



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 07:08 pm GMT

PDB ID : 4U51
Title : Crystal structure of Narciclasine 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (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) : 2.36

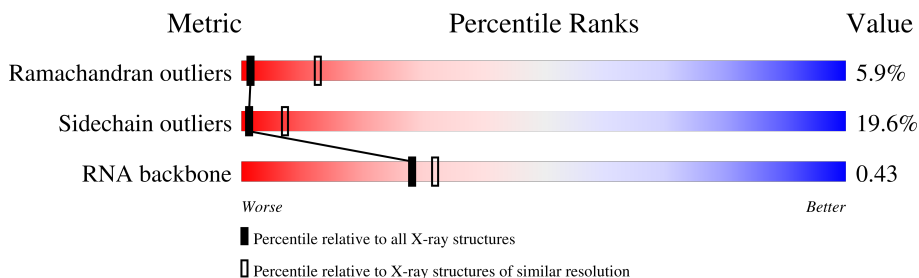
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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 of 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	
1	6	1800	
2	S0	251	
2	s0	251	
3	S1	254	
3	s1	254	
4	S2	253	
4	s2	253	









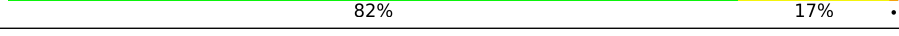

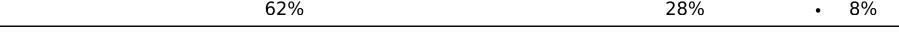
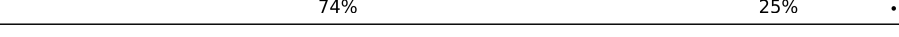

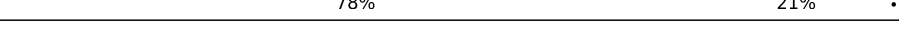


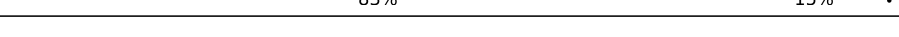

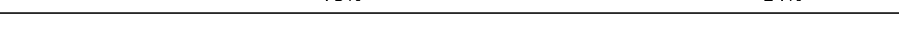






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Mol	Chain	Length	Quality of chain
5	S3	239	 74% 18% 7%
5	s3	239	 71% 21% 7%
6	S4	260	 80% 18%
6	s4	260	 78% 20%
7	S5	224	 73% 19% 8%
7	s5	224	 71% 21% 8%
8	S6	236	 75% 20%
8	s6	236	 77% 15% 8%
9	S7	189	 75% 21%
9	s7	189	 74% 22%
10	S8	200	 77% 15% 6%
10	s8	200	 78% 16% 6%
11	S9	196	 70% 22% 6%
11	s9	196	 70% 23% 6%
12	C0	105	 70% 21% 9%
12	c0	105	 66% 22% 9%
13	C1	155	 81% 18%
13	c1	155	 74% 19% 6%
14	C2	142	 64% 20% 13%
14	c2	142	 60% 25% 13%
15	C3	150	 79% 18%
15	c3	150	 79% 19%
16	C4	136	 71% 19% 7%
16	c4	136	 68% 22% 6%
17	C5	141	 69% 16% 12%

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Mol	Chain	Length	Quality of chain
17	c5	141	 71% 23% . .
18	C6	142	 78% 19% ..
18	c6	142	 80% 19% .
19	C7	136	 70% 12% 6% 12%
19	c7	136	 65% 18% . 14%
20	C8	145	 70% 26% .
20	c8	145	 73% 26% .
21	C9	143	 77% 22% .
21	c9	143	 82% 17% .
22	D0	120	 72% 18% 11%
22	d0	120	 62% 28% . 8%
23	D1	87	 74% 25% .
23	d1	87	 70% 28% .
24	D2	129	 78% 21% .
24	d2	129	 85% 14% .
25	D3	144	 83% 13% .
25	d3	144	 83% 15% .
26	D4	134	 86% 13% .
26	d4	134	 75% 24% .
27	D5	107	 39% 23% . 35%
27	d5	107	 50% 15% 36%
28	D6	97	 66% 28% 6%
28	d6	97	 76% 24%
29	D7	81	 86% 12% .
29	d7	81	 77% 23%












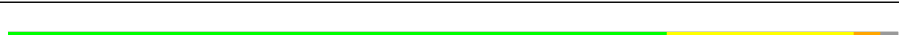

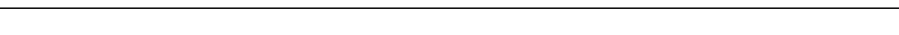
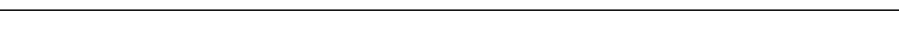
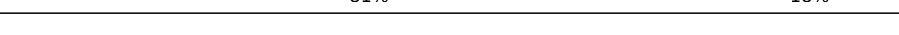

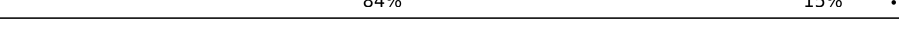







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Mol	Chain	Length	Quality of chain
30	D8	66	67% 29% 5%
30	d8	66	74% 20% 5%
31	D9	55	69% 25% 5%
31	d9	55	71% 25% 5%
32	E0	60	82% 17% 1%
33	E1	76	53% 34% 7% 7%
33	e1	76	59% 36% 5%
34	SR	318	86% 14%
34	sR	318	87% 13% 1%
35	SM	273	44% 14% 42%
35	sM	273	29% 9% 62%
36	1	3396	49% 37% 7% 7%
36	5	3396	47% 39% 8% 7%
37	3	121	68% 27% 5%
37	7	121	62% 31% 7%
38	4	158	47% 48% 5%
38	8	158	62% 32% 6%
39	L2	253	80% 19% 1%
39	l2	253	79% 20% 1%
40	L3	386	79% 20% 1%
40	l3	386	78% 21% 1% 1%
41	L4	361	79% 20% 1%
41	l4	361	78% 20% 1% 1%
42	L5	296	81% 18% 1%
42	l5	296	82% 17% 1% 1%

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Mol	Chain	Length	Quality of chain
43	L6	175	 74% 14% • 11%
43	l6	175	 75% 14% •• 10%
44	L7	243	 79% 11% • 9%
44	l7	243	 78% 12% • 8%
45	L8	255	 73% 17% • 9%
45	l8	255	 73% 17% 9%
46	L9	191	 79% 20% •
46	l9	191	 74% 25% •
47	M0	220	 76% 18% ••
47	m0	220	 77% 19% ••
48	M1	173	 73% 20% ••
48	m1	173	 74% 21% ••
49	M3	198	 79% 17% ••
49	m3	198	 78% 18% ••
50	M4	137	 81% 18% ••
50	m4	137	 79% 20% •
51	M5	203	 84% 15% •
51	m5	203	 82% 17% •
52	M6	198	 86% 13% ••
52	m6	198	 79% 18% •••
53	M7	183	 80% 18% ••
53	m7	183	 67% 17% • 15%
54	M8	185	 85% 14% ••
54	m8	185	 80% 19% •
55	M9	188	 86% 14%

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Mol	Chain	Length	Quality of chain
55	m9	188	85% 14% .
56	N0	172	80% 18% .
56	n0	172	74% 26%
57	N1	159	79% 21%
57	n1	159	77% 23% .
58	N2	120	62% 20% . 17%
58	n2	120	68% 13% . 18%
59	N3	136	81% 19%
59	n3	136	85% 15%
60	N4	155	54% 10% 37%
60	n4	155	68% 18% . 13%
61	N5	141	68% 16% . 14%
61	n5	141	68% 15% . 15%
62	N6	126	83% 15% .
62	n6	126	80% 20%
63	N7	135	79% 19% .
63	n7	135	73% 25% .
64	N8	148	83% 15% .
64	n8	148	79% 20% .
65	N9	58	79% 19% .
65	n9	58	67% 29% .
66	O0	104	81% 12% . 7%
66	o0	104	78% 18% .
67	O1	112	78% 20% .
67	o1	112	69% 28% . .

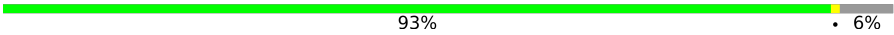

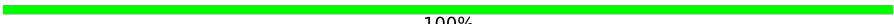

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Mol	Chain	Length	Quality of chain	
68	O2	129	80%	19%
68	o2	129	78%	19%
69	O3	106	80%	19%
69	o3	106	84%	16%
70	O4	120	78%	13%
70	o4	120	77%	17%
71	O5	119	81%	17%
71	o5	119	75%	25%
72	O6	99	79%	17%
72	o6	99	74%	25%
73	O7	87	78%	21%
73	o7	87	87%	13%
74	O8	77	66%	34%
74	o8	77	79%	18%
75	O9	50	82%	18%
75	o9	50	76%	24%
76	Q0	52	81%	17%
76	q0	52	75%	21%
77	Q1	25	76%	24%
77	q1	25	64%	36%
78	Q2	105	73%	23%
78	q2	105	76%	21%
79	Q3	91	80%	19%
79	q3	91	85%	15%
80	e0	62	74%	24%

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Mol	Chain	Length	Quality of chain
81	m2	160	 93% • 6%
82	p0	311	 38% 8% 54%
83	p1	47	 100%
84	p2	46	 100%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411178 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
			Total	C	N	O	P			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
5	S3	223	Total 1734	C 1101	N 313	O 314	S 6	0	0	0
5	s3	223	Total 1734	C 1101	N 313	O 314	S 6	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
13	C1	155	1213	774	230	206	3	0	0	0
13	c1	146	1168	747	221	197	3	0	0	0

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	c7	117	906	563	174	167	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	D7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
29	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	12	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	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	18	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	19	191	1518	963	274	277	4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	S			
53	M7	183	Total	C	N	O	S	0	0	0
			1420	882	281	257				
53	m7	155	Total	C	N	O	S	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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
55	M9	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				
55	m9	188	Total	C	N	O	S	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
			Total	C	N	O	S			
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	S	0	0	0
			796	516	131	149				
58	n2	98	Total	C	N	O	S	0	0	0
			778	505	127	146				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called unknown protein chain m2.

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

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

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

- Molecule 83 is a protein called unknown protein chain p1.

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

- 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	2	125	Total	Mg	0	0
			125	125		
85	S2	1	Total	Mg	0	0
			1	1		
85	D0	1	Total	Mg	0	0
			1	1		
85	D3	1	Total	Mg	0	0
			1	1		
85	SM	1	Total	Mg	0	0
			1	1		
85	1	472	Total	Mg	0	0
			472	472		
85	3	14	Total	Mg	0	0
			14	14		
85	4	20	Total	Mg	0	0
			20	20		
85	L2	1	Total	Mg	0	0
			1	1		
85	L3	1	Total	Mg	0	0
			1	1		
85	L4	1	Total	Mg	0	0
			1	1		
85	L5	1	Total	Mg	0	0
			1	1		
85	L7	4	Total	Mg	0	0
			4	4		
85	L8	1	Total	Mg	0	0
			1	1		
85	M0	2	Total	Mg	0	0
			2	2		
85	M1	1	Total	Mg	0	0
			1	1		
85	M3	3	Total	Mg	0	0
			3	3		
85	M5	2	Total	Mg	0	0
			2	2		
85	M6	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	M7	5	Total 5	Mg 5	0	0
85	M9	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0
85	N3	3	Total 3	Mg 3	0	0
85	N5	2	Total 2	Mg 2	0	0
85	N6	1	Total 1	Mg 1	0	0
85	N8	4	Total 4	Mg 4	0	0
85	O2	1	Total 1	Mg 1	0	0
85	O7	3	Total 3	Mg 3	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	6	144	Total 144	Mg 144	0	0
85	s1	1	Total 1	Mg 1	0	0
85	s6	1	Total 1	Mg 1	0	0
85	s8	3	Total 3	Mg 3	0	0
85	c1	1	Total 1	Mg 1	0	0
85	c4	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	d3	2	Total 2	Mg 2	0	0
85	d4	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0

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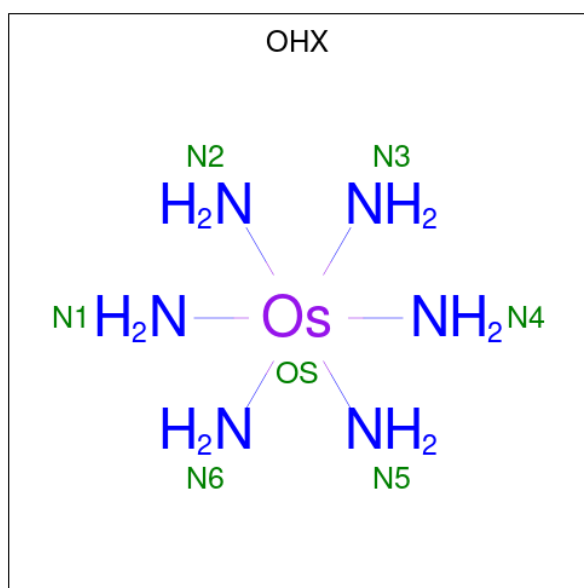
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	sM	2	Total 2	Mg 2	0	0
85	5	501	Total 501	Mg 501	0	0
85	7	17	Total 17	Mg 17	0	0
85	8	13	Total 13	Mg 13	0	0
85	12	2	Total 2	Mg 2	0	0
85	13	2	Total 2	Mg 2	0	0
85	14	1	Total 1	Mg 1	0	0
85	15	1	Total 1	Mg 1	0	0
85	17	1	Total 1	Mg 1	0	0
85	19	1	Total 1	Mg 1	0	0
85	m5	3	Total 3	Mg 3	0	0
85	m6	3	Total 3	Mg 3	0	0
85	m7	5	Total 5	Mg 5	0	0
85	n0	3	Total 3	Mg 3	0	0
85	n3	2	Total 2	Mg 2	0	0
85	n6	2	Total 2	Mg 2	0	0
85	n8	4	Total 4	Mg 4	0	0
85	n9	1	Total 1	Mg 1	0	0
85	o1	2	Total 2	Mg 2	0	0
85	o3	1	Total 1	Mg 1	0	0
85	o4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	o7	1	Total Mg 1 1	0	0
85	o9	1	Total Mg 1 1	0	0
85	q0	1	Total Mg 1 1	0	0
85	q1	1	Total Mg 1 1	0	0
85	q3	2	Total Mg 2 2	0	0

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	S8	1	7	6	1	0	0
86	C3	1	7	6	1	0	0
86	C5	1	7	6	1	0	0
86	C8	1	7	6	1	0	0
86	D9	1	7	6	1	0	0
86	SR	1	7	6	1	0	0
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86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	L3	1	7	6	1	0	0
86	L3	1	7	6	1	0	0
86	L4	1	7	6	1	0	0
86	M0	1	7	6	1	0	0
86	M5	1	7	6	1	0	0
86	M7	1	7	6	1	0	0
86	M7	1	7	6	1	0	0
86	M8	1	7	6	1	0	0
86	M9	1	7	6	1	0	0
86	N1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	N9	1	7	6	1	0	0
86	O3	1	7	6	1	0	0
86	O7	1	7	6	1	0	0
86	O7	1	7	6	1	0	0
86	Q2	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	s1	1	7	6	1	0	0
86	s1	1	7	6	1	0	0
86	s4	1	7	6	1	0	0
86	s8	1	7	6	1	0	0
86	s9	1	7	6	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	8	1	7	6	1	0	0
86	8	1	7	6	1	0	0
86	8	1	7	6	1	0	0
86	8	1	7	6	1	0	0
86	8	1	7	6	1	0	0
86	8	1	7	6	1	0	0
86	8	1	7	6	1	0	0
86	13	1	7	6	1	0	0
86	13	1	7	6	1	0	0
86	14	1	7	6	1	0	0
86	14	1	7	6	1	0	0
86	15	1	7	6	1	0	0
86	15	1	7	6	1	0	0
86	15	1	7	6	1	0	0
86	19	1	7	6	1	0	0
86	m0	1	7	6	1	0	0
86	m0	1	7	6	1	0	0
86	m1	1	7	6	1	0	0
86	m4	1	7	6	1	0	0
86	m5	1	7	6	1	0	0
86	m6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	m7	1	7	6	1	0	0
86	m8	1	7	6	1	0	0
86	n3	1	7	6	1	0	0
86	n3	1	7	6	1	0	0
86	n5	1	7	6	1	0	0
86	n9	1	7	6	1	0	0
86	o2	1	7	6	1	0	0
86	o3	1	7	6	1	0	0
86	q1	1	7	6	1	0	0
86	q2	1	7	6	1	0	0

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

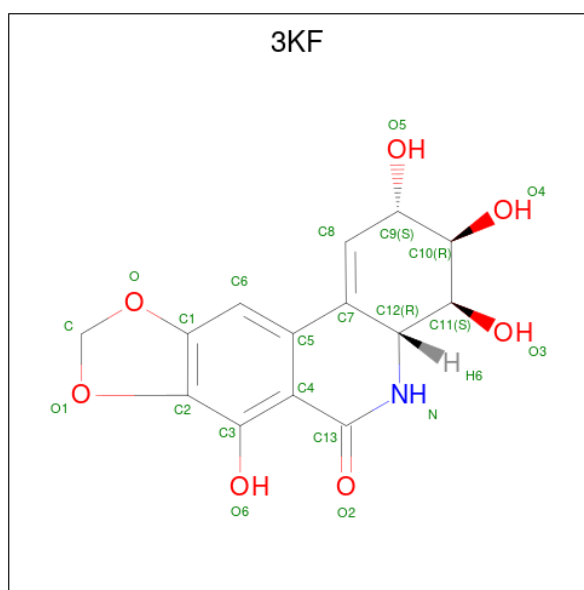
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
87	D6	1	1	1	0	0
87	D7	1	1	1	0	0
87	D9	1	1	1	0	0
87	E1	1	1	1	0	0
87	O7	1	1	1	0	0
87	Q0	1	1	1	0	0
87	Q2	1	1	1	0	0
87	Q3	1	1	1	0	0
87	d6	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	d7	1	Total	Zn	0	0
			1	1		
87	d9	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	o7	1	Total	Zn	0	0
			1	1		
87	q0	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		
87	q3	1	Total	Zn	0	0
			1	1		

- Molecule 88 is (2S,3R,4S,4aR)-2,3,4,7-tetrahydroxy-3,4,4a,5-tetrahydro[1,3]dioxolo[4,5-j]phenanthridin-6(2H)-one (three-letter code: 3KF) (formula: C₁₄H₁₃NO₇).



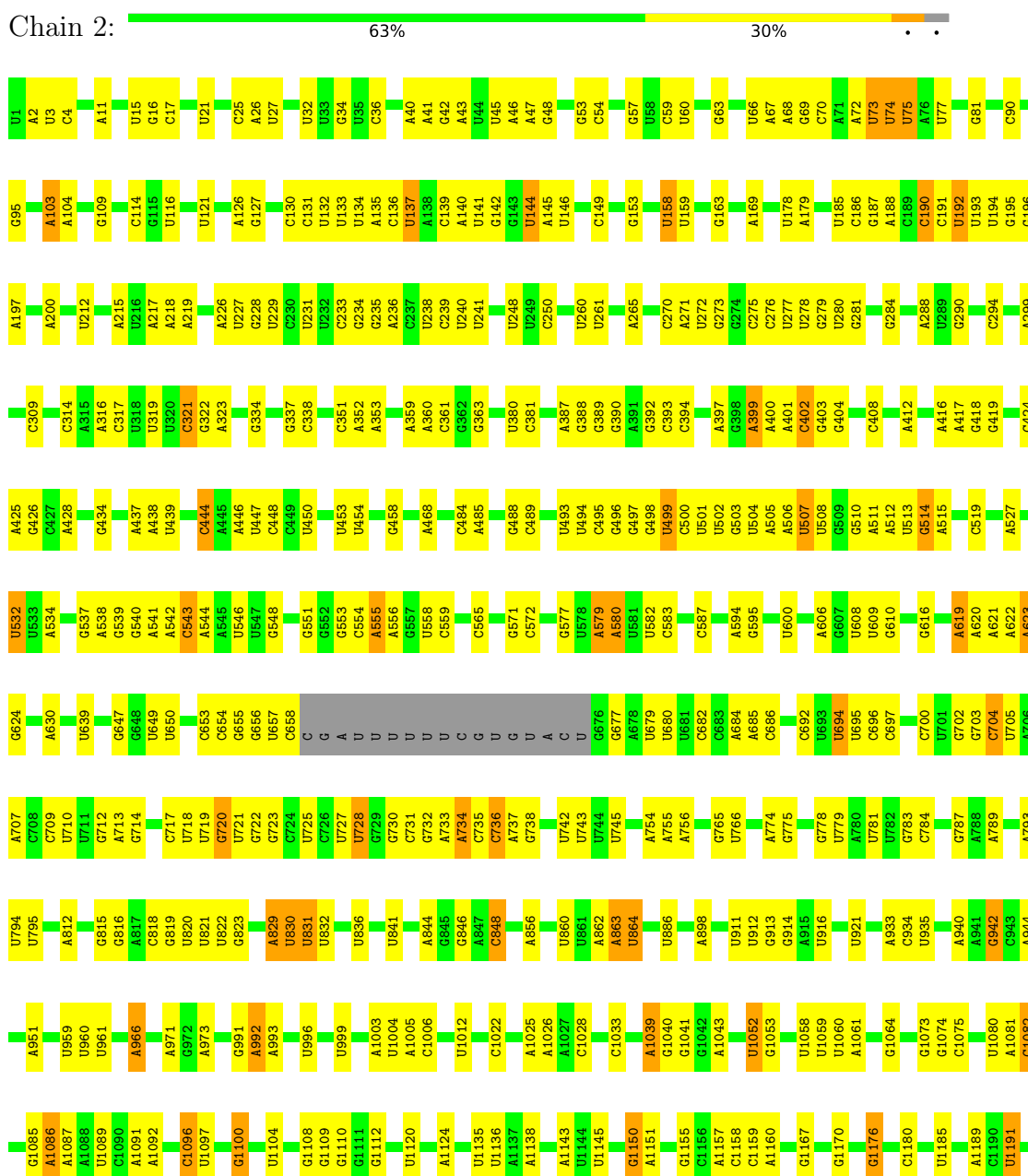
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	1	1	Total	C	N	O	0	0
			22	14	1	7		
88	5	1	Total	C	N	O	0	0
			22	14	1	7		

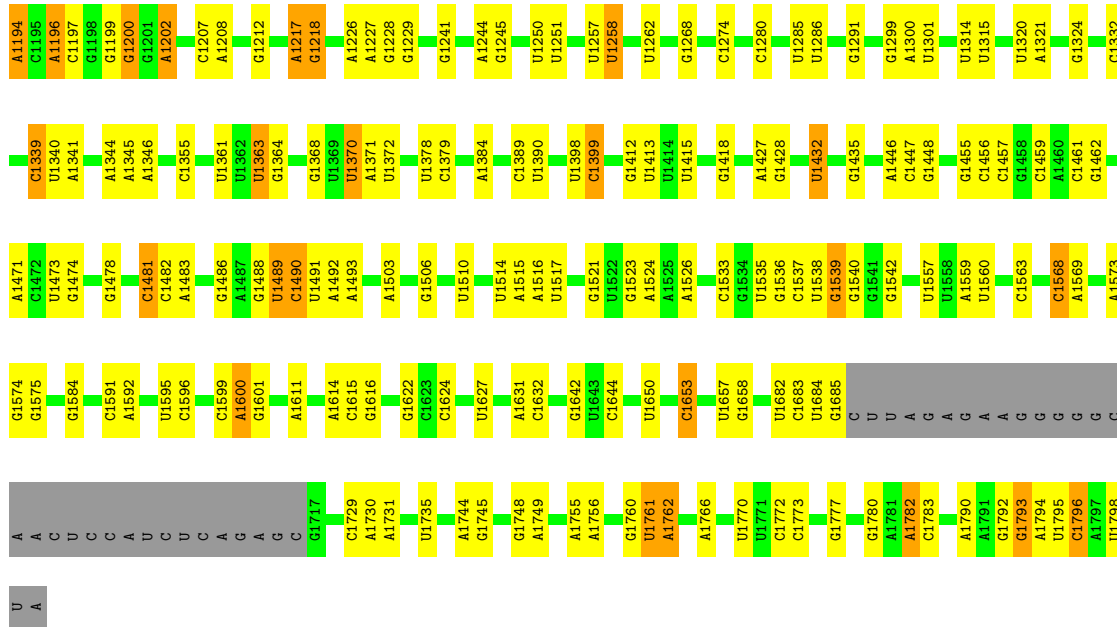
3 Residue-property plots

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

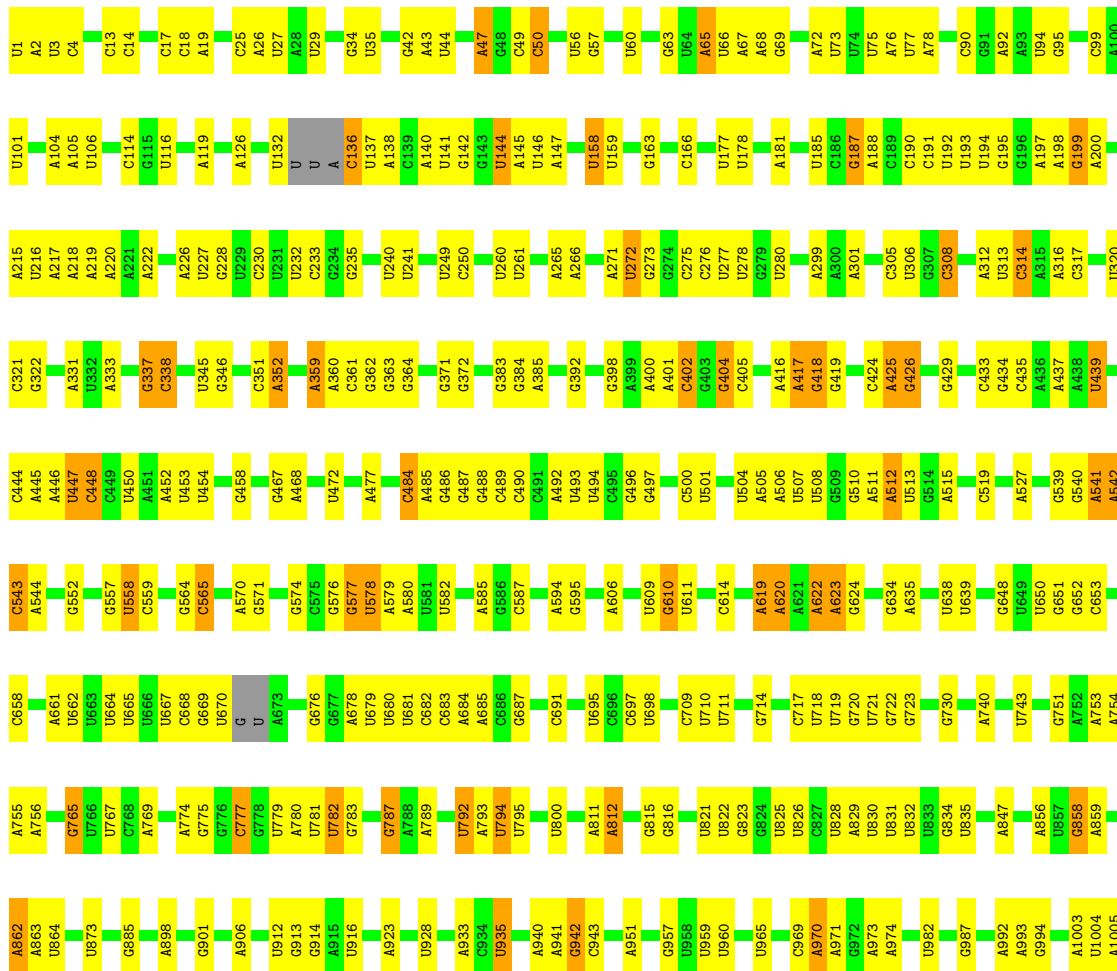
Note EDS failed to run properly.

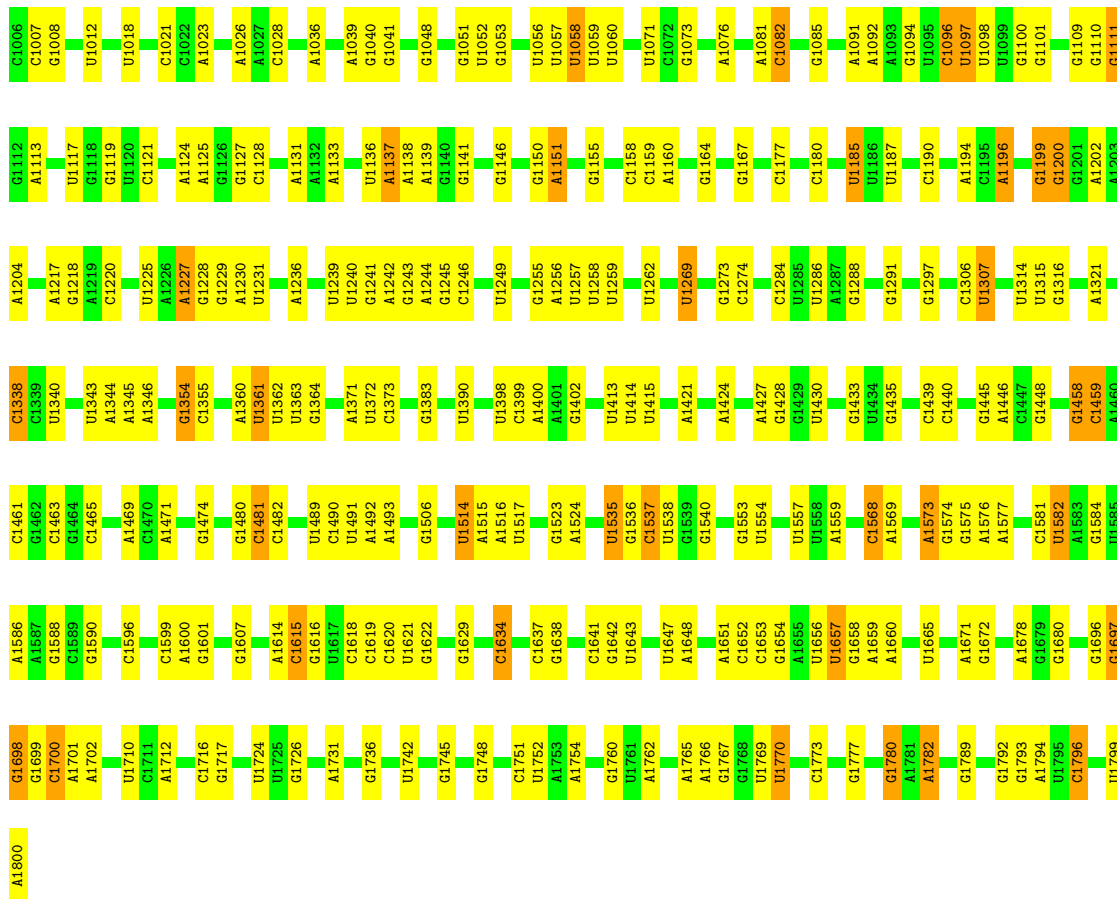
- Molecule 1: 18S ribosomal RNA



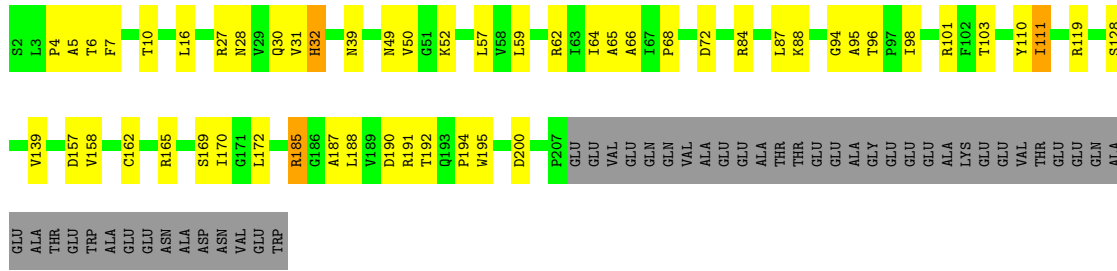


• Molecule 1: 18S ribosomal RNA

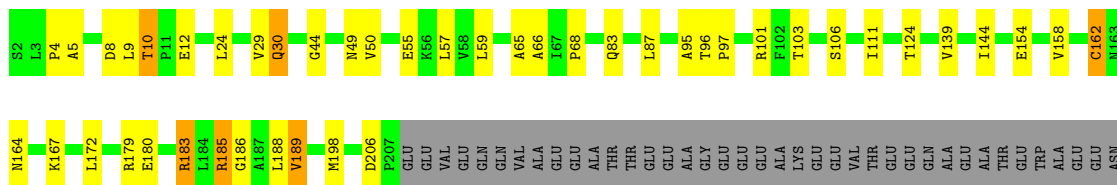




- Molecule 2: 40S ribosomal protein S0-A

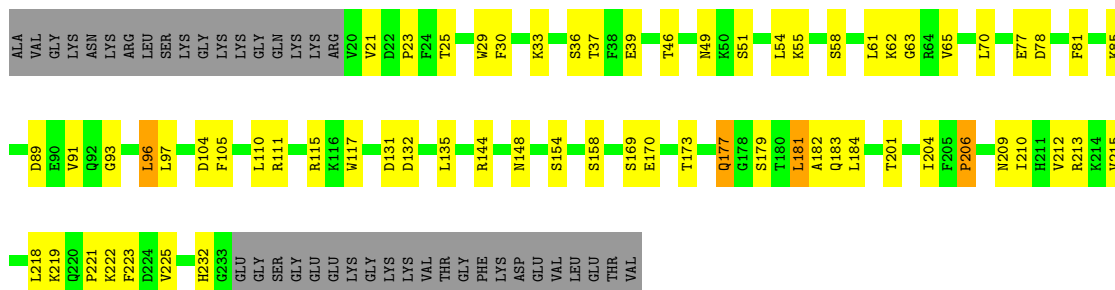


- Molecule 2: 40S ribosomal protein S0-A

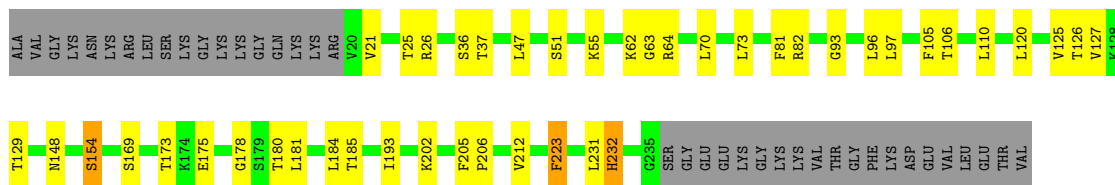


ALA
ASP
ASN
VAL
GLU
TRP

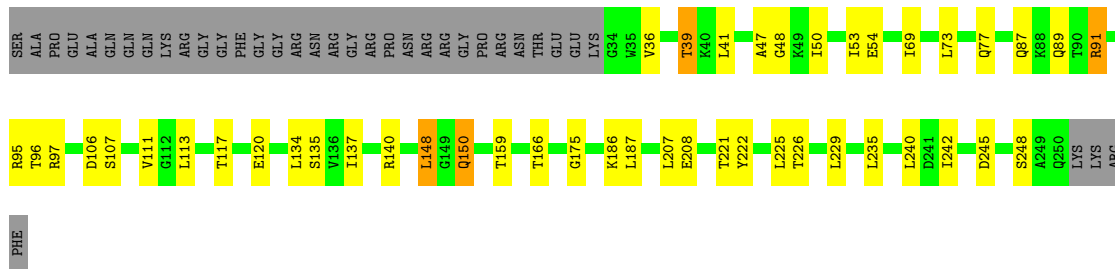
• Molecule 3: 40S ribosomal protein S1-A



• Molecule 3: 40S ribosomal protein S1-A

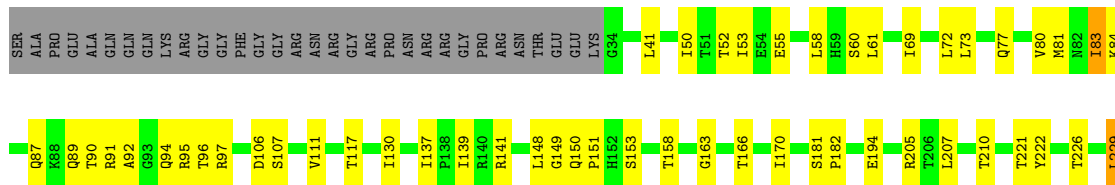


• Molecule 4: 40S ribosomal protein S2



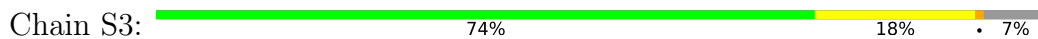
PHE

• Molecule 4: 40S ribosomal protein S2

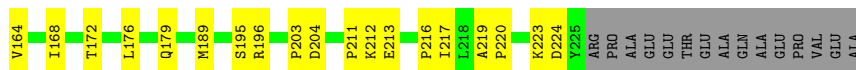




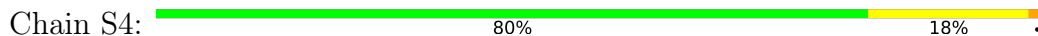
• Molecule 5: 40S ribosomal protein S3



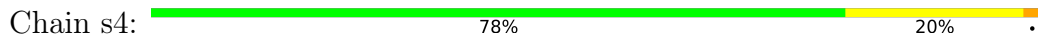
• Molecule 5: 40S ribosomal protein S3



• Molecule 6: 40S ribosomal protein S4-A



• Molecule 6: 40S ribosomal protein S4-A



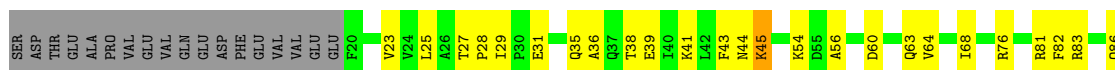
• Molecule 7: 40S ribosomal protein S5





- Molecule 7: 40S ribosomal protein S5

Chain s5: 71% 21% 8%



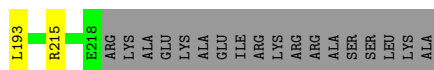
- Molecule 8: 40S ribosomal protein S6-A

Chain S6: 75% 20%



- Molecule 8: 40S ribosomal protein S6-A

Chain s6: 77% 15% 8%



- Molecule 9: 40S ribosomal protein S7-A

Chain S7: 75% 21%



- Molecule 9: 40S ribosomal protein S7-A

Chain s7: 74% 22%





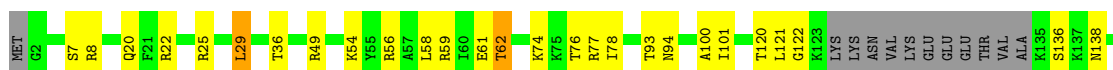
- Molecule 10: 40S ribosomal protein S8-A

Chain S8: 77% 15% • 6%



- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 78% 16% • 6%



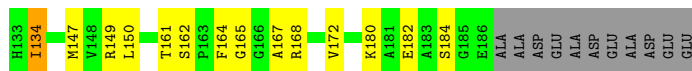
- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 70% 22% • 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 70% 23% • 6%

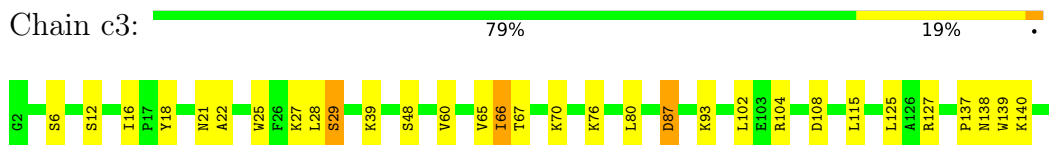


- Molecule 12: 40S ribosomal protein S10-A

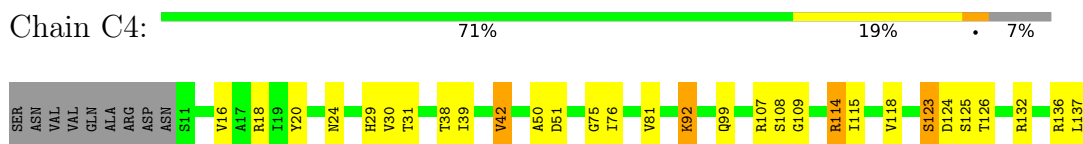
Chain C0: 70% 21% • 9%



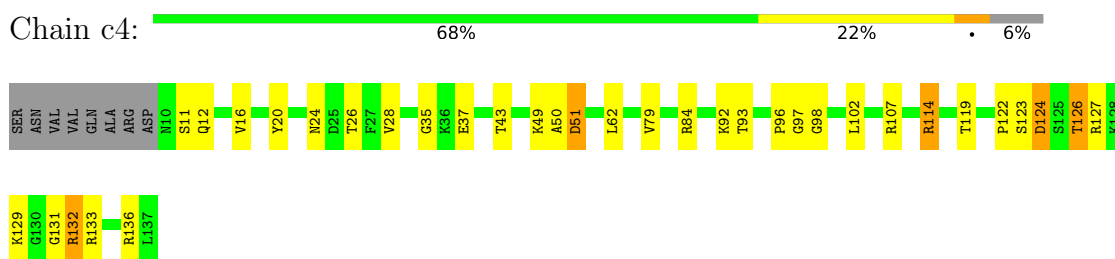
• Molecule 15: 40S ribosomal protein S13



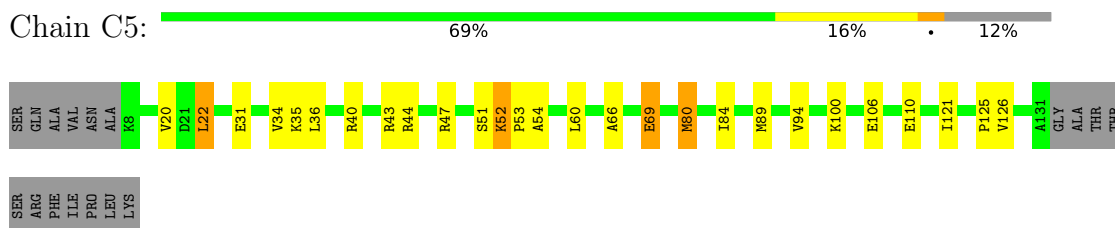
• Molecule 16: 40S ribosomal protein S14-A



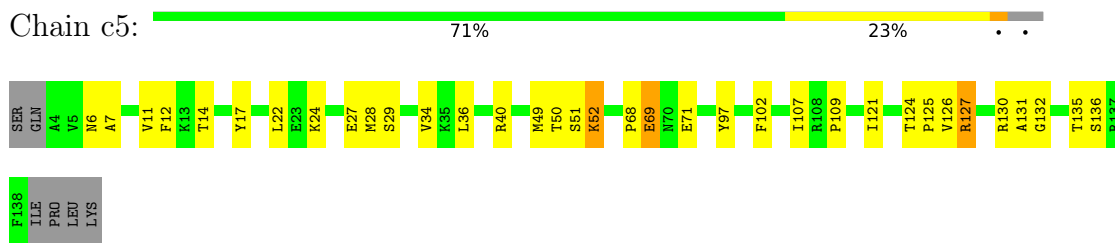
• Molecule 16: 40S ribosomal protein S14-A



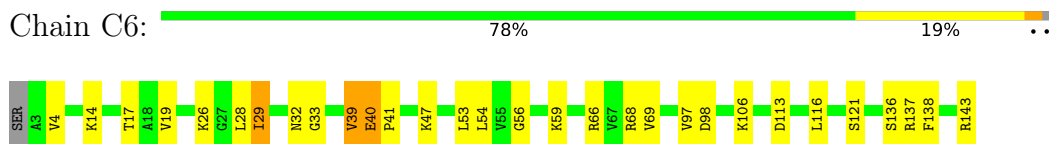
• Molecule 17: 40S ribosomal protein S15




• Molecule 17: 40S ribosomal protein S15

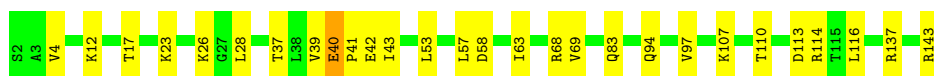


• Molecule 18: 40S ribosomal protein S16-A



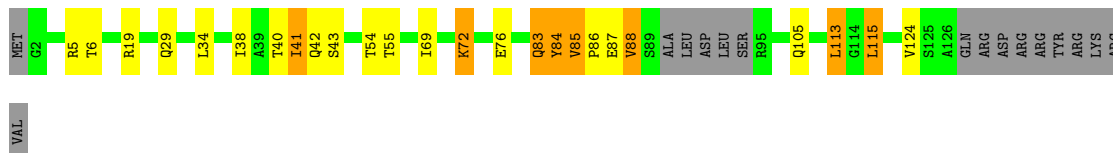
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:  80% 19%



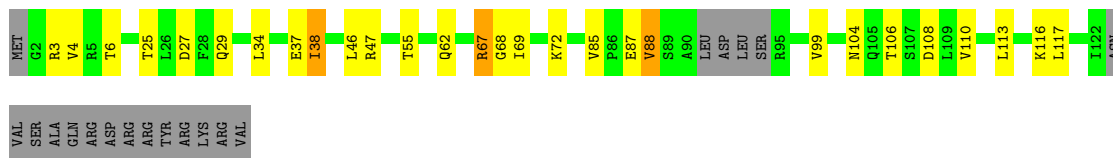
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:  70% 12% 6% 12%



- Molecule 19: 40S ribosomal protein S17-A

Chain c7:  65% 18% 14%



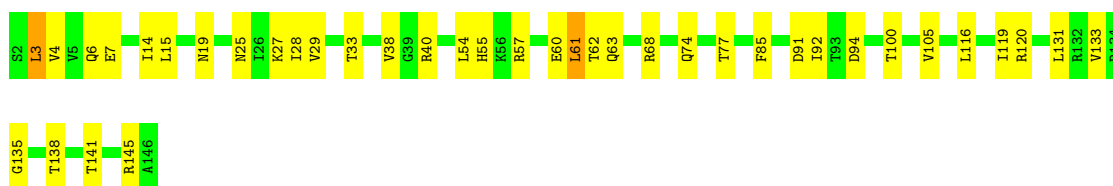
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:  70% 26%




- Molecule 20: 40S ribosomal protein S18-A

Chain c8:  73% 26%

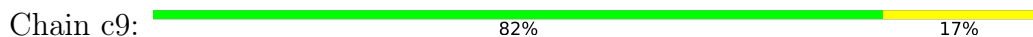


- Molecule 21: 40S ribosomal protein S19-A

Chain C9:  77% 22%



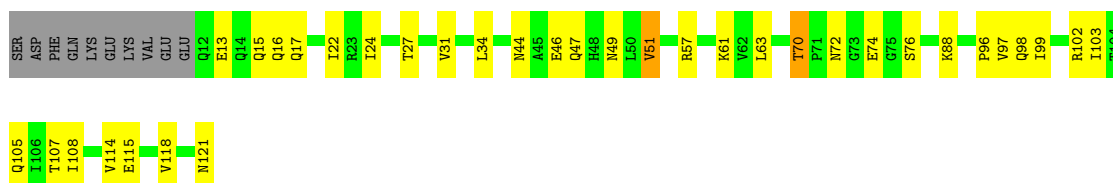
- Molecule 21: 40S ribosomal protein S19-A



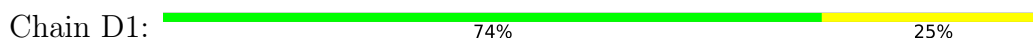
- Molecule 22: 40S ribosomal protein S20



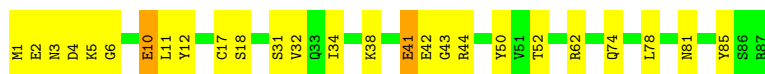
- Molecule 22: 40S ribosomal protein S20



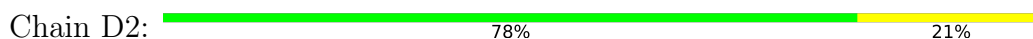
- Molecule 23: 40S ribosomal protein S21-A




- Molecule 23: 40S ribosomal protein S21-A



- Molecule 24: 40S ribosomal protein S22-A




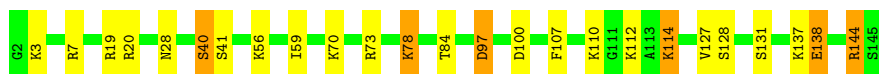
- Molecule 24: 40S ribosomal protein S22-A

Chain d2:  85% 14%




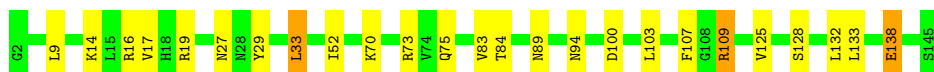
- Molecule 25: 40S ribosomal protein S23-A

Chain D3:  83% 13%




- Molecule 25: 40S ribosomal protein S23-A

Chain d3:  83% 15%




- Molecule 26: 40S ribosomal protein S24-A

Chain D4:  86% 13%



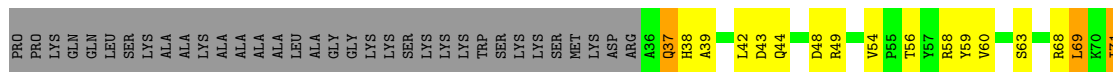
- Molecule 26: 40S ribosomal protein S24-A

Chain d4:  75% 24%



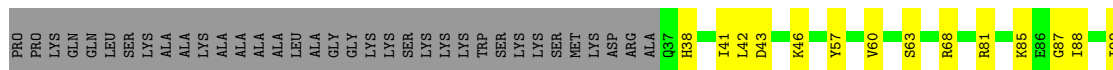
- Molecule 27: 40S ribosomal protein S25-A

Chain D5:  39% 23% 35%



- Molecule 27: 40S ribosomal protein S25-A

Chain d5:  50% 15% 36%





- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 66% 28% 6%



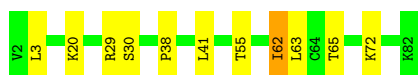
- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 76% 24%



- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 86% 12%



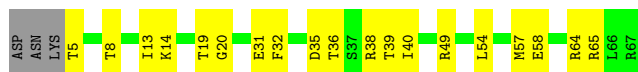
- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 77% 23%



- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 67% 29% 5%



- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 74% 20% 5%

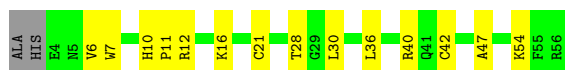


- Molecule 31: 40S ribosomal protein S29-A

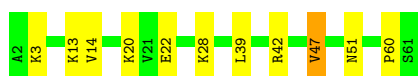
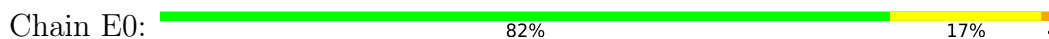
Chain D9: 69% 25%



- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A



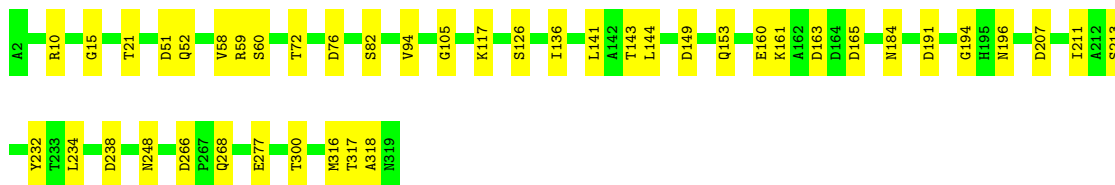
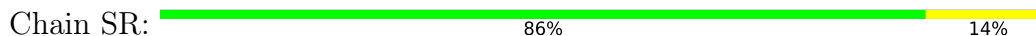
- Molecule 33: Ubiquitin-40S ribosomal protein S31



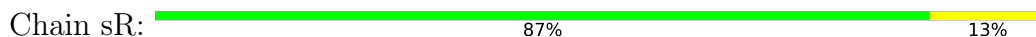
- Molecule 33: Ubiquitin-40S ribosomal protein S31



