3-C2-O2	-5.35	118.16	121.90
36	1	2699	G	C5-C6-O6	-5.34	125.39	128.60
36	5	1410	U	C6-N1-C2	5.34	124.21	121.00
36	5	1817	G	O4'-C1'-N9	5.34	112.48	108.20
36	5	2333	C	OP2-P-O3'	5.34	116.96	105.20
36	1	2159	U	N3-C4-C5	5.34	117.81	114.60
36	1	2295	A	C8-N9-C4	-5.34	103.66	105.80
36	1	2612	U	N3-C4-O4	-5.34	115.66	119.40
36	5	1238	C	P-O3'-C3'	5.34	126.11	119.70
36	5	1370	G	N1-C2-N3	5.34	127.11	123.90
36	5	2372	A	C2-N3-C4	5.34	113.27	110.60
1	2	1052	U	C2-N1-C1'	5.34	124.11	117.70
36	1	360	G	N3-C4-N9	5.34	129.21	126.00
36	1	1852	G	N1-C6-O6	5.34	123.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2237	C	C6-N1-C2	5.34	122.44	120.30
36	1	2395	G	N1-C6-O6	5.34	123.11	119.90
36	1	2993	G	N3-C2-N2	5.34	123.64	119.90
36	1	3101	G	N1-C6-O6	-5.34	116.69	119.90
1	6	1649	G	N3-C4-N9	5.34	129.21	126.00
36	5	1898	G	N1-C6-O6	5.34	123.11	119.90
36	5	2188	A	O5'-P-OP1	-5.34	100.89	105.70
36	5	2890	A	N1-C6-N6	5.34	121.81	118.60
36	1	859	G	C4-C5-C6	5.34	122.00	118.80
36	5	275	U	OP2-P-O3'	5.34	116.95	105.20
36	5	1112	A	C6-N1-C2	-5.34	115.40	118.60
36	1	93	C	O5'-P-OP2	-5.34	100.89	105.70
36	1	1492	G	O5'-P-OP2	-5.34	100.90	105.70
1	6	1649	G	C8-N9-C4	5.34	108.53	106.40
36	5	1143	A	N1-C2-N3	5.34	131.97	129.30
36	1	357	A	C8-N9-C4	-5.34	103.67	105.80
36	1	1000	C	C6-N1-C1'	-5.34	114.40	120.80
36	1	1144	U	N1-C2-O2	-5.34	119.06	122.80
1	6	1773	C	N3-C2-O2	5.34	125.64	121.90
36	5	51	A	N1-C6-N6	5.34	121.80	118.60
36	5	204	A	N1-C6-N6	-5.34	115.40	118.60
36	1	965	A	OP1-P-O3'	5.33	116.94	105.20
36	1	1412	G	C5-C6-N1	-5.33	108.83	111.50
36	1	1417	G	C2-N3-C4	-5.33	109.23	111.90
36	1	1440	G	C8-N9-C4	5.33	108.53	106.40
37	3	111	U	O5'-P-OP1	-5.33	100.90	105.70
36	5	821	U	C5-C6-N1	-5.33	120.03	122.70
36	5	908	G	C5-C6-O6	-5.33	125.40	128.60
36	1	1375	G	C6-C5-N7	-5.33	127.20	130.40
36	1	1655	G	C8-N9-C1'	-5.33	120.07	127.00
36	1	2802	A	OP2-P-O3'	5.33	116.93	105.20
36	1	2879	C	N3-C2-O2	5.33	125.63	121.90
36	1	3087	A	OP2-P-O3'	5.33	116.93	105.20
36	5	670	C	N1-C2-O2	-5.33	115.70	118.90
36	5	1310	G	OP1-P-O3'	5.33	116.93	105.20
36	5	3362	A	C5-C6-N1	-5.33	115.03	117.70
36	5	1116	G	C4-N9-C1'	5.33	133.43	126.50
38	8	39	G	C8-N9-C4	-5.33	104.27	106.40
36	1	198	A	C5-C6-N6	-5.33	119.44	123.70
36	1	1334	U	C6-N1-C2	-5.33	117.80	121.00
36	1	2379	U	C5-C6-N1	5.33	125.36	122.70
38	4	113	U	N1-C2-N3	5.33	118.10	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	767	U	C5-C4-O4	5.33	129.10	125.90
1	6	1602	C	N3-C2-O2	-5.33	118.17	121.90
36	5	86	G	O5'-P-OP1	5.33	117.09	110.70
36	5	2811	A	N7-C8-N9	-5.33	111.14	113.80
36	5	3197	G	C2-N3-C4	-5.33	109.23	111.90
37	7	104	A	O5'-P-OP2	-5.33	100.91	105.70
1	2	587	C	N3-C4-C5	-5.33	119.77	121.90
36	1	718	G	C8-N9-C4	-5.33	104.27	106.40
36	1	958	C	N3-C2-O2	-5.33	118.17	121.90
36	5	1866	C	O4'-C1'-N1	-5.33	103.94	108.20
36	5	2950	G	C8-N9-C4	-5.33	104.27	106.40
36	1	692	A	C4-C5-C6	5.33	119.66	117.00
36	1	845	G	OP1-P-O3'	5.33	116.92	105.20
36	1	1445	U	C2-N1-C1'	-5.33	111.31	117.70
36	1	1468	A	N1-C2-N3	5.33	131.96	129.30
36	1	3054	U	C4-C5-C6	5.33	122.90	119.70
51	M5	188	ARG	NE-CZ-NH1	-5.33	117.64	120.30
36	5	324	A	OP1-P-O3'	5.33	116.92	105.20
36	5	634	C	OP2-P-O3'	5.33	116.92	105.20
36	5	715	A	C5-C6-N1	5.33	120.36	117.70
36	5	3153	U	N3-C2-O2	-5.33	118.47	122.20
1	2	1277	G	N3-C4-N9	-5.32	122.81	126.00
36	1	1166	G	N9-C4-C5	-5.32	103.27	105.40
36	1	2411	U	C2-N3-C4	-5.32	123.81	127.00
36	1	2959	C	N1-C2-O2	-5.32	115.71	118.90
1	6	65	A	N1-C6-N6	5.32	121.80	118.60
38	8	51	G	C5-C6-O6	-5.32	125.41	128.60
36	5	1409	G	N1-C6-O6	-5.32	116.71	119.90
36	1	407	A	C5-C6-N6	-5.32	119.44	123.70
36	1	2384	A	C8-N9-C4	-5.32	103.67	105.80
36	1	3100	U	N3-C4-O4	5.32	123.12	119.40
36	5	279	U	C6-N1-C2	5.32	124.19	121.00
36	5	1158	A	N1-C6-N6	5.32	121.79	118.60
36	5	1327	C	C6-N1-C2	5.32	122.43	120.30
37	3	74	C	C6-N1-C2	5.32	122.43	120.30
36	1	922	U	C6-N1-C1'	-5.32	113.76	121.20
36	1	1203	A	N1-C6-N6	5.32	121.79	118.60
36	5	1604	G	C4-N9-C1'	5.32	133.41	126.50
36	5	1844	C	N3-C4-C5	5.32	124.03	121.90
36	1	81	C	C2-N3-C4	-5.32	117.24	119.90
36	5	1191	U	C5-C6-N1	-5.32	120.04	122.70
36	5	2642	A	N1-C6-N6	-5.32	115.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1633	A	N9-C4-C5	5.31	107.92	105.80
1	6	308	C	C4-C5-C6	5.31	120.06	117.40
1	6	1697	G	N3-C4-N9	5.31	129.19	126.00
36	5	579	G	O5'-P-OP1	5.31	117.08	110.70
36	5	1305	U	N3-C4-C5	-5.31	111.41	114.60
36	5	1903	U	C5-C6-N1	5.31	125.36	122.70
38	8	102	U	N3-C4-O4	5.31	123.12	119.40
1	2	751	G	C8-N9-C4	5.31	108.53	106.40
1	2	864	U	C5-C4-O4	5.31	129.09	125.90
36	1	1843	C	C2-N3-C4	-5.31	117.24	119.90
1	6	145	A	O4'-C1'-N9	5.31	112.45	108.20
36	1	170	G	O5'-P-OP1	-5.31	100.92	105.70
36	1	2859	U	O5'-P-OP1	-5.31	100.92	105.70
1	6	1537	C	N1-C2-O2	-5.31	115.71	118.90
36	5	1469	C	N1-C2-O2	-5.31	115.71	118.90
36	5	3229	G	N1-C6-O6	-5.31	116.71	119.90
38	8	71	A	C8-N9-C4	5.31	107.92	105.80
1	2	186	C	C5-C6-N1	5.31	123.66	121.00
36	1	1116	G	C8-N9-C4	-5.31	104.28	106.40
36	1	1389	G	N1-C6-O6	5.31	123.08	119.90
36	1	1448	U	OP2-P-O3'	5.31	116.88	105.20
1	6	1382	A	O4'-C1'-N9	5.31	112.45	108.20
1	6	1748	G	OP2-P-O3'	5.31	116.88	105.20
36	5	656	A	N9-C4-C5	-5.31	103.68	105.80
36	5	800	G	N9-C4-C5	5.31	107.52	105.40
1	2	278	U	O5'-P-OP1	-5.31	100.92	105.70
36	1	1300	G	C4-C5-N7	5.31	112.92	110.80
36	1	2153	U	C6-N1-C2	-5.31	117.82	121.00
36	1	2314	U	C6-N1-C2	5.31	124.18	121.00
1	6	1481	C	OP1-P-O3'	5.31	116.88	105.20
36	5	1878	G	N1-C6-O6	-5.31	116.72	119.90
36	1	1514	G	O5'-P-OP2	-5.31	100.92	105.70
36	1	2351	U	N1-C2-N3	5.30	118.08	114.90
1	6	1027	A	N1-C6-N6	5.30	121.78	118.60
38	8	18	U	C5-C4-O4	5.30	129.08	125.90
36	1	898	U	N1-C2-N3	-5.30	111.72	114.90
36	1	961	C	N3-C4-C5	5.30	124.02	121.90
36	1	2287	C	N1-C2-O2	-5.30	115.72	118.90
36	1	2926	A	N1-C6-N6	5.30	121.78	118.60
41	L4	313	LEU	CA-CB-CG	5.30	127.50	115.30
36	5	283	G	C4-C5-N7	5.30	112.92	110.80
36	1	371	G	C4-C5-N7	5.30	112.92	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1840	U	OP1-P-O3'	5.30	116.86	105.20
1	6	363	G	C8-N9-C4	5.30	108.52	106.40
36	5	672	A	C5-N7-C8	-5.30	101.25	103.90
36	5	1113	G	C2-N3-C4	-5.30	109.25	111.90
36	5	2391	G	C2-N3-C4	5.30	114.55	111.90
36	5	2685	C	C6-N1-C2	5.30	122.42	120.30
36	5	3058	U	C2-N1-C1'	5.30	124.06	117.70
1	2	1596	C	N3-C2-O2	-5.30	118.19	121.90
36	1	936	A	O4'-C1'-N9	5.30	112.44	108.20
36	1	2402	A	C4-C5-C6	5.30	119.65	117.00
36	1	2692	A	N1-C6-N6	5.30	121.78	118.60
36	1	2808	A	N1-C2-N3	5.30	131.95	129.30
36	5	2351	U	N3-C2-O2	-5.30	118.49	122.20
36	5	3129	A	N9-C4-C5	-5.30	103.68	105.80
36	5	3218	A	P-O3'-C3'	5.30	126.06	119.70
36	1	267	G	O4'-C1'-N9	-5.30	103.96	108.20
36	1	2249	G	C8-N9-C1'	-5.30	120.11	127.00
36	5	807	A	C6-N1-C2	-5.30	115.42	118.60
1	2	1634	C	C6-N1-C2	5.30	122.42	120.30
36	1	608	A	C5-C6-N6	-5.30	119.46	123.70
36	1	667	C	N3-C4-C5	5.30	124.02	121.90
36	1	1528	G	O5'-P-OP1	-5.30	100.93	105.70
36	1	3059	G	C8-N9-C4	5.30	108.52	106.40
36	5	31	C	C5-C4-N4	-5.30	116.49	120.20
36	5	1593	A	C5-C6-N6	-5.30	119.46	123.70
36	5	2685	C	N1-C2-O2	-5.30	115.72	118.90
37	7	103	A	C5-C6-N1	5.30	120.35	117.70
36	5	436	A	OP1-P-OP2	-5.29	111.66	119.60
36	5	1060	U	C5-C6-N1	-5.29	120.05	122.70
36	1	636	C	N3-C4-C5	5.29	124.02	121.90
36	1	933	A	C6-N1-C2	-5.29	115.42	118.60
36	1	2953	U	C5-C4-O4	-5.29	122.72	125.90
38	4	103	G	N3-C4-C5	-5.29	125.95	128.60
36	5	283	G	O4'-C1'-N9	-5.29	103.97	108.20
36	5	1344	G	N3-C4-C5	5.29	131.25	128.60
36	5	1422	G	C4-C5-N7	5.29	112.92	110.80
59	n3	48	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	2	393	C	N3-C4-C5	5.29	124.02	121.90
1	2	795	U	C4-C5-C6	5.29	122.88	119.70
1	2	1196	A	P-O3'-C3'	5.29	126.05	119.70
36	1	1726	C	N3-C4-N4	-5.29	114.30	118.00
36	1	1795	U	N3-C2-O2	-5.29	118.50	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3214	U	O4'-C1'-N1	5.29	112.43	108.20
36	5	31	C	N3-C4-C5	5.29	124.02	121.90
36	5	1119	C	C5-C6-N1	-5.29	118.35	121.00
37	7	104	A	N1-C6-N6	5.29	121.77	118.60
36	1	54	C	C5-C6-N1	-5.29	118.36	121.00
36	1	1343	A	C6-C5-N7	-5.29	128.60	132.30
36	1	2987	A	N1-C2-N3	5.29	131.94	129.30
36	5	2185	G	C2-N3-C4	-5.29	109.25	111.90
36	1	1330	A	C5-C6-N1	-5.29	115.06	117.70
36	1	1433	A	N7-C8-N9	5.29	116.44	113.80
36	1	1903	U	C2-N3-C4	5.29	130.17	127.00
36	1	3173	G	N1-C6-O6	5.29	123.07	119.90
1	6	5	U	OP2-P-O3'	5.29	116.83	105.20
36	5	416	A	OP2-P-O3'	5.29	116.84	105.20
36	5	1137	C	C6-N1-C2	5.29	122.42	120.30
36	5	1825	G	O5'-P-OP1	5.29	117.05	110.70
36	5	2829	U	C5-C6-N1	5.29	125.34	122.70
36	5	3115	C	N1-C2-N3	5.29	122.90	119.20
36	5	3195	U	OP1-P-O3'	5.29	116.83	105.20
1	2	728	U	N1-C2-O2	5.29	126.50	122.80
36	1	158	G	C6-C5-N7	-5.29	127.23	130.40
36	1	2636	A	N7-C8-N9	5.29	116.44	113.80
1	6	15	U	N1-C2-N3	5.29	118.07	114.90
1	6	369	A	O5'-P-OP2	-5.29	100.94	105.70
1	6	1747	G	N7-C8-N9	-5.29	110.46	113.10
36	5	511	G	O5'-P-OP2	-5.29	100.94	105.70
36	5	793	C	C5-C4-N4	-5.29	116.50	120.20
36	5	1174	G	C5-C6-O6	-5.29	125.43	128.60
36	5	1483	G	N1-C6-O6	-5.29	116.73	119.90
36	5	2682	C	C5-C6-N1	-5.29	118.36	121.00
1	2	619	A	N1-C6-N6	-5.28	115.43	118.60
36	1	3204	C	N3-C2-O2	-5.28	118.20	121.90
38	4	91	C	C6-N1-C2	-5.28	118.19	120.30
37	7	75	G	N1-C6-O6	5.28	123.07	119.90
38	8	25	G	O5'-P-OP2	-5.28	100.94	105.70
36	1	2298	U	C5-C6-N1	-5.28	120.06	122.70
1	6	364	G	N9-C4-C5	-5.28	103.29	105.40
36	1	1134	G	C5-C6-O6	-5.28	125.43	128.60
36	1	2594	C	O5'-P-OP2	-5.28	100.95	105.70
36	5	2283	G	N1-C6-O6	5.28	123.07	119.90
36	5	2820	A	C6-N1-C2	-5.28	115.43	118.60
38	8	26	U	OP1-P-OP2	5.28	127.52	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	357	A	C5-N7-C8	-5.28	101.26	103.90
36	1	419	G	OP2-P-O3'	5.28	116.81	105.20
36	1	423	A	N1-C2-N3	5.28	131.94	129.30
36	1	699	A	C2-N3-C4	-5.28	107.96	110.60
36	1	2887	A	C8-N9-C4	-5.28	103.69	105.80
73	O7	65	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	6	68	A	N1-C6-N6	5.28	121.77	118.60
36	5	281	G	C5-C6-O6	-5.28	125.43	128.60
1	2	622	A	C8-N9-C4	5.28	107.91	105.80
36	1	881	C	N1-C2-O2	5.28	122.07	118.90
36	1	2375	G	O4'-C1'-N9	5.28	112.42	108.20
36	1	3181	C	N1-C2-N3	5.28	122.89	119.20
36	5	201	A	C2-N3-C4	-5.28	107.96	110.60
36	5	740	G	C5-C6-N1	5.28	114.14	111.50
36	5	880	G	N7-C8-N9	-5.28	110.46	113.10
36	5	964	G	N3-C4-C5	-5.28	125.96	128.60
36	5	971	G	C5-N7-C8	5.28	106.94	104.30
36	5	1589	A	C8-N9-C4	-5.28	103.69	105.80
36	5	2121	G	C5-C6-O6	-5.28	125.43	128.60
1	2	1463	C	C6-N1-C2	5.28	122.41	120.30
36	1	398	A	N1-C6-N6	5.28	121.77	118.60
36	1	1103	A	C2-N3-C4	5.28	113.24	110.60
36	1	1194	G	N9-C4-C5	5.28	107.51	105.40
36	1	1635	G	C5-C6-O6	-5.28	125.44	128.60
1	6	454	U	C2-N1-C1'	-5.28	111.37	117.70
36	5	398	A	OP1-P-OP2	5.28	127.51	119.60
1	2	1182	U	N3-C2-O2	-5.27	118.51	122.20
36	1	883	A	O5'-P-OP2	5.27	117.03	110.70
36	5	1710	C	C5-C6-N1	-5.27	118.36	121.00
36	5	3303	G	OP1-P-OP2	5.27	127.51	119.60
36	1	689	U	C2-N3-C4	-5.27	123.84	127.00
36	1	925	A	N9-C4-C5	5.27	107.91	105.80
36	1	1429	G	C8-N9-C4	5.27	108.51	106.40
36	5	24	G	C5-C6-N1	5.27	114.14	111.50
36	5	97	U	OP2-P-O3'	5.27	116.80	105.20
36	5	668	G	C5-C6-N1	5.27	114.14	111.50
36	5	931	C	N3-C4-C5	5.27	124.01	121.90
1	2	933	A	C8-N9-C4	-5.27	103.69	105.80
36	1	2808	A	C4-C5-C6	5.27	119.64	117.00
36	1	2815	G	N9-C4-C5	-5.27	103.29	105.40
36	5	2632	G	OP1-P-O3'	5.27	116.80	105.20
36	1	940	G	C6-N1-C2	-5.27	121.94	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1693	C	N3-C4-C5	-5.27	119.79	121.90
1	6	1134	C	O5'-P-OP2	-5.27	100.96	105.70
36	5	965	A	O5'-P-OP2	-5.27	100.96	105.70
36	5	1828	A	N1-C6-N6	5.27	121.76	118.60
36	5	1847	A	O5'-P-OP2	-5.27	100.96	105.70
36	5	2818	U	P-O3'-C3'	5.27	126.02	119.70
36	1	1116	G	O4'-C1'-N9	5.27	112.41	108.20
36	1	1399	A	N3-C4-N9	-5.27	123.19	127.40
38	4	115	C	C6-N1-C2	5.27	122.41	120.30
1	6	315	A	C2-N3-C4	5.27	113.23	110.60
1	6	350	U	N1-C2-O2	-5.27	119.11	122.80
36	5	587	U	N1-C2-N3	-5.27	111.74	114.90
36	5	801	A	N1-C2-N3	5.27	131.93	129.30
36	5	981	U	C5-C6-N1	5.27	125.33	122.70
36	5	1316	C	N3-C4-C5	-5.27	119.79	121.90
1	2	647	G	N3-C2-N2	-5.26	116.21	119.90
1	2	825	U	C5-C6-N1	5.26	125.33	122.70
36	1	1131	G	C4-C5-N7	5.26	112.91	110.80
36	1	1349	G	C4-N9-C1'	5.26	133.34	126.50
36	1	3362	A	C4-C5-C6	5.26	119.63	117.00
49	M3	7	LEU	CB-CG-CD2	-5.26	102.05	111.00
36	5	971	G	OP2-P-O3'	5.26	116.78	105.20
36	5	2121	G	C4-C5-N7	5.26	112.91	110.80
36	5	3067	C	C5-C6-N1	-5.26	118.37	121.00
36	1	87	U	N3-C4-O4	5.26	123.08	119.40
36	1	2554	A	P-O3'-C3'	5.26	126.02	119.70
36	1	2772	C	O4'-C1'-N1	5.26	112.41	108.20
37	3	87	G	N9-C4-C5	-5.26	103.30	105.40
1	6	543	C	C4-C5-C6	-5.26	114.77	117.40
1	6	1165	G	OP2-P-O3'	5.26	116.78	105.20
36	5	299	G	O5'-P-OP2	-5.26	100.96	105.70
36	5	917	A	O5'-P-OP2	-5.26	100.96	105.70
36	5	2412	G	C6-N1-C2	-5.26	121.94	125.10
38	8	33	A	N1-C6-N6	5.26	121.76	118.60
1	6	1716	C	O4'-C1'-N1	5.26	112.41	108.20
36	5	1550	C	N1-C2-O2	-5.26	115.74	118.90
36	5	2296	A	C5-C6-N1	5.26	120.33	117.70
36	5	2375	G	C4-C5-N7	-5.26	108.69	110.80
36	1	24	G	C8-N9-C1'	-5.26	120.16	127.00
36	1	642	U	N3-C2-O2	-5.26	118.52	122.20
36	1	1041	U	O5'-P-OP2	-5.26	100.97	105.70
1	6	765	G	O4'-C1'-N9	-5.26	103.99	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1458	G	C4-N9-C1'	5.26	133.34	126.50
36	5	1428	A	C4-C5-C6	-5.26	114.37	117.00
36	5	1839	A	O5'-P-OP1	-5.26	100.97	105.70
36	5	2704	A	C8-N9-C4	5.26	107.90	105.80
36	1	304	G	C5-N7-C8	5.26	106.93	104.30
36	1	676	G	C4-C5-C6	5.26	121.95	118.80
36	1	912	G	N3-C4-C5	-5.26	125.97	128.60
36	1	2192	C	C5-C6-N1	-5.26	118.37	121.00
36	1	2400	G	N1-C2-N2	-5.26	111.47	116.20
36	5	349	A	O4'-C1'-N9	-5.26	104.00	108.20
36	5	404	G	O5'-P-OP2	-5.26	100.97	105.70
36	5	65	A	O5'-P-OP2	-5.25	100.97	105.70
36	5	212	G	OP1-P-O3'	5.25	116.76	105.20
36	5	645	A	C4-C5-C6	5.25	119.63	117.00
36	5	1317	A	N9-C4-C5	-5.25	103.70	105.80
36	5	1805	C	C6-N1-C2	5.25	122.40	120.30
36	5	3319	U	C6-N1-C2	-5.25	117.85	121.00
48	m1	12	LEU	CA-CB-CG	5.25	127.39	115.30
1	2	554	C	C2-N1-C1'	5.25	124.58	118.80
36	1	778	U	N3-C2-O2	-5.25	118.52	122.20
36	1	1363	A	C5-C6-N1	5.25	120.33	117.70
36	1	2611	U	O5'-P-OP1	5.25	117.00	110.70
1	6	607	G	C4-C5-C6	5.25	121.95	118.80
36	5	2379	U	C2-N3-C4	-5.25	123.85	127.00
36	5	3176	G	C4-N9-C1'	5.25	133.33	126.50
36	5	3181	C	N1-C2-O2	-5.25	115.75	118.90
36	1	930	U	N3-C4-C5	5.25	117.75	114.60
36	1	1304	A	N1-C6-N6	-5.25	115.45	118.60
36	1	2257	C	O4'-C1'-N1	5.25	112.40	108.20
36	1	2606	G	C4-C5-C6	5.25	121.95	118.80
41	L4	326	ARG	NE-CZ-NH2	-5.25	117.67	120.30
36	5	632	G	C5-N7-C8	5.25	106.92	104.30
36	5	1167	U	OP1-P-OP2	-5.25	111.72	119.60
36	5	1496	C	C6-N1-C1'	-5.25	114.50	120.80
36	5	3044	G	O4'-C1'-N9	5.25	112.40	108.20
36	1	23	A	C5-N7-C8	-5.25	101.28	103.90
36	1	148	G	C6-C5-N7	-5.25	127.25	130.40
36	1	666	A	OP1-P-O3'	5.25	116.75	105.20
36	1	2371	G	C6-C5-N7	-5.25	127.25	130.40
36	5	672	A	N3-C4-N9	5.25	131.60	127.40
1	2	408	C	N1-C2-O2	-5.25	115.75	118.90
36	1	420	G	N3-C4-C5	-5.25	125.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1178	G	C5-N7-C8	-5.25	101.68	104.30
36	5	1589	A	C5-C6-N6	-5.25	119.50	123.70
36	5	1655	G	C5-C6-O6	-5.25	125.45	128.60
36	1	798	G	N1-C2-N3	5.25	127.05	123.90
36	5	383	G	N3-C4-C5	5.25	131.22	128.60
36	5	2314	U	C2-N1-C1'	5.25	124.00	117.70
36	5	3311	C	N1-C2-O2	-5.25	115.75	118.90
36	1	2912	G	C2-N3-C4	5.25	114.52	111.90
36	5	365	A	N1-C6-N6	5.25	121.75	118.60
36	5	2597	U	N1-C2-N3	-5.25	111.75	114.90
38	8	42	G	C4-N9-C1'	-5.25	119.68	126.50
1	2	1324	G	N1-C2-N2	5.24	120.92	116.20
36	1	346	C	O5'-P-OP2	-5.24	100.98	105.70
36	1	883	A	OP1-P-OP2	-5.24	111.73	119.60
36	5	942	U	C6-N1-C2	-5.24	117.85	121.00
36	5	2144	A	OP1-P-O3'	5.24	116.74	105.20
36	5	2398	A	C5-C6-N1	5.24	120.32	117.70
36	5	2777	G	C4-C5-N7	-5.24	108.70	110.80
36	1	2243	A	C8-N9-C4	5.24	107.90	105.80
36	1	2919	A	N1-C2-N3	-5.24	126.68	129.30
1	6	1696	G	P-O3'-C3'	5.24	125.99	119.70
36	5	3059	G	C8-N9-C4	5.24	108.50	106.40
36	1	1063	G	C8-N9-C4	-5.24	104.30	106.40
36	1	1496	C	C6-N1-C2	-5.24	118.20	120.30
36	1	2139	A	N1-C6-N6	-5.24	115.46	118.60
37	3	80	G	C5-C6-N1	-5.24	108.88	111.50
36	5	941	G	OP1-P-O3'	5.24	116.73	105.20
36	5	2820	A	C5-C6-N1	5.24	120.32	117.70
36	5	2938	G	OP1-P-OP2	5.24	127.46	119.60
1	2	317	C	C5-C4-N4	-5.24	116.53	120.20
1	2	1781	A	C5-C6-N1	-5.24	115.08	117.70
36	1	1148	G	OP1-P-O3'	5.24	116.72	105.20
36	1	1305	U	N3-C2-O2	-5.24	118.53	122.20
36	1	1434	G	C2-N3-C4	5.24	114.52	111.90
36	1	1453	A	C8-N9-C4	-5.24	103.70	105.80
36	1	2763	U	C5-C4-O4	-5.24	122.76	125.90
36	5	2918	G	C8-N9-C4	5.24	108.50	106.40
1	2	334	G	N3-C4-N9	-5.24	122.86	126.00
36	1	793	C	N1-C2-O2	-5.24	115.76	118.90
36	1	1807	G	C4-N9-C1'	5.24	133.31	126.50
36	5	1159	A	C2-N3-C4	-5.24	107.98	110.60
36	5	1469	C	C4-C5-C6	5.24	120.02	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	33	G	C5-C6-N1	-5.24	108.88	111.50
36	1	590	G	N1-C6-O6	5.24	123.04	119.90
36	1	2169	G	C2-N3-C4	5.24	114.52	111.90
36	1	2216	G	C5-C6-O6	5.24	131.74	128.60
36	5	1876	U	N3-C4-O4	-5.24	115.73	119.40
36	5	2627	C	N1-C2-N3	5.24	122.86	119.20
36	5	2741	C	N1-C2-O2	-5.24	115.76	118.90
36	1	2162	U	OP1-P-OP2	5.23	127.45	119.60
36	1	2375	G	O5'-P-OP2	5.23	116.98	110.70
36	1	3241	G	N3-C4-N9	-5.23	122.86	126.00
36	5	1348	U	N3-C4-C5	-5.23	111.46	114.60
36	5	1370	G	C6-N1-C2	-5.23	121.96	125.10
36	5	2799	A	N1-C6-N6	-5.23	115.46	118.60
36	5	3343	G	N3-C2-N2	5.23	123.56	119.90
37	7	97	A	N1-C2-N3	5.23	131.92	129.30
1	2	1642	G	C6-C5-N7	-5.23	127.26	130.40
36	1	2806	U	C5-C4-O4	5.23	129.04	125.90
36	1	2899	C	C2-N1-C1'	5.23	124.56	118.80
56	N0	24	LEU	CA-CB-CG	5.23	127.34	115.30
36	5	1495	U	C2-N1-C1'	5.23	123.98	117.70
36	5	2664	C	N3-C2-O2	5.23	125.56	121.90
38	8	68	G	N1-C6-O6	5.23	123.04	119.90
42	15	75	LEU	CA-CB-CG	5.23	127.33	115.30
36	1	800	G	N3-C2-N2	-5.23	116.24	119.90
41	L4	327	LEU	CA-CB-CG	5.23	127.33	115.30
1	6	874	C	C6-N1-C1'	-5.23	114.52	120.80
38	8	26	U	N3-C2-O2	-5.23	118.54	122.20
36	1	2250	G	C8-N9-C4	5.23	108.49	106.40
36	5	876	A	OP2-P-O3'	5.23	116.70	105.20
36	5	1163	A	N1-C2-N3	5.23	131.91	129.30
36	5	1344	G	C8-N9-C4	5.23	108.49	106.40
36	5	3032	A	N1-C6-N6	-5.23	115.46	118.60
37	7	71	G	OP2-P-O3'	5.23	116.70	105.20
1	2	447	U	C5-C6-N1	5.23	125.31	122.70
36	1	2739	A	N1-C6-N6	5.23	121.74	118.60
1	6	542	A	C5-N7-C8	-5.23	101.29	103.90
36	5	959	C	O5'-P-OP1	5.23	116.97	110.70
36	5	1126	G	C5-C6-N1	-5.23	108.89	111.50
36	5	1178	G	C4-C5-N7	5.23	112.89	110.80
36	5	1364	C	OP2-P-O3'	5.23	116.70	105.20
36	5	1422	G	C5-C6-O6	-5.23	125.46	128.60
36	5	2639	G	C6-C5-N7	-5.23	127.26	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3045	G	C5-C6-O6	-5.23	125.46	128.60
36	5	3116	G	C5-C6-N1	5.23	114.11	111.50
36	1	1414	G	C5-C6-O6	-5.23	125.46	128.60
38	4	9	A	N9-C4-C5	5.23	107.89	105.80
1	6	1596	C	N3-C4-N4	-5.23	114.34	118.00
1	2	1657	U	N1-C2-O2	5.22	126.46	122.80
36	1	652	G	N3-C4-C5	-5.22	125.99	128.60
36	1	914	A	C5-C6-N6	5.22	127.88	123.70
36	1	1061	A	N1-C6-N6	5.22	121.73	118.60
36	1	1795	U	O5'-P-OP1	-5.22	101.00	105.70
36	1	2396	G	C4-C5-C6	5.22	121.94	118.80
36	1	2723	U	C2-N3-C4	-5.22	123.87	127.00
1	6	1503	A	C8-N9-C4	-5.22	103.71	105.80
36	5	410	U	N3-C4-O4	5.22	123.06	119.40
36	5	1471	U	N3-C4-O4	-5.22	115.74	119.40
36	5	2116	G	N1-C6-O6	5.22	123.03	119.90
36	5	2886	U	C4-C5-C6	5.22	122.83	119.70
36	1	806	A	N9-C4-C5	-5.22	103.71	105.80
36	1	928	C	N1-C2-N3	5.22	122.86	119.20
57	N1	89	LEU	CA-CB-CG	5.22	127.31	115.30
1	6	418	G	C4-C5-N7	5.22	112.89	110.80
36	5	694	C	C6-N1-C2	-5.22	118.21	120.30
36	5	2246	G	C2-N3-C4	5.22	114.51	111.90
36	5	2375	G	O4'-C1'-N9	5.22	112.38	108.20
36	5	2838	A	O5'-P-OP1	5.22	116.97	110.70
36	5	2869	U	C5-C4-O4	5.22	129.03	125.90
36	1	878	G	C5-C6-N1	-5.22	108.89	111.50
36	5	889	U	C2-N3-C4	-5.22	123.87	127.00
36	5	2777	G	C5-C6-O6	5.22	131.73	128.60
36	5	2801	A	N1-C6-N6	-5.22	115.47	118.60
36	1	325	A	C5-C6-N1	5.22	120.31	117.70
36	1	573	C	C2-N3-C4	-5.22	117.29	119.90
36	1	582	G	N3-C4-N9	-5.22	122.87	126.00
36	1	994	G	N3-C2-N2	5.22	123.55	119.90
36	1	1331	U	O4'-C1'-N1	-5.22	104.02	108.20
36	5	3035	A	N7-C8-N9	-5.22	111.19	113.80
36	5	3244	A	C2-N3-C4	-5.22	107.99	110.60
52	m6	84	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	2	44	U	N1-C2-O2	-5.22	119.15	122.80
36	5	984	G	N3-C4-C5	-5.22	125.99	128.60
1	2	453	U	C6-N1-C1'	-5.22	113.90	121.20
36	1	2145	A	C5-C6-N6	-5.22	119.53	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3256	G	N1-C6-O6	5.22	123.03	119.90
1	6	1093	A	C8-N9-C4	-5.22	103.71	105.80
1	6	1129	U	C2-N1-C1'	-5.22	111.44	117.70
36	5	1331	U	C6-N1-C2	5.22	124.13	121.00
36	5	1339	C	N3-C4-C5	-5.22	119.81	121.90
36	5	3335	A	N1-C6-N6	5.22	121.73	118.60
38	8	4	C	N3-C4-N4	-5.22	114.35	118.00
1	2	73	U	P-O3'-C3'	5.21	125.96	119.70
1	2	992	A	N3-C4-C5	5.21	130.45	126.80
1	2	1107	G	C5-C6-N1	-5.21	108.89	111.50
36	1	656	A	C4-C5-C6	5.21	119.61	117.00
36	1	663	C	N3-C4-N4	5.21	121.65	118.00
36	1	2192	C	O5'-P-OP2	-5.21	101.01	105.70
36	1	2739	A	C5-C6-N6	-5.21	119.53	123.70
38	4	78	G	N3-C4-N9	5.21	129.13	126.00
1	6	112	A	C8-N9-C4	5.21	107.89	105.80
1	6	514	G	C8-N9-C4	5.21	108.48	106.40
1	6	1658	G	C8-N9-C4	5.21	108.49	106.40
36	5	1316	C	C5-C4-N4	-5.21	116.55	120.20
36	5	1545	A	C6-C5-N7	-5.21	128.65	132.30
36	5	2364	G	N3-C4-N9	-5.21	122.87	126.00
36	5	2625	C	C5-C4-N4	-5.21	116.55	120.20
36	5	3198	U	N1-C2-O2	5.21	126.45	122.80
1	2	1673	G	C6-C5-N7	-5.21	127.27	130.40
1	6	982	U	C5-C6-N1	-5.21	120.09	122.70
1	6	1560	U	O5'-P-OP1	-5.21	101.01	105.70
36	5	589	A	C8-N9-C4	5.21	107.89	105.80
36	5	2875	U	OP2-P-O3'	-5.21	93.73	105.20
36	1	1385	C	C6-N1-C2	5.21	122.38	120.30
36	1	2800	G	N1-C2-N3	5.21	127.03	123.90
1	6	542	A	P-O3'-C3'	5.21	125.95	119.70
1	6	542	A	C4-N9-C1'	5.21	135.68	126.30
1	6	1458	G	C8-N9-C1'	-5.21	120.22	127.00
1	6	1532	U	C5-C6-N1	-5.21	120.09	122.70
36	5	2421	U	N1-C2-O2	-5.21	119.15	122.80
36	1	942	U	OP1-P-OP2	-5.21	111.78	119.60
1	2	115	G	O5'-P-OP2	-5.21	101.01	105.70
35	SM	134	ASP	CB-CG-OD2	5.21	122.99	118.30
36	1	185	C	N1-C2-N3	5.21	122.85	119.20
36	1	635	G	C6-C5-N7	-5.21	127.28	130.40
36	1	1296	C	N1-C2-N3	5.21	122.84	119.20
36	1	1334	U	C4-C5-C6	5.21	122.83	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2623	G	N3-C2-N2	5.21	123.55	119.90
1	6	901	G	N7-C8-N9	5.21	115.70	113.10
1	6	1767	G	N3-C4-C5	5.21	131.20	128.60
36	5	1685	C	N1-C2-O2	5.21	122.03	118.90
36	5	2800	G	C5-C6-O6	-5.21	125.47	128.60
36	5	2978	U	N3-C2-O2	-5.21	118.55	122.20
36	1	283	G	O4'-C1'-N9	-5.21	104.03	108.20
36	1	701	G	C4-C5-C6	5.21	121.92	118.80
36	1	2403	G	O5'-P-OP1	5.21	116.95	110.70
36	1	2537	U	P-O3'-C3'	5.21	125.95	119.70
38	4	12	A	N1-C2-N3	-5.21	126.70	129.30
1	6	804	A	C8-N9-C4	5.21	107.88	105.80
36	5	630	A	N9-C4-C5	-5.21	103.72	105.80
36	5	931	C	C2-N3-C4	-5.21	117.30	119.90
36	5	2579	G	N3-C4-C5	-5.21	126.00	128.60
36	5	2636	A	O5'-P-OP2	5.21	116.95	110.70
64	n8	46	ASP	N-CA-C	-5.21	96.94	111.00
36	1	2621	G	N9-C4-C5	5.21	107.48	105.40
36	5	395	A	C5-C6-N6	-5.21	119.54	123.70
1	2	250	C	O5'-P-OP1	-5.20	101.02	105.70
36	1	206	G	C5-C6-N1	5.20	114.10	111.50
36	1	1154	A	C6-N1-C2	-5.20	115.48	118.60
36	1	1269	U	N3-C2-O2	-5.20	118.56	122.20
36	1	2956	A	N1-C6-N6	5.20	121.72	118.60
37	3	81	U	N1-C2-O2	5.20	126.44	122.80
1	6	1653	C	N3-C4-C5	-5.20	119.82	121.90
36	5	1870	C	C5-C4-N4	-5.20	116.56	120.20
36	5	2763	U	N3-C4-C5	5.20	117.72	114.60
56	n0	113	ARG	NE-CZ-NH1	-5.20	117.70	120.30
36	1	355	A	C8-N9-C4	5.20	107.88	105.80
36	1	1060	U	C6-N1-C2	5.20	124.12	121.00
36	1	1165	A	N1-C6-N6	5.20	121.72	118.60
36	1	1351	U	C5-C6-N1	5.20	125.30	122.70
36	5	630	A	N1-C2-N3	5.20	131.90	129.30
1	2	145	A	N7-C8-N9	5.20	116.40	113.80
36	1	794	U	N3-C2-O2	5.20	125.84	122.20
36	1	816	A	N9-C4-C5	5.20	107.88	105.80
36	1	921	A	O4'-C1'-N9	-5.20	104.04	108.20
36	1	2136	C	N1-C2-O2	-5.20	115.78	118.90
36	1	2380	U	N3-C4-C5	5.20	117.72	114.60
36	5	884	A	C5-N7-C8	-5.20	101.30	103.90
36	5	968	G	C8-N9-C4	5.20	108.48	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1083	G	OP1-P-OP2	5.20	127.40	119.60
36	5	1171	G	OP1-P-OP2	-5.20	111.80	119.60
36	5	3244	A	O4'-C1'-N9	-5.20	104.04	108.20
36	5	3287	U	C6-N1-C2	-5.20	117.88	121.00
36	1	22	G	C5-C6-O6	-5.20	125.48	128.60
36	1	424	G	O5'-P-OP2	-5.20	101.02	105.70
36	1	830	A	O5'-P-OP1	-5.20	101.02	105.70
37	3	108	A	O5'-P-OP1	-5.20	101.02	105.70
36	5	610	G	C4-C5-N7	-5.20	108.72	110.80
36	5	2723	U	N1-C2-N3	5.20	118.02	114.90
38	8	19	C	N1-C2-O2	-5.20	115.78	118.90
1	2	396	G	N3-C4-C5	5.20	131.20	128.60
1	2	1164	G	C5-C6-O6	-5.20	125.48	128.60
36	1	1207	G	N3-C4-N9	5.20	129.12	126.00
36	1	1392	G	N3-C4-C5	-5.20	126.00	128.60
36	5	2425	G	N3-C4-N9	-5.20	122.88	126.00
1	2	1777	G	C6-C5-N7	-5.20	127.28	130.40
36	1	190	U	C2-N1-C1'	-5.20	111.47	117.70
36	1	815	G	C4-N9-C1'	5.20	133.25	126.50
36	1	861	C	O5'-P-OP1	5.20	116.94	110.70
36	1	1386	A	C4-C5-C6	5.20	119.60	117.00
59	n3	45	ARG	NE-CZ-NH1	-5.20	117.70	120.30
36	1	2916	U	N1-C2-O2	5.19	126.44	122.80
1	6	163	G	C8-N9-C4	-5.19	104.32	106.40
36	5	2381	G	C2-N3-C4	5.19	114.50	111.90
36	5	3003	G	C5-C6-N1	5.19	114.10	111.50
36	1	83	U	C5-C4-O4	-5.19	122.78	125.90
36	1	1849	C	N1-C2-O2	-5.19	115.78	118.90
36	1	2355	G	N3-C2-N2	-5.19	116.27	119.90
36	1	2551	U	C2-N1-C1'	5.19	123.93	117.70
1	6	1596	C	N3-C2-O2	-5.19	118.27	121.90
36	5	1149	G	N3-C4-C5	-5.19	126.00	128.60
36	5	1424	C	N1-C2-O2	-5.19	115.78	118.90
36	5	2867	C	N1-C2-O2	-5.19	115.78	118.90
36	5	3225	C	N1-C2-O2	5.19	122.02	118.90
1	2	1650	U	C5-C6-N1	-5.19	120.11	122.70
36	1	2612	U	C2-N3-C4	-5.19	123.89	127.00
36	5	104	G	C5-C6-O6	-5.19	125.49	128.60
36	5	1304	A	OP1-P-OP2	5.19	127.39	119.60
36	5	1431	G	C2-N3-C4	5.19	114.50	111.90
1	6	536	C	C6-N1-C2	-5.19	118.22	120.30
36	5	1056	U	OP2-P-O3'	5.19	116.62	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2887	A	C4-C5-C6	5.19	119.59	117.00
1	2	1100	G	N3-C4-N9	5.19	129.11	126.00
36	1	2151	C	N3-C2-O2	5.19	125.53	121.90
36	1	2358	A	N1-C2-N3	5.19	131.89	129.30
36	1	2915	U	C2-N3-C4	-5.19	123.89	127.00
37	3	86	U	C2-N3-C4	-5.19	123.89	127.00
36	5	538	G	C5-C6-N1	-5.19	108.91	111.50
36	5	648	C	OP1-P-OP2	5.19	127.38	119.60
36	5	903	U	OP1-P-O3'	5.19	116.61	105.20
36	5	1329	U	N1-C2-O2	-5.19	119.17	122.80
36	5	2394	G	C6-C5-N7	-5.19	127.29	130.40
1	2	1744	A	N1-C2-N3	5.19	131.89	129.30
1	6	884	A	C8-N9-C4	5.19	107.87	105.80
36	5	1285	G	C8-N9-C4	5.19	108.47	106.40
36	1	1371	G	C5-C6-O6	-5.18	125.49	128.60
36	1	1857	C	N1-C2-O2	-5.18	115.79	118.90
36	1	2541	U	P-O3'-C3'	5.18	125.92	119.70
68	O2	66	LEU	CB-CG-CD1	-5.18	102.19	111.00
36	5	831	G	C2-N3-C4	5.18	114.49	111.90
36	5	883	A	N1-C2-N3	5.18	131.89	129.30
36	5	1738	C	N1-C2-O2	-5.18	115.79	118.90
36	5	2345	A	N3-C4-N9	5.18	131.55	127.40
36	5	2615	G	C2-N3-C4	-5.18	109.31	111.90
36	5	3008	A	N1-C2-N3	5.18	131.89	129.30
36	5	3098	G	O5'-P-OP2	-5.18	101.03	105.70
36	5	3141	A	OP1-P-OP2	5.18	127.38	119.60
1	2	1486	G	C6-C5-N7	-5.18	127.29	130.40
36	1	205	C	C6-N1-C2	5.18	122.37	120.30
36	1	231	G	N9-C4-C5	5.18	107.47	105.40
36	1	1480	G	N1-C6-O6	5.18	123.01	119.90
1	6	565	C	C6-N1-C1'	-5.18	114.58	120.80
36	5	1306	G	C8-N9-C1'	-5.18	120.26	127.00
36	5	1413	G	C5-C6-N1	5.18	114.09	111.50
36	5	2761	G	N1-C6-O6	5.18	123.01	119.90
36	1	1394	A	C4-C5-C6	-5.18	114.41	117.00
38	4	66	A	C4-C5-C6	5.18	119.59	117.00
1	2	4	C	O5'-P-OP1	-5.18	101.04	105.70
36	1	2412	G	N3-C4-C5	-5.18	126.01	128.60
36	1	2710	C	N1-C2-O2	-5.18	115.79	118.90
36	5	1476	G	C5-C6-O6	5.18	131.71	128.60
1	2	971	A	C4-C5-C6	5.18	119.59	117.00
36	1	210	U	O5'-P-OP1	5.18	116.91	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	M6	28	LEU	CB-CG-CD1	-5.18	102.20	111.00
1	6	435	C	C6-N1-C1'	-5.18	114.59	120.80
36	5	424	G	C8-N9-C4	5.18	108.47	106.40
36	5	1400	G	N3-C4-C5	-5.18	126.01	128.60
36	5	1495	U	N3-C4-C5	-5.18	111.49	114.60
36	1	396	A	C8-N9-C4	-5.17	103.73	105.80
36	1	635	G	N3-C4-C5	-5.17	126.01	128.60
36	5	963	G	N3-C2-N2	5.17	123.52	119.90
36	5	1646	G	C5-C6-O6	-5.17	125.50	128.60
36	5	1757	A	C8-N9-C4	-5.17	103.73	105.80
1	2	730	G	C4-N9-C1'	5.17	133.22	126.50
36	1	757	C	C2-N1-C1'	-5.17	113.11	118.80
36	1	3361	G	N1-C2-N2	-5.17	111.55	116.20
36	1	1131	G	C6-C5-N7	-5.17	127.30	130.40
36	1	2801	A	C8-N9-C4	5.17	107.87	105.80
37	3	82	G	C6-N1-C2	-5.17	122.00	125.10
47	M0	21	ARG	NE-CZ-NH1	-5.17	117.71	120.30