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

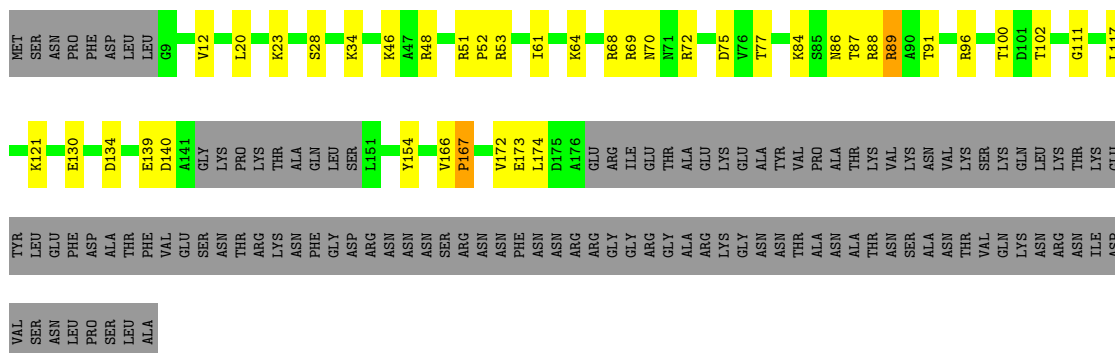


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

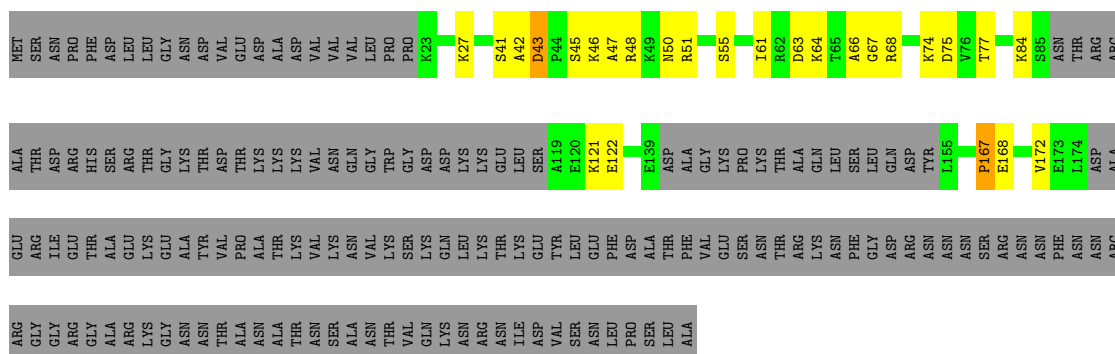




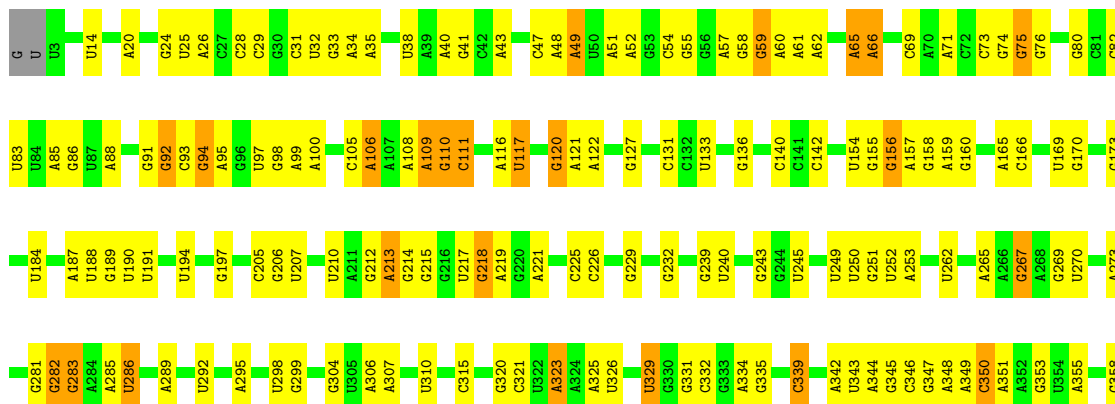
• Molecule 35: Suppressor protein STM1



• Molecule 35: Suppressor protein STM1

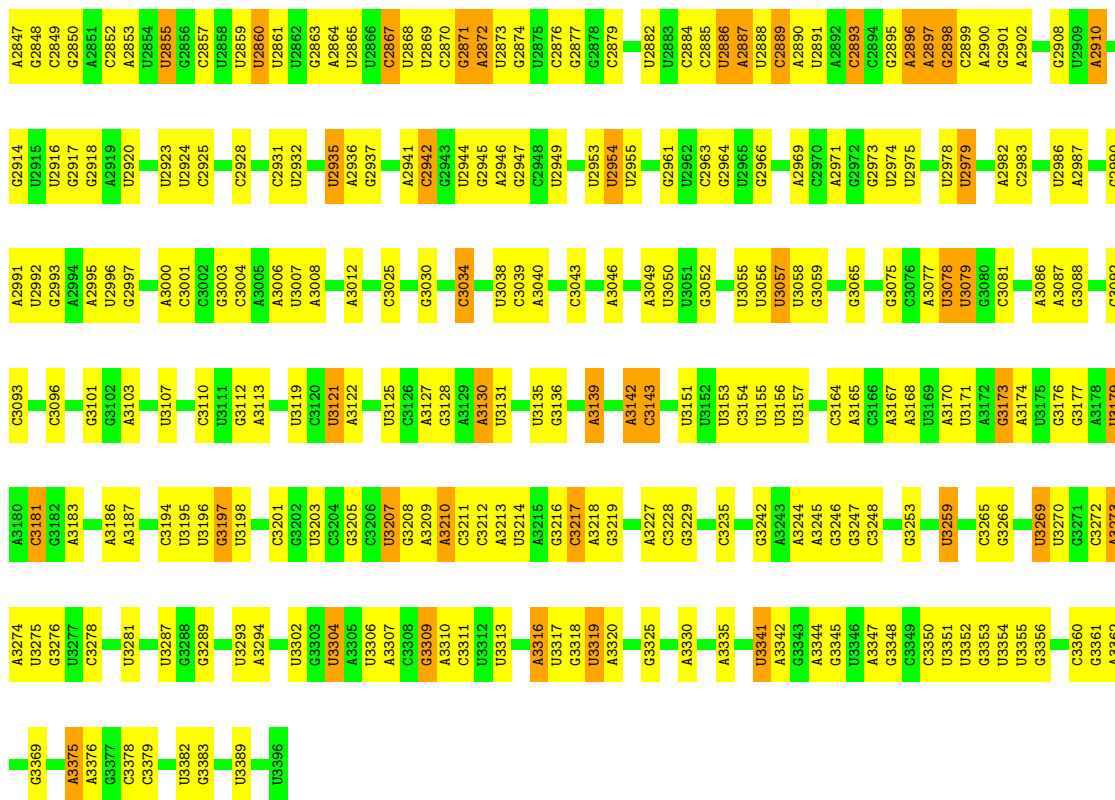


• Molecule 36: 25S ribosomal RNA



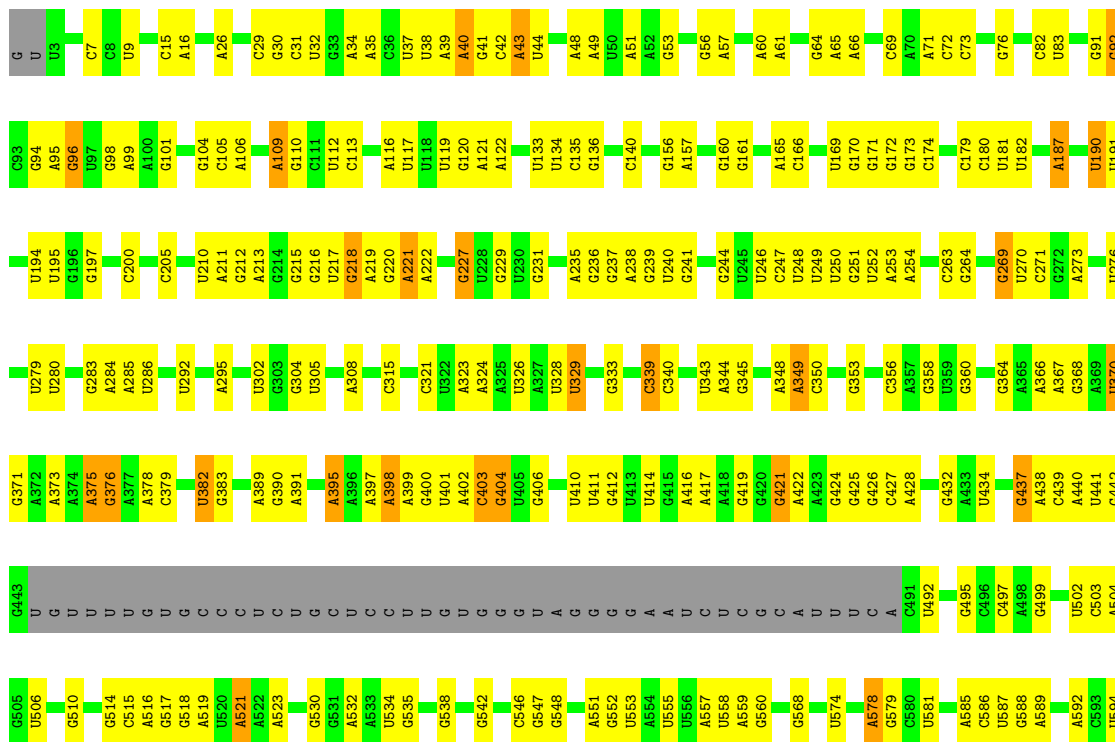
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A1507	G1417	G1349	A1263	G1185	C1119	A1036	C949	A862	G792	A693	G614	A519	U
C1508	A1418	U1350	G1264	C1186	A1120	C1037	G950	A883	C793	C694	A619	A520	G
A1509	A1419	U1351	U1265	C1187	U1121	U1038	A951	A884	U794	C695	U620	A521	U
G1510	C1420	A1352	G1266	U1188	U1122	U1041	A952	U885	U797	A699	A621	G368	G
U1511	G1421	U1353	U1267	C1189	U1123	U1042	G953	C886	G798	C700	G625	G369	C
U1425	U1454	G1354	G1268	A1190	U1124	U1043	C957	C887	C799	G701	A626	G370	C
C1426	U1355	U1356	A1269	U1191	G1126	C1043	C958	A888	A801	U704	A628	G535	C
G1513	C1427	C1192	U1270	C1192	G1127	A1046	C959	C890	C802	U705	U541	G372	C
G1514	A1428	G1357	A1271	A1193	U1128	A1047	A960	C891	C803	A706	A629	A373	U
A1515	G1428	C1358	C1272	G1194	U1129	U1048	C961	C892	C804	U707	G632	A374	U
C1516	G429	C1359	A1273	A1195	A1129	C1049	A962	C893	A806	U708	C544	A375	U
U1430	A1274	C1360	A1274	C1196	A1130	U1050	G963	A895	A807	A709	U545	G376	G
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A1433	G1362	C1199	A1278	C1198	C1132	U1052	G965	A897	G809	A711	C634	A397	U
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U1436	G1365	A1201	A1286	A1204	U1138	A1055	A970	G900	A817	U714	U552	A391	U
C1437	A1366	A1287	A1287	A1205	G1139	U1056	G971	G901	U821	U715	U553	G392	U
U1438	G1367	A1287	A1287	A1206	U1140	A1057	A972	G902	U822	A716	A557	A395	G
A1535	U1440	A1369	C1292	A1207	C1141	U1058	G974	G903	C824	U717	U642	A396	G
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U1547	U1442	G1298	U1208	U1209	A1143	A1065	G978	G905	A827	U719	G644	A398	U
C1548	G1443	G1298	G1209	U1210	U1144	A1065	U979	G906	A827	A720	A645	A399	A
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U1445	U1445	A1303	A1303	G1213	C1146	A990	A981	A913	G722	A647	C573	U401	G
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U1447	G1377	A1304	A1304	G1214	G1148	A983	A983	A915	A831	A649	A578	C403	G
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G1450	G1382	A1308	A1308	G1222	A1153	G1083	G994	A920	A846	A653	G584	U411	C
C1451	G1383	U1309	U1309	G1222	C1154	U1084	G995	A921	A847	C654	A585	U414	C
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A1453	U1387	C1314	C1314	C1227	C1156	U1093	A997	A922	U850	G658	U587	U414	C
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A1455	U1388	U1315	U1315	G1233	A1158	U1094	A999	C924	C852	U766	C586	A422	U
A1456	G1389	C1316	C1316	U1234	A1159	U1095	C1000	A925	G854	U767	U587	A423	U
U1457	A1390	G1316	G1316	G1234	U1159	U1096	G1001	A926	U855	U768	G588	G426	A
U1458	C1391	C1320	C1320	U1236	C1160	U1097	G1002	A927	G857	G664	A592	A426	A
A1467	G1392	U1321	U1321	G1236	A1163	A1099	A1005	C928	A858	U664	C593	A438	C
A1468	A1393	U1324	U1324	G1237	G1164	A1099	A1006	C929	A859	A665	A602	A439	C
U1569	G1395	U1325	U1325	U1241	A1165	U1100	A1006	C930	G860	A666	A603	A440	C
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G1487	A1399	U1329	U1329	A1244	A1169	G1104	U1014	A936	U865	U776	G607	A507	G
G1488	G1400	U1331	U1331	C1246	U1173	A1105	U1014	A937	U866	U777	A608	A507	G
A1489	C1403	A1332	A1332	U1247	U1174	U1108	C1017	C938	U871	A780	A609	A507	G
G1492	G1404	U1336	U1336	C1248	G1175	U1108	G1018	C939	U872	A676	G610	G610	U
A1580	U1405	U1336	U1336	G1249	C1176	U1111	G1019	A940	U873	A677	G611	G611	U
C1581	A1406	G1250	G1250	G1250	C1177	A1112	G1020	G941	C873	A678	U607	G612	U
C1582	A1407	A1251	A1251	A1251	G1177	A1113	G1021	U942	U874	G785	A607	G613	G
U1495	G1340	A1251	A1251	G1254	G1178	G1114	G1021	U943	C875	A786	A608	G614	G
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G1576	G1414	G1345	G1345	U1258	U1180	G1115	A1025	U945	U879	A789	G610	U512	U
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G1579	U1415	U1347	U1347	U1258	U1182	G1117	A1025	U947	G880	U790	G611	U513	U
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C1582	U1415	U1347	U1347	U1258	U1182	G1117	A1025	U947	G880	U790	G611	U513	U
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G1586	U1415	U1347	U1347	U1258	U1182	G1117	A1025	U947	G880	U790	G611	U513	U
A1587	U1415	U1347	U1347	U1258	U1182	G1117	A1025	U947	G880	U790	G611	U513	U

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C2772	A2689	G2614	C2512	C2374	U2297	G2210	G2130	A1911	A1838	A1741	G1592
C2773	G2690	G2615	U2513	G2375	U2298	A2219	C2132	A1915	U1840	U1742	U1595
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G2779	A2692	G2617	A2515	C2378	U2301	A2224	U2134	G1923	A1842	A1750	U1601
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G2787	G2698	G2623	G2525	A2384	A2308	A2229	U2140	G1935	C1848	C1767	C1609
A2790	G2699	G2624	C2531	G2385	U2310	C2230	U2141	G1935	C1849	U1765	U1607
U2795	G2700	C2625	U2532	A2386	U2310	C2231	U2142	G1935	A1850	G1766	C1608
G2796	U2701	C2626	G2533	A2387	U2310	C2231	A2142	G1935	G1851	C1767	C1609
G2796	C2702	C2627	G2533	U2388	A2313	G2234	U2143	G1935	G1852	G1770	G1610
A2799	A2704	U2631	U2537	C2392	A2314	G2234	A2144	C1951	U1855	A1770	U1620
G2800	A2705	G2632	U2538	G2393	G2315	C2237	A2145	C1952	C1856	G1775	A1621
A2801	C2707	U2633	C2539	G2394	G2316	U2241	C2146	C1953	C1857	G1776	G1624
A2802	C2708	G2634	A2540	G2394	A2317	A2242	A2147	C1954	A1858	G1776	G1624
A2803	A2714	U2635	U2541	G2395	U2318	A2243	G2150	U1955	A1858	G1776	G1624
A2808	U2718	A2636	U2542	A2397	A2321	A2244	C2151	A	C1866	G1780	U1629
C2809	U2719	C2638	U2544	A2398	A2326	G2246	U2152	G	A1867	G1781	U1629
C2810	U2720	G2639	G2547	A2399	A2326	G2247	U2153	G	C1868	U1782	G1635
A2811	A2721	A2640	C2548	G2400	C2330	G2248	U2154	G	C1869	G1783	G1635
A2812	U2722	G2641	U2549	A2401	C2330	C2248	A2158	G	C1870	G1784	C1639
A2813	U2723	U2642	G2550	G2402	C2333	G2249	U2159	G	U1871	G1790	C1639
G2814	U2723	A2643	U2551	G2403	C2334	G2250	C2163	G	C1872	G1791	U1641
G2815	C2726	C2644	U2552	A2404	G2335	G2251	A2164	G	U1873	C1792	A1642
A2816	A2727	G2645	U2553	C2405	U2336	G2253	A2164	G	A1874	C1793	A1643
A2817	G2728	C2646	A2554	C2407	C2339	U2254	A2166	G	U1877	C1794	U1644
U2818	U2729	G2647	G2555	U2408	U2340	A2255	A2166	G	A1879	U1795	U1645
A2819	U2733	A2648	A2555	G2409	U2341	A2256	A2166	G	U1880	G1796	U1645
C2821	A2734	G2649	A2556	U2410	U2342	C2257	G2169	G	A1881	A1797	G1653
G2823	U2735	U2650	A2557	G2412	U2344	C2257	A2172	G	A1882	U1801	A1654
G2828	C2741	A2656	C2572	U2416	C2344	C2257	A2172	G	U1888	A1809	A1656
U2829	C2742	G2657	G2573	U2417	C2346	G2272	A2183	G	G1889	A1810	A1657
U2830	A2747	G2658	U2581	G2418	U2349	A2275	G2187	G	U1890	G1812	A1683
G2831	A2748	G2659	G2585	A2419	C2350	G2276	A2188	G	A1891	A1813	U1684
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G2834	G2754	A2673	A2593	C2422	A2352	A2279	U2191	G	A1896	U1815	U1689
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C2836	C2756	A2675	U2596	G2424	A2356	A2281	U2193	G	U1898	G1817	U1695
G2839	U2757	A2676	A2601	U2425	A2361	U2282	G2194	G	G1899	U1819	A1696
U2842	U2758	A2677	A2363	U2426	C2362	G2283	C2197	G	A1900	U1820	A1696
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	U2767		U2504	A2444	G2370	U2294	A2207	G	G1906	U1834	C1725
				A2445	G2371			G	A1908	A1835	C1726

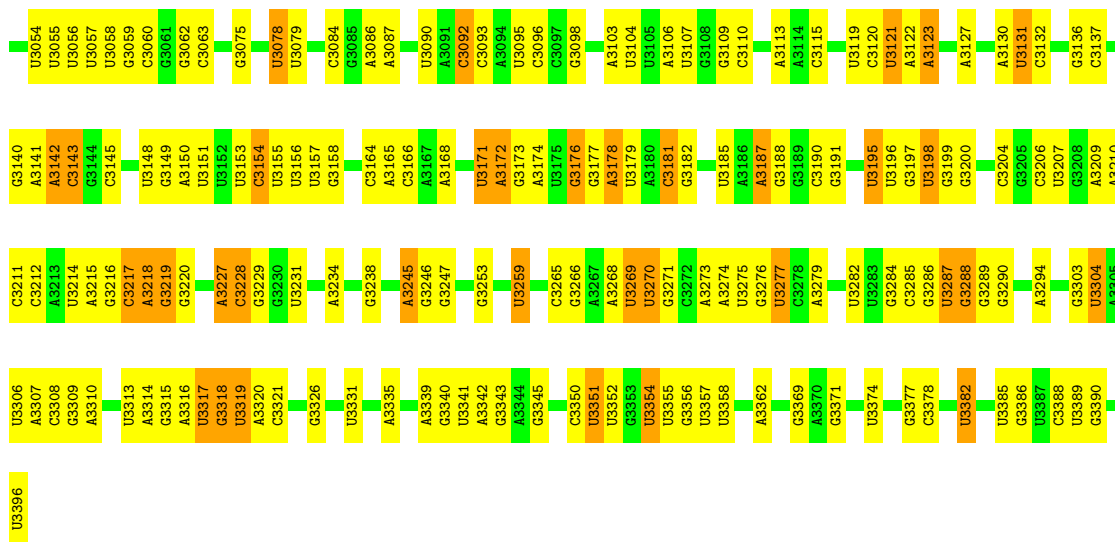


● Molecule 36: 25S ribosomal RNA

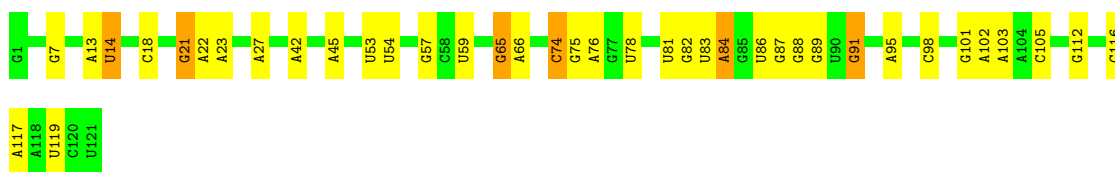
Chain 5: 47% 39% 8% 7%



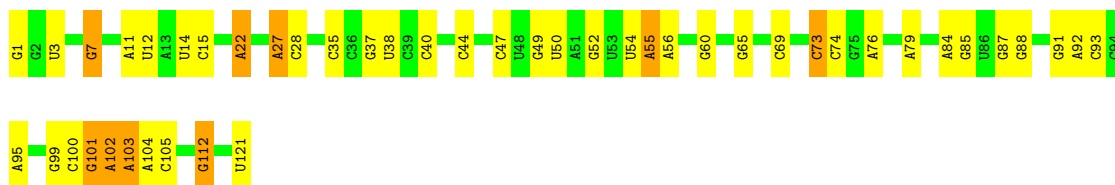
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A1153 C1154 U1155 G1156 A1157 C1158 U1159 G1160 A1161 U1162 C1163 A1164 G1165 U1166	C1016 U1017 G1018 U1019 A1020 C1021 U1022 G1023 C1024 A1025 U1026 G1027 U1028 C1029 G1035 U1041 A1046 U1047 A1048 C1049 U1052 G1060 C1063 A1064 U1065 C1066 U1067 C1068 U1071 G1072 C1076 U1077 A1078 U1079 A1080 U1081 C1082 U1088 A1093 U1094 C1095 U1096 G1097 A1098 U1099 U1100 A1101 C1102 A1103	G941 U942 C944 U945 G946 C947 U948 C949 G950 U951 A952 G953 U954 C955 G956 U957 A958 C959 G960 U961 A962 G963 C964 U965 A966 U967 G968 C969 A970 U971 G972 C973 U974 A975 G976 C977 U978 A979 G980 C981 U982 A983 G984 C985 U986 A987 G988 C989 A989 U990 G991 C992 A993 G994 U995 A996 G997 C998 U999 A1000 G1001 C1002 U1003 A1004 G1007 U1008 A1009 U1010 C1011 A1012 G1013 U1014	C873 U874 G875 G878 U879 C880 G881 A882 U883 C884 G885 U886 A887 C888 U889 G890 A891 C892 U893 G894 C895 A896 U897 G898 C899 A899 U900 G901 C902 A903 U904 G905 A906 U907 C908 A909 U910 G911 C912 A913 U914 G915 A916 U917 C918 U919 A920 U921 C922 G923 A924 U925 C928 U929 G933 A934 U935 C936 G937 U938 A939 C940 G941 U942	U867 C868 U872 U876 U877 G881 A884 U885 A886 C887 G888 U889 C890 A891 U892 C893 G894 U895 C896 A897 G898 U899 C900 A901 U902 C903 G904 A905 U906 C907 G908 U909 A910 C911 G912 A913 U914 G915 A916 U917 C918 U919 A920 U921 C922 G923 A924 U925 C928 U929 G933 A934 U935 C936 G937 U938 A939 C940 G941 U942	G600 G604 U605 C606 A607 U608 G609 A610 U611 C612 G613 U614 A619 C620 U621 G624 A630 U631 C632 G633 U634 A635 C636 U637 G640 A641 C642 U643 A644 C645 U646 A647 C648 A649 U650 G651 C652 A653 U654 G655 C658 A659 U660 G664 A665 U666 C667 G668 U669 C670 U673	A677 G680 U681 C682 A683 G686 U687 C688 A689 U690 G691 C692 A693 U694 G695 C696 A697 U698 G702 A705 U706 G712 A715 U716 C717 U718 A719 C720 G725 U726 A727 C735 U736 G739 U741 C740 A744 C748 A751 C752 U756 A757 C758 U765 A766 U767 C768 U772 U776 U777 G781 A784 U785 A786 G787 C788 U800 A801 C802 G803 U804 A805 U806 C807 G808 U821 A822 C823 G826 A830 U834 G835 C835 U851 G854 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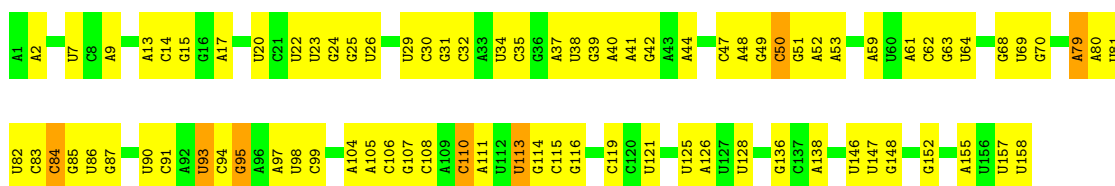
• Molecule 37: 5S ribosomal RNA



• Molecule 37: 5S ribosomal RNA

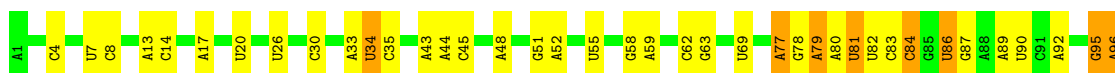


• Molecule 38: 5.8S ribosomal RNA

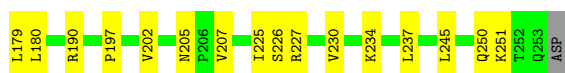
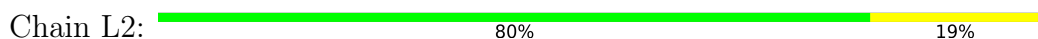


• Molecule 38: 5.8S ribosomal RNA

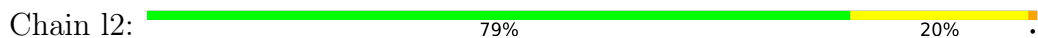




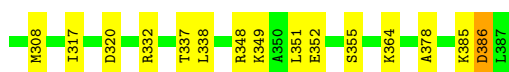
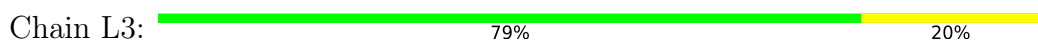
- Molecule 39: 60S ribosomal protein L2-A



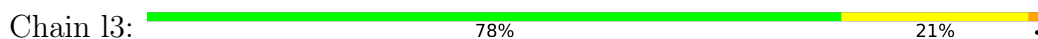
- Molecule 39: 60S ribosomal protein L2-A



- Molecule 40: 60S ribosomal protein L3

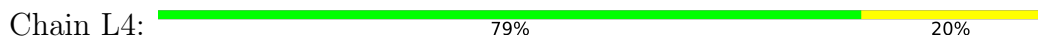


- Molecule 40: 60S ribosomal protein L3

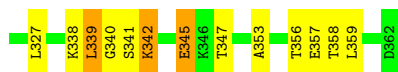
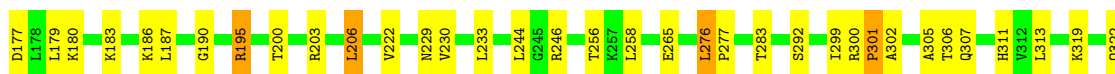
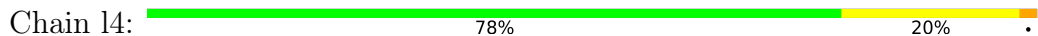




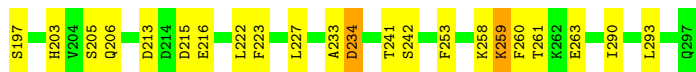
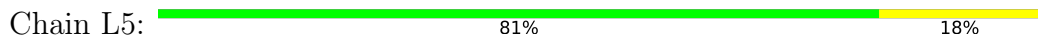
• Molecule 41: 60S ribosomal protein L4-A



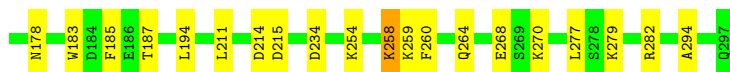
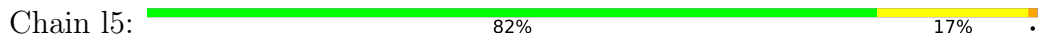
• Molecule 41: 60S ribosomal protein L4-A



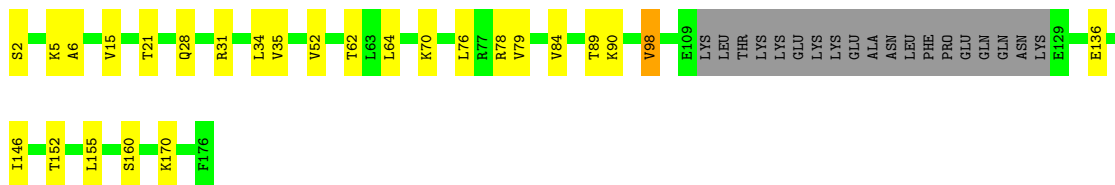
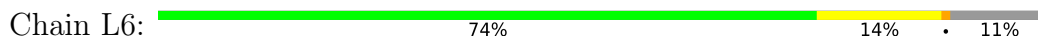
• Molecule 42: 60S ribosomal protein L5



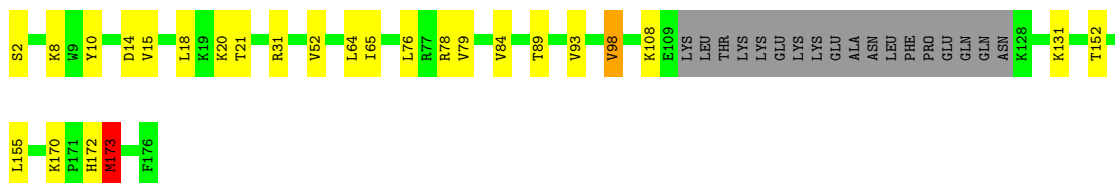
• Molecule 42: 60S ribosomal protein L5



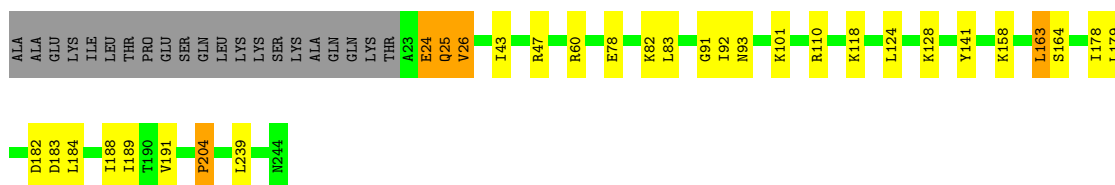
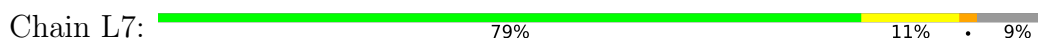
• Molecule 43: 60S ribosomal protein L6-A



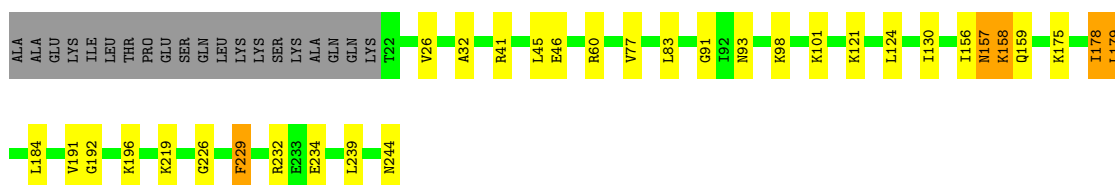
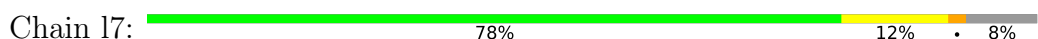
• Molecule 43: 60S ribosomal protein L6-A



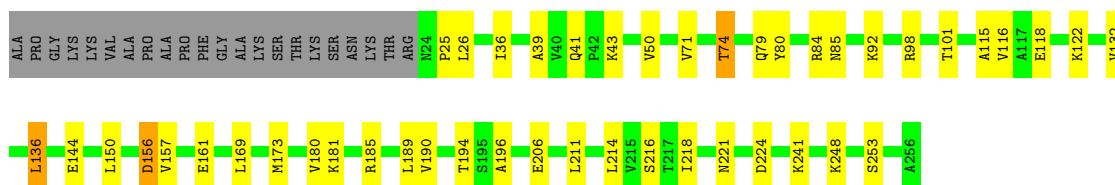
• Molecule 44: 60S ribosomal protein L7-A



• Molecule 44: 60S ribosomal protein L7-A

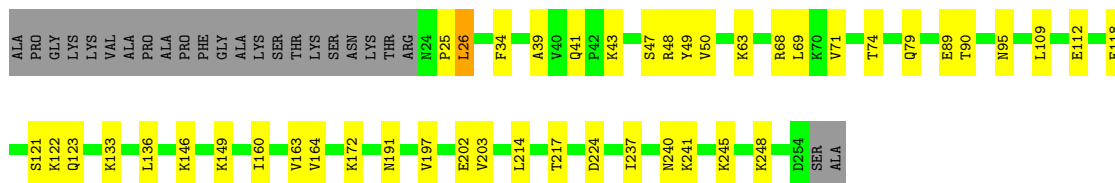


• Molecule 45: 60S ribosomal protein L8-A




- Molecule 45: 60S ribosomal protein L8-A

Chain l8:  73% 17% 9%



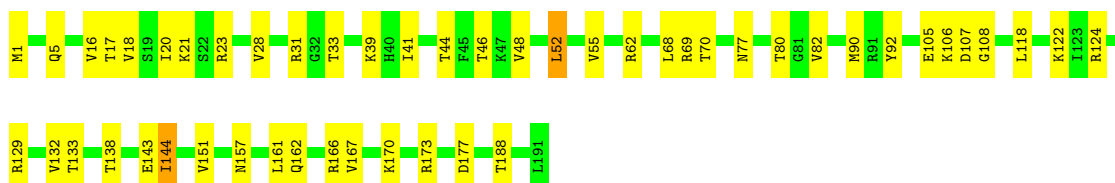
- Molecule 46: 60S ribosomal protein L9-A

Chain L9:  79% 20%




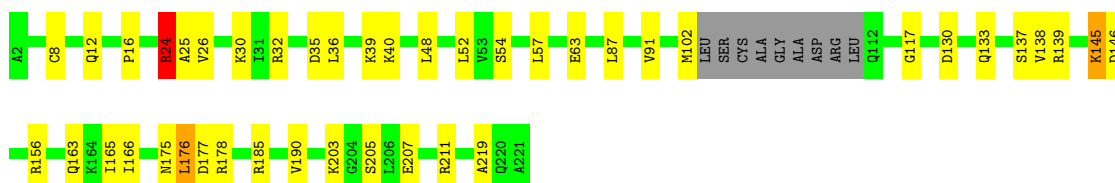
- Molecule 46: 60S ribosomal protein L9-A

Chain l9:  74% 25%




- Molecule 47: 60S ribosomal protein L10

Chain M0:  76% 18%




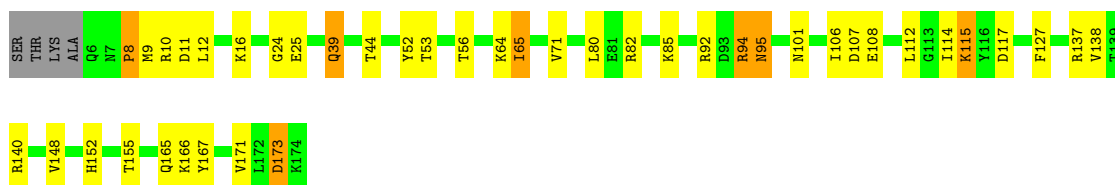
- Molecule 47: 60S ribosomal protein L10

Chain m0:  77% 19%




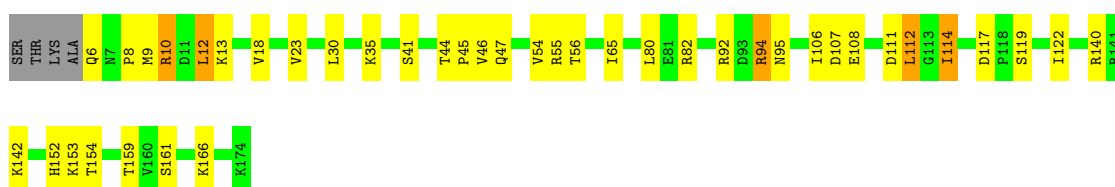
- Molecule 48: 60S ribosomal protein L11-B

Chain M1:  73% 20%




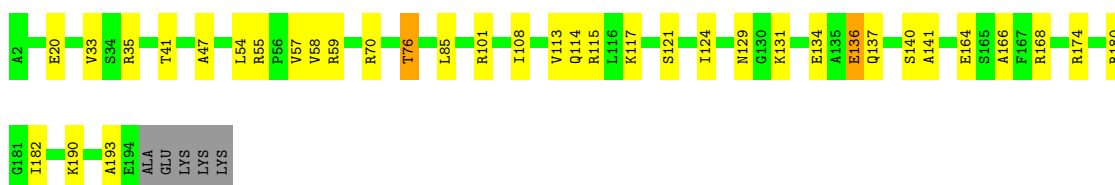
- Molecule 48: 60S ribosomal protein L11-B

Chain m1:  74% 21%




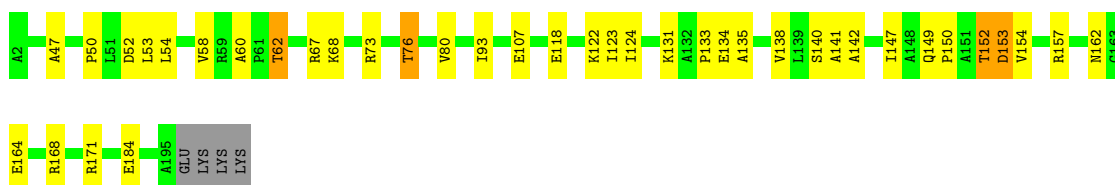
- Molecule 49: 60S ribosomal protein L13-A

Chain M3:  79% 17%




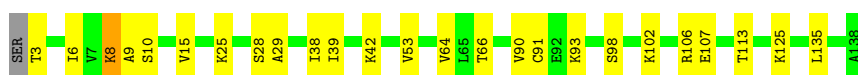
- Molecule 49: 60S ribosomal protein L13-A

Chain m3:  78% 18%




- Molecule 50: 60S ribosomal protein L14-A

Chain M4:  81% 18%




- Molecule 50: 60S ribosomal protein L14-A

Chain m4:  79% 20%




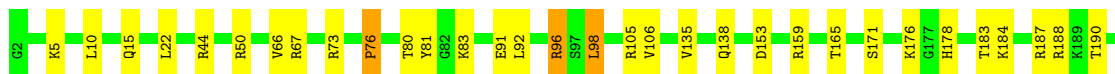
- Molecule 51: 60S ribosomal protein L15-A

Chain M5:  84% 15%




- Molecule 51: 60S ribosomal protein L15-A

Chain m5:  82% 17%




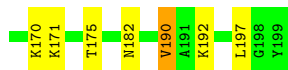
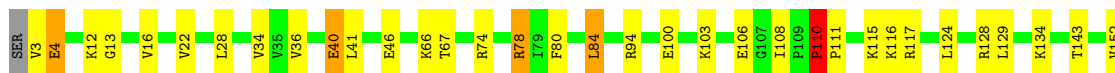
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:  86% 13%




- Molecule 52: 60S ribosomal protein L16-A

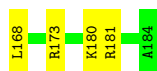
Chain m6:  79% 18%



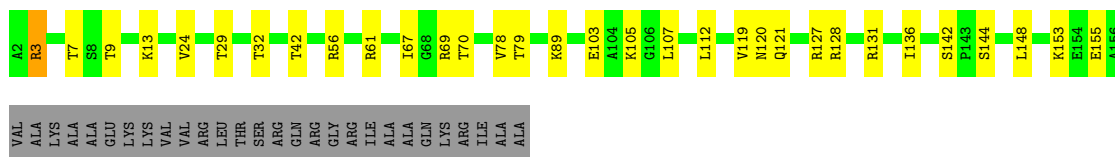
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:  80% 18%

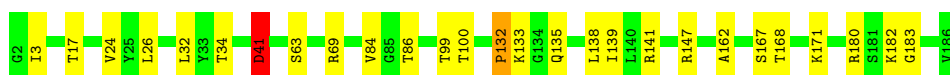
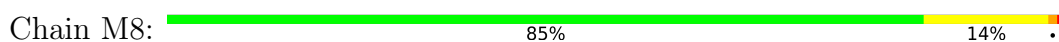




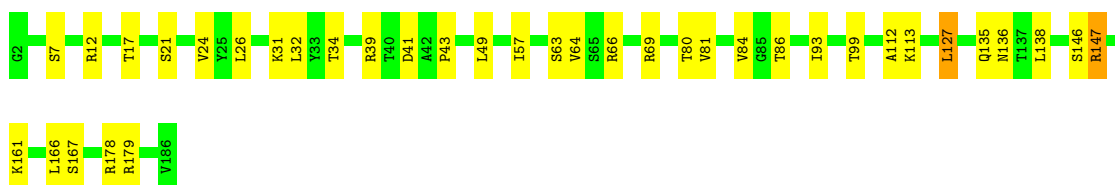
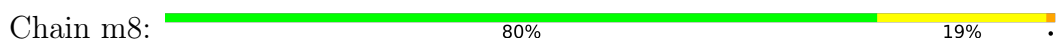
- Molecule 53: 60S ribosomal protein L17-A



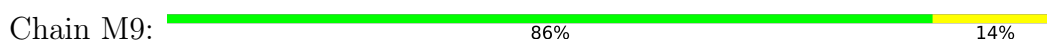
- Molecule 54: 60S ribosomal protein L18-A



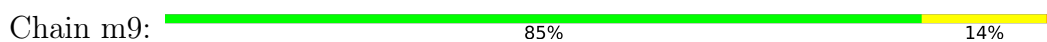
- Molecule 54: 60S ribosomal protein L18-A



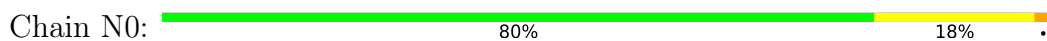
- Molecule 55: 60S ribosomal protein L19-A



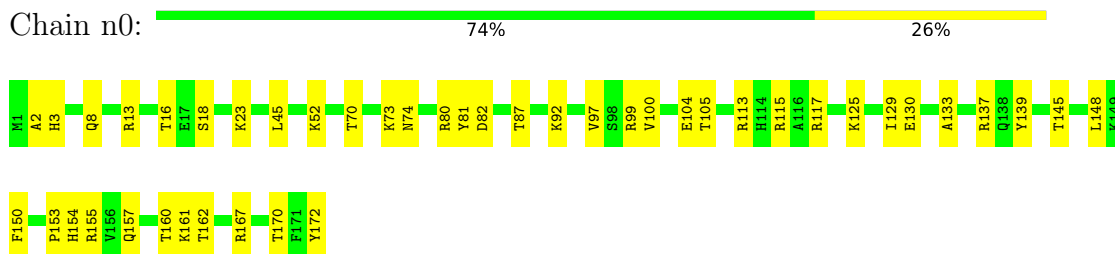
>
- Molecule 55: 60S ribosomal protein L19-A



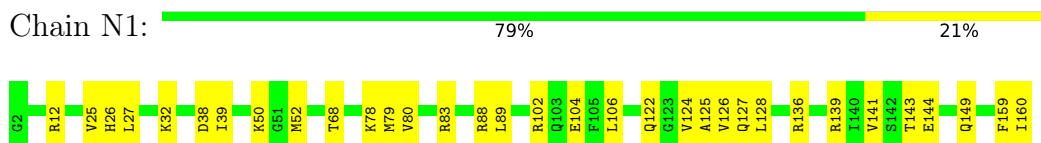
- Molecule 56: 60S ribosomal protein L20-A



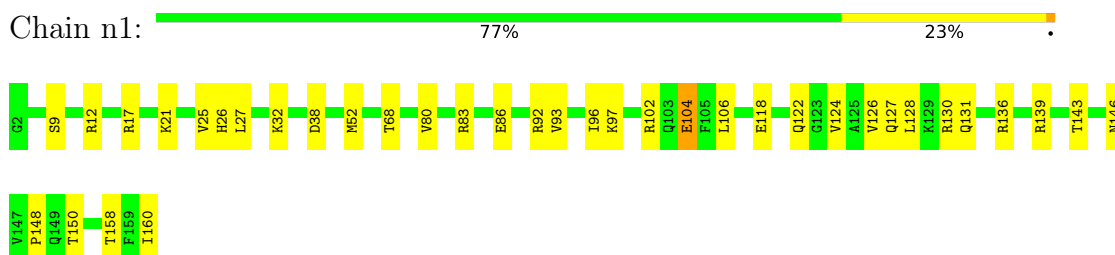
- Molecule 56: 60S ribosomal protein L20-A



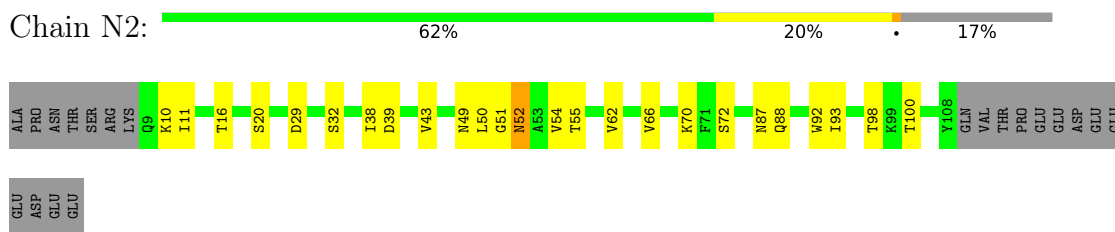
- Molecule 57: 60S ribosomal protein L21-A



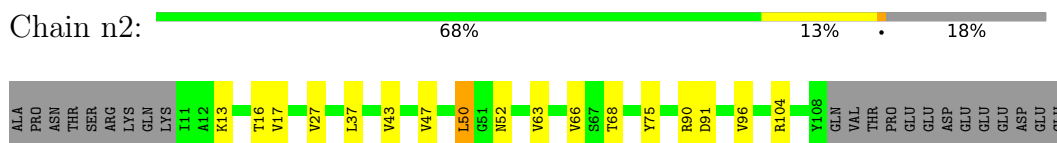
- Molecule 57: 60S ribosomal protein L21-A



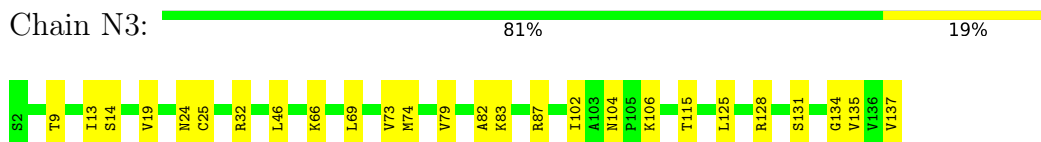
- Molecule 58: 60S ribosomal protein L22-A



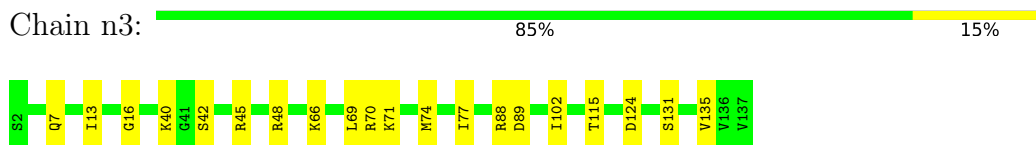
- Molecule 58: 60S ribosomal protein L22-A



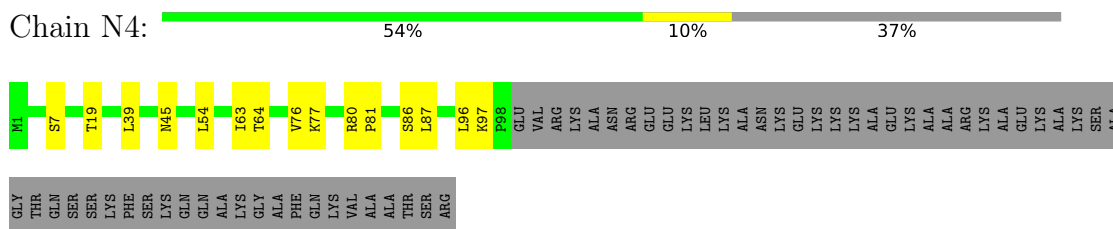
- Molecule 59: 60S ribosomal protein L23-A



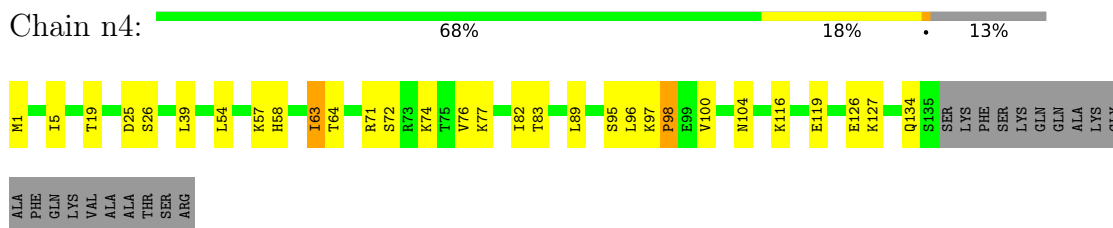
- Molecule 59: 60S ribosomal protein L23-A



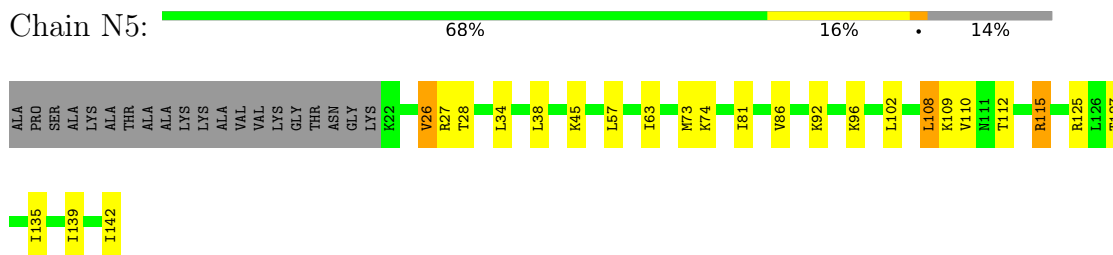
- Molecule 60: 60S ribosomal protein L24-A



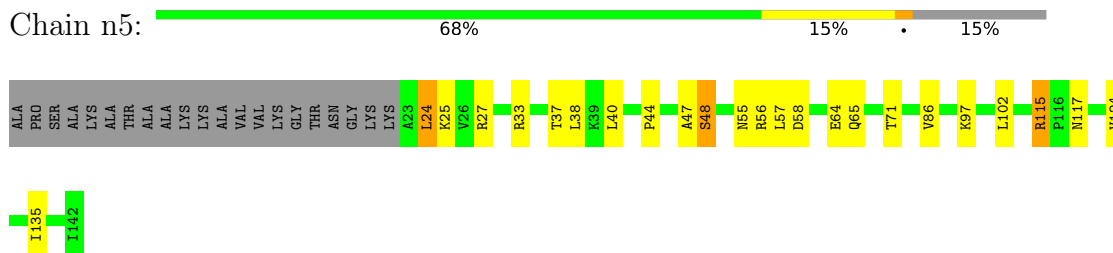
- Molecule 60: 60S ribosomal protein L24-A



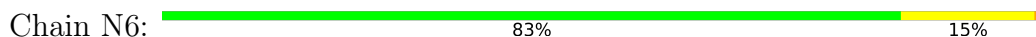
- Molecule 61: 60S ribosomal protein L25



- Molecule 61: 60S ribosomal protein L25

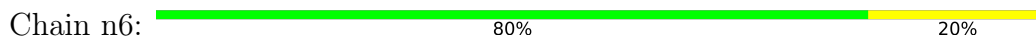


- Molecule 62: 60S ribosomal protein L26-A

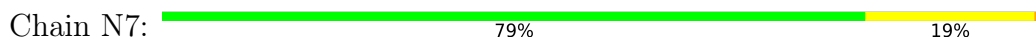




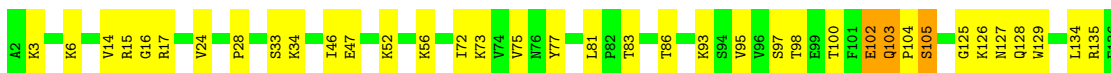
- Molecule 62: 60S ribosomal protein L26-A



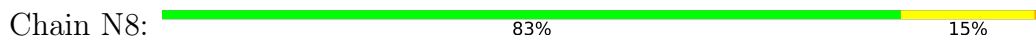
- Molecule 63: 60S ribosomal protein L27-A



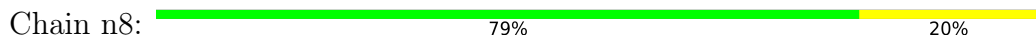
- Molecule 63: 60S ribosomal protein L27-A



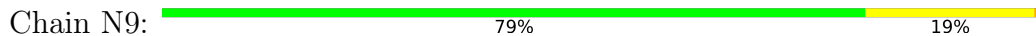
- Molecule 64: 60S ribosomal protein L28



- Molecule 64: 60S ribosomal protein L28



- Molecule 65: 60S ribosomal protein L29

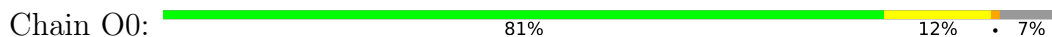


- Molecule 65: 60S ribosomal protein L29

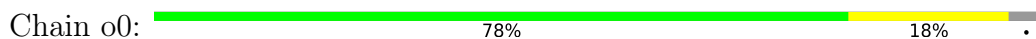




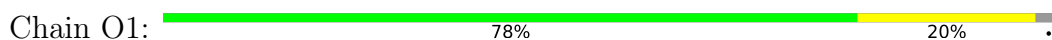
- Molecule 66: 60S ribosomal protein L30



- Molecule 66: 60S ribosomal protein L30



- Molecule 67: 60S ribosomal protein L31-A



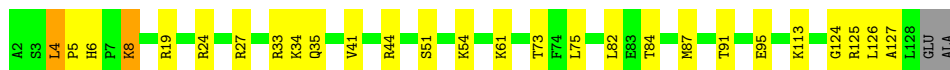
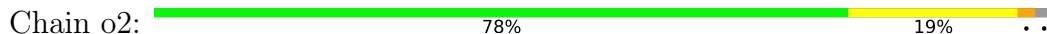
- Molecule 67: 60S ribosomal protein L31-A



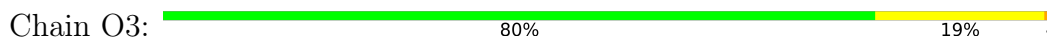
- Molecule 68: 60S ribosomal protein L32



- Molecule 68: 60S ribosomal protein L32

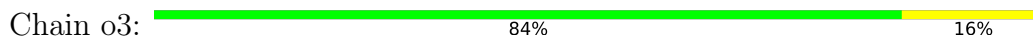


- Molecule 69: 60S ribosomal protein L33-A

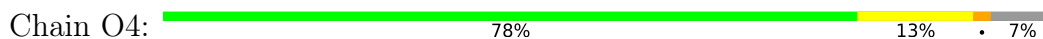




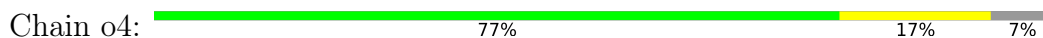
- Molecule 69: 60S ribosomal protein L33-A



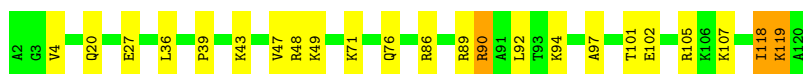
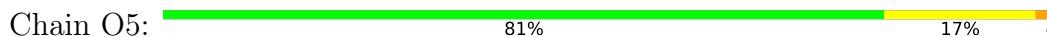
- Molecule 70: 60S ribosomal protein L34-A



- Molecule 70: 60S ribosomal protein L34-A



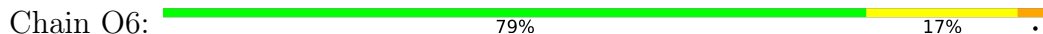
- Molecule 71: 60S ribosomal protein L35-A



- Molecule 71: 60S ribosomal protein L35-A

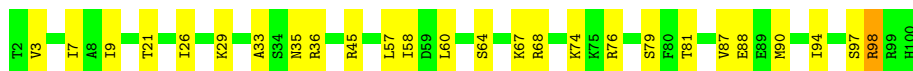


- Molecule 72: 60S ribosomal protein L36-A

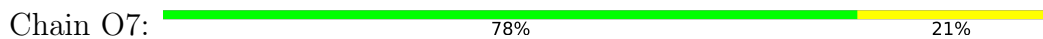


- Molecule 72: 60S ribosomal protein L36-A

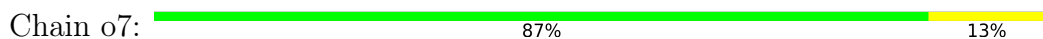




- Molecule 73: 60S ribosomal protein L37-A



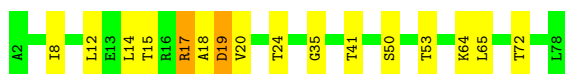
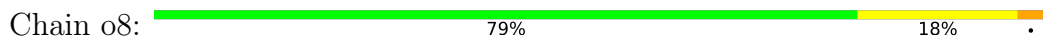
- Molecule 73: 60S ribosomal protein L37-A



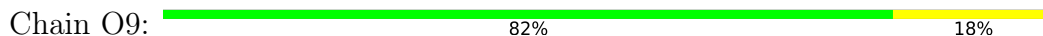
- Molecule 74: 60S ribosomal protein L38



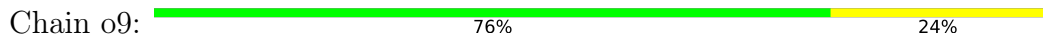
- Molecule 74: 60S ribosomal protein L38



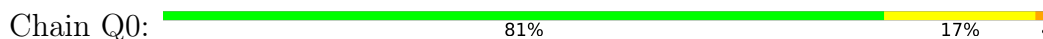
- Molecule 75: 60S ribosomal protein L39

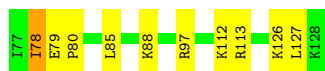


- Molecule 75: 60S ribosomal protein L39

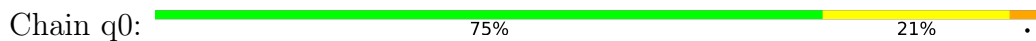


- Molecule 76: Ubiquitin-60S ribosomal protein L40

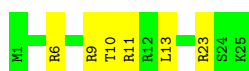
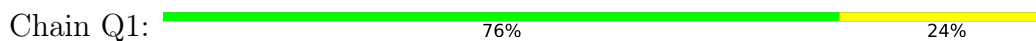




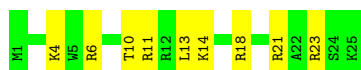
- Molecule 76: Ubiquitin-60S ribosomal protein L40



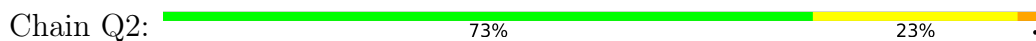
- Molecule 77: 60S ribosomal protein L41-A



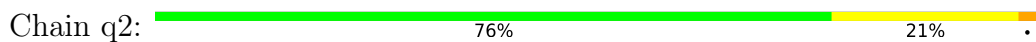
- Molecule 77: 60S ribosomal protein L41-A



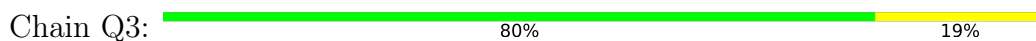
- Molecule 78: 60S ribosomal protein L42-A