36	5	1116	G	OP2-P-O3'	5.17	116.58	105.20
36	5	1848	G	O4'-C1'-N9	5.17	112.34	108.20
36	5	2556	C	N1-C2-O2	5.17	122.00	118.90
36	5	3074	G	C2-N3-C4	5.17	114.49	111.90
37	7	73	C	N3-C4-N4	5.17	121.62	118.00
36	1	994	G	OP1-P-O3'	5.17	116.57	105.20
36	5	1329	U	C3'-C2'-C1'	5.17	105.64	101.50
36	5	2932	U	C5-C6-N1	-5.17	120.11	122.70
1	2	426	G	C8-N9-C1'	-5.17	120.28	127.00
36	1	3205	G	C2-N3-C4	-5.17	109.31	111.90
36	5	1314	C	C2-N1-C1'	5.17	124.48	118.80
36	5	2380	U	O5'-P-OP2	-5.17	101.05	105.70
36	1	97	U	OP2-P-O3'	5.17	116.56	105.20
36	1	635	G	N3-C4-N9	5.17	129.10	126.00
36	1	1049	C	N3-C4-C5	5.17	123.97	121.90
36	1	2416	U	N3-C4-C5	-5.17	111.50	114.60
36	1	3362	A	C4-N9-C1'	5.17	135.60	126.30
1	6	1119	G	N3-C4-C5	-5.17	126.02	128.60
36	5	2878	G	C5-C6-N1	5.17	114.08	111.50
36	5	3177	G	C8-N9-C4	5.17	108.47	106.40
36	1	2871	G	C2-N3-C4	5.17	114.48	111.90
46	L9	31	ARG	NE-CZ-NH1	-5.17	117.72	120.30
36	1	847	A	C5-C6-N6	-5.16	119.57	123.70
36	1	1461	A	N1-C6-N6	5.16	121.70	118.60
36	1	2314	U	O5'-P-OP1	5.16	116.90	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2870	C	N3-C4-C5	5.16	123.97	121.90
36	1	2952	G	N9-C4-C5	-5.16	103.33	105.40
36	1	3303	G	O4'-C1'-N9	5.16	112.33	108.20
1	6	1775	U	C2-N3-C4	-5.16	123.90	127.00
36	5	1861	G	C8-N9-C4	-5.16	104.33	106.40
37	7	51	A	C5-N7-C8	-5.16	101.32	103.90
36	1	1886	A	N1-C6-N6	-5.16	115.50	118.60
36	5	1534	A	C8-N9-C1'	-5.16	118.41	127.70
38	8	5	U	C5-C4-O4	-5.16	122.80	125.90
38	8	45	C	N3-C4-C5	-5.16	119.84	121.90
1	2	1740	A	N9-C4-C5	-5.16	103.74	105.80
36	1	887	G	N3-C4-N9	5.16	129.10	126.00
36	1	2782	U	C5-C6-N1	-5.16	120.12	122.70
1	6	151	G	N3-C4-C5	5.16	131.18	128.60
36	5	2895	G	N1-C6-O6	5.16	123.00	119.90
36	5	704	U	N3-C2-O2	5.16	125.81	122.20
36	1	398	A	N9-C4-C5	-5.16	103.74	105.80
36	1	439	C	N3-C2-O2	-5.16	118.29	121.90
36	1	1869	C	C2-N3-C4	5.16	122.48	119.90
36	5	1304	A	C8-N9-C4	-5.16	103.74	105.80
36	5	1730	G	O5'-P-OP1	-5.16	101.06	105.70
36	5	1865	A	C2-N3-C4	-5.16	108.02	110.60
36	5	2396	G	C8-N9-C4	-5.16	104.34	106.40
36	5	2861	U	O5'-P-OP2	5.16	116.89	110.70
1	2	1782	A	N9-C4-C5	5.15	107.86	105.80
36	1	2177	G	N1-C2-N2	-5.15	111.56	116.20
36	1	1325	U	P-O3'-C3'	-5.15	113.52	119.70
38	4	107	G	N7-C8-N9	-5.15	110.52	113.10
1	6	25	C	OP2-P-O3'	5.15	116.54	105.20
1	6	163	G	C4-N9-C1'	-5.15	119.80	126.50
1	6	1674	C	N3-C2-O2	5.15	125.51	121.90
36	5	804	C	C5-C6-N1	-5.15	118.42	121.00
37	7	39	C	C2-N1-C1'	5.15	124.47	118.80
36	1	397	A	N9-C4-C5	5.15	107.86	105.80
36	1	2369	G	N3-C4-C5	-5.15	126.03	128.60
38	4	99	C	C6-N1-C2	5.15	122.36	120.30
36	5	354	U	C6-N1-C1'	-5.15	113.99	121.20
36	5	1184	A	C5-C6-N6	5.15	127.82	123.70
36	5	1866	C	C2-N1-C1'	5.15	124.47	118.80
36	5	2385	G	C5-C6-N1	-5.15	108.92	111.50
36	5	2820	A	C8-N9-C4	-5.15	103.74	105.80
1	2	139	C	P-O3'-C3'	5.15	125.88	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	874	U	O5'-P-OP1	-5.15	101.07	105.70
41	L4	98	ARG	NE-CZ-NH2	5.15	122.87	120.30
36	5	2950	G	C6-C5-N7	-5.15	127.31	130.40
36	1	878	G	N1-C2-N2	-5.15	111.57	116.20
36	1	1371	G	N3-C4-N9	5.15	129.09	126.00
36	1	1399	A	N3-C4-C5	5.15	130.40	126.80
36	1	2625	C	C2-N3-C4	-5.15	117.33	119.90
36	5	323	A	OP1-P-O3'	5.15	116.52	105.20
36	5	805	G	C5-C6-O6	-5.15	125.51	128.60
36	5	2613	U	OP1-P-O3'	5.15	116.52	105.20
36	5	3368	U	N1-C2-O2	-5.15	119.20	122.80
36	1	984	G	N1-C2-N2	-5.14	111.57	116.20
36	1	2153	U	N1-C2-N3	5.14	117.99	114.90
1	6	578	U	C5-C6-N1	-5.14	120.13	122.70
1	6	1346	A	O4'-C1'-N9	5.14	112.32	108.20
1	6	1354	G	C4-N9-C1'	5.14	133.19	126.50
36	5	225	C	N1-C2-O2	-5.14	115.81	118.90
36	5	2721	A	O5'-P-OP1	-5.14	101.07	105.70
36	5	3153	U	C2-N1-C1'	5.14	123.87	117.70
36	1	332	C	C5-C6-N1	-5.14	118.43	121.00
36	1	395	A	N9-C4-C5	5.14	107.86	105.80
36	1	900	G	C4-C5-N7	-5.14	108.74	110.80
36	1	1194	G	C8-N9-C4	-5.14	104.34	106.40
36	1	2400	G	N1-C6-O6	5.14	122.98	119.90
36	5	1117	G	N3-C4-C5	5.14	131.17	128.60
36	5	1298	C	N1-C2-O2	-5.14	115.81	118.90
36	5	1662	G	N1-C6-O6	5.14	122.99	119.90
36	1	2114	C	O5'-P-OP2	-5.14	101.07	105.70
1	6	29	U	C4-C5-C6	5.14	122.78	119.70
36	5	963	G	N1-C6-O6	-5.14	116.81	119.90
36	5	1075	A	C8-N9-C4	5.14	107.86	105.80
73	O7	5	THR	C-N-CD	5.14	139.19	128.40
36	5	806	A	C8-N9-C4	5.14	107.86	105.80
36	5	806	A	N3-C4-C5	5.14	130.40	126.80
36	5	935	U	N3-C4-O4	5.14	123.00	119.40
36	5	1885	U	C5-C6-N1	-5.14	120.13	122.70
36	5	3105	U	C2-N1-C1'	-5.14	111.53	117.70
1	2	409	C	N1-C2-O2	-5.14	115.82	118.90
36	1	3207	U	C6-N1-C1'	5.14	128.39	121.20
38	4	31	G	N1-C6-O6	5.14	122.98	119.90
36	1	1103	A	P-O3'-C3'	5.14	125.86	119.70
36	1	2298	U	O4'-C1'-N1	5.14	112.31	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2873	U	N1-C2-N3	5.14	117.98	114.90
36	5	394	G	C5-C6-O6	5.14	131.68	128.60
36	5	1226	G	C5-C6-O6	-5.14	125.52	128.60
36	5	1456	A	OP1-P-O3'	5.14	116.50	105.20
36	5	1483	G	C6-C5-N7	5.14	133.48	130.40
36	5	2145	A	N3-C4-C5	-5.14	123.20	126.80
36	5	2617	U	C6-N1-C2	-5.14	117.92	121.00
36	5	2940	A	C6-N1-C2	-5.14	115.52	118.60
36	1	364	G	N1-C2-N3	-5.13	120.82	123.90
36	1	609	G	C5-C6-N1	5.13	114.07	111.50
36	1	632	G	N9-C4-C5	-5.13	103.35	105.40
36	1	1316	C	N3-C4-C5	-5.13	119.85	121.90
36	1	2891	U	C5-C4-O4	-5.13	122.82	125.90
1	6	1758	U	C2-N1-C1'	5.13	123.86	117.70
36	5	2950	G	C5-C6-O6	-5.13	125.52	128.60
36	5	2263	C	C5-C6-N1	5.13	123.57	121.00
1	2	1096	C	N3-C2-O2	-5.13	118.31	121.90
36	1	639	G	N3-C4-N9	5.13	129.08	126.00
36	1	971	G	C5-C6-N1	5.13	114.07	111.50
36	1	2860	U	O5'-P-OP1	5.13	116.86	110.70
1	6	280	U	N1-C2-O2	5.13	126.39	122.80
36	5	35	A	C4-C5-C6	5.13	119.57	117.00
36	5	1214	U	C6-N1-C2	-5.13	117.92	121.00
36	1	249	U	C6-N1-C2	-5.13	117.92	121.00
36	1	1436	U	N1-C2-O2	-5.13	119.21	122.80
36	1	3362	A	C4-C5-N7	5.13	113.27	110.70
36	5	3099	C	C6-N1-C1'	5.13	126.95	120.80
1	2	616	G	C4-C5-N7	-5.13	108.75	110.80
36	1	2728	G	O5'-P-OP1	-5.13	101.08	105.70
1	6	1162	C	C6-N1-C2	-5.13	118.25	120.30
1	6	1615	C	N1-C2-O2	-5.13	115.82	118.90
36	5	636	C	C5-C6-N1	-5.13	118.44	121.00
36	5	1187	C	OP2-P-O3'	5.13	116.48	105.20
36	5	1214	U	N3-C4-O4	5.13	122.99	119.40
36	5	1437	C	C6-N1-C2	-5.13	118.25	120.30
36	5	1848	G	OP2-P-O3'	5.13	116.48	105.20
36	5	3370	A	C2-N3-C4	5.13	113.16	110.60
1	2	1345	A	O5'-P-OP2	-5.13	101.09	105.70
1	2	1389	C	N1-C2-O2	5.13	121.98	118.90
41	L4	316	ASN	C-N-CD	5.13	139.17	128.40
1	6	937	C	N3-C4-C5	-5.13	119.85	121.90
36	5	1667	A	N9-C4-C5	-5.13	103.75	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2191	U	C5-C4-O4	5.13	128.98	125.90
36	5	2920	U	C2-N3-C4	-5.13	123.92	127.00
38	8	2	A	C5-N7-C8	-5.13	101.34	103.90
36	1	1133	A	N9-C4-C5	-5.12	103.75	105.80
1	6	359	A	N3-C4-N9	-5.12	123.30	127.40
36	5	655	C	C2-N3-C4	-5.12	117.34	119.90
1	2	323	A	N7-C8-N9	5.12	116.36	113.80
36	1	21	G	C5-C6-O6	5.12	131.67	128.60
36	1	1414	G	C6-C5-N7	-5.12	127.33	130.40
36	1	2847	A	C5-C6-N6	-5.12	119.60	123.70
36	1	3298	C	C6-N1-C2	5.12	122.35	120.30
36	5	2968	G	O4'-C1'-N9	-5.12	104.10	108.20
1	2	1274	C	C6-N1-C1'	-5.12	114.65	120.80
36	1	1146	C	C6-N1-C2	5.12	122.35	120.30
36	1	2385	G	O5'-P-OP2	-5.12	101.09	105.70
36	1	2773	C	OP1-P-OP2	5.12	127.28	119.60
36	1	2966	G	N9-C4-C5	-5.12	103.35	105.40
37	3	82	G	C6-C5-N7	-5.12	127.33	130.40
36	5	27	C	C2-N1-C1'	-5.12	113.17	118.80
36	5	403	C	OP2-P-O3'	5.12	116.47	105.20
36	5	2405	C	N3-C4-C5	-5.12	119.85	121.90
38	8	90	U	N1-C2-N3	-5.12	111.83	114.90
36	1	1556	C	C6-N1-C1'	-5.12	114.66	120.80
36	1	2177	G	N1-C6-O6	-5.12	116.83	119.90
36	1	2871	G	C5-C6-N1	5.12	114.06	111.50
36	5	704	U	N1-C2-O2	-5.12	119.22	122.80
1	2	570	A	C5-C6-N6	-5.12	119.61	123.70
36	1	98	G	C8-N9-C4	5.12	108.45	106.40
36	1	1486	G	C5-C6-O6	-5.12	125.53	128.60
36	1	1877	U	N3-C2-O2	5.12	125.78	122.20
36	1	2705	A	OP2-P-O3'	5.12	116.46	105.20
36	1	2710	C	N3-C4-C5	5.12	123.95	121.90
36	5	1319	G	C5-N7-C8	5.12	106.86	104.30
36	5	2393	G	O5'-P-OP2	-5.12	101.09	105.70
37	7	12	U	C5-C4-O4	-5.12	122.83	125.90
37	7	75	G	C6-C5-N7	-5.12	127.33	130.40
36	1	1180	A	C2-N3-C4	-5.12	108.04	110.60
36	1	2351	U	C6-N1-C2	-5.12	117.93	121.00
36	5	639	G	N9-C1'-C2'	-5.12	106.37	112.00
36	5	1386	A	OP1-P-OP2	5.12	127.28	119.60
61	n5	34	LEU	CA-CB-CG	5.12	127.07	115.30
38	4	95	G	C4-N9-C1'	-5.12	119.85	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	251	A	C8-N9-C4	5.12	107.85	105.80
1	6	1615	C	C3'-C2'-C1'	5.12	105.59	101.50
36	5	934	G	N1-C6-O6	5.12	122.97	119.90
36	5	2816	G	C6-N1-C2	-5.12	122.03	125.10
1	2	590	C	C6-N1-C2	-5.11	118.25	120.30
36	1	1190	A	C4-N9-C1'	5.11	135.50	126.30
36	1	2200	U	N3-C4-O4	5.11	122.98	119.40
1	6	426	G	C5-C6-O6	5.11	131.67	128.60
36	5	250	U	C5-C6-N1	5.11	125.26	122.70
36	5	512	U	N1-C2-N3	5.11	117.97	114.90
36	1	1790	G	N3-C2-N2	-5.11	116.32	119.90
36	1	2165	G	OP1-P-OP2	5.11	127.27	119.60
36	1	2586	G	N1-C6-O6	-5.11	116.83	119.90
68	O2	27	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	6	901	G	C6-C5-N7	-5.11	127.33	130.40
1	6	1744	A	C5-C6-N6	-5.11	119.61	123.70
36	1	612	U	C5-C6-N1	-5.11	120.14	122.70
36	1	1858	A	N7-C8-N9	5.11	116.36	113.80
37	3	39	C	OP1-P-OP2	5.11	127.27	119.60
36	5	635	G	C2-N3-C4	-5.11	109.34	111.90
36	5	1534	A	N1-C6-N6	5.11	121.67	118.60
36	5	1897	G	N7-C8-N9	5.11	115.66	113.10
36	1	48	A	O4'-C1'-N9	5.11	112.29	108.20
36	1	1405	U	C2-N3-C4	-5.11	123.94	127.00
46	L9	41	ILE	N-CA-C	5.11	124.79	111.00
1	6	1767	G	C4-N9-C1'	-5.11	119.86	126.50
36	5	2121	G	N3-C4-N9	5.11	129.06	126.00
36	5	3245	A	C4-C5-C6	5.11	119.55	117.00
1	2	158	U	P-O3'-C3'	5.11	125.83	119.70
36	1	1340	G	N9-C4-C5	-5.11	103.36	105.40
36	1	1556	C	C5-C6-N1	5.11	123.55	121.00
36	1	1654	A	C8-N9-C4	5.11	107.84	105.80
36	1	2949	U	C6-N1-C2	5.11	124.06	121.00
1	6	915	A	C8-N9-C4	-5.11	103.76	105.80
36	5	561	C	C2-N3-C4	5.11	122.45	119.90
36	5	916	G	O5'-P-OP1	-5.11	101.10	105.70
36	5	2198	A	C6-N1-C2	-5.11	115.53	118.60
36	1	282	G	N1-C6-O6	-5.11	116.84	119.90
36	1	999	G	C8-N9-C4	5.11	108.44	106.40
36	5	2848	G	C5-C6-N1	-5.11	108.95	111.50
36	1	676	G	N1-C6-O6	5.10	122.96	119.90
36	1	2572	C	C5-C6-N1	5.10	123.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	3	82	G	C8-N9-C1'	-5.10	120.36	127.00
36	5	1540	U	N3-C2-O2	-5.10	118.63	122.20
36	5	2338	C	N3-C4-N4	5.10	121.57	118.00
36	5	2805	G	C8-N9-C4	5.10	108.44	106.40
36	5	3378	C	C2-N3-C4	-5.10	117.35	119.90
1	2	142	G	N1-C6-O6	5.10	122.96	119.90
1	2	1465	C	C4-C5-C6	5.10	119.95	117.40
36	1	901	G	C5-C6-O6	-5.10	125.54	128.60
36	1	937	G	O5'-P-OP2	-5.10	101.11	105.70
36	1	1334	U	N3-C4-O4	5.10	122.97	119.40
36	1	2290	C	N3-C4-C5	-5.10	119.86	121.90
1	6	187	G	P-O3'-C3'	5.10	125.82	119.70
36	5	1113	G	N1-C6-O6	5.10	122.96	119.90
36	5	1902	G	O5'-P-OP2	5.10	116.82	110.70
36	5	2296	A	N7-C8-N9	5.10	116.35	113.80
36	5	2372	A	OP1-P-OP2	5.10	127.25	119.60
36	5	2395	G	OP2-P-O3'	5.10	116.43	105.20
36	5	3195	U	N1-C2-O2	5.10	126.37	122.80
37	7	32	U	C5-C4-O4	-5.10	122.84	125.90
36	1	1386	A	N1-C6-N6	5.10	121.66	118.60
36	5	2616	C	N1-C2-O2	-5.10	115.84	118.90
36	1	935	U	C4-C5-C6	5.10	122.76	119.70
36	1	1395	G	N7-C8-N9	-5.10	110.55	113.10
36	1	2343	C	C2-N3-C4	-5.10	117.35	119.90
1	6	1185	U	N1-C2-O2	5.10	126.37	122.80
9	s7	141	ARG	NE-CZ-NH1	5.10	122.85	120.30
36	5	112	U	C2-N1-C1'	5.10	123.82	117.70
36	5	768	C	C6-N1-C2	-5.10	118.26	120.30
36	5	878	G	C6-C5-N7	-5.10	127.34	130.40
36	5	2320	A	C2-N3-C4	-5.10	108.05	110.60
38	8	114	G	O5'-P-OP1	-5.10	101.11	105.70
1	2	992	A	O4'-C1'-N9	5.10	112.28	108.20
36	1	1056	U	C6-N1-C2	-5.10	117.94	121.00
36	1	1827	C	C6-N1-C2	5.10	122.34	120.30
36	1	2914	G	N7-C8-N9	-5.10	110.55	113.10
36	1	2986	U	C6-N1-C2	-5.10	117.94	121.00
1	6	347	G	N3-C4-C5	-5.10	126.05	128.60
36	5	2980	U	N1-C2-N3	5.10	117.96	114.90
36	5	3323	A	C2-N3-C4	-5.10	108.05	110.60
1	6	639	U	N3-C4-O4	-5.10	115.83	119.40
36	5	354	U	C2-N1-C1'	5.10	123.82	117.70
36	5	2725	U	C4-C5-C6	-5.10	116.64	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	969	C	N3-C4-C5	5.09	123.94	121.90
36	1	3140	G	C5-C6-O6	-5.09	125.54	128.60
64	N8	9	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	6	598	U	N1-C2-N3	5.09	117.96	114.90
36	5	61	A	C2-N3-C4	-5.09	108.05	110.60
36	5	358	G	C5-C6-O6	-5.09	125.54	128.60
36	5	682	U	O5'-P-OP1	-5.09	101.11	105.70
38	8	90	U	C6-N1-C1'	-5.09	114.07	121.20
36	1	949	C	N3-C4-C5	-5.09	119.86	121.90
36	1	3121	U	OP1-P-O3'	5.09	116.41	105.20
36	5	3039	C	C4-C5-C6	5.09	119.95	117.40
36	1	1124	U	OP1-P-O3'	5.09	116.40	105.20
36	1	1386	A	C6-C5-N7	-5.09	128.74	132.30
36	1	2749	G	N3-C4-C5	5.09	131.15	128.60
1	6	314	C	N3-C4-N4	5.09	121.56	118.00
1	6	943	C	O5'-P-OP1	-5.09	101.12	105.70
36	5	659	G	OP2-P-O3'	5.09	116.40	105.20
36	5	883	A	C2-N3-C4	-5.09	108.06	110.60
36	5	1872	C	N3-C4-N4	-5.09	114.44	118.00
36	5	2419	A	C5-N7-C8	-5.09	101.35	103.90
36	5	2728	G	C8-N9-C4	-5.09	104.36	106.40
36	5	3080	G	N1-C6-O6	5.09	122.95	119.90
36	5	3243	A	C4-C5-C6	5.09	119.55	117.00
1	2	1458	G	C8-N9-C1'	-5.09	120.39	127.00
36	1	297	G	N1-C6-O6	-5.09	116.85	119.90
36	1	2785	A	C8-N9-C4	5.09	107.84	105.80
36	1	3055	U	C5-C4-O4	-5.09	122.85	125.90
1	6	1000	C	C4-C5-C6	5.09	119.94	117.40
36	5	405	U	C5-C4-O4	-5.09	122.85	125.90
36	5	638	C	C6-N1-C2	-5.09	118.26	120.30
36	5	923	C	C6-N1-C1'	-5.09	114.69	120.80
36	5	1199	C	O5'-P-OP2	-5.09	101.12	105.70
36	5	3287	U	N1-C2-O2	5.09	126.36	122.80
1	2	74	U	O5'-P-OP1	-5.09	101.12	105.70
36	1	159	A	C2-N3-C4	-5.09	108.06	110.60
36	1	500	C	C4-C5-C6	5.09	119.94	117.40
36	1	3264	G	N7-C8-N9	-5.09	110.56	113.10
36	5	574	U	C2-N1-C1'	-5.09	111.59	117.70
1	2	1324	G	N9-C4-C5	5.09	107.43	105.40
15	C3	22	ALA	C-N-CA	5.09	143.36	122.00
36	1	939	U	C2-N3-C4	-5.09	123.95	127.00
36	1	2295	A	N7-C8-N9	5.09	116.34	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	102	C	N3-C4-N4	5.09	121.56	118.00
36	5	893	C	N1-C2-O2	5.09	121.95	118.90
36	5	1373	A	N9-C4-C5	-5.09	103.77	105.80
36	5	3137	C	C6-N1-C1'	5.09	126.90	120.80
36	1	1445	U	OP2-P-O3'	5.08	116.39	105.20
38	4	121	U	C5-C4-O4	5.08	128.95	125.90
1	6	116	U	N3-C4-O4	5.08	122.96	119.40
1	2	118	U	C5-C6-N1	-5.08	120.16	122.70
1	2	1633	A	C8-N9-C4	-5.08	103.77	105.80
1	2	1755	A	N1-C6-N6	5.08	121.65	118.60
36	1	2712	U	N3-C4-O4	-5.08	115.84	119.40
1	6	403	G	C2-N3-C4	-5.08	109.36	111.90
1	6	965	U	N3-C2-O2	-5.08	118.64	122.20
36	5	366	A	OP1-P-O3'	5.08	116.39	105.20
36	5	1389	G	C6-C5-N7	-5.08	127.35	130.40
36	5	2813	A	C6-C5-N7	-5.08	128.74	132.30
1	2	1462	G	C4-C5-N7	5.08	112.83	110.80
36	1	1480	G	C6-C5-N7	-5.08	127.35	130.40
36	1	2249	G	N9-C4-C5	-5.08	103.37	105.40
1	6	435	C	N3-C2-O2	-5.08	118.34	121.90
1	6	557	G	P-O3'-C3'	5.08	125.80	119.70
36	5	1407	A	C6-N1-C2	5.08	121.65	118.60
36	5	1837	U	N3-C4-O4	5.08	122.96	119.40
36	5	2884	C	C4-C5-C6	-5.08	114.86	117.40
1	2	1272	U	OP2-P-O3'	5.08	116.37	105.20
36	1	69	C	N1-C2-O2	-5.08	115.85	118.90
36	1	217	U	OP1-P-OP2	5.08	127.22	119.60
36	1	757	C	N3-C2-O2	5.08	125.45	121.90
1	6	392	G	C5-C6-O6	-5.08	125.55	128.60
1	6	1267	G	C8-N9-C4	5.08	108.43	106.40
36	5	631	U	C5-C6-N1	-5.08	120.16	122.70
36	5	1130	A	OP1-P-OP2	5.08	127.22	119.60
36	5	1226	G	C6-C5-N7	-5.08	127.35	130.40
36	5	2647	A	C6-N1-C2	-5.08	115.55	118.60
1	6	1119	G	N1-C6-O6	-5.08	116.85	119.90
36	5	567	G	C5-C6-O6	-5.08	125.55	128.60
1	2	830	U	C2-N1-C1'	5.08	123.79	117.70
36	1	712	G	OP1-P-OP2	5.08	127.21	119.60
36	1	3206	C	C2-N1-C1'	-5.08	113.22	118.80
36	5	1480	G	P-O3'-C3'	-5.08	113.61	119.70
36	5	2330	C	O5'-P-OP2	-5.08	101.13	105.70
36	1	906	A	N3-C4-C5	-5.07	123.25	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1313	G	C5-N7-C8	-5.07	101.76	104.30
36	1	1444	G	N1-C6-O6	5.07	122.94	119.90
1	6	199	G	O4'-C1'-N9	5.07	112.26	108.20
36	5	2818	U	C4-C5-C6	-5.07	116.66	119.70
36	5	2859	U	N1-C2-O2	-5.07	119.25	122.80
36	5	2900	A	N1-C6-N6	-5.07	115.56	118.60
37	7	39	C	N3-C4-N4	5.07	121.55	118.00
38	8	20	U	N1-C2-O2	-5.07	119.25	122.80
1	2	1174	C	N1-C2-O2	5.07	121.94	118.90
36	1	898	U	C2-N1-C1'	5.07	123.79	117.70
36	1	1053	A	C8-N9-C4	5.07	107.83	105.80
36	1	1906	G	C5-C6-O6	-5.07	125.56	128.60
36	5	2128	C	C2-N1-C1'	5.07	124.38	118.80
68	o2	47	ARG	NE-CZ-NH1	5.07	122.84	120.30
36	1	785	G	C2-N3-C4	5.07	114.44	111.90
36	1	2805	G	C8-N9-C4	5.07	108.43	106.40
36	1	2987	A	C8-N9-C1'	-5.07	118.57	127.70
38	4	82	U	C6-N1-C2	-5.07	117.96	121.00
1	6	1636	C	N3-C4-N4	5.07	121.55	118.00
36	5	964	G	N7-C8-N9	5.07	115.64	113.10
36	5	2398	A	C6-N1-C2	-5.07	115.56	118.60
36	5	2877	G	C5-N7-C8	5.07	106.83	104.30
36	1	100	A	C2-N3-C4	-5.07	108.07	110.60
36	1	520	U	N1-C2-O2	-5.07	119.25	122.80
36	1	1328	C	N1-C2-O2	-5.07	115.86	118.90
36	1	1420	C	C5-C4-N4	5.07	123.75	120.20
36	1	277	G	C2-N3-C4	5.07	114.43	111.90
36	1	1133	A	C8-N9-C4	5.07	107.83	105.80
36	1	1507	G	C4-N9-C1'	5.07	133.09	126.50
36	1	2314	U	O5'-P-OP2	-5.07	101.14	105.70
68	O2	47	ARG	NE-CZ-NH1	-5.07	117.77	120.30
11	s9	116	LEU	CA-CB-CG	-5.07	103.64	115.30
36	5	991	G	C2-N3-C4	5.07	114.43	111.90
36	5	1004	U	C5-C6-N1	5.07	125.23	122.70
36	1	292	U	N1-C2-O2	-5.07	119.25	122.80
36	1	1126	G	N1-C6-O6	5.07	122.94	119.90
36	1	3205	G	N1-C2-N2	-5.07	111.64	116.20
38	4	20	U	N3-C4-C5	5.07	117.64	114.60
38	4	115	C	N3-C4-C5	5.07	123.93	121.90
1	6	1133	A	O5'-P-OP2	5.07	116.78	110.70
36	5	170	G	C4-N9-C1'	5.07	133.09	126.50
36	5	353	G	O5'-P-OP1	-5.07	101.14	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2297	U	C2-N1-C1'	-5.07	111.62	117.70
36	5	2829	U	N3-C4-O4	5.07	122.95	119.40
1	6	1097	U	P-O3'-C3'	5.06	125.78	119.70
36	5	3296	A	OP2-P-O3'	5.06	116.34	105.20
36	1	87	U	C6-N1-C2	-5.06	117.96	121.00
36	1	1578	C	C6-N1-C2	-5.06	118.28	120.30
36	1	2920	U	C6-N1-C2	5.06	124.04	121.00
36	1	2961	G	N1-C6-O6	5.06	122.94	119.90
1	6	1013	A	C4-C5-N7	5.06	113.23	110.70
36	5	971	G	C6-N1-C2	-5.06	122.06	125.10
36	5	3172	A	C2-N3-C4	-5.06	108.07	110.60
1	2	1241	G	C5-N7-C8	-5.06	101.77	104.30
1	2	1675	C	N3-C2-O2	-5.06	118.36	121.90
36	1	201	A	C5-C6-N1	-5.06	115.17	117.70
36	1	498	A	O5'-P-OP1	5.06	116.77	110.70
36	1	703	G	N9-C4-C5	5.06	107.42	105.40
36	1	2866	U	OP1-P-O3'	5.06	116.33	105.20
36	5	2626	A	OP1-P-OP2	-5.06	112.01	119.60
36	5	2880	U	C6-N1-C2	-5.06	117.96	121.00
36	1	326	U	N3-C4-C5	-5.06	111.56	114.60
36	1	573	C	C5-C6-N1	-5.06	118.47	121.00
36	1	648	C	C2-N1-C1'	5.06	124.36	118.80
36	1	1113	G	C6-C5-N7	-5.06	127.36	130.40
36	1	1456	A	OP1-P-O3'	5.06	116.33	105.20
36	1	1838	G	C4-N9-C1'	5.06	133.08	126.50
36	1	2165	G	O5'-P-OP2	-5.06	101.15	105.70
36	1	2435	G	C2-N3-C4	-5.06	109.37	111.90
36	1	2999	U	C2-N1-C1'	-5.06	111.63	117.70
1	6	1648	A	N9-C4-C5	-5.06	103.78	105.80
36	5	1226	G	C4-C5-N7	5.06	112.82	110.80
36	5	3022	G	O5'-P-OP1	-5.06	101.15	105.70
1	2	1431	C	C6-N1-C2	5.06	122.32	120.30
36	1	357	A	N7-C8-N9	5.06	116.33	113.80
36	1	588	G	N3-C4-C5	-5.06	126.07	128.60
38	8	6	U	C6-N1-C2	5.06	124.03	121.00
36	5	2146	C	O5'-P-OP2	-5.06	101.15	105.70
36	1	54	C	C5-C4-N4	-5.05	116.66	120.20
36	1	1166	G	C6-C5-N7	-5.05	127.37	130.40
36	1	2800	G	O5'-P-OP1	5.05	116.77	110.70
36	1	2870	C	O5'-P-OP2	-5.05	101.15	105.70
37	3	81	U	N3-C2-O2	-5.05	118.66	122.20
1	6	976	G	N1-C2-N2	-5.05	111.65	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1748	G	C5-C6-O6	-5.05	125.57	128.60
36	5	833	G	C5-C6-O6	-5.05	125.57	128.60
36	5	949	C	C2-N3-C4	-5.05	117.37	119.90
36	5	1312	C	N3-C4-C5	-5.05	119.88	121.90
36	5	2342	U	OP2-P-O3'	5.05	116.32	105.20
36	5	2948	C	N3-C4-C5	5.05	123.92	121.90
36	1	2995	A	C5-C6-N1	-5.05	115.17	117.70
36	1	3101	G	C8-N9-C4	5.05	108.42	106.40
36	5	2697	A	C6-C5-N7	-5.05	128.76	132.30
36	5	2984	C	C6-N1-C2	5.05	122.32	120.30
36	5	3309	G	N3-C4-N9	5.05	129.03	126.00
1	2	169	A	C5-C6-N6	-5.05	119.66	123.70
1	2	969	C	C6-N1-C2	5.05	122.32	120.30
36	1	1192	C	C2-N3-C4	5.05	122.42	119.90
36	1	2167	A	OP2-P-O3'	5.05	116.31	105.20
36	1	2227	C	C4-C5-C6	5.05	119.92	117.40
36	1	2376	G	C5-N7-C8	-5.05	101.77	104.30
36	5	1379	G	C6-C5-N7	-5.05	127.37	130.40
36	5	1409	G	N3-C4-C5	-5.05	126.07	128.60
1	2	1611	A	N1-C2-N3	5.05	131.82	129.30
36	1	1001	G	C8-N9-C1'	-5.05	120.44	127.00
36	1	2378	C	C2-N3-C4	-5.05	117.38	119.90
36	1	2880	U	C5-C6-N1	5.05	125.22	122.70
36	5	2605	G	OP2-P-O3'	5.05	116.31	105.20
36	5	2979	U	C2-N1-C1'	-5.05	111.64	117.70
36	1	3079	U	C5-C6-N1	-5.05	120.18	122.70
1	6	1022	C	N3-C2-O2	5.05	125.43	121.90
36	5	1634	G	C8-N9-C4	5.05	108.42	106.40
1	2	499	U	C3'-C2'-C1'	5.05	105.54	101.50
36	1	632	G	OP2-P-O3'	5.05	116.30	105.20
36	1	1174	G	C8-N9-C1'	-5.05	120.44	127.00
36	1	2391	G	C6-N1-C2	-5.05	122.07	125.10
36	5	336	A	N1-C6-N6	-5.05	115.57	118.60
36	5	3382	U	C5-C6-N1	5.05	125.22	122.70
38	8	2	A	C8-N9-C4	-5.05	103.78	105.80
36	1	1310	G	N1-C6-O6	-5.04	116.87	119.90
36	1	2401	A	C8-N9-C4	-5.04	103.78	105.80
37	3	67	G	C8-N9-C4	5.04	108.42	106.40
1	6	435	C	C2-N1-C1'	5.04	124.35	118.80
1	6	616	G	N9-C4-C5	5.04	107.42	105.40
36	5	1766	G	C8-N9-C4	-5.04	104.38	106.40
1	2	359	A	N1-C2-N3	-5.04	126.78	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	794	U	N1-C2-O2	5.04	126.33	122.80
36	1	999	G	O5'-P-OP2	5.04	116.75	110.70
36	1	1307	G	N3-C4-N9	-5.04	122.97	126.00
36	1	1355	A	P-O3'-C3'	5.04	125.75	119.70
36	1	2179	C	N1-C2-O2	5.04	121.92	118.90
36	1	2873	U	N3-C4-O4	-5.04	115.87	119.40
36	1	2954	U	C6-N1-C2	5.04	124.02	121.00
36	1	3275	U	C6-N1-C2	-5.04	117.97	121.00
36	5	834	U	C4-C5-C6	-5.04	116.67	119.70
36	5	1466	G	C8-N9-C4	5.04	108.42	106.40
36	5	1941	C	N3-C2-O2	5.04	125.43	121.90
36	1	320	G	N1-C6-O6	5.04	122.92	119.90
36	1	2723	U	N3-C4-C5	5.04	117.62	114.60
36	5	696	C	N3-C4-N4	5.04	121.53	118.00
56	n0	13	ARG	NE-CZ-NH2	-5.04	117.78	120.30
36	1	665	A	C5-C6-N1	5.04	120.22	117.70
36	1	916	G	P-O3'-C3'	5.04	125.75	119.70
36	1	1429	G	C4-N9-C1'	5.04	133.05	126.50
36	1	1480	G	N3-C2-N2	5.04	123.43	119.90
36	1	2612	U	N3-C4-C5	5.04	117.62	114.60
1	6	100	A	C8-N9-C4	5.04	107.82	105.80
36	5	1083	G	N9-C4-C5	5.04	107.42	105.40
36	5	1302	A	OP1-P-OP2	-5.04	112.04	119.60
36	5	2366	C	C2-N1-C1'	5.04	124.34	118.80
36	5	2645	G	C4-C5-N7	-5.04	108.78	110.80
38	8	3	A	N1-C6-N6	-5.04	115.58	118.60
36	1	1002	A	C8-N9-C4	5.04	107.81	105.80
36	5	1387	G	N3-C4-N9	-5.04	122.98	126.00
36	5	2145	A	C4-C5-C6	5.04	119.52	117.00
36	5	2215	A	C2-N3-C4	-5.04	108.08	110.60
37	7	12	U	C4-C5-C6	-5.04	116.68	119.70
36	1	788	C	C6-N1-C1'	5.04	126.84	120.80
36	1	1139	G	C5-C6-N1	-5.04	108.98	111.50
36	1	1836	C	N1-C2-O2	5.04	121.92	118.90
36	1	1903	U	O5'-P-OP1	-5.04	101.17	105.70
37	3	84	A	C5-C6-N6	-5.04	119.67	123.70
36	5	189	G	N1-C6-O6	-5.04	116.88	119.90
36	5	2386	A	N1-C2-N3	5.04	131.82	129.30
36	5	3167	A	C8-N9-C4	-5.04	103.78	105.80
36	1	910	G	C4-C5-C6	5.03	121.82	118.80
36	1	2763	U	N3-C2-O2	5.03	125.72	122.20
36	5	938	C	C6-N1-C1'	-5.03	114.76	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1214	U	C5-C6-N1	5.03	125.22	122.70
36	5	2296	A	O5'-P-OP1	-5.03	101.17	105.70
37	7	5	G	N1-C2-N3	5.03	126.92	123.90
36	1	3174	A	C5-N7-C8	-5.03	101.38	103.90
1	2	1536	G	C4-N9-C1'	5.03	133.04	126.50
36	1	79	U	N1-C2-O2	-5.03	119.28	122.80
36	1	859	G	N1-C6-O6	5.03	122.92	119.90
36	1	898	U	C6-N1-C1'	-5.03	114.16	121.20
38	4	47	C	C6-N1-C2	5.03	122.31	120.30
1	6	959	U	O4'-C1'-N1	-5.03	104.17	108.20
36	5	73	C	C5-C4-N4	-5.03	116.68	120.20
36	5	337	G	C4-C5-N7	-5.03	108.79	110.80
36	5	716	A	N9-C4-C5	-5.03	103.79	105.80
36	5	1306	G	N1-C2-N3	5.03	126.92	123.90
36	5	2689	A	N3-C4-N9	5.03	131.43	127.40
50	m4	74	ARG	NE-CZ-NH2	-5.03	117.78	120.30
36	1	1507	G	C4-C5-C6	5.03	121.82	118.80
36	1	2985	C	N1-C2-O2	-5.03	115.88	118.90
36	5	1493	G	O4'-C1'-N9	5.03	112.22	108.20
36	5	1662	G	C5-C6-N1	-5.03	108.99	111.50
36	5	2222	A	OP2-P-O3'	5.03	116.26	105.20
36	5	2393	G	N3-C4-N9	5.03	129.02	126.00
1	2	75	U	C6-N1-C1'	-5.03	114.16	121.20
1	2	1339	C	C2-N1-C1'	5.03	124.33	118.80
36	1	89	A	C6-N1-C2	-5.03	115.58	118.60
38	4	35	C	OP1-P-OP2	-5.03	112.06	119.60
38	4	125	U	O4'-C1'-N1	5.03	112.22	108.20
62	N6	75	ARG	NE-CZ-NH1	-5.03	117.79	120.30
36	5	348	A	N9-C4-C5	-5.03	103.79	105.80
36	5	407	A	C4-N9-C1'	5.03	135.34	126.30
36	5	758	C	N3-C4-N4	-5.03	114.48	118.00
36	5	912	G	C5-C6-N1	5.03	114.01	111.50
36	5	1438	U	N3-C4-O4	5.03	122.92	119.40
36	5	2426	U	N1-C2-O2	5.03	126.32	122.80
36	5	2754	G	N3-C2-N2	5.03	123.42	119.90
36	5	2860	U	OP1-P-OP2	5.03	127.14	119.60
36	5	3214	U	N1-C2-O2	5.03	126.32	122.80
36	1	973	A	N1-C2-N3	5.02	131.81	129.30
36	5	34	A	OP2-P-O3'	5.02	116.25	105.20
36	5	190	U	O4'-C1'-N1	5.02	112.22	108.20
36	5	1115	G	P-O3'-C3'	5.02	125.73	119.70
36	5	2371	G	N1-C2-N2	-5.02	111.68	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	150	U	O5'-P-OP1	-5.02	101.18	105.70
1	2	1740	A	C5-C6-N6	-5.02	119.68	123.70
36	1	1431	G	C4-C5-N7	-5.02	108.79	110.80
38	4	74	U	C2-N3-C4	-5.02	123.99	127.00
44	L7	129	LEU	CB-CG-CD2	-5.02	102.46	111.00
51	M5	96	ARG	NE-CZ-NH1	5.02	122.81	120.30
36	5	878	G	N3-C4-C5	-5.02	126.09	128.60
36	5	2212	C	C5-C6-N1	5.02	123.51	121.00
44	17	229	PHE	CB-CG-CD2	-5.02	117.28	120.80
1	6	119	A	N1-C6-N6	5.02	121.61	118.60
36	5	343	U	N3-C4-C5	-5.02	111.59	114.60
36	5	796	U	C6-N1-C2	-5.02	117.99	121.00
36	5	2932	U	C6-N1-C1'	-5.02	114.17	121.20
1	2	389	G	C5-C6-O6	-5.02	125.59	128.60
36	1	1384	U	OP2-P-O3'	5.02	116.24	105.20
36	1	2197	C	N1-C2-N3	-5.02	115.69	119.20
36	1	2824	G	C8-N9-C4	5.02	108.41	106.40
36	5	437	G	N7-C8-N9	5.02	115.61	113.10
36	5	1306	G	C4-N9-C1'	5.02	133.02	126.50
36	1	2607	G	O5'-P-OP2	-5.02	101.18	105.70
36	1	2823	G	C4-C5-N7	-5.02	108.79	110.80
36	1	3111	U	C6-N1-C2	5.02	124.01	121.00
1	6	1503	A	C5-N7-C8	-5.02	101.39	103.90
36	5	341	G	N3-C4-N9	-5.02	122.99	126.00
36	5	2632	G	C5-C6-O6	5.02	131.61	128.60
36	5	2792	A	C4-C5-C6	5.02	119.51	117.00
36	5	3351	U	N1-C2-O2	5.02	126.31	122.80
36	1	2772	C	C3'-C2'-C1'	-5.02	97.49	101.50
36	1	1322	U	N3-C2-O2	5.01	125.71	122.20
36	1	3201	C	C4-C5-C6	5.01	119.91	117.40
38	4	136	G	C5-C6-O6	-5.01	125.59	128.60
1	6	1140	G	C5-C6-O6	-5.01	125.59	128.60
36	5	1447	G	N3-C4-C5	-5.01	126.09	128.60
36	5	2257	C	C6-N1-C2	-5.01	118.29	120.30
36	5	2266	U	N3-C2-O2	-5.01	118.69	122.20
36	5	3362	A	OP2-P-O3'	5.01	116.23	105.20
37	7	27	A	C6-N1-C2	-5.01	115.59	118.60
1	2	57	G	O5'-P-OP2	-5.01	101.19	105.70
36	1	814	U	C2-N3-C4	5.01	130.01	127.00
36	5	637	C	O5'-P-OP1	-5.01	101.19	105.70
36	5	1481	A	O5'-P-OP2	-5.01	101.19	105.70
36	5	2303	A	C2-N3-C4	-5.01	108.09	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	90	U	C6-N1-C2	5.01	124.01	121.00
1	2	44	U	C2-N3-C4	-5.01	123.99	127.00
36	1	2247	G	N3-C2-N2	-5.01	116.39	119.90
36	1	2687	G	C5-C6-O6	5.01	131.61	128.60
36	1	2779	A	C8-N9-C4	5.01	107.80	105.80
1	6	1743	U	N3-C4-C5	-5.01	111.59	114.60
20	c8	116	LEU	CA-CB-CG	5.01	126.83	115.30
36	5	1184	A	C6-C5-N7	5.01	135.81	132.30
36	5	1452	A	N9-C4-C5	-5.01	103.80	105.80
36	5	2615	G	N1-C2-N3	5.01	126.91	123.90
36	5	2625	C	OP1-P-O3'	5.01	116.22	105.20
36	5	2675	C	O5'-P-OP1	-5.01	101.19	105.70
36	1	1128	U	C2-N3-C4	-5.01	123.99	127.00
36	1	1176	C	N1-C2-O2	-5.01	115.89	118.90
36	1	2904	U	O5'-P-OP1	5.01	116.71	110.70
1	6	371	G	N3-C4-C5	-5.01	126.10	128.60
36	5	716	A	N1-C6-N6	5.01	121.61	118.60
36	5	1316	C	N3-C2-O2	5.01	125.41	121.90
37	7	10	C	C6-N1-C2	5.01	122.30	120.30
1	2	310	C	C6-N1-C2	-5.01	118.30	120.30
1	2	777	C	N1-C2-O2	5.01	121.91	118.90
36	1	720	A	C5-C6-N6	-5.01	119.69	123.70
1	6	1614	A	C5-C6-N1	-5.01	115.20	117.70
36	1	407	A	C4-C5-N7	5.01	113.20	110.70
36	1	887	G	N3-C4-C5	-5.01	126.10	128.60
36	1	1109	U	C2-N3-C4	5.01	130.00	127.00
36	1	1393	A	C2-N3-C4	5.01	113.10	110.60
36	1	2914	G	C5-N7-C8	5.01	106.80	104.30
1	6	430	G	N1-C6-O6	-5.01	116.90	119.90
36	5	1316	C	C4-C5-C6	5.01	119.90	117.40
36	5	2606	G	N1-C6-O6	-5.01	116.90	119.90
36	5	2931	C	C2-N1-C1'	-5.01	113.29	118.80
36	5	3080	G	C6-C5-N7	-5.01	127.40	130.40
36	5	3231	U	C5-C4-O4	5.01	128.90	125.90
1	2	1745	G	C6-C5-N7	-5.00	127.40	130.40
36	1	1392	G	C5-C6-N1	5.00	114.00	111.50
36	1	2125	A	C8-N9-C4	5.00	107.80	105.80
36	1	2606	G	C5-C6-O6	-5.00	125.60	128.60
36	1	2980	U	N1-C2-N3	5.00	117.90	114.90
1	6	15	U	C6-N1-C2	-5.00	118.00	121.00
1	6	1113	A	N1-C2-N3	5.00	131.80	129.30
36	5	2945	G	O5'-P-OP1	-5.00	101.20	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2968	G	N7-C8-N9	-5.00	110.60	113.10
36	1	31	C	C2-N3-C4	-5.00	117.40	119.90
36	1	1670	C	C6-N1-C2	5.00	122.30	120.30
1	6	1119	G	C8-N9-C4	-5.00	104.40	106.40
36	5	2357	A	C8-N9-C4	5.00	107.80	105.80
37	7	85	G	OP1-P-OP2	-5.00	112.10	119.60

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
16	C4	38	THR	Peptide
18	C6	113	ASP	Peptide
19	C7	85	VAL	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
27	D5	96	SER	Peptide
28	D6	85	ARG	Peptide
39	L2	19	HIS	Peptide
46	L9	189	GLU	Peptide
48	M1	8	PRO	Peptide
52	M6	110	PRO	Peptide
56	N0	22	PRO	Peptide
57	N1	16	GLN	Peptide
64	N8	30	GLY	Peptide
64	N8	54	GLY	Peptide
65	N9	19	ASN	Peptide
67	O1	5	LYS	Peptide
7	S5	44	ASN	Peptide
9	S7	131	PHE	Peptide
9	S7	31	SER	Peptide
10	S8	147	ALA	Peptide
16	c4	124	ASP	Peptide
17	c5	52	LYS	Peptide
18	c6	40	GLU	Peptide
24	d2	54	ASP	Peptide
26	d4	59	GLY	Peptide
80	e0	51	ASN	Peptide
39	l2	143	GLU	Peptide
39	l2	212	GLY	Peptide

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Mol	Chain	Res	Type	Group
39	l2	215	ASN	Peptide
39	l2	247	ARG	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
82	m2	29	UNK	Peptide
52	m6	110	PRO	Peptide
56	n0	133	ALA	Peptide
59	n3	136	VAL	Peptide
64	n8	18	GLY	Peptide
64	n8	26	ARG	Peptide
64	n8	66	ALA	Peptide
2	s0	72	ASP	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide
9	s7	130	VAL	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%)	148 (72%)	39 (19%)	17 (8%)	1	5
2	s0	204/251 (81%)	148 (72%)	32 (16%)	24 (12%)	0	2
3	S1	212/254 (84%)	149 (70%)	34 (16%)	29 (14%)	0	1
3	s1	214/254 (84%)	178 (83%)	23 (11%)	13 (6%)	1	12
4	S2	215/253 (85%)	178 (83%)	26 (12%)	11 (5%)	2	15
4	s2	215/253 (85%)	169 (79%)	30 (14%)	16 (7%)	1	7
5	S3	221/239 (92%)	173 (78%)	28 (13%)	20 (9%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	s3	221/239 (92%)	176 (80%)	29 (13%)	16 (7%)	1	7
6	S4	258/260 (99%)	203 (79%)	38 (15%)	17 (7%)	1	9
6	s4	258/260 (99%)	209 (81%)	29 (11%)	20 (8%)	1	6
7	S5	204/224 (91%)	155 (76%)	28 (14%)	21 (10%)	0	3
7	s5	204/224 (91%)	156 (76%)	26 (13%)	22 (11%)	0	2
8	S6	224/236 (95%)	191 (85%)	22 (10%)	11 (5%)	2	17
8	s6	216/236 (92%)	179 (83%)	22 (10%)	15 (7%)	1	8
9	S7	182/189 (96%)	137 (75%)	25 (14%)	20 (11%)	0	2
9	s7	184/189 (97%)	140 (76%)	28 (15%)	16 (9%)	1	4
10	S8	184/200 (92%)	154 (84%)	21 (11%)	9 (5%)	2	17
10	s8	184/200 (92%)	161 (88%)	12 (6%)	11 (6%)	1	12
11	S9	183/196 (93%)	147 (80%)	24 (13%)	12 (7%)	1	9
11	s9	183/196 (93%)	149 (81%)	26 (14%)	8 (4%)	2	19
12	C0	94/105 (90%)	70 (74%)	18 (19%)	6 (6%)	1	10
12	c0	92/105 (88%)	66 (72%)	11 (12%)	15 (16%)	0	0
13	C1	153/155 (99%)	118 (77%)	17 (11%)	18 (12%)	0	2
13	c1	144/155 (93%)	114 (79%)	24 (17%)	6 (4%)	3	20
14	C2	122/142 (86%)	75 (62%)	21 (17%)	26 (21%)	0	0
14	c2	122/142 (86%)	71 (58%)	31 (25%)	20 (16%)	0	0
15	C3	148/150 (99%)	123 (83%)	12 (8%)	13 (9%)	1	4
15	c3	148/150 (99%)	115 (78%)	22 (15%)	11 (7%)	1	7
16	C4	125/136 (92%)	95 (76%)	15 (12%)	15 (12%)	0	2
16	c4	126/136 (93%)	104 (82%)	16 (13%)	6 (5%)	2	17
17	C5	122/141 (86%)	81 (66%)	28 (23%)	13 (11%)	0	2
17	c5	133/141 (94%)	90 (68%)	26 (20%)	17 (13%)	0	1
18	C6	139/142 (98%)	109 (78%)	20 (14%)	10 (7%)	1	7
18	c6	140/142 (99%)	112 (80%)	16 (11%)	12 (9%)	1	4
19	C7	116/136 (85%)	82 (71%)	25 (22%)	9 (8%)	1	6
19	c7	113/136 (83%)	87 (77%)	14 (12%)	12 (11%)	0	2
20	C8	143/145 (99%)	115 (80%)	15 (10%)	13 (9%)	1	3
20	c8	143/145 (99%)	117 (82%)	20 (14%)	6 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	C9	141/143 (99%)	115 (82%)	20 (14%)	6 (4%)	2	20
21	c9	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	5	29
22	D0	105/120 (88%)	82 (78%)	20 (19%)	3 (3%)	4	28
22	d0	108/120 (90%)	84 (78%)	14 (13%)	10 (9%)	0	3
23	D1	85/87 (98%)	64 (75%)	15 (18%)	6 (7%)	1	8
23	d1	85/87 (98%)	70 (82%)	8 (9%)	7 (8%)	1	5
24	D2	127/129 (98%)	105 (83%)	20 (16%)	2 (2%)	9	43
24	d2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	19	58
25	D3	142/144 (99%)	115 (81%)	14 (10%)	13 (9%)	1	3
25	d3	142/144 (99%)	123 (87%)	13 (9%)	6 (4%)	3	20
26	D4	132/134 (98%)	107 (81%)	19 (14%)	6 (4%)	2	18
26	d4	132/134 (98%)	100 (76%)	21 (16%)	11 (8%)	1	5
27	D5	68/107 (64%)	45 (66%)	13 (19%)	10 (15%)	0	1
27	d5	67/107 (63%)	52 (78%)	12 (18%)	3 (4%)	2	18
28	D6	95/97 (98%)	61 (64%)	17 (18%)	17 (18%)	0	0
28	d6	95/97 (98%)	71 (75%)	16 (17%)	8 (8%)	1	5
29	D7	79/81 (98%)	62 (78%)	11 (14%)	6 (8%)	1	7
29	d7	79/81 (98%)	59 (75%)	15 (19%)	5 (6%)	1	10
30	D8	61/66 (92%)	45 (74%)	11 (18%)	5 (8%)	1	5
30	d8	61/66 (92%)	46 (75%)	10 (16%)	5 (8%)	1	5
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	1	12
31	d9	51/55 (93%)	37 (72%)	8 (16%)	6 (12%)	0	2
32	E0	58/60 (97%)	42 (72%)	12 (21%)	4 (7%)	1	8
33	E1	69/76 (91%)	34 (49%)	11 (16%)	24 (35%)	0	0
33	e1	74/76 (97%)	34 (46%)	22 (30%)	18 (24%)	0	0
34	SR	316/318 (99%)	238 (75%)	56 (18%)	22 (7%)	1	8
34	sR	316/318 (99%)	261 (83%)	39 (12%)	16 (5%)	2	15
35	SM	155/273 (57%)	109 (70%)	26 (17%)	20 (13%)	0	1
35	sM	98/273 (36%)	61 (62%)	23 (24%)	14 (14%)	0	1
39	L2	250/253 (99%)	218 (87%)	22 (9%)	10 (4%)	3	21
39	l2	250/253 (99%)	209 (84%)	26 (10%)	15 (6%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	L3	384/386 (100%)	333 (87%)	34 (9%)	17 (4%)	2	19
40	l3	384/386 (100%)	339 (88%)	32 (8%)	13 (3%)	3	24
41	L4	359/361 (99%)	302 (84%)	40 (11%)	17 (5%)	2	17
41	l4	359/361 (99%)	293 (82%)	40 (11%)	26 (7%)	1	7
42	L5	294/296 (99%)	239 (81%)	34 (12%)	21 (7%)	1	8
42	l5	292/296 (99%)	252 (86%)	32 (11%)	8 (3%)	5	30
43	L6	152/175 (87%)	134 (88%)	16 (10%)	2 (1%)	12	47
43	l6	153/175 (87%)	127 (83%)	23 (15%)	3 (2%)	7	38
44	L7	220/243 (90%)	195 (89%)	19 (9%)	6 (3%)	5	30
44	l7	221/243 (91%)	193 (87%)	23 (10%)	5 (2%)	6	34
45	L8	231/255 (91%)	188 (81%)	36 (16%)	7 (3%)	4	28
45	l8	229/255 (90%)	181 (79%)	31 (14%)	17 (7%)	1	7
46	L9	189/191 (99%)	156 (82%)	25 (13%)	8 (4%)	3	20
46	l9	189/191 (99%)	162 (86%)	23 (12%)	4 (2%)	7	37
47	M0	207/220 (94%)	172 (83%)	21 (10%)	14 (7%)	1	9
47	m0	209/220 (95%)	165 (79%)	30 (14%)	14 (7%)	1	9
48	M1	167/173 (96%)	127 (76%)	24 (14%)	16 (10%)	0	3
48	m1	167/173 (96%)	142 (85%)	10 (6%)	15 (9%)	1	4
49	M3	191/198 (96%)	156 (82%)	23 (12%)	12 (6%)	1	10
49	m3	192/198 (97%)	149 (78%)	25 (13%)	18 (9%)	0	3
50	M4	134/137 (98%)	115 (86%)	12 (9%)	7 (5%)	2	15
50	m4	135/137 (98%)	120 (89%)	13 (10%)	2 (2%)	10	44
51	M5	201/203 (99%)	179 (89%)	17 (8%)	5 (2%)	5	32
51	m5	201/203 (99%)	175 (87%)	17 (8%)	9 (4%)	2	18
52	M6	195/198 (98%)	176 (90%)	14 (7%)	5 (3%)	5	31
52	m6	195/198 (98%)	170 (87%)	18 (9%)	7 (4%)	3	23
53	M7	181/183 (99%)	150 (83%)	22 (12%)	9 (5%)	2	16
53	m7	153/183 (84%)	136 (89%)	12 (8%)	5 (3%)	4	25
54	M8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	4	25
54	m8	183/185 (99%)	158 (86%)	23 (13%)	2 (1%)	14	51
55	M9	186/188 (99%)	158 (85%)	23 (12%)	5 (3%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	m9	186/188 (99%)	165 (89%)	20 (11%)	1 (0%)	29	67
56	N0	170/172 (99%)	150 (88%)	17 (10%)	3 (2%)	8	41
56	n0	170/172 (99%)	154 (91%)	15 (9%)	1 (1%)	25	64
57	N1	157/159 (99%)	132 (84%)	19 (12%)	6 (4%)	3	22
57	n1	157/159 (99%)	143 (91%)	13 (8%)	1 (1%)	25	64
58	N2	98/120 (82%)	77 (79%)	17 (17%)	4 (4%)	3	21
58	n2	96/120 (80%)	76 (79%)	14 (15%)	6 (6%)	1	10
59	N3	134/136 (98%)	120 (90%)	12 (9%)	2 (2%)	10	44
59	n3	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	6	35
60	N4	96/155 (62%)	69 (72%)	17 (18%)	10 (10%)	0	3
60	n4	133/155 (86%)	106 (80%)	17 (13%)	10 (8%)	1	7
61	N5	119/141 (84%)	103 (87%)	10 (8%)	6 (5%)	2	16
61	n5	118/141 (84%)	94 (80%)	15 (13%)	9 (8%)	1	7
62	N6	124/126 (98%)	110 (89%)	11 (9%)	3 (2%)	6	34
62	n6	124/126 (98%)	112 (90%)	7 (6%)	5 (4%)	3	21
63	N7	133/135 (98%)	108 (81%)	12 (9%)	13 (10%)	0	3
63	n7	133/135 (98%)	101 (76%)	21 (16%)	11 (8%)	1	5
64	N8	146/148 (99%)	120 (82%)	19 (13%)	7 (5%)	2	17
64	n8	146/148 (99%)	117 (80%)	21 (14%)	8 (6%)	2	14
65	N9	56/58 (97%)	47 (84%)	5 (9%)	4 (7%)	1	8
65	n9	56/58 (97%)	37 (66%)	13 (23%)	6 (11%)	0	2
66	O0	95/104 (91%)	86 (90%)	8 (8%)	1 (1%)	14	51
66	o0	98/104 (94%)	88 (90%)	9 (9%)	1 (1%)	15	54
67	O1	107/112 (96%)	96 (90%)	5 (5%)	6 (6%)	2	14
67	o1	107/112 (96%)	84 (78%)	15 (14%)	8 (8%)	1	7
68	O2	125/129 (97%)	106 (85%)	14 (11%)	5 (4%)	3	21
68	o2	125/129 (97%)	105 (84%)	15 (12%)	5 (4%)	3	21
69	O3	104/106 (98%)	94 (90%)	6 (6%)	4 (4%)	3	22
69	o3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	4	28
70	O4	110/120 (92%)	90 (82%)	19 (17%)	1 (1%)	17	56
70	o4	110/120 (92%)	97 (88%)	10 (9%)	3 (3%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	O5	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	5	31
71	o5	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	5	31
72	O6	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	1	5
72	o6	97/99 (98%)	81 (84%)	11 (11%)	5 (5%)	2	15
73	O7	85/87 (98%)	72 (85%)	12 (14%)	1 (1%)	13	49
73	o7	85/87 (98%)	68 (80%)	12 (14%)	5 (6%)	1	12
74	O8	75/77 (97%)	61 (81%)	12 (16%)	2 (3%)	5	30
74	o8	75/77 (97%)	64 (85%)	8 (11%)	3 (4%)	3	21
75	O9	48/50 (96%)	42 (88%)	5 (10%)	1 (2%)	7	37
75	o9	48/50 (96%)	40 (83%)	8 (17%)	0	100	100
76	Q0	50/52 (96%)	44 (88%)	4 (8%)	2 (4%)	3	21
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	7	38
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	20
78	Q2	103/105 (98%)	76 (74%)	19 (18%)	8 (8%)	1	6
78	q2	103/105 (98%)	86 (84%)	14 (14%)	3 (3%)	4	28
79	Q3	89/91 (98%)	76 (85%)	10 (11%)	3 (3%)	3	24
79	q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	14	51
80	e0	60/62 (97%)	44 (73%)	8 (13%)	8 (13%)	0	1
81	p0	139/311 (45%)	110 (79%)	21 (15%)	8 (6%)	1	13
All	All	22333/24143 (92%)	18176 (81%)	2788 (12%)	1369 (6%)	1	12

All (1369) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	66	ALA
2	S0	139	VAL
2	S0	158	VAL
2	S0	185	ARG
2	S0	190	ASP
2	S0	191	ARG
3	S1	49	ASN
3	S1	58	SER

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Mol	Chain	Res	Type
3	S1	63	GLY
3	S1	93	GLY
3	S1	132	ASP
3	S1	158	SER
3	S1	179	SER
3	S1	206	PRO
4	S2	91	ARG
4	S2	248	SER
5	S3	44	THR
5	S3	65	ARG
5	S3	93	ASP
5	S3	211	PRO
5	S3	216	PRO
5	S3	220	PRO
6	S4	3	ARG
6	S4	96	ASN
6	S4	104	ASP
6	S4	167	GLY
6	S4	227	VAL
6	S4	228	ILE
6	S4	258	GLN
7	S5	35	GLN
7	S5	39	GLU
7	S5	51	VAL
7	S5	58	LEU
7	S5	63	GLN
7	S5	101	GLY
7	S5	154	ALA
8	S6	173	PRO
8	S6	174	LYS
9	S7	30	SER
9	S7	31	SER
9	S7	64	VAL
9	S7	85	PHE
9	S7	110	GLN
9	S7	112	ARG
9	S7	131	PHE
9	S7	134	GLU
9	S7	159	VAL
10	S8	82	VAL
10	S8	155	SER
11	S9	98	ALA

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Mol	Chain	Res	Type
11	S9	118	LEU
11	S9	134	ILE
11	S9	171	ARG
12	C0	87	VAL
12	C0	88	PRO
12	C0	89	ALA
13	C1	3	THR
13	C1	7	VAL
13	C1	29	LYS
13	C1	72	THR
13	C1	139	VAL
13	C1	140	VAL
13	C1	144	ALA
13	C1	154	ALA
14	C2	25	GLU
14	C2	91	VAL
14	C2	93	ASP
14	C2	126	TRP
15	C3	27	LYS
15	C3	28	LEU
15	C3	68	GLY
16	C4	38	THR
16	C4	39	ILE
16	C4	42	VAL
16	C4	50	ALA
16	C4	92	LYS
16	C4	124	ASP
16	C4	125	SER
17	C5	22	LEU
17	C5	54	ALA
17	C5	125	PRO
17	C5	126	VAL
18	C6	41	PRO
18	C6	58	ASP
18	C6	59	LYS
19	C7	23	LYS
19	C7	26	LEU
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
20	C8	7	GLU
20	C8	14	ILE

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Mol	Chain	Res	Type
20	C8	61	LEU
20	C8	82	PRO
20	C8	91	ASP
20	C8	92	ILE
20	C8	134	ARG
21	C9	31	PRO
21	C9	53	TRP
23	D1	4	ASP
23	D1	6	GLY
24	D2	57	ARG
24	D2	83	ILE
25	D3	11	SER
25	D3	53	VAL
25	D3	54	LEU
25	D3	144	ARG
26	D4	6	THR
26	D4	60	PHE
27	D5	39	ALA
27	D5	56	THR
27	D5	71	ILE
27	D5	86	GLU
28	D6	5	ARG
28	D6	45	VAL
28	D6	47	ALA
28	D6	65	PRO
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
29	D7	38	PRO
29	D7	62	ILE
30	D8	36	THR
32	E0	47	VAL
32	E0	51	ASN
33	E1	85	TYR
33	E1	87	THR
33	E1	98	VAL
33	E1	99	LYS
33	E1	102	VAL
33	E1	103	LEU
33	E1	138	ARG
34	SR	113	VAL

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Mol	Chain	Res	Type
34	SR	155	ARG
34	SR	161	LYS
34	SR	188	ILE
34	SR	231	MET
34	SR	270	LEU
34	SR	271	VAL
35	SM	17	VAL
35	SM	18	VAL
35	SM	87	THR
35	SM	89	ARG
35	SM	102	THR
35	SM	139	GLU
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
39	L2	47	GLN
40	L3	3	HIS
40	L3	4	ARG
40	L3	5	LYS
40	L3	113	GLU
40	L3	140	ASP
40	L3	188	ILE
40	L3	347	SER
40	L3	385	LYS
41	L4	131	VAL
41	L4	292	SER
41	L4	338	LYS
42	L5	107	ARG
42	L5	108	ARG
42	L5	137	ASP
42	L5	233	ALA
42	L5	234	ASP
42	L5	258	LYS
43	L6	98	VAL
44	L7	24	GLU
44	L7	26	VAL
45	L8	25	PRO
46	L9	50	ASN
47	M0	145	LYS
47	M0	207	GLU
48	M1	8	PRO
48	M1	9	MET