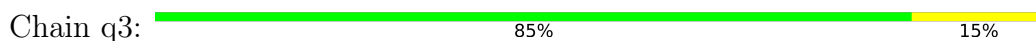
- Molecule 78: 60S ribosomal protein L42-A

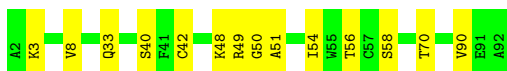


- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A





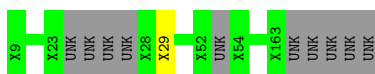
- Molecule 80: 40S ribosomal protein S30-A

Chain e0: 74% 24%



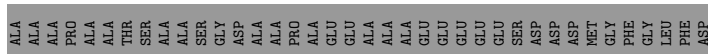
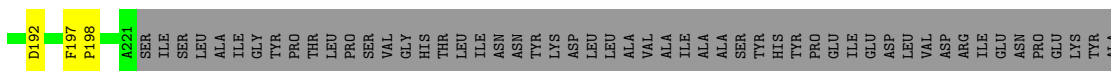
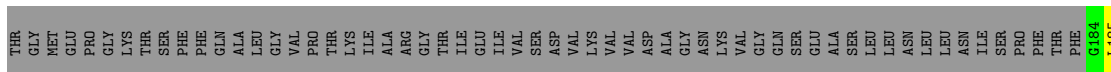
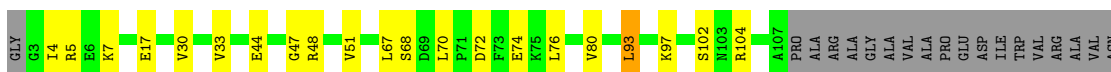
- Molecule 81: unknown protein chain m2

Chain m2: 93% 6%



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0: 38% 8% 54%



- 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	435.34Å 287.00Å 303.36Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	49.18 – 3.20	Depositor
% Data completeness (in resolution range)	99.9 (49.18-3.20)	Depositor
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.204 , 0.253	Depositor
Wilson B-factor (Å ²)	80.8	Xtrriage
Anisotropy	0.212	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	411178	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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 i

5.1 Standard geometry i

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

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	0.71	5/41698 (0.0%)	1.31	312/64972 (0.5%)
1	6	0.78	12/42765 (0.0%)	1.35	404/66634 (0.6%)
2	S0	0.44	0/1617	0.66	0/2215
2	s0	0.44	0/1623	0.65	0/2222
3	S1	0.39	0/1735	0.66	2/2335 (0.1%)
3	s1	0.49	0/1748	0.68	0/2352
4	S2	0.51	1/1665 (0.1%)	0.66	0/2263
4	s2	0.56	0/1665	0.75	1/2263 (0.0%)
5	S3	0.49	0/1759	0.68	0/2368
5	s3	0.41	0/1759	0.60	0/2368
6	S4	0.47	0/2109	0.72	2/2839 (0.1%)
6	s4	0.49	0/2109	0.72	0/2839
7	S5	0.38	0/1629	0.60	0/2202
7	s5	0.41	0/1629	0.61	0/2202
8	S6	0.47	0/1823	0.66	0/2439
8	s6	0.53	0/1779	0.69	0/2379
9	S7	0.43	0/1506	0.64	0/2028
9	s7	0.44	0/1516	0.63	0/2043
10	S8	0.54	0/1514	0.70	0/2021
10	s8	0.59	0/1514	0.75	3/2021 (0.1%)
11	S9	0.49	0/1519	0.69	1/2035 (0.0%)
11	s9	0.52	0/1519	0.72	2/2035 (0.1%)
12	C0	0.45	0/790	0.71	1/1069 (0.1%)
12	c0	0.36	0/777	0.64	3/1049 (0.3%)
13	C1	0.56	0/1239	0.66	0/1673
13	c1	0.57	0/1194	0.74	1/1610 (0.1%)
14	C2	0.37	0/900	0.66	0/1224
14	c2	0.31	0/900	0.58	0/1224
15	C3	0.50	0/1215	0.66	2/1638 (0.1%)
15	c3	0.53	0/1215	0.70	0/1638
16	C4	0.40	0/901	0.66	0/1217
16	c4	0.51	0/960	0.73	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.46	0/998	0.66	0/1341
17	c5	0.47	0/1060	0.69	0/1426
18	C6	0.44	0/1125	0.68	2/1510 (0.1%)
18	c6	0.44	0/1131	0.65	0/1518
19	C7	0.43	0/935	0.65	0/1254
19	c7	0.45	0/914	0.68	0/1224
20	C8	0.43	0/1211	0.65	1/1628 (0.1%)
20	c8	0.45	0/1211	0.66	1/1628 (0.1%)
21	C9	0.41	0/1130	0.60	0/1517
21	c9	0.46	0/1130	0.66	0/1517
22	D0	0.43	0/865	0.65	0/1169
22	d0	0.43	0/892	0.65	0/1205
23	D1	0.42	0/693	0.63	0/935
23	d1	0.50	0/693	0.70	0/935
24	D2	0.53	0/1038	0.72	0/1395
24	d2	0.56	0/1038	0.73	1/1395 (0.1%)
25	D3	0.60	0/1139	0.77	0/1518
25	d3	0.66	0/1139	0.81	2/1518 (0.1%)
26	D4	0.45	0/1087	0.61	0/1449
26	d4	0.51	0/1087	0.71	0/1449
27	D5	0.39	0/571	0.72	0/768
27	d5	0.41	0/566	0.65	0/761
28	D6	0.46	0/782	0.71	0/1047
28	d6	0.57	0/782	0.73	0/1047
29	D7	0.44	0/620	0.66	0/838
29	d7	0.47	0/620	0.74	0/838
30	D8	0.37	0/499	0.60	0/670
30	d8	0.40	0/499	0.64	0/670
31	D9	0.53	0/452	0.70	1/600 (0.2%)
31	d9	0.46	0/452	0.61	0/600
32	E0	0.47	0/483	0.62	0/643
33	E1	0.47	0/577	0.79	0/770
33	e1	0.39	0/619	0.71	0/822
34	SR	0.36	0/2494	0.57	0/3393
34	sR	0.35	0/2495	0.56	0/3395
35	SM	0.51	0/1113	0.71	2/1502 (0.1%)
35	sM	0.46	0/683	0.68	1/923 (0.1%)
36	1	1.08	102/75394 (0.1%)	1.68	1977/117545 (1.7%)
36	5	1.10	107/75414 (0.1%)	1.70	2076/117575 (1.8%)
37	3	0.91	3/2883 (0.1%)	1.45	38/4491 (0.8%)
37	7	1.04	3/2883 (0.1%)	1.64	63/4491 (1.4%)
38	4	1.03	0/3746	1.64	78/5832 (1.3%)
38	8	0.95	0/3746	1.54	62/5832 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.70	0/1948	0.84	1/2617 (0.0%)
39	l2	0.65	0/1946	0.85	1/2614 (0.0%)
40	L3	0.72	1/3146 (0.0%)	0.80	0/4228
40	l3	0.78	0/3146	0.86	2/4228 (0.0%)
41	L4	0.76	0/2800	0.90	3/3790 (0.1%)
41	l4	0.75	1/2800 (0.0%)	0.92	5/3790 (0.1%)
42	L5	0.56	0/2425	0.69	0/3271
42	l5	0.70	0/2408	0.80	1/3248 (0.0%)
43	L6	0.72	0/1260	0.81	1/1694 (0.1%)
43	l6	0.77	0/1269	0.82	2/1705 (0.1%)
44	L7	0.79	0/1821	0.87	2/2451 (0.1%)
44	l7	0.83	0/1828	0.91	4/2461 (0.2%)
45	L8	0.54	0/1836	0.68	0/2481
45	l8	0.49	0/1795	0.65	0/2429
46	L9	0.68	0/1539	0.79	0/2073
46	l9	0.77	0/1539	0.83	1/2073 (0.0%)
47	M0	0.71	1/1741 (0.1%)	0.84	3/2335 (0.1%)
47	m0	0.72	1/1758 (0.1%)	0.81	1/2358 (0.0%)
48	M1	0.50	0/1374	0.72	0/1842
48	m1	0.63	0/1374	0.80	2/1842 (0.1%)
49	M3	0.74	0/1568	0.84	0/2106
49	m3	0.69	0/1573	0.79	0/2113
50	M4	0.74	0/1068	0.83	0/1438
50	m4	0.78	0/1074	0.81	1/1446 (0.1%)
51	M5	0.73	0/1757	0.90	2/2354 (0.1%)
51	m5	0.65	0/1757	0.83	3/2354 (0.1%)
52	M6	0.84	0/1585	0.88	3/2128 (0.1%)
52	m6	0.95	2/1585 (0.1%)	0.94	4/2128 (0.2%)
53	M7	0.77	0/1443	0.86	2/1944 (0.1%)
53	m7	0.91	0/1250	0.88	0/1683
54	M8	0.75	0/1465	0.88	1/1965 (0.1%)
54	m8	0.75	0/1465	0.88	1/1965 (0.1%)
55	M9	0.56	0/1538	0.65	0/2050
55	m9	0.56	0/1538	0.67	0/2050
56	N0	0.75	0/1481	0.81	0/1990
56	n0	0.86	0/1481	0.89	1/1990 (0.1%)
57	N1	0.72	0/1300	0.78	0/1743
57	n1	0.79	1/1300 (0.1%)	0.84	1/1743 (0.1%)
58	N2	0.45	0/812	0.59	0/1099
58	n2	0.46	0/794	0.69	0/1076
59	N3	0.69	0/1018	0.82	0/1369
59	n3	0.78	0/1018	0.85	1/1369 (0.1%)
60	N4	0.56	0/712	0.68	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.62	0/1052	0.73	0/1398
61	N5	0.65	0/979	0.82	1/1321 (0.1%)
61	n5	0.64	0/974	0.80	1/1314 (0.1%)
62	N6	0.68	0/1004	0.87	1/1341 (0.1%)
62	n6	0.67	0/1004	0.84	0/1341
63	N7	0.53	0/1118	0.65	0/1497
63	n7	0.53	0/1118	0.68	0/1497
64	N8	0.76	0/1204	0.90	2/1612 (0.1%)
64	n8	0.77	0/1204	0.86	1/1612 (0.1%)
65	N9	0.66	0/473	0.75	0/629
65	n9	0.71	0/473	0.96	1/629 (0.2%)
66	O0	0.50	0/751	0.69	0/1008
66	o0	0.49	0/775	0.66	0/1040
67	O1	0.63	0/890	0.72	0/1196
67	o1	0.73	0/897	0.86	0/1205
68	O2	0.82	0/1041	0.90	0/1394
68	o2	0.81	0/1041	0.90	1/1394 (0.1%)
69	O3	0.87	0/868	0.94	2/1168 (0.2%)
69	o3	0.87	0/868	0.91	2/1168 (0.2%)
70	O4	0.60	0/890	0.77	2/1189 (0.2%)
70	o4	0.58	0/890	0.79	0/1189
71	O5	0.71	0/978	0.81	1/1301 (0.1%)
71	o5	0.58	0/974	0.72	1/1297 (0.1%)
72	O6	0.63	0/778	0.77	0/1034
72	o6	0.56	0/777	0.68	0/1033
73	O7	0.76	0/696	0.95	2/923 (0.2%)
73	o7	0.68	0/696	0.84	0/923
74	O8	0.55	0/618	0.67	0/826
74	o8	0.53	0/614	0.66	0/822
75	O9	0.77	0/443	0.91	0/588
75	o9	0.67	0/443	0.85	0/588
76	Q0	0.72	0/423	0.82	0/562
76	q0	0.86	0/423	0.93	0/562
77	Q1	0.62	0/234	0.81	0/300
77	q1	0.80	0/234	1.02	0/300
78	Q2	0.80	1/860 (0.1%)	0.84	2/1136 (0.2%)
78	q2	0.75	1/860 (0.1%)	0.82	2/1136 (0.2%)
79	Q3	0.70	0/701	0.80	0/934
79	q3	0.70	0/701	0.82	1/934 (0.1%)
80	e0	0.53	0/499	0.74	0/665
82	p0	0.45	0/1091	0.60	0/1472
All	All	0.84	242/430072 (0.1%)	1.32	5111/631360 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	s3	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
11	s9	0	1
16	C4	0	2
18	c6	0	1
19	C7	0	1
19	c7	0	1
22	d0	0	1
25	D3	0	1
27	D5	0	2
33	E1	0	1
39	L2	0	2
40	l3	0	1
41	L4	0	1
44	l7	0	2
45	L8	0	1
48	M1	0	1
50	m4	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	1
56	n0	0	3
64	n8	0	1
65	N9	0	1
69	o3	0	1
72	O6	0	1
75	O9	0	1
81	m2	0	1
All	All	0	37

All (242) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	12.79	2.04	1.82
36	5	1152	G	N9-C4	-11.94	1.28	1.38
36	1	3181	C	N3-C4	-9.75	1.27	1.33
36	1	895	A	C5-C6	-9.41	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	9.34	1.98	1.82
36	1	2404	A	N7-C5	9.31	1.44	1.39
36	5	2411	U	C2-N3	-8.15	1.32	1.37
36	5	924	G	N3-C4	-8.00	1.29	1.35
36	1	1394	A	N9-C4	-7.92	1.33	1.37
36	1	2406	C	N1-C6	-7.89	1.32	1.37
36	5	2971	A	N9-C4	7.87	1.42	1.37
36	1	1116	G	N3-C4	-7.61	1.30	1.35
36	5	945	C	N1-C6	-7.60	1.32	1.37
36	1	925	A	N3-C4	-7.48	1.30	1.34
36	5	2726	C	N3-C4	-7.43	1.28	1.33
36	5	1152	G	N9-C8	7.35	1.43	1.37
36	5	996	A	N9-C4	-7.27	1.33	1.37
36	5	2903	A	N9-C4	-7.18	1.33	1.37
36	1	1891	A	N9-C4	-7.13	1.33	1.37
36	5	1366	A	N3-C4	-6.98	1.30	1.34
36	5	2943	G	N7-C5	-6.97	1.35	1.39
36	5	2358	A	N9-C4	-6.92	1.33	1.37
52	m6	40	GLU	CG-CD	6.91	1.62	1.51
36	1	1148	G	N7-C5	-6.87	1.35	1.39
36	5	2372	A	N7-C5	-6.73	1.35	1.39
36	1	2401	A	C6-N1	6.69	1.40	1.35
1	6	623	A	N9-C4	-6.56	1.33	1.37
36	5	1148	G	N9-C8	-6.56	1.33	1.37
36	1	653	A	C5-C6	-6.53	1.35	1.41
36	1	1103	A	N9-C4	6.51	1.41	1.37
36	1	2983	C	N3-C4	-6.50	1.29	1.33
36	1	2404	A	C5-C6	6.44	1.46	1.41
47	m0	8	CYS	CB-SG	-6.40	1.71	1.82
36	5	1148	G	N7-C5	-6.40	1.35	1.39
36	1	716	A	N9-C4	-6.39	1.34	1.37
36	5	609	G	C2-N3	-6.35	1.27	1.32
36	5	1136	A	N9-C4	-6.34	1.34	1.37
36	1	2147	A	N9-C4	-6.32	1.34	1.37
36	5	94	G	C6-N1	-6.27	1.35	1.39
36	1	952	A	N9-C4	-6.26	1.34	1.37
36	1	884	A	N7-C5	-6.26	1.35	1.39
36	5	3008	A	N9-C4	-6.26	1.34	1.37
36	5	883	A	N3-C4	-6.25	1.31	1.34
36	5	2385	G	N9-C4	-6.20	1.32	1.38
36	5	960	U	N1-C2	6.18	1.44	1.38
36	5	1143	A	N9-C4	-6.18	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2147	A	C5-C6	-6.18	1.35	1.41
36	5	2399	A	N9-C4	-6.16	1.34	1.37
36	1	2326	A	N9-C4	-6.16	1.34	1.37
36	5	1152	G	C2-N3	-6.12	1.27	1.32
36	1	367	A	N9-C4	-6.12	1.34	1.37
36	1	2601	A	N9-C4	-6.11	1.34	1.37
36	5	2619	G	C5-C4	-6.10	1.34	1.38
36	1	884	A	N9-C4	-6.10	1.34	1.37
36	5	2637	A	N9-C4	-6.08	1.34	1.37
36	1	936	A	N9-C4	-6.08	1.34	1.37
36	5	1152	G	N3-C4	-6.07	1.31	1.35
36	5	61	A	N3-C4	-6.06	1.31	1.34
1	6	1131	A	N3-C4	-5.99	1.31	1.34
36	1	2409	G	C5-C4	-5.99	1.34	1.38
36	5	3209	A	C5-C4	5.99	1.43	1.38
36	1	2333	C	N3-C4	-5.98	1.29	1.33
57	n1	104	GLU	CB-CG	5.98	1.63	1.52
36	5	1897	G	N3-C4	-5.97	1.31	1.35
36	1	952	A	N3-C4	-5.92	1.31	1.34
36	1	92	G	N1-C2	-5.92	1.33	1.37
36	1	2198	A	N3-C4	-5.91	1.31	1.34
36	5	2640	A	N9-C4	-5.90	1.34	1.37
36	1	2147	A	C5-C4	-5.90	1.34	1.38
36	1	585	A	N9-C4	-5.89	1.34	1.37
36	1	653	A	C6-N1	-5.89	1.31	1.35
36	1	962	A	N7-C5	-5.89	1.35	1.39
36	1	2640	A	N9-C4	-5.89	1.34	1.37
41	14	94	CYS	CB-SG	-5.88	1.72	1.81
1	2	992	A	N9-C4	-5.87	1.34	1.37
36	1	92	G	C5-C4	-5.87	1.34	1.38
37	3	86	U	C2-N3	-5.87	1.33	1.37
36	5	955	U	C2-N3	-5.87	1.33	1.37
4	S2	120	GLU	CG-CD	5.86	1.60	1.51
36	1	343	U	N1-C6	-5.85	1.32	1.38
37	3	88	G	C6-N1	-5.84	1.35	1.39
36	5	2892	A	C5-C6	-5.84	1.35	1.41
36	5	2139	A	N3-C4	-5.84	1.31	1.34
36	1	3209	A	C5-C4	5.83	1.42	1.38
36	5	1432	C	N3-C4	-5.82	1.29	1.33
1	6	1137	A	N9-C4	-5.82	1.34	1.37
36	1	2333	C	N1-C6	-5.80	1.33	1.37
1	2	334	G	N9-C4	-5.80	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	651	G	C6-N1	-5.80	1.35	1.39
36	5	2397	A	N9-C4	-5.79	1.34	1.37
36	1	2363	A	C6-N1	-5.78	1.31	1.35
36	5	924	G	C6-N1	-5.78	1.35	1.39
36	5	2970	C	N1-C6	-5.77	1.33	1.37
36	5	2243	A	N3-C4	-5.77	1.31	1.34
36	1	1429	G	N9-C8	-5.76	1.33	1.37
36	5	884	A	N9-C4	-5.76	1.34	1.37
36	5	3362	A	N3-C4	-5.75	1.31	1.34
36	1	35	A	C5-C6	-5.75	1.35	1.41
36	5	941	G	C6-N1	-5.73	1.35	1.39
1	6	1137	A	C5-C4	-5.71	1.34	1.38
36	1	895	A	N7-C5	-5.71	1.35	1.39
37	7	102	A	N9-C4	-5.67	1.34	1.37
36	5	428	A	N7-C5	-5.66	1.35	1.39
36	1	2626	A	N3-C4	-5.66	1.31	1.34
36	1	2931	C	N1-C6	-5.64	1.33	1.37
36	1	1379	G	C6-N1	-5.64	1.35	1.39
36	1	2138	A	N9-C4	-5.63	1.34	1.37
36	5	924	G	C2-N3	-5.61	1.28	1.32
37	7	88	G	C6-N1	-5.61	1.35	1.39
36	1	2617	U	C4-C5	5.61	1.48	1.43
1	6	163	G	N9-C4	-5.61	1.33	1.38
36	5	924	G	N9-C4	-5.60	1.33	1.38
36	1	744	A	N9-C4	-5.60	1.34	1.37
36	1	422	A	N7-C5	-5.57	1.35	1.39
36	5	2813	A	N7-C5	-5.57	1.35	1.39
36	1	659	G	C5-C4	-5.56	1.34	1.38
36	5	2138	A	N7-C5	-5.55	1.35	1.39
36	1	1099	A	N9-C4	-5.55	1.34	1.37
36	1	3173	G	C8-N7	-5.54	1.27	1.30
47	M0	8	CYS	CB-SG	-5.53	1.72	1.81
36	5	1587	A	N9-C4	-5.53	1.34	1.37
36	5	1454	A	N9-C4	-5.53	1.34	1.37
36	1	1100	U	C2-N3	-5.52	1.33	1.37
36	5	2132	C	N3-C4	-5.51	1.30	1.33
36	5	1868	G	N7-C5	-5.50	1.35	1.39
36	1	3130	A	N7-C5	-5.50	1.35	1.39
36	1	1103	A	N7-C5	5.49	1.42	1.39
36	5	1149	G	C2-N3	5.49	1.37	1.32
36	5	1152	G	N1-C2	5.47	1.42	1.37
36	1	3142	A	N3-C4	-5.45	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	645	A	C5-C6	5.45	1.46	1.41
1	2	1291	G	N3-C4	-5.44	1.31	1.35
36	5	3033	A	N9-C4	-5.44	1.34	1.37
36	1	1391	C	N1-C6	-5.44	1.33	1.37
36	5	2896	A	N9-C4	-5.44	1.34	1.37
36	1	1394	A	N3-C4	-5.43	1.31	1.34
36	5	1868	G	C5-C6	-5.43	1.36	1.42
40	L3	200	GLU	CG-CD	5.41	1.60	1.51
36	5	2643	A	N9-C4	-5.40	1.34	1.37
36	1	402	A	N9-C4	-5.38	1.34	1.37
36	1	2341	A	N3-C4	-5.38	1.31	1.34
36	1	3306	U	N3-C4	-5.38	1.33	1.38
36	5	345	G	N9-C8	-5.37	1.34	1.37
36	1	1547	G	C5-C4	-5.37	1.34	1.38
36	1	49	A	N9-C4	-5.36	1.34	1.37
36	5	367	A	N9-C4	-5.34	1.34	1.37
36	5	883	A	C6-N1	-5.33	1.31	1.35
36	1	92	G	C6-N1	-5.33	1.35	1.39
36	1	1304	A	N9-C4	-5.33	1.34	1.37
36	5	953	G	N7-C5	-5.33	1.36	1.39
36	1	1116	G	N7-C5	-5.32	1.36	1.39
36	1	3006	A	N9-C4	-5.31	1.34	1.37
36	1	402	A	C5-C4	-5.31	1.35	1.38
36	1	1320	C	N1-C6	-5.31	1.33	1.37
36	5	1116	G	N3-C4	-5.30	1.31	1.35
36	5	3033	A	N7-C5	-5.29	1.36	1.39
1	6	1659	A	N9-C4	-5.29	1.34	1.37
36	5	2392	C	C2-N3	-5.29	1.31	1.35
36	1	658	G	C8-N7	-5.29	1.27	1.30
1	2	1730	A	N9-C4	-5.28	1.34	1.37
36	5	1456	A	N9-C4	-5.28	1.34	1.37
36	1	2868	U	C4-O4	5.28	1.27	1.23
36	1	585	A	N3-C4	-5.26	1.31	1.34
36	5	2878	G	C6-O6	-5.26	1.19	1.24
36	5	1177	G	C6-N1	-5.25	1.35	1.39
36	1	924	G	C8-N7	-5.25	1.27	1.30
36	5	585	A	N9-C4	-5.25	1.34	1.37
36	5	922	U	N1-C2	5.24	1.43	1.38
36	1	699	A	N9-C4	-5.24	1.34	1.37
1	6	1137	A	N3-C4	-5.24	1.31	1.34
36	1	422	A	C5-C4	-5.23	1.35	1.38
36	1	2910	A	N9-C4	-5.23	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	34	A	N9-C4	-5.22	1.34	1.37
36	5	706	A	N9-C4	-5.22	1.34	1.37
36	5	3087	A	N7-C5	-5.22	1.36	1.39
36	1	655	C	N3-C4	-5.22	1.30	1.33
36	1	1153	A	C5-C6	-5.22	1.36	1.41
36	5	808	A	N3-C4	-5.22	1.31	1.34
36	1	609	G	C5-C4	-5.21	1.34	1.38
36	5	1332	A	N9-C4	-5.21	1.34	1.37
36	1	887	G	N9-C8	-5.20	1.34	1.37
36	5	2954	U	N1-C2	5.20	1.43	1.38
36	1	1154	A	N7-C5	-5.20	1.36	1.39
36	5	3362	A	N9-C4	-5.19	1.34	1.37
36	5	1406	A	N3-C4	-5.18	1.31	1.34
36	5	822	G	C2-N3	-5.17	1.28	1.32
36	5	948	C	N1-C6	-5.16	1.34	1.37
36	1	649	A	N9-C4	-5.16	1.34	1.37
36	5	947	G	C6-N1	-5.16	1.35	1.39
36	1	1140	G	C6-N1	-5.15	1.35	1.39
36	5	1310	G	N9-C8	-5.14	1.34	1.37
36	1	1157	G	C6-N1	-5.13	1.35	1.39
36	5	2291	A	N9-C4	-5.13	1.34	1.37
36	5	2419	A	P-O5'	5.13	1.64	1.59
1	2	1749	A	N9-C4	-5.12	1.34	1.37
36	1	1116	G	C6-N1	-5.12	1.35	1.39
52	m6	80	PHE	CB-CG	-5.12	1.42	1.51
36	1	2146	C	N3-C4	-5.12	1.30	1.33
36	1	3273	A	N3-C4	-5.12	1.31	1.34
36	5	421	G	C6-N1	-5.12	1.35	1.39
36	1	282	G	C6-N1	-5.12	1.35	1.39
36	5	2983	C	N3-C4	-5.12	1.30	1.33
36	5	1454	A	C5-C6	-5.11	1.36	1.41
36	5	646	A	C6-N1	-5.11	1.31	1.35
36	5	2404	A	C6-N6	5.11	1.38	1.33
36	5	636	C	N3-C4	-5.10	1.30	1.33
36	5	1152	G	C5-C6	-5.10	1.37	1.42
1	6	337	G	C2-N3	5.09	1.36	1.32
36	1	1308	A	C6-N1	-5.09	1.31	1.35
36	5	416	A	N7-C5	-5.08	1.36	1.39
37	3	66	A	N9-C4	-5.08	1.34	1.37
36	1	189	G	C5-C4	-5.08	1.34	1.38
1	6	417	A	N9-C4	5.07	1.40	1.37
36	5	375	A	N9-C4	-5.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2916	U	C2-O2	5.07	1.26	1.22
36	5	2375	G	C6-N1	-5.07	1.36	1.39
36	5	2636	A	C6-N1	-5.06	1.32	1.35
36	1	1589	A	N9-C4	-5.06	1.34	1.37
36	1	951	A	N9-C4	-5.05	1.34	1.37
36	5	2399	A	N3-C4	-5.05	1.31	1.34
36	1	206	G	C5-C4	-5.04	1.34	1.38
36	1	421	G	N1-C2	-5.04	1.33	1.37
36	1	913	A	N7-C5	-5.04	1.36	1.39
36	5	2627	C	N1-C6	-5.04	1.34	1.37
36	5	426	G	C5-C4	-5.04	1.34	1.38
36	5	3136	G	C6-N1	-5.04	1.36	1.39
36	5	2983	C	N1-C6	-5.04	1.34	1.37
1	6	1113	A	N3-C4	-5.03	1.31	1.34
36	5	1592	G	C6-O6	5.03	1.28	1.24
36	1	1326	A	N9-C4	-5.03	1.34	1.37
36	1	984	G	N7-C5	-5.03	1.36	1.39
1	6	923	A	N9-C4	-5.02	1.34	1.37
36	5	1905	G	C5-C4	-5.02	1.34	1.38
36	5	2878	G	C6-N1	-5.02	1.36	1.39
36	1	2401	A	N3-C4	5.01	1.37	1.34
36	5	428	A	N9-C8	-5.01	1.33	1.37
36	5	519	A	N9-C4	-5.01	1.34	1.37
36	5	1303	A	N9-C4	-5.01	1.34	1.37
36	1	2409	G	N7-C5	-5.00	1.36	1.39
1	6	541	A	N9-C4	5.00	1.40	1.37
37	7	56	A	N9-C4	-5.00	1.34	1.37
36	1	1495	U	N1-C2	-5.00	1.34	1.38