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Mol	Chain	Res	Type
48	M1	11	ASP
48	M1	39	GLN
48	M1	74	PRO
48	M1	94	ARG
48	M1	165	GLN
49	M3	47	ALA
49	M3	76	THR
49	M3	129	ASN
49	M3	141	ALA
50	M4	8	LYS
50	M4	9	ALA
50	M4	10	SER
51	M5	74	PRO
51	M5	75	VAL
51	M5	91	GLU
52	M6	111	PRO
53	M7	110	THR
53	M7	157	VAL
54	M8	41	ASP
54	M8	99	THR
57	N1	126	VAL
57	N1	159	PHE
58	N2	51	GLY
60	N4	64	THR
60	N4	81	PRO
60	N4	86	SER
60	N4	97	LYS
61	N5	44	PRO
62	N6	52	ARG
62	N6	92	GLY
63	N7	17	ARG
63	N7	125	GLY
63	N7	129	TRP
64	N8	76	ASP
67	O1	5	LYS
68	O2	27	ARG
68	O2	127	ALA
71	O5	119	LYS
72	O6	28	TYR
72	O6	33	ALA
75	O9	4	GLN
76	Q0	78	ILE

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Mol	Chain	Res	Type
78	Q2	60	LYS
78	Q2	100	LYS
2	s0	4	PRO
2	s0	29	VAL
2	s0	66	ALA
2	s0	103	THR
2	s0	158	VAL
2	s0	164	ASN
2	s0	186	GLY
2	s0	191	ARG
2	s0	203	PHE
2	s0	206	ASP
3	s1	106	THR
3	s1	107	THR
3	s1	147	ALA
3	s1	154	SER
3	s1	206	PRO
4	s2	92	ALA
4	s2	146	THR
4	s2	234	PRO
5	s3	115	ILE
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	12	LEU
6	s4	24	SER
6	s4	95	THR
6	s4	104	ASP
6	s4	117	GLU
6	s4	195	ILE
6	s4	196	VAL
7	s5	28	PRO
7	s5	35	GLN
7	s5	36	ALA
7	s5	126	ASP
7	s5	127	GLN
7	s5	184	PHE
7	s5	204	GLY
8	s6	21	GLU
8	s6	68	LEU
8	s6	153	VAL

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Mol	Chain	Res	Type
8	s6	154	ARG
8	s6	173	PRO
8	s6	174	LYS
9	s7	30	SER
9	s7	63	PRO
9	s7	64	VAL
9	s7	67	LEU
9	s7	106	SER
9	s7	131	PHE
9	s7	155	ASP
9	s7	163	ASP
10	s8	62	THR
12	c0	32	HIS
12	c0	82	LEU
12	c0	83	PRO
12	c0	88	PRO
12	c0	92	ILE
12	c0	97	PRO
13	c1	133	LYS
14	c2	22	VAL
14	c2	101	ALA
14	c2	115	VAL
15	c3	19	SER
15	c3	66	ILE
15	c3	139	TRP
15	c3	140	LYS
16	c4	132	ARG
17	c5	9	LYS
17	c5	17	TYR
17	c5	51	SER
17	c5	126	VAL
18	c6	39	VAL
18	c6	42	GLU
18	c6	116	LEU
19	c7	67	ARG
19	c7	86	PRO
19	c7	88	VAL
19	c7	99	VAL
19	c7	104	ASN
20	c8	91	ASP
20	c8	92	ILE
21	c9	34	VAL

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Mol	Chain	Res	Type
22	d0	15	GLN
22	d0	51	VAL
22	d0	97	VAL
23	d1	4	ASP
25	d3	138	GLU
26	d4	30	PRO
26	d4	33	ALA
26	d4	53	ASP
27	d5	85	LYS
29	d7	38	PRO
29	d7	59	CYS
29	d7	60	SER
29	d7	75	GLU
31	d9	7	TRP
31	d9	19	ARG
80	e0	51	ASN
33	e1	84	VAL
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	102	VAL
33	e1	103	LEU
33	e1	106	TYR
33	e1	146	SER
34	sR	4	ASN
34	sR	163	ASP
34	sR	165	ASP
34	sR	279	ALA
34	sR	318	ALA
35	sM	50	ASN
35	sM	122	GLU
39	l2	56	ALA
39	l2	96	LEU
39	l2	194	ASN
39	l2	213	GLY
39	l2	238	ILE
40	l3	3	HIS
40	l3	129	ALA
40	l3	140	ASP
40	l3	142	ALA
40	l3	347	SER
41	l4	15	ALA

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Mol	Chain	Res	Type
41	l4	90	PHE
41	l4	142	VAL
41	l4	145	ILE
41	l4	270	SER
41	l4	301	PRO
41	l4	302	ALA
41	l4	329	PRO
41	l4	330	TYR
41	l4	339	LEU
41	l4	342	LYS
41	l4	345	GLU
42	l5	115	LEU
42	l5	260	PHE
42	l5	270	LYS
43	l6	98	VAL
44	l7	159	GLN
45	l8	25	PRO
45	l8	26	LEU
45	l8	34	PHE
45	l8	122	LYS
45	l8	223	ALA
45	l8	240	ASN
46	l9	167	VAL
47	m0	23	ASN
47	m0	220	GLN
48	m1	8	PRO
48	m1	9	MET
48	m1	10	ARG
48	m1	94	ARG
48	m1	95	ASN
48	m1	108	GLU
48	m1	115	LYS
48	m1	165	GLN
49	m3	47	ALA
49	m3	93	ILE
49	m3	134	GLU
49	m3	141	ALA
49	m3	152	THR
49	m3	162	ASN
50	m4	136	ALA
51	m5	184	LYS
52	m6	16	VAL

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Mol	Chain	Res	Type
52	m6	110	PRO
52	m6	111	PRO
52	m6	177	LYS
53	m7	67	ILE
54	m8	99	THR
57	n1	122	GLN
58	n2	50	LEU
59	n3	42	SER
59	n3	68	GLU
60	n4	25	ASP
60	n4	71	ARG
60	n4	76	VAL
60	n4	133	THR
61	n5	40	LEU
61	n5	55	ASN
62	n6	84	LYS
62	n6	85	VAL
62	n6	125	LYS
63	n7	56	LYS
63	n7	105	SER
63	n7	127	ASN
64	n8	6	THR
64	n8	76	ASP
65	n9	5	LYS
65	n9	21	ILE
65	n9	23	LYS
65	n9	39	PHE
66	o0	100	ILE
67	o1	7	VAL
68	o2	6	HIS
71	o5	119	LYS
72	o6	4	LYS
72	o6	64	SER
72	o6	98	ARG
73	o7	84	SER
79	q3	51	ALA
81	p0	93	LEU
81	p0	102	SER
81	p0	198	PRO
2	S0	5	ALA
2	S0	49	ASN
2	S0	94	GLY

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Mol	Chain	Res	Type
2	S0	202	TYR
3	S1	37	THR
3	S1	54	LEU
3	S1	79	HIS
3	S1	81	PHE
3	S1	221	PRO
4	S2	148	LEU
5	S3	36	GLY
5	S3	40	ARG
5	S3	218	LEU
6	S4	26	CYS
7	S5	26	ALA
7	S5	43	PHE
7	S5	60	ASP
7	S5	64	VAL
7	S5	81	ARG
7	S5	127	GLN
7	S5	156	ARG
8	S6	20	ASP
8	S6	54	GLY
8	S6	59	GLN
9	S7	29	ASN
9	S7	32	PRO
9	S7	36	ALA
9	S7	111	LYS
9	S7	132	PRO
9	S7	156	SER
10	S8	40	ALA
10	S8	120	THR
10	S8	152	ILE
10	S8	199	LYS
11	S9	117	GLY
11	S9	150	LEU
11	S9	170	GLY
12	C0	81	ASN
13	C1	55	ASP
13	C1	74	THR
13	C1	145	ALA
13	C1	146	ALA
14	C2	21	GLU
14	C2	66	VAL
14	C2	113	ARG

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Mol	Chain	Res	Type
14	C2	127	GLY
15	C3	3	ARG
15	C3	13	SER
15	C3	19	SER
15	C3	22	ALA
15	C3	31	GLU
15	C3	138	ASN
16	C4	40	ALA
16	C4	86	THR
16	C4	126	THR
17	C5	80	MET
17	C5	101	ALA
18	C6	39	VAL
18	C6	113	ASP
18	C6	116	LEU
19	C7	87	GLU
20	C8	8	GLN
20	C8	60	GLU
20	C8	83	ALA
20	C8	142	GLY
20	C8	144	ARG
21	C9	69	LYS
21	C9	126	GLU
23	D1	10	GLU
23	D1	11	LEU
23	D1	43	GLY
25	D3	4	GLY
25	D3	46	SER
25	D3	114	LYS
27	D5	43	ASP
27	D5	55	PRO
27	D5	62	VAL
27	D5	88	ILE
27	D5	97	LYS
28	D6	46	GLU
28	D6	63	ALA
29	D7	24	LEU
29	D7	63	LEU
31	D9	8	PHE
33	E1	84	VAL
33	E1	94	LYS
33	E1	106	TYR

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Mol	Chain	Res	Type
33	E1	111	GLU
33	E1	118	ARG
33	E1	127	GLY
33	E1	128	ALA
34	SR	114	ASP
34	SR	189	GLU
34	SR	228	LYS
34	SR	295	SER
35	SM	154	TYR
39	L2	13	GLY
39	L2	234	LYS
39	L2	250	GLN
40	L3	83	PRO
40	L3	134	SER
40	L3	351	LEU
41	L4	146	PRO
41	L4	190	GLY
41	L4	232	SER
41	L4	268	ALA
41	L4	320	ASN
42	L5	57	ASN
42	L5	178	ASN
42	L5	260	PHE
44	L7	175	LYS
45	L8	157	VAL
45	L8	209	ALA
46	L9	164	ILE
47	M0	117	GLY
47	M0	211	ARG
47	M0	220	GLN
48	M1	24	GLY
48	M1	114	ILE
48	M1	115	LYS
48	M1	151	SER
48	M1	152	HIS
48	M1	167	TYR
48	M1	173	ASP
49	M3	193	ALA
52	M6	16	VAL
52	M6	90	HIS
53	M7	159	LYS
53	M7	162	GLU

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Mol	Chain	Res	Type
54	M8	98	LYS
54	M8	158	HIS
55	M9	146	LYS
56	N0	2	ALA
56	N0	167	ARG
57	N1	123	GLY
57	N1	124	VAL
58	N2	60	GLY
59	N3	69	LEU
60	N4	76	VAL
61	N5	23	ALA
61	N5	45	LYS
62	N6	84	LYS
63	N7	3	LYS
63	N7	30	ASP
63	N7	35	SER
63	N7	126	LYS
63	N7	128	GLN
64	N8	66	ALA
65	N9	25	LYS
67	O1	6	ASP
67	O1	82	GLU
68	O2	12	LYS
68	O2	126	LEU
71	O5	40	SER
72	O6	27	SER
72	O6	34	SER
72	O6	64	SER
72	O6	78	GLY
73	O7	86	ALA
74	O8	18	ALA
74	O8	33	LYS
78	Q2	34	SER
78	Q2	104	LEU
79	Q3	51	ALA
2	s0	30	GLN
2	s0	81	PHE
2	s0	92	HIS
2	s0	95	ALA
2	s0	111	ILE
2	s0	185	ARG
2	s0	189	VAL

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Mol	Chain	Res	Type
3	s1	43	VAL
3	s1	93	GLY
4	s2	95	ARG
4	s2	149	GLY
4	s2	163	GLY
5	s3	61	GLU
5	s3	90	ARG
5	s3	179	GLN
5	s3	221	SER
6	s4	3	ARG
6	s4	164	LEU
7	s5	37	GLN
7	s5	84	LYS
8	s6	25	ARG
9	s7	8	ILE
9	s7	74	GLN
9	s7	111	LYS
9	s7	156	SER
10	s8	94	ASN
10	s8	100	ALA
10	s8	101	ILE
10	s8	147	ALA
11	s9	150	LEU
11	s9	167	ALA
12	c0	2	LEU
12	c0	94	GLU
13	c1	7	VAL
14	c2	54	ARG
14	c2	66	VAL
14	c2	89	ILE
14	c2	131	ASP
16	c4	51	ASP
17	c5	7	ALA
17	c5	11	VAL
17	c5	49	MET
17	c5	50	THR
17	c5	117	GLY
17	c5	127	ARG
18	c6	57	LEU
18	c6	113	ASP
18	c6	120	ASP
19	c7	63	LYS

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Mol	Chain	Res	Type
19	c7	116	LYS
19	c7	120	SER
20	c8	135	GLY
21	c9	28	LEU
22	d0	52	LYS
22	d0	96	PRO
22	d0	118	VAL
23	d1	42	GLU
23	d1	43	GLY
26	d4	35	VAL
26	d4	121	THR
28	d6	8	ASN
28	d6	13	LYS
28	d6	24	VAL
30	d8	57	MET
31	d9	6	VAL
31	d9	16	LYS
80	e0	45	VAL
33	e1	83	LYS
34	sR	75	ALA
34	sR	78	ALA
34	sR	271	VAL
35	sM	47	ALA
35	sM	63	ASP
35	sM	67	GLY
35	sM	79	SER
39	l2	14	SER
39	l2	215	ASN
40	l3	4	ARG
41	l4	220	ARG
41	l4	233	LEU
41	l4	311	HIS
41	l4	352	ALA
41	l4	361	HIS
43	l6	10	TYR
44	l7	217	PRO
45	l8	39	ALA
45	l8	121	SER
45	l8	133	LYS
45	l8	188	THR
45	l8	203	VAL
46	l9	144	ILE

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Mol	Chain	Res	Type
46	l9	189	GLU
47	m0	25	ALA
47	m0	194	GLY
47	m0	207	GLU
48	m1	116	TYR
49	m3	76	THR
49	m3	101	ARG
49	m3	121	SER
49	m3	129	ASN
49	m3	135	ALA
51	m5	76	PRO
51	m5	81	TYR
51	m5	182	ASN
51	m5	185	ALA
52	m6	176	LYS
54	m8	167	SER
56	n0	129	ILE
58	n2	32	SER
58	n2	44	GLU
59	n3	3	GLY
60	n4	63	ILE
60	n4	95	SER
62	n6	126	LEU
63	n7	5	LEU
63	n7	16	GLY
63	n7	104	PRO
64	n8	84	GLU
67	o1	45	GLY
67	o1	91	SER
67	o1	99	ALA
68	o2	27	ARG
68	o2	124	GLY
70	o4	59	PRO
70	o4	79	SER
72	o6	33	ALA
73	o7	87	SER
78	q2	60	LYS
81	p0	68	SER
2	S0	195	TRP
3	S1	35	PRO
3	S1	51	SER
3	S1	78	ASP

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Mol	Chain	Res	Type
3	S1	90	GLU
3	S1	209	ASN
3	S1	213	ARG
3	S1	218	LEU
4	S2	106	ASP
4	S2	108	ASN
4	S2	235	LEU
5	S3	37	VAL
5	S3	64	ARG
5	S3	81	PRO
5	S3	90	ARG
5	S3	112	GLY
5	S3	143	ARG
5	S3	217	ILE
6	S4	195	ILE
6	S4	223	ASN
6	S4	245	LYS
7	S5	21	THR
7	S5	59	VAL
7	S5	206	SER
8	S6	70	PRO
8	S6	122	GLU
8	S6	152	ASP
8	S6	165	GLY
9	S7	14	THR
9	S7	98	ILE
11	S9	120	LYS
11	S9	121	SER
12	C0	60	SER
13	C1	30	ARG
13	C1	73	GLY
13	C1	147	ALA
14	C2	101	ALA
14	C2	106	ILE
14	C2	112	ALA
14	C2	118	ALA
14	C2	119	SER
14	C2	125	ASN
14	C2	130	THR
14	C2	131	ASP
15	C3	32	SER
16	C4	108	SER

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Mol	Chain	Res	Type
17	C5	11	VAL
17	C5	51	SER
17	C5	69	GLU
18	C6	29	ILE
18	C6	33	GLY
18	C6	142	TYR
19	C7	25	THR
21	C9	130	ARG
23	D1	82	VAL
25	D3	3	LYS
25	D3	92	CYS
25	D3	112	LYS
26	D4	5	VAL
28	D6	11	ASN
28	D6	62	TYR
29	D7	57	GLU
32	E0	13	LYS
33	E1	83	LYS
33	E1	97	LYS
33	E1	144	CYS
34	SR	153	GLN
34	SR	318	ALA
35	SM	52	PRO
35	SM	53	ARG
35	SM	88	ARG
35	SM	174	LEU
39	L2	143	GLU
40	L3	155	ALA
40	L3	300	ARG
41	L4	4	PRO
41	L4	143	GLU
41	L4	265	GLU
41	L4	311	HIS
41	L4	317	PRO
42	L5	72	ASP
42	L5	115	LEU
42	L5	215	ASP
42	L5	253	PHE
42	L5	259	LYS
43	L6	108	LYS
44	L7	163	LEU
45	L8	85	ASN

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Mol	Chain	Res	Type
45	L8	156	ASP
46	L9	59	ASN
46	L9	190	ASP
47	M0	24	ARG
47	M0	189	GLU
49	M3	136	GLU
49	M3	166	ALA
50	M4	29	ALA
51	M5	81	TYR
52	M6	196	ALA
53	M7	3	ARG
53	M7	164	LYS
55	M9	53	LYS
55	M9	120	TYR
56	N0	50	LYS
60	N4	16	GLY
60	N4	69	LYS
60	N4	77	LYS
61	N5	25	LYS
61	N5	26	VAL
63	N7	18	TYR
63	N7	102	GLU
64	N8	79	TRP
64	N8	96	LYS
64	N8	117	ARG
66	O0	96	GLY
68	O2	13	HIS
69	O3	59	VAL
72	O6	21	THR
78	Q2	15	LYS
78	Q2	94	GLY
79	Q3	7	LYS
79	Q3	84	ARG
2	s0	10	THR
2	s0	49	ASN
2	s0	139	VAL
2	s0	162	CYS
3	s1	26	ARG
3	s1	223	PHE
3	s1	232	HIS
4	s2	106	ASP
4	s2	107	SER

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Mol	Chain	Res	Type
5	s3	43	PRO
5	s3	44	THR
5	s3	195	SER
6	s4	245	LYS
7	s5	43	PHE
7	s5	45	LYS
7	s5	100	ASN
7	s5	151	GLY
7	s5	154	ALA
7	s5	209	TYR
8	s6	209	ALA
10	s8	27	PHE
10	s8	148	ALA
11	s9	121	SER
11	s9	183	ALA
12	c0	3	MET
12	c0	23	ALA
12	c0	24	LYS
12	c0	30	ALA
13	c1	55	ASP
14	c2	26	ASP
14	c2	40	GLY
14	c2	58	LEU
14	c2	106	ILE
14	c2	108	ARG
14	c2	119	SER
15	c3	61	THR
16	c4	90	ARG
17	c5	69	GLU
17	c5	135	THR
18	c6	97	VAL
19	c7	68	GLY
19	c7	113	LEU
20	c8	14	ILE
20	c8	61	LEU
21	c9	33	TYR
22	d0	17	GLN
22	d0	39	SER
22	d0	45	ALA
22	d0	49	ASN
23	d1	44	ARG
24	d2	31	SER

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Mol	Chain	Res	Type
25	d3	3	LYS
25	d3	70	LYS
25	d3	109	ARG
25	d3	128	SER
26	d4	49	LYS
26	d4	58	PHE
26	d4	78	SER
28	d6	61	GLU
29	d7	20	LYS
30	d8	58	GLU
30	d8	61	ARG
31	d9	11	PRO
31	d9	17	GLY
80	e0	53	LYS
80	e0	60	PRO
33	e1	85	TYR
33	e1	100	LEU
33	e1	111	GLU
33	e1	128	ALA
34	sR	149	ASP
34	sR	160	GLU
34	sR	186	PHE
35	sM	171	LYS
39	l2	80	GLU
40	l3	188	ILE
40	l3	385	LYS
40	l3	386	ASP
41	l4	146	PRO
42	l5	72	ASP
42	l5	178	ASN
42	l5	258	LYS
42	l5	266	ALA
44	l7	191	VAL
45	l8	118	GLU
45	l8	196	ALA
47	m0	193	ASP
47	m0	196	PHE
49	m3	60	ALA
49	m3	150	PRO
55	m9	36	ASN
58	n2	51	GLY
58	n2	91	ASP

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Mol	Chain	Res	Type
60	n4	72	SER
60	n4	77	LYS
60	n4	134	GLN
61	n5	38	LEU
61	n5	47	ALA
63	n7	34	LYS
63	n7	102	GLU
64	n8	120	ASN
65	n9	37	PRO
67	o1	83	GLU
68	o2	17	PHE
71	o5	40	SER
71	o5	82	ALA
72	o6	34	SER
73	o7	86	ALA
74	o8	16	ARG
76	q0	78	ILE
78	q2	74	CYS
81	p0	197	PHE
81	p0	203	ASP
2	S0	103	THR
2	S0	187	ALA
2	S0	194	PRO
3	S1	23	PRO
3	S1	55	LYS
3	S1	147	ALA
4	S2	47	ALA
4	S2	150	GLN
5	S3	38	GLU
5	S3	72	LEU
5	S3	196	ARG
6	S4	157	ASN
6	S4	242	LYS
7	S5	65	ARG
7	S5	100	ASN
8	S6	146	GLY
9	S7	155	ASP
11	S9	16	LYS
11	S9	99	LEU
13	C1	4	GLU
13	C1	5	LEU
14	C2	107	ASP

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Mol	Chain	Res	Type
14	C2	108	ARG
14	C2	128	ALA
15	C3	64	ARG
16	C4	88	GLY
17	C5	29	SER
17	C5	52	LYS
17	C5	127	ARG
19	C7	72	LYS
22	D0	17	GLN
26	D4	53	ASP
27	D5	93	SER
28	D6	9	GLY
28	D6	36	ILE
28	D6	53	LEU
28	D6	64	LEU
28	D6	88	SER
29	D7	75	GLU
30	D8	14	LYS
30	D8	37	SER
31	D9	6	VAL
33	E1	86	THR
33	E1	93	HIS
33	E1	110	ALA
33	E1	137	ASP
34	SR	3	SER
34	SR	72	THR
34	SR	163	ASP
34	SR	230	ALA
34	SR	237	GLN
34	SR	242	SER
35	SM	12	VAL
35	SM	83	LYS
35	SM	85	SER
35	SM	172	VAL
39	L2	130	SER
39	L2	246	LEU
40	L3	141	GLY
40	L3	386	ASP
41	L4	90	PHE
42	L5	6	ASP
42	L5	188	GLU
42	L5	292	ALA

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Mol	Chain	Res	Type
46	L9	110	LYS
47	M0	7	ARG
47	M0	23	ASN
47	M0	91	VAL
49	M3	128	ARG
50	M4	28	SER
50	M4	113	THR
53	M7	158	ALA
53	M7	160	ALA
58	N2	11	ILE
58	N2	31	ALA
60	N4	26	SER
61	N5	128	ALA
63	N7	36	HIS
63	N7	93	LYS
63	N7	103	GLN
64	N8	47	LYS
70	O4	46	ASP
72	O6	3	VAL
76	Q0	79	GLU
78	Q2	8	ARG
4	s2	150	GLN
4	s2	152	HIS
4	s2	235	LEU
4	s2	238	SER
5	s3	93	ASP
5	s3	196	ARG
6	s4	11	ARG
6	s4	31	PRO
6	s4	90	ILE
6	s4	168	LYS
7	s5	21	THR
7	s5	29	ILE
7	s5	56	ALA
8	s6	11	GLY
8	s6	58	LYS
8	s6	69	LEU
8	s6	156	PHE
9	s7	9	LEU
9	s7	185	ILE
10	s8	136	SER
11	s9	5	PRO

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Mol	Chain	Res	Type
11	s9	134	ILE
11	s9	162	SER
12	c0	31	LYS
13	c1	3	THR
14	c2	21	GLU
14	c2	45	LEU
14	c2	90	LYS
14	c2	107	ASP
15	c3	12	SER
16	c4	32	ASP
16	c4	92	LYS
17	c5	125	PRO
18	c6	142	TYR
21	c9	88	VAL
23	d1	10	GLU
25	d3	131	SER
26	d4	50	ALA
26	d4	52	LYS
28	d6	59	TYR
28	d6	62	TYR
28	d6	82	ARG
30	d8	51	ASN
80	e0	61	SER
33	e1	79	LYS
33	e1	131	PHE
33	e1	145	HIS
34	sR	194	GLY
34	sR	237	GLN
34	sR	281	TYR
35	sM	42	ALA
35	sM	48	ARG
35	sM	84	LYS
35	sM	168	GLU
39	l2	13	GLY
39	l2	32	LEU
39	l2	125	ALA
39	l2	227	ARG
41	l4	14	GLU
41	l4	24	ALA
41	l4	338	LYS
45	l8	69	LEU
46	l9	110	LYS

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Mol	Chain	Res	Type
47	m0	7	ARG
47	m0	102	MET
48	m1	114	ILE
48	m1	167	TYR
49	m3	140	SER
50	m4	135	LEU
51	m5	104	GLU
51	m5	183	THR
53	m7	66	SER
53	m7	72	GLN
61	n5	24	LEU
63	n7	28	PRO
63	n7	103	GLN
64	n8	78	LEU
64	n8	135	GLU
67	o1	90	PHE
67	o1	97	LEU
69	o3	90	PRO
70	o4	82	ALA
73	o7	85	LYS
77	q1	22	ALA
81	p0	33	VAL
4	S2	39	THR
4	S2	107	SER
4	S2	145	GLY
5	S3	4	LEU
6	S4	164	LEU
9	S7	53	GLY
10	S8	10	LYS
10	S8	81	VAL
12	C0	34	GLU
14	C2	39	ASP
14	C2	115	VAL
17	C5	87	PRO
22	D0	21	LYS
25	D3	131	SER
26	D4	4	ALA
26	D4	83	LYS
30	D8	22	ARG
32	E0	27	PRO
33	E1	113	LYS
33	E1	148	TYR

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Mol	Chain	Res	Type
34	SR	38	ARG
34	SR	244	ALA
35	SM	64	LYS
35	SM	173	GLU
39	L2	34	TYR
41	L4	14	GLU
41	L4	193	LYS
42	L5	7	ALA
42	L5	125	VAL
44	L7	25	GLN
45	L8	36	ILE
45	L8	39	ALA
46	L9	2	LYS
46	L9	96	HIS
47	M0	16	PRO
47	M0	146	ASP
47	M0	186	GLU
48	M1	111	ASP
48	M1	117	ASP
49	M3	130	GLY
49	M3	140	SER
50	M4	6	ILE
51	M5	94	TYR
53	M7	163	LYS
54	M8	160	GLY
54	M8	162	ALA
57	N1	121	ALA
64	N8	78	LEU
65	N9	53	ALA
67	O1	7	VAL
67	O1	60	TRP
67	O1	84	ASP
69	O3	91	ALA
71	O5	75	TYR
78	Q2	48	SER
2	s0	36	TYR
2	s0	54	TRP
3	s1	22	ASP
3	s1	77	GLU
3	s1	207	LEU
4	s2	244	SER
6	s4	141	THR

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Mol	Chain	Res	Type
6	s4	163	ASP
6	s4	260	GLY
7	s5	42	LEU
7	s5	55	ASP
7	s5	57	SER
7	s5	60	ASP
9	s7	11	GLN
9	s7	112	ARG
10	s8	52	ASN
10	s8	78	ILE
11	s9	147	MET
12	c0	35	ILE
12	c0	95	ARG
14	c2	39	ASP
14	c2	82	PRO
15	c3	22	ALA
15	c3	87	ASP
16	c4	114	ARG
17	c5	6	ASN
17	c5	68	PRO
18	c6	100	GLN
23	d1	6	GLY
26	d4	96	LEU
80	e0	54	ARG
33	e1	81	LYS
34	sR	247	PRO
35	sM	43	ASP
35	sM	46	LYS
39	l2	249	SER
40	l3	10	ARG
40	l3	155	ALA
40	l3	206	ASP
41	l4	5	GLN
41	l4	328	ASN
44	l7	178	ILE
45	l8	80	TYR
47	m0	3	ARG
47	m0	195	ALA
47	m0	204	GLY
48	m1	12	LEU
48	m1	152	HIS
48	m1	153	LYS

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Mol	Chain	Res	Type
49	m3	62	THR
49	m3	122	LYS
49	m3	130	GLY
51	m5	68	ARG
52	m6	170	LYS
52	m6	183	ALA
53	m7	3	ARG
61	n5	48	SER
62	n6	83	ASP
63	n7	41	ALA
64	n8	48	TYR
65	n9	22	LYS
67	o1	46	THR
73	o7	25	ARG
74	o8	18	ALA
3	S1	62	LYS
3	S1	207	LEU
3	S1	224	ASP
6	S4	12	LEU
7	S5	163	SER
9	S7	73	VAL
11	S9	163	PRO
13	C1	75	VAL
16	C4	18	ARG
19	C7	124	VAL
20	C8	79	TYR
21	C9	116	ILE
25	D3	97	ASP
33	E1	100	LEU
39	L2	35	ALA
39	L2	251	LYS
42	L5	295	GLY
44	L7	178	ILE
49	M3	13	HIS
49	M3	165	SER
55	M9	154	ALA
57	N1	18	ASP
5	s3	33	GLY
6	s4	30	ARG
6	s4	93	ASP
8	s6	70	PRO
8	s6	104	PRO

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Mol	Chain	Res	Type
13	c1	119	VAL
14	c2	87	PRO
15	c3	29	SER
15	c3	60	VAL
17	c5	14	THR
17	c5	52	LYS
18	c6	106	LYS
19	c7	15	ALA
20	c8	9	GLY
23	d1	82	VAL
27	d5	83	LEU
27	d5	103	ARG
28	d6	16	GLY
30	d8	6	PRO
80	e0	47	VAL
33	e1	112	GLY
34	sR	248	ASN
39	l2	240	ALA
40	l3	289	ASP
41	l4	43	ASN
41	l4	144	LYS
44	l7	228	SER
45	l8	237	ILE
47	m0	170	LYS
47	m0	176	LEU
53	m7	37	ASN
61	n5	57	LEU
68	o2	5	PRO
74	o8	37	PRO
78	q2	78	LYS
8	S6	69	LEU
14	C2	89	ILE
25	D3	41	SER
34	SR	67	ILE
40	L3	185	GLY
46	L9	98	PRO
65	N9	21	ILE
10	s8	50	GLY
18	c6	40	GLU
43	l6	171	PRO
51	m5	74	PRO
2	S0	189	VAL

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Mol	Chain	Res	Type
3	S1	215	VAL
6	S4	233	LYS
10	S8	50	GLY
14	C2	22	VAL
14	C2	37	VAL
16	C4	109	GLY
18	C6	40	GLU
22	D0	106	ILE
40	L3	317	ILE
41	L4	181	VAL
59	N3	3	GLY
69	O3	25	PRO
4	s2	83	ILE
8	s6	165	GLY
15	c3	82	PRO
18	c6	4	VAL
35	sM	172	VAL
39	l2	141	PRO
49	m3	50	PRO
61	n5	44	PRO
61	n5	115	ARG
64	n8	70	LYS
3	S1	210	ILE
3	S1	226	GLY
6	S4	193	GLY
14	C2	87	PRO
15	C3	122	ILE
15	C3	137	PRO
31	D9	11	PRO
47	M0	114	GLY
55	M9	129	GLY
69	O3	90	PRO
5	s3	180	GLY
13	c1	113	PRO
80	e0	50	VAL
42	l5	125	VAL
45	l8	239	GLY
48	m1	7	ASN
58	n2	27	VAL
7	S5	153	GLY
16	C4	96	PRO
30	D8	20	GLY

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Mol	Chain	Res	Type
42	L5	148	ILE
52	M6	110	PRO
60	N4	10	GLY
65	N9	29	TYR
2	s0	152	PRO
4	s2	93	GLY
6	s4	243	GLY
19	c7	117	LEU
60	n4	132	GLY
69	o3	59	VAL
81	p0	70	LEU
14	C2	116	VAL
4	s2	182	PRO
41	l4	277	PRO
69	o3	61	GLY

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%)	135 (82%)	29 (18%)	2	9
2	s0	165/209 (79%)	134 (81%)	31 (19%)	1	8
3	S1	191/223 (86%)	154 (81%)	37 (19%)	1	7
3	s1	192/223 (86%)	155 (81%)	37 (19%)	1	8
4	S2	176/204 (86%)	138 (78%)	38 (22%)	1	5
4	s2	176/204 (86%)	131 (74%)	45 (26%)	0	2
5	S3	182/194 (94%)	145 (80%)	37 (20%)	1	6
5	s3	182/194 (94%)	141 (78%)	41 (22%)	1	4
6	S4	221/221 (100%)	170 (77%)	51 (23%)	1	3
6	s4	221/221 (100%)	183 (83%)	38 (17%)	2	10
7	S5	173/190 (91%)	137 (79%)	36 (21%)	1	6
7	s5	173/190 (91%)	141 (82%)	32 (18%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	S6	188/201 (94%)	154 (82%)	34 (18%)	1	8
8	s6	187/201 (93%)	153 (82%)	34 (18%)	1	8
9	S7	165/169 (98%)	136 (82%)	29 (18%)	2	9
9	s7	165/169 (98%)	142 (86%)	23 (14%)	3	16
10	S8	150/161 (93%)	129 (86%)	21 (14%)	3	16
10	s8	150/161 (93%)	124 (83%)	26 (17%)	2	10
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	3
11	s9	158/165 (96%)	128 (81%)	30 (19%)	1	8
12	C0	77/98 (79%)	66 (86%)	11 (14%)	3	15
12	c0	73/98 (74%)	58 (80%)	15 (20%)	1	6
13	C1	129/136 (95%)	111 (86%)	18 (14%)	3	16
13	c1	129/136 (95%)	99 (77%)	30 (23%)	1	3
14	C2	88/118 (75%)	69 (78%)	19 (22%)	1	5
14	c2	88/118 (75%)	62 (70%)	26 (30%)	0	1
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	6
15	c3	127/127 (100%)	102 (80%)	25 (20%)	1	7
16	C4	81/104 (78%)	58 (72%)	23 (28%)	0	1
16	c4	97/104 (93%)	77 (79%)	20 (21%)	1	6
17	C5	101/117 (86%)	87 (86%)	14 (14%)	3	16
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	9
18	C6	117/118 (99%)	92 (79%)	25 (21%)	1	5
18	c6	118/118 (100%)	95 (80%)	23 (20%)	1	7
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1	4
19	c7	92/124 (74%)	73 (79%)	19 (21%)	1	6
20	C8	128/128 (100%)	97 (76%)	31 (24%)	0	2
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	3
21	C9	115/115 (100%)	87 (76%)	28 (24%)	0	2
21	c9	115/115 (100%)	97 (84%)	18 (16%)	2	12
22	D0	100/113 (88%)	80 (80%)	20 (20%)	1	6
22	d0	103/113 (91%)	77 (75%)	26 (25%)	0	2
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	d1	74/74 (100%)	55 (74%)	19 (26%)	0	2
24	D2	110/110 (100%)	89 (81%)	21 (19%)	1	8
24	d2	110/110 (100%)	95 (86%)	15 (14%)	3	17
25	D3	119/119 (100%)	95 (80%)	24 (20%)	1	6
25	d3	119/119 (100%)	97 (82%)	22 (18%)	1	8
26	D4	112/112 (100%)	95 (85%)	17 (15%)	3	13
26	d4	112/112 (100%)	94 (84%)	18 (16%)	2	11
27	D5	61/88 (69%)	49 (80%)	12 (20%)	1	7
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	11
28	D6	83/83 (100%)	65 (78%)	18 (22%)	1	5
28	d6	83/83 (100%)	73 (88%)	10 (12%)	5	22
29	D7	70/70 (100%)	59 (84%)	11 (16%)	2	12
29	d7	70/70 (100%)	60 (86%)	10 (14%)	3	15
30	D8	56/59 (95%)	41 (73%)	15 (27%)	0	2
30	d8	56/59 (95%)	42 (75%)	14 (25%)	0	2
31	D9	47/48 (98%)	38 (81%)	9 (19%)	1	8
31	d9	47/48 (98%)	36 (77%)	11 (23%)	1	3
32	E0	51/51 (100%)	43 (84%)	8 (16%)	2	12
33	E1	62/66 (94%)	47 (76%)	15 (24%)	0	2
33	e1	66/66 (100%)	47 (71%)	19 (29%)	0	1
34	SR	260/261 (100%)	213 (82%)	47 (18%)	1	8
34	sR	260/261 (100%)	232 (89%)	28 (11%)	6	27
35	SM	97/228 (42%)	69 (71%)	28 (29%)	0	1
35	sM	54/228 (24%)	40 (74%)	14 (26%)	0	2
39	L2	193/195 (99%)	153 (79%)	40 (21%)	1	6
39	l2	192/195 (98%)	149 (78%)	43 (22%)	1	4
40	L3	320/322 (99%)	251 (78%)	69 (22%)	1	5
40	l3	320/322 (99%)	258 (81%)	62 (19%)	1	7
41	L4	288/288 (100%)	225 (78%)	63 (22%)	1	5
41	l4	288/288 (100%)	230 (80%)	58 (20%)	1	6
42	L5	244/244 (100%)	197 (81%)	47 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	l5	243/244 (100%)	191 (79%)	52 (21%)	1	5
43	L6	134/152 (88%)	118 (88%)	16 (12%)	5	22
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	10
44	L7	186/204 (91%)	165 (89%)	21 (11%)	6	25
44	l7	187/204 (92%)	158 (84%)	29 (16%)	2	12
45	L8	187/207 (90%)	151 (81%)	36 (19%)	1	8
45	l8	177/207 (86%)	141 (80%)	36 (20%)	1	6
46	L9	171/171 (100%)	137 (80%)	34 (20%)	1	6
46	l9	171/171 (100%)	123 (72%)	48 (28%)	0	1
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	5
47	m0	179/186 (96%)	145 (81%)	34 (19%)	1	8
48	M1	147/150 (98%)	123 (84%)	24 (16%)	2	11
48	m1	147/150 (98%)	115 (78%)	32 (22%)	1	5
49	M3	154/158 (98%)	123 (80%)	31 (20%)	1	6
49	m3	154/158 (98%)	124 (80%)	30 (20%)	1	7
50	M4	107/108 (99%)	87 (81%)	20 (19%)	1	8
50	m4	108/108 (100%)	81 (75%)	27 (25%)	0	2
51	M5	175/175 (100%)	143 (82%)	32 (18%)	1	8
51	m5	175/175 (100%)	142 (81%)	33 (19%)	1	8
52	M6	160/161 (99%)	141 (88%)	19 (12%)	5	22
52	m6	160/161 (99%)	130 (81%)	30 (19%)	1	8
53	M7	140/145 (97%)	107 (76%)	33 (24%)	1	3
53	m7	125/145 (86%)	100 (80%)	25 (20%)	1	6
54	M8	150/150 (100%)	126 (84%)	24 (16%)	2	11
54	m8	150/150 (100%)	122 (81%)	28 (19%)	1	8
55	M9	153/153 (100%)	121 (79%)	32 (21%)	1	6
55	m9	153/153 (100%)	123 (80%)	30 (20%)	1	7
56	N0	156/156 (100%)	127 (81%)	29 (19%)	1	8
56	n0	156/156 (100%)	122 (78%)	34 (22%)	1	5
57	N1	136/136 (100%)	111 (82%)	25 (18%)	1	8
57	n1	136/136 (100%)	108 (79%)	28 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	N2	87/106 (82%)	70 (80%)	17 (20%)	1	7
58	n2	85/106 (80%)	70 (82%)	15 (18%)	2	9
59	N3	104/104 (100%)	87 (84%)	17 (16%)	2	11
59	n3	104/104 (100%)	89 (86%)	15 (14%)	3	15
60	N4	57/129 (44%)	51 (90%)	6 (10%)	7	28
60	n4	100/129 (78%)	82 (82%)	18 (18%)	1	9
61	N5	104/117 (89%)	84 (81%)	20 (19%)	1	8
61	n5	104/117 (89%)	82 (79%)	22 (21%)	1	5
62	N6	109/109 (100%)	85 (78%)	24 (22%)	1	5
62	n6	109/109 (100%)	86 (79%)	23 (21%)	1	6
63	N7	115/115 (100%)	93 (81%)	22 (19%)	1	8
63	n7	115/115 (100%)	89 (77%)	26 (23%)	1	4
64	N8	118/118 (100%)	95 (80%)	23 (20%)	1	7
64	n8	118/118 (100%)	99 (84%)	19 (16%)	2	11
65	N9	46/46 (100%)	33 (72%)	13 (28%)	0	1
65	n9	46/46 (100%)	32 (70%)	14 (30%)	0	0
66	O0	81/87 (93%)	64 (79%)	17 (21%)	1	6
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1	6
67	O1	92/96 (96%)	74 (80%)	18 (20%)	1	7
67	o1	94/96 (98%)	68 (72%)	26 (28%)	0	1
68	O2	109/110 (99%)	88 (81%)	21 (19%)	1	8
68	o2	109/110 (99%)	81 (74%)	28 (26%)	0	2
69	O3	90/90 (100%)	75 (83%)	15 (17%)	2	10
69	o3	90/90 (100%)	75 (83%)	15 (17%)	2	10
70	O4	95/102 (93%)	74 (78%)	21 (22%)	1	4
70	o4	95/102 (93%)	77 (81%)	18 (19%)	1	8
71	O5	104/104 (100%)	81 (78%)	23 (22%)	1	4
71	o5	103/104 (99%)	78 (76%)	25 (24%)	0	2
72	O6	81/81 (100%)	59 (73%)	22 (27%)	0	1
72	o6	80/81 (99%)	51 (64%)	29 (36%)	0	0
73	O7	70/70 (100%)	52 (74%)	18 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	o7	70/70 (100%)	57 (81%)	13 (19%)	1	8
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	3
74	o8	67/68 (98%)	51 (76%)	16 (24%)	0	3
75	O9	45/45 (100%)	38 (84%)	7 (16%)	2	12
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	9
76	Q0	47/47 (100%)	36 (77%)	11 (23%)	1	3
76	q0	47/47 (100%)	35 (74%)	12 (26%)	0	2
77	Q1	23/23 (100%)	18 (78%)	5 (22%)	1	5
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	0
78	Q2	90/90 (100%)	69 (77%)	21 (23%)	1	3
78	q2	90/90 (100%)	74 (82%)	16 (18%)	2	9
79	Q3	71/71 (100%)	55 (78%)	16 (22%)	1	4
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1	4
80	e0	53/53 (100%)	40 (76%)	13 (24%)	0	2
81	p0	105/253 (42%)	85 (81%)	20 (19%)	1	8
All	All	18728/20241 (92%)	15006 (80%)	3722 (20%)	1	6

All (3722) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	9	LEU
2	S0	12	GLU
2	S0	28	ASN
2	S0	32	HIS
2	S0	37	VAL
2	S0	41	ARG
2	S0	56	LYS
2	S0	72	ASP
2	S0	76	ILE
2	S0	80	THR
2	S0	84	ARG
2	S0	86	VAL
2	S0	88	LYS
2	S0	96	THR
2	S0	103	THR
2	S0	110	TYR
2	S0	111	ILE

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Mol	Chain	Res	Type
2	S0	119	ARG
2	S0	123	VAL
2	S0	146	LEU
2	S0	157	ASP
2	S0	165	ARG
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	39	GLU
3	S1	42	ASN
3	S1	46	THR
3	S1	47	LEU
3	S1	51	SER
3	S1	61	LEU
3	S1	65	VAL
3	S1	70	LEU
3	S1	77	GLU
3	S1	81	PHE
3	S1	89	ASP
3	S1	96	LEU
3	S1	97	LEU
3	S1	101	HIS
3	S1	105	PHE
3	S1	111	ARG
3	S1	115	ARG
3	S1	117	TRP
3	S1	125	VAL
3	S1	135	LEU
3	S1	144	ARG
3	S1	154	SER
3	S1	170	GLU
3	S1	181	LEU
3	S1	184	LEU
3	S1	202	LYS

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Mol	Chain	Res	Type
3	S1	214	LYS
3	S1	215	VAL
3	S1	218	LEU
3	S1	219	LYS
3	S1	220	GLN
3	S1	223	PHE
3	S1	231	LEU
4	S2	41	LEU
4	S2	54	GLU
4	S2	69	ILE
4	S2	70	ASP
4	S2	72	LEU
4	S2	73	LEU
4	S2	76	LEU
4	S2	77	GLN
4	S2	89	GLN
4	S2	91	ARG
4	S2	94	GLN
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	99	LYS
4	S2	106	ASP
4	S2	111	VAL
4	S2	113	LEU
4	S2	117	THR
4	S2	134	LEU
4	S2	137	ILE
4	S2	139	ILE
4	S2	148	LEU
4	S2	153	SER
4	S2	157	LYS
4	S2	159	THR
4	S2	166	THR
4	S2	195	ASP
4	S2	198	THR
4	S2	207	LEU
4	S2	221	THR
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	235	LEU

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Mol	Chain	Res	Type
4	S2	237	VAL
4	S2	245	ASP
4	S2	250	GLN
5	S3	4	LEU
5	S3	6	SER
5	S3	7	LYS
5	S3	9	ARG
5	S3	21	LEU
5	S3	26	THR
5	S3	27	ARG
5	S3	37	VAL
5	S3	65	ARG
5	S3	66	ILE
5	S3	76	ARG
5	S3	84	ILE
5	S3	89	GLU
5	S3	90	ARG
5	S3	94	ARG
5	S3	103	GLU
5	S3	105	MET
5	S3	110	LEU
5	S3	111	ASN
5	S3	113	LEU
5	S3	116	ARG
5	S3	117	ARG
5	S3	124	ARG
5	S3	134	CYS
5	S3	137	VAL
5	S3	141	LYS
5	S3	146	ARG
5	S3	148	LYS
5	S3	151	LYS
5	S3	158	ILE
5	S3	172	THR
5	S3	174	HIS
5	S3	176	LEU
5	S3	178	ARG
5	S3	200	LYS
5	S3	209	ILE
5	S3	218	LEU
6	S4	5	PRO
6	S4	9	LEU

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Mol	Chain	Res	Type
6	S4	12	LEU
6	S4	21	ASP
6	S4	23	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	42	LEU
6	S4	48	LEU
6	S4	56	LEU
6	S4	67	GLN
6	S4	70	VAL
6	S4	77	ARG
6	S4	78	THR
6	S4	92	LEU
6	S4	93	ASP
6	S4	95	THR
6	S4	102	VAL
6	S4	113	ARG
6	S4	116	ASP
6	S4	117	GLU
6	S4	123	LEU
6	S4	131	LEU
6	S4	133	LYS
6	S4	134	LYS
6	S4	153	ASN
6	S4	158	ASP
6	S4	160	VAL
6	S4	176	ASP
6	S4	179	LYS
6	S4	180	LEU
6	S4	181	VAL
6	S4	182	TYR
6	S4	187	ARG
6	S4	192	ILE
6	S4	197	HIS
6	S4	202	ASP
6	S4	206	ASP
6	S4	210	ILE
6	S4	211	LYS
6	S4	215	ASP
6	S4	221	ARG
6	S4	226	PHE
6	S4	227	VAL

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Mol	Chain	Res	Type
6	S4	228	ILE
6	S4	236	ILE
6	S4	240	LYS
6	S4	242	LYS
6	S4	247	SER
6	S4	248	ILE
6	S4	259	GLN
7	S5	25	LEU
7	S5	32	GLU
7	S5	38	THR
7	S5	42	LEU
7	S5	43	PHE
7	S5	45	LYS
7	S5	46	TRP
7	S5	48	PHE
7	S5	53	VAL
7	S5	63	GLN
7	S5	65	ARG
7	S5	66	GLN
7	S5	79	ASN
7	S5	86	GLN
7	S5	89	ILE
7	S5	90	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	97	LEU
7	S5	99	MET
7	S5	122	ASN
7	S5	128	ASN
7	S5	137	ILE
7	S5	139	ASN
7	S5	146	THR
7	S5	147	THR
7	S5	148	ARG
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	162	VAL
7	S5	186	ASN
7	S5	190	ILE
7	S5	194	LEU
7	S5	203	LYS

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Mol	Chain	Res	Type
7	S5	216	GLU
8	S6	5	ILE
8	S6	6	SER
8	S6	25	ARG
8	S6	29	ASP
8	S6	44	GLU
8	S6	56	ASN
8	S6	59	GLN
8	S6	65	GLN
8	S6	67	VAL
8	S6	78	THR
8	S6	79	LYS
8	S6	81	VAL
8	S6	82	SER
8	S6	89	ASP
8	S6	94	ARG
8	S6	109	LEU
8	S6	120	GLU
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	129	VAL
8	S6	133	LEU
8	S6	143	LYS
8	S6	151	ASP
8	S6	154	ARG
8	S6	162	VAL
8	S6	169	TYR
8	S6	170	THR
8	S6	175	ILE
8	S6	177	ARG
8	S6	190	GLN
8	S6	210	GLN
8	S6	211	LEU
8	S6	223	LYS
9	S7	14	THR
9	S7	15	GLU
9	S7	16	LEU
9	S7	22	GLN
9	S7	37	GLU
9	S7	38	LEU
9	S7	50	ASP

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Mol	Chain	Res	Type
9	S7	51	VAL
9	S7	60	ILE
9	S7	70	PHE
9	S7	75	THR
9	S7	77	LEU
9	S7	85	PHE
9	S7	97	ARG
9	S7	99	LEU
9	S7	104	ARG
9	S7	110	GLN
9	S7	114	ARG
9	S7	116	ARG
9	S7	117	THR
9	S7	126	LEU
9	S7	130	VAL
9	S7	133	THR
9	S7	136	VAL
9	S7	141	ARG
9	S7	144	VAL
9	S7	147	ASN
9	S7	149	ILE
9	S7	184	GLU
10	S8	4	SER
10	S8	8	ARG
10	S8	14	THR
10	S8	21	PHE
10	S8	22	ARG
10	S8	29	LEU
10	S8	36	THR
10	S8	56	ARG
10	S8	58	LEU
10	S8	66	SER
10	S8	69	SER
10	S8	70	GLU
10	S8	72	ILE
10	S8	82	VAL
10	S8	97	THR
10	S8	138	ASN
10	S8	152	ILE
10	S8	164	ARG
10	S8	184	LEU
10	S8	187	GLU

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Mol	Chain	Res	Type
10	S8	196	LEU
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR
11	S9	9	SER
11	S9	14	THR
11	S9	28	LEU
11	S9	30	LEU
11	S9	33	GLU
11	S9	39	LYS
11	S9	46	SER
11	S9	62	ARG
11	S9	63	ASP
11	S9	78	ARG
11	S9	79	ARG
11	S9	82	ARG
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	97	LEU
11	S9	99	LEU
11	S9	101	VAL
11	S9	118	LEU
11	S9	121	SER
11	S9	126	ARG
11	S9	130	THR
11	S9	134	ILE
11	S9	138	LYS
11	S9	140	ILE
11	S9	143	ILE
11	S9	149	ARG
11	S9	155	HIS
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	7	ASP
12	C0	20	VAL
12	C0	27	PHE
12	C0	32	HIS

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Mol	Chain	Res	Type
12	C0	49	LEU
12	C0	55	VAL
12	C0	56	LYS
12	C0	58	GLN
12	C0	76	LEU
12	C0	78	GLU
12	C0	82	LEU
13	C1	8	GLN
13	C1	21	ASN
13	C1	25	VAL
13	C1	29	LYS
13	C1	40	LEU
13	C1	44	THR
13	C1	67	ARG
13	C1	69	LYS
13	C1	74	THR
13	C1	79	LYS
13	C1	83	THR
13	C1	91	LEU
13	C1	94	ILE
13	C1	99	ARG
13	C1	100	TYR
13	C1	112	SER
13	C1	118	GLN
13	C1	140	VAL
14	C2	33	ARG
14	C2	36	LEU
14	C2	37	VAL
14	C2	43	ARG
14	C2	46	ARG
14	C2	50	LYS
14	C2	52	LEU
14	C2	54	ARG
14	C2	66	VAL
14	C2	71	ILE
14	C2	74	LEU
14	C2	89	ILE
14	C2	103	LEU
14	C2	121	VAL
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU

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Mol	Chain	Res	Type
14	C2	138	GLU
14	C2	139	HIS
15	C3	6	SER
15	C3	12	SER
15	C3	13	SER
15	C3	16	ILE
15	C3	27	LYS
15	C3	32	SER
15	C3	39	LYS
15	C3	42	ARG
15	C3	45	LEU
15	C3	46	THR
15	C3	64	ARG
15	C3	66	ILE
15	C3	76	LYS
15	C3	83	GLU
15	C3	88	LEU
15	C3	102	LEU
15	C3	107	LYS
15	C3	110	ASP
15	C3	114	ARG
15	C3	115	LEU
15	C3	125	LEU
15	C3	131	THR
15	C3	140	LYS
15	C3	143	SER
15	C3	149	LEU
15	C3	151	ASN
16	C4	11	SER
16	C4	13	VAL
16	C4	16	VAL
16	C4	20	TYR
16	C4	22	SER
16	C4	24	ASN
16	C4	29	HIS
16	C4	30	VAL
16	C4	31	THR
16	C4	42	VAL
16	C4	43	THR
16	C4	51	ASP
16	C4	76	ILE
16	C4	89	THR

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Mol	Chain	Res	Type
16	C4	92	LYS
16	C4	93	THR
16	C4	102	LEU
16	C4	103	ARG
16	C4	118	VAL
16	C4	123	SER
16	C4	125	SER
16	C4	136	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	22	LEU
17	C5	26	LEU
17	C5	36	LEU
17	C5	43	ARG
17	C5	44	ARG
17	C5	47	ARG
17	C5	52	LYS
17	C5	80	MET
17	C5	94	VAL
17	C5	110	GLU
17	C5	121	ILE
17	C5	124	THR
17	C5	130	ARG
18	C6	15	SER
18	C6	26	LYS
18	C6	29	ILE
18	C6	40	GLU
18	C6	43	ILE
18	C6	54	LEU
18	C6	58	ASP
18	C6	65	ILE
18	C6	66	ARG
18	C6	68	ARG
18	C6	69	VAL
18	C6	98	ASP
18	C6	104	GLU
18	C6	106	LYS
18	C6	114	ARG
18	C6	115	THR
18	C6	116	LEU
18	C6	118	ILE
18	C6	121	SER

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Mol	Chain	Res	Type
18	C6	123	ARG
18	C6	128	LYS
18	C6	137	ARG
18	C6	138	PHE
18	C6	139	GLN
18	C6	143	ARG
19	C7	6	THR
19	C7	10	LYS
19	C7	25	THR
19	C7	26	LEU
19	C7	34	LEU
19	C7	38	ILE
19	C7	40	THR
19	C7	46	LEU
19	C7	49	LYS
19	C7	54	THR
19	C7	55	THR
19	C7	69	ILE
19	C7	72	LYS
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	88	VAL
19	C7	105	GLN
19	C7	113	LEU
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	6	GLN
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	17	LEU
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	36	LYS
20	C8	40	ARG
20	C8	54	LEU
20	C8	60	GLU

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Mol	Chain	Res	Type
20	C8	61	LEU
20	C8	71	GLN
20	C8	80	LYS
20	C8	82	PRO
20	C8	89	GLN
20	C8	92	ILE
20	C8	101	LEU
20	C8	108	LYS
20	C8	114	GLU
20	C8	120	ARG
20	C8	132	ARG
20	C8	133	VAL
20	C8	136	GLN
20	C8	138	THR
20	C8	141	THR
20	C8	143	ARG
21	C9	4	VAL
21	C9	6	VAL
21	C9	18	TYR
21	C9	22	LEU
21	C9	25	GLN
21	C9	27	LYS
21	C9	28	LEU
21	C9	29	GLU
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	38	LYS
21	C9	57	ARG
21	C9	63	ARG
21	C9	67	MET
21	C9	68	ARG
21	C9	70	GLN
21	C9	84	LYS
21	C9	94	ILE
21	C9	97	SER
21	C9	105	LEU
21	C9	122	ARG
21	C9	123	ARG
21	C9	130	ARG
21	C9	131	ASP

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Mol	Chain	Res	Type
21	C9	132	LEU
21	C9	133	ASP
22	D0	23	ARG
22	D0	25	THR
22	D0	27	THR
22	D0	30	LYS
22	D0	47	GLN
22	D0	50	LEU
22	D0	51	VAL
22	D0	57	ARG
22	D0	61	LYS
22	D0	66	SER
22	D0	67	THR
22	D0	68	ARG
22	D0	72	ASN
22	D0	74	GLU
22	D0	81	THR
22	D0	82	TYR
22	D0	89	ARG
22	D0	99	ILE
22	D0	103	ILE
22	D0	117	VAL
23	D1	3	ASN
23	D1	5	LYS
23	D1	7	GLN
23	D1	11	LEU
23	D1	12	TYR
23	D1	18	SER
23	D1	33	GLN
23	D1	36	VAL
23	D1	41	GLU
23	D1	49	GLU
23	D1	52	THR
23	D1	68	SER
23	D1	69	LEU
23	D1	72	LEU
23	D1	78	LEU
23	D1	82	VAL
24	D2	2	THR
24	D2	12	ASN
24	D2	15	ASN
24	D2	24	GLN

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Mol	Chain	Res	Type
24	D2	25	VAL
24	D2	26	LEU
24	D2	27	ILE
24	D2	37	PHE
24	D2	53	ILE
24	D2	65	LEU
24	D2	74	VAL
24	D2	81	VAL
24	D2	87	GLU
24	D2	93	LEU
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR
24	D2	106	THR
24	D2	121	VAL
24	D2	129	VAL
25	D3	7	ARG
25	D3	9	LEU
25	D3	19	ARG
25	D3	26	GLU
25	D3	28	ASN
25	D3	33	LEU
25	D3	41	SER
25	D3	47	SER
25	D3	69	ARG
25	D3	72	VAL
25	D3	78	LYS
25	D3	79	ASN
25	D3	84	THR
25	D3	96	VAL
25	D3	97	ASP
25	D3	102	VAL
25	D3	103	LEU
25	D3	107	PHE
25	D3	110	LYS
25	D3	114	LYS
25	D3	125	VAL
25	D3	127	VAL
25	D3	132	LEU
25	D3	136	TRP
26	D4	2	SER

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Mol	Chain	Res	Type
26	D4	14	SER
26	D4	28	LEU
26	D4	34	ASN
26	D4	36	SER
26	D4	40	LEU
26	D4	51	GLU
26	D4	52	LYS
26	D4	61	ARG
26	D4	62	THR
26	D4	74	LEU
26	D4	81	GLU
26	D4	83	LYS
26	D4	88	THR
26	D4	102	LYS
26	D4	124	ARG
26	D4	127	LYS
27	D5	37	GLN
27	D5	42	LEU
27	D5	63	SER
27	D5	67	ASP
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	78	ILE
27	D5	85	LYS
27	D5	92	ILE
27	D5	95	HIS
27	D5	96	SER
28	D6	4	LYS
28	D6	19	LYS
28	D6	32	LYS
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	44	ILE
28	D6	45	VAL
28	D6	46	GLU
28	D6	61	GLU
28	D6	66	LYS
28	D6	67	THR
28	D6	68	TYR
28	D6	70	LYS

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Mol	Chain	Res	Type
28	D6	82	ARG
28	D6	83	ILE
28	D6	85	ARG
28	D6	88	SER
29	D7	3	LEU
29	D7	17	ARG
29	D7	24	LEU
29	D7	29	ARG
29	D7	33	LEU
29	D7	34	ASP
29	D7	41	LEU
29	D7	43	ILE
29	D7	62	ILE
29	D7	65	THR
29	D7	72	LYS
30	D8	12	VAL
30	D8	13	ILE
30	D8	19	THR
30	D8	28	VAL
30	D8	30	VAL
30	D8	32	PHE
30	D8	34	GLU
30	D8	36	THR
30	D8	38	ARG
30	D8	40	ILE
30	D8	49	ARG
30	D8	57	MET
30	D8	58	GLU
30	D8	61	ARG
30	D8	64	ARG
31	D9	5	ASN
31	D9	7	TRP
31	D9	12	ARG
31	D9	19	ARG
31	D9	25	SER
31	D9	28	THR
31	D9	32	ARG
31	D9	36	LEU
31	D9	39	CYS
32	E0	3	LYS
32	E0	20	LYS
32	E0	21	VAL

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Mol	Chain	Res	Type
32	E0	22	GLU
32	E0	41	THR
32	E0	42	ARG
32	E0	47	VAL
32	E0	49	LEU
33	E1	84	VAL
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	94	LYS
33	E1	97	LYS
33	E1	100	LEU
33	E1	108	VAL
33	E1	113	LYS
33	E1	118	ARG
33	E1	120	GLU
33	E1	137	ASP
33	E1	139	LEU
33	E1	140	TYR
33	E1	146	SER
34	SR	21	THR
34	SR	29	GLN
34	SR	37	SER
34	SR	39	ASP
34	SR	52	GLN
34	SR	58	VAL
34	SR	59	ARG
34	SR	62	LYS
34	SR	72	THR
34	SR	76	ASP
34	SR	81	LEU
34	SR	82	SER
34	SR	88	THR
34	SR	94	VAL
34	SR	98	GLU
34	SR	108	SER
34	SR	117	LYS
34	SR	136	ILE
34	SR	141	LEU
34	SR	144	LEU
34	SR	145	LEU
34	SR	148	ASN

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Mol	Chain	Res	Type
34	SR	149	ASP
34	SR	153	GLN
34	SR	154	VAL
34	SR	159	ASN
34	SR	165	ASP
34	SR	184	ASN
34	SR	187	GLN
34	SR	188	ILE
34	SR	193	ILE
34	SR	199	ILE
34	SR	200	ASN
34	SR	201	THR
34	SR	213	SER
34	SR	231	MET
34	SR	232	TYR
34	SR	235	SER
34	SR	238	ASP
34	SR	242	SER
34	SR	248	ASN
34	SR	258	THR
34	SR	266	ASP
34	SR	268	GLN
34	SR	300	THR
34	SR	309	VAL
34	SR	312	VAL
35	SM	23	LYS
35	SM	24	GLU
35	SM	27	LYS
35	SM	28	SER
35	SM	41	SER
35	SM	45	SER
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	72	ARG
35	SM	74	LYS
35	SM	77	THR
35	SM	83	LYS
35	SM	84	LYS

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Mol	Chain	Res	Type
35	SM	89	ARG
35	SM	91	THR
35	SM	94	HIS
35	SM	100	THR
35	SM	105	LYS
35	SM	106	VAL
35	SM	116	GLU
35	SM	122	GLU
35	SM	130	GLU
35	SM	133	GLU
35	SM	139	GLU
39	L2	18	SER
39	L2	20	THR
39	L2	23	ARG
39	L2	28	LYS
39	L2	31	THR
39	L2	32	LEU
39	L2	42	ARG
39	L2	44	ILE
39	L2	45	VAL
39	L2	49	VAL
39	L2	62	VAL
39	L2	70	ARG
39	L2	71	LEU
39	L2	73	GLU
39	L2	74	GLU
39	L2	82	VAL
39	L2	95	SER
39	L2	101	VAL
39	L2	104	LEU
39	L2	106	SER
39	L2	114	SER
39	L2	116	VAL
39	L2	134	VAL
39	L2	143	GLU
39	L2	165	VAL
39	L2	169	ILE
39	L2	175	VAL
39	L2	177	LYS
39	L2	179	LEU
39	L2	180	LEU
39	L2	188	LYS

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Mol	Chain	Res	Type
39	L2	190	ARG
39	L2	192	LYS
39	L2	202	VAL
39	L2	204	MET
39	L2	207	VAL
39	L2	225	ILE
39	L2	227	ARG
39	L2	230	VAL
39	L2	247	ARG
40	L3	7	GLU
40	L3	10	ARG
40	L3	17	LEU
40	L3	19	ARG
40	L3	24	SER
40	L3	25	ILE
40	L3	30	LYS
40	L3	37	ARG
40	L3	39	LYS
40	L3	46	PHE
40	L3	47	LEU
40	L3	56	ILE
40	L3	65	SER
40	L3	66	LYS
40	L3	70	ARG
40	L3	81	THR
40	L3	83	PRO
40	L3	84	VAL
40	L3	85	VAL
40	L3	86	VAL
40	L3	87	VAL
40	L3	100	ARG
40	L3	103	THR
40	L3	114	VAL
40	L3	115	LYS
40	L3	128	LYS
40	L3	134	SER
40	L3	139	GLN
40	L3	140	ASP
40	L3	146	ARG
40	L3	148	LEU
40	L3	156	SER
40	L3	167	ARG

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Mol	Chain	Res	Type
40	L3	169	THR
40	L3	173	GLN
40	L3	183	LEU
40	L3	188	ILE
40	L3	192	VAL
40	L3	196	ARG
40	L3	200	GLU
40	L3	202	THR
40	L3	208	VAL
40	L3	210	GLU
40	L3	211	GLN
40	L3	212	ASN
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	237	LYS
40	L3	238	LEU
40	L3	241	LYS
40	L3	252	ILE
40	L3	263	SER
40	L3	264	VAL
40	L3	266	ARG
40	L3	275	ARG
40	L3	284	ARG
40	L3	287	LYS
40	L3	289	ASP
40	L3	291	GLU
40	L3	305	ILE
40	L3	308	MET
40	L3	324	VAL
40	L3	332	ARG
40	L3	347	SER
40	L3	354	VAL
40	L3	355	SER
40	L3	361	THR
40	L3	382	THR
41	L4	3	ARG
41	L4	4	PRO
41	L4	18	ASN
41	L4	20	LEU
41	L4	34	ILE
41	L4	36	HIS

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Mol	Chain	Res	Type
41	L4	37	THR
41	L4	55	LYS
41	L4	60	THR
41	L4	64	SER
41	L4	71	VAL
41	L4	73	ARG
41	L4	74	ILE
41	L4	84	ARG
41	L4	85	SER
41	L4	93	MET
41	L4	108	LYS
41	L4	112	LYS
41	L4	120	TYR
41	L4	124	SER
41	L4	138	ARG
41	L4	142	VAL
41	L4	144	LYS
41	L4	147	GLU
41	L4	148	ILE
41	L4	150	LEU
41	L4	152	VAL
41	L4	156	LEU
41	L4	161	LYS
41	L4	170	LYS
41	L4	172	VAL
41	L4	179	LEU
41	L4	182	LEU
41	L4	186	LYS
41	L4	187	LEU
41	L4	188	ARG
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	206	LEU
41	L4	211	GLU
41	L4	222	VAL
41	L4	230	VAL
41	L4	246	ARG
41	L4	256	THR
41	L4	258	LEU
41	L4	265	GLU
41	L4	266	THR

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Mol	Chain	Res	Type
41	L4	267	VAL
41	L4	270	SER
41	L4	287	THR
41	L4	292	SER
41	L4	306	THR
41	L4	307	GLN
41	L4	311	HIS
41	L4	313	LEU
41	L4	319	LYS
41	L4	321	LYS
41	L4	323	VAL
41	L4	339	LEU
41	L4	346	LYS
41	L4	350	LYS
41	L4	354	VAL
42	L5	4	GLN
42	L5	5	LYS
42	L5	10	SER
42	L5	22	ARG
42	L5	23	ARG
42	L5	32	GLN
42	L5	35	ARG
42	L5	41	LYS
42	L5	66	SER
42	L5	69	ILE
42	L5	92	LEU
42	L5	105	ILE
42	L5	109	THR
42	L5	112	LYS
42	L5	115	LEU
42	L5	118	THR
42	L5	122	VAL
42	L5	131	LEU
42	L5	132	THR
42	L5	140	ARG
42	L5	146	LEU
42	L5	148	ILE
42	L5	151	GLN
42	L5	152	ARG
42	L5	154	THR
42	L5	155	THR
42	L5	158	ARG

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Mol	Chain	Res	Type
42	L5	159	VAL
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE
42	L5	187	THR
42	L5	190	ILE
42	L5	193	GLU
42	L5	196	ARG
42	L5	197	SER
42	L5	203	HIS
42	L5	216	GLU
42	L5	222	LEU
42	L5	242	SER
42	L5	257	GLU
42	L5	258	LYS
42	L5	268	GLU
42	L5	273	ARG
42	L5	275	THR
42	L5	290	ILE
42	L5	297	GLN
43	L6	5	LYS
43	L6	19	LYS
43	L6	21	THR
43	L6	31	ARG
43	L6	35	VAL
43	L6	48	ARG
43	L6	52	VAL
43	L6	64	LEU
43	L6	65	ILE
43	L6	77	ARG
43	L6	78	ARG
43	L6	89	THR
43	L6	93	VAL
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	30	ARG
44	L7	43	ILE
44	L7	60	ARG

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Mol	Chain	Res	Type
44	L7	82	LYS
44	L7	92	ILE
44	L7	93	ASN
44	L7	100	ARG
44	L7	101	LYS
44	L7	110	ARG
44	L7	118	LYS
44	L7	124	LEU
44	L7	158	LYS
44	L7	178	ILE
44	L7	179	LEU
44	L7	180	SER
44	L7	184	LEU
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	27	THR
45	L8	38	GLN
45	L8	41	GLN
45	L8	47	SER
45	L8	51	LYS
45	L8	63	LYS
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	84	ARG
45	L8	92	LYS
45	L8	101	THR
45	L8	106	LYS
45	L8	108	ARG
45	L8	118	GLU
45	L8	132	VAL
45	L8	136	LEU
45	L8	147	LYS
45	L8	149	LYS
45	L8	150	LEU
45	L8	156	ASP
45	L8	160	ILE
45	L8	169	LEU
45	L8	180	VAL
45	L8	185	ARG
45	L8	194	THR

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Mol	Chain	Res	Type
45	L8	197	VAL
45	L8	203	VAL
45	L8	206	GLU
45	L8	218	ILE
45	L8	221	ASN
45	L8	227	ASP
45	L8	241	LYS
45	L8	246	MET
45	L8	248	LYS
46	L9	5	GLN
46	L9	7	GLU
46	L9	9	GLN
46	L9	16	VAL
46	L9	19	SER
46	L9	36	LYS
46	L9	41	ILE
46	L9	49	ASN
46	L9	52	LEU
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	72	LYS
46	L9	73	SER
46	L9	80	THR
46	L9	82	VAL
46	L9	90	MET
46	L9	106	LYS
46	L9	118	LEU
46	L9	121	LYS
46	L9	124	ARG
46	L9	132	VAL
46	L9	133	THR
46	L9	138	THR
46	L9	149	ASN
46	L9	151	VAL
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	164	ILE
46	L9	173	ARG
46	L9	188	THR
46	L9	189	GLU

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Mol	Chain	Res	Type
46	L9	190	ASP
47	M0	3	ARG
47	M0	7	ARG
47	M0	15	LYS
47	M0	24	ARG
47	M0	30	LYS
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
47	M0	52	LEU
47	M0	57	LEU
47	M0	63	GLU
47	M0	74	LYS
47	M0	76	MET
47	M0	78	THR
47	M0	87	LEU
47	M0	90	ARG
47	M0	102	MET
47	M0	116	ARG
47	M0	129	VAL
47	M0	130	ASP
47	M0	137	SER
47	M0	138	VAL
47	M0	139	ARG
47	M0	145	LYS
47	M0	156	ARG
47	M0	163	GLN
47	M0	165	ILE
47	M0	167	LEU
47	M0	174	THR
47	M0	176	LEU
47	M0	177	ASP
47	M0	178	ARG
47	M0	200	LEU
47	M0	205	SER
48	M1	9	MET
48	M1	10	ARG
48	M1	11	ASP

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Mol	Chain	Res	Type
48	M1	12	LEU
48	M1	19	LEU
48	M1	20	ASN
48	M1	28	ASP
48	M1	44	THR
48	M1	46	VAL
48	M1	65	ILE
48	M1	70	THR
48	M1	80	LEU
48	M1	94	ARG
48	M1	106	ILE
48	M1	110	ILE
48	M1	112	LEU
48	M1	119	SER
48	M1	137	ARG
48	M1	138	VAL
48	M1	140	ARG
48	M1	158	ASP
48	M1	161	SER
48	M1	165	GLN
48	M1	166	LYS
49	M3	23	LYS
49	M3	24	VAL
49	M3	34	SER
49	M3	35	ARG
49	M3	37	ASN
49	M3	41	THR
49	M3	46	ILE
49	M3	54	LEU
49	M3	55	ARG
49	M3	58	VAL
49	M3	59	ARG
49	M3	67	ARG
49	M3	70	ARG
49	M3	76	THR
49	M3	85	LEU
49	M3	114	GLN
49	M3	115	ARG
49	M3	118	GLU
49	M3	124	ILE
49	M3	129	ASN
49	M3	131	LYS

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Mol	Chain	Res	Type
49	M3	134	GLU
49	M3	144	THR
49	M3	164	GLU
49	M3	165	SER
49	M3	168	ARG
49	M3	169	THR
49	M3	170	LEU
49	M3	171	ARG
49	M3	172	LEU
49	M3	192	GLU
50	M4	3	THR
50	M4	5	SER
50	M4	20	VAL
50	M4	46	ILE
50	M4	50	LYS
50	M4	53	VAL
50	M4	58	ILE
50	M4	62	GLN
50	M4	63	VAL
50	M4	64	VAL
50	M4	69	THR
50	M4	72	LEU
50	M4	90	VAL
50	M4	91	CYS
50	M4	93	LYS
50	M4	102	LYS
50	M4	105	GLN
50	M4	132	LYS
50	M4	135	LEU
50	M4	137	LYS
51	M5	5	LYS
51	M5	10	LEU
51	M5	18	VAL
51	M5	22	LEU
51	M5	38	ARG
51	M5	50	ARG
51	M5	51	LEU
51	M5	54	LYS
51	M5	77	LYS
51	M5	80	THR
51	M5	83	LYS
51	M5	85	THR

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Mol	Chain	Res	Type
51	M5	96	ARG
51	M5	97	SER
51	M5	106	VAL
51	M5	109	ARG
51	M5	123	GLN
51	M5	124	ASP
51	M5	133	ILE
51	M5	138	GLN
51	M5	142	ILE
51	M5	153	ASP
51	M5	155	VAL
51	M5	157	LYS
51	M5	159	ARG
51	M5	167	THR
51	M5	170	LYS
51	M5	171	SER
51	M5	184	LYS
51	M5	187	ARG
51	M5	190	THR
51	M5	198	SER
52	M6	34	VAL
52	M6	44	SER
52	M6	51	LYS
52	M6	58	LEU
52	M6	78	ARG
52	M6	85	ARG
52	M6	94	ARG
52	M6	106	GLU
52	M6	117	ARG
52	M6	122	GLN
52	M6	126	VAL
52	M6	128	ARG
52	M6	143	THR
52	M6	152	VAL
52	M6	166	GLU
52	M6	180	SER
52	M6	184	THR
52	M6	187	GLU
52	M6	190	VAL
53	M7	3	ARG
53	M7	7	THR
53	M7	9	THR

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Mol	Chain	Res	Type
53	M7	14	SER
53	M7	18	ARG
53	M7	20	SER
53	M7	23	ARG
53	M7	24	VAL
53	M7	29	THR
53	M7	32	THR
53	M7	36	ILE
53	M7	52	LEU
53	M7	53	ASP
53	M7	56	ARG
53	M7	66	SER
53	M7	67	ILE
53	M7	78	VAL
53	M7	79	THR
53	M7	112	LEU
53	M7	115	SER
53	M7	119	VAL
53	M7	126	ARG
53	M7	127	ARG
53	M7	128	ARG
53	M7	138	LYS
53	M7	142	SER
53	M7	144	SER
53	M7	157	VAL
53	M7	168	LEU
53	M7	173	ARG
53	M7	180	LYS
53	M7	181	ARG
53	M7	182	ILE
54	M8	7	SER
54	M8	17	THR
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	34	THR
54	M8	46	LYS
54	M8	50	LYS
54	M8	57	ILE
54	M8	63	SER
54	M8	64	VAL
54	M8	66	ARG