All (5111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-26.30	110.22	126.00
36	5	1152	G	N3-C4-C5	25.75	141.47	128.60
36	5	1152	G	C2-N3-C4	-18.79	102.51	111.90
36	5	929	A	O5'-P-OP2	-14.22	92.90	105.70
36	1	2420	C	O5'-P-OP1	-13.73	93.34	105.70
36	5	2400	G	N1-C6-O6	13.63	128.08	119.90
36	5	218	G	O5'-P-OP2	-13.42	93.62	105.70
36	5	963	G	O5'-P-OP2	-13.37	93.67	105.70
36	5	1152	G	C8-N9-C1'	13.34	144.34	127.00
36	1	2617	U	N1-C2-N3	13.19	122.81	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2283	G	O5'-P-OP2	-12.91	94.08	105.70
36	1	1377	G	C5-C6-O6	-12.71	120.97	128.60
36	1	282	G	O5'-P-OP1	-12.69	94.28	105.70
36	1	895	A	N1-C6-N6	12.69	126.22	118.60
36	1	1175	C	C6-N1-C2	12.60	125.34	120.30
36	1	802	C	O5'-P-OP1	-12.58	94.38	105.70
36	5	2818	U	O5'-P-OP1	-12.52	94.44	105.70
36	5	2857	C	N3-C4-C5	12.51	126.90	121.90
36	1	895	A	C2-N3-C4	-12.48	104.36	110.60
36	1	2617	U	N3-C2-O2	-12.43	113.50	122.20
36	5	1869	C	C6-N1-C2	12.33	125.23	120.30
36	1	1450	G	O5'-P-OP1	-12.32	94.61	105.70
36	1	435	C	C6-N1-C2	12.29	125.22	120.30
36	5	3050	U	C5-C4-O4	12.21	133.22	125.90
36	1	3269	U	O5'-P-OP2	-12.03	94.88	105.70
36	1	2355	G	N1-C6-O6	11.85	127.01	119.90
36	5	222	A	O5'-P-OP2	-11.85	95.03	105.70
36	1	1495	U	C5-C6-N1	-11.83	116.78	122.70
36	5	922	U	N3-C2-O2	-11.82	113.93	122.20
36	5	1316	C	N3-C4-N4	11.81	126.27	118.00
38	8	80	A	C8-N9-C4	-11.74	101.10	105.80
1	2	1200	G	N1-C6-O6	11.74	126.94	119.90
36	5	640	U	N1-C2-O2	-11.73	114.59	122.80
36	1	1896	A	O5'-P-OP1	-11.63	95.24	105.70
36	1	2874	G	C5-C6-N1	-11.62	105.69	111.50
36	1	2617	U	C5-C4-O4	11.59	132.85	125.90
36	5	1152	G	C5-N7-C8	-11.53	98.53	104.30
36	1	942	U	O5'-P-OP2	-11.48	95.36	105.70
38	4	94	C	C6-N1-C2	11.48	124.89	120.30
36	5	1897	G	N1-C6-O6	11.45	126.77	119.90
36	5	2186	U	O5'-P-OP2	-11.42	95.42	105.70
1	6	144	U	N3-C2-O2	-11.40	114.22	122.20
36	5	2117	A	N1-C6-N6	-11.35	111.79	118.60
36	1	3278	C	N1-C2-O2	11.31	125.69	118.90
36	5	1152	G	C4-N9-C1'	-11.30	111.81	126.50
37	7	92	A	N1-C6-N6	11.29	125.37	118.60
1	2	553	G	N1-C6-O6	11.28	126.67	119.90
36	1	3306	U	C5-C4-O4	11.28	132.66	125.90
36	1	3181	C	C5-C4-N4	11.25	128.08	120.20
36	1	1153	A	N1-C6-N6	11.17	125.30	118.60
36	5	3218	A	N1-C6-N6	11.06	125.24	118.60
36	1	304	G	N9-C4-C5	11.04	109.81	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2372	A	C8-N9-C4	-10.99	101.40	105.80
36	1	2281	A	O5'-P-OP2	-10.98	95.82	105.70
36	5	1426	C	C6-N1-C2	10.96	124.68	120.30
36	5	2943	G	C6-C5-N7	-10.92	123.85	130.40
36	1	3306	U	N3-C4-O4	-10.91	111.76	119.40
36	1	2371	G	O5'-P-OP2	-10.85	95.93	105.70
36	1	895	A	C6-C5-N7	-10.75	124.78	132.30
1	6	1773	C	N3-C4-C5	-10.71	117.61	121.90
36	5	2379	U	C5-C6-N1	-10.67	117.36	122.70
36	5	640	U	C5-C4-O4	-10.62	119.53	125.90
36	5	2400	G	C5-C6-O6	-10.59	122.24	128.60
36	1	2617	U	C4-C5-C6	10.58	126.05	119.70
36	5	1316	C	N3-C4-C5	-10.58	117.67	121.90
36	5	2822	U	N3-C4-O4	-10.58	111.99	119.40
36	5	2283	G	N1-C6-O6	10.56	126.24	119.90
36	1	1308	A	C8-N9-C4	-10.54	101.58	105.80
36	1	86	G	O5'-P-OP2	-10.50	96.25	105.70
36	1	2874	G	C2-N3-C4	-10.48	106.66	111.90
36	1	3181	C	N3-C4-N4	-10.46	110.68	118.00
36	1	1308	A	O5'-P-OP2	-10.46	96.29	105.70
36	5	3092	C	N1-C2-O2	10.46	125.17	118.90
36	1	2827	U	N1-C2-N3	10.44	121.17	114.90
36	5	3245	A	C2-N3-C4	-10.44	105.38	110.60
36	5	424	G	C5-C6-O6	-10.43	122.34	128.60
44	17	232	ARG	NE-CZ-NH1	-10.43	115.08	120.30
1	2	623	A	O5'-P-OP1	-10.42	96.32	105.70
36	5	2309	A	N1-C6-N6	-10.42	112.35	118.60
36	1	1377	G	N1-C6-O6	10.39	126.14	119.90
36	1	1367	G	N1-C6-O6	10.38	126.12	119.90
36	1	2819	A	O5'-P-OP2	-10.37	96.37	105.70
36	1	304	G	C4-C5-N7	-10.37	106.65	110.80
36	5	2819	A	O5'-P-OP2	-10.28	96.45	105.70
36	5	683	U	O5'-P-OP2	-10.27	96.46	105.70
36	5	2147	A	N1-C6-N6	10.27	124.76	118.60
36	5	2943	G	N1-C6-O6	10.24	126.05	119.90
36	5	2283	G	C5-C6-O6	-10.21	122.47	128.60
36	5	1445	U	N1-C2-O2	-10.18	115.67	122.80
36	5	2822	U	C5-C4-O4	10.14	131.99	125.90
36	5	1303	A	N1-C6-N6	10.14	124.69	118.60
36	5	922	U	N1-C2-O2	10.14	129.90	122.80
1	6	163	G	N3-C4-N9	-10.09	119.95	126.00
36	1	2714	G	N3-C4-N9	-10.09	119.95	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2714	G	N3-C4-C5	10.07	133.63	128.60
36	1	2868	U	N3-C2-O2	-10.04	115.17	122.20
1	2	334	G	N3-C4-C5	10.03	133.62	128.60
36	1	2920	U	C5-C6-N1	-10.00	117.70	122.70
36	1	2619	G	O5'-P-OP1	-9.98	96.72	105.70
36	5	587	U	C6-N1-C2	9.98	126.99	121.00
36	1	1377	G	C4-C5-N7	9.96	114.78	110.80
36	1	1381	A	N1-C6-N6	9.94	124.56	118.60
36	1	2401	A	N1-C6-N6	9.94	124.56	118.60
36	5	1868	G	C6-C5-N7	-9.93	124.44	130.40
36	1	699	A	O5'-P-OP2	-9.87	96.81	105.70
36	1	611	A	O5'-P-OP2	-9.87	96.82	105.70
36	5	640	U	N3-C4-O4	9.86	126.30	119.40
36	5	1390	A	N1-C6-N6	-9.84	112.70	118.60
36	1	637	C	N1-C2-O2	9.84	124.80	118.90
36	1	2374	C	N3-C2-O2	-9.83	115.02	121.90
36	1	2767	U	O5'-P-OP2	-9.80	96.88	105.70
1	6	426	G	O5'-P-OP2	-9.79	96.89	105.70
36	1	2827	U	C5-C4-O4	9.79	131.77	125.90
36	5	869	G	N1-C6-O6	-9.79	114.03	119.90
36	5	1306	G	C5-C6-O6	-9.78	122.73	128.60
1	2	1560	U	N3-C2-O2	-9.77	115.36	122.20
36	5	636	C	C6-N1-C2	9.73	124.19	120.30
36	5	1142	G	O5'-P-OP2	-9.73	96.94	105.70
36	1	895	A	C4-C5-N7	9.72	115.56	110.70
1	6	352	A	N1-C6-N6	-9.72	112.77	118.60
36	5	861	C	C6-N1-C2	9.71	124.19	120.30
1	6	1137	A	C8-N9-C4	9.71	109.68	105.80
38	8	26	U	N1-C2-O2	9.70	129.59	122.80
36	5	2799	A	O5'-P-OP2	-9.70	96.97	105.70
1	2	334	G	C2-N3-C4	-9.68	107.06	111.90
36	5	2983	C	O5'-P-OP1	-9.68	96.98	105.70
36	5	1437	C	C6-N1-C2	-9.68	116.43	120.30
36	5	2857	C	C6-N1-C2	9.68	124.17	120.30
36	5	834	U	C6-N1-C2	9.68	126.81	121.00
36	5	1390	A	C8-N9-C4	-9.68	101.93	105.80
36	5	1303	A	N9-C4-C5	-9.67	101.93	105.80
1	6	163	G	N3-C4-C5	9.67	133.43	128.60
36	1	1379	G	C2-N3-C4	-9.66	107.07	111.90
36	5	1316	C	N1-C2-O2	-9.65	113.11	118.90
36	1	1403	C	C6-N1-C2	9.63	124.15	120.30
36	1	2606	G	C6-C5-N7	-9.63	124.62	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2363	A	N1-C6-N6	-9.61	112.83	118.60
36	1	914	A	N1-C6-N6	-9.61	112.84	118.60
36	5	2872	A	O5'-P-OP1	9.61	122.22	110.70
36	1	948	C	N1-C2-O2	-9.60	113.14	118.90
36	5	1192	C	N1-C2-O2	9.60	124.66	118.90
36	1	2996	U	C2-N1-C1'	9.60	129.21	117.70
36	1	2942	C	N3-C4-C5	9.59	125.74	121.90
36	5	3050	U	N3-C2-O2	-9.56	115.51	122.20
36	5	3140	G	C4-C5-N7	9.55	114.62	110.80
36	1	1142	G	O5'-P-OP2	-9.52	97.13	105.70
1	2	553	G	C5-C6-O6	-9.51	122.89	128.60
36	5	1793	C	O5'-P-OP1	-9.50	97.15	105.70
36	1	1509	A	C8-N9-C4	9.48	109.59	105.80
36	1	2870	C	C2-N1-C1'	-9.48	108.37	118.80
1	2	73	U	O4'-C1'-N1	9.46	115.77	108.20
36	5	3137	C	C6-N1-C2	9.45	124.08	120.30
36	5	1152	G	N3-C2-N2	-9.45	113.29	119.90
1	2	1745	G	N3-C4-N9	9.44	131.66	126.00
36	5	2726	C	N3-C4-N4	-9.41	111.42	118.00
36	1	1495	U	C2-N1-C1'	-9.40	106.42	117.70
38	8	80	A	N7-C8-N9	9.39	118.50	113.80
36	5	2872	A	O5'-P-OP2	-9.39	97.25	105.70
36	1	406	G	O4'-C1'-N9	9.38	115.71	108.20
36	1	704	U	N3-C4-O4	9.38	125.97	119.40
36	1	282	G	C8-N9-C4	-9.37	102.65	106.40
36	1	2361	A	O5'-P-OP1	-9.36	97.28	105.70
36	1	2865	U	C5-C4-O4	-9.36	120.29	125.90
36	1	1367	G	N9-C4-C5	-9.35	101.66	105.40
36	5	2892	A	N1-C6-N6	9.35	124.21	118.60
36	1	3306	U	N3-C2-O2	-9.34	115.66	122.20
36	5	2245	C	C6-N1-C2	-9.32	116.57	120.30
36	1	2726	C	N3-C4-N4	-9.32	111.48	118.00
36	1	2636	A	C8-N9-C4	-9.31	102.08	105.80
36	1	922	U	N1-C2-O2	9.29	129.30	122.80
36	1	933	A	N1-C2-N3	9.29	133.94	129.30
36	5	2333	C	C6-N1-C2	9.27	124.01	120.30
36	1	188	U	N1-C2-O2	-9.27	116.31	122.80
36	1	2147	A	C8-N9-C4	9.26	109.50	105.80
36	1	1428	A	N1-C6-N6	9.25	124.15	118.60
36	1	3212	C	C6-N1-C2	9.24	124.00	120.30
36	5	1331	U	C5-C6-N1	-9.23	118.08	122.70
36	5	2971	A	C2-N3-C4	9.23	115.22	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2644	C	O5'-P-OP1	-9.22	97.40	105.70
36	1	218	G	O5'-P-OP2	-9.22	97.40	105.70
36	5	2572	C	N1-C2-O2	9.22	124.43	118.90
36	5	2978	U	C5-C6-N1	-9.21	118.09	122.70
36	5	2978	U	C4-C5-C6	9.21	125.23	119.70
36	5	2406	C	C6-N1-C2	9.21	123.98	120.30
36	5	1313	G	O5'-P-OP2	-9.19	97.43	105.70
36	1	2643	A	O5'-P-OP1	-9.19	97.43	105.70
36	5	41	G	C5-C6-O6	-9.19	123.09	128.60
36	1	1100	U	C5-C6-N1	-9.18	118.11	122.70
36	1	346	C	N1-C2-O2	-9.16	113.40	118.90
36	5	2245	C	N3-C4-C5	-9.15	118.24	121.90
36	5	2403	G	O5'-P-OP2	-9.15	97.47	105.70
36	5	2726	C	C5-C4-N4	9.13	126.59	120.20
36	5	1119	C	N3-C4-C5	9.12	125.55	121.90
36	5	776	U	N3-C2-O2	-9.09	115.84	122.20
36	5	2147	A	C5-C6-N6	-9.09	116.43	123.70
36	5	3188	G	N1-C6-O6	-9.08	114.45	119.90
36	1	363	G	N1-C6-O6	9.08	125.35	119.90
36	1	1428	A	C5-C6-N6	-9.08	116.44	123.70
36	5	1303	A	C5-C6-N6	-9.07	116.44	123.70
36	5	1151	U	N1-C2-O2	-9.07	116.45	122.80
36	1	2621	G	N1-C6-O6	9.05	125.33	119.90
36	5	1481	A	C8-N9-C4	-9.04	102.18	105.80
36	5	974	G	N3-C4-C5	-9.04	124.08	128.60
36	5	3154	C	C2-N1-C1'	9.04	128.74	118.80
36	5	1885	U	C5-C6-N1	-9.03	118.19	122.70
36	5	514	G	C5-C6-O6	-9.02	123.19	128.60
36	5	660	A	N1-C6-N6	-9.01	113.19	118.60
36	1	3143	C	N1-C2-O2	-8.99	113.50	118.90
36	1	2885	C	C6-N1-C2	8.99	123.89	120.30
36	1	1192	C	N1-C2-O2	8.98	124.29	118.90
36	1	2643	A	C8-N9-C4	8.98	109.39	105.80
36	1	2812	C	O5'-P-OP2	8.98	121.47	110.70
36	1	363	G	C5-C6-O6	-8.97	123.22	128.60
36	5	1303	A	C8-N9-C4	8.95	109.38	105.80
36	1	1001	G	N9-C4-C5	-8.93	101.83	105.40
36	5	2343	C	C6-N1-C2	8.92	123.87	120.30
36	1	2413	A	C8-N9-C4	8.91	109.37	105.80
36	5	3078	U	N3-C2-O2	-8.90	115.97	122.20
36	1	2617	U	C5-C6-N1	-8.90	118.25	122.70
36	5	2334	U	N1-C2-N3	8.89	120.24	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1507	G	N1-C6-O6	8.89	125.23	119.90
36	1	2410	U	N3-C2-O2	8.88	128.41	122.20
36	1	881	C	N1-C2-O2	8.87	124.22	118.90
36	5	3093	C	N1-C2-O2	-8.87	113.58	118.90
36	1	1367	G	C8-N9-C4	8.87	109.95	106.40
36	5	933	A	C4-C5-C6	8.85	121.42	117.00
38	8	34	U	C5-C6-N1	-8.85	118.28	122.70
36	5	2808	A	C8-N9-C4	8.84	109.34	105.80
36	1	1386	A	N1-C6-N6	8.83	123.90	118.60
36	1	1429	G	N3-C4-N9	8.83	131.30	126.00
36	1	2243	A	O5'-P-OP2	-8.83	97.75	105.70
36	5	1430	U	C6-N1-C2	8.83	126.30	121.00
38	8	26	U	N3-C2-O2	-8.83	116.02	122.20
36	1	1157	G	C8-N9-C4	-8.82	102.87	106.40
36	5	2860	U	O5'-P-OP2	-8.82	97.76	105.70
36	1	304	G	C6-C5-N7	8.82	135.69	130.40
36	5	1137	C	C6-N1-C2	8.81	123.83	120.30
36	1	2811	A	N1-C6-N6	-8.81	113.31	118.60
36	5	3137	C	C5-C6-N1	-8.81	116.60	121.00
36	5	3245	A	N7-C8-N9	8.79	118.19	113.80
36	1	3362	A	O4'-C1'-N9	8.77	115.21	108.20
36	5	2937	G	C8-N9-C4	8.77	109.91	106.40
36	5	504	A	C8-N9-C4	8.76	109.31	105.80
1	6	1773	C	N3-C4-N4	8.76	124.13	118.00
36	1	776	U	C4-C5-C6	8.74	124.95	119.70
36	5	3211	C	C6-N1-C2	8.74	123.80	120.30
36	1	1365	G	N3-C4-C5	-8.74	124.23	128.60
1	2	389	G	C5-C6-O6	-8.73	123.36	128.60
36	5	1390	A	N9-C4-C5	8.73	109.29	105.80
36	5	2866	U	N1-C2-O2	8.73	128.91	122.80
36	1	1001	G	N1-C6-O6	8.72	125.13	119.90
36	5	640	U	N3-C2-O2	8.72	128.30	122.20
37	7	92	A	N9-C4-C5	-8.71	102.32	105.80
36	1	372	A	O5'-P-OP2	-8.70	97.87	105.70
36	5	966	U	N3-C2-O2	-8.68	116.12	122.20
36	5	3154	C	N1-C2-O2	8.68	124.11	118.90
1	2	75	U	N1-C2-O2	8.66	128.86	122.80
73	O7	65	ARG	NE-CZ-NH1	8.66	124.63	120.30
36	1	884	A	N1-C6-N6	8.65	123.79	118.60
36	5	1598	G	N1-C6-O6	-8.63	114.72	119.90
1	6	453	U	C2-N1-C1'	8.63	128.06	117.70
36	1	2944	U	N1-C2-O2	8.62	128.84	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1329	U	C2-N1-C1'	8.62	128.04	117.70
36	1	1179	A	O5'-P-OP1	-8.61	97.95	105.70
36	1	2808	A	N1-C6-N6	8.61	123.76	118.60
36	1	1405	U	C5-C6-N1	-8.61	118.40	122.70
36	1	933	A	C4-C5-C6	8.60	121.30	117.00
36	5	1389	G	C4-C5-N7	8.60	114.24	110.80
38	4	94	C	N3-C4-C5	8.56	125.32	121.90
36	5	1152	G	C5-C6-N1	-8.56	107.22	111.50
36	5	3014	U	C5-C4-O4	-8.56	120.77	125.90
36	1	2884	C	C6-N1-C2	8.56	123.72	120.30
36	5	1149	G	N3-C4-N9	8.54	131.13	126.00
36	5	971	G	C8-N9-C4	8.54	109.82	106.40
36	5	2342	U	C5-C6-N1	-8.54	118.43	122.70
36	5	1151	U	N3-C4-O4	8.54	125.38	119.40
36	5	1110	U	N1-C2-O2	8.54	128.78	122.80
36	5	2704	A	O5'-P-OP1	-8.53	98.02	105.70
36	5	960	U	C5-C4-O4	-8.53	120.78	125.90
36	5	2797	C	N1-C2-O2	-8.53	113.78	118.90
36	5	2848	G	C6-C5-N7	-8.53	125.28	130.40
36	5	2411	U	C5-C6-N1	-8.53	118.44	122.70
36	5	2683	U	C5-C6-N1	8.53	126.96	122.70
36	5	3204	C	C6-N1-C2	8.53	123.71	120.30
1	2	1039	A	O4'-C1'-N9	8.52	115.02	108.20
36	1	3310	A	C8-N9-C4	8.52	109.21	105.80
36	1	2314	U	C5-C4-O4	-8.51	120.79	125.90
36	1	304	G	N1-C6-O6	-8.50	114.80	119.90
1	2	15	U	C6-N1-C2	-8.49	115.90	121.00
36	1	1534	A	N1-C6-N6	8.49	123.70	118.60
36	5	969	C	C5-C6-N1	-8.49	116.76	121.00
36	5	1313	G	C8-N9-C4	8.48	109.79	106.40
36	5	650	C	N1-C2-O2	-8.47	113.81	118.90
36	5	411	U	C5-C6-N1	-8.46	118.47	122.70
36	1	1182	A	C8-N9-C4	8.46	109.19	105.80
36	5	2621	G	N3-C2-N2	-8.46	113.98	119.90
36	5	612	U	O5'-P-OP1	-8.45	98.09	105.70
36	5	2402	A	N9-C4-C5	8.45	109.18	105.80
36	5	2402	A	N1-C6-N6	-8.44	113.53	118.60
1	2	553	G	C6-C5-N7	-8.44	125.34	130.40
36	5	960	U	C6-N1-C1'	-8.44	109.39	121.20
36	5	2383	C	C6-N1-C2	-8.43	116.93	120.30
36	1	2833	A	C8-N9-C4	8.43	109.17	105.80
36	1	1414	G	N1-C6-O6	8.43	124.95	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2726	C	C6-N1-C2	-8.42	116.93	120.30
38	8	96	A	C8-N9-C4	8.42	109.17	105.80
36	1	1076	C	C6-N1-C2	8.41	123.67	120.30
36	5	3137	C	C2-N3-C4	-8.41	115.69	119.90
36	5	2870	C	N3-C4-C5	8.41	125.26	121.90
36	1	1791	C	N1-C2-O2	-8.40	113.86	118.90
36	5	2832	C	C6-N1-C2	8.39	123.66	120.30
36	1	1585	C	C6-N1-C2	8.39	123.66	120.30
36	5	2524	A	O4'-C1'-N9	8.39	114.91	108.20
36	5	3245	A	N1-C2-N3	8.39	133.49	129.30
36	1	2606	G	C4-C5-N7	8.37	114.15	110.80
36	5	2398	A	C5-C6-N1	8.37	121.89	117.70
36	5	1187	C	C6-N1-C2	8.37	123.65	120.30
36	5	3145	C	C6-N1-C2	8.36	123.64	120.30
36	1	1495	U	N1-C2-O2	-8.36	116.95	122.80
36	1	304	G	N3-C2-N2	-8.34	114.06	119.90
36	5	963	G	O5'-P-OP1	8.34	120.71	110.70
36	5	727	G	O5'-P-OP1	-8.34	98.20	105.70
36	5	2983	C	C4-C5-C6	8.33	121.56	117.40
36	1	54	C	C6-N1-C2	8.33	123.63	120.30
36	1	92	G	C5-C6-N1	8.33	115.66	111.50
36	1	1308	A	N7-C8-N9	8.32	117.96	113.80
36	5	217	U	C5-C6-N1	-8.31	118.54	122.70
36	1	2795	U	O5'-P-OP1	-8.31	98.22	105.70
36	1	1367	G	C5-C6-O6	-8.30	123.62	128.60
36	1	1379	G	N1-C2-N3	8.30	128.88	123.90
36	1	2333	C	C5-C6-N1	-8.29	116.85	121.00
37	7	93	C	N3-C2-O2	-8.29	116.09	121.90
36	5	2978	U	N3-C2-O2	-8.28	116.40	122.20
36	5	2354	C	N3-C4-C5	-8.28	118.59	121.90
36	1	2758	A	N7-C8-N9	-8.28	109.66	113.80
36	1	2343	C	C6-N1-C2	8.27	123.61	120.30
36	1	1346	G	O5'-P-OP2	-8.27	98.26	105.70
36	5	1380	G	C8-N9-C4	8.27	109.71	106.40
36	5	2811	A	O5'-P-OP1	-8.27	98.26	105.70
36	1	282	G	N1-C6-O6	-8.27	114.94	119.90
36	5	1389	G	C5-C6-O6	-8.27	123.64	128.60
36	1	1556	C	N3-C2-O2	-8.26	116.12	121.90
1	2	577	G	N1-C6-O6	8.25	124.85	119.90
36	5	1124	U	N3-C4-O4	-8.25	113.62	119.40
36	1	2408	U	O5'-P-OP1	-8.25	98.27	105.70
36	5	1165	A	N1-C6-N6	8.25	123.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2983	C	N3-C4-N4	-8.24	112.23	118.00
36	5	3245	A	C5-N7-C8	-8.24	99.78	103.90
36	1	2867	C	C2-N3-C4	-8.24	115.78	119.90
36	5	1155	C	O5'-P-OP1	-8.24	98.29	105.70
36	1	3278	C	N3-C2-O2	-8.23	116.14	121.90
36	1	2139	A	C5-C6-N1	8.23	121.81	117.70
36	1	3344	A	C5-N7-C8	-8.23	99.78	103.90
36	1	2209	U	C5-C6-N1	8.22	126.81	122.70
1	6	437	A	N1-C6-N6	-8.22	113.67	118.60
36	1	2139	A	C6-N1-C2	-8.22	113.67	118.60
36	5	1592	G	C5-C6-N1	-8.22	107.39	111.50
36	1	1175	C	C5-C6-N1	-8.21	116.89	121.00
36	1	2846	U	N3-C2-O2	-8.21	116.45	122.20
36	5	216	G	N1-C6-O6	8.21	124.83	119.90
36	5	1513	G	C8-N9-C4	-8.20	103.12	106.40
36	5	2852	C	C6-N1-C2	8.21	123.58	120.30
1	2	1212	G	C5-C6-O6	-8.20	123.68	128.60
1	6	1634	C	C6-N1-C2	-8.19	117.03	120.30
36	1	3217	C	C6-N1-C2	-8.16	117.03	120.30
37	3	98	C	N1-C2-O2	-8.16	114.00	118.90
36	5	1924	U	C6-N1-C2	8.16	125.90	121.00
36	1	2802	A	OP2-P-O3'	8.15	123.14	105.20
37	3	88	G	N1-C6-O6	-8.15	115.01	119.90
36	5	895	A	N1-C2-N3	8.15	133.38	129.30
36	1	2886	U	N3-C4-O4	8.15	125.11	119.40
44	17	229	PHE	CB-CG-CD1	8.15	126.51	120.80
36	1	1116	G	N9-C4-C5	8.15	108.66	105.40
36	1	282	G	C5-C6-O6	8.14	133.49	128.60
36	1	35	A	N1-C6-N6	8.14	123.48	118.60
36	5	2764	C	N3-C4-C5	8.13	125.15	121.90
36	5	784	A	N1-C6-N6	8.13	123.48	118.60
36	5	1129	A	O5'-P-OP2	-8.13	98.39	105.70
36	1	639	G	N1-C6-O6	8.11	124.77	119.90
36	5	1897	G	N3-C2-N2	-8.11	114.22	119.90
36	5	3154	C	C5-C6-N1	8.10	125.05	121.00
36	5	2333	C	N3-C4-C5	8.10	125.14	121.90
36	1	1429	G	N3-C4-C5	-8.09	124.56	128.60
1	6	1568	C	P-O3'-C3'	8.09	129.41	119.70
36	5	2797	C	N3-C4-C5	-8.09	118.67	121.90
36	1	2983	C	C5-C4-N4	8.07	125.85	120.20
36	1	2364	G	C4-C5-N7	-8.07	107.57	110.80
36	5	329	U	N3-C2-O2	-8.07	116.55	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	28	C	C6-N1-C2	8.06	123.53	120.30
36	1	901	G	N1-C6-O6	8.06	124.74	119.90
36	5	1316	C	N3-C2-O2	8.06	127.54	121.90
1	2	334	G	C8-N9-C4	8.04	109.62	106.40
36	1	1157	G	N1-C2-N3	8.04	128.73	123.90
36	1	55	G	C8-N9-C4	8.03	109.61	106.40
36	1	2376	G	C8-N9-C4	-8.03	103.19	106.40
38	8	4	C	N3-C2-O2	-8.03	116.28	121.90
36	5	510	G	C5-C6-O6	8.03	133.42	128.60
1	6	1748	G	C8-N9-C4	8.02	109.61	106.40
36	5	2234	G	C5-C6-O6	-8.02	123.79	128.60
1	2	1600	A	C2-N3-C4	-8.02	106.59	110.60
36	1	635	G	C5-C6-O6	-8.02	123.79	128.60
36	5	1119	C	C2-N3-C4	-8.01	115.89	119.90
38	8	33	A	N1-C6-N6	8.01	123.40	118.60
36	1	3311	C	C6-N1-C2	8.00	123.50	120.30
36	1	2827	U	N3-C4-O4	-8.00	113.80	119.40
36	1	3217	C	C2-N1-C1'	8.00	127.60	118.80
1	6	453	U	N3-C2-O2	-8.00	116.60	122.20
44	17	232	ARG	NE-CZ-NH2	8.00	124.30	120.30
36	1	2726	C	N3-C2-O2	-7.99	116.31	121.90
36	5	1151	U	N3-C2-O2	7.99	127.79	122.20
36	5	1907	C	O5'-P-OP2	-7.99	98.51	105.70
36	1	28	C	N3-C4-C5	7.98	125.09	121.90
36	1	2726	C	C5-C4-N4	7.98	125.79	120.20
36	1	2121	G	N3-C2-N2	7.98	125.48	119.90
36	5	2988	C	N3-C4-N4	-7.98	112.42	118.00
36	5	41	G	C4-C5-N7	7.97	113.99	110.80
36	5	1192	C	N3-C2-O2	-7.97	116.32	121.90
36	5	2393	G	C8-N9-C4	7.97	109.59	106.40
36	5	3218	A	C6-C5-N7	-7.96	126.73	132.30
1	6	610	G	C8-N9-C1'	-7.96	116.65	127.00
36	1	54	C	N3-C4-C5	7.96	125.08	121.90
36	1	2623	G	N9-C4-C5	-7.96	102.22	105.40
36	1	836	A	O5'-P-OP2	-7.96	98.54	105.70
36	1	435	C	C5-C6-N1	-7.95	117.02	121.00
36	1	62	A	O5'-P-OP2	-7.94	98.55	105.70
36	1	58	G	N1-C6-O6	7.94	124.66	119.90
36	1	699	A	C2-N3-C4	-7.94	106.63	110.60
36	1	1136	A	N1-C6-N6	7.94	123.36	118.60
36	5	343	U	O5'-P-OP1	-7.93	98.56	105.70
1	2	389	G	N3-C4-N9	7.93	130.76	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1274	C	C6-N1-C2	-7.93	117.13	120.30
36	5	664	U	N3-C4-C5	-7.93	109.84	114.60
36	5	644	G	C4-C5-N7	-7.92	107.63	110.80
1	2	1280	C	N3-C4-C5	-7.91	118.73	121.90
36	5	706	A	C8-N9-C4	7.91	108.97	105.80
36	1	2987	A	C4-C5-C6	7.91	120.95	117.00
36	5	3123	A	C8-N9-C4	7.91	108.96	105.80
36	5	2572	C	C2-N1-C1'	7.91	127.50	118.80
36	5	53	G	C8-N9-C4	7.90	109.56	106.40
36	5	348	A	O5'-P-OP1	-7.90	98.59	105.70
36	5	3154	C	C6-N1-C2	-7.90	117.14	120.30
36	5	2796	G	O5'-P-OP2	-7.89	98.59	105.70
36	1	131	C	C6-N1-C2	-7.89	117.14	120.30
1	6	1110	G	C5-C6-O6	7.89	133.33	128.60
36	5	1905	G	C5-C6-O6	-7.88	123.87	128.60
1	6	383	G	C8-N9-C4	-7.88	103.25	106.40
36	1	1165	A	C8-N9-C4	7.87	108.95	105.80
1	2	1212	G	N1-C6-O6	7.87	124.62	119.90
36	1	3181	C	N3-C2-O2	-7.86	116.39	121.90
36	1	1433	A	O5'-P-OP1	-7.86	98.63	105.70
36	1	1316	C	N1-C2-O2	-7.86	114.19	118.90
36	1	3079	U	C2-N1-C1'	-7.86	108.27	117.70
1	6	558	U	N1-C2-O2	7.86	128.30	122.80
36	5	1837	U	N1-C2-O2	-7.85	117.31	122.80
1	6	1745	G	N9-C4-C5	-7.84	102.26	105.40
1	2	453	U	C2-N1-C1'	7.83	127.10	117.70
1	2	1124	A	O5'-P-OP1	-7.83	98.65	105.70
36	1	1204	A	O5'-P-OP1	-7.83	98.65	105.70
1	2	1096	C	N1-C2-O2	7.83	123.60	118.90
36	5	2823	G	O5'-P-OP2	-7.83	98.66	105.70
36	5	2991	A	N1-C6-N6	-7.83	113.91	118.60
36	5	195	U	O5'-P-OP2	-7.82	98.66	105.70
36	5	1116	G	O5'-P-OP1	-7.82	98.66	105.70
36	5	3140	G	C5-C6-O6	-7.82	123.91	128.60
36	1	1313	G	C5-C6-O6	-7.81	123.91	128.60
36	1	1205	A	C8-N9-C4	7.81	108.92	105.80
1	6	1125	A	C2-N3-C4	-7.81	106.70	110.60
36	5	2849	C	N1-C2-O2	-7.80	114.22	118.90
37	7	87	G	N3-C2-N2	-7.80	114.44	119.90
37	7	84	A	OP1-P-O3'	7.80	122.36	105.20
1	6	435	C	N1-C2-O2	7.80	123.58	118.90
36	1	2283	G	N1-C6-O6	7.80	124.58	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1300	G	N9-C4-C5	-7.79	102.28	105.40
36	1	2815	G	C8-N9-C4	7.79	109.52	106.40
36	5	2411	U	N3-C4-O4	-7.79	113.95	119.40
1	2	1773	C	N1-C2-O2	-7.78	114.23	118.90
36	1	2885	C	C5-C6-N1	-7.78	117.11	121.00
36	1	2836	C	C4-C5-C6	7.78	121.29	117.40
36	1	2756	C	N1-C2-O2	-7.78	114.23	118.90
36	5	410	U	N3-C4-C5	-7.78	109.93	114.60
36	5	3306	U	C5-C4-O4	-7.78	121.23	125.90
1	6	19	A	N1-C6-N6	7.77	123.26	118.60
36	5	2961	G	C5-C6-N1	-7.76	107.62	111.50
1	2	1200	G	C6-C5-N7	-7.76	125.75	130.40
36	1	320	G	C5-C6-O6	-7.75	123.95	128.60
36	1	2661	G	C5-C6-O6	-7.75	123.95	128.60
36	1	69	C	N1-C2-O2	-7.75	114.25	118.90
36	1	1001	G	C5-C6-O6	-7.75	123.95	128.60
36	5	706	A	N1-C6-N6	7.75	123.25	118.60
36	5	1869	C	C5-C6-N1	-7.75	117.12	121.00
36	5	1885	U	C6-N1-C2	7.75	125.65	121.00
36	1	2942	C	C6-N1-C2	7.75	123.40	120.30
36	1	2114	C	O5 ¹ -P-OP2	-7.74	98.74	105.70
36	1	218	G	C5-C6-O6	-7.74	123.96	128.60
36	1	922	U	C5-C4-O4	7.74	130.54	125.90
36	1	282	G	N9-C4-C5	7.73	108.49	105.40
36	1	221	A	O5 ¹ -P-OP2	-7.73	98.74	105.70
36	1	1414	G	C5-C6-O6	-7.73	123.96	128.60
36	1	2416	U	O5 ¹ -P-OP1	-7.73	98.74	105.70
36	1	142	C	C6-N1-C2	-7.73	117.21	120.30
36	5	2957	G	O5 ¹ -P-OP1	-7.72	98.75	105.70
36	5	1389	G	N9-C4-C5	-7.72	102.31	105.40
36	1	1547	G	N7-C8-N9	-7.72	109.24	113.10
38	8	7	U	O5 ¹ -P-OP2	-7.71	98.76	105.70
36	1	2870	C	C6-N1-C1'	7.71	130.05	120.80
36	1	2572	C	N1-C2-O2	7.71	123.53	118.90
36	5	609	G	N3-C2-N2	-7.71	114.50	119.90
36	5	1308	A	N1-C6-N6	-7.71	113.97	118.60
36	1	1882	G	N1-C6-O6	7.71	124.52	119.90
36	5	205	C	N3-C4-C5	7.71	124.98	121.90
36	1	2996	U	C6-N1-C1'	-7.70	110.42	121.20
36	5	2147	A	C6-C5-N7	-7.70	126.91	132.30
36	1	2355	G	C6-C5-N7	-7.69	125.78	130.40
1	6	1121	C	C6-N1-C2	7.69	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1149	G	N3-C4-C5	-7.69	124.75	128.60
36	5	2923	U	O5'-P-OP1	-7.69	98.78	105.70
36	5	1113	G	C2-N3-C4	-7.68	108.06	111.90
36	1	1906	G	N1-C6-O6	7.68	124.51	119.90
1	2	75	U	N3-C2-O2	-7.67	116.83	122.20
37	7	84	A	N1-C6-N6	7.67	123.20	118.60
36	5	2870	C	C2-N1-C1'	-7.67	110.36	118.80
1	6	622	A	O5'-P-OP1	-7.67	98.80	105.70
1	6	1137	A	N7-C8-N9	-7.67	109.97	113.80
36	5	2425	G	N3-C2-N2	-7.67	114.53	119.90
36	5	3140	G	C6-C5-N7	-7.67	125.80	130.40
36	1	1303	A	C8-N9-C4	7.67	108.87	105.80
36	5	3382	U	C5-C6-N1	7.66	126.53	122.70
36	1	2363	A	C5-C6-N6	7.66	129.83	123.70
36	5	2400	G	C8-N9-C4	7.65	109.46	106.40
36	5	776	U	C5-C6-N1	-7.65	118.87	122.70
36	5	1292	C	C6-N1-C2	7.65	123.36	120.30
36	5	3140	G	N1-C6-O6	7.64	124.49	119.90
36	5	940	G	O5'-P-OP1	-7.64	98.82	105.70
1	6	305	C	N1-C2-O2	-7.64	114.31	118.90
36	5	2892	A	C6-C5-N7	-7.64	126.95	132.30
36	1	1138	U	C5-C6-N1	-7.64	118.88	122.70
36	5	2385	G	N1-C6-O6	7.64	124.48	119.90
36	1	922	U	N3-C2-O2	-7.64	116.85	122.20
36	1	2814	G	O5'-P-OP2	7.64	119.86	110.70
36	1	2860	U	N3-C4-O4	-7.63	114.06	119.40
36	1	2869	U	O5'-P-OP1	-7.63	98.83	105.70
36	5	3145	C	C5-C6-N1	-7.63	117.19	121.00
36	5	3245	A	C8-N9-C4	-7.63	102.75	105.80
36	5	942	U	N1-C2-O2	-7.62	117.46	122.80
36	5	3004	C	C6-N1-C2	7.62	123.35	120.30
36	1	798	G	C8-N9-C4	-7.62	103.35	106.40
36	1	1379	G	N1-C2-N2	-7.62	109.34	116.20
36	1	2661	G	N1-C6-O6	7.62	124.47	119.90
36	5	2893	C	N1-C2-O2	-7.62	114.33	118.90
36	1	676	G	C6-C5-N7	-7.62	125.83	130.40
36	1	1094	U	C5-C6-N1	7.62	126.51	122.70
36	1	3217	C	N3-C2-O2	-7.61	116.57	121.90
1	2	864	U	N3-C2-O2	-7.61	116.87	122.20
36	1	2893	C	C2-N3-C4	-7.61	116.09	119.90
36	5	2295	A	C5-C6-N1	7.61	121.51	117.70
1	6	101	U	N3-C2-O2	-7.61	116.88	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2978	U	O4'-C1'-N1	7.61	114.28	108.20
36	5	2309	A	N9-C4-C5	7.61	108.84	105.80
36	5	2820	A	C8-N9-C4	-7.61	102.76	105.80
38	8	84	C	C6-N1-C2	-7.61	117.26	120.30
36	1	1421	G	OP2-P-O3'	7.60	121.93	105.20
36	5	1116	G	N9-C4-C5	7.60	108.44	105.40
36	5	1119	C	C5-C6-N1	-7.60	117.20	121.00
36	1	2963	C	C5-C6-N1	-7.59	117.20	121.00
36	5	1052	U	O5'-P-OP2	-7.59	98.87	105.70
36	1	924	G	C4-C5-N7	7.59	113.84	110.80
36	1	1386	A	C4-C5-C6	7.59	120.79	117.00
36	5	190	U	N3-C2-O2	-7.58	116.89	122.20
36	1	2821	C	C6-N1-C2	-7.58	117.27	120.30
36	1	1313	G	C4-C5-N7	7.58	113.83	110.80
36	1	3362	A	N7-C8-N9	7.58	117.59	113.80
36	1	608	A	N1-C6-N6	7.57	123.14	118.60
36	5	636	C	C5-C6-N1	-7.57	117.21	121.00
36	5	503	C	C6-N1-C2	7.57	123.33	120.30
36	5	2921	U	N1-C2-O2	-7.57	117.50	122.80
36	1	2298	U	C5-C4-O4	7.57	130.44	125.90
36	1	2777	G	C5-C6-O6	7.57	133.14	128.60
36	1	2850	G	C4-C5-N7	7.56	113.83	110.80
36	5	694	C	N3-C2-O2	-7.56	116.61	121.90
1	6	1141	G	C5-C6-O6	-7.56	124.07	128.60
36	5	510	G	N1-C6-O6	-7.56	115.36	119.90
1	6	1177	C	C6-N1-C2	7.55	123.32	120.30
36	5	812	G	C5-N7-C8	7.55	108.08	104.30
36	5	2881	C	C6-N1-C2	7.55	123.32	120.30
36	5	3214	U	N3-C2-O2	-7.55	116.92	122.20
36	5	2943	G	C4-C5-N7	7.55	113.82	110.80
1	2	830	U	N1-C2-O2	7.55	128.08	122.80
36	1	718	G	C4-C5-N7	7.54	113.82	110.80
36	5	2727	A	C8-N9-C4	-7.54	102.78	105.80
36	1	2814	G	O5'-P-OP1	-7.54	98.91	105.70
1	6	1537	C	C6-N1-C2	-7.54	117.28	120.30
36	5	2315	G	O5'-P-OP1	-7.54	98.91	105.70
36	1	1405	U	C2-N3-C4	-7.54	122.48	127.00
36	1	2121	G	N1-C2-N2	-7.54	109.42	116.20
36	5	2305	G	C6-C5-N7	-7.54	125.88	130.40
36	5	2899	C	C2-N3-C4	-7.54	116.13	119.90
1	2	36	C	C6-N1-C2	7.53	123.31	120.30
1	6	1119	G	O5'-P-OP2	-7.53	98.92	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2385	G	N3-C4-C5	7.53	132.37	128.60
36	1	940	G	O5'-P-OP1	-7.53	98.92	105.70
36	1	2342	U	C2-N1-C1'	-7.53	108.67	117.70
36	1	961	C	C2-N3-C4	-7.53	116.14	119.90
36	5	2885	C	C5-C4-N4	-7.53	114.93	120.20
36	1	2860	U	C5-C4-O4	7.52	130.41	125.90
36	5	3218	A	C4-C5-N7	7.52	114.46	110.70
36	1	1433	A	C8-N9-C4	-7.51	102.79	105.80
38	4	136	G	N1-C6-O6	7.51	124.41	119.90
36	5	2400	G	N3-C4-C5	7.51	132.36	128.60
36	1	1386	A	C5-C6-N6	-7.51	117.69	123.70
36	5	1311	G	O5'-P-OP2	-7.51	98.94	105.70
1	2	1762	A	C2-N3-C4	-7.51	106.85	110.60
36	5	2906	C	O5'-P-OP1	7.51	119.71	110.70
36	1	1146	C	N3-C4-C5	7.50	124.90	121.90
36	5	1838	G	N1-C6-O6	7.50	124.40	119.90
36	1	886	C	N1-C2-O2	-7.50	114.40	118.90
36	1	24	G	C8-N9-C1'	-7.50	117.25	127.00
36	5	871	U	C5-C4-O4	7.50	130.40	125.90
36	1	645	A	C6-N1-C2	-7.50	114.10	118.60
36	1	650	C	OP2-P-O3'	7.50	121.69	105.20
36	1	661	G	C8-N9-C4	-7.50	103.40	106.40
36	5	1340	G	C8-N9-C4	7.49	109.40	106.40
36	1	1547	G	C5-N7-C8	7.49	108.05	104.30
36	5	2699	G	N9-C4-C5	-7.49	102.41	105.40
36	1	2634	U	C2-N3-C4	-7.49	122.51	127.00
36	1	59	G	C6-C5-N7	-7.48	125.91	130.40
36	1	2572	C	C2-N1-C1'	7.48	127.02	118.80
36	1	2147	A	N7-C8-N9	-7.48	110.06	113.80
36	1	974	G	N3-C4-N9	7.47	130.48	126.00
36	1	776	U	N1-C2-N3	7.47	119.38	114.90
36	5	3136	G	N1-C2-N3	7.47	128.38	123.90
36	1	2924	U	C6-N1-C2	7.47	125.48	121.00
36	1	2121	G	N3-C4-C5	-7.47	124.87	128.60
36	1	2867	C	C5-C6-N1	-7.47	117.27	121.00
38	4	107	G	N1-C6-O6	-7.46	115.42	119.90
36	1	1606	U	N3-C2-O2	7.46	127.42	122.20
36	5	2309	A	C5-C6-N6	7.46	129.67	123.70
36	1	857	G	C5-C6-N1	-7.46	107.77	111.50
36	5	2412	G	N3-C4-C5	-7.45	124.87	128.60
37	7	88	G	O5'-P-OP1	-7.45	98.99	105.70
36	1	1269	U	C2-N1-C1'	7.45	126.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2868	U	N1-C2-O2	7.44	128.01	122.80
1	6	371	G	C6-C5-N7	-7.44	125.93	130.40
36	1	369	A	C2-N3-C4	7.44	114.32	110.60
1	6	1085	G	N1-C6-O6	-7.44	115.44	119.90
36	5	3185	U	C5-C6-N1	-7.44	118.98	122.70
36	1	801	A	O4'-C1'-N9	-7.44	102.25	108.20
36	1	1741	A	C2-N3-C4	-7.44	106.88	110.60
36	1	2192	C	O5'-P-OP2	-7.44	99.01	105.70
36	1	2402	A	O5'-P-OP2	-7.43	99.02	105.70
36	5	1438	U	N3-C4-O4	7.43	124.60	119.40
36	5	1127	G	O5'-P-OP2	-7.42	99.03	105.70
36	5	2333	C	C5-C6-N1	-7.41	117.30	121.00
36	1	2689	A	N1-C6-N6	-7.41	114.16	118.60
36	1	3025	C	C6-N1-C2	7.41	123.26	120.30
36	5	664	U	C4-C5-C6	7.41	124.14	119.70
36	5	2856	G	N1-C6-O6	7.41	124.34	119.90
37	7	73	C	C6-N1-C2	-7.41	117.34	120.30
36	5	2699	G	C8-N9-C4	7.40	109.36	106.40
36	5	3084	C	C6-N1-C2	7.40	123.26	120.30
36	1	2335	G	N1-C6-O6	-7.40	115.46	119.90
36	1	621	A	C8-N9-C4	-7.40	102.84	105.80
36	1	3208	G	N3-C4-C5	-7.40	124.90	128.60
37	7	101	G	N1-C6-O6	7.40	124.34	119.90
1	2	830	U	N3-C2-O2	-7.39	117.02	122.20
36	1	1192	C	C2-N1-C1'	7.39	126.94	118.80
36	1	2944	U	N3-C4-C5	7.39	119.04	114.60
1	6	144	U	C2-N1-C1'	7.39	126.57	117.70
36	5	995	U	O5'-P-OP1	-7.39	99.05	105.70
36	1	1332	A	O5'-P-OP1	-7.39	99.05	105.70
36	5	2329	C	C2-N3-C4	-7.38	116.21	119.90
36	1	1376	C	C4-C5-C6	7.38	121.09	117.40
36	5	1119	C	C6-N1-C2	7.38	123.25	120.30
36	5	1158	A	C2-N3-C4	-7.38	106.91	110.60
36	1	504	A	C5-C6-N6	-7.37	117.80	123.70
36	1	1386	A	C6-C5-N7	-7.37	127.14	132.30
36	1	3001	C	C6-N1-C2	7.37	123.25	120.30
36	1	2374	C	N1-C2-O2	7.37	123.32	118.90
36	5	1132	C	O5'-P-OP1	-7.37	99.07	105.70
36	1	908	G	O4'-C1'-N9	-7.37	102.31	108.20
36	1	1904	C	C6-N1-C2	-7.37	117.35	120.30
1	6	194	U	C2-N1-C1'	7.37	126.54	117.70
36	5	960	U	C2-N1-C1'	7.36	126.54	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	90	C	C6-N1-C2	-7.36	117.36	120.30
36	5	1004	U	N3-C2-O2	-7.36	117.05	122.20
36	5	644	G	C5-C6-O6	7.36	133.02	128.60
36	5	3271	G	N1-C6-O6	-7.36	115.48	119.90
36	5	644	G	N9-C4-C5	7.35	108.34	105.40
38	4	25	G	C5-C6-O6	7.35	133.01	128.60
36	5	2938	G	C5-C6-N1	7.35	115.17	111.50
36	5	712	G	O5'-P-OP2	-7.35	99.09	105.70
37	3	119	U	C5-C4-O4	7.34	130.31	125.90
36	5	1303	A	C4-C5-N7	7.34	114.37	110.70
1	2	1100	G	C6-C5-N7	-7.34	125.99	130.40
1	6	1200	G	N1-C6-O6	7.34	124.30	119.90
36	5	2941	A	O4'-C1'-N9	-7.34	102.33	108.20
48	m1	112	LEU	CA-CB-CG	7.34	132.18	115.30
36	1	2197	C	C6-N1-C2	7.34	123.23	120.30
36	5	1931	U	C2-N1-C1'	-7.33	108.90	117.70
36	1	267	G	N1-C6-O6	7.33	124.30	119.90
36	1	1199	C	N1-C2-O2	7.32	123.29	118.90
1	6	973	A	O5'-P-OP2	-7.32	99.11	105.70
36	1	3344	A	C2-N3-C4	-7.32	106.94	110.60
38	4	136	G	C6-C5-N7	-7.32	126.01	130.40
1	2	1200	G	C5-C6-O6	-7.32	124.21	128.60
38	8	33	A	N9-C4-C5	-7.31	102.87	105.80
36	1	802	C	O5'-P-OP2	7.31	119.47	110.70
36	1	2811	A	C5-C6-N1	7.31	121.36	117.70
36	5	665	A	C5-C6-N6	-7.31	117.85	123.70
36	5	3362	A	C2-N3-C4	-7.31	106.94	110.60
36	5	3103	A	O5'-P-OP2	-7.31	99.12	105.70
36	1	3214	U	N3-C2-O2	-7.30	117.09	122.20
36	1	1849	C	C5-C4-N4	-7.30	115.09	120.20
36	5	182	U	C5-C6-N1	7.30	126.35	122.70
36	1	2718	U	C5-C6-N1	-7.30	119.05	122.70
1	6	144	U	N1-C2-O2	7.29	127.91	122.80
36	1	2969	A	N1-C6-N6	7.29	122.97	118.60
36	1	883	A	C6-N1-C2	-7.29	114.23	118.60
36	1	1160	C	O5'-P-OP1	-7.29	99.14	105.70
36	1	1495	U	C4-C5-C6	7.29	124.07	119.70
38	4	38	U	N3-C2-O2	-7.29	117.10	122.20
36	5	2777	G	C5-C6-N1	-7.29	107.86	111.50
36	5	1101	G	C8-N9-C4	7.28	109.31	106.40
36	5	2857	C	C2-N3-C4	-7.28	116.26	119.90
36	1	3275	U	C5-C6-N1	7.28	126.34	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	17	C	N1-C2-O2	7.27	123.26	118.90
36	5	1152	G	N9-C4-C5	7.27	108.31	105.40
36	5	938	C	C5-C4-N4	-7.26	115.11	120.20
36	5	2572	C	N3-C2-O2	-7.26	116.81	121.90
36	5	2400	G	C4-C5-N7	7.26	113.70	110.80
36	1	997	A	C8-N9-C4	-7.26	102.90	105.80
36	5	1116	G	N1-C2-N3	7.26	128.25	123.90
36	1	2830	G	N3-C2-N2	-7.25	114.82	119.90
36	5	1888	U	C5-C6-N1	-7.25	119.07	122.70
37	7	92	A	C5-C6-N6	-7.25	117.90	123.70
37	7	101	G	C6-C5-N7	-7.25	126.05	130.40
36	5	2980	U	N3-C2-O2	-7.25	117.13	122.20
36	1	2996	U	N1-C2-O2	7.25	127.87	122.80
1	2	1176	G	C6-C5-N7	-7.24	126.05	130.40
36	1	1434	G	N3-C2-N2	-7.24	114.83	119.90
1	6	116	U	C6-N1-C2	-7.24	116.66	121.00
36	5	2400	G	N9-C4-C5	-7.24	102.50	105.40
1	6	610	G	C8-N9-C4	7.24	109.30	106.40
36	5	2707	C	C6-N1-C2	7.24	123.19	120.30
36	5	2808	A	N9-C4-C5	-7.24	102.91	105.80
36	1	2400	G	C2-N3-C4	-7.24	108.28	111.90
36	5	971	G	N1-C2-N3	7.24	128.24	123.90
36	5	665	A	N1-C6-N6	7.23	122.94	118.60
36	1	432	G	C2-N3-C4	-7.23	108.28	111.90
36	1	2973	G	N1-C6-O6	7.23	124.24	119.90
36	1	3101	G	N1-C6-O6	-7.23	115.56	119.90
36	1	197	G	C5-C6-O6	-7.23	124.26	128.60
36	1	1838	G	N1-C6-O6	7.23	124.24	119.90
36	1	2916	U	N1-C2-N3	-7.23	110.56	114.90
36	5	1403	C	C2-N3-C4	-7.23	116.29	119.90
36	1	2169	G	N1-C6-O6	-7.23	115.56	119.90
36	1	2144	A	C5-C6-N1	7.22	121.31	117.70
36	5	105	C	C6-N1-C2	7.22	123.19	120.30
36	5	834	U	N3-C4-C5	7.22	118.93	114.60
36	1	609	G	C2-N3-C4	7.22	115.51	111.90
36	5	2816	G	C5-C6-O6	-7.22	124.27	128.60
36	5	3055	U	C5-C4-O4	-7.22	121.57	125.90
1	6	1465	C	C6-N1-C2	-7.22	117.41	120.30
38	8	79	A	C8-N9-C4	-7.22	102.91	105.80
36	1	1192	C	C5-C6-N1	7.21	124.61	121.00
36	5	2345	A	C8-N9-C4	7.21	108.69	105.80
37	7	40	C	C6-N1-C2	7.21	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	24	G	N1-C2-N2	-7.21	109.71	116.20
1	6	1141	G	O5'-P-OP1	-7.21	99.21	105.70
36	5	776	U	N1-C2-N3	7.21	119.22	114.90
36	1	1492	G	N3-C2-N2	7.21	124.94	119.90
36	1	1724	U	O5'-P-OP2	-7.21	99.21	105.70
36	1	883	A	C5-C6-N1	7.21	121.30	117.70
1	2	389	G	N1-C6-O6	7.20	124.22	119.90
36	1	1210	U	C5-C6-N1	-7.20	119.10	122.70
37	7	92	A	C6-C5-N7	-7.20	127.26	132.30
36	5	578	A	N1-C6-N6	7.20	122.92	118.60
36	5	3010	U	N3-C2-O2	-7.20	117.16	122.20
36	5	2134	G	C5-C6-O6	7.19	132.92	128.60
41	14	313	LEU	CA-CB-CG	7.19	131.85	115.30
36	1	2621	G	C2-N3-C4	-7.19	108.30	111.90
36	1	3212	C	C5-C6-N1	-7.19	117.40	121.00
36	5	1308	A	OP1-P-OP2	-7.19	108.81	119.60
36	1	3379	C	C6-N1-C2	7.19	123.18	120.30
36	5	516	A	C8-N9-C4	7.19	108.67	105.80
36	5	280	U	O5'-P-OP2	-7.19	99.23	105.70
1	6	1187	U	C5-C6-N1	7.18	126.29	122.70
36	5	937	G	O5'-P-OP1	-7.18	99.24	105.70
36	5	2329	C	C5-C6-N1	-7.18	117.41	121.00
36	5	2899	C	N1-C2-N3	7.18	124.22	119.20
1	6	95	G	N9-C4-C5	7.17	108.27	105.40
36	1	776	U	C5-C6-N1	-7.17	119.11	122.70
37	7	73	C	C5-C6-N1	7.17	124.58	121.00
36	5	2892	A	C5-C6-N6	-7.16	117.97	123.70
36	5	3137	C	N3-C4-C5	7.16	124.77	121.90
36	1	2874	G	N1-C6-O6	7.16	124.20	119.90
36	1	2995	A	C8-N9-C4	7.16	108.66	105.80
36	1	1149	G	N1-C6-O6	7.16	124.19	119.90
36	1	3362	A	C6-C5-N7	-7.16	127.29	132.30
36	5	2621	G	N1-C6-O6	7.16	124.19	119.90
36	1	919	U	O5'-P-OP1	7.16	119.29	110.70
36	1	2901	G	N1-C6-O6	7.16	124.19	119.90
36	5	3140	G	N9-C4-C5	-7.16	102.54	105.40
36	5	3096	C	C6-N1-C2	7.15	123.16	120.30
1	2	1082	C	C2-N1-C1'	7.15	126.67	118.80
36	1	1001	G	C4-C5-N7	7.15	113.66	110.80
36	1	2606	G	N9-C4-C5	-7.15	102.54	105.40
36	1	1403	C	N3-C4-C5	7.15	124.76	121.90
36	1	2634	U	C5-C6-N1	-7.15	119.12	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	100	U	C2-N1-C1'	7.15	126.28	117.70
36	5	1868	G	N1-C6-O6	7.15	124.19	119.90
1	6	116	U	N1-C2-N3	7.14	119.19	114.90
36	5	3374	U	N3-C4-O4	-7.14	114.40	119.40
37	7	14	U	C5-C6-N1	-7.14	119.13	122.70
36	1	1175	C	N3-C4-C5	7.14	124.76	121.90
36	1	2852	C	C6-N1-C2	7.14	123.16	120.30
36	5	2395	G	C5-C6-O6	-7.14	124.32	128.60
1	2	1761	U	P-O3'-C3'	7.14	128.27	119.70
36	1	2333	C	C6-N1-C2	7.14	123.16	120.30
1	2	577	G	C4-C5-N7	7.14	113.66	110.80
36	1	2121	G	N3-C4-N9	7.14	130.28	126.00
36	5	2978	U	O4'-C1'-N1	7.14	113.91	108.20
12	C0	88	PRO	N-CA-CB	7.13	111.86	103.30
36	5	2825	C	C6-N1-C2	7.13	123.15	120.30
36	5	1868	G	C4-C5-N7	7.13	113.65	110.80
36	5	1885	U	O5'-P-OP2	-7.13	99.28	105.70
36	1	895	A	C5-N7-C8	-7.13	100.33	103.90
36	1	1507	G	C6-C5-N7	-7.13	126.12	130.40
36	1	3344	A	N7-C8-N9	7.13	117.36	113.80
36	5	3042	U	C5-C6-N1	-7.13	119.14	122.70
36	5	389	A	O5'-P-OP1	-7.13	99.29	105.70
1	2	16	G	N3-C4-N9	7.12	130.27	126.00
1	6	994	G	C6-C5-N7	-7.12	126.13	130.40
36	5	2880	U	C6-N1-C2	-7.12	116.73	121.00
36	1	2550	U	C5-C4-O4	7.11	130.17	125.90
36	1	3043	C	N3-C4-C5	7.11	124.74	121.90
36	1	1372	C	C5-C6-N1	-7.10	117.45	121.00
36	5	1308	A	C5-C6-N6	7.10	129.38	123.70
36	1	3004	C	O5'-P-OP1	-7.10	99.31	105.70
52	m6	28	LEU	CA-CB-CG	-7.10	98.97	115.30
36	1	659	G	C5-C6-N1	7.10	115.05	111.50
36	5	645	A	N1-C6-N6	-7.10	114.34	118.60
36	5	868	C	C6-N1-C2	7.10	123.14	120.30
36	5	970	A	C8-N9-C4	7.10	108.64	105.80
36	1	1329	U	N3-C2-O2	-7.10	117.23	122.20
36	5	1323	G	N1-C2-N2	-7.10	109.81	116.20
36	1	347	G	C4-C5-N7	7.10	113.64	110.80
36	1	1151	U	C6-N1-C2	-7.09	116.74	121.00
36	5	1852	G	C8-N9-C4	-7.09	103.56	106.40
36	1	2621	G	C5-C6-N1	-7.09	107.95	111.50
36	5	3000	A	C8-N9-C4	7.09	108.64	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1560	U	C5-C4-O4	7.09	130.16	125.90
36	5	812	G	N7-C8-N9	-7.09	109.56	113.10
36	5	382	U	N1-C2-N3	7.09	119.15	114.90
36	1	1790	G	N1-C6-O6	7.09	124.15	119.90
36	1	29	C	C5-C4-N4	-7.08	115.24	120.20