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Mol	Chain	Res	Type
54	M8	67	ILE
54	M8	74	GLU
54	M8	95	GLU
54	M8	100	THR
54	M8	113	LYS
54	M8	135	GLN
54	M8	138	LEU
54	M8	159	LYS
54	M8	174	ARG
54	M8	178	ARG
54	M8	180	ARG
54	M8	181	SER
55	M9	5	ARG
55	M9	29	THR
55	M9	31	GLU
55	M9	41	ILE
55	M9	44	LEU
55	M9	46	LYS
55	M9	47	ASN
55	M9	55	VAL
55	M9	69	SER
55	M9	70	LYS
55	M9	72	GLU
55	M9	75	HIS
55	M9	81	ARG
55	M9	99	LEU
55	M9	103	ARG
55	M9	104	ARG
55	M9	105	LEU
55	M9	106	LEU
55	M9	108	LYS
55	M9	110	ARG
55	M9	115	ILE
55	M9	116	ASP
55	M9	126	GLU
55	M9	133	LYS
55	M9	134	HIS
55	M9	138	LEU
55	M9	153	LYS
55	M9	164	LEU
55	M9	165	LYS
55	M9	175	GLN

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Mol	Chain	Res	Type
55	M9	176	ARG
55	M9	180	LYS
56	N0	1	MET
56	N0	8	GLN
56	N0	13	ARG
56	N0	16	THR
56	N0	40	ARG
56	N0	45	LEU
56	N0	47	LYS
56	N0	61	ILE
56	N0	71	LYS
56	N0	77	VAL
56	N0	79	VAL
56	N0	80	ARG
56	N0	87	THR
56	N0	92	LYS
56	N0	97	VAL
56	N0	105	THR
56	N0	115	ARG
56	N0	117	ARG
56	N0	122	HIS
56	N0	130	GLU
56	N0	132	THR
56	N0	137	ARG
56	N0	141	LYS
56	N0	145	THR
56	N0	155	ARG
56	N0	156	VAL
56	N0	158	LYS
56	N0	167	ARG
56	N0	171	PHE
57	N1	9	SER
57	N1	25	VAL
57	N1	27	LEU
57	N1	32	LYS
57	N1	38	ASP
57	N1	69	LYS
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	80	VAL
57	N1	83	ARG

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Mol	Chain	Res	Type
57	N1	88	ARG
57	N1	92	ARG
57	N1	96	ILE
57	N1	104	GLU
57	N1	106	LEU
57	N1	110	LYS
57	N1	124	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	136	ARG
57	N1	139	ARG
57	N1	140	ILE
57	N1	141	VAL
57	N1	143	THR
58	N2	10	LYS
58	N2	14	THR
58	N2	27	VAL
58	N2	29	ASP
58	N2	38	ILE
58	N2	39	ASP
58	N2	43	VAL
58	N2	52	ASN
58	N2	62	VAL
58	N2	66	VAL
58	N2	80	THR
58	N2	82	LYS
58	N2	88	GLN
58	N2	92	TRP
58	N2	93	ILE
58	N2	95	PHE
58	N2	100	THR
59	N3	9	THR
59	N3	13	ILE
59	N3	14	SER
59	N3	32	ARG
59	N3	48	ARG
59	N3	64	LYS
59	N3	72	LYS
59	N3	73	VAL
59	N3	79	VAL
59	N3	81	GLN
59	N3	83	LYS

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Mol	Chain	Res	Type
59	N3	102	ILE
59	N3	110	LYS
59	N3	112	SER
59	N3	115	THR
59	N3	120	LYS
59	N3	135	VAL
60	N4	1	MET
60	N4	4	GLU
60	N4	5	ILE
60	N4	39	LEU
60	N4	43	ARG
60	N4	64	THR
61	N5	27	ARG
61	N5	34	LEU
61	N5	37	THR
61	N5	38	LEU
61	N5	39	LYS
61	N5	42	ARG
61	N5	44	PRO
61	N5	45	LYS
61	N5	59	SER
61	N5	63	ILE
61	N5	71	THR
61	N5	92	LYS
61	N5	96	LYS
61	N5	108	LEU
61	N5	115	ARG
61	N5	125	ARG
61	N5	127	THR
61	N5	134	ASP
61	N5	139	ILE
61	N5	142	ILE
62	N6	5	SER
62	N6	8	VAL
62	N6	13	ARG
62	N6	36	SER
62	N6	37	LYS
62	N6	38	GLU
62	N6	39	LEU
62	N6	42	GLN
62	N6	45	ILE
62	N6	50	ILE

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Mol	Chain	Res	Type
62	N6	51	ARG
62	N6	56	VAL
62	N6	57	LEU
62	N6	60	ARG
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	83	ASP
62	N6	86	THR
62	N6	88	GLU
62	N6	105	VAL
62	N6	115	ARG
62	N6	126	LEU
62	N6	127	GLU
63	N7	14	VAL
63	N7	21	LYS
63	N7	24	VAL
63	N7	26	VAL
63	N7	30	ASP
63	N7	34	LYS
63	N7	46	ILE
63	N7	52	LYS
63	N7	64	LYS
63	N7	65	ARG
63	N7	81	LEU
63	N7	83	THR
63	N7	89	VAL
63	N7	93	LYS
63	N7	95	VAL
63	N7	99	GLU
63	N7	102	GLU
63	N7	107	ARG
63	N7	109	GLU
63	N7	116	LYS
63	N7	134	LEU
63	N7	135	ARG
64	N8	4	ARG
64	N8	8	THR
64	N8	10	LYS
64	N8	16	SER
64	N8	26	ARG
64	N8	29	PRO

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Mol	Chain	Res	Type
64	N8	34	MET
64	N8	42	ARG
64	N8	46	ASP
64	N8	47	LYS
64	N8	60	TYR
64	N8	65	GLN
64	N8	78	LEU
64	N8	80	THR
64	N8	88	ASP
64	N8	91	LEU
64	N8	92	LYS
64	N8	118	ILE
64	N8	120	ASN
64	N8	123	VAL
64	N8	133	LEU
64	N8	135	GLU
64	N8	144	VAL
65	N9	12	GLN
65	N9	13	THR
65	N9	14	ARG
65	N9	18	ARG
65	N9	21	ILE
65	N9	22	LYS
65	N9	23	LYS
65	N9	25	LYS
65	N9	33	LYS
65	N9	35	VAL
65	N9	38	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	10	ILE
66	O0	14	LEU
66	O0	16	LEU
66	O0	24	THR
66	O0	30	THR
66	O0	36	GLN
66	O0	40	LYS
66	O0	54	SER
66	O0	57	GLU
66	O0	61	MET
66	O0	66	LYS
66	O0	83	LYS

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Mol	Chain	Res	Type
66	O0	87	VAL
66	O0	93	LEU
66	O0	99	ASP
66	O0	100	ILE
66	O0	101	LEU
67	O1	8	VAL
67	O1	13	THR
67	O1	16	LEU
67	O1	26	LYS
67	O1	31	ARG
67	O1	46	THR
67	O1	64	VAL
67	O1	68	GLU
67	O1	73	LEU
67	O1	76	SER
67	O1	79	ARG
67	O1	84	ASP
67	O1	86	LYS
67	O1	94	GLU
67	O1	100	SER
67	O1	105	GLN
67	O1	106	THR
67	O1	107	VAL
68	O2	4	LEU
68	O2	15	LYS
68	O2	19	ARG
68	O2	24	ARG
68	O2	33	ARG
68	O2	34	LYS
68	O2	35	GLN
68	O2	41	VAL
68	O2	52	GLN
68	O2	54	LYS
68	O2	60	ASN
68	O2	61	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	82	LEU
68	O2	84	THR
68	O2	91	THR
68	O2	101	SER
68	O2	106	VAL

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Mol	Chain	Res	Type
68	O2	125	ARG
68	O2	128	LEU
69	O3	4	SER
69	O3	12	LYS
69	O3	14	LEU
69	O3	15	SER
69	O3	31	LYS
69	O3	49	ILE
69	O3	59	VAL
69	O3	67	MET
69	O3	70	LYS
69	O3	74	THR
69	O3	80	VAL
69	O3	81	VAL
69	O3	93	THR
69	O3	98	VAL
69	O3	106	ASN
70	O4	8	ARG
70	O4	20	ILE
70	O4	21	LYS
70	O4	24	LYS
70	O4	29	ILE
70	O4	51	LEU
70	O4	52	GLN
70	O4	56	THR
70	O4	57	LEU
70	O4	58	ARG
70	O4	65	VAL
70	O4	71	THR
70	O4	74	ARG
70	O4	81	CYS
70	O4	86	LYS
70	O4	87	GLU
70	O4	90	ILE
70	O4	102	LYS
70	O4	103	LYS
70	O4	104	VAL
70	O4	107	GLU
71	O5	10	ARG
71	O5	21	LEU
71	O5	27	GLU
71	O5	38	ARG

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Mol	Chain	Res	Type
71	O5	42	PRO
71	O5	43	LYS
71	O5	46	THR
71	O5	48	ARG
71	O5	49	LYS
71	O5	50	SER
71	O5	60	GLU
71	O5	62	GLN
71	O5	68	GLN
71	O5	71	LYS
71	O5	73	LYS
71	O5	86	ARG
71	O5	89	ARG
71	O5	90	ARG
71	O5	101	THR
71	O5	102	GLU
71	O5	107	LYS
71	O5	115	LYS
71	O5	119	LYS
72	O6	17	VAL
72	O6	18	THR
72	O6	19	SER
72	O6	21	THR
72	O6	26	ILE
72	O6	28	TYR
72	O6	36	ARG
72	O6	41	ARG
72	O6	42	SER
72	O6	45	ARG
72	O6	46	GLU
72	O6	57	LEU
72	O6	58	ILE
72	O6	62	ARG
72	O6	70	ARG
72	O6	72	VAL
72	O6	76	ARG
72	O6	81	THR
72	O6	86	LYS
72	O6	88	GLU
72	O6	90	MET
72	O6	98	ARG
73	O7	5	THR

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Mol	Chain	Res	Type
73	O7	10	LYS
73	O7	12	HIS
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	36	SER
73	O7	44	THR
73	O7	46	SER
73	O7	55	ARG
73	O7	58	THR
73	O7	59	THR
73	O7	65	ARG
73	O7	67	LEU
73	O7	71	SER
73	O7	80	THR
73	O7	85	LYS
74	O8	5	ILE
74	O8	12	LEU
74	O8	22	THR
74	O8	24	THR
74	O8	32	ASN
74	O8	41	THR
74	O8	46	ARG
74	O8	53	THR
74	O8	61	LYS
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	21	ARG
75	O9	23	LEU
75	O9	25	GLN
75	O9	28	ARG
75	O9	34	THR
75	O9	36	ARG
75	O9	51	ILE
76	Q0	77	ILE
76	Q0	78	ILE

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Mol	Chain	Res	Type
76	Q0	80	PRO
76	Q0	85	LEU
76	Q0	92	ASP
76	Q0	98	LYS
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	126	LYS
76	Q0	127	LEU
77	Q1	6	ARG
77	Q1	9	ARG
77	Q1	10	THR
77	Q1	11	ARG
77	Q1	20	VAL
78	Q2	13	LYS
78	Q2	22	GLN
78	Q2	23	HIS
78	Q2	26	THR
78	Q2	29	LYS
78	Q2	35	LEU
78	Q2	38	GLN
78	Q2	45	ARG
78	Q2	48	SER
78	Q2	60	LYS
78	Q2	64	THR
78	Q2	70	LEU
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
79	Q3	10	ILE
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	25	GLN
79	Q3	33	GLN
79	Q3	36	ARG
79	Q3	45	LYS

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Mol	Chain	Res	Type
79	Q3	46	THR
79	Q3	56	THR
79	Q3	59	CYS
79	Q3	60	CYS
79	Q3	73	THR
79	Q3	81	SER
79	Q3	88	GLU
79	Q3	90	VAL
79	Q3	91	GLU
2	s0	10	THR
2	s0	12	GLU
2	s0	28	ASN
2	s0	30	GLN
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	76	ILE
2	s0	78	SER
2	s0	87	LEU
2	s0	93	THR
2	s0	101	ARG
2	s0	106	SER
2	s0	108	THR
2	s0	111	ILE
2	s0	119	ARG
2	s0	124	THR
2	s0	144	ILE
2	s0	154	GLU
2	s0	157	ASP
2	s0	169	SER
2	s0	172	LEU
2	s0	179	ARG
2	s0	183	ARG
2	s0	184	LEU
2	s0	185	ARG
2	s0	189	VAL
2	s0	202	TYR
3	s1	25	THR
3	s1	36	SER

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Mol	Chain	Res	Type
3	s1	37	THR
3	s1	43	VAL
3	s1	47	LEU
3	s1	51	SER
3	s1	62	LYS
3	s1	70	LEU
3	s1	73	LEU
3	s1	81	PHE
3	s1	83	LYS
3	s1	96	LEU
3	s1	97	LEU
3	s1	105	PHE
3	s1	106	THR
3	s1	112	SER
3	s1	125	VAL
3	s1	126	THR
3	s1	127	VAL
3	s1	129	THR
3	s1	137	ILE
3	s1	159	SER
3	s1	169	SER
3	s1	177	GLN
3	s1	179	SER
3	s1	180	THR
3	s1	181	LEU
3	s1	185	THR
3	s1	195	LYS
3	s1	196	GLU
3	s1	202	LYS
3	s1	203	ASP
3	s1	208	GLN
3	s1	217	LEU
3	s1	222	LYS
3	s1	229	MET
3	s1	231	LEU
4	s2	41	LEU
4	s2	52	THR
4	s2	53	ILE
4	s2	55	GLU
4	s2	58	LEU
4	s2	60	SER
4	s2	69	ILE

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Mol	Chain	Res	Type
4	s2	70	ASP
4	s2	73	LEU
4	s2	77	GLN
4	s2	83	ILE
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	94	GLN
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	113	LEU
4	s2	116	LYS
4	s2	117	THR
4	s2	120	GLU
4	s2	137	ILE
4	s2	139	ILE
4	s2	141	ARG
4	s2	146	THR
4	s2	150	GLN
4	s2	153	SER
4	s2	161	LYS
4	s2	164	SER
4	s2	166	THR
4	s2	170	ILE
4	s2	178	ILE
4	s2	185	LYS
4	s2	194	GLU
4	s2	206	THR
4	s2	207	LEU
4	s2	210	THR
4	s2	221	THR
4	s2	222	TYR
4	s2	225	LEU
4	s2	226	THR
4	s2	229	LEU
4	s2	232	GLU
4	s2	248	SER
5	s3	7	LYS
5	s3	11	LEU
5	s3	21	LEU
5	s3	23	GLU

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Mol	Chain	Res	Type
5	s3	34	TYR
5	s3	35	SER
5	s3	39	VAL
5	s3	41	VAL
5	s3	44	THR
5	s3	54	ARG
5	s3	61	GLU
5	s3	69	LEU
5	s3	70	THR
5	s3	76	ARG
5	s3	84	ILE
5	s3	86	LEU
5	s3	87	TYR
5	s3	90	ARG
5	s3	93	ASP
5	s3	113	LEU
5	s3	115	ILE
5	s3	117	ARG
5	s3	125	TYR
5	s3	127	MET
5	s3	128	GLU
5	s3	134	CYS
5	s3	139	SER
5	s3	142	LEU
5	s3	143	ARG
5	s3	148	LYS
5	s3	157	LEU
5	s3	158	ILE
5	s3	162	GLN
5	s3	164	VAL
5	s3	169	ASP
5	s3	176	LEU
5	s3	177	MET
5	s3	179	GLN
5	s3	212	LYS
5	s3	213	GLU
5	s3	223	LYS
6	s4	6	LYS
6	s4	12	LEU
6	s4	23	LEU
6	s4	24	SER
6	s4	29	PRO

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Mol	Chain	Res	Type
6	s4	38	LEU
6	s4	41	SER
6	s4	42	LEU
6	s4	45	ILE
6	s4	48	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	56	LEU
6	s4	67	GLN
6	s4	68	ARG
6	s4	70	VAL
6	s4	93	ASP
6	s4	95	THR
6	s4	98	ASN
6	s4	104	ASP
6	s4	108	ARG
6	s4	113	ARG
6	s4	116	ASP
6	s4	146	THR
6	s4	148	ARG
6	s4	159	THR
6	s4	176	ASP
6	s4	180	LEU
6	s4	182	TYR
6	s4	184	THR
6	s4	210	ILE
6	s4	219	VAL
6	s4	221	ARG
6	s4	222	LEU
6	s4	236	ILE
6	s4	245	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	45	LYS
7	s5	59	VAL
7	s5	63	GLN
7	s5	66	GLN

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Mol	Chain	Res	Type
7	s5	68	ILE
7	s5	73	THR
7	s5	79	ASN
7	s5	83	ARG
7	s5	89	ILE
7	s5	90	ILE
7	s5	93	LEU
7	s5	99	MET
7	s5	119	ASP
7	s5	122	ASN
7	s5	125	THR
7	s5	127	GLN
7	s5	130	ILE
7	s5	148	ARG
7	s5	156	ARG
7	s5	157	ARG
7	s5	160	VAL
7	s5	162	VAL
7	s5	163	SER
7	s5	190	ILE
7	s5	194	LEU
7	s5	203	LYS
7	s5	216	GLU
8	s6	17	GLU
8	s6	22	HIS
8	s6	31	ARG
8	s6	59	GLN
8	s6	65	GLN
8	s6	67	VAL
8	s6	69	LEU
8	s6	71	THR
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU
8	s6	120	GLU
8	s6	121	LEU
8	s6	125	THR
8	s6	126	ASP
8	s6	127	THR
8	s6	128	THR
8	s6	132	ARG
8	s6	143	LYS

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Mol	Chain	Res	Type
8	s6	151	ASP
8	s6	153	VAL
8	s6	154	ARG
8	s6	155	ASP
8	s6	156	PHE
8	s6	164	LYS
8	s6	168	THR
8	s6	171	LYS
8	s6	175	ILE
8	s6	179	VAL
8	s6	180	THR
8	s6	182	GLN
8	s6	193	LEU
8	s6	212	LEU
8	s6	215	ARG
9	s7	28	GLU
9	s7	33	GLU
9	s7	38	LEU
9	s7	55	LYS
9	s7	64	VAL
9	s7	67	LEU
9	s7	75	THR
9	s7	77	LEU
9	s7	80	GLU
9	s7	86	GLN
9	s7	97	ARG
9	s7	99	LEU
9	s7	114	ARG
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	134	GLU
9	s7	141	ARG
9	s7	143	LEU
9	s7	149	ILE
9	s7	165	LYS
9	s7	166	LEU
9	s7	185	ILE
10	s8	7	SER
10	s8	8	ARG
10	s8	9	HIS
10	s8	10	LYS

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Mol	Chain	Res	Type
10	s8	18	ARG
10	s8	20	GLN
10	s8	22	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	46	VAL
10	s8	54	LYS
10	s8	59	ARG
10	s8	61	GLU
10	s8	62	THR
10	s8	74	LYS
10	s8	76	THR
10	s8	89	GLU
10	s8	120	THR
10	s8	121	LEU
10	s8	138	ASN
10	s8	151	LYS
10	s8	152	ILE
10	s8	155	SER
10	s8	161	SER
10	s8	168	CYS
10	s8	183	ILE
11	s9	3	ARG
11	s9	6	ARG
11	s9	7	THR
11	s9	9	SER
11	s9	16	LYS
11	s9	20	GLU
11	s9	28	LEU
11	s9	29	LYS
11	s9	41	GLU
11	s9	46	SER
11	s9	49	LEU
11	s9	78	ARG
11	s9	82	ARG
11	s9	93	LEU
11	s9	101	VAL
11	s9	105	LEU
11	s9	109	LEU
11	s9	111	THR
11	s9	120	LYS
11	s9	130	THR

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Mol	Chain	Res	Type
11	s9	133	HIS
11	s9	134	ILE
11	s9	149	ARG
11	s9	150	LEU
11	s9	161	THR
11	s9	168	ARG
11	s9	179	ARG
11	s9	180	LYS
11	s9	182	GLU
11	s9	186	GLU
12	c0	2	LEU
12	c0	5	LYS
12	c0	15	LEU
12	c0	20	VAL
12	c0	22	VAL
12	c0	27	PHE
12	c0	33	GLU
12	c0	36	ASP
12	c0	37	THR
12	c0	40	LEU
12	c0	47	GLN
12	c0	55	VAL
12	c0	57	THR
12	c0	71	GLU
12	c0	76	LEU
13	c1	2	SER
13	c1	5	LEU
13	c1	10	GLU
13	c1	18	HIS
13	c1	22	ASN
13	c1	27	THR
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	56	LYS
13	c1	60	PHE
13	c1	67	ARG
13	c1	69	LYS
13	c1	72	THR

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Mol	Chain	Res	Type
13	c1	74	THR
13	c1	76	VAL
13	c1	77	SER
13	c1	79	LYS
13	c1	80	MET
13	c1	83	THR
13	c1	99	ARG
13	c1	112	SER
13	c1	129	ARG
13	c1	133	LYS
13	c1	138	ASN
13	c1	140	VAL
13	c1	143	SER
14	c2	28	LEU
14	c2	30	VAL
14	c2	36	LEU
14	c2	38	HIS
14	c2	43	ARG
14	c2	45	LEU
14	c2	53	THR
14	c2	59	LEU
14	c2	62	LEU
14	c2	66	VAL
14	c2	71	ILE
14	c2	74	LEU
14	c2	85	LYS
14	c2	89	ILE
14	c2	97	LEU
14	c2	103	LEU
14	c2	116	VAL
14	c2	119	SER
14	c2	120	VAL
14	c2	121	VAL
14	c2	132	GLU
14	c2	136	ILE
14	c2	137	MET
14	c2	138	GLU
14	c2	140	PHE
14	c2	142	GLN
15	c3	6	SER
15	c3	12	SER
15	c3	14	SER

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Mol	Chain	Res	Type
15	c3	16	ILE
15	c3	20	ARG
15	c3	21	ASN
15	c3	33	VAL
15	c3	39	LYS
15	c3	46	THR
15	c3	60	VAL
15	c3	61	THR
15	c3	65	VAL
15	c3	66	ILE
15	c3	70	LYS
15	c3	80	LEU
15	c3	84	ILE
15	c3	87	ASP
15	c3	93	LYS
15	c3	97	SER
15	c3	102	LEU
15	c3	115	LEU
15	c3	119	GLU
15	c3	125	LEU
15	c3	138	ASN
15	c3	140	LYS
16	c4	18	ARG
16	c4	26	THR
16	c4	31	THR
16	c4	39	ILE
16	c4	49	LYS
16	c4	51	ASP
16	c4	61	MET
16	c4	76	ILE
16	c4	81	VAL
16	c4	102	LEU
16	c4	107	ARG
16	c4	114	ARG
16	c4	115	ILE
16	c4	118	VAL
16	c4	123	SER
16	c4	124	ASP
16	c4	129	LYS
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU

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Mol	Chain	Res	Type
17	c5	12	PHE
17	c5	24	LYS
17	c5	28	MET
17	c5	34	VAL
17	c5	36	LEU
17	c5	40	ARG
17	c5	52	LYS
17	c5	69	GLU
17	c5	71	GLU
17	c5	92	SER
17	c5	103	ASN
17	c5	107	ILE
17	c5	110	GLU
17	c5	111	MET
17	c5	122	THR
17	c5	123	TYR
17	c5	124	THR
17	c5	127	ARG
18	c6	17	THR
18	c6	23	LYS
18	c6	26	LYS
18	c6	28	LEU
18	c6	34	SER
18	c6	37	THR
18	c6	43	ILE
18	c6	47	LYS
18	c6	48	VAL
18	c6	53	LEU
18	c6	54	LEU
18	c6	57	LEU
18	c6	63	ILE
18	c6	68	ARG
18	c6	69	VAL
18	c6	81	ILE
18	c6	85	ILE
18	c6	110	THR
18	c6	114	ARG
18	c6	115	THR
18	c6	118	ILE
18	c6	137	ARG
18	c6	143	ARG
19	c7	3	ARG

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Mol	Chain	Res	Type
19	c7	5	ARG
19	c7	6	THR
19	c7	29	GLN
19	c7	34	LEU
19	c7	45	ARG
19	c7	46	LEU
19	c7	55	THR
19	c7	62	GLN
19	c7	69	ILE
19	c7	83	GLN
19	c7	85	VAL
19	c7	87	GLU
19	c7	88	VAL
19	c7	100	LEU
19	c7	105	GLN
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	12	GLN
20	c8	13	HIS
20	c8	20	THR
20	c8	25	ASN
20	c8	26	ILE
20	c8	28	ILE
20	c8	33	THR
20	c8	36	LYS
20	c8	40	ARG
20	c8	51	ASP
20	c8	57	ARG
20	c8	63	GLN
20	c8	68	ARG
20	c8	77	THR
20	c8	92	ILE
20	c8	105	VAL
20	c8	112	ASP
20	c8	116	LEU
20	c8	119	ILE
20	c8	120	ARG
20	c8	126	ARG

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Mol	Chain	Res	Type
20	c8	136	GLN
20	c8	138	THR
20	c8	140	THR
20	c8	141	THR
20	c8	144	ARG
20	c8	145	ARG
21	c9	6	VAL
21	c9	12	GLN
21	c9	27	LYS
21	c9	28	LEU
21	c9	37	VAL
21	c9	57	ARG
21	c9	70	GLN
21	c9	71	VAL
21	c9	75	LYS
21	c9	86	ARG
21	c9	102	ARG
21	c9	111	ILE
21	c9	117	SER
21	c9	123	ARG
21	c9	139	THR
21	c9	140	LEU
21	c9	141	GLU
21	c9	142	GLU
22	d0	16	GLN
22	d0	22	ILE
22	d0	25	THR
22	d0	27	THR
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	61	LYS
22	d0	63	LEU
22	d0	66	SER
22	d0	70	THR
22	d0	74	GLU
22	d0	88	LYS
22	d0	99	ILE

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Mol	Chain	Res	Type
22	d0	103	ILE
22	d0	105	GLN
22	d0	107	THR
22	d0	108	ILE
22	d0	113	ASP
22	d0	115	GLU
22	d0	116	VAL
22	d0	121	ASN
23	d1	2	GLU
23	d1	3	ASN
23	d1	5	LYS
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	25	LYS
23	d1	34	ILE
23	d1	36	VAL
23	d1	44	ARG
23	d1	49	GLU
23	d1	52	THR
23	d1	62	ARG
23	d1	68	SER
23	d1	69	LEU
23	d1	78	LEU
23	d1	82	VAL
23	d1	85	TYR
23	d1	87	ARG
24	d2	7	LEU
24	d2	23	ARG
24	d2	25	VAL
24	d2	26	LEU
24	d2	31	SER
24	d2	33	VAL
24	d2	47	ILE
24	d2	65	LEU
24	d2	71	LYS
24	d2	88	LYS
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	124	LYS
24	d2	129	VAL

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Mol	Chain	Res	Type
25	d3	9	LEU
25	d3	14	LYS
25	d3	19	ARG
25	d3	28	ASN
25	d3	33	LEU
25	d3	40	SER
25	d3	73	ARG
25	d3	75	GLN
25	d3	82	LYS
25	d3	84	THR
25	d3	96	VAL
25	d3	97	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	109	ARG
25	d3	123	LYS
25	d3	125	VAL
25	d3	128	SER
25	d3	131	SER
25	d3	133	LEU
25	d3	137	LYS
25	d3	144	ARG
26	d4	5	VAL
26	d4	10	ARG
26	d4	13	ILE
26	d4	14	SER
26	d4	21	LYS
26	d4	43	LYS
26	d4	44	LEU
26	d4	49	LYS
26	d4	62	THR
26	d4	74	LEU
26	d4	77	ASN
26	d4	88	THR
26	d4	91	LEU
26	d4	92	VAL
26	d4	98	GLU
26	d4	107	GLN
26	d4	128	LYS
26	d4	133	ASN
27	d5	41	ILE
27	d5	51	LEU

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Mol	Chain	Res	Type
27	d5	53	GLU
27	d5	60	VAL
27	d5	62	VAL
27	d5	71	ILE
27	d5	81	ARG
27	d5	88	ILE
27	d5	90	LYS
27	d5	93	SER
28	d6	3	LYS
28	d6	4	LYS
28	d6	10	ARG
28	d6	18	VAL
28	d6	38	ARG
28	d6	51	ARG
28	d6	53	LEU
28	d6	82	ARG
28	d6	85	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	14	SER
29	d7	29	ARG
29	d7	40	CYS
29	d7	43	ILE
29	d7	46	VAL
29	d7	52	THR
29	d7	75	GLU
29	d7	77	THR
29	d7	81	ARG
30	d8	16	LEU
30	d8	22	ARG
30	d8	26	THR
30	d8	27	GLN
30	d8	30	VAL
30	d8	32	PHE
30	d8	33	LEU
30	d8	40	ILE
30	d8	52	ASP
30	d8	54	LEU
30	d8	56	LEU
30	d8	58	GLU
30	d8	62	GLU
30	d8	65	ARG

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Mol	Chain	Res	Type
31	d9	4	GLU
31	d9	10	HIS
31	d9	16	LYS
31	d9	19	ARG
31	d9	23	VAL
31	d9	26	SER
31	d9	32	ARG
31	d9	36	LEU
31	d9	40	ARG
31	d9	49	ASP
31	d9	54	LYS
80	e0	4	VAL
80	e0	14	VAL
80	e0	21	VAL
80	e0	22	GLU
80	e0	25	GLU
80	e0	26	LYS
80	e0	29	LYS
80	e0	39	LEU
80	e0	41	THR
80	e0	43	ARG
80	e0	45	VAL
80	e0	46	ASN
80	e0	49	LEU
33	e1	78	LYS
33	e1	89	LYS
33	e1	90	LYS
33	e1	96	LYS
33	e1	97	LYS
33	e1	98	VAL
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	113	LYS
33	e1	115	THR
33	e1	116	LYS
33	e1	120	GLU
33	e1	135	HIS
33	e1	137	ASP
33	e1	140	TYR
33	e1	148	TYR
33	e1	149	LYS

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Mol	Chain	Res	Type
33	e1	151	ASN
34	sR	21	THR
34	sR	25	THR
34	sR	29	GLN
34	sR	51	ASP
34	sR	58	VAL
34	sR	59	ARG
34	sR	64	HIS
34	sR	65	SER
34	sR	66	HIS
34	sR	70	ASP
34	sR	98	GLU
34	sR	108	SER
34	sR	115	ILE
34	sR	123	ILE
34	sR	145	LEU
34	sR	168	THR
34	sR	176	LYS
34	sR	178	VAL
34	sR	184	ASN
34	sR	199	ILE
34	sR	203	THR
34	sR	228	LYS
34	sR	232	TYR
34	sR	258	THR
34	sR	275	ARG
34	sR	286	GLU
34	sR	297	ASP
34	sR	314	GLN
35	sM	23	LYS
35	sM	30	THR
35	sM	33	LYS
35	sM	38	PRO
35	sM	41	SER
35	sM	43	ASP
35	sM	49	LYS
35	sM	50	ASN
35	sM	61	ILE
35	sM	68	ARG
35	sM	71	ASN
35	sM	74	LYS
35	sM	77	THR

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Mol	Chain	Res	Type
35	sM	82	THR
39	l2	15	ILE
39	l2	19	HIS
39	l2	23	ARG
39	l2	28	LYS
39	l2	30	ARG
39	l2	32	LEU
39	l2	42	ARG
39	l2	44	ILE
39	l2	45	VAL
39	l2	48	ILE
39	l2	49	VAL
39	l2	54	ARG
39	l2	61	VAL
39	l2	62	VAL
39	l2	71	LEU
39	l2	74	GLU
39	l2	80	GLU
39	l2	82	VAL
39	l2	96	LEU
39	l2	101	VAL
39	l2	112	ILE
39	l2	128	ARG
39	l2	134	VAL
39	l2	135	ILE
39	l2	137	ILE
39	l2	144	ASN
39	l2	147	ARG
39	l2	158	ILE
39	l2	159	SER
39	l2	165	VAL
39	l2	168	VAL
39	l2	169	ILE
39	l2	179	LEU
39	l2	191	LEU
39	l2	192	LYS
39	l2	193	ARG
39	l2	204	MET
39	l2	205	ASN
39	l2	207	VAL
39	l2	227	ARG
39	l2	230	VAL

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Mol	Chain	Res	Type
39	l2	231	SER
39	l2	246	LEU
40	l3	5	LYS
40	l3	10	ARG
40	l3	17	LEU
40	l3	19	ARG
40	l3	44	THR
40	l3	47	LEU
40	l3	50	LYS
40	l3	56	ILE
40	l3	69	LYS
40	l3	70	ARG
40	l3	81	THR
40	l3	85	VAL
40	l3	101	SER
40	l3	103	THR
40	l3	104	THR
40	l3	111	SER
40	l3	114	VAL
40	l3	116	ARG
40	l3	120	LYS
40	l3	139	GLN
40	l3	146	ARG
40	l3	148	LEU
40	l3	150	ARG
40	l3	156	SER
40	l3	157	VAL
40	l3	160	VAL
40	l3	167	ARG
40	l3	169	THR
40	l3	183	LEU
40	l3	188	ILE
40	l3	196	ARG
40	l3	197	GLU
40	l3	202	THR
40	l3	205	VAL
40	l3	210	GLU
40	l3	211	GLN
40	l3	213	GLU
40	l3	232	ARG
40	l3	235	THR
40	l3	238	LEU

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Mol	Chain	Res	Type
40	l3	242	THR
40	l3	249	VAL
40	l3	252	ILE
40	l3	274	SER
40	l3	284	ARG
40	l3	296	THR
40	l3	297	SER
40	l3	302	LYS
40	l3	304	THR
40	l3	308	MET
40	l3	324	VAL
40	l3	325	LYS
40	l3	328	ILE
40	l3	332	ARG
40	l3	338	LEU
40	l3	340	LYS
40	l3	341	SER
40	l3	346	THR
40	l3	347	SER
40	l3	354	VAL
40	l3	363	SER
40	l3	364	LYS
41	l4	3	ARG
41	l4	14	GLU
41	l4	16	THR
41	l4	20	LEU
41	l4	25	VAL
41	l4	27	SER
41	l4	53	SER
41	l4	55	LYS
41	l4	64	SER
41	l4	73	ARG
41	l4	93	MET
41	l4	99	MET
41	l4	120	TYR
41	l4	131	VAL
41	l4	144	LYS
41	l4	145	ILE
41	l4	150	LEU
41	l4	151	VAL
41	l4	154	THR
41	l4	156	LEU

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Mol	Chain	Res	Type
41	14	169	LEU
41	14	170	LYS
41	14	172	VAL
41	14	179	LEU
41	14	182	LEU
41	14	186	LYS
41	14	187	LEU
41	14	193	LYS
41	14	203	ARG
41	14	220	ARG
41	14	222	VAL
41	14	230	VAL
41	14	246	ARG
41	14	256	THR
41	14	258	LEU
41	14	265	GLU
41	14	266	THR
41	14	267	VAL
41	14	284	SER
41	14	295	ILE
41	14	299	ILE
41	14	300	ARG
41	14	301	PRO
41	14	304	GLN
41	14	306	THR
41	14	307	GLN
41	14	313	LEU
41	14	316	ASN
41	14	319	LYS
41	14	323	VAL
41	14	327	LEU
41	14	333	VAL
41	14	339	LEU
41	14	345	GLU
41	14	346	LYS
41	14	347	THR
41	14	356	THR
41	14	360	LYS
42	15	4	GLN
42	15	9	SER
42	15	10	SER
42	15	13	SER

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Mol	Chain	Res	Type
42	15	15	ARG
42	15	34	LYS
42	15	35	ARG
42	15	51	LEU
42	15	57	ASN
42	15	61	ILE
42	15	64	ILE
42	15	70	THR
42	15	74	VAL
42	15	75	LEU
42	15	79	TYR
42	15	89	THR
42	15	109	THR
42	15	110	LEU
42	15	112	LYS
42	15	113	LEU
42	15	118	THR
42	15	120	LYS
42	15	128	GLU
42	15	131	LEU
42	15	132	THR
42	15	133	GLU
42	15	135	VAL
42	15	136	GLU
42	15	140	ARG
42	15	146	LEU
42	15	151	GLN
42	15	152	ARG
42	15	154	THR
42	15	155	THR
42	15	158	ARG
42	15	185	PHE
42	15	194	LEU
42	15	196	ARG
42	15	211	LEU
42	15	227	LEU
42	15	239	ILE
42	15	241	THR
42	15	254	LYS
42	15	257	GLU
42	15	258	LYS
42	15	259	LYS

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Mol	Chain	Res	Type
42	15	268	GLU
42	15	271	LYS
42	15	273	ARG
42	15	280	GLU
42	15	281	GLU
42	15	297	GLN
43	16	4	GLN
43	16	8	LYS
43	16	14	ASP
43	16	15	VAL
43	16	20	LYS
43	16	21	THR
43	16	31	ARG
43	16	50	LYS
43	16	64	LEU
43	16	65	ILE
43	16	76	LEU
43	16	78	ARG
43	16	89	THR
43	16	91	VAL
43	16	93	VAL
43	16	98	VAL
43	16	109	GLU
43	16	131	LYS
43	16	133	GLU
43	16	143	LYS
43	16	151	LYS
43	16	152	THR
43	16	155	LEU
44	17	40	LYS
44	17	45	LEU
44	17	46	GLU
44	17	56	GLU
44	17	60	ARG
44	17	62	ILE
44	17	82	LYS
44	17	83	LEU
44	17	98	LYS
44	17	113	SER
44	17	119	VAL
44	17	124	LEU
44	17	128	LYS

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Mol	Chain	Res	Type
44	17	150	LYS
44	17	156	ILE
44	17	157	ASN
44	17	158	LYS
44	17	159	GLN
44	17	175	LYS
44	17	178	ILE
44	17	179	LEU
44	17	181	ILE
44	17	184	LEU
44	17	196	LYS
44	17	206	LYS
44	17	219	LYS
44	17	224	ILE
44	17	229	PHE
44	17	239	LEU
45	18	26	LEU
45	18	41	GLN
45	18	46	LEU
45	18	50	VAL
45	18	55	TYR
45	18	63	LYS
45	18	64	ILE
45	18	65	LEU
45	18	67	ILE
45	18	68	ARG
45	18	74	THR
45	18	77	GLN
45	18	79	GLN
45	18	93	LEU
45	18	95	ASN
45	18	101	THR
45	18	111	LYS
45	18	132	VAL
45	18	134	TYR
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	172	LYS

Continued on next page...