1	6	337	G	C4-N9-C1'	7.08	135.71	126.50
36	5	2152	A	N1-C6-N6	7.08	122.85	118.60
36	5	1879	A	C8-N9-C4	-7.08	102.97	105.80
36	1	1381	A	O5'-P-OP2	7.08	119.19	110.70
36	1	1547	G	C6-C5-N7	7.07	134.64	130.40
1	6	13	C	C6-N1-C2	-7.07	117.47	120.30
36	1	1116	G	C8-N9-C4	-7.07	103.57	106.40
36	1	2649	A	C5-C6-N1	7.07	121.24	117.70
36	5	2192	C	N3-C2-O2	-7.07	116.95	121.90
36	1	970	A	C6-N1-C2	-7.07	114.36	118.60
36	1	3278	C	C2-N1-C1'	7.07	126.57	118.80
1	2	389	G	C6-C5-N7	-7.06	126.16	130.40
36	5	3177	G	C8-N9-C4	7.06	109.22	106.40
36	5	3209	A	N7-C8-N9	7.06	117.33	113.80
36	5	504	A	N9-C4-C5	-7.06	102.98	105.80
36	1	1906	G	C5-C6-O6	-7.06	124.36	128.60
36	1	1846	C	N1-C2-O2	-7.06	114.67	118.90
36	5	2272	G	O4'-C1'-N9	7.05	113.84	108.20
36	5	41	G	N1-C6-O6	7.05	124.13	119.90
36	1	2886	U	C5-C4-O4	-7.05	121.67	125.90
36	1	52	A	O5'-P-OP2	-7.05	99.36	105.70
36	1	951	A	N1-C6-N6	7.05	122.83	118.60
36	1	968	G	C5-C6-O6	-7.05	124.37	128.60
36	1	2400	G	N1-C6-O6	7.04	124.13	119.90
37	7	44	C	N3-C4-C5	-7.04	119.08	121.90
1	2	1600	A	C5-C6-N1	-7.04	114.18	117.70
36	5	673	U	C5-C6-N1	-7.04	119.18	122.70
36	1	948	C	N3-C2-O2	7.04	126.83	121.90
36	5	2805	G	N1-C6-O6	7.04	124.12	119.90
38	8	13	A	O5'-P-OP2	-7.04	99.37	105.70
36	5	2993	G	C4-C5-N7	7.04	113.61	110.80
36	1	2889	C	N3-C2-O2	-7.04	116.98	121.90
36	5	2643	A	C8-N9-C4	7.04	108.61	105.80
36	1	292	U	C5-C6-N1	-7.03	119.18	122.70
36	5	2857	C	C5-C4-N4	-7.03	115.28	120.20
36	1	1795	U	O5'-P-OP1	-7.03	99.38	105.70
36	1	3310	A	N9-C4-C5	-7.03	102.99	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2192	C	N1-C2-O2	7.03	123.11	118.90
36	5	3182	G	O5'-P-OP2	7.03	119.13	110.70
36	1	2406	C	N3-C4-N4	7.02	122.92	118.00
36	1	2623	G	C8-N9-C4	7.02	109.21	106.40
1	2	499	U	P-O3'-C3'	7.02	128.13	119.70
36	5	3234	A	C8-N9-C4	7.02	108.61	105.80
37	7	40	C	N3-C4-C5	7.02	124.71	121.90
36	1	1834	U	N3-C4-C5	-7.02	110.39	114.60
1	6	19	A	C8-N9-C4	7.02	108.61	105.80
36	5	2376	G	N3-C2-N2	-7.02	114.99	119.90
36	1	286	U	N3-C2-O2	-7.02	117.29	122.20
36	1	972	A	C8-N9-C4	7.02	108.61	105.80
36	5	2840	C	C6-N1-C2	7.02	123.11	120.30
18	C6	40	GLU	C-N-CD	-7.01	105.17	120.60
36	1	2758	A	N1-C6-N6	-7.01	114.39	118.60
36	1	66	A	O5'-P-OP1	-7.01	99.39	105.70
36	1	695	C	N3-C4-N4	-7.01	113.09	118.00
36	1	304	G	C5-C6-O6	7.01	132.81	128.60
36	5	1909	A	C8-N9-C4	7.01	108.60	105.80
36	5	2134	G	N1-C6-O6	-7.01	115.69	119.90
36	5	906	A	N3-C4-C5	-7.01	121.89	126.80
36	5	2183	A	N1-C6-N6	7.01	122.80	118.60
36	1	2400	G	C6-C5-N7	-7.00	126.20	130.40
1	6	1700	C	C2-N1-C1'	7.00	126.50	118.80
36	1	659	G	C4-C5-N7	7.00	113.60	110.80
36	5	2871	G	O5'-P-OP2	-7.00	99.40	105.70
36	5	1878	G	C4-N9-C1'	6.99	135.59	126.50
36	1	934	G	C8-N9-C1'	-6.99	117.91	127.00
36	1	1376	C	C5-C6-N1	-6.99	117.50	121.00
36	5	3000	A	N1-C6-N6	6.99	122.80	118.60
36	5	3218	A	C5-N7-C8	-6.99	100.40	103.90
36	1	2305	G	C6-C5-N7	-6.99	126.21	130.40
36	5	2942	C	N3-C4-N4	6.99	122.89	118.00
1	6	609	U	C5-C6-N1	-6.99	119.21	122.70
36	5	1380	G	N9-C4-C5	-6.99	102.60	105.40
36	5	1837	U	N3-C4-O4	6.99	124.29	119.40
36	5	1198	C	C5-C4-N4	6.98	125.09	120.20
36	1	637	C	N3-C4-N4	-6.98	113.11	118.00
1	6	1111	G	C4-C5-N7	6.98	113.59	110.80
36	5	1121	U	N1-C2-N3	6.98	119.09	114.90
36	5	2372	A	P-O3'-C3'	6.98	128.08	119.70
36	5	1848	G	C5-C6-O6	-6.98	124.41	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2409	G	N9-C4-C5	6.98	108.19	105.40
36	1	97	U	OP1-P-OP2	-6.97	109.14	119.60
36	1	2376	G	N9-C4-C5	6.97	108.19	105.40
36	5	2905	U	C5-C6-N1	-6.97	119.21	122.70
36	5	906	A	C6-N1-C2	-6.97	114.42	118.60
36	1	938	C	C5-C4-N4	-6.97	115.32	120.20
36	1	2314	U	N1-C2-N3	-6.97	110.72	114.90
1	6	619	A	N1-C6-N6	-6.97	114.42	118.60
36	5	648	C	O5'-P-OP1	-6.97	99.43	105.70
36	5	2953	U	N3-C4-O4	6.97	124.28	119.40
36	5	2805	G	C5-C6-O6	-6.97	124.42	128.60
36	1	984	G	N3-C4-N9	6.97	130.18	126.00
36	1	1124	U	N3-C2-O2	-6.97	117.32	122.20
36	5	94	G	N1-C6-O6	-6.97	115.72	119.90
36	5	1450	G	C5-C6-O6	-6.97	124.42	128.60
36	5	1187	C	C5-C6-N1	-6.96	117.52	121.00
36	5	1884	A	C2-N3-C4	-6.96	107.12	110.60
36	1	833	G	C8-N9-C4	6.96	109.19	106.40
36	5	1403	C	C6-N1-C2	6.96	123.08	120.30
1	6	1700	C	N1-C2-O2	6.96	123.08	118.90
36	5	1158	A	C4-C5-C6	6.96	120.48	117.00
36	5	1841	A	O5'-P-OP1	-6.96	99.44	105.70
36	1	2821	C	N3-C2-O2	-6.96	117.03	121.90
36	1	957	C	N1-C2-O2	-6.96	114.73	118.90
36	5	2748	A	C8-N9-C4	6.96	108.58	105.80
36	5	587	U	N1-C2-N3	-6.95	110.73	114.90
36	5	2295	A	C6-N1-C2	-6.95	114.43	118.60
36	5	3245	A	C5-C6-N1	-6.95	114.22	117.70
36	1	718	G	C5-N7-C8	-6.95	100.82	104.30
36	1	1320	C	N3-C4-C5	-6.95	119.12	121.90
36	1	3177	G	C5-C6-O6	-6.95	124.43	128.60
36	5	655	C	C6-N1-C2	-6.95	117.52	120.30
36	1	1105	A	C8-N9-C4	6.95	108.58	105.80
37	7	84	A	C5-C6-N6	-6.95	118.14	123.70
36	1	586	C	C6-N1-C2	6.94	123.08	120.30
36	1	919	U	N3-C4-O4	-6.94	114.54	119.40
1	6	1641	C	N1-C2-O2	-6.94	114.73	118.90
36	5	1403	C	C5-C6-N1	-6.94	117.53	121.00
36	5	1305	U	N3-C4-O4	6.94	124.26	119.40
36	1	646	A	C4-C5-C6	6.94	120.47	117.00
36	5	953	G	C4-C5-N7	6.94	113.58	110.80
36	1	884	A	C6-C5-N7	-6.94	127.44	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2342	U	C5-C6-N1	-6.94	119.23	122.70
36	5	2937	G	N7-C8-N9	-6.94	109.63	113.10
36	5	2425	G	N3-C4-N9	-6.94	121.84	126.00
36	1	504	A	N1-C6-N6	6.93	122.76	118.60
36	5	1869	C	N3-C4-C5	6.93	124.67	121.90
36	1	307	A	O5'-P-OP2	-6.93	99.46	105.70
36	1	335	G	C5-C6-N1	6.93	114.96	111.50
36	1	363	G	C6-C5-N7	-6.93	126.24	130.40
36	1	1607	U	P-O3'-C3'	6.93	128.01	119.70
36	1	1489	A	N1-C6-N6	6.92	122.75	118.60
36	1	2607	G	N1-C6-O6	-6.92	115.75	119.90
36	5	2199	G	C5-N7-C8	-6.92	100.84	104.30
1	6	158	U	P-O3'-C3'	6.92	128.00	119.70
36	1	58	G	C5-C6-O6	-6.92	124.45	128.60
1	2	704	C	C2-N1-C1'	6.92	126.41	118.80
36	5	2333	C	C2-N3-C4	-6.92	116.44	119.90
36	1	335	G	C5-C6-O6	-6.91	124.45	128.60
36	1	2823	G	N3-C4-C5	-6.91	125.14	128.60
36	1	1124	U	N3-C4-O4	-6.91	114.56	119.40
36	5	2726	C	N3-C2-O2	-6.91	117.06	121.90
36	1	513	G	O5'-P-OP1	-6.91	99.48	105.70
36	1	2636	A	N9-C4-C5	6.91	108.56	105.80
36	1	1136	A	C5-C6-N6	-6.91	118.18	123.70
36	1	790	U	N1-C2-N3	6.90	119.04	114.90
36	1	1509	A	C2-N3-C4	-6.90	107.15	110.60
36	1	2376	G	N1-C6-O6	-6.90	115.76	119.90
36	5	434	U	O5'-P-OP2	-6.90	99.49	105.70
36	5	2379	U	C2-N3-C4	-6.90	122.86	127.00
36	1	432	G	C5-C6-N1	-6.90	108.05	111.50
1	2	942	G	N1-C6-O6	-6.89	115.77	119.90
36	1	2423	U	N3-C2-O2	6.89	127.03	122.20
36	1	2758	A	C5-N7-C8	6.89	107.35	103.90
36	5	2197	C	C6-N1-C2	6.89	123.06	120.30
36	1	2874	G	C6-C5-N7	-6.89	126.27	130.40
1	6	610	G	N9-C4-C5	-6.89	102.64	105.40
36	1	2606	G	N3-C4-N9	6.88	130.13	126.00
36	5	2418	G	C5-C6-O6	-6.88	124.47	128.60
36	1	1118	C	C6-N1-C2	-6.88	117.55	120.30
36	1	410	U	C6-N1-C2	-6.88	116.87	121.00
1	6	1745	G	N3-C4-N9	6.88	130.13	126.00
36	1	880	G	N1-C6-O6	-6.88	115.77	119.90
36	1	1304	A	C5-C6-N6	-6.88	118.20	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	38	U	C6-N1-C2	6.88	125.13	121.00
36	5	2376	G	C5-C6-O6	-6.88	124.47	128.60
36	1	1414	G	C6-C5-N7	-6.87	126.28	130.40
36	1	3209	A	C5-C6-N1	-6.87	114.26	117.70
36	5	1307	G	P-O3'-C3'	6.87	127.95	119.70
36	5	947	G	N1-C6-O6	-6.87	115.78	119.90
36	5	3054	U	N3-C4-C5	-6.87	110.48	114.60
36	5	1828	A	N1-C6-N6	6.87	122.72	118.60
36	1	111	C	C6-N1-C2	6.87	123.05	120.30
36	1	1434	G	C5-C6-O6	-6.87	124.48	128.60
1	2	408	C	O5'-P-OP2	-6.86	99.52	105.70
1	6	1600	A	O4'-C1'-N9	6.86	113.69	108.20
36	5	2409	G	O5'-P-OP2	-6.86	99.52	105.70
36	5	2727	A	N9-C4-C5	6.86	108.55	105.80
36	5	2989	U	O5'-P-OP2	6.86	118.94	110.70
36	5	39	A	C2-N3-C4	-6.86	107.17	110.60
36	5	2512	C	N1-C2-O2	-6.86	114.78	118.90
36	5	2137	U	C6-N1-C2	6.86	125.11	121.00
36	1	2279	A	N9-C4-C5	-6.86	103.06	105.80
36	1	2409	G	N3-C4-N9	6.86	130.11	126.00
36	5	1628	C	C6-N1-C2	-6.86	117.56	120.30
36	5	3227	A	N1-C6-N6	6.86	122.71	118.60
36	1	2368	A	N1-C2-N3	6.85	132.73	129.30
36	5	2874	G	C5-C6-O6	6.85	132.71	128.60
36	5	2147	A	C4-C5-N7	6.85	114.12	110.70
36	1	65	A	P-O3'-C3'	6.84	127.91	119.70
36	1	1377	G	N9-C4-C5	-6.84	102.66	105.40
36	1	2404	A	N1-C6-N6	-6.84	114.50	118.60
36	5	3382	U	C2-N1-C1'	6.84	125.91	117.70
36	5	1374	G	O5'-P-OP2	-6.84	99.54	105.70
36	5	2350	C	OP1-P-OP2	-6.84	109.34	119.60
36	1	1116	G	N3-C4-C5	-6.84	125.18	128.60
36	1	1405	U	O5'-P-OP2	-6.84	99.55	105.70
36	5	2137	U	N3-C4-C5	6.83	118.70	114.60
1	2	1176	G	N1-C6-O6	6.83	124.00	119.90
36	1	1295	G	N1-C6-O6	-6.83	115.80	119.90
36	1	2827	U	C5-C6-N1	-6.83	119.28	122.70
36	1	2983	C	C5-C6-N1	-6.83	117.58	121.00
36	5	205	C	O5'-P-OP1	-6.83	99.55	105.70
36	1	1820	U	P-O3'-C3'	6.83	127.89	119.70
36	5	64	G	C8-N9-C4	-6.83	103.67	106.40
36	5	197	G	C6-C5-N7	-6.83	126.30	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1158	A	N1-C2-N3	6.83	132.71	129.30
25	d3	132	LEU	CA-CB-CG	-6.83	99.60	115.30
36	1	2679	A	O4'-C1'-N9	6.83	113.66	108.20
36	5	1844	C	C6-N1-C2	-6.83	117.57	120.30
36	5	2893	C	N3-C4-N4	6.83	122.78	118.00
1	6	453	U	N1-C2-O2	6.82	127.58	122.80
36	5	1454	A	N1-C6-N6	6.82	122.69	118.60
36	5	889	U	C5-C6-N1	-6.82	119.29	122.70
36	5	2871	G	N3-C4-C5	-6.82	125.19	128.60
1	2	1456	C	O4'-C1'-N1	6.82	113.66	108.20
36	5	2860	U	C5-C4-O4	6.82	129.99	125.90
1	2	321	C	C6-N1-C2	-6.82	117.57	120.30
36	1	1458	U	C5-C6-N1	-6.81	119.29	122.70
36	5	585	A	O5'-P-OP2	-6.81	99.57	105.70
36	5	907	G	N9-C4-C5	-6.81	102.67	105.40
36	5	2772	C	P-O3'-C3'	6.81	127.87	119.70
36	1	857	G	N1-C6-O6	6.81	123.99	119.90
36	1	86	G	O5'-P-OP1	6.81	118.87	110.70
38	4	79	A	C8-N9-C4	-6.81	103.08	105.80
36	5	504	A	N1-C6-N6	6.81	122.69	118.60
36	5	888	A	N1-C6-N6	6.81	122.69	118.60
36	5	2856	G	C5-C6-O6	-6.81	124.51	128.60
36	1	614	C	N3-C4-C5	6.81	124.62	121.90
36	1	637	C	N3-C4-C5	6.81	124.62	121.90
36	1	937	G	O5'-P-OP2	-6.81	99.57	105.70
36	1	1874	A	O5'-P-OP1	-6.81	99.57	105.70
36	5	411	U	C6-N1-C2	6.81	125.08	121.00
36	5	776	U	C5-C4-O4	6.81	129.99	125.90
36	1	905	U	O5'-P-OP2	-6.81	99.57	105.70
36	1	353	G	N1-C6-O6	6.80	123.98	119.90
36	5	2817	A	C5-C6-N6	-6.80	118.26	123.70
36	1	1189	C	N1-C2-O2	-6.80	114.82	118.90
36	1	2884	C	N3-C4-C5	6.80	124.62	121.90
36	5	1116	G	C4-C5-N7	-6.80	108.08	110.80
36	1	933	A	C6-N1-C2	-6.80	114.52	118.60
36	1	1094	U	C6-N1-C2	-6.80	116.92	121.00
36	5	3143	C	N3-C4-C5	-6.80	119.18	121.90
36	1	3096	C	N3-C4-C5	-6.80	119.18	121.90
36	1	3344	A	C4-C5-N7	6.80	114.10	110.70
36	5	2425	G	N1-C2-N2	6.80	122.32	116.20
36	1	1411	C	C5-C6-N1	-6.79	117.60	121.00
36	1	1547	G	C4-C5-N7	-6.79	108.08	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2816	G	N1-C6-O6	6.79	123.98	119.90
41	14	276	LEU	CA-CB-CG	6.79	130.93	115.30
36	5	2191	U	N3-C2-O2	-6.79	117.45	122.20
36	5	329	U	N1-C2-O2	6.79	127.55	122.80
38	4	136	G	C5-C6-O6	-6.79	124.53	128.60
36	1	2760	C	N1-C2-O2	-6.78	114.83	118.90
36	5	3177	G	N9-C4-C5	-6.78	102.69	105.40
38	8	51	G	C8-N9-C4	-6.78	103.69	106.40
37	3	75	G	O5'-P-OP1	-6.78	99.60	105.70
36	5	2980	U	N1-C2-N3	6.78	118.97	114.90
36	5	3204	C	C5-C6-N1	-6.78	117.61	121.00
36	1	394	G	N9-C4-C5	6.78	108.11	105.40
36	1	3209	A	N1-C6-N6	6.78	122.67	118.60
36	5	1803	C	C6-N1-C2	6.78	123.01	120.30
36	1	2979	U	C5-C6-N1	-6.77	119.31	122.70
36	5	2884	C	N3-C4-N4	6.77	122.74	118.00
36	1	2964	G	O5'-P-OP2	-6.77	99.60	105.70
36	5	1417	G	N3-C4-C5	-6.77	125.22	128.60
36	5	806	A	N1-C6-N6	-6.77	114.54	118.60
36	5	2913	C	N3-C4-C5	-6.77	119.19	121.90
36	1	1176	C	C5-C4-N4	-6.77	115.46	120.20
36	1	699	A	O5'-P-OP1	6.76	118.82	110.70
36	1	1741	A	N1-C2-N3	6.76	132.68	129.30
36	1	3201	C	N3-C4-C5	-6.76	119.19	121.90
36	5	2392	C	C6-N1-C2	6.76	123.00	120.30
36	1	3209	A	O5'-P-OP1	-6.76	99.61	105.70
36	1	2636	A	N1-C6-N6	-6.76	114.55	118.60
38	4	44	A	O5'-P-OP2	6.76	118.81	110.70
36	1	1898	G	N1-C6-O6	6.76	123.95	119.90
36	1	1153	A	N9-C4-C5	-6.75	103.10	105.80
36	5	2345	A	N1-C6-N6	6.75	122.65	118.60
36	1	2661	G	C6-C5-N7	-6.75	126.35	130.40
36	5	2948	C	C6-N1-C2	6.75	123.00	120.30
36	1	2864	A	O5'-P-OP1	-6.75	99.62	105.70
36	1	695	C	N3-C4-C5	6.75	124.60	121.90
36	5	421	G	OP1-P-O3'	6.75	120.05	105.20
36	5	1549	U	C5-C6-N1	-6.75	119.33	122.70
1	2	75	U	C2-N1-C1'	6.75	125.80	117.70
1	2	1560	U	N3-C4-O4	-6.75	114.68	119.40
36	1	2624	G	N1-C6-O6	6.75	123.95	119.90
36	5	1149	G	C5-C6-O6	-6.75	124.55	128.60
36	5	3362	A	N1-C2-N3	6.75	132.67	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	994	G	N1-C2-N2	-6.74	110.13	116.20
36	5	607	A	N1-C6-N6	-6.74	114.56	118.60
36	5	1437	C	C2-N1-C1'	6.74	126.22	118.80
36	5	1116	G	OP2-P-O3'	6.74	120.03	105.20
36	1	1053	A	C8-N9-C4	6.74	108.50	105.80
36	5	1208	U	N3-C2-O2	-6.74	117.48	122.20
36	1	2639	G	C6-C5-N7	-6.74	126.36	130.40
36	1	2643	A	O5'-P-OP2	6.74	118.78	110.70
36	5	2385	G	C2-N3-C4	-6.74	108.53	111.90
36	5	2409	G	C8-N9-C4	-6.74	103.71	106.40
36	5	2822	U	N1-C2-O2	6.74	127.51	122.80
36	5	2994	A	C6-N1-C2	-6.74	114.56	118.60
36	1	2873	U	N1-C2-O2	-6.73	118.09	122.80
36	5	1710	C	C6-N1-C2	6.73	122.99	120.30
1	2	16	G	N3-C4-C5	-6.73	125.23	128.60
36	1	3143	C	N3-C2-O2	6.73	126.61	121.90
36	5	2369	G	C8-N9-C4	6.73	109.09	106.40
38	8	52	A	O5'-P-OP1	-6.73	99.64	105.70
36	5	2136	C	C5-C6-N1	-6.73	117.64	121.00
1	2	453	U	N3-C2-O2	-6.73	117.49	122.20
37	3	86	U	N3-C4-O4	-6.73	114.69	119.40
36	5	784	A	C5-C6-N6	-6.73	118.32	123.70
36	5	2977	G	C5-C6-N1	6.73	114.86	111.50
36	1	1344	G	N1-C6-O6	6.73	123.94	119.90
36	5	1476	G	N1-C6-O6	-6.73	115.86	119.90
36	5	3092	C	N3-C2-O2	-6.73	117.19	121.90
36	1	2917	G	C5-C6-O6	-6.72	124.56	128.60
36	1	637	C	P-O3'-C3'	6.72	127.77	119.70
1	6	163	G	C2-N3-C4	-6.72	108.54	111.90
36	1	1152	G	O4'-C1'-N9	6.72	113.58	108.20
36	1	1492	G	N3-C4-N9	6.72	130.03	126.00
41	L4	182	LEU	CA-CB-CG	6.72	130.75	115.30
1	2	1280	C	C6-N1-C2	-6.71	117.61	120.30
36	1	344	A	N1-C6-N6	-6.71	114.57	118.60
36	5	3287	U	N1-C2-O2	6.71	127.50	122.80
36	5	718	G	C4-N9-C1'	6.71	135.23	126.50
36	1	1149	G	C4-C5-C6	6.71	122.83	118.80
36	1	2847	A	N1-C6-N6	6.71	122.63	118.60
36	1	640	U	N3-C4-O4	6.71	124.09	119.40
36	5	3197	G	N3-C4-N9	-6.70	121.98	126.00
36	1	2679	A	C2-N3-C4	-6.70	107.25	110.60
36	5	2342	U	C2-N3-C4	-6.70	122.98	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1745	G	C4-C5-N7	6.70	113.48	110.80
36	5	1875	G	C8-N9-C4	6.70	109.08	106.40
36	5	2345	A	C5-C6-N6	-6.70	118.34	123.70
36	5	2944	U	N1-C2-O2	6.70	127.49	122.80
36	1	3361	G	N3-C4-N9	6.70	130.02	126.00
38	4	84	C	C6-N1-C2	6.70	122.98	120.30
36	5	43	A	N1-C6-N6	6.70	122.62	118.60
36	5	1885	U	C2-N1-C1'	-6.70	109.66	117.70
36	1	2889	C	N1-C2-O2	6.70	122.92	118.90
36	5	1481	A	N7-C8-N9	6.69	117.15	113.80
36	1	621	A	N7-C8-N9	6.69	117.15	113.80
36	1	810	A	C5-C6-N1	6.69	121.05	117.70
36	5	424	G	C5-C6-N1	6.69	114.85	111.50
36	5	609	G	N1-C2-N2	6.69	122.22	116.20
36	5	2404	A	C8-N9-C4	6.69	108.47	105.80
1	2	323	A	C8-N9-C4	-6.68	103.13	105.80
1	2	507	U	N1-C2-O2	6.68	127.48	122.80
36	5	1924	U	N3-C2-O2	6.68	126.88	122.20
36	5	3351	U	N3-C2-O2	-6.68	117.52	122.20
36	1	212	G	N3-C4-N9	6.68	130.01	126.00
36	1	2554	A	C8-N9-C4	6.68	108.47	105.80
36	1	2688	U	N1-C2-N3	-6.68	110.89	114.90
36	5	2392	C	C5-C6-N1	-6.68	117.66	121.00
36	1	1304	A	N1-C6-N6	6.68	122.61	118.60
36	1	1515	A	N1-C6-N6	6.68	122.61	118.60
36	1	2313	A	O5'-P-OP1	-6.68	99.69	105.70
36	5	1589	A	C5-C6-N6	-6.68	118.36	123.70
36	1	801	A	N9-C4-C5	-6.68	103.13	105.80
36	5	1152	G	C4-C5-N7	6.68	113.47	110.80
36	5	2939	G	C6-C5-N7	6.68	134.41	130.40
1	2	1112	G	C6-C5-N7	-6.67	126.39	130.40
36	1	1279	C	C6-N1-C2	-6.67	117.63	120.30
36	1	585	A	O5'-P-OP2	-6.67	99.69	105.70
36	1	3107	U	C5-C6-N1	-6.67	119.36	122.70
36	5	2710	C	N3-C2-O2	6.67	126.57	121.90
36	5	2823	G	OP1-P-OP2	6.67	129.61	119.60
36	5	2939	G	C4-C5-N7	-6.67	108.13	110.80
1	2	577	G	C5-C6-O6	-6.67	124.60	128.60
36	5	2889	C	N3-C2-O2	-6.67	117.23	121.90
36	1	900	G	C4-C5-N7	-6.67	108.13	110.80
36	5	2950	G	O4'-C1'-N9	6.67	113.53	108.20
36	1	641	C	N1-C2-O2	-6.67	114.90	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	3	95	A	N1-C6-N6	6.67	122.60	118.60
36	5	216	G	C6-C5-N7	-6.67	126.40	130.40
36	5	2917	G	C6-C5-N7	-6.66	126.40	130.40
36	5	3388	C	C5-C6-N1	-6.66	117.67	121.00
1	2	1761	U	N1-C2-N3	6.66	118.90	114.90
36	1	2130	G	N9-C4-C5	6.66	108.06	105.40
36	1	1119	C	C6-N1-C2	6.66	122.97	120.30
36	1	1307	G	P-O3'-C3'	6.66	127.69	119.70
36	5	2944	U	N3-C2-O2	-6.66	117.54	122.20
1	2	1241	G	C4-C5-N7	6.66	113.46	110.80
36	1	106	A	C8-N9-C4	6.66	108.46	105.80
36	1	426	G	N3-C4-N9	6.66	130.00	126.00
36	5	2989	U	O5'-P-OP1	-6.66	99.71	105.70
36	1	205	C	C6-N1-C2	6.66	122.96	120.30
36	1	1445	U	C5-C6-N1	-6.66	119.37	122.70
37	3	88	G	C5-C6-O6	6.66	132.59	128.60
36	5	1407	A	C8-N9-C4	6.66	108.46	105.80
36	5	2307	G	N3-C2-N2	6.66	124.56	119.90
36	5	2383	C	N1-C2-O2	-6.66	114.91	118.90
36	5	2421	U	N3-C2-O2	-6.66	117.54	122.20
36	5	2718	U	O5'-P-OP2	-6.66	99.71	105.70
1	6	638	U	N3-C2-O2	-6.65	117.54	122.20
35	SM	167	PRO	N-CA-CB	6.65	111.28	103.30
36	1	35	A	C4-C5-N7	6.65	114.02	110.70
36	5	996	A	C2-N3-C4	-6.65	107.28	110.60
36	5	2653	C	N3-C2-O2	-6.65	117.25	121.90
36	1	2961	G	C4-C5-N7	6.64	113.46	110.80
36	1	914	A	C5-C6-N6	6.64	129.01	123.70
36	1	1507	G	C5-C6-O6	-6.64	124.61	128.60
36	5	669	U	C5-C6-N1	-6.64	119.38	122.70
36	5	1499	C	C2-N1-C1'	-6.64	111.49	118.80
1	2	992	A	C2-N3-C4	-6.64	107.28	110.60
1	2	1082	C	C6-N1-C2	-6.64	117.65	120.30
36	1	2130	G	C4-C5-N7	-6.63	108.15	110.80
38	4	20	U	O5'-P-OP2	-6.63	99.73	105.70
1	6	1648	A	C8-N9-C4	6.63	108.45	105.80
36	1	1160	C	N1-C2-O2	6.63	122.88	118.90
36	5	326	U	N3-C2-O2	6.63	126.84	122.20
36	5	1394	A	C5-C6-N6	-6.63	118.40	123.70
36	1	3008	A	N1-C6-N6	-6.63	114.62	118.60
36	5	1101	G	N9-C4-C5	-6.63	102.75	105.40
36	5	2808	A	N1-C6-N6	6.63	122.58	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1151	U	N3-C4-C5	-6.62	110.63	114.60
36	1	1367	G	C6-C5-N7	-6.62	126.43	130.40
38	4	22	U	C5-C6-N1	-6.62	119.39	122.70
36	5	826	G	N1-C6-O6	6.62	123.87	119.90
38	8	33	A	C5-C6-N6	-6.62	118.40	123.70
36	1	651	G	N1-C2-N2	-6.62	110.24	116.20
37	7	15	C	C6-N1-C2	6.62	122.95	120.30
1	2	577	G	C6-C5-N7	-6.62	126.43	130.40
36	1	1157	G	N9-C4-C5	6.62	108.05	105.40
36	1	1489	A	N9-C4-C5	-6.62	103.15	105.80
36	1	1881	A	C8-N9-C4	6.62	108.45	105.80
36	1	2406	C	C4-C5-C6	6.62	120.71	117.40
38	4	24	G	C5-C6-O6	-6.62	124.63	128.60
1	2	393	C	N3-C4-C5	6.61	124.55	121.90
36	1	1381	A	C5-C6-N6	-6.61	118.41	123.70
1	6	965	U	N1-C2-O2	6.61	127.43	122.80
36	1	2412	G	C5-C6-O6	-6.61	124.63	128.60
36	5	1484	U	C6-N1-C2	6.61	124.97	121.00
36	1	2827	U	O5'-P-OP2	-6.60	99.76	105.70
36	5	2814	G	N3-C2-N2	6.60	124.52	119.90
36	1	2900	A	C8-N9-C4	6.60	108.44	105.80
36	5	2405	C	N3-C4-C5	6.60	124.54	121.90
36	1	159	A	C8-N9-C4	6.60	108.44	105.80
36	5	1203	A	N1-C6-N6	6.60	122.56	118.60
36	5	2813	A	C4-C5-C6	6.60	120.30	117.00
36	1	3135	U	C5-C6-N1	-6.59	119.40	122.70
37	3	116	C	C6-N1-C2	-6.59	117.66	120.30
36	5	56	G	N1-C6-O6	-6.59	115.94	119.90
36	1	398	A	C8-N9-C4	6.59	108.44	105.80
36	1	1081	U	C5-C6-N1	6.59	126.00	122.70
36	5	2904	U	C5-C6-N1	-6.59	119.40	122.70
36	1	1330	A	C2-N3-C4	-6.59	107.31	110.60
36	1	2403	G	C6-C5-N7	-6.59	126.45	130.40
1	6	1	U	C2-N1-C1'	6.59	125.60	117.70
36	5	2870	C	C2-N3-C4	-6.58	116.61	119.90
36	1	1516	C	N1-C2-O2	-6.58	114.95	118.90
36	5	907	G	O5'-P-OP1	-6.58	99.78	105.70
36	5	1897	G	C5-C6-O6	-6.58	124.65	128.60
36	5	2307	G	N1-C6-O6	-6.58	115.95	119.90
36	5	902	G	N9-C4-C5	-6.58	102.77	105.40
36	1	1153	A	C6-C5-N7	-6.58	127.69	132.30
36	1	2355	G	C5-C6-O6	-6.58	124.65	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2409	G	C5-C6-O6	-6.58	124.65	128.60
36	1	2949	U	C6-N1-C2	6.58	124.95	121.00
1	6	1082	C	N3-C4-C5	-6.58	119.27	121.90
36	5	816	A	N9-C4-C5	6.58	108.43	105.80
1	2	1100	G	N3-C4-N9	6.57	129.94	126.00
36	1	410	U	N1-C2-N3	6.57	118.84	114.90
36	1	2364	G	N9-C4-C5	6.57	108.03	105.40
37	3	82	G	N3-C4-C5	-6.57	125.31	128.60
36	5	651	G	OP2-P-O3'	6.57	119.66	105.20
36	5	1848	G	C4-C5-N7	6.57	113.43	110.80
36	1	2827	U	N3-C2-O2	-6.57	117.60	122.20
36	5	2885	C	N3-C4-C5	6.57	124.53	121.90
36	5	2849	C	N3-C4-C5	-6.57	119.27	121.90
37	7	102	A	C8-N9-C4	6.57	108.43	105.80
36	5	2876	C	N3-C4-N4	-6.56	113.41	118.00
36	1	765	C	N1-C2-O2	6.56	122.84	118.90
36	5	1495	U	N3-C4-C5	-6.56	110.66	114.60
36	5	1837	U	C5-C4-O4	-6.56	121.96	125.90
36	1	2144	A	C6-N1-C2	-6.56	114.66	118.60
36	5	1454	A	C2-N3-C4	-6.56	107.32	110.60
38	8	86	U	C5-C6-N1	6.56	125.98	122.70
36	5	2389	C	N1-C2-O2	6.55	122.83	118.90
36	1	2651	G	C4-C5-N7	-6.55	108.18	110.80
1	2	1560	U	N1-C2-O2	6.55	127.39	122.80
36	1	1849	C	N3-C4-N4	6.55	122.58	118.00
38	8	95	G	C4-N9-C1'	-6.55	117.98	126.50
36	1	968	G	C6-N1-C2	-6.55	121.17	125.10
36	1	1468	A	O5'-P-OP1	-6.55	99.81	105.70
36	1	1294	A	O4'-C1'-N9	6.55	113.44	108.20
36	1	1365	G	N3-C4-N9	6.55	129.93	126.00
36	5	1445	U	C2-N1-C1'	-6.55	109.84	117.70
36	5	1372	C	C6-N1-C2	6.54	122.92	120.30
36	5	2320	A	C2-N3-C4	-6.54	107.33	110.60
36	1	2121	G	N1-C6-O6	-6.54	115.97	119.90
36	5	344	A	C5-C6-N1	-6.54	114.43	117.70
36	5	1300	G	C6-C5-N7	-6.54	126.47	130.40
36	1	2823	G	C6-N1-C2	-6.54	121.17	125.10
36	1	3361	G	N3-C2-N2	6.54	124.48	119.90
36	5	3127	A	C6-N1-C2	-6.54	114.68	118.60
1	2	507	U	N3-C2-O2	-6.54	117.62	122.20
1	6	101	U	N1-C2-O2	6.54	127.38	122.80
1	6	338	C	C6-N1-C2	-6.54	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1348	U	C6-N1-C2	-6.54	117.08	121.00
36	5	1407	A	C2-N3-C4	-6.54	107.33	110.60
38	4	91	C	C6-N1-C2	-6.54	117.69	120.30
1	6	1023	A	N1-C6-N6	6.54	122.52	118.60
36	1	1495	U	C6-N1-C1'	6.54	130.35	121.20
37	7	105	C	C6-N1-C2	-6.54	117.69	120.30
36	1	671	U	N1-C2-O2	-6.53	118.23	122.80
38	4	93	U	O5'-P-OP2	-6.53	99.82	105.70
36	5	2142	A	N1-C6-N6	-6.53	114.68	118.60
36	5	510	G	N3-C4-C5	-6.53	125.33	128.60
38	8	33	A	C8-N9-C4	6.53	108.41	105.80
15	C3	22	ALA	C-N-CD	-6.53	106.24	120.60
36	5	3078	U	N1-C2-O2	6.53	127.37	122.80
36	1	3362	A	C5-N7-C8	-6.53	100.64	103.90
36	5	1896	A	O5'-P-OP1	-6.53	99.83	105.70
36	5	2278	C	N1-C2-O2	6.52	122.81	118.90
36	5	2917	G	N3-C4-N9	6.52	129.91	126.00
36	1	401	U	N3-C2-O2	-6.52	117.63	122.20
36	1	2247	G	N1-C6-O6	6.52	123.81	119.90
36	5	960	U	N1-C2-O2	6.52	127.36	122.80
1	6	452	A	N1-C6-N6	6.52	122.51	118.60
1	6	1782	A	C8-N9-C4	-6.52	103.19	105.80
36	5	1298	C	O5'-P-OP1	-6.52	99.83	105.70
56	n0	113	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	2	1082	C	N3-C2-O2	-6.52	117.34	121.90
36	5	1481	A	P-O3'-C3'	6.52	127.52	119.70
1	2	334	G	N3-C4-N9	-6.52	122.09	126.00
36	1	3248	C	C6-N1-C2	-6.52	117.69	120.30
36	1	1433	A	C5-C6-N1	6.51	120.96	117.70
36	1	2937	G	C8-N9-C4	6.51	109.00	106.40
1	6	337	G	N3-C4-N9	6.51	129.91	126.00
1	6	1581	C	N3-C4-C5	6.51	124.50	121.90
36	1	936	A	O5'-P-OP2	-6.51	99.84	105.70
36	5	914	A	C2-N3-C4	-6.51	107.34	110.60
36	5	1008	U	C5-C6-N1	-6.51	119.44	122.70
36	5	2805	G	N9-C4-C5	-6.51	102.80	105.40
36	1	2410	U	C6-N1-C2	6.51	124.91	121.00
36	1	2698	G	C4-C5-N7	-6.51	108.20	110.80
36	5	2299	A	C8-N9-C4	6.51	108.40	105.80
37	7	69	C	C6-N1-C2	6.51	122.90	120.30
1	2	1730	A	C8-N9-C4	6.51	108.40	105.80
1	6	1150	G	N3-C4-C5	6.51	131.85	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1202	A	N1-C6-N6	-6.51	114.70	118.60
36	1	2823	G	C4-C5-N7	-6.51	108.20	110.80
36	1	2372	A	C4-C5-C6	6.50	120.25	117.00
1	2	1761	U	C6-N1-C2	-6.50	117.10	121.00
36	1	2813	A	C4-C5-C6	6.50	120.25	117.00
36	1	2610	G	N1-C6-O6	6.50	123.80	119.90
36	5	568	G	C5-C6-O6	-6.50	124.70	128.60
37	7	93	C	C6-N1-C2	-6.50	117.70	120.30
36	1	1269	U	N1-C2-O2	6.50	127.35	122.80
36	5	1158	A	N1-C6-N6	6.50	122.50	118.60
36	1	1108	U	C6-N1-C2	6.49	124.90	121.00
52	M6	78	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	6	558	U	C2-N1-C1'	6.49	125.49	117.70
36	1	948	C	N3-C4-N4	6.49	122.54	118.00
1	2	1745	G	N9-C4-C5	-6.49	102.80	105.40
36	5	633	C	N1-C2-O2	-6.49	115.01	118.90
36	5	971	G	C6-N1-C2	-6.49	121.21	125.10
36	5	2143	A	C8-N9-C4	-6.49	103.20	105.80
36	1	1351	U	N1-C2-O2	6.49	127.34	122.80
36	1	1380	G	O5'-P-OP1	6.49	118.49	110.70
36	5	1335	C	N1-C2-O2	-6.49	115.01	118.90
36	5	2727	A	N1-C6-N6	-6.49	114.71	118.60
36	1	47	C	C6-N1-C2	6.49	122.89	120.30
36	1	51	A	C2-N3-C4	6.49	113.84	110.60
36	1	2772	C	C2-N1-C1'	6.49	125.94	118.80
36	5	610	G	C8-N9-C4	-6.49	103.81	106.40
36	5	1166	G	C8-N9-C4	6.49	108.99	106.40
36	5	1848	G	N9-C4-C5	-6.49	102.81	105.40
36	1	666	A	C8-N9-C4	6.48	108.39	105.80
36	1	2624	G	N7-C8-N9	6.48	116.34	113.10
36	1	2813	A	C5-C6-N1	-6.48	114.46	117.70
36	5	119	U	C5-C6-N1	-6.48	119.46	122.70
36	5	2978	U	N1-C2-N3	6.48	118.79	114.90
36	5	510	G	C8-N9-C4	-6.48	103.81	106.40
36	1	1445	U	C2-N1-C1'	-6.48	109.93	117.70
36	1	803	C	O5'-P-OP2	-6.47	99.87	105.70
36	1	2142	A	C6-N1-C2	-6.47	114.72	118.60
36	1	2356	A	C4-C5-N7	6.47	113.94	110.70
36	5	1496	C	C2-N1-C1'	6.47	125.92	118.80
1	6	1581	C	C6-N1-C2	6.47	122.89	120.30
36	5	680	G	N3-C4-C5	6.47	131.84	128.60
36	5	718	G	O4'-C1'-N9	6.47	113.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	704	C	N1-C2-O2	6.47	122.78	118.90
36	5	1426	C	N3-C4-C5	6.47	124.49	121.90
36	1	1406	A	C5-C6-N6	-6.47	118.53	123.70
37	3	91	G	N1-C6-O6	6.47	123.78	119.90
38	4	9	A	N1-C6-N6	-6.47	114.72	118.60
37	7	11	A	N1-C6-N6	6.47	122.48	118.60
36	5	787	G	C2-N3-C4	-6.47	108.67	111.90
1	6	305	C	N3-C2-O2	6.46	126.43	121.90
36	5	1848	G	C8-N9-C4	6.46	108.99	106.40
36	5	2988	C	N3-C4-C5	6.46	124.48	121.90
36	5	1152	G	C8-N9-C4	-6.46	103.81	106.40
36	5	2700	G	C5-C6-O6	-6.46	124.72	128.60
36	5	1495	U	C2-N1-C1'	6.46	125.45	117.70
36	5	2430	A	C2-N3-C4	-6.46	107.37	110.60
1	6	1111	G	C6-C5-N7	-6.46	126.52	130.40
36	1	1405	U	C6-N1-C2	6.46	124.88	121.00
36	1	2649	A	C2-N3-C4	6.46	113.83	110.60
36	5	2797	C	C4-C5-C6	6.46	120.63	117.40
36	5	2884	C	C5-C4-N4	-6.46	115.68	120.20
52	m6	94	ARG	NE-CZ-NH1	-6.46	117.07	120.30
36	5	933	A	N1-C2-N3	6.45	132.53	129.30
36	5	945	C	N1-C2-O2	6.45	122.77	118.90
36	5	3310	A	C8-N9-C4	6.45	108.38	105.80
1	2	553	G	C4-C5-N7	6.45	113.38	110.80
36	1	98	G	C8-N9-C4	6.45	108.98	106.40
36	1	934	G	C4-N9-C1'	6.45	134.89	126.50
36	1	2249	G	N3-C4-C5	-6.45	125.37	128.60
36	5	2375	G	N1-C6-O6	-6.45	116.03	119.90
36	1	1453	A	C8-N9-C4	-6.45	103.22	105.80
1	6	901	G	C4-C5-N7	6.45	113.38	110.80
36	5	2948	C	N3-C4-C5	6.45	124.48	121.90
36	1	2385	G	C5-C6-O6	-6.45	124.73	128.60
36	5	883	A	N1-C6-N6	-6.45	114.73	118.60
1	2	1180	C	N1-C2-O2	6.45	122.77	118.90
36	5	866	A	N1-C6-N6	6.45	122.47	118.60
36	5	1617	G	C8-N9-C4	6.45	108.98	106.40
36	1	1124	U	OP1-P-O3'	6.44	119.38	105.20
36	1	1138	U	C2-N3-C4	-6.44	123.13	127.00
36	5	1119	C	C5-C4-N4	-6.44	115.69	120.20
36	5	1875	G	N1-C6-O6	-6.44	116.03	119.90
36	5	2866	U	N3-C2-O2	-6.44	117.69	122.20
36	5	2876	C	OP1-P-OP2	6.44	129.26	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	424	G	C4-C5-N7	6.44	113.38	110.80
1	6	542	A	O4'-C1'-N9	6.44	113.35	108.20
36	5	1907	C	N1-C2-O2	-6.44	115.04	118.90
1	2	1773	C	N3-C4-C5	-6.44	119.33	121.90
36	1	392	G	C5-C6-O6	-6.44	124.74	128.60
36	5	1206	G	C8-N9-C4	-6.44	103.83	106.40
36	1	1365	G	C8-N9-C4	-6.43	103.83	106.40
36	5	3219	G	N3-C2-N2	6.43	124.40	119.90
36	5	1060	U	N3-C4-O4	-6.43	114.90	119.40
1	6	864	U	C2-N1-C1'	6.43	125.42	117.70
1	6	1274	C	N3-C4-C5	-6.43	119.33	121.90
36	5	3033	A	N1-C6-N6	6.43	122.46	118.60
36	5	2896	A	N1-C6-N6	-6.43	114.74	118.60
1	2	190	C	O4'-C1'-N1	6.43	113.34	108.20
36	5	1306	G	C4-C5-N7	6.43	113.37	110.80
36	5	2831	G	C6-N1-C2	-6.42	121.25	125.10
36	5	3362	A	O4'-C1'-N9	6.42	113.34	108.20
38	8	14	C	O5'-P-OP2	-6.42	99.92	105.70
1	2	1100	G	C5-C6-O6	-6.42	124.75	128.60
36	1	589	A	C5-N7-C8	6.42	107.11	103.90
1	6	1765	A	C8-N9-C4	6.42	108.37	105.80
36	5	1149	G	C5-C6-N1	6.42	114.71	111.50
36	1	33	G	N3-C2-N2	-6.42	115.41	119.90
36	1	958	C	N3-C2-O2	-6.42	117.41	121.90
36	5	1903	U	N3-C4-C5	-6.42	110.75	114.60
36	5	3218	A	N9-C4-C5	-6.42	103.23	105.80
36	5	1392	G	C5-C6-O6	-6.41	124.75	128.60
36	5	2754	G	N1-C6-O6	-6.41	116.05	119.90
36	1	801	A	N1-C2-N3	-6.41	126.09	129.30
36	1	2828	G	N3-C2-N2	6.41	124.39	119.90
36	1	2859	U	C5-C6-N1	-6.41	119.50	122.70
1	2	1773	C	C6-N1-C2	-6.41	117.74	120.30
36	1	881	C	C2-N3-C4	6.41	123.10	119.90
36	1	25	U	O5'-P-OP2	6.41	118.39	110.70
36	5	1891	A	N1-C6-N6	6.41	122.44	118.60
36	5	2334	U	N3-C2-O2	-6.41	117.72	122.20
36	1	1001	G	C6-C5-N7	-6.40	126.56	130.40
36	1	2343	C	C5-C4-N4	-6.40	115.72	120.20
36	5	586	C	C5-C6-N1	-6.40	117.80	121.00
36	1	1419	A	C5'-C4'-O4'	6.40	116.78	109.10
36	1	1425	U	N1-C2-N3	6.40	118.74	114.90
36	1	2282	U	O5'-P-OP1	6.40	118.38	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1153	A	C5-C6-N1	6.40	120.90	117.70
36	1	2891	U	O5'-P-OP1	6.40	118.38	110.70
36	1	860	G	N1-C6-O6	6.40	123.74	119.90
36	5	2138	A	C2-N3-C4	-6.40	107.40	110.60
36	1	498	A	C8-N9-C4	-6.40	103.24	105.80
36	1	775	A	N1-C6-N6	6.40	122.44	118.60
36	5	718	G	N3-C4-C5	-6.40	125.40	128.60
1	2	1596	C	N3-C2-O2	-6.39	117.42	121.90
36	1	984	G	N3-C4-C5	-6.39	125.40	128.60
36	1	2643	A	N9-C4-C5	-6.39	103.24	105.80
36	5	2211	U	C4-C5-C6	6.39	123.54	119.70
36	1	1041	U	O5'-P-OP2	-6.39	99.95	105.70
36	1	3316	A	N1-C6-N6	6.39	122.44	118.60
38	4	25	G	N1-C6-O6	-6.39	116.06	119.90
36	5	969	C	N3-C4-N4	-6.39	113.53	118.00
36	5	1685	C	N1-C2-O2	6.39	122.74	118.90
36	5	2889	C	C2-N3-C4	-6.39	116.70	119.90
36	1	2426	U	C5-C4-O4	6.39	129.74	125.90
1	2	934	C	C2-N1-C1'	6.39	125.83	118.80
36	1	1407	A	C8-N9-C4	6.39	108.36	105.80
36	5	1513	G	N3-C4-C5	-6.39	125.41	128.60
36	5	1587	A	C8-N9-C4	6.39	108.36	105.80
36	5	1851	G	C6-C5-N7	-6.39	126.57	130.40
36	5	3136	G	C2-N3-C4	-6.39	108.70	111.90
36	5	587	U	C5-C4-O4	-6.39	122.07	125.90
36	5	1126	G	C8-N9-C4	-6.39	103.85	106.40
36	5	1853	U	C5-C4-O4	6.39	129.73	125.90
36	5	1911	A	C2-N3-C4	-6.39	107.41	110.60
36	1	2993	G	N3-C2-N2	6.38	124.37	119.90
36	5	2376	G	N1-C6-O6	6.38	123.73	119.90
36	5	3039	C	C4-C5-C6	6.38	120.59	117.40
36	1	1450	G	O5'-P-OP2	6.38	118.36	110.70
36	5	1116	G	C5-C6-N1	-6.38	108.31	111.50
1	2	144	U	N3-C2-O2	-6.38	117.73	122.20
36	1	2870	C	N1-C2-O2	-6.38	115.07	118.90
10	s8	8	ARG	NE-CZ-NH1	6.38	123.49	120.30
36	5	2405	C	O5'-P-OP2	-6.38	99.96	105.70
36	1	1905	G	N3-C2-N2	-6.38	115.44	119.90
36	1	2418	G	OP1-P-O3'	6.38	119.23	105.20
36	5	2434	U	C5-C4-O4	6.38	129.73	125.90
36	1	25	U	N3-C4-O4	6.37	123.86	119.40
36	1	2409	G	C5-C6-N1	6.37	114.69	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	353	G	C4-N9-C1'	-6.37	118.22	126.50
1	6	19	A	N9-C4-C5	-6.37	103.25	105.80
36	5	2935	U	O5'-P-OP2	-6.37	99.97	105.70
1	2	453	U	N1-C2-O2	6.37	127.26	122.80
36	5	2991	A	N9-C4-C5	6.37	108.35	105.80
36	1	3362	A	C8-N9-C4	-6.37	103.25	105.80
1	6	1131	A	N1-C2-N3	6.37	132.48	129.30
36	5	2982	A	C2-N3-C4	6.37	113.78	110.60
36	5	2608	G	OP2-P-O3'	6.37	119.21	105.20
36	1	628	A	N1-C6-N6	6.36	122.42	118.60
36	5	3270	U	O5'-P-OP1	-6.36	99.97	105.70
54	m8	127	LEU	CA-CB-CG	6.36	129.93	115.30
36	1	229	G	N1-C6-O6	6.36	123.72	119.90
36	1	712	G	O5'-P-OP1	-6.36	99.97	105.70
36	1	1377	G	C6-C5-N7	-6.36	126.58	130.40
36	1	2257	C	O4'-C1'-N1	6.36	113.29	108.20
36	1	2874	G	N3-C4-C5	6.36	131.78	128.60
1	6	426	G	C8-N9-C4	-6.36	103.86	106.40
36	5	2215	A	C2-N3-C4	-6.36	107.42	110.60
36	5	3218	A	P-O3'-C3'	6.36	127.33	119.70
36	1	2200	U	C4-C5-C6	6.36	123.52	119.70
36	5	1475	A	N1-C6-N6	6.36	122.42	118.60
1	2	1189	A	C8-N9-C4	6.36	108.34	105.80
36	1	3101	G	C5-C6-N1	6.36	114.68	111.50
1	6	1745	G	C5-C6-O6	-6.36	124.79	128.60
36	5	1906	G	N9-C4-C5	-6.36	102.86	105.40
36	5	2831	G	C5-C6-O6	-6.35	124.79	128.60
36	5	3190	C	C6-N1-C2	-6.35	117.76	120.30
1	6	317	C	C2-N3-C4	-6.35	116.72	119.90
36	5	1847	A	C8-N9-C4	6.35	108.34	105.80
37	7	91	G	C6-N1-C2	-6.35	121.29	125.10
1	2	1600	A	N9-C4-C5	-6.35	103.26	105.80
36	1	24	G	C4-N9-C1'	6.35	134.76	126.50
36	1	680	G	C8-N9-C4	6.35	108.94	106.40
36	1	1116	G	C4-C5-C6	6.35	122.61	118.80
1	6	1651	A	N1-C6-N6	6.35	122.41	118.60
36	5	2411	U	C2-N3-C4	-6.35	123.19	127.00
36	1	984	G	N1-C2-N2	-6.35	110.49	116.20
36	5	644	G	C8-N9-C4	-6.35	103.86	106.40
1	6	1361	U	C2-N1-C1'	6.34	125.31	117.70
36	1	1495	U	N1-C2-N3	6.34	118.71	114.90
36	1	2622	C	C6-N1-C2	-6.34	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	941	G	C5-C6-N1	6.34	114.67	111.50
36	1	972	A	N7-C8-N9	-6.34	110.63	113.80
1	6	543	C	C6-N1-C2	-6.34	117.76	120.30
36	1	1156	C	C5-C6-N1	-6.34	117.83	121.00
1	6	965	U	N3-C2-O2	-6.34	117.76	122.20
36	5	756	U	C5-C6-N1	-6.34	119.53	122.70
36	5	2887	A	N1-C6-N6	6.34	122.40	118.60
1	2	600	U	C6-N1-C2	-6.34	117.20	121.00
36	5	2999	U	C5-C6-N1	-6.34	119.53	122.70
36	5	3209	A	O4'-C1'-N9	6.34	113.27	108.20
36	1	363	G	N9-C4-C5	-6.34	102.86	105.40
36	1	631	U	C5-C4-O4	-6.34	122.10	125.90
36	1	3214	U	C5-C4-O4	6.34	129.70	125.90
36	1	58	G	C6-C5-N7	-6.33	126.60	130.40
36	1	878	G	C2-N3-C4	-6.33	108.73	111.90
35	sM	167	PRO	N-CA-CB	6.33	110.90	103.30
36	5	1143	A	C2-N3-C4	-6.33	107.43	110.60
36	1	2355	G	C5-C6-N1	-6.33	108.33	111.50
36	1	3052	G	N1-C6-O6	6.33	123.70	119.90
36	5	751	A	O5'-P-OP2	-6.33	100.00	105.70
36	5	2404	A	C5-C6-N1	-6.33	114.53	117.70
36	5	1184	A	N1-C6-N6	-6.33	114.80	118.60
36	1	2596	U	C6-N1-C2	6.33	124.80	121.00
36	5	1114	U	OP1-P-O3'	6.33	119.12	105.20
36	1	285	A	N1-C6-N6	6.33	122.39	118.60
1	2	1082	C	N1-C2-O2	6.32	122.69	118.90
36	5	419	G	N3-C4-N9	6.32	129.79	126.00
36	5	2994	A	C5-C6-N6	-6.32	118.64	123.70
36	1	1433	A	C2-N3-C4	6.32	113.76	110.60
1	6	782	U	N3-C2-O2	-6.32	117.78	122.20
36	1	2661	G	O5'-P-OP1	-6.32	100.01	105.70
36	5	2762	A	O5'-P-OP2	-6.32	100.01	105.70
36	1	1112	A	N9-C4-C5	-6.32	103.27	105.80
36	1	2136	C	N1-C2-O2	-6.32	115.11	118.90
36	1	2405	C	N3-C4-C5	-6.32	119.37	121.90
36	5	358	G	N1-C6-O6	6.32	123.69	119.90
1	2	600	U	N3-C2-O2	-6.32	117.78	122.20
36	5	1158	A	C6-C5-N7	-6.32	127.88	132.30
36	5	2849	C	N3-C4-N4	6.32	122.42	118.00
36	5	1888	U	C2-N3-C4	-6.31	123.21	127.00
36	1	2898	G	O4'-C1'-N9	-6.31	103.15	108.20
36	5	1128	U	N1-C2-N3	6.31	118.69	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1390	A	C5-C6-N6	6.31	128.75	123.70
36	5	1837	U	N3-C2-O2	6.31	126.62	122.20
36	1	2706	G	C5-C6-O6	-6.31	124.81	128.60
36	1	611	A	N1-C6-N6	6.31	122.39	118.60
36	1	1103	A	C2-N3-C4	6.31	113.75	110.60
36	1	2831	G	C5-C6-O6	-6.31	124.81	128.60
36	5	328	U	C5-C4-O4	6.31	129.69	125.90
36	5	1301	A	N1-C6-N6	6.31	122.39	118.60
36	5	2903	A	C8-N9-C4	6.31	108.32	105.80
36	1	649	A	C2-N3-C4	-6.31	107.45	110.60
36	1	2973	G	C5-C6-O6	-6.31	124.81	128.60
1	6	1582	U	C5-C6-N1	-6.31	119.55	122.70
12	c0	83	PRO	N-CA-CB	6.31	110.87	103.30
36	1	3306	U	N1-C2-N3	6.31	118.68	114.90
1	6	1150	G	C2-N3-C4	-6.31	108.75	111.90
36	5	2764	C	C6-N1-C2	6.31	122.82	120.30
37	7	93	C	N1-C2-O2	6.31	122.68	118.90
36	1	878	G	N1-C2-N3	6.30	127.68	123.90
36	1	2343	C	C2-N3-C4	-6.30	116.75	119.90
36	5	1010	G	O5'-P-OP2	-6.30	100.03	105.70
36	5	1194	G	C4-C5-N7	-6.30	108.28	110.80
36	1	672	A	N1-C6-N6	6.30	122.38	118.60
36	5	2314	U	C2-N1-C1'	6.30	125.26	117.70
36	1	716	A	C2-N3-C4	-6.30	107.45	110.60
36	5	2140	U	C4-C5-C6	6.30	123.48	119.70
38	8	30	C	N1-C2-O2	-6.30	115.12	118.90
1	2	32	U	N3-C2-O2	-6.30	117.79	122.20
41	14	340	GLY	N-CA-C	-6.30	97.35	113.10
36	1	369	A	C8-N9-C4	-6.30	103.28	105.80
36	1	1581	C	C6-N1-C2	-6.30	117.78	120.30
36	5	1157	G	O5'-P-OP1	-6.30	100.03	105.70
36	5	1367	G	C5-C6-N1	-6.30	108.35	111.50
36	5	1494	U	C6-N1-C2	6.30	124.78	121.00
36	5	3199	G	N1-C6-O6	-6.30	116.12	119.90
1	2	959	U	N3-C2-O2	-6.29	117.79	122.20
36	5	1178	G	C4-C5-N7	6.29	113.32	110.80
36	5	2942	C	C5-C4-N4	-6.29	115.79	120.20
1	2	95	G	C5-C6-O6	6.29	132.38	128.60
36	5	1937	U	C5-C6-N1	-6.29	119.55	122.70
36	5	2836	C	O5'-P-OP2	-6.29	100.04	105.70
36	5	3215	A	N1-C6-N6	6.29	122.38	118.60
36	1	2400	G	N9-C4-C5	-6.29	102.88	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2857	C	N3-C4-C5	6.29	124.42	121.90
36	1	3201	C	C4-C5-C6	6.29	120.55	117.40
36	1	3208	G	C4-C5-C6	6.29	122.57	118.80
36	5	720	A	N1-C6-N6	6.29	122.37	118.60
36	5	2211	U	N1-C2-N3	6.29	118.67	114.90
1	2	1170	G	N1-C6-O6	6.29	123.67	119.90
36	1	1175	C	C2-N3-C4	-6.29	116.75	119.90
1	6	1599	C	N1-C2-O2	6.29	122.67	118.90
36	5	368	G	C5-C6-O6	6.29	132.37	128.60
36	5	586	C	C6-N1-C2	6.29	122.82	120.30
38	8	17	A	N1-C6-N6	6.29	122.37	118.60
36	1	518	G	O4'-C1'-N9	6.29	113.23	108.20
36	1	651	G	N3-C4-C5	-6.29	125.46	128.60
36	5	2116	G	N1-C6-O6	6.29	123.67	119.90
36	1	155	G	N3-C4-N9	6.28	129.77	126.00
36	1	2758	A	C6-C5-N7	6.28	136.70	132.30
38	4	99	C	C6-N1-C2	6.28	122.81	120.30
36	5	587	U	N3-C2-O2	6.28	126.60	122.20
36	5	942	U	N1-C2-N3	6.28	118.67	114.90
36	5	1429	G	N1-C2-N3	6.28	127.67	123.90
36	1	3208	G	C6-C5-N7	-6.28	126.63	130.40
36	5	2298	U	C5-C6-N1	-6.28	119.56	122.70
36	1	212	G	C5-C6-O6	-6.28	124.83	128.60
36	1	875	G	N3-C4-C5	-6.28	125.46	128.60
36	1	1116	G	OP2-P-O3'	6.28	119.02	105.20
1	2	1744	A	O5'-P-OP1	-6.28	100.05	105.70
36	5	1476	G	C5-C6-O6	6.28	132.37	128.60
52	m6	78	ARG	NE-CZ-NH1	6.28	123.44	120.30
36	1	2249	G	N9-C1'-C2'	-6.28	105.09	112.00
36	1	2822	U	N3-C4-O4	-6.28	115.01	119.40
36	5	2939	G	C5-N7-C8	6.28	107.44	104.30
36	5	3027	A	N1-C2-N3	6.28	132.44	129.30
36	1	2827	U	C6-N1-C1'	6.28	129.99	121.20
36	5	636	C	N1-C2-O2	6.28	122.67	118.90
36	5	3050	U	N3-C4-O4	-6.28	115.01	119.40
1	2	412	A	O5'-P-OP1	6.27	118.23	110.70
37	3	87	G	O5'-P-OP1	-6.27	100.06	105.70
36	5	1885	U	C2-N3-C4	-6.27	123.24	127.00
36	5	2819	A	OP2-P-O3'	6.27	119.00	105.20
38	8	139	U	N3-C2-O2	-6.27	117.81	122.20
1	6	1273	G	O4'-C1'-N9	6.27	113.22	108.20
36	5	398	A	O5'-P-OP2	-6.27	100.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	747	A	O5'-P-OP2	-6.27	100.06	105.70
36	5	3110	C	C6-N1-C2	6.27	122.81	120.30
36	1	969	C	N1-C2-O2	-6.27	115.14	118.90
1	2	616	G	N1-C6-O6	-6.27	116.14	119.90
36	1	2996	U	C5-C6-N1	6.27	125.83	122.70
36	5	969	C	C6-N1-C2	6.27	122.81	120.30
1	2	74	U	O5'-P-OP1	-6.26	100.06	105.70
36	1	2395	G	C5-C6-O6	-6.26	124.84	128.60
36	1	3310	A	N1-C6-N6	6.26	122.36	118.60
38	4	53	A	C2-N3-C4	6.26	113.73	110.60
1	6	56	U	C5-C6-N1	-6.26	119.57	122.70
1	2	438	A	O5'-P-OP1	-6.26	100.06	105.70
36	1	1116	G	O5'-P-OP1	-6.26	100.06	105.70
36	5	104	G	N1-C6-O6	6.26	123.66	119.90
36	5	666	A	C8-N9-C4	6.26	108.30	105.80
36	5	1099	A	N1-C6-N6	6.26	122.36	118.60
36	5	2187	G	C6-C5-N7	-6.26	126.64	130.40
36	1	785	G	C2-N3-C4	6.26	115.03	111.90
36	1	2301	U	O5'-P-OP2	-6.26	100.07	105.70
1	2	1052	U	C2-N1-C1'	6.26	125.21	117.70
36	5	1193	A	C2-N3-C4	-6.26	107.47	110.60
36	1	1150	A	N1-C6-N6	-6.25	114.85	118.60
36	1	58	G	C4-C5-N7	6.25	113.30	110.80
36	1	1142	G	O5'-P-OP1	6.25	118.20	110.70
36	1	1793	C	C2-N3-C4	-6.25	116.77	119.90
36	1	1911	A	N1-C6-N6	6.25	122.35	118.60
1	6	1340	U	N3-C2-O2	-6.25	117.82	122.20
36	5	1080	A	N7-C8-N9	-6.25	110.67	113.80
1	2	587	C	N3-C4-C5	-6.25	119.40	121.90
1	2	830	U	C2-N1-C1'	6.25	125.20	117.70
1	6	800	U	C6-N1-C2	-6.25	117.25	121.00
1	6	1643	U	C2-N3-C4	-6.25	123.25	127.00
36	5	190	U	N1-C2-O2	6.25	127.17	122.80
37	7	103	A	C5-C6-N1	6.25	120.83	117.70
36	1	1104	G	O5'-P-OP1	-6.25	100.08	105.70
36	1	411	U	O5'-P-OP1	-6.25	100.08	105.70
36	5	51	A	N1-C6-N6	6.25	122.35	118.60
36	5	939	U	C5-C4-O4	-6.25	122.15	125.90
36	5	1481	A	O5'-P-OP2	-6.25	100.08	105.70
36	5	39	A	N1-C6-N6	6.25	122.35	118.60
36	1	1326	A	C8-N9-C4	6.24	108.30	105.80
1	6	1586	A	C8-N9-C4	6.24	108.30	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1399	A	N1-C6-N6	6.24	122.34	118.60
43	16	18	LEU	CA-CB-CG	-6.24	100.94	115.30
36	1	334	A	C8-N9-C4	-6.24	103.30	105.80
36	1	1495	U	C5-C4-O4	6.24	129.64	125.90
36	5	1875	G	N7-C8-N9	-6.24	109.98	113.10
36	1	2371	G	N3-C2-N2	6.24	124.27	119.90
1	6	982	U	C6-N1-C2	6.24	124.74	121.00
36	5	48	A	C8-N9-C4	-6.24	103.31	105.80
36	5	826	G	C4-C5-N7	6.24	113.29	110.80
36	5	1373	A	N1-C6-N6	6.24	122.34	118.60
52	m6	84	LEU	CA-CB-CG	-6.23	100.96	115.30
1	2	619	A	N1-C6-N6	-6.23	114.86	118.60
36	5	340	C	C5-C6-N1	-6.23	117.88	121.00
36	5	1301	A	C6-C5-N7	-6.23	127.94	132.30
36	5	1452	A	C4-C5-N7	6.23	113.82	110.70
1	6	163	G	C8-N9-C1'	6.23	135.10	127.00
36	1	1269	U	N3-C2-O2	-6.23	117.84	122.20
36	5	514	G	C4-C5-N7	6.23	113.29	110.80
36	5	971	G	C5-C6-O6	-6.23	124.86	128.60
36	5	1429	G	N1-C2-N2	-6.23	110.60	116.20
36	5	3131	U	C6-N1-C2	6.23	124.74	121.00
36	1	1167	U	O5'-P-OP1	6.23	118.17	110.70
36	5	739	G	O5'-P-OP1	-6.22	100.10	105.70
36	1	225	C	N3-C4-C5	-6.22	119.41	121.90
36	1	2188	A	C8-N9-C4	6.22	108.29	105.80
1	6	1654	G	C4-C5-N7	6.22	113.29	110.80
36	1	2692	A	C5-C6-N6	-6.22	118.72	123.70
36	5	1110	U	N3-C2-O2	-6.22	117.84	122.20
36	1	35	A	O5'-P-OP1	6.22	118.16	110.70
1	6	92	A	N1-C6-N6	6.22	122.33	118.60
1	2	577	G	C5-N7-C8	-6.22	101.19	104.30
36	5	1115	G	C4-N9-C1'	6.22	134.58	126.50
1	2	1176	G	C4-C5-N7	6.22	113.29	110.80
36	1	3057	U	N1-C2-N3	6.22	118.63	114.90
36	5	2402	A	C5-C6-N6	6.22	128.67	123.70
36	1	49	A	C8-N9-C4	6.21	108.29	105.80
36	1	369	A	N3-C4-C5	-6.21	122.45	126.80
36	1	1351	U	N3-C2-O2	-6.21	117.85	122.20
38	4	68	G	N1-C6-O6	6.21	123.63	119.90
36	1	397	A	N1-C6-N6	-6.21	114.87	118.60
36	5	1725	C	N1-C2-O2	-6.21	115.17	118.90
1	2	554	C	N1-C2-O2	6.21	122.63	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2718	U	C2-N3-C4	-6.21	123.27	127.00
36	5	644	G	N3-C4-C5	-6.21	125.49	128.60
1	2	1761	U	C5-C4-O4	6.21	129.63	125.90
36	5	2395	G	C4-C5-N7	6.21	113.28	110.80
38	8	81	U	P-O3'-C3'	6.21	127.15	119.70
36	1	3216	G	N9-C4-C5	6.21	107.88	105.40
36	5	1495	U	C6-N1-C2	-6.21	117.28	121.00
36	1	2585	G	N3-C4-C5	-6.21	125.50	128.60
36	5	2379	U	C4-C5-C6	6.21	123.42	119.70
36	1	2861	U	N3-C2-O2	-6.21	117.86	122.20
36	5	333	G	N1-C2-N3	6.21	127.62	123.90
36	5	660	A	C6-C5-N7	6.21	136.64	132.30
36	5	2211	U	N3-C2-O2	-6.21	117.86	122.20
1	2	394	C	C6-N1-C2	-6.20	117.82	120.30
36	1	2298	U	N3-C4-O4	-6.20	115.06	119.40
1	2	1596	C	N1-C2-O2	6.20	122.62	118.90
36	1	668	G	N7-C8-N9	-6.20	110.00	113.10
36	1	1838	G	C6-C5-N7	-6.20	126.68	130.40
36	1	3050	U	N1-C2-O2	6.20	127.14	122.80
1	2	380	U	N3-C2-O2	-6.20	117.86	122.20
36	1	2729	U	N1-C2-O2	6.19	127.14	122.80
36	5	1338	C	C4-C5-C6	6.19	120.50	117.40
36	1	1369	A	O5'-P-OP1	-6.19	100.13	105.70
36	1	2607	G	C5-C6-O6	6.19	132.32	128.60
1	6	398	G	C5-C6-O6	6.19	132.31	128.60
36	1	2867	C	N3-C2-O2	-6.19	117.57	121.90
36	5	1426	C	O5'-P-OP2	-6.19	100.13	105.70
36	5	2282	U	C5-C6-N1	-6.19	119.61	122.70
36	5	3047	U	C5-C6-N1	-6.19	119.61	122.70
36	1	1434	G	N1-C6-O6	6.19	123.61	119.90
36	5	2211	U	C5-C4-O4	6.19	129.61	125.90
36	1	2111	G	O5'-P-OP1	-6.18	100.14	105.70
36	1	1589	A	O5'-P-OP2	-6.18	100.14	105.70
36	1	2393	G	C5-C6-O6	-6.18	124.89	128.60
36	5	269	G	N1-C6-O6	6.18	123.61	119.90
36	5	364	G	C2-N3-C4	-6.18	108.81	111.90
36	5	1300	G	N3-C4-N9	6.18	129.71	126.00
36	1	933	A	N3-C4-C5	-6.18	122.47	126.80
36	5	1156	C	N1-C2-O2	-6.18	115.19	118.90
36	1	1154	A	C8-N9-C4	-6.18	103.33	105.80
36	5	2199	G	N7-C8-N9	6.18	116.19	113.10
36	5	2531	C	N1-C2-O2	6.18	122.61	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2710	C	C6-N1-C2	6.18	122.77	120.30
1	2	1241	G	O4'-C1'-N9	6.18	113.14	108.20
36	1	2572	C	N3-C2-O2	-6.18	117.58	121.90
1	2	1762	A	O5'-P-OP1	-6.18	100.14	105.70
36	5	953	G	C5-C6-O6	-6.18	124.89	128.60
36	5	1389	G	C6-C5-N7	-6.18	126.69	130.40
36	5	2351	U	N3-C2-O2	-6.18	117.88	122.20
36	5	2871	G	N3-C4-N9	6.18	129.71	126.00
36	5	3154	C	N3-C2-O2	-6.18	117.58	121.90
36	1	908	G	C4-N9-C1'	6.17	134.53	126.50
36	1	2343	C	C5-C6-N1	-6.17	117.91	121.00
36	1	2758	A	C4-C5-N7	-6.17	107.61	110.70
38	4	30	C	C2-N1-C1'	-6.17	112.01	118.80
36	5	3377	G	C2-N3-C4	6.17	114.99	111.90
36	1	229	G	N3-C2-N2	-6.17	115.58	119.90
36	1	937	G	N1-C6-O6	6.17	123.60	119.90
36	1	2130	G	C5-C6-O6	6.17	132.30	128.60
36	1	2385	G	N1-C6-O6	6.17	123.60	119.90
36	5	2862	U	N3-C4-O4	-6.17	115.08	119.40
36	5	2117	A	C5-C6-N6	6.17	128.64	123.70
36	5	2183	A	C5-C6-N6	-6.17	118.76	123.70
1	6	119	A	C2-N3-C4	-6.17	107.52	110.60
36	1	790	U	N3-C2-O2	-6.17	117.88	122.20
36	1	1793	C	O5'-P-OP1	-6.17	100.15	105.70
36	5	1534	A	C4-C5-C6	6.17	120.08	117.00
1	2	1568	C	P-O3'-C3'	6.17	127.10	119.70
36	1	1140	G	N1-C2-N2	-6.17	110.65	116.20
1	6	308	C	C5-C4-N4	6.17	124.52	120.20
1	2	736	C	C5-C6-N1	6.17	124.08	121.00
1	6	337	G	N3-C4-C5	-6.17	125.52	128.60
36	5	1152	G	N1-C2-N2	6.17	121.75	116.20
36	1	2808	A	C5-N7-C8	-6.16	100.82	103.90
36	5	283	G	O4'-C1'-N9	-6.16	103.27	108.20
36	5	217	U	OP1-P-O3'	6.16	118.75	105.20
36	1	941	G	OP1-P-O3'	6.16	118.75	105.20
36	1	1141	C	C2-N3-C4	-6.16	116.82	119.90
36	1	1182	A	N1-C6-N6	6.16	122.30	118.60
36	1	1909	A	C2-N3-C4	-6.16	107.52	110.60
1	2	1258	U	N3-C2-O2	-6.16	117.89	122.20
36	1	14	U	C5-C6-N1	-6.16	119.62	122.70
36	1	557	A	C8-N9-C4	6.16	108.26	105.80
36	1	3344	A	N1-C6-N6	6.16	122.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	875	G	N3-C4-C5	-6.16	125.52	128.60
36	5	2627	C	C4-C5-C6	6.16	120.48	117.40
36	1	29	C	N3-C4-N4	6.16	122.31	118.00
1	6	364	G	C8-N9-C1'	-6.16	119.00	127.00
36	5	339	C	C6-N1-C2	-6.16	117.84	120.30
36	5	974	G	C8-N9-C4	-6.16	103.94	106.40
36	5	1101	G	N3-C2-N2	6.16	124.21	119.90
36	5	3028	G	N1-C2-N2	-6.16	110.66	116.20
36	5	1452	A	C5-C6-N6	-6.15	118.78	123.70
36	5	3200	G	N1-C6-O6	6.15	123.59	119.90
1	2	1745	G	N3-C4-C5	-6.15	125.52	128.60
36	1	2768	U	O5'-P-OP2	-6.15	100.16	105.70
1	6	194	U	N1-C2-O2	6.15	127.11	122.80
36	5	1392	G	C8-N9-C4	6.15	108.86	106.40
36	5	2288	G	O5'-P-OP1	-6.15	100.16	105.70
36	1	2636	A	N7-C8-N9	6.15	116.88	113.80
36	1	2867	C	C4-C5-C6	6.15	120.47	117.40
1	6	1097	U	P-O3'-C3'	6.15	127.08	119.70
36	5	906	A	C2-N3-C4	6.15	113.67	110.60
36	5	2996	U	N1-C2-O2	6.15	127.11	122.80
36	5	3120	C	C6-N1-C2	-6.15	117.84	120.30
36	1	1296	C	N3-C4-C5	-6.15	119.44	121.90
36	5	706	A	N9-C4-C5	-6.15	103.34	105.80
36	5	1588	A	O5'-P-OP1	-6.15	100.17	105.70
36	5	2364	G	N9-C4-C5	6.15	107.86	105.40
36	5	3050	U	N1-C2-O2	6.15	127.10	122.80
36	1	188	U	C6-N1-C1'	6.14	129.80	121.20
36	1	1725	C	C6-N1-C2	6.14	122.76	120.30
36	5	30	G	O5'-P-OP2	6.14	118.07	110.70
36	5	924	G	N3-C4-N9	-6.14	122.31	126.00
36	5	2125	A	C5-C6-N6	-6.14	118.78	123.70
36	1	1216	C	O5'-P-OP2	-6.14	100.17	105.70
36	1	2313	A	N1-C6-N6	-6.14	114.92	118.60
36	5	2968	G	C4-C5-N7	-6.14	108.34	110.80
36	1	573	C	N3-C2-O2	-6.14	117.60	121.90
36	5	1444	G	O5'-P-OP2	6.14	118.06	110.70
36	1	2368	A	C6-N1-C2	-6.14	114.92	118.60
36	1	2762	A	N1-C6-N6	-6.14	114.92	118.60
1	6	364	G	N1-C6-O6	6.14	123.58	119.90
36	1	878	G	C5-C6-N1	-6.13	108.43	111.50
36	1	2404	A	C6-C5-N7	6.13	136.59	132.30
36	1	3046	A	O5'-P-OP1	-6.13	100.18	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1438	U	C4-C5-C6	6.13	123.38	119.70
36	5	2402	A	C8-N9-C4	-6.13	103.35	105.80
36	5	3362	A	C5-N7-C8	-6.13	100.83	103.90
36	1	2401	A	C5-C6-N6	-6.13	118.79	123.70
36	1	2836	C	N1-C2-N3	6.13	123.49	119.20
36	5	693	A	O5'-P-OP1	-6.13	100.18	105.70
36	1	347	G	N9-C4-C5	-6.13	102.95	105.40
36	1	1849	C	O5'-P-OP1	-6.13	100.18	105.70
37	3	82	G	N1-C2-N3	6.13	127.58	123.90
36	5	2379	U	N1-C2-N3	6.13	118.58	114.90
1	6	957	G	N1-C6-O6	6.13	123.58	119.90
1	2	1745	G	C8-N9-C1'	-6.13	119.04	127.00
36	5	518	G	C5-C6-N1	6.13	114.56	111.50
37	7	103	A	C2-N3-C4	6.13	113.66	110.60
36	1	2150	G	C6-C5-N7	-6.12	126.72	130.40
36	5	929	A	O5'-P-OP1	6.12	118.05	110.70
36	1	636	C	C5-C6-N1	-6.12	117.94	121.00
36	1	2372	A	C6-C5-N7	-6.12	128.01	132.30
36	5	1308	A	N9-C4-C5	6.12	108.25	105.80
36	5	1362	G	N1-C6-O6	-6.12	116.23	119.90
36	5	1483	G	O4'-C1'-N9	6.12	113.10	108.20
36	1	1304	A	N9-C4-C5	-6.12	103.35	105.80
36	1	2855	U	C5-C6-N1	-6.12	119.64	122.70
1	6	362	G	N3-C4-C5	-6.12	125.54	128.60
1	6	1463	C	C6-N1-C2	6.12	122.75	120.30
36	1	1100	U	C6-N1-C2	6.12	124.67	121.00
36	1	1114	U	C4-C5-C6	-6.12	116.03	119.70
36	5	1670	C	C6-N1-C2	6.12	122.75	120.30
36	5	2911	A	C8-N9-C4	-6.12	103.35	105.80
36	5	3314	A	C8-N9-C4	6.12	108.25	105.80
36	1	310	U	C5-C6-N1	-6.12	119.64	122.70
36	1	1057	A	C8-N9-C4	6.12	108.25	105.80
36	1	2808	A	C4-C5-N7	6.12	113.76	110.70
36	1	590	G	C4-C5-N7	6.12	113.25	110.80
36	1	2406	C	C6-N1-C2	6.12	122.75	120.30
36	5	3033	A	C2-N3-C4	-6.12	107.54	110.60
36	1	948	C	C6-N1-C2	6.11	122.75	120.30
36	1	2200	U	N3-C4-C5	-6.11	110.93	114.60
36	1	648	C	C2-N1-C1'	6.11	125.52	118.80
1	6	14	C	C6-N1-C2	-6.11	117.86	120.30
36	5	947	G	C6-N1-C2	-6.11	121.43	125.10
36	5	3141	A	N1-C2-N3	6.11	132.36	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2249	G	C5-C6-N1	6.11	114.56	111.50
1	6	372	G	C5-C6-O6	-6.11	124.93	128.60
10	s8	8	ARG	NE-CZ-NH2	-6.11	117.25	120.30
36	5	878	G	C4-C5-N7	6.11	113.24	110.80
36	5	2411	U	N3-C4-C5	6.11	118.27	114.60
36	1	94	G	O4'-C1'-N9	6.11	113.09	108.20
36	1	2345	A	C5-C6-N6	-6.11	118.81	123.70
36	5	2353	G	N3-C2-N2	-6.11	115.62	119.90
36	5	686	G	C8-N9-C4	6.11	108.84	106.40
36	1	1178	G	C6-C5-N7	-6.11	126.74	130.40
36	5	1152	G	C4-C5-C6	-6.11	115.14	118.80
36	5	2400	G	C2-N3-C4	-6.11	108.85	111.90
38	8	34	U	N1-C2-N3	6.11	118.56	114.90
38	8	139	U	C5-C4-O4	6.11	129.56	125.90
36	5	417	A	C8-N9-C4	6.10	108.24	105.80
36	1	2846	U	C5-C4-O4	6.10	129.56	125.90
36	5	1496	C	C5-C6-N1	6.10	124.05	121.00
36	5	2892	A	C4-C5-C6	6.10	120.05	117.00
36	5	2953	U	N3-C2-O2	6.10	126.47	122.20
36	1	1381	A	N9-C4-C5	-6.10	103.36	105.80
36	5	92	G	N1-C6-O6	-6.10	116.24	119.90
36	5	952	A	O5'-P-OP2	-6.10	100.21	105.70
36	1	658	G	C8-N9-C1'	-6.10	119.07	127.00
36	1	1365	G	C4-N9-C1'	6.10	134.43	126.50
36	1	2986	U	N1-C2-O2	-6.10	118.53	122.80
36	5	1360	C	N1-C2-O2	-6.10	115.24	118.90
36	1	654	C	C6-N1-C2	6.10	122.74	120.30
36	1	1351	U	C2-N1-C1'	6.10	125.02	117.70
36	1	2406	C	C5-C6-N1	-6.10	117.95	121.00
36	1	2617	U	C2-N3-C4	-6.10	123.34	127.00
38	4	115	C	C5-C6-N1	-6.10	117.95	121.00
1	6	1745	G	C6-C5-N7	-6.10	126.74	130.40
36	5	41	G	N9-C4-C5	-6.10	102.96	105.40
36	5	881	C	N1-C2-O2	6.10	122.56	118.90
36	5	2422	C	C5-C6-N1	-6.10	117.95	121.00
36	5	2849	C	N3-C2-O2	6.10	126.17	121.90
36	1	658	G	N1-C6-O6	6.10	123.56	119.90
36	1	694	C	N3-C4-C5	6.10	124.34	121.90
1	6	308	C	C6-N1-C1'	6.10	128.12	120.80
36	5	3215	A	C2-N3-C4	-6.10	107.55	110.60
36	1	938	C	C2-N1-C1'	6.09	125.50	118.80
1	6	418	G	O5'-P-OP1	-6.09	100.22	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2341	A	C8-N9-C4	6.09	108.24	105.80
37	3	82	G	N3-C4-N9	6.09	129.66	126.00
36	1	1434	G	N1-C2-N2	6.09	121.68	116.20
1	6	136	C	C2-N1-C1'	6.09	125.50	118.80
36	5	1149	G	C6-N1-C2	-6.09	121.45	125.10
1	6	1297	G	O5'-P-OP2	-6.09	100.22	105.70
36	5	2345	A	N9-C4-C5	-6.09	103.36	105.80
36	5	2920	U	C2-N3-C4	-6.09	123.35	127.00
36	5	3245	A	C6-C5-N7	-6.09	128.04	132.30
36	1	978	G	C4-C5-N7	6.09	113.23	110.80
36	1	1513	G	C5-C6-O6	-6.09	124.95	128.60
36	5	698	U	C4-C5-C6	6.09	123.35	119.70
36	5	1382	G	C8-N9-C4	6.09	108.83	106.40
78	Q2	93	LEU	CA-CB-CG	6.08	129.29	115.30
36	1	636	C	C2-N3-C4	-6.08	116.86	119.90
36	5	417	A	N7-C8-N9	-6.08	110.76	113.80
36	5	1140	G	OP1-P-O3'	6.08	118.58	105.20
36	5	1833	G	N1-C6-O6	-6.08	116.25	119.90
36	5	2244	A	O5'-P-OP2	-6.08	100.22	105.70
37	7	37	G	C5-C6-O6	-6.08	124.95	128.60
1	2	1599	C	N1-C2-O2	-6.08	115.25	118.90
36	1	24	G	C6-C5-N7	-6.08	126.75	130.40
36	1	1153	A	C8-N9-C4	6.08	108.23	105.80
36	5	1851	G	N1-C6-O6	6.08	123.55	119.90
36	5	3171	U	N3-C4-O4	-6.08	115.14	119.40
37	7	87	G	N1-C6-O6	6.08	123.55	119.90
36	1	1163	A	OP1-P-OP2	6.08	128.72	119.60
36	5	1292	C	OP1-P-OP2	6.08	128.72	119.60
36	1	586	C	N3-C2-O2	6.08	126.16	121.90
36	1	587	U	C2-N3-C4	-6.08	123.35	127.00
36	1	666	A	O5'-P-OP1	-6.08	100.23	105.70
1	6	1665	U	C5-C4-O4	-6.08	122.25	125.90
36	5	2890	A	O5'-P-OP2	6.08	117.99	110.70
64	N8	42	ARG	NE-CZ-NH1	6.08	123.34	120.30
24	d2	93	LEU	CA-CB-CG	6.08	129.28	115.30
36	5	364	G	N3-C4-C5	6.08	131.64	128.60
38	8	55	U	C5-C6-N1	6.08	125.74	122.70
36	1	1407	A	N7-C8-N9	-6.08	110.76	113.80
36	1	1894	U	C5-C6-N1	-6.08	119.66	122.70
36	1	2945	G	C6-C5-N7	-6.08	126.75	130.40
38	4	32	C	O5'-P-OP2	-6.08	100.23	105.70
36	5	1331	U	C2-N3-C4	-6.08	123.36	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	953	G	OP1-P-O3'	6.07	118.56	105.20
36	5	1448	U	N1-C2-O2	6.07	127.05	122.80
36	1	1846	C	O5'-P-OP1	-6.07	100.23	105.70
36	1	1907	C	N3-C2-O2	-6.07	117.65	121.90
36	1	2412	G	C6-C5-N7	-6.07	126.76	130.40
36	1	2944	U	C4-C5-C6	-6.07	116.06	119.70
36	1	3003	G	C8-N9-C4	6.07	108.83	106.40
36	1	590	G	N9-C4-C5	-6.07	102.97	105.40
36	1	984	G	C6-C5-N7	-6.07	126.76	130.40
36	5	356	C	N3-C4-N4	-6.07	113.75	118.00
36	5	378	A	C8-N9-C4	6.07	108.23	105.80
36	5	397	A	N1-C6-N6	-6.07	114.96	118.60
1	2	1196	A	P-O3'-C3'	6.07	126.98	119.70
36	1	919	U	C5-C4-O4	6.07	129.54	125.90
36	1	2627	C	C5-C6-N1	-6.07	117.97	121.00
36	5	664	U	N1-C2-N3	6.07	118.54	114.90
36	5	2295	A	C5-C6-N6	-6.07	118.84	123.70
36	1	1606	U	N1-C2-O2	-6.07	118.55	122.80
37	3	14	U	C6-N1-C2	6.07	124.64	121.00
36	5	31	C	N3-C4-C5	6.07	124.33	121.90
36	5	3109	G	C8-N9-C4	-6.07	103.97	106.40
36	1	939	U	C5-C4-O4	-6.07	122.26	125.90
36	5	2943	G	C5-N7-C8	-6.07	101.27	104.30
36	5	410	U	C6-N1-C2	-6.06	117.36	121.00
36	1	964	G	C5-C6-O6	-6.06	124.96	128.60
36	5	940	G	N1-C6-O6	-6.06	116.26	119.90
36	5	2943	G	C5-C6-O6	-6.06	124.96	128.60
36	5	3351	U	N1-C2-O2	6.06	127.04	122.80
36	1	3217	C	N1-C2-O2	6.06	122.54	118.90
36	5	1450	G	N1-C2-N2	6.06	121.66	116.20
36	5	1842	A	N9-C4-C5	-6.06	103.38	105.80
36	5	406	G	O4'-C1'-N9	6.06	113.05	108.20
36	5	3287	U	N3-C2-O2	-6.06	117.96	122.20
36	5	803	C	OP1-P-OP2	-6.06	110.51	119.60
36	5	890	C	O5'-P-OP2	-6.06	100.25	105.70
36	5	1321	G	N1-C6-O6	6.06	123.53	119.90
36	5	2954	U	N3-C2-O2	-6.06	117.96	122.20
36	1	325	A	OP2-P-O3'	6.05	118.52	105.20
1	6	447	U	N1-C2-N3	6.05	118.53	114.90
36	5	1331	U	C6-N1-C2	6.05	124.63	121.00
36	1	948	C	O5'-P-OP1	6.05	117.96	110.70
37	3	21	G	C8-N9-C4	6.05	108.82	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1773	C	N1-C2-O2	-6.05	115.27	118.90
36	5	1047	A	N1-C6-N6	6.05	122.23	118.60
36	5	1403	C	N3-C4-C5	6.05	124.32	121.90
36	5	2902	A	N1-C6-N6	6.05	122.23	118.60
36	5	3041	U	N3-C4-O4	-6.05	115.17	119.40
36	5	3190	C	N3-C4-C5	-6.05	119.48	121.90
38	8	20	U	N1-C2-N3	6.05	118.53	114.90
36	1	2727	A	O5'-P-OP1	-6.05	100.25	105.70
36	1	2831	G	N1-C6-O6	6.05	123.53	119.90
36	5	974	G	C6-N1-C2	-6.05	121.47	125.10
36	5	2117	A	C4-C5-N7	-6.05	107.67	110.70
36	5	3343	G	N3-C4-N9	6.05	129.63	126.00
38	4	13	A	O5'-P-OP1	-6.05	100.26	105.70
36	1	1100	U	N3-C4-O4	-6.05	115.17	119.40
36	1	2361	A	N1-C6-N6	-6.05	114.97	118.60
36	1	2371	G	N1-C2-N2	-6.04	110.76	116.20
36	1	651	G	N3-C4-N9	6.04	129.63	126.00
36	5	680	G	C8-N9-C4	6.04	108.82	106.40
36	5	2878	G	C8-N9-C4	6.04	108.82	106.40
36	1	386	A	C5-C6-N1	-6.04	114.68	117.70
36	1	3205	G	C8-N9-C4	6.04	108.82	106.40
36	5	957	C	N3-C2-O2	-6.04	117.67	121.90
36	5	2943	G	C4-N9-C1'	6.04	134.35	126.50
36	5	3382	U	C6-N1-C2	-6.04	117.38	121.00
36	1	3362	A	N1-C6-N6	6.04	122.22	118.60
1	2	571	G	C4-C5-N7	-6.04	108.39	110.80
36	1	31	C	C6-N1-C2	6.04	122.72	120.30
36	1	2606	G	C8-N9-C1'	-6.04	119.15	127.00
36	5	804	C	N3-C4-C5	-6.04	119.48	121.90
1	2	1773	C	N3-C4-N4	6.04	122.22	118.00
36	5	37	U	N1-C2-N3	6.04	118.52	114.90
36	5	3143	C	N1-C2-O2	-6.04	115.28	118.90
36	1	939	U	N1-C2-O2	-6.03	118.58	122.80
36	5	637	C	O5'-P-OP1	-6.03	100.27	105.70
36	5	1494	U	C5-C6-N1	-6.03	119.68	122.70
1	2	1490	C	C6-N1-C2	-6.03	117.89	120.30
36	1	2993	G	N1-C6-O6	-6.03	116.28	119.90
36	1	798	G	N9-C4-C5	6.03	107.81	105.40
36	1	2550	U	N3-C2-O2	-6.03	117.98	122.20
36	1	2918	G	C6-C5-N7	-6.03	126.78	130.40
1	6	402	C	O5'-P-OP2	-6.03	100.27	105.70
1	6	1653	C	C4-C5-C6	6.03	120.42	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1124	U	C5-C4-O4	6.03	129.52	125.90
36	1	2402	A	C6-N1-C2	-6.03	114.98	118.60
36	5	1081	U	C5-C6-N1	6.03	125.72	122.70
36	5	1389	G	N1-C6-O6	6.03	123.52	119.90
36	5	2891	U	C2-N3-C4	-6.03	123.38	127.00
38	4	97	A	O5'-P-OP2	-6.03	100.28	105.70
36	5	1049	C	N1-C2-O2	6.03	122.52	118.90
36	5	1294	A	O4'-C1'-N9	6.03	113.02	108.20
36	5	2814	G	N1-C2-N2	-6.03	110.78	116.20
36	1	2305	G	N1-C6-O6	6.02	123.52	119.90
36	5	2882	U	O5'-P-OP2	-6.02	100.28	105.70
1	2	192	U	C2-N1-C1'	6.02	124.93	117.70
36	5	1447	G	C4-C5-N7	-6.02	108.39	110.80
36	5	2833	A	C6-N1-C2	-6.02	114.99	118.60
36	5	2891	U	N3-C4-C5	6.02	118.21	114.60
36	1	1520	G	N7-C8-N9	-6.02	110.09	113.10
36	5	1499	C	N3-C4-N4	-6.02	113.79	118.00
36	1	1381	A	OP1-P-O3'	6.02	118.44	105.20
36	5	2140	U	N1-C2-N3	6.02	118.51	114.90
36	5	3218	A	C2-N3-C4	-6.02	107.59	110.60
36	1	1169	A	OP2-P-O3'	6.02	118.44	105.20
36	1	2372	A	N1-C6-N6	6.02	122.21	118.60
36	1	2993	G	N3-C4-N9	6.02	129.61	126.00
36	1	289	A	C8-N9-C4	6.01	108.21	105.80
36	1	1392	G	N3-C4-C5	-6.01	125.59	128.60
36	1	1852	G	C5-C6-O6	-6.01	124.99	128.60
1	6	144	U	C6-N1-C2	-6.01	117.39	121.00
36	1	865	U	C5-C6-N1	-6.01	119.69	122.70
36	1	1386	A	C6-N1-C2	-6.01	114.99	118.60
36	5	2584	G	C8-N9-C4	-6.01	104.00	106.40
36	1	1296	C	C4-C5-C6	6.01	120.41	117.40
36	1	1443	G	C8-N9-C4	-6.01	104.00	106.40
36	5	889	U	C6-N1-C2	6.01	124.61	121.00
36	5	1442	U	OP1-P-O3'	6.01	118.43	105.20
36	5	1842	A	O5'-P-OP2	-6.01	100.29	105.70
1	2	163	G	C8-N9-C4	-6.01	104.00	106.40
1	2	1777	G	C6-C5-N7	-6.01	126.79	130.40
36	1	1199	C	N3-C2-O2	-6.01	117.69	121.90
36	1	2987	A	N1-C2-N3	6.01	132.31	129.30
1	6	565	C	C5-C6-N1	-6.01	118.00	121.00
36	5	1152	G	C6-N1-C2	6.01	128.71	125.10
36	5	2693	C	C2-N3-C4	-6.01	116.90	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	961	C	C5-C6-N1	-6.01	118.00	121.00
36	1	2374	C	C4-C5-C6	6.01	120.40	117.40
36	1	2873	U	O5'-P-OP2	-6.01	100.30	105.70
36	5	1369	A	N1-C6-N6	6.01	122.20	118.60
36	5	2899	C	C4-C5-C6	6.00	120.40	117.40
36	1	2850	G	C5-C6-O6	-6.00	125.00	128.60
36	5	1454	A	C4-C5-N7	6.00	113.70	110.70
36	1	880	G	C4-C5-N7	-6.00	108.40	110.80
36	1	1152	G	O5'-P-OP1	-6.00	100.30	105.70
36	5	1884	A	OP2-P-O3'	6.00	118.40	105.20
36	1	925	A	N1-C2-N3	6.00	132.30	129.30
36	5	776	U	N3-C4-O4	-6.00	115.20	119.40
36	1	2622	C	O5'-P-OP1	6.00	117.90	110.70
36	5	35	A	C5-C6-N6	-6.00	118.90	123.70
1	6	404	G	N3-C2-N2	-6.00	115.70	119.90
36	5	217	U	C6-N1-C2	6.00	124.60	121.00
36	5	345	G	N1-C6-O6	6.00	123.50	119.90
36	5	1426	C	C5-C4-N4	-6.00	116.00	120.20
36	5	2871	G	N3-C2-N2	6.00	124.10	119.90
36	1	1552	G	N1-C6-O6	6.00	123.50	119.90
36	1	3052	G	C5-C6-O6	-6.00	125.00	128.60
36	1	1386	A	N3-C4-N9	5.99	132.19	127.40
1	6	308	C	N1-C2-N3	5.99	123.39	119.20
1	6	542	A	O5'-P-OP1	-5.99	100.31	105.70
36	1	504	A	C8-N9-C4	5.99	108.20	105.80
36	1	229	G	C5-C6-O6	-5.99	125.01	128.60
1	6	1085	G	C5-C6-O6	5.99	132.19	128.60
36	5	1549	U	C6-N1-C2	5.99	124.59	121.00
69	O3	89	LEU	CB-CG-CD2	-5.99	100.82	111.00
36	1	994	G	N3-C2-N2	5.99	124.09	119.90
36	1	2276	G	N3-C2-N2	-5.99	115.71	119.90
41	L4	313	LEU	CA-CB-CG	5.99	129.07	115.30
1	6	1773	C	C6-N1-C2	-5.99	117.91	120.30
36	1	423	A	C4-C5-C6	5.98	119.99	117.00
36	5	35	A	N1-C6-N6	5.98	122.19	118.60
36	5	2962	U	C6-N1-C2	-5.98	117.41	121.00
36	1	646	A	N1-C2-N3	5.98	132.29	129.30
36	1	1429	G	N1-C2-N2	-5.98	110.82	116.20
36	1	1436	U	OP1-P-OP2	-5.98	110.62	119.60
36	1	1620	U	O5'-P-OP2	-5.98	100.32	105.70
36	1	2138	A	C2-N3-C4	-5.98	107.61	110.60
37	3	81	U	C5-C6-N1	-5.98	119.71	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1274	C	C6-N1-C2	-5.98	117.91	120.30
36	1	1419	A	O5'-P-OP1	5.98	117.88	110.70
36	5	220	G	O5'-P-OP2	-5.98	100.32	105.70
36	1	3361	G	N3-C4-C5	-5.98	125.61	128.60
1	6	1600	A	N9-C1'-C2'	5.98	121.77	114.00
36	5	1337	A	N1-C6-N6	5.98	122.19	118.60
36	1	636	C	C5-C4-N4	-5.97	116.02	120.20
36	1	2385	G	N3-C4-C5	5.97	131.59	128.60
36	1	2897	A	C8-N9-C4	5.97	108.19	105.80
1	6	1200	G	N3-C2-N2	-5.97	115.72	119.90
36	5	1115	G	C8-N9-C1'	-5.97	119.23	127.00
1	2	971	A	C4-C5-C6	5.97	119.99	117.00
36	1	659	G	C6-C5-N7	-5.97	126.82	130.40
36	1	937	G	C5-C6-O6	-5.97	125.02	128.60
36	1	2369	G	N3-C2-N2	-5.97	115.72	119.90
36	5	726	G	N1-C6-O6	5.97	123.48	119.90
36	5	2372	A	N7-C8-N9	5.97	116.79	113.80
36	1	95	A	C2-N3-C4	-5.97	107.61	110.60
36	1	1429	G	C8-N9-C1'	-5.97	119.24	127.00
36	5	40	A	O5'-P-OP1	-5.97	100.33	105.70
36	1	2699	G	C6-C5-N7	-5.97	126.82	130.40
70	O4	51	LEU	CA-CB-CG	5.97	129.03	115.30
1	6	564	G	C8-N9-C4	-5.97	104.01	106.40
36	5	823	C	C6-N1-C2	5.97	122.69	120.30
36	5	694	C	N1-C2-O2	5.97	122.48	118.90
36	1	1329	U	C6-N1-C2	-5.97	117.42	121.00
20	c8	15	LEU	CA-CB-CG	5.97	129.02	115.30
36	5	908	G	C5-C6-O6	-5.97	125.02	128.60
36	5	1528	G	C6-C5-N7	-5.97	126.82	130.40
36	5	2186	U	O5'-P-OP1	5.97	117.86	110.70
36	5	2395	G	C5-C6-N1	5.97	114.48	111.50
36	5	2758	A	O4'-C1'-N9	5.97	112.97	108.20
36	1	1002	A	C8-N9-C4	5.96	108.19	105.80
36	5	812	G	C4-C5-N7	-5.96	108.41	110.80
36	5	3211	C	C5-C6-N1	-5.96	118.02	121.00
36	1	1205	A	N9-C4-C5	-5.96	103.42	105.80
36	5	974	G	C5-C6-N1	5.96	114.48	111.50
36	5	994	G	OP1-P-O3'	5.96	118.32	105.20
36	5	2853	A	C8-N9-C4	5.96	108.19	105.80
36	1	2417	U	C5-C6-N1	-5.96	119.72	122.70
36	5	1392	G	N1-C6-O6	5.96	123.48	119.90
36	1	895	A	C5-C6-N6	-5.96	118.93	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	803	C	C6-N1-C2	-5.96	117.92	120.30
36	5	2852	C	N3-C2-O2	5.96	126.07	121.90
36	1	2364	G	C5-N7-C8	5.96	107.28	104.30
36	5	1302	A	O5'-P-OP2	5.96	117.85	110.70
36	1	3269	U	N3-C2-O2	-5.96	118.03	122.20
36	5	3178	A	C2-N3-C4	-5.96	107.62	110.60
36	1	2632	G	OP1-P-O3'	5.96	118.30	105.20
36	5	2400	G	C6-C5-N7	-5.96	126.83	130.40
36	1	55	G	N7-C8-N9	-5.95	110.12	113.10
36	5	1146	C	C6-N1-C2	5.95	122.68	120.30
36	5	1136	A	C2-N3-C4	-5.95	107.62	110.60
1	2	572	C	O5'-P-OP1	-5.95	100.34	105.70
36	1	1520	G	C8-N9-C4	5.95	108.78	106.40
36	1	2963	C	C2-N3-C4	-5.95	116.92	119.90
61	N5	115	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	6	458	G	C8-N9-C4	-5.95	104.02	106.40
36	5	1165	A	N9-C4-C5	-5.95	103.42	105.80
36	5	2306	C	O5'-P-OP2	-5.95	100.34	105.70
36	5	2685	C	C2-N3-C4	-5.95	116.92	119.90
1	2	73	U	OP1-P-O3'	5.95	118.29	105.20
52	M6	110	PRO	C-N-CD	-5.95	107.52	120.60
36	5	834	U	N3-C4-O4	-5.95	115.24	119.40
36	1	608	A	C6-C5-N7	-5.95	128.14	132.30
36	1	3274	A	C8-N9-C4	-5.95	103.42	105.80
36	1	2300	G	O5'-P-OP1	-5.95	100.35	105.70
36	1	2920	U	C2-N3-C4	-5.94	123.43	127.00
36	1	3075	G	N1-C6-O6	5.94	123.47	119.90
36	1	339	C	N3-C4-N4	-5.94	113.84	118.00
36	1	353	G	C5-C6-O6	-5.94	125.03	128.60
36	5	2834	G	N1-C6-O6	5.94	123.47	119.90
36	5	2848	G	N1-C6-O6	5.94	123.47	119.90
36	5	3288	G	C5-C6-N1	5.94	114.47	111.50
1	6	1634	C	N3-C2-O2	-5.94	117.74	121.90
36	1	110	G	O4'-C1'-N9	5.94	112.95	108.20
36	1	2758	A	C8-N9-C4	5.94	108.18	105.80
36	5	666	A	N7-C8-N9	-5.94	110.83	113.80
36	5	875	G	N1-C2-N3	5.94	127.46	123.90
36	5	2297	U	C5-C4-O4	5.94	129.46	125.90
1	2	70	C	C6-N1-C2	5.94	122.67	120.30
36	1	895	A	N9-C4-C5	-5.94	103.42	105.80
36	1	2356	A	C5-N7-C8	-5.94	100.93	103.90
1	6	1007	C	C6-N1-C2	5.94	122.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1121	U	C5-C6-N1	-5.94	119.73	122.70
36	5	2339	C	OP1-P-O3'	5.94	118.26	105.20
36	1	3001	C	C2-N1-C1'	-5.94	112.27	118.80
38	8	92	A	N1-C6-N6	5.94	122.16	118.60
1	2	1796	C	C4-C5-C6	5.93	120.37	117.40
1	6	1121	C	C5-C6-N1	-5.93	118.03	121.00
1	6	1141	G	N1-C6-O6	5.93	123.46	119.90
36	5	2907	G	C8-N9-C4	-5.93	104.03	106.40
36	5	3269	U	P-O3'-C3'	5.93	126.82	119.70
36	5	2320	A	C5-C6-N6	5.93	128.45	123.70
36	5	2364	G	N1-C6-O6	-5.93	116.34	119.90
36	1	1931	U	C2-N1-C1'	-5.93	110.58	117.70
36	1	2130	G	N1-C2-N3	5.93	127.46	123.90
36	1	2379	U	N1-C2-O2	-5.93	118.65	122.80
36	1	3207	U	C2-N1-C1'	-5.93	110.58	117.70
1	6	1164	G	C5-C6-O6	-5.93	125.04	128.60
36	5	945	C	C6-N1-C1'	-5.93	113.68	120.80
36	5	1395	G	OP2-P-O3'	5.93	118.25	105.20
36	5	2943	G	C8-N9-C1'	-5.93	119.29	127.00
36	5	3107	U	C5-C4-O4	-5.93	122.34	125.90
36	5	1211	U	O5'-P-OP2	-5.93	100.36	105.70
36	5	1417	G	N3-C4-N9	5.93	129.56	126.00
36	1	431	U	C5-C4-O4	-5.93	122.34	125.90
36	1	1487	G	O5'-P-OP1	-5.93	100.37	105.70
1	6	1765	A	N1-C6-N6	-5.93	115.04	118.60
36	5	43	A	C2-N3-C4	-5.93	107.64	110.60
36	5	2728	G	O5'-P-OP2	-5.93	100.37	105.70
36	1	2159	U	C6-N1-C2	5.92	124.56	121.00
36	1	2620	G	C8-N9-C4	5.92	108.77	106.40
36	5	2357	A	O5'-P-OP1	-5.92	100.37	105.70
36	5	2902	A	C5-C6-N6	-5.92	118.96	123.70
36	5	1306	G	C5-C6-N1	5.92	114.46	111.50
1	2	458	G	C5-C6-N1	-5.92	108.54	111.50
1	2	1300	A	N1-C6-N6	-5.92	115.05	118.60
36	5	744	A	N1-C6-N6	5.92	122.15	118.60
36	5	3014	U	C2-N3-C4	-5.92	123.45	127.00
36	1	945	C	C2-N3-C4	-5.92	116.94	119.90
36	5	1911	A	N1-C2-N3	5.92	132.26	129.30
36	1	1128	U	N3-C4-C5	5.92	118.15	114.60
36	1	2136	C	N3-C2-O2	5.92	126.04	121.90
36	1	3203	U	C5-C4-O4	5.92	129.45	125.90
1	2	1600	A	N1-C6-N6	5.92	122.15	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	3	88	G	N3-C4-C5	-5.92	125.64	128.60
36	5	3028	G	N3-C2-N2	5.92	124.04	119.90
36	1	3079	U	C6-N1-C1'	5.92	129.48	121.20
36	5	979	U	C6-N1-C2	-5.92	117.45	121.00
36	5	1433	A	O5'-P-OP2	5.92	117.80	110.70
36	1	908	G	C8-N9-C1'	-5.91	119.31	127.00
36	5	834	U	C5-C6-N1	-5.91	119.74	122.70
36	5	1048	A	C8-N9-C4	5.91	108.17	105.80
36	5	2389	C	O5'-P-OP1	-5.91	100.38	105.70
36	5	2643	A	N9-C4-C5	-5.91	103.44	105.80
36	5	1130	A	C8-N9-C4	5.91	108.17	105.80
36	5	3209	A	C5-N7-C8	-5.91	100.94	103.90
36	1	960	U	C6-N1-C2	5.91	124.55	121.00
36	1	984	G	N3-C2-N2	5.91	124.04	119.90
1	6	512	A	P-O3'-C3'	5.91	126.79	119.70
1	2	1089	U	N3-C2-O2	-5.91	118.06	122.20
36	1	2706	G	C6-C5-N7	-5.91	126.86	130.40
36	1	2949	U	N3-C2-O2	5.91	126.33	122.20
1	6	795	U	N3-C2-O2	-5.91	118.06	122.20
36	5	1316	C	C5-C4-N4	-5.91	116.06	120.20
36	1	2924	U	N3-C2-O2	5.91	126.33	122.20
36	1	3344	A	C6-C5-N7	-5.91	128.17	132.30
36	1	1324	U	C5-C6-N1	-5.90	119.75	122.70
1	2	720	G	OP1-P-O3'	5.90	118.18	105.20
36	1	1909	A	N1-C6-N6	5.90	122.14	118.60
1	6	333	A	N1-C2-N3	5.90	132.25	129.30
1	6	371	G	C4-N9-C1'	5.90	134.17	126.50
38	8	103	G	N3-C4-N9	5.90	129.54	126.00
36	5	42	C	N1-C2-O2	5.90	122.44	118.90
36	5	2775	U	C5-C6-N1	-5.90	119.75	122.70
38	8	79	A	N7-C8-N9	5.90	116.75	113.80
36	1	666	A	N7-C8-N9	-5.90	110.85	113.80
36	1	2871	G	O5'-P-OP2	-5.90	100.39	105.70
36	5	971	G	N1-C6-O6	5.90	123.44	119.90
36	5	2707	C	N3-C4-C5	5.90	124.26	121.90
36	1	2314	U	N3-C4-C5	5.90	118.14	114.60
36	1	3001	C	C5-C6-N1	-5.89	118.05	121.00
38	4	7	U	C5-C6-N1	-5.89	119.75	122.70
36	5	140	C	N1-C2-O2	-5.89	115.36	118.90
36	5	2396	G	N3-C2-N2	-5.89	115.77	119.90
36	5	3093	C	C5-C6-N1	-5.89	118.05	121.00
1	2	582	U	C2-N1-C1'	5.89	124.77	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1241	G	C6-C5-N7	-5.89	126.86	130.40
36	1	909	G	N1-C6-O6	-5.89	116.36	119.90
36	1	1344	G	C4-C5-N7	5.89	113.16	110.80
36	1	1585	C	N3-C4-C5	5.89	124.26	121.90
38	4	108	C	N3-C4-C5	-5.89	119.54	121.90
36	5	718	G	N3-C4-N9	5.89	129.54	126.00
36	5	1339	C	C6-N1-C2	-5.89	117.94	120.30
36	5	1445	U	N1-C2-N3	5.89	118.44	114.90
36	5	2385	G	C8-N9-C4	5.89	108.76	106.40
36	5	2943	G	C4-C5-C6	5.89	122.33	118.80
36	1	111	C	N3-C4-C5	5.89	124.26	121.90
1	6	337	G	C8-N9-C1'	-5.89	119.34	127.00
36	5	504	A	C5-C6-N6	-5.89	118.99	123.70
36	5	1394	A	C5-C6-N1	5.89	120.64	117.70
36	1	49	A	O5'-P-OP1	-5.89	100.40	105.70
36	1	716	A	N3-C4-C5	5.89	130.92	126.80
36	1	1609	C	O5'-P-OP1	-5.89	100.40	105.70
36	5	2870	C	C6-N1-C1'	5.89	127.87	120.80
36	1	1199	C	C6-N1-C2	5.89	122.65	120.30
36	1	1405	U	OP1-P-OP2	5.89	128.43	119.60
36	5	1100	U	C5-C6-N1	-5.89	119.76	122.70
36	5	2191	U	N1-C2-O2	5.89	126.92	122.80
36	1	2351	U	N3-C4-O4	-5.88	115.28	119.40
36	1	2935	U	OP2-P-O3'	5.88	118.14	105.20
36	1	1047	A	O5'-P-OP1	5.88	117.76	110.70
1	6	1012	U	N3-C4-O4	-5.88	115.28	119.40
36	5	1152	G	N1-C6-O6	5.88	123.43	119.90
1	6	1537	C	C6-N1-C1'	5.88	127.86	120.80
36	5	589	A	O4'-C1'-N9	-5.88	103.50	108.20
36	5	2404	A	N1-C6-N6	5.88	122.13	118.60
36	1	82	C	C6-N1-C2	5.88	122.65	120.30
1	6	116	U	N3-C4-C5	-5.88	111.07	114.60
36	5	187	A	C6-N1-C2	-5.88	115.07	118.60
36	5	1513	G	OP1-P-O3'	5.88	118.13	105.20
1	2	48	G	O5'-P-OP2	-5.88	100.41	105.70
36	1	861	C	O5'-P-OP1	5.88	117.75	110.70
36	5	895	A	C6-N1-C2	-5.88	115.07	118.60
36	5	2709	C	C6-N1-C2	5.88	122.65	120.30
36	5	2927	C	OP2-P-O3'	5.88	118.13	105.20
37	7	28	C	C4-C5-C6	5.88	120.34	117.40
36	1	716	A	C4-C5-N7	5.88	113.64	110.70
1	2	1456	C	C2-N1-C1'	5.87	125.26	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2723	U	C5-C6-N1	-5.87	119.76	122.70
36	5	2158	A	C5-C6-N1	5.87	120.64	117.70
36	5	2424	A	N1-C6-N6	5.87	122.12	118.60
1	2	1370	U	P-O3'-C3'	5.87	126.75	119.70
36	5	641	C	C2-N3-C4	-5.87	116.96	119.90
36	5	2145	A	C6-N1-C2	-5.87	115.08	118.60
37	7	27	A	N1-C6-N6	5.87	122.12	118.60
38	4	29	U	C5-C4-O4	-5.87	122.38	125.90
1	2	81	G	N1-C6-O6	5.87	123.42	119.90
1	2	831	U	C5-C6-N1	5.87	125.64	122.70
1	2	1761	U	N3-C2-O2	-5.87	118.09	122.20
36	1	2371	G	OP2-P-O3'	5.87	118.11	105.20
1	6	352	A	C6-C5-N7	5.87	136.41	132.30
36	5	1162	U	OP1-P-OP2	5.87	128.40	119.60
1	2	1110	G	N3-C4-C5	5.87	131.53	128.60
36	1	1177	G	O5'-P-OP1	-5.87	100.42	105.70
36	1	2910	A	C2-N3-C4	-5.87	107.67	110.60
36	1	3079	U	N1-C2-O2	-5.87	118.69	122.80
36	1	3110	C	C6-N1-C2	-5.87	117.95	120.30
36	1	92	G	N1-C6-O6	-5.87	116.38	119.90
36	1	676	G	C4-N9-C1'	5.87	134.12	126.50
36	1	959	C	C6-N1-C2	5.87	122.65	120.30
36	1	2305	G	C5-C6-O6	-5.87	125.08	128.60
36	1	3125	U	C6-N1-C2	5.87	124.52	121.00
36	5	813	G	N9-C4-C5	-5.87	103.05	105.40
1	2	587	C	C6-N1-C2	-5.86	117.95	120.30
36	1	2417	U	C2-N3-C4	-5.86	123.48	127.00
36	1	2606	G	N3-C2-N2	5.86	124.00	119.90
36	1	2889	C	C6-N1-C2	-5.86	117.95	120.30
1	6	1724	U	N3-C4-O4	-5.86	115.30	119.40
36	5	437	G	C8-N9-C4	-5.86	104.06	106.40
36	5	786	A	N1-C6-N6	5.86	122.12	118.60
51	M5	159	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	6	1634	C	C2-N1-C1'	5.86	125.25	118.80
36	5	668	G	N1-C6-O6	-5.86	116.38	119.90
36	1	2855	U	C2-N3-C4	-5.86	123.48	127.00
1	6	1653	C	N3-C4-C5	-5.86	119.56	121.90
36	5	218	G	OP1-P-OP2	5.86	128.39	119.60
36	5	969	C	C2-N3-C4	-5.86	116.97	119.90
36	5	1116	G	C4-C5-C6	5.86	122.32	118.80
36	5	3103	A	C5-C6-N1	5.86	120.63	117.70
36	5	3306	U	O5'-P-OP2	-5.86	100.42	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	m0	90	ARG	NE-CZ-NH1	-5.86	117.37	120.30
36	1	1601	U	C5-C6-N1	-5.86	119.77	122.70
36	1	3181	C	C6-N1-C2	-5.86	117.96	120.30
36	5	1367	G	C6-C5-N7	-5.86	126.89	130.40
36	5	1897	G	C5-C6-N1	-5.86	108.57	111.50
36	5	2953	U	OP2-P-O3'	5.86	118.09	105.20
36	1	2309	A	N1-C6-N6	5.86	122.11	118.60
36	1	2641	U	C6-N1-C2	5.86	124.51	121.00
36	5	2598	G	N1-C6-O6	5.86	123.41	119.90
36	5	3043	C	C5-C6-N1	-5.86	118.07	121.00
1	2	1100	G	N1-C6-O6	5.85	123.41	119.90
36	5	1189	C	N1-C2-O2	-5.85	115.39	118.90
36	1	2726	C	C6-N1-C2	-5.85	117.96	120.30
1	6	1440	C	C6-N1-C2	-5.85	117.96	120.30
36	5	1433	A	C8-N9-C4	-5.85	103.46	105.80
36	5	3321	C	C6-N1-C2	5.85	122.64	120.30
37	7	85	G	O5'-P-OP2	5.85	117.72	110.70
36	1	709	A	C8-N9-C4	5.85	108.14	105.80
36	1	2286	U	O5'-P-OP2	-5.85	100.44	105.70
1	6	1136	U	O5'-P-OP1	-5.85	100.44	105.70
36	5	48	A	N9-C4-C5	5.85	108.14	105.80
36	5	1134	G	O5'-P-OP2	-5.85	100.44	105.70
36	1	968	G	N3-C4-C5	-5.85	125.68	128.60
36	1	981	U	C5-C6-N1	5.85	125.62	122.70
1	2	1104	U	N3-C4-O4	-5.85	115.31	119.40
36	1	913	A	C8-N9-C4	-5.85	103.46	105.80
36	5	400	G	C8-N9-C4	-5.85	104.06	106.40
36	1	1097	G	P-O3'-C3'	5.84	126.71	119.70
36	5	2110	G	C8-N9-C4	5.84	108.74	106.40
1	2	389	G	C4-N9-C1'	5.84	134.09	126.50
1	6	1058	U	OP1-P-O3'	5.84	118.05	105.20
36	1	267	G	C2-N3-C4	-5.84	108.98	111.90
36	1	1192	C	C2-N3-C4	5.84	122.82	119.90
1	2	389	G	N3-C4-C5	-5.84	125.68	128.60
1	2	864	U	C5-C4-O4	5.84	129.40	125.90
36	1	1509	A	N7-C8-N9	-5.84	110.88	113.80
36	5	776	U	C4-C5-C6	5.84	123.20	119.70
36	5	1482	A	O5'-P-OP2	-5.84	100.44	105.70
37	3	82	G	C4-N9-C1'	5.84	134.09	126.50
36	5	3141	A	O5'-P-OP1	-5.84	100.45	105.70
36	1	362	U	C5-C6-N1	-5.83	119.78	122.70
36	1	924	G	O5'-P-OP1	-5.83	100.45	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	635	A	C2-N3-C4	-5.83	107.68	110.60
36	5	969	C	C2-N1-C1'	-5.83	112.38	118.80
36	5	1121	U	OP2-P-O3'	5.83	118.03	105.20
38	8	55	U	C6-N1-C2	-5.83	117.50	121.00
36	1	1001	G	C8-N9-C4	5.83	108.73	106.40
36	1	1503	A	P-O3'-C3'	-5.83	112.70	119.70
36	5	2350	C	N3-C4-C5	5.83	124.23	121.90
36	1	3194	C	C2-N1-C1'	-5.83	112.39	118.80
36	5	3042	U	N3-C4-O4	-5.83	115.32	119.40
1	6	1657	U	C5-C6-N1	5.83	125.61	122.70
36	1	215	G	N3-C4-C5	-5.83	125.69	128.60
36	1	3242	G	C8-N9-C4	5.83	108.73	106.40
1	6	1128	C	N1-C2-O2	-5.83	115.40	118.90
36	1	2406	C	C5-C4-N4	-5.83	116.12	120.20
37	3	89	G	C5-C6-O6	-5.83	125.11	128.60
36	5	658	G	N1-C6-O6	5.83	123.40	119.90
36	5	718	G	C8-N9-C1'	-5.83	119.43	127.00
36	5	945	C	C4-C5-C6	5.83	120.31	117.40
36	5	1340	G	N9-C4-C5	-5.83	103.07	105.40
36	5	2351	U	N1-C2-N3	5.83	118.39	114.90
36	1	120	G	N9-C4-C5	-5.82	103.07	105.40
36	1	1149	G	C6-C5-N7	-5.82	126.91	130.40
36	1	1365	G	C4-C5-C6	5.82	122.29	118.80
36	1	1898	G	C8-N9-C4	5.82	108.73	106.40
36	1	2241	U	C2-N1-C1'	-5.82	110.71	117.70
1	6	1200	G	N3-C4-C5	5.82	131.51	128.60
36	1	304	G	N3-C4-N9	-5.82	122.51	126.00
36	1	950	G	C5-C6-O6	-5.82	125.11	128.60
36	1	3078	U	C5-C6-N1	5.82	125.61	122.70
36	1	31	C	N3-C4-C5	5.82	124.23	121.90
36	1	587	U	C5-C6-N1	-5.82	119.79	122.70
36	1	922	U	N3-C4-O4	-5.82	115.33	119.40
36	5	3371	G	N1-C6-O6	5.82	123.39	119.90
36	1	2850	G	C6-C5-N7	-5.82	126.91	130.40
65	n9	23	LYS	C-N-CD	5.82	140.62	128.40
36	1	704	U	C5-C4-O4	-5.82	122.41	125.90
36	1	1132	C	O5'-P-OP1	-5.82	100.46	105.70
36	5	1712	G	C5-C6-O6	-5.82	125.11	128.60
36	5	1838	G	C5-C6-O6	-5.82	125.11	128.60
36	1	1128	U	N3-C4-O4	-5.82	115.33	119.40