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Mol	Chain	Res	Type
45	18	190	VAL
45	18	211	LEU
45	18	213	LYS
45	18	214	LEU
45	18	222	PHE
45	18	224	ASP
45	18	238	LEU
45	18	241	LYS
45	18	245	LYS
45	18	248	LYS
46	19	1	MET
46	19	5	GLN
46	19	6	THR
46	19	16	VAL
46	19	17	THR
46	19	18	VAL
46	19	19	SER
46	19	24	ILE
46	19	28	VAL
46	19	31	ARG
46	19	33	THR
46	19	34	LEU
46	19	37	ASN
46	19	39	LYS
46	19	44	THR
46	19	46	THR
46	19	47	LYS
46	19	48	VAL
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	71	VAL
46	19	80	THR
46	19	82	VAL
46	19	91	ARG
46	19	92	TYR
46	19	105	GLU
46	19	106	LYS
46	19	107	ASP

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Mol	Chain	Res	Type
46	l9	113	GLU
46	l9	128	VAL
46	l9	129	ARG
46	l9	130	ASP
46	l9	133	THR
46	l9	138	THR
46	l9	143	GLU
46	l9	144	ILE
46	l9	149	ASN
46	l9	151	VAL
46	l9	157	ASN
46	l9	162	GLN
46	l9	163	GLN
46	l9	166	ARG
46	l9	177	ASP
46	l9	188	THR
47	m0	22	TYR
47	m0	24	ARG
47	m0	26	VAL
47	m0	39	LYS
47	m0	42	THR
47	m0	48	LEU
47	m0	52	LEU
47	m0	57	LEU
47	m0	58	GLU
47	m0	63	GLU
47	m0	74	LYS
47	m0	77	THR
47	m0	78	THR
47	m0	87	LEU
47	m0	91	VAL
47	m0	99	ILE
47	m0	113	GLN
47	m0	116	ARG
47	m0	139	ARG
47	m0	143	SER
47	m0	144	ASN
47	m0	153	ARG
47	m0	156	ARG
47	m0	169	LYS
47	m0	170	LYS
47	m0	177	ASP

Continued on next page...

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Mol	Chain	Res	Type
47	m0	178	ARG
47	m0	182	LEU
47	m0	197	VAL
47	m0	200	LEU
47	m0	206	LEU
47	m0	208	ASN
47	m0	211	ARG
47	m0	217	PHE
48	m1	6	GLN
48	m1	10	ARG
48	m1	11	ASP
48	m1	12	LEU
48	m1	13	LYS
48	m1	14	ILE
48	m1	16	LYS
48	m1	17	LEU
48	m1	23	VAL
48	m1	30	LEU
48	m1	35	LYS
48	m1	37	LEU
48	m1	44	THR
48	m1	46	VAL
48	m1	54	VAL
48	m1	56	THR
48	m1	71	VAL
48	m1	80	LEU
48	m1	106	ILE
48	m1	107	ASP
48	m1	108	GLU
48	m1	112	LEU
48	m1	130	VAL
48	m1	140	ARG
48	m1	145	LYS
48	m1	152	HIS
48	m1	156	LYS
48	m1	158	ASP
48	m1	159	THR
48	m1	160	VAL
48	m1	161	SER
48	m1	166	LYS
49	m3	36	ARG
49	m3	53	LEU

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Mol	Chain	Res	Type
49	m3	54	LEU
49	m3	58	VAL
49	m3	59	ARG
49	m3	67	ARG
49	m3	68	LYS
49	m3	69	VAL
49	m3	75	PHE
49	m3	76	THR
49	m3	80	VAL
49	m3	100	ARG
49	m3	104	ARG
49	m3	107	GLU
49	m3	113	VAL
49	m3	118	GLU
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	172	LEU
49	m3	183	ARG
49	m3	184	GLU
49	m3	194	GLU
50	m4	2	SER
50	m4	3	THR
50	m4	8	LYS
50	m4	12	TRP
50	m4	15	VAL
50	m4	16	GLU
50	m4	20	VAL
50	m4	28	SER
50	m4	53	VAL
50	m4	55	ARG
50	m4	62	GLN
50	m4	63	VAL
50	m4	64	VAL
50	m4	66	THR

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Mol	Chain	Res	Type
50	m4	74	ARG
50	m4	80	THR
50	m4	82	SER
50	m4	85	TRP
50	m4	103	ILE
50	m4	107	GLU
50	m4	108	ARG
50	m4	113	THR
50	m4	123	LEU
50	m4	124	ARG
50	m4	128	ARG
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	10	LEU
51	m5	12	ARG
51	m5	18	VAL
51	m5	24	ARG
51	m5	49	ARG
51	m5	50	ARG
51	m5	54	LYS
51	m5	56	LYS
51	m5	73	ARG
51	m5	76	PRO
51	m5	80	THR
51	m5	85	THR
51	m5	87	GLN
51	m5	92	LEU
51	m5	96	ARG
51	m5	98	LEU
51	m5	105	ARG
51	m5	106	VAL
51	m5	109	ARG
51	m5	138	GLN
51	m5	142	ILE
51	m5	153	ASP
51	m5	155	VAL
51	m5	159	ARG
51	m5	165	THR
51	m5	171	SER
51	m5	176	LYS
51	m5	182	ASN

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Mol	Chain	Res	Type
51	m5	183	THR
51	m5	184	LYS
51	m5	190	THR
51	m5	199	LEU
52	m6	12	LYS
52	m6	22	VAL
52	m6	41	LEU
52	m6	49	ARG
52	m6	58	LEU
52	m6	66	LYS
52	m6	67	THR
52	m6	78	ARG
52	m6	79	ILE
52	m6	85	ARG
52	m6	87	MET
52	m6	94	ARG
52	m6	100	GLU
52	m6	101	ARG
52	m6	106	GLU
52	m6	108	ILE
52	m6	116	LYS
52	m6	117	ARG
52	m6	124	LEU
52	m6	126	VAL
52	m6	144	SER
52	m6	152	VAL
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	194	LEU
52	m6	197	LEU
53	m7	7	THR
53	m7	9	THR
53	m7	16	SER
53	m7	23	ARG
53	m7	24	VAL
53	m7	29	THR
53	m7	32	THR
53	m7	41	LEU

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Mol	Chain	Res	Type
53	m7	42	THR
53	m7	47	TYR
53	m7	52	LEU
53	m7	53	ASP
53	m7	69	ARG
53	m7	70	THR
53	m7	78	VAL
53	m7	79	THR
53	m7	86	LYS
53	m7	94	LEU
53	m7	105	LYS
53	m7	114	VAL
53	m7	119	VAL
53	m7	121	GLN
53	m7	128	ARG
53	m7	138	LYS
53	m7	144	SER
54	m8	3	ILE
54	m8	7	SER
54	m8	12	ARG
54	m8	22	ASP
54	m8	26	LEU
54	m8	31	LYS
54	m8	32	LEU
54	m8	34	THR
54	m8	46	LYS
54	m8	57	ILE
54	m8	63	SER
54	m8	64	VAL
54	m8	69	ARG
54	m8	74	GLU
54	m8	80	THR
54	m8	81	VAL
54	m8	82	VAL
54	m8	93	ILE
54	m8	135	GLN
54	m8	138	LEU
54	m8	147	ARG
54	m8	150	VAL
54	m8	159	LYS
54	m8	165	ILE
54	m8	166	LEU

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Mol	Chain	Res	Type
54	m8	167	SER
54	m8	178	ARG
54	m8	180	ARG
55	m9	5	ARG
55	m9	6	THR
55	m9	7	GLN
55	m9	8	LYS
55	m9	9	ARG
55	m9	10	LEU
55	m9	20	ARG
55	m9	29	THR
55	m9	31	GLU
55	m9	36	ASN
55	m9	37	SER
55	m9	38	ARG
55	m9	49	THR
55	m9	52	LYS
55	m9	63	THR
55	m9	88	ARG
55	m9	94	VAL
55	m9	98	ARG
55	m9	99	LEU
55	m9	116	ASP
55	m9	126	GLU
55	m9	138	LEU
55	m9	146	LYS
55	m9	153	LYS
55	m9	156	ASN
55	m9	158	GLU
55	m9	163	ARG
55	m9	166	ASN
55	m9	173	ARG
55	m9	177	VAL
56	n0	13	ARG
56	n0	16	THR
56	n0	45	LEU
56	n0	50	LYS
56	n0	52	LYS
56	n0	61	ILE
56	n0	63	GLN
56	n0	70	THR
56	n0	73	LYS

Continued on next page...

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Mol	Chain	Res	Type
56	n0	79	VAL
56	n0	80	ARG
56	n0	87	THR
56	n0	89	ASN
56	n0	96	ASP
56	n0	97	VAL
56	n0	100	VAL
56	n0	104	GLU
56	n0	106	LEU
56	n0	115	ARG
56	n0	117	ARG
56	n0	120	SER
56	n0	123	ILE
56	n0	130	GLU
56	n0	132	THR
56	n0	137	ARG
56	n0	148	LEU
56	n0	149	LYS
56	n0	155	ARG
56	n0	160	THR
56	n0	162	THR
56	n0	167	ARG
56	n0	170	THR
56	n0	171	PHE
56	n0	172	TYR
57	n1	12	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	36	VAL
57	n1	68	THR
57	n1	71	SER
57	n1	75	ILE
57	n1	78	LYS
57	n1	80	VAL
57	n1	83	ARG
57	n1	88	ARG
57	n1	96	ILE
57	n1	97	LYS
57	n1	102	ARG
57	n1	103	GLN
57	n1	104	GLU

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Mol	Chain	Res	Type
57	n1	122	GLN
57	n1	124	VAL
57	n1	126	VAL
57	n1	127	GLN
57	n1	129	LYS
57	n1	139	ARG
57	n1	141	VAL
57	n1	143	THR
57	n1	150	THR
57	n1	151	LEU
57	n1	158	THR
58	n2	19	VAL
58	n2	21	SER
58	n2	27	VAL
58	n2	43	VAL
58	n2	47	VAL
58	n2	57	THR
58	n2	62	VAL
58	n2	63	VAL
58	n2	74	LYS
58	n2	75	TYR
58	n2	85	LYS
58	n2	90	ARG
58	n2	94	ARG
58	n2	96	VAL
58	n2	100	THR
59	n3	7	GLN
59	n3	13	ILE
59	n3	40	LYS
59	n3	45	ARG
59	n3	48	ARG
59	n3	58	VAL
59	n3	70	ARG
59	n3	73	VAL
59	n3	79	VAL
59	n3	88	ARG
59	n3	91	VAL
59	n3	93	LEU
59	n3	102	ILE
59	n3	106	LYS
59	n3	115	THR
60	n4	1	MET

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Mol	Chain	Res	Type
60	n4	5	ILE
60	n4	39	LEU
60	n4	41	LYS
60	n4	54	LEU
60	n4	57	LYS
60	n4	59	HIS
60	n4	63	ILE
60	n4	82	ILE
60	n4	87	LEU
60	n4	89	LEU
60	n4	93	ARG
60	n4	96	LEU
60	n4	97	LYS
60	n4	100	VAL
60	n4	104	ASN
60	n4	105	ARG
60	n4	127	LYS
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	42	ARG
61	n5	52	PRO
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	70	GLU
61	n5	71	THR
61	n5	75	LYS
61	n5	78	ASP
61	n5	86	VAL
61	n5	87	SER
61	n5	108	LEU
61	n5	109	LYS
61	n5	114	VAL
61	n5	115	ARG
61	n5	117	ASN
61	n5	125	ARG
61	n5	135	ILE
62	n6	4	GLN
62	n6	5	SER
62	n6	9	SER

Continued on next page...

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Mol	Chain	Res	Type
62	n6	12	ARG
62	n6	13	ARG
62	n6	17	LYS
62	n6	37	LYS
62	n6	45	ILE
62	n6	50	ILE
62	n6	51	ARG
62	n6	52	ARG
62	n6	56	VAL
62	n6	57	LEU
62	n6	63	LYS
62	n6	66	GLN
62	n6	69	LYS
62	n6	71	SER
62	n6	74	TYR
62	n6	83	ASP
62	n6	90	VAL
62	n6	94	SER
62	n6	99	LEU
62	n6	120	GLN
63	n7	3	LYS
63	n7	17	ARG
63	n7	28	PRO
63	n7	31	GLU
63	n7	33	SER
63	n7	34	LYS
63	n7	36	HIS
63	n7	46	ILE
63	n7	47	GLU
63	n7	52	LYS
63	n7	65	ARG
63	n7	72	ILE
63	n7	77	TYR
63	n7	81	LEU
63	n7	83	THR
63	n7	90	GLU
63	n7	93	LYS
63	n7	95	VAL
63	n7	97	SER
63	n7	99	GLU
63	n7	106	GLN
63	n7	113	VAL

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Mol	Chain	Res	Type
63	n7	120	GLU
63	n7	123	GLN
63	n7	134	LEU
63	n7	135	ARG
64	n8	8	THR
64	n8	10	LYS
64	n8	15	VAL
64	n8	25	HIS
64	n8	26	ARG
64	n8	34	MET
64	n8	42	ARG
64	n8	60	TYR
64	n8	73	LEU
64	n8	91	LEU
64	n8	98	THR
64	n8	123	VAL
64	n8	128	ARG
64	n8	131	SER
64	n8	132	LYS
64	n8	133	LEU
64	n8	135	GLU
64	n8	139	ARG
64	n8	148	ILE
65	n9	3	LYS
65	n9	13	THR
65	n9	14	ARG
65	n9	19	ASN
65	n9	21	ILE
65	n9	22	LYS
65	n9	26	THR
65	n9	28	LYS
65	n9	33	LYS
65	n9	38	LYS
65	n9	42	ASN
65	n9	54	LEU
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	10	ILE
66	o0	19	LYS
66	o0	32	LYS
66	o0	34	LEU

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Mol	Chain	Res	Type
66	o0	40	LYS
66	o0	41	LEU
66	o0	48	THR
66	o0	61	MET
66	o0	66	LYS
66	o0	68	TYR
66	o0	74	ASN
66	o0	79	THR
66	o0	86	ARG
66	o0	99	ASP
66	o0	101	LEU
66	o0	103	THR
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	31	ARG
67	o1	41	LYS
67	o1	44	MET
67	o1	46	THR
67	o1	54	GLU
67	o1	55	LEU
67	o1	57	GLN
67	o1	62	ARG
67	o1	64	VAL
67	o1	76	SER
67	o1	82	GLU
67	o1	83	GLU
67	o1	84	ASP
67	o1	91	SER
67	o1	94	GLU
67	o1	96	VAL
67	o1	98	VAL
67	o1	100	SER
67	o1	102	LYS
67	o1	106	THR
67	o1	107	VAL
67	o1	110	GLU
67	o1	112	ASP
68	o2	4	LEU
68	o2	5	PRO
68	o2	14	THR
68	o2	15	LYS

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Mol	Chain	Res	Type
68	o2	21	HIS
68	o2	24	ARG
68	o2	33	ARG
68	o2	34	LYS
68	o2	35	GLN
68	o2	36	LYS
68	o2	41	VAL
68	o2	51	SER
68	o2	62	LYS
68	o2	64	LYS
68	o2	71	HIS
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	87	MET
68	o2	89	THR
68	o2	91	THR
68	o2	95	GLU
68	o2	101	SER
68	o2	109	LEU
68	o2	111	ARG
68	o2	123	LYS
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	19	SER
69	o3	31	LYS
69	o3	42	GLN
69	o3	49	ILE
69	o3	56	SER
69	o3	57	LYS
69	o3	59	VAL
69	o3	63	LYS
69	o3	70	LYS
69	o3	74	THR
69	o3	84	THR
69	o3	93	THR
69	o3	98	VAL
69	o3	107	ILE
70	o4	5	VAL
70	o4	20	ILE
70	o4	22	VAL

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Mol	Chain	Res	Type
70	o4	24	LYS
70	o4	33	GLN
70	o4	35	VAL
70	o4	37	LYS
70	o4	40	THR
70	o4	47	CYS
70	o4	57	LEU
70	o4	58	ARG
70	o4	71	THR
70	o4	79	SER
70	o4	83	ASN
70	o4	87	GLU
70	o4	88	ARG
70	o4	98	GLN
70	o4	104	VAL
71	o5	4	VAL
71	o5	11	THR
71	o5	15	GLU
71	o5	20	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	30	GLU
71	o5	36	LEU
71	o5	45	LYS
71	o5	46	THR
71	o5	47	VAL
71	o5	48	ARG
71	o5	53	CYS
71	o5	62	GLN
71	o5	69	LEU
71	o5	80	LEU
71	o5	81	ARG
71	o5	86	ARG
71	o5	89	ARG
71	o5	90	ARG
71	o5	94	LYS
71	o5	101	THR
71	o5	107	LYS
71	o5	113	GLN
71	o5	119	LYS
72	o6	3	VAL
72	o6	7	ILE

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Mol	Chain	Res	Type
72	o6	9	ILE
72	o6	11	LEU
72	o6	15	LYS
72	o6	21	THR
72	o6	26	ILE
72	o6	27	SER
72	o6	29	LYS
72	o6	34	SER
72	o6	36	ARG
72	o6	37	THR
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	59	ASP
72	o6	60	LEU
72	o6	62	ARG
72	o6	66	GLU
72	o6	67	LYS
72	o6	68	ARG
72	o6	71	LYS
72	o6	74	LYS
72	o6	76	ARG
72	o6	81	THR
72	o6	88	GLU
72	o6	94	ILE
72	o6	98	ARG
73	o7	3	LYS
73	o7	17	THR
73	o7	19	CYS
73	o7	21	ARG
73	o7	25	ARG
73	o7	33	THR
73	o7	36	SER
73	o7	55	ARG
73	o7	59	THR
73	o7	65	ARG
73	o7	67	LEU
73	o7	74	PHE
73	o7	75	LYS
74	o8	12	LEU
74	o8	13	GLU

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Mol	Chain	Res	Type
74	o8	17	ARG
74	o8	27	ILE
74	o8	38	PHE
74	o8	41	THR
74	o8	46	ARG
74	o8	50	SER
74	o8	53	THR
74	o8	54	LEU
74	o8	61	LYS
74	o8	63	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	67	GLN
74	o8	72	THR
75	o9	4	GLN
75	o9	15	LYS
75	o9	21	ARG
75	o9	23	LEU
75	o9	27	ILE
75	o9	28	ARG
75	o9	29	LEU
75	o9	47	THR
76	q0	79	GLU
76	q0	85	LEU
76	q0	88	LYS
76	q0	93	LYS
76	q0	94	SER
76	q0	99	CYS
76	q0	106	ARG
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	127	LEU
76	q0	128	LYS
77	q1	2	ARG
77	q1	6	ARG
77	q1	9	ARG
77	q1	11	ARG
77	q1	13	LEU
77	q1	21	ARG
77	q1	23	ARG
78	q2	6	LYS

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Mol	Chain	Res	Type
78	q2	7	THR
78	q2	8	ARG
78	q2	16	THR
78	q2	18	ARG
78	q2	22	GLN
78	q2	45	ARG
78	q2	46	LYS
78	q2	61	LYS
78	q2	71	ARG
78	q2	78	LYS
78	q2	83	LEU
78	q2	85	LEU
78	q2	93	LEU
78	q2	98	LYS
78	q2	99	GLN
79	q3	3	LYS
79	q3	16	VAL
79	q3	20	SER
79	q3	33	GLN
79	q3	40	SER
79	q3	42	CYS
79	q3	45	LYS
79	q3	48	LYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	59	CYS
79	q3	70	THR
79	q3	81	SER
79	q3	84	ARG
79	q3	90	VAL
81	p0	4	ILE
81	p0	5	ARG
81	p0	15	LEU
81	p0	30	VAL
81	p0	31	ASP
81	p0	39	HIS
81	p0	42	ARG
81	p0	43	LYS
81	p0	48	ARG
81	p0	52	LEU
81	p0	55	LYS

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Mol	Chain	Res	Type
81	p0	57	THR
81	p0	67	LEU
81	p0	70	LEU
81	p0	76	LEU
81	p0	93	LEU
81	p0	94	THR
81	p0	97	LYS
81	p0	101	VAL
81	p0	104	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
3	S1	209	ASN
3	S1	232	HIS
4	S2	152	HIS
12	C0	58	GLN
13	C1	110	HIS
13	C1	118	GLN
18	C6	77	GLN
20	C8	75	ASN
20	C8	78	HIS
22	D0	48	HIS
23	D1	74	GLN
24	D2	56	HIS
25	D3	79	ASN
40	L3	139	GLN
42	L5	40	HIS
42	L5	264	GLN
43	L6	28	GLN
44	L7	244	ASN
46	L9	49	ASN
47	M0	144	ASN
53	M7	179	GLN
58	N2	87	ASN
62	N6	120	GLN
64	N8	74	ASN
69	O3	26	ASN
70	O4	3	GLN
75	O9	50	ASN
11	s9	110	GLN
11	s9	124	HIS

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Mol	Chain	Res	Type
20	c8	89	GLN
24	d2	15	ASN
24	d2	24	GLN
24	d2	56	HIS
26	d4	22	GLN
29	d7	19	HIS
40	l3	184	ASN
44	l7	80	GLN
45	l8	192	GLN
47	m0	51	HIS
47	m0	144	ASN
55	m9	7	GLN
62	n6	4	GLN
63	n7	57	HIS
68	o2	88	HIS
72	o6	63	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	509 (29%)	56 (3%)
1	6	1793/1800 (99%)	472 (26%)	48 (2%)
36	1	3145/3396 (92%)	704 (22%)	78 (2%)
36	5	3145/3396 (92%)	688 (21%)	76 (2%)
37	3	120/121 (99%)	17 (14%)	2 (1%)
37	7	120/121 (99%)	24 (20%)	2 (1%)
38	4	157/158 (99%)	36 (22%)	5 (3%)
38	8	157/158 (99%)	38 (24%)	2 (1%)
All	All	10384/10950 (94%)	2488 (23%)	269 (2%)

All (2488) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	40	A
1	2	41	A

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Mol	Chain	Res	Type
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	77	U
1	2	100	A
1	2	104	A
1	2	114	C
1	2	116	U
1	2	125	U
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	152	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	169	A
1	2	178	U
1	2	185	U
1	2	186	C
1	2	187	G
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U

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Mol	Chain	Res	Type
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	212	U
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	226	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	231	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	249	U
1	2	250	C
1	2	256	A
1	2	260	U
1	2	261	U
1	2	265	A
1	2	270	C
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	284	G
1	2	288	A
1	2	290	G

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Mol	Chain	Res	Type
1	2	299	A
1	2	308	C
1	2	313	U
1	2	314	C
1	2	316	A
1	2	319	U
1	2	321	C
1	2	322	G
1	2	337	G
1	2	338	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	363	G
1	2	368	U
1	2	369	A
1	2	381	C
1	2	387	A
1	2	390	G
1	2	393	C
1	2	397	A
1	2	399	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	403	G
1	2	404	G
1	2	416	A
1	2	418	G
1	2	419	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	434	G
1	2	439	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	452	A
1	2	454	U

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Mol	Chain	Res	Type
1	2	464	A
1	2	468	A
1	2	471	A
1	2	480	G
1	2	484	C
1	2	485	A
1	2	486	G
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	514	G
1	2	515	A
1	2	516	G
1	2	518	A
1	2	519	C
1	2	520	A
1	2	524	U
1	2	527	A
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

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Mol	Chain	Res	Type
1	2	544	A
1	2	546	U
1	2	547	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	578	U
1	2	579	A
1	2	580	A
1	2	582	U
1	2	585	A
1	2	594	A
1	2	595	G
1	2	597	G
1	2	598	U
1	2	606	A
1	2	609	U
1	2	610	G
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	630	A
1	2	639	U
1	2	640	U
1	2	648	G
1	2	649	U
1	2	650	U
1	2	653	C
1	2	654	C
1	2	656	G
1	2	658	C
1	2	677	G
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C

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Mol	Chain	Res	Type
1	2	692	C
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	711	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	724	C
1	2	725	U
1	2	727	U
1	2	728	U
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	744	U
1	2	753	A
1	2	754	A

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Mol	Chain	Res	Type
1	2	755	A
1	2	756	A
1	2	758	U
1	2	759	U
1	2	765	G
1	2	766	U
1	2	768	C
1	2	774	A
1	2	775	G
1	2	778	G
1	2	779	U
1	2	781	U
1	2	783	G
1	2	784	C
1	2	787	G
1	2	789	A
1	2	790	U
1	2	793	A
1	2	794	U
1	2	795	U
1	2	807	A
1	2	812	A
1	2	814	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	838	G
1	2	840	U
1	2	846	G
1	2	848	C
1	2	854	U
1	2	860	U

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Mol	Chain	Res	Type
1	2	861	U
1	2	862	A
1	2	863	A
1	2	864	U
1	2	865	A
1	2	876	G
1	2	886	U
1	2	892	A
1	2	898	A
1	2	912	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	916	U
1	2	921	U
1	2	933	A
1	2	935	U
1	2	942	G
1	2	951	A
1	2	960	U
1	2	961	U
1	2	966	A
1	2	971	A
1	2	982	U
1	2	992	A
1	2	993	A
1	2	995	A
1	2	1002	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1021	C
1	2	1026	A
1	2	1028	C
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1057	U
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	1066	C
1	2	1067	C
1	2	1073	G
1	2	1074	G
1	2	1081	A
1	2	1082	C
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1101	G
1	2	1109	G
1	2	1111	G
1	2	1138	A
1	2	1139	A
1	2	1150	G
1	2	1151	A
1	2	1155	G
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1168	U
1	2	1185	U
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	1212	G
1	2	1217	A
1	2	1218	G
1	2	1226	A

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Mol	Chain	Res	Type
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1258	U
1	2	1262	U
1	2	1276	U
1	2	1284	C
1	2	1286	U
1	2	1290	U
1	2	1314	U
1	2	1315	U
1	2	1319	A
1	2	1320	U
1	2	1321	A
1	2	1338	C
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1342	C
1	2	1344	A
1	2	1345	A
1	2	1354	G
1	2	1355	C
1	2	1361	U
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1378	U
1	2	1383	G
1	2	1384	A
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1412	G

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Mol	Chain	Res	Type
1	2	1413	U
1	2	1415	U
1	2	1424	A
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1432	U
1	2	1445	G
1	2	1446	A
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1461	C
1	2	1469	A
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1478	G
1	2	1481	C
1	2	1482	C
1	2	1485	C
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1503	A
1	2	1506	G
1	2	1515	A
1	2	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1526	A
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1540	G
1	2	1542	G

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Mol	Chain	Res	Type
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
1	2	1616	G
1	2	1619	C
1	2	1631	A
1	2	1634	C
1	2	1639	C
1	2	1657	U
1	2	1658	G
1	2	1663	G
1	2	1680	G
1	2	1681	A
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1731	A
1	2	1747	G
1	2	1756	A
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1789	G
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	15	C
36	1	16	A
36	1	18	G

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Mol	Chain	Res	Type
36	1	26	A
36	1	40	A
36	1	45	A
36	1	49	A
36	1	54	C
36	1	57	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	73	C
36	1	74	G
36	1	76	G
36	1	83	U
36	1	85	A
36	1	87	U
36	1	92	G
36	1	93	C
36	1	94	G
36	1	99	A
36	1	102	C
36	1	103	G
36	1	105	C
36	1	109	A
36	1	110	G
36	1	111	C
36	1	120	G
36	1	121	A
36	1	122	A
36	1	126	U
36	1	133	U
36	1	135	C
36	1	136	G
36	1	142	C
36	1	147	U
36	1	156	G
36	1	157	A
36	1	163	C
36	1	166	C
36	1	169	U
36	1	170	G
36	1	173	G

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Mol	Chain	Res	Type
36	1	187	A
36	1	190	U
36	1	191	U
36	1	210	U
36	1	211	A
36	1	218	G
36	1	219	A
36	1	235	A
36	1	239	G
36	1	240	U
36	1	243	G
36	1	245	U
36	1	247	C
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	256	G
36	1	269	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	296	A
36	1	305	U
36	1	323	A
36	1	329	U
36	1	339	C
36	1	344	A
36	1	349	A
36	1	350	C
36	1	351	A
36	1	352	A
36	1	376	G
36	1	397	A
36	1	398	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	420	G
36	1	421	G
36	1	422	A
36	1	438	A

Continued on next page...

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Mol	Chain	Res	Type
36	1	439	C
36	1	440	A
36	1	495	G
36	1	503	C
36	1	507	U
36	1	520	U
36	1	521	A
36	1	531	G
36	1	532	A
36	1	533	A
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	557	A
36	1	558	U
36	1	559	A
36	1	569	A
36	1	578	A
36	1	579	G
36	1	592	A
36	1	593	C
36	1	601	U
36	1	604	G
36	1	607	A
36	1	609	G
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A
36	1	625	G
36	1	636	C
36	1	638	C
36	1	647	A
36	1	649	A
36	1	660	A
36	1	661	G

Continued on next page...

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Mol	Chain	Res	Type
36	1	667	C
36	1	677	A
36	1	681	U
36	1	683	U
36	1	691	A
36	1	692	A
36	1	699	A
36	1	705	A
36	1	708	G
36	1	712	G
36	1	715	A
36	1	716	A
36	1	718	G
36	1	719	U
36	1	725	G
36	1	744	A
36	1	763	G
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	780	A
36	1	781	G
36	1	785	G
36	1	792	G
36	1	804	C
36	1	806	A
36	1	817	A
36	1	828	A
36	1	830	A
36	1	849	C
36	1	861	C
36	1	874	U
36	1	878	G
36	1	879	U
36	1	882	A
36	1	883	A
36	1	890	C
36	1	896	A
36	1	897	U

Continued on next page...

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Mol	Chain	Res	Type
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	919	U
36	1	921	A
36	1	923	C
36	1	924	G
36	1	926	A
36	1	937	G
36	1	938	C
36	1	944	C
36	1	959	C
36	1	960	U
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
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	1015	U
36	1	1016	C
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1037	C
36	1	1041	U
36	1	1047	A
36	1	1049	C
36	1	1051	U
36	1	1063	G
36	1	1064	A
36	1	1065	A

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Mol	Chain	Res	Type
36	1	1069	C
36	1	1070	U
36	1	1072	G
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1087	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1129	A
36	1	1131	G
36	1	1144	U
36	1	1153	A
36	1	1159	A
36	1	1160	C
36	1	1161	G
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1191	U
36	1	1192	C
36	1	1196	C
36	1	1197	A
36	1	1201	C
36	1	1209	G
36	1	1212	A
36	1	1213	G
36	1	1216	C
36	1	1217	A
36	1	1218	U
36	1	1221	A
36	1	1222	G
36	1	1225	A
36	1	1227	C

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Mol	Chain	Res	Type
36	1	1232	C
36	1	1233	G
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	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	1298	C
36	1	1303	A
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1310	G
36	1	1313	G
36	1	1330	A
36	1	1331	U
36	1	1345	G
36	1	1348	U
36	1	1349	G
36	1	1350	A
36	1	1351	U
36	1	1352	A

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Mol	Chain	Res	Type
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1379	G
36	1	1386	A
36	1	1392	G
36	1	1398	U
36	1	1399	A
36	1	1400	G
36	1	1419	A
36	1	1421	G
36	1	1431	G
36	1	1433	A
36	1	1434	G
36	1	1437	C
36	1	1438	U
36	1	1446	A
36	1	1450	G
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1508	C
36	1	1523	U
36	1	1527	C
36	1	1528	G
36	1	1533	U
36	1	1535	A
36	1	1536	G
36	1	1554	U
36	1	1555	U
36	1	1556	C
36	1	1558	A
36	1	1560	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1565	G
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U

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Mol	Chain	Res	Type
36	1	1570	U
36	1	1572	U
36	1	1576	G
36	1	1579	C
36	1	1580	A
36	1	1581	C
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1606	U
36	1	1607	U
36	1	1612	A
36	1	1620	U
36	1	1621	A
36	1	1628	C
36	1	1629	U
36	1	1639	C
36	1	1643	A
36	1	1645	U
36	1	1657	C
36	1	1658	G
36	1	1683	A
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1742	U
36	1	1749	A
36	1	1750	A
36	1	1751	G
36	1	1761	C
36	1	1762	C
36	1	1764	U
36	1	1765	U
36	1	1767	C
36	1	1769	G
36	1	1770	G
36	1	1776	G
36	1	1779	C
36	1	1780	G
36	1	1797	A
36	1	1801	U

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Mol	Chain	Res	Type
36	1	1809	A
36	1	1810	A
36	1	1814	A
36	1	1815	U
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1839	A
36	1	1840	U
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	1851	G
36	1	1855	U
36	1	1866	C
36	1	1871	U
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1906	G
36	1	1911	A
36	1	1912	U
36	1	1931	U
36	1	1935	G
36	1	1950	U
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	1954	G
36	1	2094	C
36	1	2097	U
36	1	2101	C
36	1	2102	U
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2121	G

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Mol	Chain	Res	Type
36	1	2122	G
36	1	2131	A
36	1	2134	G
36	1	2139	A
36	1	2140	U
36	1	2144	A
36	1	2158	A
36	1	2169	G
36	1	2177	G
36	1	2205	U
36	1	2206	G
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2239	G
36	1	2244	A
36	1	2245	C
36	1	2246	G
36	1	2249	G
36	1	2254	U
36	1	2255	A
36	1	2256	A
36	1	2263	C
36	1	2264	U
36	1	2268	U
36	1	2272	G
36	1	2273	G
36	1	2279	A
36	1	2280	A
36	1	2281	A
36	1	2282	U
36	1	2284	C
36	1	2286	U
36	1	2298	U
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2331	C
36	1	2334	U
36	1	2336	U

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Mol	Chain	Res	Type
36	1	2339	C
36	1	2343	C
36	1	2361	A
36	1	2366	C
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	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2405	C
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2435	G
36	1	2437	G
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	2514	U
36	1	2515	A
36	1	2519	A
36	1	2520	A
36	1	2522	G
36	1	2523	A
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

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Mol	Chain	Res	Type
36	1	2544	U
36	1	2546	C
36	1	2547	A
36	1	2549	G
36	1	2550	U
36	1	2551	U
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2561	A
36	1	2562	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	2581	U
36	1	2582	C
36	1	2585	G
36	1	2586	G
36	1	2593	A
36	1	2594	C
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2628	A
36	1	2637	A
36	1	2638	C
36	1	2652	U
36	1	2656	A
36	1	2657	A
36	1	2674	A
36	1	2677	G
36	1	2689	A
36	1	2690	G
36	1	2691	A
36	1	2694	A
36	1	2696	A
36	1	2705	A
36	1	2706	G
36	1	2712	U

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Mol	Chain	Res	Type
36	1	2714	G
36	1	2719	U
36	1	2720	G
36	1	2727	A
36	1	2728	G
36	1	2729	U
36	1	2737	C
36	1	2753	G
36	1	2755	C
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	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2810	C
36	1	2815	G
36	1	2817	A
36	1	2818	U
36	1	2829	U
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2847	A
36	1	2853	A
36	1	2856	G
36	1	2860	U
36	1	2863	G
36	1	2871	G
36	1	2872	A
36	1	2873	U
36	1	2886	U
36	1	2887	A
36	1	2889	C
36	1	2898	G
36	1	2899	C

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Mol	Chain	Res	Type
36	1	2914	G
36	1	2923	U
36	1	2935	U
36	1	2936	A
36	1	2937	G
36	1	2942	C
36	1	2945	G
36	1	2947	G
36	1	2951	G
36	1	2955	U
36	1	2971	A
36	1	2974	U
36	1	2977	G
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	3002	C
36	1	3006	A
36	1	3012	A
36	1	3040	A
36	1	3054	U
36	1	3056	U
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3070	A
36	1	3076	C
36	1	3078	U
36	1	3079	U
36	1	3086	A
36	1	3087	A
36	1	3092	C
36	1	3104	U
36	1	3113	A
36	1	3122	A
36	1	3130	A
36	1	3131	U
36	1	3136	G
36	1	3142	A

Continued on next page...

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Mol	Chain	Res	Type
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	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	3190	C
36	1	3191	G
36	1	3196	U
36	1	3206	C
36	1	3207	U
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3229	G
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	3276	G
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3288	G

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Mol	Chain	Res	Type
36	1	3289	G
36	1	3294	A
36	1	3295	A
36	1	3304	U
36	1	3313	U
36	1	3316	A
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3335	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3346	U
36	1	3347	A
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3360	C
36	1	3363	U
36	1	3368	U
36	1	3369	G
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
37	3	7	G
37	3	13	A
37	3	14	U
37	3	21	G
37	3	22	A
37	3	44	C
37	3	45	A
37	3	54	U
37	3	65	G
37	3	74	C
37	3	76	A
37	3	89	G
37	3	91	G

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Mol	Chain	Res	Type
37	3	95	A
37	3	102	A
37	3	112	G
37	3	121	U
38	4	2	A
38	4	9	A
38	4	21	C
38	4	26	U
38	4	34	U
38	4	35	C
38	4	43	A
38	4	52	A
38	4	58	G
38	4	59	A
38	4	62	C
38	4	63	G
38	4	79	A
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	104	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	148	G
38	4	152	G
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C

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Mol	Chain	Res	Type
1	6	6	G
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	47	A
1	6	50	C
1	6	57	G
1	6	60	U
1	6	61	A
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	78	A
1	6	80	A
1	6	103	A
1	6	104	A
1	6	114	C
1	6	115	G
1	6	125	U
1	6	129	U
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	142	G
1	6	144	U
1	6	145	A
1	6	158	U
1	6	159	U
1	6	161	U
1	6	166	C
1	6	177	U
1	6	178	U
1	6	185	U
1	6	188	A

Continued on next page...