47	M0	24	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	6	901	G	C5-C6-O6	-5.82	125.11	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2930	A	O4'-C1'-N9	5.82	112.85	108.20
62	N6	57	LEU	CA-CB-CG	5.81	128.67	115.30
1	6	1514	U	N3-C4-O4	-5.81	115.33	119.40
1	2	1022	C	C6-N1-C2	5.81	122.62	120.30
36	1	639	G	N3-C2-N2	-5.81	115.83	119.90
36	1	2287	C	N1-C2-O2	-5.81	115.41	118.90
36	1	2953	U	N1-C2-O2	-5.81	118.73	122.80
36	5	933	A	C6-N1-C2	-5.81	115.11	118.60
36	5	1121	U	C2-N3-C4	-5.81	123.51	127.00
36	5	1669	C	C6-N1-C2	5.81	122.62	120.30
36	5	1751	G	C8-N9-C4	5.81	108.72	106.40
36	5	3307	A	C8-N9-C4	5.81	108.12	105.80
37	7	12	U	N3-C4-C5	5.81	118.09	114.60
36	1	395	A	C8-N9-C4	-5.81	103.47	105.80
1	6	941	A	C2-N3-C4	5.81	113.50	110.60
36	5	1365	G	C6-C5-N7	-5.81	126.92	130.40
36	5	2283	G	C4-C5-N7	5.81	113.12	110.80
36	1	2393	G	N3-C2-N2	-5.81	115.83	119.90
36	1	2823	G	N9-C4-C5	5.81	107.72	105.40
36	1	3065	G	N1-C6-O6	5.81	123.39	119.90
1	6	18	C	N3-C4-C5	-5.81	119.58	121.90
36	5	3288	G	N1-C6-O6	-5.81	116.42	119.90
36	1	2914	G	OP1-P-OP2	5.81	128.31	119.60
36	1	3034	C	O5'-P-OP2	-5.80	100.48	105.70
36	5	2813	A	N1-C2-N3	5.80	132.20	129.30
1	6	308	C	C2-N1-C1'	-5.80	112.42	118.80
36	5	962	A	C4-C5-C6	5.80	119.90	117.00
36	5	2125	A	N1-C6-N6	5.80	122.08	118.60
36	1	2785	A	C8-N9-C4	5.80	108.12	105.80
36	5	3172	A	C2-N3-C4	-5.80	107.70	110.60
1	6	1648	A	N9-C4-C5	-5.80	103.48	105.80
36	5	1198	C	N3-C2-O2	-5.80	117.84	121.90
36	1	661	G	N7-C8-N9	5.80	116.00	113.10
36	5	2964	G	O5'-P-OP2	-5.80	100.48	105.70
36	5	1194	G	N9-C4-C5	5.80	107.72	105.40
3	S1	96	LEU	CA-CB-CG	5.79	128.63	115.30
36	1	1907	C	C6-N1-C2	-5.79	117.98	120.30
36	5	376	G	C8-N9-C4	-5.79	104.08	106.40
1	2	137	U	O5'-P-OP1	-5.79	100.49	105.70
36	1	584	G	C5-C6-O6	5.79	132.08	128.60
36	1	1321	G	C8-N9-C4	-5.79	104.08	106.40
36	1	1329	U	C6-N1-C1'	-5.79	113.09	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2643	A	N1-C6-N6	5.79	122.08	118.60
36	5	2234	G	C8-N9-C4	5.79	108.72	106.40
36	1	24	G	N3-C4-N9	5.79	129.47	126.00
36	5	534	U	N3-C2-O2	-5.79	118.15	122.20
36	5	660	A	C4-C5-N7	-5.79	107.80	110.70
36	1	1381	A	C6-C5-N7	-5.79	128.25	132.30
36	1	3000	A	C8-N9-C4	5.79	108.12	105.80
37	3	103	A	C5-C6-N6	-5.79	119.07	123.70
36	1	951	A	C2-N3-C4	-5.79	107.70	110.60
36	1	2402	A	C5-C6-N6	-5.79	119.07	123.70
36	1	3319	U	P-O3'-C3'	5.79	126.65	119.70
1	6	90	C	N1-C2-O2	5.79	122.37	118.90
36	5	868	C	N3-C2-O2	5.79	125.95	121.90
36	5	2234	G	N9-C4-C5	-5.79	103.08	105.40
36	5	2627	C	N3-C2-O2	-5.79	117.85	121.90
1	2	1432	U	C6-N1-C2	5.79	124.47	121.00
36	1	2309	A	C5-C6-N6	-5.79	119.07	123.70
36	1	2901	G	C5-C6-O6	-5.79	125.13	128.60
36	5	1869	C	C2-N1-C1'	-5.79	112.44	118.80
36	5	2145	A	N1-C2-N3	5.79	132.19	129.30
36	5	2524	A	N9-C1'-C2'	5.79	121.52	114.00
36	5	3326	G	N9-C4-C5	-5.79	103.09	105.40
1	2	1073	G	C8-N9-C4	5.78	108.71	106.40
1	2	1280	C	N3-C4-N4	5.78	122.05	118.00
1	2	1611	A	N7-C8-N9	5.78	116.69	113.80
36	1	207	U	N1-C2-O2	-5.78	118.75	122.80
36	1	659	G	C5-C6-O6	-5.78	125.13	128.60
36	5	416	A	C4-C5-C6	5.78	119.89	117.00
36	5	2584	G	N7-C8-N9	5.78	115.99	113.10
37	3	91	G	N3-C2-N2	-5.78	115.85	119.90
36	5	2834	G	C4-C5-N7	5.78	113.11	110.80
36	1	1076	C	C5-C6-N1	-5.78	118.11	121.00
36	5	2136	C	C6-N1-C2	5.78	122.61	120.30
36	5	3000	A	N9-C4-C5	-5.78	103.49	105.80
36	5	1910	A	C8-N9-C4	5.78	108.11	105.80
36	1	212	G	N1-C6-O6	5.78	123.37	119.90
36	1	2355	G	C2-N3-C4	-5.78	109.01	111.90
36	1	3065	G	C5-C6-O6	-5.78	125.13	128.60
36	5	2239	G	C4-C5-N7	5.78	113.11	110.80
36	5	2647	A	C6-N1-C2	-5.78	115.13	118.60
36	5	3343	G	N3-C2-N2	5.78	123.94	119.90
1	2	95	G	N1-C6-O6	-5.78	116.44	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1202	A	C2-N3-C4	5.78	113.49	110.60
36	1	1178	G	C5-C6-O6	-5.78	125.14	128.60
36	1	2961	G	C6-C5-N7	-5.78	126.93	130.40
36	5	1499	C	C6-N1-C1'	5.78	127.73	120.80
36	1	960	U	C5-C4-O4	-5.77	122.44	125.90
36	5	1348	U	N3-C2-O2	-5.77	118.16	122.20
36	1	721	G	C6-C5-N7	-5.77	126.94	130.40
36	1	1635	G	C5-C6-O6	-5.77	125.14	128.60
36	5	945	C	N3-C2-O2	-5.77	117.86	121.90
36	5	2170	U	C5-C6-N1	-5.77	119.81	122.70
37	7	91	G	N1-C2-N3	5.77	127.36	123.90
36	1	2901	G	C6-C5-N7	-5.77	126.94	130.40
36	5	610	G	C5-C6-O6	5.77	132.06	128.60
36	5	1434	G	C5-C6-N1	5.77	114.39	111.50
1	2	580	A	C8-N9-C4	-5.77	103.49	105.80
36	1	611	A	O5'-P-OP1	5.77	117.62	110.70
36	1	1916	U	C5-C6-N1	-5.77	119.81	122.70
36	1	3269	U	C5-C4-O4	5.77	129.36	125.90
1	6	542	A	N1-C6-N6	5.77	122.06	118.60
36	5	2323	G	C8-N9-C4	-5.77	104.09	106.40
36	5	2848	G	C4-C5-C6	5.77	122.26	118.80
38	8	103	G	C5-C6-O6	-5.77	125.14	128.60
36	1	2375	G	O4'-C1'-N9	5.77	112.81	108.20
36	5	1198	C	N3-C4-N4	-5.77	113.96	118.00
36	5	2392	C	C2-N1-C1'	-5.77	112.45	118.80
36	5	2597	U	N1-C2-N3	-5.77	111.44	114.90
36	5	2634	U	C5-C4-O4	-5.77	122.44	125.90
38	8	8	C	C6-N1-C2	-5.77	117.99	120.30
36	5	1878	G	C8-N9-C1'	-5.76	119.51	127.00
1	2	580	A	N9-C4-C5	5.76	108.11	105.80
36	1	395	A	OP1-P-OP2	5.76	128.25	119.60
36	1	1330	A	C5-C6-N1	-5.76	114.82	117.70
36	1	1844	C	C6-N1-C2	5.76	122.61	120.30
36	1	2624	G	C8-N9-C4	-5.76	104.09	106.40
36	5	2351	U	C6-N1-C2	-5.76	117.54	121.00
1	2	992	A	N3-C4-C5	5.76	130.83	126.80
36	1	884	A	C5-C6-N6	-5.76	119.09	123.70
36	1	3302	U	O5'-P-OP1	-5.76	100.52	105.70
1	6	44	U	N1-C2-O2	-5.76	118.77	122.80
1	6	1094	G	N1-C6-O6	-5.76	116.44	119.90
36	5	938	C	OP1-P-O3'	5.76	117.87	105.20
36	1	120	G	C8-N9-C4	5.76	108.70	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	734	A	P-O3'-C3'	5.76	126.61	119.70
36	1	2364	G	C6-C5-N7	5.76	133.85	130.40
36	5	221	A	N1-C6-N6	-5.76	115.15	118.60
1	6	610	G	C4-N9-C1'	5.75	133.98	126.50
36	1	1367	G	O5'-P-OP1	-5.75	100.52	105.70
36	5	2662	G	N1-C6-O6	-5.75	116.45	119.90
1	2	1191	U	N3-C2-O2	-5.75	118.17	122.20
41	L4	206	LEU	CA-CB-CG	5.75	128.53	115.30
36	5	1906	G	C5-C6-O6	-5.75	125.15	128.60
36	1	2304	C	C6-N1-C2	-5.75	118.00	120.30
36	1	3214	U	N1-C2-O2	5.75	126.83	122.80
36	5	57	A	C2-N3-C4	-5.75	107.72	110.60
36	5	1138	U	C5-C6-N1	-5.75	119.83	122.70
36	5	2900	A	N1-C6-N6	-5.75	115.15	118.60
36	5	3050	U	C4-C5-C6	5.75	123.15	119.70
39	12	3	ARG	NE-CZ-NH1	-5.75	117.42	120.30
36	1	105	C	N1-C2-O2	-5.75	115.45	118.90
36	1	879	U	N3-C4-O4	-5.75	115.38	119.40
36	1	915	A	N1-C6-N6	-5.75	115.15	118.60
1	6	331	A	C8-N9-C4	5.75	108.10	105.80
1	6	558	U	N3-C2-O2	-5.75	118.18	122.20
36	5	1842	A	N1-C6-N6	5.75	122.05	118.60
36	5	2758	A	C2-N3-C4	5.75	113.47	110.60
36	1	974	G	N3-C4-C5	-5.75	125.73	128.60
36	1	1050	U	N3-C2-O2	-5.75	118.18	122.20
36	1	1329	U	N1-C2-O2	5.75	126.82	122.80
36	1	2961	G	N9-C4-C5	-5.75	103.10	105.40
36	5	645	A	C6-N1-C2	-5.75	115.15	118.60
36	5	955	U	N3-C4-O4	-5.75	115.38	119.40
37	7	1	G	N3-C4-C5	-5.75	125.73	128.60
36	1	2817	A	C6-N1-C2	-5.75	115.15	118.60
36	5	197	G	C4-C5-N7	5.75	113.10	110.80
36	5	1445	U	C5-C6-N1	-5.75	119.83	122.70
1	2	704	C	C6-N1-C1'	-5.74	113.91	120.80
36	1	925	A	C6-N1-C2	-5.74	115.15	118.60
36	1	931	C	C6-N1-C2	5.74	122.60	120.30
36	5	1138	U	N1-C2-O2	-5.74	118.78	122.80
37	7	35	C	C6-N1-C2	5.74	122.60	120.30
41	14	339	LEU	CA-CB-CG	5.74	128.51	115.30
36	1	1556	C	N1-C2-O2	5.74	122.34	118.90
36	1	2275	A	O5'-P-OP1	-5.74	100.53	105.70
37	7	79	A	N1-C6-N6	5.74	122.05	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	325	A	C5-C6-N1	5.74	120.57	117.70
36	1	2721	A	N1-C6-N6	5.74	122.04	118.60
1	6	1765	A	O5'-P-OP1	-5.74	100.53	105.70
36	5	642	U	O5'-P-OP2	-5.74	100.53	105.70
36	1	2172	A	N1-C6-N6	5.74	122.04	118.60
36	1	3341	U	C2-N1-C1'	5.74	124.59	117.70
36	5	2385	G	N3-C2-N2	-5.74	115.88	119.90
36	1	2661	G	C4-C5-N7	5.74	113.09	110.80
36	5	2891	U	C5-C6-N1	-5.74	119.83	122.70
36	1	716	A	O5'-P-OP1	-5.73	100.54	105.70
36	5	2660	G	C8-N9-C4	5.73	108.69	106.40
36	1	606	C	C6-N1-C2	5.73	122.59	120.30
36	1	1321	G	N9-C4-C5	5.73	107.69	105.40
36	1	1404	G	N1-C2-N2	-5.73	111.04	116.20
36	5	229	G	O5'-P-OP2	5.73	117.58	110.70
36	5	997	A	N1-C6-N6	-5.73	115.16	118.60
6	S4	246	LEU	CA-CB-CG	5.73	128.48	115.30
36	1	640	U	C5-C4-O4	-5.73	122.46	125.90
1	6	611	U	C2-N1-C1'	5.73	124.58	117.70
36	5	589	A	C8-N9-C4	5.73	108.09	105.80
36	5	953	G	O5'-P-OP1	5.73	117.57	110.70
36	5	1534	A	C6-N1-C2	-5.73	115.16	118.60
36	5	2978	U	OP1-P-O3'	5.73	117.80	105.20
36	5	3078	U	C2-N1-C1'	5.73	124.57	117.70
1	2	1041	G	C8-N9-C4	-5.73	104.11	106.40
36	5	2948	C	C5-C4-N4	-5.73	116.19	120.20
36	1	282	G	C2'-C3'-O3'	5.72	122.86	113.70
36	1	1645	U	N1-C2-O2	5.72	126.81	122.80
36	1	2585	G	N3-C4-N9	5.72	129.44	126.00
36	5	1313	G	N7-C8-N9	-5.72	110.24	113.10
36	5	2512	C	N3-C2-O2	5.72	125.91	121.90
36	5	3127	A	N3-C4-C5	-5.72	122.79	126.80
36	1	2549	G	N3-C4-N9	5.72	129.43	126.00
36	5	1130	A	N9-C4-C5	-5.72	103.51	105.80
36	5	2412	G	N3-C4-N9	5.72	129.43	126.00
1	2	3	U	N1-C2-O2	5.72	126.81	122.80
36	5	3234	A	N7-C8-N9	-5.72	110.94	113.80
36	1	2817	A	C5-C6-N1	5.72	120.56	117.70
36	1	3183	A	O5'-P-OP1	-5.72	100.55	105.70
36	5	984	G	C6-C5-N7	-5.72	126.97	130.40
36	5	2185	G	C2-N3-C4	-5.72	109.04	111.90
1	2	1389	C	N1-C2-O2	5.72	122.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1329	U	C5-C6-N1	5.72	125.56	122.70
36	1	1049	C	N1-C2-O2	5.72	122.33	118.90
36	1	1425	U	N3-C2-O2	-5.72	118.20	122.20
36	5	880	G	C4-N9-C1'	-5.72	119.07	126.50
36	5	1592	G	C5-C6-O6	5.72	132.03	128.60
36	5	2944	U	C5-C6-N1	5.72	125.56	122.70
79	q3	50	GLY	N-CA-C	-5.72	98.81	113.10
36	1	961	C	N3-C4-C5	5.71	124.19	121.90
36	5	2340	U	O5'-P-OP1	-5.71	100.56	105.70
36	5	2411	U	N3-C2-O2	-5.71	118.20	122.20
36	5	2895	G	C5-N7-C8	5.71	107.16	104.30
36	1	1419	A	N3-C4-C5	-5.71	122.80	126.80
1	2	1096	C	C2-N1-C1'	5.71	125.08	118.80
36	1	1194	G	C4-C5-N7	-5.71	108.52	110.80
36	1	1445	U	C2-N3-C4	-5.71	123.57	127.00
36	1	2658	G	C8-N9-C4	5.71	108.69	106.40
36	1	2795	U	OP1-P-OP2	5.71	128.16	119.60
36	1	1604	G	C4-N9-C1'	5.71	133.92	126.50
36	1	3341	U	C5-C6-N1	5.71	125.55	122.70
36	5	2750	U	C5-C6-N1	-5.71	119.85	122.70
36	1	1453	A	N9-C4-C5	5.71	108.08	105.80
36	1	2963	C	C4-C5-C6	5.71	120.25	117.40
38	4	70	G	N9-C4-C5	-5.71	103.12	105.40
36	5	1307	G	C2-N3-C4	5.71	114.75	111.90
36	5	1657	C	N1-C2-O2	5.71	122.32	118.90
1	2	1145	U	N3-C4-O4	5.70	123.39	119.40
36	1	304	G	N1-C2-N2	5.70	121.33	116.20
36	1	1359	C	C6-N1-C2	5.70	122.58	120.30
36	5	872	U	C5-C4-O4	-5.70	122.48	125.90
36	5	921	A	OP2-P-O3'	5.70	117.75	105.20
36	1	2321	A	C5-C6-N6	5.70	128.26	123.70
40	l3	275	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	2	388	G	C5-C6-O6	-5.70	125.18	128.60
11	S9	93	LEU	CA-CB-CG	5.70	128.41	115.30
36	1	426	G	N3-C4-C5	-5.70	125.75	128.60
36	1	883	A	N1-C6-N6	-5.70	115.18	118.60
36	5	358	G	N3-C4-C5	5.70	131.45	128.60
36	5	1000	C	N3-C4-C5	5.70	124.18	121.90
36	5	1338	C	C5-C6-N1	-5.70	118.15	121.00
1	6	65	A	C2-N3-C4	-5.70	107.75	110.60
1	6	858	G	O4'-C1'-N9	5.70	112.76	108.20
36	5	333	G	C2-N3-C4	-5.70	109.05	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2943	G	N9-C4-C5	-5.70	103.12	105.40
36	5	3374	U	N3-C4-C5	5.70	118.02	114.60
1	2	1399	C	C5-C6-N1	5.70	123.85	121.00
36	1	343	U	C4-C5-C6	5.70	123.12	119.70
36	1	895	A	C5-C6-N1	-5.70	114.85	117.70
36	1	2918	G	N1-C6-O6	5.70	123.32	119.90
38	4	113	U	C4-C5-C6	5.70	123.12	119.70
36	5	1222	G	P-O3'-C3'	5.70	126.53	119.70
36	5	2314	U	N1-C2-N3	5.70	118.32	114.90
36	5	2908	G	C5-C6-O6	-5.70	125.18	128.60
36	1	369	A	C6-N1-C2	-5.69	115.18	118.60
36	5	665	A	N3-C4-N9	5.69	131.96	127.40
1	2	606	A	N9-C4-C5	-5.69	103.52	105.80
1	2	1104	U	C5-C6-N1	-5.69	119.85	122.70
1	6	163	G	N3-C2-N2	-5.69	115.92	119.90
36	5	106	A	C8-N9-C4	5.69	108.08	105.80
36	1	770	G	O4'-C1'-N9	5.69	112.75	108.20
36	1	1552	G	C5-C6-O6	-5.69	125.19	128.60
1	6	359	A	N3-C4-N9	-5.69	122.85	127.40
36	5	610	G	N1-C6-O6	-5.69	116.49	119.90
36	5	1365	G	C4-C5-N7	5.69	113.08	110.80
36	5	1408	G	OP2-P-O3'	5.69	117.72	105.20
36	5	3055	U	C6-N1-C1'	-5.69	113.23	121.20
38	8	95	G	C8-N9-C1'	5.69	134.40	127.00
36	5	3000	A	C5-C6-N6	-5.69	119.15	123.70
36	1	35	A	C5-C6-N6	-5.69	119.15	123.70
36	1	1304	A	C8-N9-C4	5.69	108.08	105.80
36	1	3344	A	O4'-C1'-N9	5.69	112.75	108.20
36	5	915	A	OP1-P-OP2	5.69	128.13	119.60
36	5	2248	C	N1-C2-N3	5.69	123.18	119.20
36	5	3388	C	C2-N3-C4	-5.69	117.06	119.90
38	8	51	G	N7-C8-N9	5.69	115.94	113.10
36	1	1609	C	C6-N1-C2	5.68	122.57	120.30
36	1	1440	G	N3-C4-C5	5.68	131.44	128.60
36	5	2550	U	C5-C4-O4	5.68	129.31	125.90
36	5	2796	G	C4-C5-N7	-5.68	108.53	110.80
36	5	2997	G	N9-C4-C5	-5.68	103.13	105.40
36	1	2644	C	N3-C4-N4	-5.68	114.02	118.00
36	5	669	U	C2-N3-C4	-5.68	123.59	127.00
36	1	2636	A	C5-C6-N6	5.68	128.24	123.70
36	5	1838	G	C6-C5-N7	-5.68	126.99	130.40
36	5	614	C	C6-N1-C2	5.68	122.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2961	G	C2-N3-C4	-5.68	109.06	111.90
1	6	571	G	C8-N9-C4	-5.68	104.13	106.40
36	5	1114	U	N3-C4-C5	-5.68	111.19	114.60
36	5	1116	G	C8-N9-C4	-5.68	104.13	106.40
36	5	2329	C	O5'-P-OP1	5.68	117.51	110.70
1	2	507	U	C2-N1-C1'	5.67	124.51	117.70
18	C6	40	GLU	C-N-CA	5.67	145.83	122.00
36	1	591	G	N1-C6-O6	5.67	123.30	119.90
36	1	1852	G	N1-C6-O6	5.67	123.31	119.90
36	1	2714	G	C2-N3-C4	-5.67	109.06	111.90
36	5	3110	C	N3-C4-C5	5.67	124.17	121.90
36	1	1414	G	C4-C5-N7	5.67	113.07	110.80
36	1	1915	A	C8-N9-C4	-5.67	103.53	105.80
36	1	2808	A	N9-C4-C5	-5.67	103.53	105.80
36	5	534	U	N1-C2-O2	5.67	126.77	122.80
36	1	1194	G	C5-C6-O6	5.67	132.00	128.60
1	6	272	U	C2-N1-C1'	5.67	124.50	117.70
36	5	834	U	N1-C2-N3	-5.67	111.50	114.90
36	5	2217	U	N3-C2-O2	-5.67	118.23	122.20
36	5	2791	G	N1-C2-N3	5.67	127.30	123.90
36	5	3127	A	C2-N3-C4	5.67	113.44	110.60
36	1	716	A	C5-N7-C8	-5.67	101.06	103.90
36	1	3065	G	C8-N9-C4	5.67	108.67	106.40
36	5	1313	G	N9-C4-C5	-5.67	103.13	105.40
36	1	2615	G	C5-C6-O6	-5.67	125.20	128.60
1	6	95	G	C5-C6-O6	5.67	132.00	128.60
1	6	384	G	C8-N9-C4	5.67	108.67	106.40
1	6	576	G	N3-C4-N9	5.67	129.40	126.00
36	5	2834	G	N9-C4-C5	-5.67	103.13	105.40
36	1	2227	C	N3-C2-O2	-5.67	117.94	121.90
36	5	996	A	N3-C4-C5	5.67	130.77	126.80
36	1	1292	C	N3-C2-O2	5.66	125.86	121.90
36	1	1369	A	C2-N3-C4	-5.66	107.77	110.60
36	5	1452	A	C5-N7-C8	-5.66	101.07	103.90
37	7	84	A	C6-C5-N7	-5.66	128.34	132.30
38	8	139	U	N3-C4-O4	-5.66	115.44	119.40
36	1	1132	C	N1-C2-N3	5.66	123.16	119.20
36	1	2954	U	OP1-P-O3'	5.66	117.66	105.20
70	O4	58	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	6	1697	G	N3-C4-C5	-5.66	125.77	128.60
36	5	324	A	OP1-P-O3'	5.66	117.66	105.20
36	5	434	U	O5'-P-OP1	5.66	117.50	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	871	U	N3-C2-O2	-5.66	118.24	122.20
36	5	3218	A	C5-C6-N6	-5.66	119.17	123.70
36	1	329	U	C6-N1-C2	-5.66	117.60	121.00
36	1	497	C	O5'-P-OP1	5.66	117.49	110.70
1	6	542	A	C6-C5-N7	-5.66	128.34	132.30
36	5	2398	A	C6-N1-C2	-5.66	115.20	118.60
1	2	11	A	O5'-P-OP1	-5.66	100.61	105.70
1	2	734	A	OP1-P-O3'	5.66	117.65	105.20
1	2	1022	C	N3-C4-C5	5.66	124.16	121.90
36	1	2995	A	N7-C8-N9	-5.66	110.97	113.80
1	6	935	U	N3-C4-C5	-5.66	111.20	114.60
36	1	75	G	O5'-P-OP2	-5.66	100.61	105.70
36	1	718	G	N7-C8-N9	5.66	115.93	113.10
36	1	2342	U	N1-C2-O2	-5.66	118.84	122.80
36	1	2420	C	C6-N1-C2	-5.66	118.04	120.30
39	L2	237	LEU	CA-CB-CG	-5.66	102.29	115.30
36	5	1165	A	C6-C5-N7	-5.66	128.34	132.30
36	1	1437	C	C4-C5-C6	5.65	120.23	117.40
36	1	2643	A	C2-N3-C4	-5.65	107.77	110.60
36	5	2754	G	C8-N9-C4	5.65	108.66	106.40
36	1	281	G	N9-C4-C5	5.65	107.66	105.40
36	1	2298	U	O4'-C1'-N1	5.65	112.72	108.20
36	5	2818	U	C5'-C4'-O4'	-5.65	102.32	109.10
37	7	14	U	N3-C4-O4	-5.65	115.44	119.40
36	1	584	G	C4-C5-N7	-5.65	108.54	110.80
36	1	1100	U	C2-N3-C4	-5.65	123.61	127.00
1	6	1048	G	C4-C5-N7	5.65	113.06	110.80
36	5	2757	U	C5-C6-N1	-5.65	119.87	122.70
36	1	2372	A	N1-C2-N3	5.65	132.12	129.30
36	5	971	G	N7-C8-N9	-5.65	110.28	113.10
36	1	262	U	N3-C2-O2	5.65	126.15	122.20
36	1	1115	G	N3-C2-N2	-5.65	115.95	119.90
36	1	1845	G	N1-C6-O6	-5.65	116.51	119.90
36	1	2351	U	N3-C2-O2	-5.65	118.25	122.20
36	1	2634	U	N3-C4-C5	5.65	117.99	114.60
1	6	50	C	N3-C4-C5	-5.65	119.64	121.90
36	5	893	C	N3-C4-C5	-5.65	119.64	121.90
36	5	1165	A	C4-C5-C6	5.65	119.82	117.00
36	5	2327	U	C5-C6-N1	-5.65	119.88	122.70
36	5	1052	U	C5-C6-N1	-5.65	119.88	122.70
36	5	2584	G	OP2-P-O3'	5.65	117.62	105.20
36	1	2870	C	C4-C5-C6	-5.64	114.58	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2902	A	O5'-P-OP2	-5.64	100.62	105.70
36	5	1403	C	C5-C4-N4	-5.64	116.25	120.20
36	1	286	U	N1-C2-N3	5.64	118.29	114.90
36	1	1136	A	C6-C5-N7	-5.64	128.35	132.30
1	6	1481	C	N3-C2-O2	-5.64	117.95	121.90
36	5	1116	G	C5-C6-O6	5.64	131.99	128.60
36	5	1314	C	C2-N3-C4	-5.64	117.08	119.90
36	5	2634	U	C2-N3-C4	-5.64	123.61	127.00
36	1	1173	U	C4-C5-C6	5.64	123.08	119.70
36	1	1366	A	C5-N7-C8	-5.64	101.08	103.90
54	M8	41	ASP	CB-CG-OD1	5.64	123.38	118.30
1	6	1180	C	C6-N1-C2	-5.64	118.04	120.30
36	5	2817	A	N1-C6-N6	5.64	121.98	118.60
36	5	2855	U	C2-N3-C4	-5.64	123.61	127.00
36	1	1441	G	C5-N7-C8	5.64	107.12	104.30
36	1	2651	G	C5-N7-C8	5.64	107.12	104.30
36	1	3211	C	OP1-P-O3'	5.64	117.61	105.20
38	4	24	G	C5-C6-N1	5.64	114.32	111.50
1	6	385	A	N1-C6-N6	-5.64	115.22	118.60
36	5	2374	C	C5-C4-N4	5.64	124.15	120.20
36	5	2720	G	O5'-P-OP2	-5.64	100.62	105.70
36	1	860	G	C5-C6-O6	-5.64	125.22	128.60
1	6	364	G	N3-C4-N9	5.64	129.38	126.00
36	5	1131	G	C2-N3-C4	-5.64	109.08	111.90
36	5	1665	C	N3-C2-O2	-5.64	117.95	121.90
36	1	1156	C	C2-N3-C4	-5.64	117.08	119.90
36	1	1381	A	O5'-P-OP1	-5.64	100.63	105.70
36	5	71	A	O5'-P-OP2	5.64	117.47	110.70
36	5	1300	G	C8-N9-C1'	-5.64	119.67	127.00
36	5	2816	G	C6-C5-N7	-5.64	127.02	130.40
36	5	3309	G	C4-N9-C1'	5.64	133.83	126.50
36	1	2316	G	C2-N3-C4	5.63	114.72	111.90
1	2	1748	G	C2-N3-C4	-5.63	109.08	111.90
36	1	3307	A	N1-C6-N6	5.63	121.98	118.60
36	5	3211	C	N3-C4-C5	5.63	124.15	121.90
38	8	77	A	C8-N9-C4	5.63	108.05	105.80
1	2	1745	G	N3-C2-N2	5.63	123.84	119.90
36	1	645	A	N1-C2-N3	5.63	132.12	129.30
36	1	1396	C	C6-N1-C2	5.63	122.55	120.30
1	6	194	U	C5-C6-N1	5.63	125.52	122.70
1	6	1726	G	C8-N9-C4	5.63	108.65	106.40
36	5	2727	A	C2-N3-C4	5.63	113.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3143	C	N3-C4-N4	5.63	121.94	118.00
36	1	2219	A	C2-N3-C4	5.63	113.42	110.60
36	1	2343	C	N3-C4-C5	5.63	124.15	121.90
36	1	794	U	C4-C5-C6	5.63	123.08	119.70
36	1	824	C	O5'-P-OP2	-5.63	100.63	105.70
36	1	1316	C	N3-C4-N4	5.63	121.94	118.00
1	6	638	U	N1-C2-O2	5.63	126.74	122.80
36	1	948	C	C5-C6-N1	-5.63	118.19	121.00
36	1	1556	C	P-O3'-C3'	5.63	126.45	119.70
36	1	2777	G	N1-C6-O6	-5.63	116.52	119.90
36	5	940	G	C6-C5-N7	5.63	133.78	130.40
36	1	948	C	C5-C4-N4	-5.62	116.26	120.20
1	6	1196	A	C8-N9-C4	5.62	108.05	105.80
36	1	589	A	N7-C8-N9	-5.62	110.99	113.80
36	5	2197	C	N3-C2-O2	5.62	125.84	121.90
36	1	1011	A	C8-N9-C4	5.62	108.05	105.80
36	1	2381	G	N1-C6-O6	5.62	123.27	119.90
1	6	352	A	OP2-P-O3'	5.62	117.57	105.20
43	16	173	MET	CB-CG-SD	-5.62	95.53	112.40
36	1	1405	U	N3-C4-C5	5.62	117.97	114.60
36	5	2169	G	N1-C6-O6	-5.62	116.53	119.90
36	1	342	A	N1-C6-N6	-5.62	115.23	118.60
36	1	1869	C	C6-N1-C2	5.62	122.55	120.30
36	5	411	U	C2-N3-C4	-5.62	123.63	127.00
36	5	3151	U	C6-N1-C2	5.62	124.37	121.00
36	5	2391	G	OP1-P-OP2	-5.62	111.17	119.60
36	1	435	C	C2-N1-C1'	-5.62	112.62	118.80
36	1	1445	U	C6-N1-C2	5.62	124.37	121.00
1	6	433	C	C5-C4-N4	-5.62	116.27	120.20
36	5	941	G	C5-C6-N1	5.62	114.31	111.50
36	1	320	G	N1-C6-O6	5.61	123.27	119.90
36	1	653	A	C2-N3-C4	-5.61	107.79	110.60
36	5	1206	G	N1-C6-O6	-5.61	116.53	119.90
36	1	1351	U	C5-C6-N1	5.61	125.51	122.70
36	1	2290	C	C6-N1-C2	5.61	122.55	120.30
36	5	105	C	N3-C4-C5	5.61	124.14	121.90
36	1	49	A	N1-C6-N6	5.61	121.97	118.60
36	1	1157	G	N3-C2-N2	-5.61	115.97	119.90
36	5	427	C	C4-C5-C6	5.61	120.20	117.40
36	5	968	G	C8-N9-C4	5.61	108.64	106.40
36	5	1154	A	C2-N3-C4	5.61	113.41	110.60
36	5	1764	U	C5-C6-N1	5.61	125.51	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2818	U	P-O3'-C3'	5.61	126.43	119.70
36	5	2860	U	N3-C4-O4	-5.61	115.47	119.40
36	5	2924	U	C2-N1-C1'	-5.61	110.97	117.70
36	5	835	G	O4'-C1'-N9	5.61	112.69	108.20
36	5	2640	A	C2-N3-C4	-5.61	107.80	110.60
36	5	3063	C	C6-N1-C2	-5.61	118.06	120.30
1	2	736	C	C2-N1-C1'	5.61	124.97	118.80
36	1	1548	C	N3-C2-O2	5.61	125.83	121.90
36	5	816	A	C8-N9-C4	-5.61	103.56	105.80
36	5	2378	C	N3-C4-C5	5.61	124.14	121.90
36	1	1415	U	C5-C6-N1	-5.61	119.90	122.70
36	1	2409	G	N3-C4-C5	-5.61	125.80	128.60
1	6	1671	A	N1-C6-N6	-5.61	115.24	118.60
36	5	664	U	N1-C2-O2	-5.61	118.88	122.80
36	5	944	C	C5-C6-N1	-5.61	118.20	121.00
36	5	2342	U	N1-C2-N3	5.61	118.26	114.90
36	5	2772	C	OP2-P-O3'	5.61	117.53	105.20
36	5	3190	C	C4-C5-C6	5.61	120.20	117.40
36	1	159	A	C2-N3-C4	-5.60	107.80	110.60
36	1	1326	A	O5'-P-OP1	5.60	117.42	110.70
1	6	1656	U	O5'-P-OP1	5.60	117.42	110.70
36	1	92	G	C6-N1-C2	-5.60	121.74	125.10
36	1	960	U	N3-C2-O2	5.60	126.12	122.20
38	4	114	G	C5-C6-O6	5.60	131.96	128.60
11	s9	3	ARG	NE-CZ-NH2	5.60	123.10	120.30
12	c0	97	PRO	N-CA-CB	5.60	110.02	103.30
37	7	1	G	N3-C4-N9	5.60	129.36	126.00
36	1	864	G	C4-C5-N7	-5.60	108.56	110.80
38	4	68	G	C5-C6-O6	-5.60	125.24	128.60
36	1	1530	U	C6-N1-C2	5.60	124.36	121.00
36	5	1166	G	N3-C4-C5	5.60	131.40	128.60
36	5	1379	G	N9-C4-C5	-5.60	103.16	105.40
36	5	1484	U	C5-C6-N1	-5.60	119.90	122.70
36	5	1879	A	N7-C8-N9	5.60	116.60	113.80
36	5	2416	U	C5-C4-O4	5.60	129.26	125.90
36	1	2828	G	N3-C4-N9	5.60	129.36	126.00
36	1	2888	U	C2-N3-C4	-5.60	123.64	127.00
1	6	364	G	C6-C5-N7	-5.60	127.04	130.40
36	5	3154	C	C6-N1-C1'	-5.60	114.08	120.80
36	1	2229	A	C5-C6-N1	5.60	120.50	117.70
36	1	2924	U	C2-N1-C1'	-5.60	110.98	117.70
36	1	1858	A	N3-C4-N9	5.59	131.88	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	376	G	C2-N3-C4	5.59	114.70	111.90
36	5	3148	U	C5-C6-N1	-5.59	119.90	122.70
38	8	106	C	C6-N1-C2	5.59	122.54	120.30
36	1	1177	G	C5-C6-O6	-5.59	125.24	128.60
36	5	34	A	OP2-P-O3'	5.59	117.50	105.20
36	5	635	G	N9-C4-C5	-5.59	103.16	105.40
36	5	2338	C	N1-C2-O2	-5.59	115.54	118.90
36	5	2373	A	O5'-P-OP2	5.59	117.41	110.70
36	1	25	U	N1-C2-O2	-5.59	118.89	122.80
36	5	1528	G	C4-C5-C6	5.59	122.16	118.80
36	5	3188	G	C5-C6-O6	5.59	131.96	128.60
41	14	206	LEU	CA-CB-CG	5.59	128.16	115.30
1	2	334	G	C4-N9-C1'	-5.59	119.23	126.50
1	2	1745	G	C6-C5-N7	-5.59	127.05	130.40
36	1	108	A	N1-C6-N6	5.59	121.95	118.60
36	1	304	G	C8-N9-C4	-5.59	104.16	106.40
36	1	1345	G	N3-C4-C5	5.59	131.40	128.60
36	1	1457	U	O5'-P-OP1	-5.59	100.67	105.70
1	6	577	G	C8-N9-C4	-5.59	104.17	106.40
36	5	813	G	N3-C4-N9	5.59	129.35	126.00
36	5	3309	G	N3-C4-C5	-5.59	125.81	128.60
1	6	1780	G	C4-C5-N7	5.59	113.03	110.80
36	5	3215	A	C5-C6-N1	-5.59	114.91	117.70
36	1	2154	U	C5-C4-O4	-5.59	122.55	125.90
36	5	3354	U	N3-C2-O2	-5.59	118.29	122.20
36	1	343	U	OP1-P-O3'	5.58	117.49	105.20
36	1	2617	U	N3-C4-O4	-5.58	115.49	119.40
36	5	1865	A	C8-N9-C4	5.58	108.03	105.80
1	2	444	C	C6-N1-C2	5.58	122.53	120.30
36	1	33	G	N1-C6-O6	5.58	123.25	119.90
36	1	614	C	C6-N1-C2	5.58	122.53	120.30
36	1	1513	G	C6-N1-C2	-5.58	121.75	125.10
36	1	2937	G	C6-C5-N7	5.58	133.75	130.40
1	6	362	G	C4-N9-C1'	5.58	133.76	126.50
1	6	864	U	O4'-C1'-N1	5.58	112.67	108.20
36	5	91	G	C8-N9-C4	5.58	108.63	106.40
36	5	632	G	C5-C6-N1	5.58	114.29	111.50
36	5	1064	A	O4'-C1'-N9	-5.58	103.73	108.20
36	5	2971	A	N3-C4-N9	5.58	131.87	127.40
36	1	905	U	N1-C2-O2	-5.58	118.89	122.80
36	1	1177	G	C6-C5-N7	-5.58	127.05	130.40
36	1	1494	U	C6-N1-C2	5.58	124.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2244	A	C8-N9-C4	5.58	108.03	105.80
1	6	29	U	C5-C4-O4	5.58	129.25	125.90
1	6	371	G	C4-C5-C6	5.58	122.15	118.80
36	5	802	C	C4-C5-C6	5.58	120.19	117.40
36	5	2612	U	N1-C2-N3	5.58	118.25	114.90
36	1	658	G	N3-C4-N9	5.58	129.35	126.00
36	5	568	G	N1-C6-O6	5.58	123.25	119.90
36	1	2893	C	C5-C6-N1	-5.58	118.21	121.00
1	6	363	G	C8-N9-C4	5.58	108.63	106.40
36	5	1080	A	C5-N7-C8	5.58	106.69	103.90
36	1	2653	C	N1-C2-O2	5.58	122.25	118.90
36	5	1552	G	C5-C6-O6	-5.58	125.25	128.60
36	5	1868	G	C5-C6-O6	-5.58	125.25	128.60
1	2	1653	C	N3-C4-C5	-5.58	119.67	121.90
36	1	1152	G	OP1-P-OP2	5.58	127.96	119.60
36	1	1909	A	C8-N9-C4	5.58	108.03	105.80
36	5	1894	U	C5-C6-N1	-5.58	119.91	122.70
36	1	596	C	N1-C2-O2	5.57	122.24	118.90
36	1	882	A	O5'-P-OP2	-5.57	100.68	105.70
36	1	1151	U	N1-C2-O2	-5.57	118.90	122.80
36	1	1303	A	N7-C8-N9	-5.57	111.01	113.80
36	1	1442	U	OP1-P-O3'	5.57	117.46	105.20
36	5	821	U	N3-C4-O4	-5.57	115.50	119.40
36	5	1121	U	OP1-P-O3'	-5.57	92.94	105.20
36	5	2374	C	N3-C4-N4	-5.57	114.10	118.00
36	5	1374	G	N1-C2-N2	-5.57	111.19	116.20
36	5	2278	C	C5-C6-N1	5.57	123.79	121.00
36	1	188	U	C2-N1-C1'	-5.57	111.02	117.70
37	3	89	G	N9-C4-C5	-5.57	103.17	105.40
38	4	107	G	C6-C5-N7	5.57	133.74	130.40
1	6	1698	G	C5-C6-O6	5.57	131.94	128.60
36	5	1004	U	C6-N1-C2	-5.57	117.66	121.00
36	5	2882	U	C5-C4-O4	-5.57	122.56	125.90
36	1	968	G	N3-C4-N9	5.57	129.34	126.00
1	2	1489	U	N3-C2-O2	-5.57	118.30	122.20
36	1	346	C	C5-C6-N1	-5.57	118.22	121.00
36	1	2249	G	N1-C6-O6	-5.57	116.56	119.90
36	5	574	U	C6-N1-C2	5.57	124.34	121.00
36	5	938	C	N3-C4-C5	5.57	124.13	121.90
36	5	2550	U	N3-C2-O2	-5.57	118.30	122.20
36	5	2908	G	N3-C2-N2	-5.57	116.00	119.90
6	S4	193	GLY	N-CA-C	5.57	127.02	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	582	G	N3-C4-N9	-5.57	122.66	126.00
36	1	635	G	N3-C4-N9	5.57	129.34	126.00
36	1	3304	U	C5-C6-N1	-5.57	119.92	122.70
1	6	272	U	N3-C2-O2	-5.57	118.30	122.20
36	5	119	U	C2-N1-C1'	-5.57	111.02	117.70
36	5	220	G	OP1-P-O3'	5.57	117.44	105.20
36	5	2160	G	C6-C5-N7	-5.57	127.06	130.40
36	5	2964	G	C4-C5-N7	-5.57	108.57	110.80
1	6	94	U	OP2-P-O3'	5.56	117.44	105.20
36	5	2373	A	OP1-P-OP2	-5.56	111.25	119.60
1	2	1363	U	C2-N1-C1'	5.56	124.38	117.70
36	1	2376	G	N7-C8-N9	5.56	115.88	113.10
36	1	2643	A	N3-C4-C5	5.56	130.69	126.80
1	6	405	C	C6-N1-C2	5.56	122.53	120.30
36	5	860	G	O5'-P-OP2	-5.56	100.69	105.70
36	5	1166	G	C4-C5-N7	5.56	113.03	110.80
36	5	3149	G	O5'-P-OP1	5.56	117.38	110.70
1	2	21	U	O5'-P-OP2	-5.56	100.69	105.70
36	1	2692	A	N1-C6-N6	5.56	121.94	118.60
1	2	1455	G	C4-C5-N7	-5.56	108.58	110.80
36	1	2142	A	N3-C4-C5	-5.56	122.91	126.80
36	1	2386	A	N1-C6-N6	5.56	121.94	118.60
36	5	2353	G	N1-C6-O6	5.56	123.24	119.90
36	5	3044	G	C6-C5-N7	-5.56	127.06	130.40
36	1	589	A	N1-C6-N6	-5.56	115.27	118.60
36	1	920	A	N1-C2-N3	5.56	132.08	129.30
36	5	53	G	N9-C4-C5	-5.56	103.18	105.40
36	1	2279	A	N1-C6-N6	5.56	121.93	118.60
36	5	2898	G	C8-N9-C4	5.56	108.62	106.40
61	n5	115	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	2	966	A	N1-C6-N6	5.55	121.93	118.60
36	1	645	A	C5-C6-N1	5.55	120.48	117.70
36	1	1367	G	N3-C4-N9	5.55	129.33	126.00
36	1	1607	U	C5-C4-O4	5.55	129.23	125.90
36	1	3194	C	N1-C2-O2	-5.55	115.57	118.90
36	5	2825	C	N3-C2-O2	5.55	125.79	121.90
36	1	358	G	N1-C6-O6	5.55	123.23	119.90
1	2	1622	G	C8-N9-C4	5.55	108.62	106.40
36	1	1441	G	C4-C5-N7	-5.55	108.58	110.80
36	1	2638	C	C5-C4-N4	5.55	124.09	120.20
36	1	2891	U	C5-C6-N1	-5.55	119.92	122.70
1	6	1780	G	N9-C4-C5	-5.55	103.18	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	949	C	OP2-P-O3'	5.55	117.41	105.20
36	5	958	C	N1-C2-O2	5.55	122.23	118.90
36	5	1836	C	C6-N1-C2	5.55	122.52	120.30
36	5	1888	U	N1-C2-O2	-5.55	118.92	122.80
36	1	606	C	O5'-P-OP2	-5.55	100.70	105.70
36	1	2408	U	O5'-P-OP2	5.55	117.36	110.70
36	1	2420	C	O5'-P-OP2	5.55	117.36	110.70
1	6	1724	U	C5-C6-N1	-5.55	119.93	122.70
1	6	1752	U	C5-C6-N1	-5.55	119.93	122.70
36	5	693	A	O5'-P-OP2	5.55	117.36	110.70
36	5	933	A	C6-C5-N7	-5.55	128.42	132.30
36	5	2865	U	N1-C2-O2	5.55	126.68	122.80
1	2	579	A	O4'-C1'-N9	5.55	112.64	108.20
36	1	999	G	C5-C6-N1	5.55	114.27	111.50
36	1	2969	A	C6-C5-N7	-5.55	128.42	132.30
36	5	411	U	C2-N1-C1'	-5.55	111.04	117.70
1	2	43	A	C5-C6-N6	5.55	128.14	123.70
1	2	1782	A	C5-C6-N1	-5.55	114.93	117.70
1	6	542	A	P-O3'-C3'	5.55	126.36	119.70
1	6	767	U	C5-C4-O4	5.55	129.23	125.90
36	5	884	A	N1-C6-N6	-5.55	115.27	118.60
36	5	2930	A	C5-C6-N1	5.55	120.47	117.70
36	1	1784	G	C6-C5-N7	5.54	133.73	130.40
36	1	1178	G	O5'-P-OP2	-5.54	100.71	105.70
36	1	2368	A	OP1-P-OP2	5.54	127.92	119.60
36	1	2631	U	OP1-P-O3'	5.54	117.39	105.20
36	5	716	A	N9-C4-C5	-5.54	103.58	105.80
36	5	971	G	N3-C2-N2	-5.54	116.02	119.90
36	5	1317	A	C5-N7-C8	-5.54	101.13	103.90
36	5	3206	C	OP1-P-OP2	5.54	127.92	119.60
36	1	350	C	C6-N1-C2	-5.54	118.08	120.30
36	1	1153	A	C4-C5-N7	5.54	113.47	110.70
36	1	1344	G	C5-C6-O6	-5.54	125.28	128.60
36	1	2296	A	C8-N9-C4	5.54	108.02	105.80
36	1	2860	U	C2-N1-C1'	-5.54	111.05	117.70
36	5	1470	U	N3-C2-O2	-5.54	118.32	122.20
38	8	44	A	C5-C6-N6	-5.54	119.27	123.70
36	5	2832	C	C5-C6-N1	-5.54	118.23	121.00
36	1	1931	U	N3-C4-O4	-5.54	115.52	119.40
36	1	2706	G	N3-C4-N9	5.54	129.32	126.00
36	5	660	A	C5-C6-N6	5.54	128.13	123.70
36	5	1128	U	C2-N3-C4	-5.54	123.68	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	15	110	LEU	CA-CB-CG	5.54	128.04	115.30
1	6	337	G	N3-C2-N2	5.54	123.78	119.90
36	5	1868	G	N9-C4-C5	-5.54	103.19	105.40
36	5	2404	A	C4-C5-C6	5.54	119.77	117.00
36	1	2525	G	C6-C5-N7	-5.54	127.08	130.40
37	3	105	C	OP2-P-O3'	5.54	117.38	105.20
36	5	2130	G	N9-C1'-C2'	-5.54	105.91	112.00
36	5	2707	C	C5-C4-N4	-5.54	116.33	120.20
36	5	2805	G	C8-N9-C4	5.54	108.61	106.40
36	1	402	A	N1-C6-N6	-5.53	115.28	118.60
36	1	1428	A	C4-C5-N7	5.53	113.47	110.70
36	1	95	A	N1-C2-N3	5.53	132.07	129.30
36	5	119	U	N3-C4-O4	-5.53	115.53	119.40
36	5	2334	U	C4-C5-C6	5.53	123.02	119.70
36	5	865	U	N1-C2-O2	-5.53	118.93	122.80
36	5	1426	C	N3-C2-O2	5.53	125.77	121.90
36	5	1882	G	C4-C5-N7	5.53	113.01	110.80
36	5	3013	U	N1-C2-O2	5.53	126.67	122.80
36	1	790	U	C5-C4-O4	5.53	129.22	125.90
36	1	2882	U	O5'-P-OP2	-5.53	100.72	105.70
36	1	3088	G	N3-C2-N2	-5.53	116.03	119.90
36	5	383	G	N3-C4-C5	5.53	131.36	128.60
36	5	2867	C	C6-N1-C2	-5.53	118.09	120.30
36	1	1156	C	N3-C2-O2	-5.53	118.03	121.90
36	5	687	U	O5'-P-OP1	5.53	117.33	110.70
36	5	1110	U	N3-C4-C5	5.52	117.91	114.60
36	5	2117	A	C5-N7-C8	5.52	106.66	103.90
36	5	3004	C	N3-C2-O2	5.52	125.77	121.90
1	2	532	U	O5'-P-OP1	-5.52	100.73	105.70
36	1	335	G	O5'-P-OP2	5.52	117.33	110.70
36	1	711	A	C8-N9-C4	5.52	108.01	105.80
36	1	1747	G	N3-C2-N2	-5.52	116.03	119.90
1	6	1421	A	C8-N9-C4	5.52	108.01	105.80
36	5	1434	G	N1-C6-O6	-5.52	116.59	119.90
36	5	1852	G	N7-C8-N9	5.52	115.86	113.10
36	5	3362	A	N1-C6-N6	5.52	121.91	118.60
38	8	14	C	N3-C4-C5	5.52	124.11	121.90
36	1	2403	G	N1-C6-O6	5.52	123.21	119.90
36	5	2757	U	C2-N3-C4	-5.52	123.69	127.00
36	5	3181	C	N3-C4-C5	-5.52	119.69	121.90
36	1	217	U	OP1-P-O3'	5.52	117.34	105.20
36	1	2393	G	C6-N1-C2	-5.52	121.79	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1662	G	C8-N9-C4	5.52	108.61	106.40
36	5	2337	C	N3-C2-O2	-5.52	118.04	121.90
38	4	94	C	C5-C6-N1	-5.52	118.24	121.00
36	5	2917	G	C5-C6-O6	-5.52	125.29	128.60
57	n1	106	LEU	CA-CB-CG	-5.52	102.61	115.30
37	3	82	G	C8-N9-C1'	-5.52	119.83	127.00
38	4	44	A	O5'-P-OP1	-5.52	100.74	105.70
1	6	1151	A	N1-C6-N6	-5.52	115.29	118.60
1	6	1796	C	C5-C6-N1	-5.52	118.24	121.00
1	2	1575	G	N1-C6-O6	-5.51	116.59	119.90
36	1	701	G	N3-C2-N2	-5.51	116.04	119.90
36	1	1417	G	C8-N9-C4	5.51	108.61	106.40
36	1	1830	G	OP1-P-O3'	5.51	117.33	105.20
1	6	1629	G	OP2-P-O3'	5.51	117.33	105.20
36	5	424	G	N9-C4-C5	-5.51	103.19	105.40
36	5	514	G	N1-C6-O6	5.51	123.21	119.90
36	5	1152	G	N7-C8-N9	5.51	115.86	113.10
36	5	2142	A	C6-N1-C2	-5.51	115.29	118.60
36	5	2234	G	N1-C6-O6	5.51	123.21	119.90
36	5	2735	U	C5-C4-O4	5.51	129.21	125.90
36	1	1696	A	C8-N9-C4	-5.51	103.60	105.80
53	M7	3	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	6	611	U	N1-C2-O2	5.51	126.66	122.80
36	5	1398	U	C5-C4-O4	5.51	129.21	125.90
36	5	1889	G	C6-C5-N7	-5.51	127.09	130.40
36	5	2572	C	C6-N1-C1'	-5.51	114.19	120.80
1	2	1481	C	C6-N1-C2	-5.51	118.10	120.30
38	4	25	G	C4-C5-N7	-5.51	108.60	110.80
36	5	343	U	OP1-P-O3'	5.51	117.32	105.20
36	5	607	A	O5'-P-OP1	-5.51	100.74	105.70
36	5	869	G	C6-C5-N7	5.51	133.71	130.40
36	5	2352	A	C2-N3-C4	5.51	113.35	110.60
36	1	639	G	C5-C6-O6	-5.51	125.30	128.60
36	5	2191	U	N3-C4-O4	-5.51	115.54	119.40
36	5	2709	C	N3-C4-C5	5.51	124.10	121.90
1	2	600	U	C5-C4-O4	5.51	129.20	125.90
36	1	75	G	C2-N3-C4	-5.51	109.15	111.90
36	1	225	C	N1-C2-O2	-5.51	115.60	118.90
36	1	653	A	C4-C5-N7	5.51	113.45	110.70
36	1	978	G	C5-C6-O6	-5.51	125.30	128.60
36	1	2231	C	C6-N1-C2	5.51	122.50	120.30
38	4	113	U	N1-C2-N3	5.51	118.20	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	56	G	C5-C6-N1	5.51	114.25	111.50
36	5	634	C	OP2-P-O3'	5.51	117.31	105.20
36	5	1339	C	O5'-P-OP1	-5.51	100.74	105.70
36	5	3123	A	N7-C8-N9	-5.51	111.05	113.80
36	1	35	A	N9-C4-C5	-5.50	103.60	105.80
36	1	808	A	C8-N9-C4	5.50	108.00	105.80
36	1	2425	G	OP2-P-O3'	5.50	117.31	105.20
36	5	1444	G	N1-C6-O6	5.50	123.20	119.90
1	2	389	G	C8-N9-C1'	-5.50	119.85	127.00
36	1	1430	U	N3-C2-O2	5.50	126.05	122.20
36	1	1595	U	C2-N1-C1'	-5.50	111.10	117.70
36	1	2726	C	N1-C2-N3	5.50	123.05	119.20
36	5	119	U	C5-C4-O4	5.50	129.20	125.90
36	5	741	U	O5'-P-OP2	5.50	117.30	110.70
36	5	2943	G	C2-N3-C4	-5.50	109.15	111.90
36	5	3188	G	N3-C4-C5	-5.50	125.85	128.60
78	q2	35	LEU	CA-CB-CG	5.50	127.96	115.30
36	1	59	G	N1-C6-O6	5.50	123.20	119.90
36	1	928	C	N3-C4-C5	5.50	124.10	121.90
36	1	1905	G	N3-C4-N9	-5.50	122.70	126.00
36	1	3038	U	N1-C2-O2	-5.50	118.95	122.80
36	1	206	G	C5-C6-N1	5.50	114.25	111.50
36	5	400	G	N9-C4-C5	5.50	107.60	105.40
1	2	1136	U	C2-N1-C1'	-5.50	111.10	117.70
36	1	2279	A	C8-N9-C4	5.50	108.00	105.80
36	1	3248	C	C5-C6-N1	5.50	123.75	121.00
36	5	1448	U	C6-N1-C2	5.50	124.30	121.00
36	5	2425	G	N3-C4-C5	5.50	131.35	128.60
36	1	951	A	N9-C4-C5	-5.50	103.60	105.80
36	1	1643	A	C8-N9-C4	5.50	108.00	105.80
36	1	2917	G	N3-C2-N2	-5.50	116.05	119.90
1	6	552	G	C4-C5-N7	5.50	113.00	110.80
36	5	581	U	C5-C6-N1	5.50	125.45	122.70
36	5	2257	C	P-O3'-C3'	5.50	126.30	119.70
36	5	2302	G	N1-C6-O6	-5.50	116.60	119.90
36	5	919	U	C5-C6-N1	-5.50	119.95	122.70
36	5	1076	C	N1-C2-O2	-5.50	115.60	118.90
1	6	1141	G	C8-N9-C4	5.49	108.60	106.40
36	5	2339	C	OP1-P-OP2	5.49	127.84	119.60
36	1	3049	A	C8-N9-C4	5.49	108.00	105.80
37	3	27	A	N1-C6-N6	5.49	121.89	118.60
36	1	792	G	C8-N9-C4	5.49	108.60	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1602	A	C2-N3-C4	-5.49	107.86	110.60
36	1	1843	C	C2-N3-C4	-5.49	117.16	119.90
36	1	2119	A	N1-C6-N6	5.49	121.89	118.60
1	6	467	G	N3-C4-N9	5.49	129.29	126.00
36	5	3093	C	N3-C2-O2	5.49	125.74	121.90
36	5	3200	G	C4-C5-N7	5.49	113.00	110.80
36	1	189	G	N1-C6-O6	-5.49	116.61	119.90
36	1	3039	C	C2-N1-C1'	5.49	124.84	118.80
1	6	862	A	C8-N9-C4	5.49	108.00	105.80
1	6	1048	G	N3-C4-C5	5.49	131.34	128.60
1	6	1535	U	O4'-C1'-N1	5.49	112.59	108.20
36	5	653	A	C4-C5-N7	5.49	113.44	110.70
36	5	1450	G	C4-C5-N7	5.49	113.00	110.80
36	5	2687	G	N3-C4-N9	5.49	129.29	126.00
36	5	3062	G	C8-N9-C4	-5.49	104.20	106.40
36	1	2891	U	C5-C4-O4	-5.49	122.61	125.90
51	M5	68	ARG	NE-CZ-NH1	5.49	123.04	120.30
36	5	1834	U	N3-C4-C5	-5.49	111.31	114.60
36	5	1905	G	C4-C5-N7	5.49	113.00	110.80
36	1	608	A	C4-C5-C6	5.49	119.74	117.00
36	1	2142	A	C2-N3-C4	5.49	113.34	110.60
36	1	2378	C	C6-N1-C2	5.49	122.49	120.30
36	1	2414	G	N1-C2-N3	5.49	127.19	123.90
36	5	530	G	N1-C6-O6	-5.49	116.61	119.90
36	1	1503	A	C8-N9-C4	5.48	107.99	105.80
36	5	37	U	C4-C5-C6	5.48	122.99	119.70
36	5	2242	A	O5'-P-OP2	-5.48	100.77	105.70
36	5	2293	C	N1-C2-O2	5.48	122.19	118.90
36	5	2377	G	N1-C6-O6	-5.48	116.61	119.90
36	5	2803	A	C8-N9-C4	5.48	107.99	105.80
1	2	1241	G	C5-N7-C8	-5.48	101.56	104.30
36	1	1898	G	N3-C4-C5	5.48	131.34	128.60
36	1	2974	U	N1-C2-N3	5.48	118.19	114.90
36	1	3179	U	N3-C4-O4	-5.48	115.56	119.40
1	2	392	G	N1-C6-O6	5.48	123.19	119.90
36	1	1136	A	C4-C5-N7	5.48	113.44	110.70
36	1	2234	G	N1-C2-N3	5.48	127.19	123.90
36	5	2416	U	C6-N1-C2	-5.48	117.71	121.00
36	1	1903	U	N3-C4-O4	5.48	123.23	119.40
38	4	23	U	N1-C2-N3	5.48	118.19	114.90
1	6	792	U	C6-N1-C2	-5.48	117.71	121.00
10	s8	29	LEU	CA-CB-CG	5.48	127.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2988	C	C5-C6-N1	-5.48	118.26	121.00
36	1	2345	A	N1-C6-N6	5.48	121.89	118.60
1	2	848	C	C6-N1-C2	-5.47	118.11	120.30
36	1	1931	U	C5-C4-O4	5.47	129.19	125.90
36	1	2870	C	N3-C2-O2	5.47	125.73	121.90
37	3	84	A	N1-C6-N6	5.47	121.89	118.60
36	5	2815	G	C8-N9-C4	5.47	108.59	106.40
36	1	392	G	N9-C4-C5	-5.47	103.21	105.40
36	1	1313	G	C5-N7-C8	-5.47	101.56	104.30
36	5	718	G	N1-C2-N2	-5.47	111.28	116.20
36	5	2405	C	C2-N3-C4	-5.47	117.16	119.90
1	2	1731	A	N1-C6-N6	5.47	121.88	118.60
36	1	3210	A	N1-C6-N6	-5.47	115.32	118.60
36	5	2339	C	O5'-P-OP2	-5.47	100.78	105.70
38	8	34	U	C2-N3-C4	-5.47	123.72	127.00