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Mol	Chain	Res	Type
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	194	U
1	6	195	G
1	6	196	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	226	A
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	234	G
1	6	240	U
1	6	241	U
1	6	242	U
1	6	249	U
1	6	250	C
1	6	257	A
1	6	260	U
1	6	261	U
1	6	265	A
1	6	269	G
1	6	270	C
1	6	271	A
1	6	272	U
1	6	273	G
1	6	277	U
1	6	278	U
1	6	280	U
1	6	285	G
1	6	287	G
1	6	299	A

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Mol	Chain	Res	Type
1	6	308	C
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	337	G
1	6	338	C
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	362	G
1	6	369	A
1	6	370	A
1	6	390	G
1	6	397	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	421	A
1	6	424	C
1	6	425	A
1	6	426	G
1	6	429	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	477	A
1	6	480	G
1	6	484	C
1	6	486	G
1	6	487	G

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Mol	Chain	Res	Type
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	515	A
1	6	519	C
1	6	525	A
1	6	527	A
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
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

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Mol	Chain	Res	Type
1	6	594	A
1	6	595	G
1	6	606	A
1	6	609	U
1	6	610	G
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	632	U
1	6	634	G
1	6	637	C
1	6	639	U
1	6	640	U
1	6	648	G
1	6	650	U
1	6	652	G
1	6	653	C
1	6	658	C
1	6	659	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	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	696	C
1	6	697	C
1	6	698	U
1	6	709	C
1	6	710	U

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Mol	Chain	Res	Type
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	743	U
1	6	745	U
1	6	753	A
1	6	754	A
1	6	755	A
1	6	756	A
1	6	762	A
1	6	764	U
1	6	765	G
1	6	766	U
1	6	767	U
1	6	774	A
1	6	775	G
1	6	777	C
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	789	A
1	6	792	U
1	6	793	A
1	6	794	U
1	6	798	C
1	6	803	A
1	6	808	U
1	6	811	A
1	6	812	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	822	U
1	6	823	G
1	6	824	G

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Mol	Chain	Res	Type
1	6	825	U
1	6	826	U
1	6	828	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	847	A
1	6	863	A
1	6	873	U
1	6	876	G
1	6	881	A
1	6	898	A
1	6	908	U
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	970	A
1	6	971	A
1	6	983	A
1	6	988	A
1	6	992	A
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1008	G
1	6	1010	C
1	6	1018	U
1	6	1020	A
1	6	1021	C
1	6	1026	A
1	6	1028	C
1	6	1039	A
1	6	1040	G

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Mol	Chain	Res	Type
1	6	1052	U
1	6	1053	G
1	6	1056	U
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1071	U
1	6	1072	C
1	6	1073	G
1	6	1076	A
1	6	1081	A
1	6	1082	C
1	6	1092	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	1137	A
1	6	1138	A
1	6	1146	G
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
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	1227	A
1	6	1228	G

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Mol	Chain	Res	Type
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	1276	U
1	6	1286	U
1	6	1294	G
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1349	G
1	6	1354	G
1	6	1355	C
1	6	1360	A
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1371	A
1	6	1372	U
1	6	1373	C
1	6	1377	U
1	6	1388	A
1	6	1390	U
1	6	1396	U
1	6	1397	U
1	6	1398	U

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Mol	Chain	Res	Type
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1412	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	1458	G
1	6	1459	C
1	6	1461	C
1	6	1469	A
1	6	1471	A
1	6	1474	G
1	6	1478	G
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	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
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	1557	U

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Mol	Chain	Res	Type
1	6	1559	A
1	6	1569	A
1	6	1573	A
1	6	1574	G
1	6	1575	G
1	6	1576	A
1	6	1577	A
1	6	1584	G
1	6	1590	G
1	6	1601	G
1	6	1615	C
1	6	1616	G
1	6	1619	C
1	6	1621	U
1	6	1635	A
1	6	1637	C
1	6	1638	G
1	6	1639	C
1	6	1657	U
1	6	1658	G
1	6	1681	A
1	6	1682	U
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	1703	C
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1731	A
1	6	1742	U
1	6	1760	G
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G

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Mol	Chain	Res	Type
1	6	1782	A
1	6	1789	G
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	16	A
36	5	21	G
36	5	26	A
36	5	40	A
36	5	43	A
36	5	44	U
36	5	49	A
36	5	58	G
36	5	59	G
36	5	60	A
36	5	62	A
36	5	65	A
36	5	66	A
36	5	72	C
36	5	73	C
36	5	76	G
36	5	82	C
36	5	83	U
36	5	86	G
36	5	92	G
36	5	93	C
36	5	96	G
36	5	99	A
36	5	105	C
36	5	109	A
36	5	110	G
36	5	111	C
36	5	113	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	126	U

Continued on next page...

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Mol	Chain	Res	Type
36	5	127	G
36	5	133	U
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	169	U
36	5	170	G
36	5	171	G
36	5	172	G
36	5	173	G
36	5	174	C
36	5	179	C
36	5	180	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	213	A
36	5	218	G
36	5	219	A
36	5	224	C
36	5	225	C
36	5	236	G
36	5	237	G
36	5	239	G
36	5	240	U
36	5	244	G
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

Continued on next page...

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Mol	Chain	Res	Type
36	5	259	C
36	5	265	A
36	5	269	G
36	5	270	U
36	5	284	A
36	5	286	U
36	5	295	A
36	5	309	U
36	5	323	A
36	5	329	U
36	5	339	C
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	421	G
36	5	422	A
36	5	436	A
36	5	437	G
36	5	439	C
36	5	440	A
36	5	441	U
36	5	442	G
36	5	492	U
36	5	495	G
36	5	498	A
36	5	507	U
36	5	510	G
36	5	520	U
36	5	521	A
36	5	523	A
36	5	531	G
36	5	535	G
36	5	546	C
36	5	547	G

Continued on next page...

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Mol	Chain	Res	Type
36	5	548	G
36	5	551	A
36	5	555	U
36	5	557	A
36	5	559	A
36	5	578	A
36	5	579	G
36	5	592	A
36	5	600	G
36	5	604	G
36	5	607	A
36	5	608	A
36	5	609	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	651	G
36	5	660	A
36	5	677	A
36	5	681	U
36	5	683	U
36	5	691	A
36	5	705	A
36	5	708	G
36	5	711	A
36	5	712	G
36	5	715	A
36	5	716	A
36	5	725	G
36	5	726	G
36	5	727	G
36	5	758	C
36	5	764	U
36	5	765	C
36	5	766	U
36	5	767	U
36	5	776	U
36	5	777	U
36	5	781	G

Continued on next page...

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Mol	Chain	Res	Type
36	5	785	G
36	5	786	A
36	5	806	A
36	5	817	A
36	5	826	G
36	5	830	A
36	5	859	G
36	5	861	C
36	5	874	U
36	5	879	U
36	5	882	A
36	5	890	C
36	5	891	G
36	5	896	A
36	5	897	U
36	5	907	G
36	5	908	G
36	5	910	G
36	5	913	A
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	944	C
36	5	959	C
36	5	960	U
36	5	964	G
36	5	979	U
36	5	980	A
36	5	983	A
36	5	993	G
36	5	994	G
36	5	1001	G
36	5	1002	A
36	5	1006	A
36	5	1010	G
36	5	1014	U
36	5	1015	U
36	5	1017	C
36	5	1019	G

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Mol	Chain	Res	Type
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1028	U
36	5	1029	G
36	5	1032	C
36	5	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	1083	G
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	1159	A
36	5	1161	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	1201	C
36	5	1202	A
36	5	1209	G
36	5	1222	G

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Mol	Chain	Res	Type
36	5	1232	C
36	5	1233	G
36	5	1235	U
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1243	G
36	5	1245	A
36	5	1246	G
36	5	1252	A
36	5	1254	C
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	1285	G
36	5	1292	C
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1311	G
36	5	1313	G
36	5	1329	U
36	5	1330	A
36	5	1331	U
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	1380	G
36	5	1385	C
36	5	1386	A

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Mol	Chain	Res	Type
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1428	A
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1455	U
36	5	1465	A
36	5	1481	A
36	5	1482	A
36	5	1490	A
36	5	1502	C
36	5	1503	A
36	5	1508	C
36	5	1517	G
36	5	1519	G
36	5	1527	C
36	5	1533	U
36	5	1536	G
36	5	1539	A
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1557	A
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1566	A
36	5	1567	U
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C

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Mol	Chain	Res	Type
36	5	1581	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1612	A
36	5	1620	U
36	5	1629	U
36	5	1633	C
36	5	1639	C
36	5	1641	U
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1657	C
36	5	1658	G
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	1735	G
36	5	1736	G
36	5	1750	A
36	5	1751	G
36	5	1760	A
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	1781	C
36	5	1793	C
36	5	1797	A
36	5	1810	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U

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Mol	Chain	Res	Type
36	5	1821	U
36	5	1839	A
36	5	1842	A
36	5	1845	G
36	5	1846	C
36	5	1849	C
36	5	1864	A
36	5	1866	C
36	5	1873	U
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1881	A
36	5	1893	A
36	5	1906	G
36	5	1907	C
36	5	1922	A
36	5	1926	C
36	5	1935	G
36	5	1947	G
36	5	1953	G
36	5	2097	U
36	5	2101	C
36	5	2102	U
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	2155	G
36	5	2158	A
36	5	2169	G
36	5	2187	G
36	5	2192	C
36	5	2198	A
36	5	2205	U
36	5	2209	U
36	5	2210	G
36	5	2219	A
36	5	2223	A

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Mol	Chain	Res	Type
36	5	2225	U
36	5	2244	A
36	5	2246	G
36	5	2250	G
36	5	2252	A
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2258	U
36	5	2261	G
36	5	2264	U
36	5	2270	A
36	5	2273	G
36	5	2278	C
36	5	2279	A
36	5	2280	A
36	5	2281	A
36	5	2288	G
36	5	2299	A
36	5	2303	A
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2319	U
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2367	A
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2382	G
36	5	2385	G
36	5	2393	G
36	5	2397	A
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A

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Mol	Chain	Res	Type
36	5	2405	C
36	5	2406	C
36	5	2410	U
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2435	G
36	5	2436	U
36	5	2437	G
36	5	2439	A
36	5	2440	G
36	5	2441	A
36	5	2443	A
36	5	2504	U
36	5	2505	U
36	5	2506	U
36	5	2507	C
36	5	2508	U
36	5	2509	U
36	5	2510	U
36	5	2511	A
36	5	2514	U
36	5	2515	A
36	5	2523	A
36	5	2524	A
36	5	2525	G
36	5	2526	C
36	5	2529	A
36	5	2530	G
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2544	U
36	5	2550	U
36	5	2552	C
36	5	2554	A
36	5	2555	G
36	5	2562	A
36	5	2564	G
36	5	2566	C

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Mol	Chain	Res	Type
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2586	G
36	5	2587	U
36	5	2588	U
36	5	2593	A
36	5	2606	G
36	5	2607	G
36	5	2608	G
36	5	2609	A
36	5	2610	G
36	5	2614	G
36	5	2628	A
36	5	2636	A
36	5	2638	C
36	5	2639	G
36	5	2652	U
36	5	2656	A
36	5	2674	A
36	5	2675	C
36	5	2676	A
36	5	2677	G
36	5	2689	A
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2705	A
36	5	2706	G
36	5	2713	U
36	5	2714	G
36	5	2716	U
36	5	2727	A
36	5	2728	G
36	5	2729	U
36	5	2740	A

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Mol	Chain	Res	Type
36	5	2748	A
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	2781	U
36	5	2783	U
36	5	2796	G
36	5	2797	C
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	2829	U
36	5	2843	U
36	5	2845	A
36	5	2849	C
36	5	2853	A
36	5	2856	G
36	5	2865	U
36	5	2871	G
36	5	2872	A
36	5	2875	U
36	5	2876	C
36	5	2887	A
36	5	2889	C
36	5	2896	A
36	5	2899	C
36	5	2914	G
36	5	2921	U
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2947	G

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Mol	Chain	Res	Type
36	5	2957	G
36	5	2971	A
36	5	2972	G
36	5	2979	U
36	5	2980	U
36	5	2982	A
36	5	2990	G
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3028	G
36	5	3030	G
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3069	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3092	C
36	5	3094	A
36	5	3102	G
36	5	3119	U
36	5	3122	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3148	U
36	5	3150	A
36	5	3153	U
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3164	C
36	5	3165	A
36	5	3166	C
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G

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Mol	Chain	Res	Type
36	5	3174	A
36	5	3175	U
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	3197	G
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	3238	G
36	5	3239	G
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3263	G
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
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	3295	A

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Mol	Chain	Res	Type
36	5	3304	U
36	5	3313	U
36	5	3316	A
36	5	3318	G
36	5	3319	U
36	5	3320	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3350	C
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3355	U
36	5	3356	G
36	5	3358	U
36	5	3369	G
36	5	3377	G
36	5	3378	C
36	5	3382	U
36	5	3383	G
36	5	3389	U
36	5	3390	G
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	33	U
37	7	38	U
37	7	49	G
37	7	50	U
37	7	51	A
37	7	53	U
37	7	54	U
37	7	57	G
37	7	60	G
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	92	A
37	7	93	C
37	7	99	G

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Mol	Chain	Res	Type
37	7	101	G
37	7	102	A
37	7	103	A
37	7	104	A
37	7	112	G
37	7	121	U
38	8	21	C
38	8	34	U
38	8	35	C
38	8	38	U
38	8	48	A
38	8	49	G
38	8	52	A
38	8	53	A
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	82	U
38	8	83	C
38	8	84	C
38	8	86	U
38	8	87	G
38	8	89	A
38	8	90	U
38	8	95	G
38	8	96	A
38	8	97	A
38	8	98	U
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	122	U
38	8	125	U
38	8	126	A
38	8	138	A
38	8	155	A
38	8	156	U

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Mol	Chain	Res	Type
38	8	157	U
38	8	158	U

All (269) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	25	C
1	2	73	U
1	2	74	U
1	2	103	A
1	2	114	C
1	2	130	C
1	2	131	C
1	2	136	C
1	2	139	C
1	2	158	U
1	2	192	U
1	2	218	A
1	2	240	U
1	2	277	U
1	2	278	U
1	2	280	U
1	2	321	C
1	2	400	A
1	2	417	A
1	2	468	A
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	555	A
1	2	558	U
1	2	606	A
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	794	U

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Mol	Chain	Res	Type
1	2	829	A
1	2	1058	U
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	1344	A
1	2	1370	U
1	2	1481	C
1	2	1489	U
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
36	1	66	A
36	1	93	C
36	1	99	A
36	1	169	U
36	1	210	U
36	1	217	U
36	1	239	G
36	1	282	G
36	1	369	A
36	1	397	A
36	1	547	G
36	1	594	U
36	1	637	C
36	1	763	G
36	1	764	U
36	1	816	A
36	1	873	C
36	1	916	G
36	1	981	U
36	1	993	G
36	1	1064	A

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Mol	Chain	Res	Type
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1160	C
36	1	1181	U
36	1	1196	C
36	1	1273	A
36	1	1307	G
36	1	1329	U
36	1	1331	U
36	1	1352	A
36	1	1355	A
36	1	1419	A
36	1	1481	A
36	1	1484	U
36	1	1554	U
36	1	1562	C
36	1	1582	C
36	1	1589	A
36	1	1716	U
36	1	1751	G
36	1	1820	U
36	1	1842	A
36	1	1846	C
36	1	2101	C
36	1	2112	U
36	1	2121	G
36	1	2209	U
36	1	2372	A
36	1	2374	C
36	1	2418	G
36	1	2522	G
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2644	C
36	1	2704	A
36	1	2728	G
36	1	2772	C
36	1	2818	U

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Mol	Chain	Res	Type
36	1	2842	U
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3195	U
36	1	3218	A
36	1	3228	C
36	1	3242	G
36	1	3269	U
36	1	3275	U
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
37	3	13	A
37	3	49	G
38	4	59	A
38	4	79	A
38	4	82	U
38	4	85	G
38	4	111	A
1	6	2	A
1	6	25	C
1	6	66	U
1	6	114	C
1	6	136	C
1	6	139	C
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	400	A
1	6	417	A
1	6	454	U
1	6	542	A
1	6	555	A
1	6	557	G
1	6	558	U
1	6	609	U
1	6	664	U

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Mol	Chain	Res	Type
1	6	678	A
1	6	697	C
1	6	717	C
1	6	755	A
1	6	815	G
1	6	829	A
1	6	1051	G
1	6	1058	U
1	6	1097	U
1	6	1098	U
1	6	1241	G
1	6	1244	A
1	6	1255	G
1	6	1344	A
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	1574	G
1	6	1615	C
1	6	1620	C
1	6	1657	U
1	6	1696	G
1	6	1698	G
1	6	1700	C
36	5	43	A
36	5	210	U
36	5	238	A
36	5	557	A
36	5	588	G
36	5	647	A
36	5	659	G
36	5	715	A
36	5	765	C
36	5	816	A
36	5	873	C
36	5	896	A
36	5	916	G
36	5	993	G
36	5	1027	A

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Mol	Chain	Res	Type
36	5	1064	A
36	5	1081	U
36	5	1093	A
36	5	1152	G
36	5	1181	U
36	5	1192	C
36	5	1236	G
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1317	A
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1507	G
36	5	1554	U
36	5	1560	G
36	5	1589	A
36	5	1643	A
36	5	1716	U
36	5	1751	G
36	5	1816	A
36	5	1841	A
36	5	1846	C
36	5	1878	G
36	5	2101	C
36	5	2112	U
36	5	2116	G
36	5	2121	G
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2257	C
36	5	2305	G
36	5	2372	A
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2539	C

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Mol	Chain	Res	Type
36	5	2586	G
36	5	2728	G
36	5	2772	C
36	5	2818	U
36	5	2887	A
36	5	2971	A
36	5	3056	U
36	5	3078	U
36	5	3121	U
36	5	3154	C
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3275	U
36	5	3289	G
36	5	3340	G
36	5	3341	U
36	5	3354	U
36	5	3357	U
37	7	49	G
37	7	111	U
38	8	89	A
38	8	111	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2559 ligands modelled in this entry, 1426 are monoatomic - leaving 1133 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	1	4208	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	1	4145	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
87	3K8	6	2205	-	32,32,32	0.55	0	44,47,47	0.87	3 (6%)
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	7	217	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	1	4004	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	1	4165	-	0,6,6	0.00	-	-		
86	OHX	m1	202	-	0,6,6	0.00	-	-		
86	OHX	5	4235	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		
86	OHX	3	217	-	0,6,6	0.00	-	-		
86	OHX	2	2138	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		
86	OHX	5	3952	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	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	4053	-	0,6,6	0.00	-	-		
86	OHX	m8	201	-	0,6,6	0.00	-	-		
86	OHX	5	4124	-	0,6,6	0.00	-	-		
86	OHX	5	3945	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	M0	304	-	0,6,6	0.00	-	-		
86	OHX	5	4018	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	O1	201	-	0,6,6	0.00	-	-		
86	OHX	1	3998	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	1	4037	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	m7	206	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	0,6,6	0.00	-	-		
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	0,6,6	0.00	-	-		
86	OHX	l3	404	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		
86	OHX	6	2163	-	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	4091	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
86	OHX	5	4214	-	0,6,6	0.00	-	-		
86	OHX	5	3955	-	0,6,6	0.00	-	-		
86	OHX	5	4253	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	O9	101	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	n9	102	-	0,6,6	0.00	-	-		
86	OHX	O2	202	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		
86	OHX	5	4057	-	0,6,6	0.00	-	-		
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	14	402	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	1	3978	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		
86	OHX	5	3904	-	0,6,6	0.00	-	-		
86	OHX	8	215	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	5	4131	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	2	2039	-	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	2195	-	0,6,6	0.00	-	-		
86	OHX	5	4249	-	0,6,6	0.00	-	-		
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	1	3934	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	8	231	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		
86	OHX	1	4168	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	1	4083	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	8	230	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	c8	202	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	1	3967	-	0,6,6	0.00	-	-		
86	OHX	n3	203	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	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	4222	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	5	3909	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	M5	302	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	5	4225	-	0,6,6	0.00	-	-		
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	0,6,6	0.00	-	-		
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	5	4251	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	1	4138	-	0,6,6	0.00	-	-		
86	OHX	4	223	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		
86	OHX	1	3874	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	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	4100	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	6	2187	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	O7	105	-	0,6,6	0.00	-	-		
86	OHX	5	4092	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	5	4211	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		
86	OHX	s1	302	-	0,6,6	0.00	-	-		
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	5	4076	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	1	3865	-	0,6,6	0.00	-	-		
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	1	4008	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	1	4012	-	0,6,6	0.00	-	-		
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	1	3920	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	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	2089	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	5	4126	-	0,6,6	0.00	-	-		
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	5	4248	-	0,6,6	0.00	-	-		
86	OHX	2	2121	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	2	2073	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	2	2054	-	0,6,6	0.00	-	-		
86	OHX	1	4206	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	1	3957	-	0,6,6	0.00	-	-		
86	OHX	5	3962	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	2	2178	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	0,6,6	0.00	-	-		
86	OHX	M9	202	-	0,6,6	0.00	-	-		
86	OHX	1	4084	-	0,6,6	0.00	-	-		
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	5	4142	-	0,6,6	0.00	-	-		
86	OHX	6	2116	-	0,6,6	0.00	-	-		
86	OHX	1	4158	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	5	4153	-	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	3928	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		
86	OHX	6	2068	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	5	3944	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	5	3996	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		
86	OHX	1	3870	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	5	4175	-	0,6,6	0.00	-	-		
86	OHX	5	3924	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		
86	OHX	1	3861	-	0,6,6	0.00	-	-		
86	OHX	2	2023	-	0,6,6	0.00	-	-		
86	OHX	2	2102	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	1	4000	-	0,6,6	0.00	-	-		
86	OHX	7	220	-	0,6,6	0.00	-	-		
86	OHX	5	4132	-	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	2056	-	0,6,6	0.00	-	-		
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	5	4241	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		
86	OHX	5	3901	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	0,6,6	0.00	-	-		
86	OHX	1	4081	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		
86	OHX	2	2134	-	0,6,6	0.00	-	-		
86	OHX	2	2163	-	0,6,6	0.00	-	-		
86	OHX	1	4061	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	6	2075	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	1	3997	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	6	2123	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	6	2085	-	0,6,6	0.00	-	-		
86	OHX	1	4150	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	1	4170	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	2	2041	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	1	4072	-	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	4035	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	2	2046	-	0,6,6	0.00	-	-		
86	OHX	1	3872	-	0,6,6	0.00	-	-		
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	2	2126	-	0,6,6	0.00	-	-		
86	OHX	1	4115	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	7	219	-	0,6,6	0.00	-	-		
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	5	4149	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	O7	106	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	5	4226	-	0,6,6	0.00	-	-		
86	OHX	5	4047	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	1	4191	-	0,6,6	0.00	-	-		
86	OHX	8	217	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	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	2093	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		
86	OHX	M8	201	-	0,6,6	0.00	-	-		
86	OHX	1	4200	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	6	2191	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		
86	OHX	1	4065	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	1	4186	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	1	4025	-	0,6,6	0.00	-	-		
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	5	3999	-	0,6,6	0.00	-	-		
86	OHX	5	3913	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	6	2177	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	n1	201	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	1	4052	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	2	2144	-	0,6,6	0.00	-	-		
86	OHX	6	2137	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	2	2172	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	5	4055	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	15	303	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	5	4160	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	5	3972	-	0,6,6	0.00	-	-		
86	OHX	5	4195	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	5	4036	-	0,6,6	0.00	-	-		
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	5	4122	-	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	4107	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	1	3871	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	2	2122	-	0,6,6	0.00	-	-		
86	OHX	5	3995	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	1	3947	-	0,6,6	0.00	-	-		
86	OHX	1	3942	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	6	2145	-	0,6,6	0.00	-	-		
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	2	2094	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	0,6,6	0.00	-	-		
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	C8	201	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	8	216	-	0,6,6	0.00	-	-		
86	OHX	5	3915	-	0,6,6	0.00	-	-		
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	6	2050	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	1	3886	-	0,6,6	0.00	-	-		
86	OHX	m9	201	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	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	3998	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	0,6,6	0.00	-	-		
86	OHX	5	3966	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	3	222	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	N9	101	-	0,6,6	0.00	-	-		
86	OHX	1	3900	-	0,6,6	0.00	-	-		
86	OHX	1	4023	-	0,6,6	0.00	-	-		
86	OHX	1	3862	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		
86	OHX	5	4198	-	0,6,6	0.00	-	-		
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	1	4087	-	0,6,6	0.00	-	-		
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	5	4246	-	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	4014	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	C1	201	-	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	1	3864	-	0,6,6	0.00	-	-		
86	OHX	6	2095	-	0,6,6	0.00	-	-		
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	M7	207	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	l5	304	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	1	4019	-	0,6,6	0.00	-	-		
86	OHX	5	4014	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	5	4125	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		
86	OHX	1	4210	-	0,6,6	0.00	-	-		
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	5	4089	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	5	4096	-	0,6,6	0.00	-	-		
86	OHX	m0	303	-	0,6,6	0.00	-	-		
86	OHX	5	4232	-	0,6,6	0.00	-	-		
86	OHX	6	2142	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	5	4168	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	4	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	1	4151	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	1	4180	-	0,6,6	0.00	-	-		
86	OHX	s4	301	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	s1	303	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	1	4085	-	0,6,6	0.00	-	-		
86	OHX	6	2135	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	1	4114	-	0,6,6	0.00	-	-		
86	OHX	5	4024	-	0,6,6	0.00	-	-		
86	OHX	6	2196	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		
86	OHX	8	229	-	0,6,6	0.00	-	-		
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	5	3942	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	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	4003	-	0,6,6	0.00	-	-		
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	m5	303	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	6	2047	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	1	3867	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	O3	201	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	6	2183	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		
86	OHX	L3	406	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	1	4207	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	2	2106	-	0,6,6	0.00	-	-		
86	OHX	1	4209	-	0,6,6	0.00	-	-		
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	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	403	-	0,6,6	0.00	-	-		
86	OHX	8	219	-	0,6,6	0.00	-	-		
86	OHX	4	225	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	s9	201	-	0,6,6	0.00	-	-		
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	1	4063	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	1	4183	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		
86	OHX	2	2175	-	0,6,6	0.00	-	-		
86	OHX	5	4250	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		
86	OHX	5	4097	-	0,6,6	0.00	-	-		
86	OHX	1	4153	-	0,6,6	0.00	-	-		
86	OHX	5	4208	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	1	4156	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	1	4116	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	5	4143	-	0,6,6	0.00	-	-		
86	OHX	1	4109	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	8	218	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	5	4038	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	s8	303	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	d4	202	-	0,6,6	0.00	-	-		
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	5	3941	-	0,6,6	0.00	-	-		
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	5	4167	-	0,6,6	0.00	-	-		
86	OHX	m6	202	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	6	2181	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	3	215	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		
86	OHX	1	3917	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	0,6,6	0.00	-	-		
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	4	222	-	0,6,6	0.00	-	-		
86	OHX	1	3889	-	0,6,6	0.00	-	-		
86	OHX	5	4228	-	0,6,6	0.00	-	-		
86	OHX	6	2082	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	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	3884	-	0,6,6	0.00	-	-		
86	OHX	2	2123	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		
86	OHX	6	2054	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	2	2080	-	0,6,6	0.00	-	-		
86	OHX	c3	201	-	0,6,6	0.00	-	-		
86	OHX	6	2174	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	0,6,6	0.00	-	-		
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	1	4045	-	0,6,6	0.00	-	-		
86	OHX	1	4082	-	0,6,6	0.00	-	-		
86	OHX	5	4254	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	5	4217	-	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	4161	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	15	305	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	2	2111	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	m4	201	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	0,6,6	0.00	-	-		
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	l3	402	-	0,6,6	0.00	-	-		
86	OHX	1	4098	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	19	202	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	6	2139	-	0,6,6	0.00	-	-		
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	5	4010	-	0,6,6	0.00	-	-		
86	OHX	6	2048	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	5	4100	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	0,6,6	0.00	-	-		
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	1	3869	-	0,6,6	0.00	-	-		
86	OHX	1	3863	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	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	6	2184	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	5	4239	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	1	3929	-	0,6,6	0.00	-	-		
86	OHX	5	4045	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	0,6,6	0.00	-	-		
86	OHX	6	2202	-	0,6,6	0.00	-	-		
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	1	3885	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		
86	OHX	5	4234	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	1	4211	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	5	4252	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	3	225	-	0,6,6	0.00	-	-		
86	OHX	2	2147	-	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	4007	-	0,6,6	0.00	-	-		
86	OHX	M7	206	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	2	2032	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	0,6,6	0.00	-	-		
86	OHX	1	3873	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	5	4023	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	5	4026	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	2	2047	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	0,6,6	0.00	-	-		
86	OHX	5	3939	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	4	224	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	0,6,6	0.00	-	-		
86	OHX	C3	201	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	1	4073	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	0,6,6	0.00	-	-		
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	1	3898	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	1	3939	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		
86	OHX	1	4086	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	2	2096	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	2	2028	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		
86	OHX	1	4009	-	0,6,6	0.00	-	-		
86	OHX	2	2149	-	0,6,6	0.00	-	-		
86	OHX	1	3866	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	L4	402	-	0,6,6	0.00	-	-		
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	1	4013	-	0,6,6	0.00	-	-		
86	OHX	6	2073	-	0,6,6	0.00	-	-		
86	OHX	5	4247	-	0,6,6	0.00	-	-		
86	OHX	L3	405	-	0,6,6	0.00	-	-		
86	OHX	1	4020	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	1	4127	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	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	2198	-	0,6,6	0.00	-	-		
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	5	4028	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	L3	404	-	0,6,6	0.00	-	-		
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	N1	201	-	0,6,6	0.00	-	-		
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	5	4178	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	0,6,6	0.00	-	-		
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	1	4175	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	5	4236	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	1	3891	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	1	4120	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	2	2176	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	5	3917	-	0,6,6	0.00	-	-		
86	OHX	6	2204	-	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	2069	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	5	3988	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	0,6,6	0.00	-	-		
86	OHX	2	2062	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	2	2035	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	2	2024	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
87	3K8	2	2179	-	32,32,32	0.79	1 (3%)	44,47,47	0.91	2 (4%)
86	OHX	5	4016	-	0,6,6	0.00	-	-		
86	OHX	5	4073	-	0,6,6	0.00	-	-		
86	OHX	5	3911	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	6	2074	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	6	2203	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	5	4227	-	0,6,6	0.00	-	-		
86	OHX	2	2170	-	0,6,6	0.00	-	-		
86	OHX	6	2151	-	0,6,6	0.00	-	-		
86	OHX	1	3868	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	5	4151	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		
86	OHX	5	4154	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	1	4030	-	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	3986	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	o3	202	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	5	3982	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	7	222	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	0,6,6	0.00	-	-		
86	OHX	6	2105	-	0,6,6	0.00	-	-		
86	OHX	2	2087	-	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
87	3K8	2	2179	-	-	0/6/25/25	0/5/5/5
87	3K8	6	2205	-	-	0/6/25/25	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	2	2179	3K8	C7-C8	3.62	1.42	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	2	2179	3K8	C15-C7-C4	-3.24	116.14	120.34
87	6	2205	3K8	C11-C10-N	3.05	118.55	110.59
87	2	2179	3K8	C11-C10-N	3.02	118.48	110.59
87	6	2205	3K8	C20-C19-C18	-2.13	117.97	120.07
87	6	2205	3K8	C17-C18-C19	2.03	122.08	120.07

There are no chirality outliers.

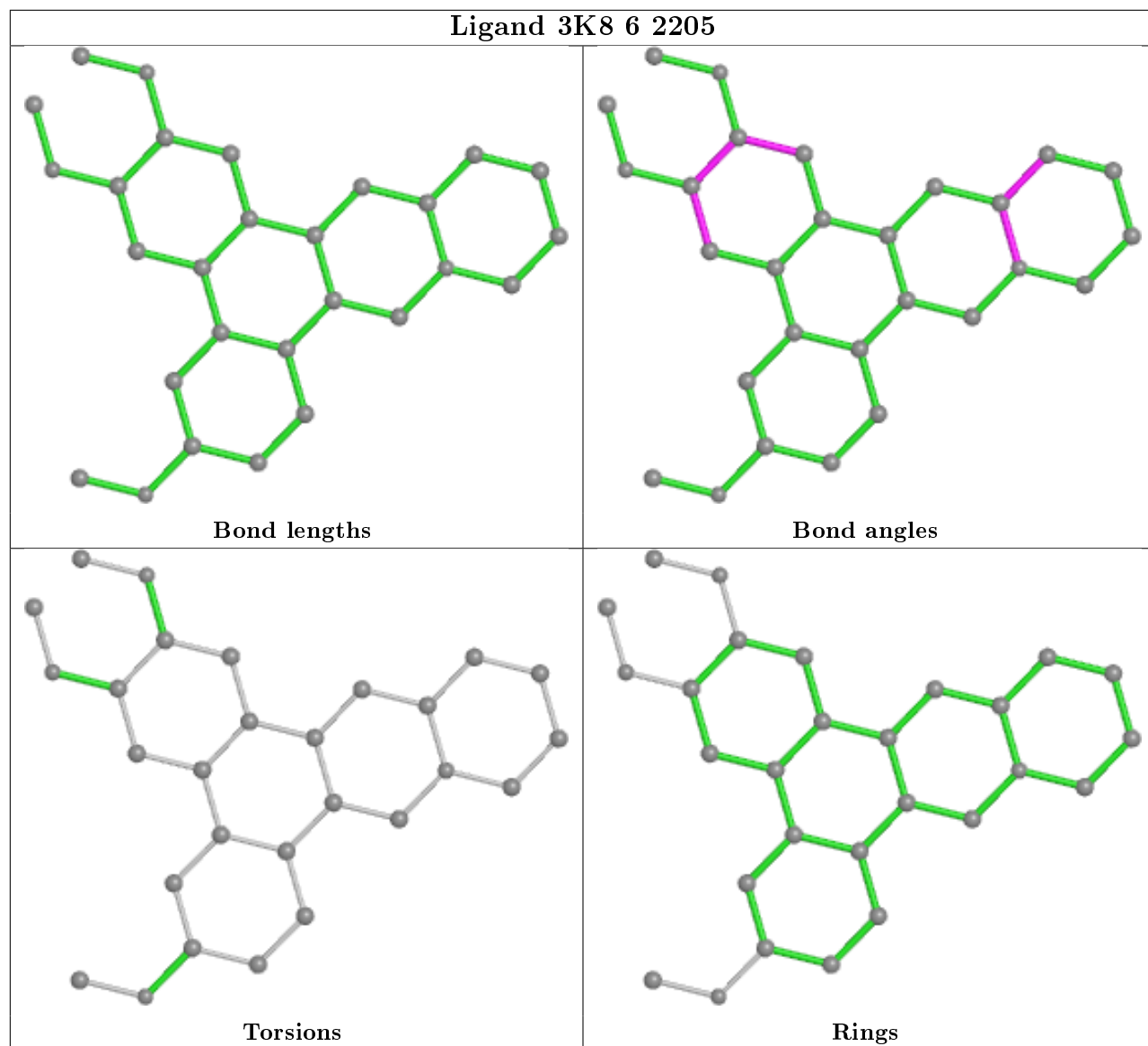
There are no torsion outliers.

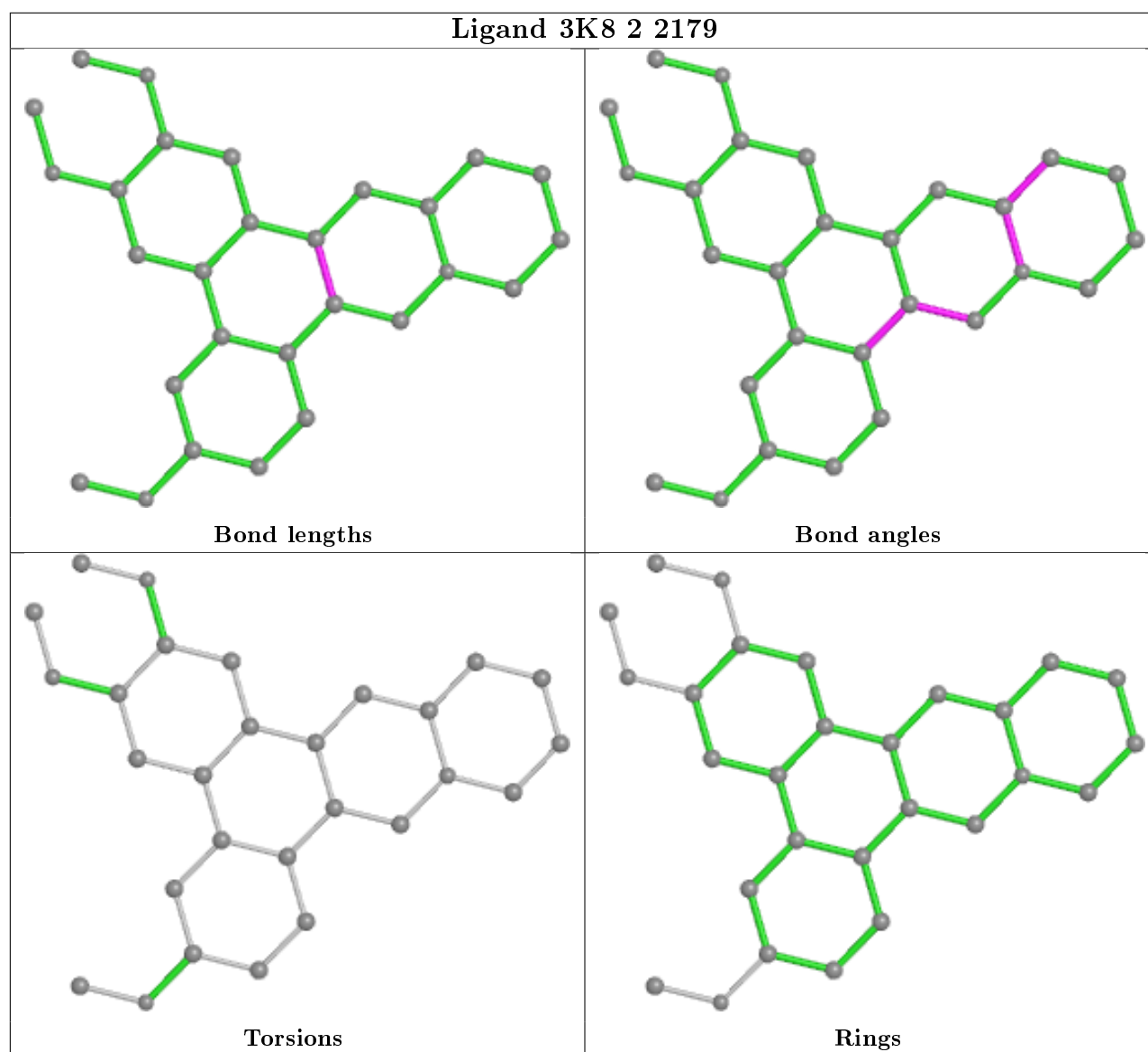
There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand 3K8 6 2205





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.