36	1	1653	G	N1-C6-O6	-5.47	116.62	119.90
36	1	1795	U	O5'-P-OP2	5.47	117.26	110.70
38	4	136	G	C4-C5-N7	5.47	112.99	110.80
1	6	364	G	C5-C6-O6	-5.47	125.32	128.60
36	5	1604	G	C8-N9-C1'	-5.47	119.89	127.00
36	5	2245	C	C2-N3-C4	5.47	122.64	119.90
36	5	2871	G	N1-C6-O6	-5.47	116.62	119.90
36	1	3101	G	C8-N9-C4	5.47	108.59	106.40
36	5	3319	U	C5-C6-N1	5.47	125.43	122.70
1	6	17	C	N3-C2-O2	-5.47	118.07	121.90
1	6	1354	G	C6-C5-N7	-5.47	127.12	130.40
36	5	984	G	N3-C4-C5	-5.47	125.87	128.60
36	5	1299	U	O5'-P-OP2	-5.47	100.78	105.70
36	5	3106	A	OP1-P-O3'	5.47	117.23	105.20
36	5	3107	U	C2-N3-C4	-5.47	123.72	127.00
44	17	179	LEU	CA-CB-CG	5.47	127.87	115.30
36	1	1166	G	N3-C4-C5	5.46	131.33	128.60
36	1	1330	A	N1-C6-N6	5.46	121.88	118.60
36	1	2200	U	N3-C4-O4	5.46	123.22	119.40
36	1	2653	C	N3-C2-O2	-5.46	118.08	121.90
36	1	2699	G	N1-C6-O6	5.46	123.18	119.90
38	4	13	A	N1-C6-N6	5.46	121.88	118.60
1	6	163	G	C4-N9-C1'	-5.46	119.40	126.50
1	6	392	G	C5-C6-O6	-5.46	125.32	128.60
1	6	453	U	C6-N1-C2	-5.46	117.72	121.00
36	5	875	G	C4-N9-C1'	5.46	133.60	126.50
36	1	1443	G	N3-C2-N2	-5.46	116.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	95	G	C8-N9-C4	-5.46	104.22	106.40
36	5	1164	G	C8-N9-C4	5.46	108.58	106.40
36	5	2764	C	C5-C4-N4	-5.46	116.38	120.20
36	5	3075	G	N1-C6-O6	5.46	123.18	119.90
1	2	54	C	N3-C4-C5	5.46	124.08	121.90
36	1	1888	U	C2-N1-C1'	-5.46	111.15	117.70
36	1	3362	A	N1-C2-N3	5.46	132.03	129.30
1	6	426	G	N3-C4-C5	-5.46	125.87	128.60
36	5	395	A	C6-N1-C2	-5.46	115.32	118.60
36	5	1190	A	C8-N9-C4	-5.46	103.62	105.80
36	5	3060	C	C5-C4-N4	-5.46	116.38	120.20
36	1	2314	U	C6-N1-C1'	-5.46	113.56	121.20
38	4	32	C	C2-N1-C1'	-5.46	112.80	118.80
36	5	61	A	N9-C4-C5	5.46	107.98	105.80
36	5	606	C	C5-C6-N1	-5.46	118.27	121.00
36	5	2980	U	C6-N1-C2	-5.46	117.72	121.00
59	n3	89	ASP	CB-CG-OD1	-5.46	113.39	118.30
36	1	2848	G	C5-C6-O6	-5.46	125.33	128.60
37	3	95	A	C6-C5-N7	-5.46	128.48	132.30
46	19	52	LEU	CA-CB-CG	5.46	127.85	115.30
36	1	2621	G	C6-C5-N7	-5.46	127.13	130.40
1	2	1749	A	C2-N3-C4	-5.45	107.87	110.60
36	1	49	A	C2-N3-C4	-5.45	107.87	110.60
36	1	154	U	C2-N1-C1'	-5.45	111.16	117.70
36	1	827	A	N1-C6-N6	-5.45	115.33	118.60
36	1	1841	A	N3-C4-C5	-5.45	122.98	126.80
36	1	1929	G	N3-C2-N2	5.45	123.72	119.90
38	4	146	U	C5-C6-N1	-5.45	119.97	122.70
1	6	187	G	P-O3'-C3'	5.45	126.24	119.70
36	5	1446	A	OP1-P-O3'	5.45	117.20	105.20
36	5	2105	G	C5-C6-O6	-5.45	125.33	128.60
36	5	2342	U	N1-C2-O2	-5.45	118.98	122.80
36	5	2376	G	C5-N7-C8	-5.45	101.57	104.30
36	5	3214	U	N3-C4-O4	-5.45	115.58	119.40
36	5	1142	G	C6-C5-N7	-5.45	127.13	130.40
36	5	2625	C	C6-N1-C2	5.45	122.48	120.30
36	1	71	A	O5'-P-OP2	5.45	117.24	110.70
36	1	765	C	C5-C6-N1	5.45	123.73	121.00
36	1	1165	A	N7-C8-N9	-5.45	111.07	113.80
36	1	2870	C	N3-C4-C5	5.45	124.08	121.90
1	6	306	U	C5-C6-N1	-5.45	119.97	122.70
36	5	2728	G	C4-C5-N7	5.45	112.98	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2757	U	N1-C2-N3	5.45	118.17	114.90
36	1	1122	U	N3-C2-O2	-5.45	118.39	122.20
1	6	47	A	O5'-P-OP1	-5.45	100.80	105.70
36	5	1300	G	C4-C5-N7	5.45	112.98	110.80
36	5	1450	G	N1-C6-O6	5.45	123.17	119.90
36	5	3339	A	N1-C6-N6	5.45	121.87	118.60
1	2	1200	G	N3-C2-N2	-5.45	116.09	119.90
36	1	117	U	N1-C2-O2	-5.45	118.99	122.80
36	1	1001	G	N3-C4-N9	5.45	129.27	126.00
36	1	3039	C	N1-C2-O2	5.45	122.17	118.90
36	5	426	G	C8-N9-C4	5.45	108.58	106.40
36	5	1878	G	N3-C4-C5	-5.45	125.88	128.60
36	5	3014	U	N1-C2-O2	-5.45	118.99	122.80
1	2	1012	U	C2-N3-C4	5.44	130.27	127.00
36	1	949	C	C4-C5-C6	5.44	120.12	117.40
36	5	83	U	OP1-P-OP2	5.44	127.77	119.60
36	5	2820	A	O5'-P-OP2	-5.44	100.80	105.70
36	5	61	A	C5-C6-N6	5.44	128.06	123.70
36	5	970	A	N1-C6-N6	5.44	121.87	118.60
36	5	2917	G	N1-C6-O6	5.44	123.17	119.90
36	5	3104	U	O5'-P-OP2	-5.44	100.80	105.70
36	1	2688	U	C6-N1-C2	5.44	124.26	121.00
36	1	2865	U	N3-C4-C5	5.44	117.86	114.60
36	1	2966	G	N3-C2-N2	5.44	123.71	119.90
36	1	3128	G	N1-C6-O6	5.44	123.16	119.90
36	5	1604	G	C4-N9-C1'	5.44	133.57	126.50
36	5	1891	A	C5-C6-N6	-5.44	119.35	123.70
1	2	43	A	N1-C6-N6	-5.44	115.34	118.60
1	2	1150	G	C8-N9-C4	5.44	108.58	106.40
36	5	412	G	N3-C4-C5	-5.44	125.88	128.60
36	5	3115	C	C6-N1-C2	-5.44	118.12	120.30
36	1	1565	G	C8-N9-C4	-5.44	104.22	106.40
36	1	1867	A	C8-N9-C4	5.44	107.97	105.80
36	5	1378	U	C5-C6-N1	-5.44	119.98	122.70
37	7	112	G	C8-N9-C4	-5.44	104.22	106.40
36	1	225	C	C4-C5-C6	5.44	120.12	117.40
36	1	821	U	C5-C6-N1	-5.44	119.98	122.70
1	6	1765	A	N7-C8-N9	-5.44	111.08	113.80
36	5	869	G	C5-C6-N1	5.44	114.22	111.50
36	5	2148	U	C2-N1-C1'	-5.44	111.18	117.70
36	5	2273	G	C4-N9-C1'	-5.44	119.43	126.50
48	m1	12	LEU	CA-CB-CG	5.44	127.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1135	U	C6-N1-C2	5.43	124.26	121.00
36	1	376	G	O5'-P-OP1	-5.43	100.81	105.70
36	1	880	G	C5-C6-O6	5.43	131.86	128.60
36	1	901	G	C5-C6-O6	-5.43	125.34	128.60
36	1	1383	G	C8-N9-C4	-5.43	104.23	106.40
1	2	294	C	C6-N1-C2	5.43	122.47	120.30
36	1	3197	G	C2-N3-C4	-5.43	109.18	111.90
36	5	364	G	N3-C4-N9	-5.43	122.74	126.00
36	5	610	G	N9-C4-C5	5.43	107.57	105.40
37	3	82	G	C6-N1-C2	-5.43	121.84	125.10
1	6	1110	G	N1-C6-O6	-5.43	116.64	119.90
38	8	132	G	O5'-P-OP2	-5.43	100.81	105.70
38	4	38	U	N1-C2-O2	5.43	126.60	122.80
1	6	994	G	N1-C6-O6	5.43	123.16	119.90
36	5	215	G	O5'-P-OP2	5.43	117.22	110.70
36	5	945	C	C2-N1-C1'	5.43	124.77	118.80
36	1	1826	C	C6-N1-C2	5.43	122.47	120.30
1	6	1307	U	N3-C2-O2	-5.43	118.40	122.20
36	5	1208	U	N1-C2-N3	5.43	118.16	114.90
37	7	37	G	N9-C4-C5	-5.43	103.23	105.40
36	1	587	U	N1-C2-O2	-5.43	119.00	122.80
36	1	1509	A	N9-C4-C5	-5.43	103.63	105.80
1	6	1724	U	C5-C4-O4	5.43	129.16	125.90
36	5	1120	A	OP1-P-OP2	5.43	127.74	119.60
36	5	1340	G	N7-C8-N9	-5.43	110.39	113.10
36	5	1460	A	C5-C6-N6	-5.43	119.36	123.70
36	5	3219	G	C4-C5-N7	5.43	112.97	110.80
38	8	58	G	C8-N9-C4	5.43	108.57	106.40
1	2	1324	G	C8-N9-C1'	5.42	134.05	127.00
36	1	265	A	N1-C6-N6	5.42	121.86	118.60
36	5	2133	U	OP1-P-OP2	-5.42	111.46	119.60
36	5	2309	A	C4-C5-N7	-5.42	107.99	110.70
1	2	103	A	P-O3'-C3'	5.42	126.21	119.70
36	1	646	A	C2-N3-C4	-5.42	107.89	110.60
36	1	936	A	P-O3'-C3'	5.42	126.21	119.70
36	5	370	U	N3-C2-O2	-5.42	118.40	122.20
36	1	32	U	C2-N3-C4	-5.42	123.75	127.00
36	1	323	A	C4-C5-C6	5.42	119.71	117.00
36	1	1155	C	O5'-P-OP1	-5.42	100.82	105.70
36	5	706	A	OP2-P-O3'	5.42	117.13	105.20
36	5	902	G	C8-N9-C4	5.42	108.57	106.40
36	5	1292	C	N3-C4-C5	5.42	124.07	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2775	U	C6-N1-C2	5.42	124.25	121.00
38	8	116	G	C5-C6-O6	-5.42	125.35	128.60
36	1	1140	G	N3-C2-N2	5.42	123.69	119.90
36	1	2245	C	N3-C2-O2	-5.42	118.11	121.90
36	1	961	C	C6-N1-C2	5.42	122.47	120.30
36	1	1851	G	N1-C6-O6	5.42	123.15	119.90
36	1	2166	A	N1-C6-N6	5.42	121.85	118.60
36	1	2932	U	C5-C6-N1	-5.42	119.99	122.70
36	5	904	A	C5-C6-N1	5.42	120.41	117.70
36	5	1420	C	OP2-P-O3'	5.42	117.12	105.20
36	5	3098	G	O5'-P-OP2	-5.42	100.82	105.70
36	5	3308	C	C2-N3-C4	-5.42	117.19	119.90
51	m5	187	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	2	399	A	N1-C6-N6	-5.42	115.35	118.60
36	1	214	G	N3-C2-N2	-5.42	116.11	119.90
36	1	2867	C	N1-C2-N3	5.42	122.99	119.20
36	5	373	A	O5'-P-OP1	-5.42	100.83	105.70
36	5	1724	U	P-O3'-C3'	5.42	126.20	119.70
36	5	2393	G	N1-C6-O6	5.42	123.15	119.90
36	5	2852	C	N1-C2-O2	-5.42	115.65	118.90
36	5	3271	G	N3-C4-C5	-5.42	125.89	128.60
36	1	1834	U	C4-C5-C6	5.42	122.95	119.70
38	4	42	G	N1-C6-O6	5.42	123.15	119.90
36	5	91	G	N9-C4-C5	-5.42	103.23	105.40
36	5	1430	U	C5-C6-N1	-5.42	119.99	122.70
36	5	2315	G	OP2-P-O3'	5.42	117.11	105.20
1	6	1459	C	O5'-P-OP2	-5.41	100.83	105.70
36	5	344	A	C2-N3-C4	-5.41	107.89	110.60
36	5	631	U	C5-C6-N1	-5.41	119.99	122.70
36	5	1181	U	N1-C2-N3	5.41	118.15	114.90
36	5	1476	G	N3-C4-C5	5.41	131.31	128.60
36	5	2238	G	O5'-P-OP2	-5.41	100.83	105.70
36	5	2876	C	P-O3'-C3'	5.41	126.20	119.70
36	1	1359	C	N3-C4-C5	5.41	124.06	121.90
36	5	908	G	O5'-P-OP1	5.41	117.19	110.70
36	5	948	C	C6-N1-C2	5.41	122.47	120.30
36	5	1662	G	N1-C6-O6	5.41	123.15	119.90
36	5	2393	G	C5-C6-O6	-5.41	125.35	128.60
36	5	3303	G	C4-C5-N7	5.41	112.96	110.80
1	2	606	A	N1-C6-N6	5.41	121.84	118.60
1	6	858	G	C4-N9-C1'	5.41	133.53	126.50
36	5	1041	U	C6-N1-C2	5.41	124.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2726	C	N1-C2-N3	5.41	122.98	119.20
36	5	3259	U	C6-N1-C2	5.41	124.25	121.00
36	1	1411	C	N3-C2-O2	-5.41	118.11	121.90
36	1	1421	G	C8-N9-C4	5.41	108.56	106.40
36	5	2139	A	N1-C2-N3	5.41	132.00	129.30
36	5	2187	G	N1-C2-N2	-5.41	111.33	116.20
36	1	1128	U	C2-N3-C4	-5.41	123.76	127.00
1	6	558	U	C5-C6-N1	5.41	125.40	122.70
36	5	404	G	N3-C4-C5	-5.41	125.90	128.60
36	5	523	A	N1-C6-N6	-5.41	115.36	118.60
36	5	949	C	C4-C5-C6	5.41	120.10	117.40
36	5	1346	G	N3-C4-C5	5.41	131.30	128.60
36	5	2186	U	N3-C2-O2	-5.41	118.42	122.20
36	5	1561	G	O4'-C1'-N9	5.40	112.52	108.20
44	L7	183	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	6	313	U	O5'-P-OP1	-5.40	100.84	105.70
1	6	439	U	C5-C6-N1	-5.40	120.00	122.70
12	c0	88	PRO	N-CA-CB	5.40	109.78	103.30
36	5	890	C	N3-C4-N4	5.40	121.78	118.00
36	5	2421	U	N1-C2-N3	5.40	118.14	114.90
1	2	1145	U	N1-C2-O2	-5.40	119.02	122.80
36	1	713	U	C5-C6-N1	-5.40	120.00	122.70
36	1	1163	A	O5'-P-OP2	-5.40	100.84	105.70
36	1	1421	G	OP1-P-OP2	-5.40	111.50	119.60
38	4	95	G	C8-N9-C1'	5.40	134.02	127.00
36	5	29	C	C6-N1-C2	5.40	122.46	120.30
36	5	283	G	C5-C6-O6	-5.40	125.36	128.60
36	5	985	U	C5-C6-N1	-5.40	120.00	122.70
36	5	1300	G	N1-C6-O6	5.40	123.14	119.90
36	5	715	A	C5-C6-N1	5.40	120.40	117.70
36	1	20	A	N1-C6-N6	-5.40	115.36	118.60
36	1	273	A	C8-N9-C4	5.40	107.96	105.80
36	1	1182	A	N9-C4-C5	-5.40	103.64	105.80
36	1	1515	A	C6-C5-N7	-5.40	128.52	132.30
1	6	163	G	C5-N7-C8	-5.40	101.60	104.30
36	1	2639	G	N1-C2-N3	5.40	127.14	123.90
1	6	923	A	C2-N3-C4	-5.40	107.90	110.60
36	5	101	G	O4'-C1'-N9	5.40	112.52	108.20
36	5	2531	C	C2-N1-C1'	5.40	124.74	118.80
1	2	394	C	N3-C2-O2	-5.39	118.12	121.90
1	2	403	G	C4-N9-C1'	5.39	133.51	126.50
36	1	283	G	O4'-C1'-N9	-5.39	103.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	421	G	C8-N9-C4	5.39	108.56	106.40
36	1	963	G	O5'-P-OP1	5.39	117.17	110.70
36	1	1427	U	C6-N1-C1'	-5.39	113.65	121.20
37	3	89	G	C8-N9-C4	5.39	108.56	106.40
38	4	23	U	C2-N1-C1'	-5.39	111.23	117.70
1	6	1036	A	O5'-P-OP2	-5.39	100.84	105.70
36	1	1372	C	N3-C4-N4	-5.39	114.22	118.00
36	5	340	C	C6-N1-C2	5.39	122.46	120.30
36	5	1365	G	N9-C4-C5	-5.39	103.24	105.40
36	5	1534	A	N1-C2-N3	5.39	132.00	129.30
36	5	2417	U	N3-C4-C5	-5.39	111.36	114.60
36	5	2994	A	C5-C6-N1	5.39	120.40	117.70
36	1	589	A	C6-C5-N7	5.39	136.07	132.30
36	1	188	U	N3-C4-C5	-5.39	111.37	114.60
38	4	116	G	C8-N9-C1'	-5.39	119.99	127.00
36	5	1536	G	N3-C2-N2	-5.39	116.13	119.90
36	5	1822	C	C6-N1-C2	5.39	122.45	120.30
36	5	1847	A	C4-C5-C6	-5.39	114.31	117.00
36	5	2415	C	N3-C4-C5	5.39	124.06	121.90
36	5	2639	G	N1-C6-O6	5.39	123.13	119.90
36	5	2625	C	N3-C2-O2	5.39	125.67	121.90
36	1	1645	U	N3-C2-O2	-5.39	118.43	122.20
36	1	1489	A	C5-C6-N6	-5.38	119.39	123.70
36	1	2508	U	C5-C6-N1	5.38	125.39	122.70
1	6	982	U	N3-C2-O2	5.38	125.97	122.20
36	5	650	C	N3-C2-O2	5.38	125.67	121.90
36	5	1004	U	C2-N1-C1'	5.38	124.16	117.70
36	5	3142	A	N1-C6-N6	5.38	121.83	118.60
36	1	2966	G	N1-C2-N2	-5.38	111.36	116.20
36	5	887	G	C2-N3-C4	-5.38	109.21	111.90
1	2	393	C	C6-N1-C2	5.38	122.45	120.30
36	1	1053	A	O5'-P-OP2	-5.38	100.86	105.70
52	M6	15	LEU	CA-CB-CG	-5.38	102.92	115.30
1	6	1458	G	C4-N9-C1'	5.38	133.50	126.50
36	5	1669	C	N3-C2-O2	5.38	125.67	121.90
36	5	1323	G	N1-C2-N3	5.38	127.13	123.90
1	2	1194	A	N1-C6-N6	5.38	121.83	118.60
36	1	392	G	N1-C6-O6	5.38	123.13	119.90
36	1	392	G	N3-C4-N9	5.38	129.23	126.00
36	1	1894	U	C2-N1-C1'	-5.38	111.25	117.70
36	1	2523	A	N1-C6-N6	5.38	121.83	118.60
36	1	2827	U	C2-N1-C1'	-5.38	111.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1133	A	N1-C6-N6	5.38	121.83	118.60
36	5	696	C	N3-C4-N4	5.38	121.77	118.00
36	5	1452	A	N1-C6-N6	5.38	121.83	118.60
36	5	2618	G	C6-N1-C2	-5.38	121.87	125.10
36	1	281	G	C5-C6-N1	5.38	114.19	111.50
36	1	1055	A	C8-N9-C4	5.38	107.95	105.80
36	1	1315	U	N3-C2-O2	-5.38	118.44	122.20
36	1	1406	A	N1-C6-N6	5.38	121.83	118.60
1	6	383	G	N7-C8-N9	5.38	115.79	113.10
36	5	2376	G	C6-N1-C2	-5.38	121.88	125.10
36	1	321	C	C4-C5-C6	5.38	120.09	117.40
1	6	313	U	C5-C6-N1	-5.38	120.01	122.70
36	5	3317	U	P-O3'-C3'	5.38	126.15	119.70
36	1	995	U	C5-C4-O4	-5.37	122.68	125.90
36	1	1194	G	N1-C6-O6	-5.37	116.68	119.90
1	6	1751	C	C6-N1-C2	5.37	122.45	120.30
36	5	875	G	C6-N1-C2	-5.37	121.88	125.10
36	5	1048	A	N9-C4-C5	-5.37	103.65	105.80
36	5	1438	U	N3-C4-C5	-5.37	111.38	114.60
1	2	694	U	N1-C2-O2	5.37	126.56	122.80
36	1	353	G	C6-C5-N7	-5.37	127.18	130.40
36	1	1428	A	C6-C5-N7	-5.37	128.54	132.30
1	6	794	U	C2-N1-C1'	5.37	124.14	117.70
36	5	805	G	C8-N9-C4	5.37	108.55	106.40
36	5	1445	U	C2-N3-C4	-5.37	123.78	127.00
36	5	2616	C	OP2-P-O3'	5.37	117.02	105.20
36	5	3127	A	C5-C6-N1	5.37	120.39	117.70
38	8	4	C	N3-C4-N4	-5.37	114.24	118.00
38	8	34	U	C4-C5-C6	5.37	122.92	119.70
3	S1	181	LEU	CA-CB-CG	5.37	127.65	115.30
36	1	830	A	N1-C6-N6	5.37	121.82	118.60
36	5	264	G	N9-C4-C5	-5.37	103.25	105.40
36	5	2140	U	N1-C2-O2	-5.37	119.04	122.80
36	5	2377	G	C5-C6-O6	5.37	131.82	128.60
36	5	3121	U	C5-C4-O4	5.37	129.12	125.90
37	7	27	A	C5-C6-N6	-5.37	119.40	123.70
36	1	1345	G	OP2-P-O3'	5.37	117.01	105.20
36	1	2811	A	C2-N3-C4	5.37	113.28	110.60
36	1	3302	U	OP1-P-OP2	5.37	127.65	119.60
36	5	2820	A	N9-C4-C5	5.37	107.95	105.80
36	5	3228	C	C2-N1-C1'	5.37	124.70	118.80
36	5	889	U	N3-C4-C5	5.37	117.82	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1198	C	C6-N1-C1'	5.37	127.24	120.80
1	2	1650	U	C5-C6-N1	-5.37	120.02	122.70
36	1	639	G	OP1-P-O3'	5.37	117.01	105.20
36	1	671	U	N3-C2-O2	5.37	125.96	122.20
36	1	979	U	C6-N1-C2	-5.37	117.78	121.00
36	1	1198	C	N3-C4-C5	-5.37	119.75	121.90
36	1	1377	G	C5-N7-C8	-5.37	101.62	104.30
36	1	2398	A	C8-N9-C4	5.37	107.95	105.80
36	1	3003	G	N9-C4-C5	-5.37	103.25	105.40
36	5	212	G	C8-N9-C4	-5.37	104.25	106.40
36	1	590	G	N1-C6-O6	5.36	123.12	119.90
36	1	1192	C	C6-N1-C1'	-5.36	114.36	120.80
36	1	1520	G	C5-N7-C8	5.36	106.98	104.30
36	1	2282	U	O5'-P-OP2	-5.36	100.87	105.70
36	1	2748	A	C2-N3-C4	-5.36	107.92	110.60
36	1	2836	C	N3-C4-C5	-5.36	119.75	121.90
36	1	2946	A	OP1-P-OP2	-5.36	111.56	119.60
36	5	645	A	C4-C5-N7	-5.36	108.02	110.70
36	5	907	G	C8-N9-C4	5.36	108.55	106.40
36	5	1874	A	C2-N3-C4	-5.36	107.92	110.60
36	5	2796	G	C5-C6-O6	5.36	131.82	128.60
1	2	863	A	N1-C6-N6	5.36	121.82	118.60
36	1	350	C	N3-C2-O2	-5.36	118.15	121.90
1	6	1700	C	C6-N1-C1'	-5.36	114.36	120.80
36	5	856	G	C8-N9-C4	-5.36	104.25	106.40
36	5	961	C	O5'-P-OP2	5.36	117.14	110.70
36	1	321	C	N3-C2-O2	-5.36	118.15	121.90
36	1	2278	C	N1-C2-O2	5.36	122.12	118.90
36	1	2418	G	OP2-P-O3'	-5.36	93.41	105.20
37	3	89	G	N1-C6-O6	5.36	123.12	119.90
1	6	1656	U	O5'-P-OP2	-5.36	100.88	105.70
36	5	1929	G	C2-N3-C4	-5.36	109.22	111.90
36	5	2147	A	N9-C4-C5	-5.36	103.66	105.80
36	1	3077	A	C2-N3-C4	-5.36	107.92	110.60
1	6	359	A	N3-C4-C5	5.36	130.55	126.80
36	5	3343	G	N3-C4-C5	-5.36	125.92	128.60
1	2	380	U	N1-C2-O2	5.36	126.55	122.80
1	2	1006	C	N1-C2-O2	-5.36	115.69	118.90
36	1	1837	U	OP2-P-O3'	5.36	116.98	105.20
36	5	2981	U	N3-C4-O4	5.36	123.15	119.40
1	2	543	C	N3-C2-O2	-5.35	118.15	121.90
1	2	864	U	C6-N1-C2	-5.35	117.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1351	U	C6-N1-C2	-5.35	117.79	121.00
36	1	2942	C	C4-C5-C6	-5.35	114.72	117.40
36	5	1317	A	N1-C6-N6	5.35	121.81	118.60
36	1	281	G	C6-N1-C2	-5.35	121.89	125.10
36	1	1434	G	C2-N3-C4	5.35	114.58	111.90
36	1	1699	A	N1-C6-N6	5.35	121.81	118.60
36	1	2790	A	O5'-P-OP2	-5.35	100.88	105.70
36	1	3112	G	C4-C5-N7	5.35	112.94	110.80
36	5	788	C	C4-C5-C6	5.35	120.08	117.40
36	5	803	C	N3-C4-N4	5.35	121.75	118.00
1	2	1120	U	C5-C4-O4	5.35	129.11	125.90
36	1	958	C	N1-C2-O2	5.35	122.11	118.90
36	1	2639	G	N3-C4-N9	5.35	129.21	126.00
36	5	807	A	O4'-C1'-N9	5.35	112.48	108.20
36	1	789	A	C2-N3-C4	-5.35	107.93	110.60
36	1	2310	U	C5-C4-O4	5.35	129.11	125.90
1	6	1119	G	N1-C2-N2	-5.35	111.39	116.20
36	1	1655	G	C8-N9-C4	5.35	108.54	106.40
36	1	2153	U	N1-C2-N3	5.35	118.11	114.90
36	1	2708	C	N1-C2-O2	5.35	122.11	118.90
36	1	2871	G	C5-C6-N1	5.35	114.17	111.50
36	1	3278	C	C6-N1-C1'	-5.35	114.38	120.80
37	3	117	A	N1-C6-N6	5.35	121.81	118.60
38	4	30	C	C6-N1-C1'	5.35	127.22	120.80
1	6	448	C	C6-N1-C2	-5.35	118.16	120.30
36	5	2774	C	N3-C4-C5	-5.35	119.76	121.90
36	1	2699	G	C4-C5-N7	5.35	112.94	110.80
1	6	1648	A	N1-C6-N6	5.35	121.81	118.60
1	2	15	U	N3-C2-O2	-5.34	118.46	122.20
36	1	24	G	N3-C2-N2	5.34	123.64	119.90
36	1	978	G	N1-C6-O6	5.34	123.11	119.90
36	1	2169	G	C2-N3-C4	5.34	114.57	111.90
36	1	3121	U	OP1-P-O3'	5.34	116.96	105.20
1	6	609	U	C4-C5-C6	5.34	122.91	119.70
1	6	622	A	O5'-P-OP2	5.34	117.11	110.70
1	6	1227	A	P-O3'-C3'	5.34	126.11	119.70
36	5	2728	G	C6-C5-N7	-5.34	127.19	130.40
36	5	3214	U	C5-C4-O4	5.34	129.11	125.90
36	1	3008	A	N9-C4-C5	5.34	107.94	105.80
36	1	3309	G	C6-C5-N7	-5.34	127.19	130.40
37	3	86	U	C5-C4-O4	5.34	129.11	125.90
36	1	821	U	C5-C4-O4	5.34	129.10	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1437	C	N3-C2-O2	-5.34	118.16	121.90
36	1	1610	G	N1-C6-O6	5.34	123.10	119.90
36	1	1784	G	N1-C6-O6	-5.34	116.69	119.90
36	5	1317	A	C4-C5-N7	5.34	113.37	110.70
36	5	2121	G	N9-C4-C5	-5.34	103.26	105.40
36	5	3382	U	N1-C2-O2	5.34	126.54	122.80
36	5	353	G	C8-N9-C1'	5.34	133.94	127.00
36	5	2245	C	N3-C2-O2	-5.34	118.16	121.90
36	5	3331	U	C6-N1-C2	5.34	124.20	121.00
36	1	655	C	C4-C5-C6	5.34	120.07	117.40
36	1	2364	G	N3-C2-N2	-5.34	116.16	119.90
36	5	2661	G	N3-C4-N9	5.34	129.20	126.00
36	1	2152	A	C5-C6-N1	5.34	120.37	117.70
1	6	1573	A	P-O3'-C3'	5.34	126.10	119.70
36	5	1716	U	P-O3'-C3'	5.34	126.10	119.70
36	5	1734	G	C8-N9-C4	5.34	108.53	106.40
36	1	100	A	C5-C6-N1	-5.33	115.03	117.70
36	1	798	G	N7-C8-N9	5.33	115.77	113.10
1	6	194	U	N3-C2-O2	-5.33	118.47	122.20
36	5	1757	A	C8-N9-C4	-5.33	103.67	105.80
36	1	638	C	N3-C2-O2	-5.33	118.17	121.90
36	1	1114	U	N1-C2-O2	5.33	126.53	122.80
36	1	1153	A	C5-C6-N1	-5.33	115.03	117.70
36	1	1429	G	C5-N7-C8	5.33	106.97	104.30
36	1	1794	G	N1-C2-N2	-5.33	111.40	116.20
36	5	875	G	N3-C4-N9	5.33	129.20	126.00
36	5	960	U	OP1-P-OP2	5.33	127.60	119.60
36	5	1170	A	N9-C4-C5	-5.33	103.67	105.80
36	5	2913	C	C5-C4-N4	5.33	123.93	120.20
36	5	3182	G	OP1-P-OP2	-5.33	111.60	119.60
36	1	945	C	C5-C6-N1	-5.33	118.33	121.00
36	1	2647	A	N9-C4-C5	5.33	107.93	105.80
36	5	950	G	N7-C8-N9	-5.33	110.43	113.10
36	5	1068	C	C2-N1-C1'	-5.33	112.94	118.80
36	5	1853	U	N1-C2-N3	5.33	118.10	114.90
36	5	2947	G	O4'-C1'-N9	5.33	112.47	108.20
36	5	2996	U	C5-C6-N1	5.33	125.37	122.70
36	1	650	C	OP1-P-O3'	-5.33	93.47	105.20
36	5	1148	G	C8-N9-C4	5.33	108.53	106.40
36	5	1450	G	C5-N7-C8	-5.33	101.64	104.30
36	1	589	A	C4-C5-N7	-5.33	108.04	110.70
36	1	631	U	C6-N1-C2	5.33	124.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	935	U	O5'-P-OP2	-5.33	100.91	105.70
36	1	1923	C	C5-C4-N4	-5.33	116.47	120.20
1	6	484	C	C5-C6-N1	5.33	123.67	121.00
36	5	982	C	N1-C2-O2	5.33	122.10	118.90
36	5	2935	U	C5-C6-N1	5.33	125.36	122.70
1	2	829	A	P-O3'-C3'	5.33	126.09	119.70
1	2	1339	C	P-O3'-C3'	5.33	126.09	119.70
36	1	649	A	N1-C2-N3	5.33	131.96	129.30
36	1	1838	G	C5-C6-O6	-5.33	125.41	128.60
36	1	2384	A	O5'-P-OP2	-5.33	100.91	105.70
1	6	1568	C	C6-N1-C2	-5.33	118.17	120.30
36	5	1931	U	C5-C6-N1	-5.33	120.04	122.70
36	5	2376	G	C6-C5-N7	-5.33	127.20	130.40
36	1	588	G	N3-C4-C5	-5.32	125.94	128.60
36	1	895	A	C4-C5-C6	5.32	119.66	117.00
36	1	2699	G	N9-C4-C5	-5.32	103.27	105.40
37	3	14	U	C5-C6-N1	-5.32	120.04	122.70
1	6	385	A	C5-C6-N6	5.32	127.96	123.70
37	7	92	A	C4-C5-N7	5.32	113.36	110.70
68	o2	4	LEU	C-N-CA	-5.32	99.64	122.00
36	1	2554	A	N9-C4-C5	-5.32	103.67	105.80
36	1	2816	G	C5-C6-O6	-5.32	125.41	128.60
36	5	1497	C	N1-C2-O2	-5.32	115.71	118.90
36	5	2699	G	N1-C2-N2	-5.32	111.41	116.20
36	1	3139	A	O5'-P-OP1	-5.32	100.91	105.70
1	6	687	G	N3-C4-N9	-5.32	122.81	126.00
37	7	88	G	N1-C6-O6	-5.32	116.71	119.90
1	6	777	C	C5-C6-N1	5.32	123.66	121.00
1	6	1125	A	C5-C6-N1	-5.32	115.04	117.70
36	5	706	A	C2-N3-C4	-5.32	107.94	110.60
36	5	1077	U	C6-N1-C2	5.32	124.19	121.00
36	1	430	U	C5-C6-N1	-5.32	120.04	122.70
36	1	1292	C	C6-N1-C2	5.32	122.43	120.30
36	1	2827	U	C2-N3-C4	-5.32	123.81	127.00
36	5	276	U	N3-C4-O4	5.32	123.12	119.40
36	5	1589	A	N1-C6-N6	5.32	121.79	118.60
36	1	1394	A	C2-N3-C4	-5.32	107.94	110.60
36	1	2606	G	C4-N9-C1'	5.32	133.41	126.50
36	1	3078	U	C2-N1-C1'	5.32	124.08	117.70
36	5	726	G	OP1-P-O3'	5.32	116.89	105.20
36	5	2376	G	N1-C2-N3	5.32	127.09	123.90
36	1	1366	A	N1-C2-N3	-5.31	126.64	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2420	C	N3-C2-O2	5.31	125.62	121.90
36	5	3090	U	OP2-P-O3'	5.31	116.89	105.20
1	2	1241	G	N7-C8-N9	5.31	115.76	113.10
36	1	2101	C	P-O3'-C3'	5.31	126.08	119.70
36	1	2198	A	N1-C2-N3	5.31	131.96	129.30
1	6	1614	A	O4'-C1'-N9	5.31	112.45	108.20
36	5	1444	G	C5-C6-O6	-5.31	125.41	128.60
1	2	1793	G	OP1-P-OP2	-5.31	111.63	119.60
36	5	1704	A	C8-N9-C4	5.31	107.92	105.80
38	4	14	C	O5'-P-OP2	-5.31	100.92	105.70
36	5	345	G	C8-N9-C4	5.31	108.52	106.40
36	5	890	C	C5-C4-N4	-5.31	116.48	120.20
36	5	1454	A	N3-C4-C5	5.31	130.52	126.80
1	2	1200	G	C5-C6-N1	-5.31	108.85	111.50
36	1	347	G	C8-N9-C1'	-5.31	120.10	127.00
36	1	895	A	N1-C2-N3	5.31	131.95	129.30
36	1	2388	U	C5-C4-O4	-5.31	122.72	125.90
1	6	472	U	N1-C2-N3	5.31	118.08	114.90
36	5	971	G	N9-C4-C5	-5.31	103.28	105.40
36	5	1480	G	N3-C4-C5	5.31	131.25	128.60
36	5	2631	U	OP1-P-O3'	5.31	116.88	105.20
36	1	350	C	N1-C2-O2	5.31	122.08	118.90
1	2	1749	A	C8-N9-C4	5.30	107.92	105.80
36	1	830	A	C4-C5-N7	5.30	113.35	110.70
36	1	897	U	C5-C6-N1	-5.30	120.05	122.70
36	1	1206	G	O5'-P-OP2	-5.30	100.92	105.70
36	1	3375	A	C5'-C4'-C3'	-5.30	107.51	116.00
36	5	366	A	C8-N9-C4	5.30	107.92	105.80
36	5	1373	A	C5-C6-N6	-5.30	119.46	123.70
36	5	1435	A	P-O3'-C3'	5.30	126.07	119.70
36	5	1939	G	OP2-P-O3'	5.30	116.87	105.20
36	5	2932	U	C6-N1-C2	5.30	124.18	121.00
1	6	35	U	N3-C2-O2	-5.30	118.49	122.20
36	5	586	C	C2-N3-C4	-5.30	117.25	119.90
36	5	1165	A	C5-C6-N6	-5.30	119.46	123.70
36	1	2293	C	N1-C2-O2	5.30	122.08	118.90
44	L7	163	LEU	CA-CB-CG	-5.30	103.11	115.30
1	6	1355	C	C6-N1-C2	-5.30	118.18	120.30
1	6	1672	G	C6-C5-N7	-5.30	127.22	130.40
36	5	502	U	C4-C5-C6	5.30	122.88	119.70
36	5	624	G	C8-N9-C4	5.30	108.52	106.40
36	5	813	G	C8-N9-C4	5.30	108.52	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1847	A	N3-C4-C5	5.30	130.51	126.80
36	1	633	C	C4-C5-C6	5.30	120.05	117.40
36	1	788	C	C5-C6-N1	-5.30	118.35	121.00
36	1	1448	U	OP2-P-O3'	5.30	116.86	105.20
36	1	2309	A	C4-C5-N7	5.30	113.35	110.70
36	5	800	G	C8-N9-C4	5.30	108.52	106.40
36	5	933	A	N3-C4-C5	-5.30	123.09	126.80
36	5	1426	C	N1-C2-N3	-5.30	115.49	119.20
36	5	1519	G	N1-C6-O6	5.30	123.08	119.90
1	2	453	U	C6-N1-C1'	-5.30	113.78	121.20
36	1	1606	U	C6-N1-C2	5.30	124.18	121.00
36	5	502	U	C5-C6-N1	-5.30	120.05	122.70
1	2	1339	C	C3'-C2'-C1'	5.30	105.74	101.50
36	1	776	U	C5-C4-O4	5.30	129.08	125.90
36	1	1601	U	N3-C4-O4	-5.30	115.69	119.40
36	1	2572	C	C6-N1-C2	-5.30	118.18	120.30
36	5	911	C	C5-C6-N1	-5.30	118.35	121.00
36	5	955	U	O5'-P-OP2	-5.30	100.93	105.70
36	5	1598	G	C5-C6-O6	5.30	131.78	128.60
36	5	2326	A	C8-N9-C4	5.30	107.92	105.80
36	5	2705	A	N9-C4-C5	-5.30	103.68	105.80
36	5	3277	U	C5-C6-N1	5.30	125.35	122.70
38	8	26	U	C2-N1-C1'	5.30	124.06	117.70
1	6	1119	G	N1-C6-O6	-5.29	116.72	119.90
36	5	3045	G	N3-C4-C5	-5.29	125.95	128.60
36	1	439	C	N1-C2-O2	5.29	122.08	118.90
36	1	2383	C	C5-C4-N4	-5.29	116.49	120.20
1	6	787	G	C8-N9-C4	-5.29	104.28	106.40
36	5	2999	U	C2-N3-C4	-5.29	123.82	127.00
36	5	3219	G	N3-C4-N9	5.29	129.18	126.00
36	1	331	G	N3-C4-C5	-5.29	125.95	128.60
36	1	346	C	C4-C5-C6	5.29	120.05	117.40
36	1	871	U	N3-C4-O4	-5.29	115.70	119.40
36	1	1587	A	N1-C6-N6	-5.29	115.42	118.60
38	4	136	G	N9-C4-C5	-5.29	103.28	105.40
1	6	767	U	N3-C2-O2	-5.29	118.50	122.20
36	5	1652	G	C8-N9-C4	5.29	108.52	106.40
37	7	7	G	N3-C4-C5	-5.29	125.95	128.60
36	1	1120	A	C5-C6-N1	5.29	120.34	117.70
1	6	312	A	OP1-P-O3'	5.29	116.84	105.20
36	5	2862	U	C5-C6-N1	-5.29	120.06	122.70
1	2	1595	U	C4-C5-C6	5.29	122.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	334	A	C4-C5-N7	5.29	113.34	110.70
36	1	347	G	C5-C6-O6	-5.29	125.43	128.60
36	1	637	C	N3-C2-O2	-5.29	118.20	121.90
36	1	1050	U	N1-C2-O2	5.29	126.50	122.80
38	4	98	U	C5-C4-O4	-5.29	122.73	125.90
36	5	419	G	N9-C4-C5	-5.29	103.28	105.40
36	5	3220	G	N3-C4-C5	-5.29	125.96	128.60
1	2	334	G	N1-C6-O6	5.29	123.07	119.90
36	1	2963	C	C6-N1-C2	5.29	122.42	120.30
38	4	119	C	C6-N1-C2	-5.29	118.19	120.30
36	5	2863	G	N3-C2-N2	5.29	123.60	119.90
36	1	38	U	O5'-P-OP2	5.29	117.04	110.70
36	1	947	G	C2-N3-C4	-5.29	109.26	111.90
36	1	996	A	C8-N9-C4	5.29	107.91	105.80
36	1	2356	A	C5-C6-N6	-5.29	119.47	123.70
36	1	2541	U	P-O3'-C3'	5.29	126.04	119.70
36	1	2896	A	C5'-C4'-O4'	-5.29	102.76	109.10
36	5	395	A	C5-C6-N6	-5.29	119.47	123.70
36	5	800	G	O4'-C1'-N9	-5.29	103.97	108.20
36	5	974	G	N1-C6-O6	-5.29	116.73	119.90
36	5	2950	G	OP1-P-O3'	5.29	116.83	105.20
36	5	3335	A	N1-C6-N6	5.29	121.77	118.60
36	1	682	U	C5-C6-N1	-5.28	120.06	122.70
36	1	1151	U	C5-C6-N1	5.28	125.34	122.70
1	6	49	C	C6-N1-C2	5.28	122.41	120.30
1	6	1141	G	N9-C4-C5	-5.28	103.29	105.40
1	6	1642	G	C5-C6-O6	-5.28	125.43	128.60
36	5	1847	A	O5'-P-OP2	-5.28	100.94	105.70
36	5	2959	C	OP2-P-O3'	5.28	116.82	105.20
36	5	3041	U	N3-C4-C5	5.28	117.77	114.60
1	2	647	G	N3-C4-N9	-5.28	122.83	126.00
36	1	105	C	C2-N3-C4	-5.28	117.26	119.90
36	1	3093	C	N1-C2-O2	-5.28	115.73	118.90
36	1	3361	G	N1-C6-O6	-5.28	116.73	119.90
36	5	326	U	C5-C4-O4	-5.28	122.73	125.90
36	5	2822	U	C2-N1-C1'	-5.28	111.36	117.70
36	1	879	U	C5-C4-O4	5.28	129.07	125.90
36	1	1907	C	N1-C2-O2	5.28	122.07	118.90
1	6	970	A	P-O3'-C3'	5.28	126.04	119.70
36	5	39	A	C5-N7-C8	-5.28	101.26	103.90
36	5	2415	C	C2-N3-C4	-5.28	117.26	119.90
36	1	2409	G	C2-N3-C4	5.28	114.54	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	142	G	N3-C2-N2	-5.28	116.21	119.90
1	2	1112	G	C4-C5-N7	5.28	112.91	110.80
36	1	71	A	N1-C2-N3	5.28	131.94	129.30
36	1	1130	A	C5-C6-N6	-5.28	119.48	123.70
36	5	82	C	C4-C5-C6	5.28	120.04	117.40
36	5	1200	A	OP1-P-O3'	5.28	116.81	105.20
36	5	2310	U	C6-N1-C2	-5.28	117.83	121.00
36	5	2761	G	N3-C4-N9	5.28	129.17	126.00
36	5	2812	C	C6-N1-C2	-5.28	118.19	120.30
36	5	3131	U	N1-C2-O2	5.28	126.50	122.80
36	1	859	G	C4-N9-C1'	5.28	133.36	126.50
36	1	1115	G	OP1-P-OP2	-5.28	111.69	119.60
36	1	2812	C	C6-N1-C2	5.28	122.41	120.30
36	1	2833	A	O5'-P-OP2	-5.28	100.95	105.70
43	L6	34	LEU	CA-CB-CG	-5.28	103.17	115.30
36	5	51	A	N9-C4-C5	-5.28	103.69	105.80
36	5	1662	G	C5-C6-N1	-5.28	108.86	111.50
36	1	48	A	N1-C2-N3	5.27	131.94	129.30
1	6	1465	C	N3-C4-C5	-5.27	119.79	121.90
37	7	1	G	C4-N9-C1'	5.27	133.36	126.50
1	2	863	A	C4-C5-N7	5.27	113.34	110.70
1	2	1745	G	C4-N9-C1'	5.27	133.35	126.50
36	1	915	A	O5'-P-OP1	-5.27	100.95	105.70
36	1	2146	C	C6-N1-C2	-5.27	118.19	120.30
36	5	360	G	C5-C6-O6	5.27	131.76	128.60
36	5	878	G	N3-C2-N2	5.27	123.59	119.90
36	5	3176	G	C4-N9-C1'	5.27	133.35	126.50
36	1	363	G	C4-C5-N7	5.27	112.91	110.80
36	1	1306	G	N1-C6-O6	5.27	123.06	119.90
1	6	943	C	O5'-P-OP1	-5.27	100.96	105.70
36	5	1473	G	C8-N9-C4	5.27	108.51	106.40
1	2	1274	C	N3-C2-O2	-5.27	118.21	121.90
36	1	31	C	C2-N3-C4	-5.27	117.27	119.90
36	1	931	C	C5-C4-N4	-5.27	116.51	120.20
36	1	1888	U	N1-C2-O2	-5.27	119.11	122.80
36	1	2187	G	N3-C2-N2	5.27	123.59	119.90
38	4	119	C	N3-C4-N4	5.27	121.69	118.00
36	5	1178	G	C6-C5-N7	-5.27	127.24	130.40
36	5	1445	U	N3-C2-O2	5.27	125.89	122.20
36	5	2893	C	C4-C5-C6	5.27	120.03	117.40
38	4	40	A	N1-C6-N6	5.27	121.76	118.60
36	5	1405	U	C5-C6-N1	-5.27	120.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1846	C	OP2-P-O3'	5.27	116.79	105.20
36	5	2231	C	O4'-C1'-N1	5.27	112.42	108.20
1	2	940	A	C8-N9-C4	-5.27	103.69	105.80
36	1	511	G	OP1-P-OP2	5.27	127.50	119.60
36	1	1315	U	C5-C6-N1	-5.27	120.07	122.70
36	5	375	A	C5-C6-N6	5.27	127.91	123.70
36	5	1150	A	O5'-P-OP2	-5.27	100.96	105.70
36	5	1335	C	N3-C4-N4	5.27	121.69	118.00
36	1	836	A	O4'-C1'-N9	-5.26	103.99	108.20
36	1	2197	C	N1-C2-N3	-5.26	115.52	119.20
36	5	1454	A	C5-N7-C8	-5.26	101.27	103.90
36	5	1851	G	C4-C5-C6	5.26	121.96	118.80
36	5	2896	A	C5'-C4'-O4'	-5.26	102.78	109.10
36	1	2330	C	N3-C4-C5	5.26	124.00	121.90
1	6	1	U	O4'-C1'-N1	5.26	112.41	108.20
36	5	963	G	N1-C6-O6	-5.26	116.74	119.90
1	2	1022	C	C2-N3-C4	-5.26	117.27	119.90
36	1	1352	A	P-O3'-C3'	5.26	126.01	119.70
36	1	2137	U	C5-C4-O4	-5.26	122.74	125.90
1	6	578	U	C5-C6-N1	-5.26	120.07	122.70
36	5	1314	C	C2-N1-C1'	5.26	124.59	118.80
36	1	109	A	OP1-P-O3'	5.26	116.77	105.20
36	1	2975	U	N1-C2-O2	5.26	126.48	122.80
1	6	1647	U	C5-C4-O4	5.26	129.06	125.90
36	5	3027	A	C6-N1-C2	-5.26	115.44	118.60
36	5	3187	A	C8-N9-C4	5.26	107.90	105.80
1	2	248	U	C2-N1-C1'	-5.26	111.39	117.70
36	1	2872	A	C8-N9-C4	-5.26	103.70	105.80
36	5	197	G	C4-N9-C1'	5.26	133.34	126.50
36	5	1124	U	OP1-P-O3'	5.26	116.77	105.20
36	5	1404	G	C8-N9-C4	5.26	108.50	106.40
36	1	728	G	OP2-P-O3'	5.26	116.76	105.20
36	1	1841	A	C4-C5-C6	5.26	119.63	117.00
36	1	2917	G	C2-N3-C4	5.26	114.53	111.90
36	1	2991	A	N1-C6-N6	-5.26	115.45	118.60
64	N8	42	ARG	NE-CZ-NH2	-5.26	117.67	120.30
36	5	2434	U	N3-C4-O4	-5.26	115.72	119.40
36	5	2526	C	N1-C2-O2	5.26	122.05	118.90
36	5	2908	G	N1-C6-O6	5.26	123.05	119.90
36	1	1419	A	O4'-C1'-N9	5.25	112.40	108.20
36	1	2747	A	N1-C6-N6	-5.25	115.45	118.60
36	5	326	U	O5'-P-OP2	-5.25	100.97	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	321	C	N3-C2-O2	-5.25	118.22	121.90
1	6	1124	A	N9-C4-C5	-5.25	103.70	105.80
36	5	717	C	N3-C4-C5	5.25	124.00	121.90
36	5	1143	A	N1-C2-N3	5.25	131.93	129.30
38	8	20	U	C5-C6-N1	-5.25	120.07	122.70
36	1	1178	G	C8-N9-C1'	-5.25	120.17	127.00
36	1	3208	G	N3-C4-N9	5.25	129.15	126.00
1	6	1023	A	OP1-P-O3'	5.25	116.75	105.20
1	6	1599	C	N3-C2-O2	-5.25	118.22	121.90
1	6	1777	G	O5'-P-OP1	-5.25	100.97	105.70
36	5	71	A	O5'-P-OP1	-5.25	100.97	105.70
36	5	578	A	C5-C6-N6	-5.25	119.50	123.70
36	5	1528	G	C4-N9-C1'	5.25	133.33	126.50
36	5	1867	A	C2-N3-C4	-5.25	107.97	110.60
36	5	2892	A	N9-C4-C5	-5.25	103.70	105.80
36	1	1507	G	C4-C5-C6	5.25	121.95	118.80
36	5	881	C	C6-N1-C2	5.25	122.40	120.30
1	2	959	U	N1-C2-O2	5.25	126.47	122.80
36	1	1445	U	N3-C4-C5	5.25	117.75	114.60
36	1	2374	C	C2-N1-C1'	5.25	124.57	118.80
38	4	32	C	N3-C4-C5	5.25	124.00	121.90
36	5	869	G	C5-C6-O6	5.25	131.75	128.60
36	5	960	U	N3-C4-C5	5.25	117.75	114.60
36	5	2621	G	C5-C6-O6	-5.25	125.45	128.60
36	5	3231	U	C5-C4-O4	5.25	129.05	125.90
37	7	22	A	N1-C6-N6	5.25	121.75	118.60
64	n8	46	ASP	CB-CG-OD1	5.25	123.02	118.30
36	1	1365	G	C6-C5-N7	-5.25	127.25	130.40
36	1	3173	G	C4-N9-C1'	5.25	133.32	126.50
36	5	2817	A	OP2-P-O3'	5.25	116.74	105.20
1	2	720	G	P-O3'-C3'	5.25	125.99	119.70
1	2	1418	G	C4-N9-C1'	5.25	133.32	126.50
36	1	1165	A	C2-N3-C4	-5.25	107.98	110.60
36	1	1313	G	C6-C5-N7	-5.25	127.25	130.40
36	1	2172	A	C4-C5-N7	5.25	113.32	110.70
36	5	273	A	C8-N9-C4	5.25	107.90	105.80
36	5	1528	G	N1-C2-N3	5.25	127.05	123.90
1	2	16	G	N1-C2-N2	-5.24	111.48	116.20
36	1	392	G	C4-C5-N7	5.24	112.90	110.80
36	1	2410	U	N1-C2-O2	-5.24	119.13	122.80
36	1	2877	G	N1-C2-N3	5.24	127.05	123.90
1	6	512	A	C2'-C3'-O3'	5.24	122.09	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2197	C	N1-C2-N3	-5.24	115.53	119.20
36	1	2525	G	C4-C5-N7	5.24	112.90	110.80
37	3	65	G	C8-N9-C1'	-5.24	120.19	127.00
1	6	199	G	O4'-C1'-N9	5.24	112.39	108.20
36	5	1293	U	N1-C2-N3	5.24	118.05	114.90
36	5	1337	A	C5-C6-N6	-5.24	119.51	123.70
36	1	2682	C	O5'-P-OP2	-5.24	100.98	105.70
36	1	2700	G	C6-C5-N7	-5.24	127.26	130.40
36	1	2931	C	C6-N1-C2	5.24	122.40	120.30
36	5	2208	A	O4'-C1'-N9	5.24	112.39	108.20
36	1	25	U	N3-C2-O2	5.24	125.87	122.20
36	1	969	C	O5'-P-OP1	-5.24	100.98	105.70
36	5	1474	A	C8-N9-C4	5.24	107.89	105.80
36	5	2815	G	C5-N7-C8	5.24	106.92	104.30
36	5	3354	U	N1-C2-O2	5.24	126.47	122.80
1	6	450	U	C6-N1-C2	5.24	124.14	121.00
36	5	1924	U	N3-C4-C5	5.24	117.74	114.60
1	2	323	A	N7-C8-N9	5.24	116.42	113.80
36	1	24	G	C4-C5-C6	5.24	121.94	118.80
36	1	646	A	C5-C6-N1	-5.24	115.08	117.70
36	5	1315	U	C5-C6-N1	-5.24	120.08	122.70
36	5	1879	A	C6-C5-N7	-5.24	128.63	132.30
36	1	2370	G	OP2-P-O3'	5.23	116.71	105.20
38	4	42	G	N9-C4-C5	-5.23	103.31	105.40
36	5	2639	G	N3-C2-N2	-5.23	116.24	119.90
36	1	857	G	C6-C5-N7	-5.23	127.26	130.40
36	1	1394	A	N3-C4-C5	5.23	130.46	126.80
36	1	2427	U	N3-C2-O2	-5.23	118.54	122.20
36	1	2941	A	O4'-C1'-N9	-5.23	104.01	108.20
36	1	3207	U	C6-N1-C1'	5.23	128.53	121.20
36	1	3213	A	C2-N3-C4	-5.23	107.98	110.60
1	6	1117	U	N1-C2-O2	-5.23	119.14	122.80
1	6	1269	U	C2-N1-C1'	5.23	123.98	117.70
36	5	302	U	N3-C4-O4	-5.23	115.74	119.40
1	2	1217	A	O4'-C1'-N9	-5.23	104.02	108.20
36	1	24	G	N9-C4-C5	-5.23	103.31	105.40
36	1	969	C	C5-C6-N1	-5.23	118.39	121.00
36	1	2098	C	C5-C6-N1	5.23	123.61	121.00
36	1	2860	U	C6-N1-C1'	5.23	128.52	121.20
36	5	899	U	N3-C2-O2	-5.23	118.54	122.20
36	5	1317	A	N1-C2-N3	-5.23	126.69	129.30
36	5	3304	U	N3-C4-O4	5.23	123.06	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2899	C	C5-C6-N1	-5.23	118.39	121.00
36	1	2346	C	N3-C4-C5	-5.23	119.81	121.90
38	4	110	C	OP2-P-O3'	5.23	116.70	105.20
1	6	13	C	C4-C5-C6	5.23	120.01	117.40
1	6	338	C	C5-C6-N1	5.23	123.61	121.00
36	1	2130	G	N1-C6-O6	-5.23	116.77	119.90
53	M7	41	LEU	CA-CB-CG	5.23	127.32	115.30
1	6	105	A	N1-C6-N6	5.23	121.73	118.60
1	6	362	G	N1-C2-N3	5.23	127.04	123.90
36	5	2584	G	C6-C5-N7	-5.23	127.26	130.40
36	5	2637	A	C8-N9-C4	5.23	107.89	105.80
71	o5	21	LEU	CA-CB-CG	5.23	127.32	115.30
1	2	973	A	C8-N9-C4	5.22	107.89	105.80
36	1	1534	A	C5-C6-N6	-5.22	119.52	123.70
36	1	2131	A	C5-C6-N1	-5.22	115.09	117.70
36	1	2762	A	C5-C6-N6	5.22	127.88	123.70
36	1	2778	G	C8-N9-C4	-5.22	104.31	106.40
1	6	614	C	C6-N1-C2	5.22	122.39	120.30
36	5	414	U	N1-C2-O2	-5.22	119.14	122.80
36	5	1060	U	N3-C4-C5	5.22	117.73	114.60
36	5	1297	C	C2-N3-C4	-5.22	117.29	119.90
36	5	1724	U	C2-N1-C1'	5.22	123.97	117.70
36	1	1367	G	C4-C5-N7	5.22	112.89	110.80
36	1	1395	G	C5-C6-N1	5.22	114.11	111.50
38	4	17	A	C8-N9-C4	5.22	107.89	105.80
1	6	1659	A	C8-N9-C4	5.22	107.89	105.80
36	5	922	U	N3-C4-O4	-5.22	115.74	119.40
1	2	416	A	C2-N3-C4	-5.22	107.99	110.60
36	5	2705	A	C8-N9-C4	5.22	107.89	105.80
1	2	1539	G	C4-N9-C1'	5.22	133.28	126.50
36	1	270	U	O5'-P-OP1	-5.22	101.00	105.70
1	6	1274	C	C5-C6-N1	5.22	123.61	121.00
36	5	308	A	O5'-P-OP1	5.22	116.96	110.70
36	5	1047	A	C6-C5-N7	-5.22	128.65	132.30
36	5	3308	C	N1-C2-N3	5.22	122.85	119.20
51	m5	96	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	2	1642	G	N1-C6-O6	5.22	123.03	119.90
36	1	2835	U	C5-C6-N1	-5.22	120.09	122.70
1	6	1117	U	N3-C4-C5	-5.22	111.47	114.60
36	1	127	G	C5-C6-O6	-5.22	125.47	128.60
36	1	2339	C	OP1-P-OP2	5.22	127.43	119.60
36	5	95	A	C4-C5-C6	-5.22	114.39	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	984	G	C4-C5-C6	5.22	121.93	118.80
36	5	2648	G	N1-C6-O6	-5.22	116.77	119.90
36	5	2917	G	O5'-P-OP2	-5.22	101.00	105.70
36	1	952	A	C2-N3-C4	-5.21	107.99	110.60
36	1	1902	G	C6-C5-N7	-5.21	127.27	130.40
36	1	2118	C	C5-C4-N4	-5.21	116.55	120.20
36	1	2735	U	N3-C4-O4	-5.21	115.75	119.40
38	4	147	U	N3-C4-O4	5.21	123.05	119.40
1	6	1698	G	N1-C6-O6	-5.21	116.77	119.90
36	5	2396	G	N9-C4-C5	5.21	107.49	105.40
36	5	2704	A	OP2-P-O3'	5.21	116.67	105.20
36	1	2549	G	N1-C2-N2	-5.21	111.51	116.20
36	5	994	G	O5'-P-OP2	-5.21	101.01	105.70
36	5	1114	U	O5'-P-OP2	-5.21	101.01	105.70
36	5	1367	G	C4-C5-C6	5.21	121.93	118.80
38	8	43	A	C8-N9-C4	-5.21	103.72	105.80
1	2	1200	G	C4-C5-C6	5.21	121.93	118.80
36	1	1365	G	N1-C2-N2	-5.21	111.51	116.20
36	5	1906	G	C4-C5-N7	5.21	112.89	110.80
36	5	971	G	OP2-P-O3'	5.21	116.66	105.20
36	5	2878	G	N7-C8-N9	-5.21	110.50	113.10
36	1	184	U	C5-C4-O4	5.21	129.03	125.90
36	1	355	A	N1-C6-N6	5.21	121.72	118.60
36	1	1126	G	C6-C5-N7	-5.21	127.28	130.40
36	1	2808	A	C6-C5-N7	-5.21	128.65	132.30
36	1	3197	G	N3-C4-N9	-5.21	122.87	126.00
36	1	619	A	N1-C6-N6	5.21	121.72	118.60
36	1	923	C	C4-C5-C6	5.21	120.00	117.40
36	1	3136	G	C6-C5-N7	-5.21	127.28	130.40
37	3	78	U	C5-C4-O4	-5.21	122.78	125.90
38	4	31	G	C8-N9-C4	5.21	108.48	106.40
38	4	95	G	C4-N9-C1'	-5.21	119.73	126.50
1	6	1096	C	C6-N1-C2	5.21	122.38	120.30
36	5	1475	A	C8-N9-C4	5.21	107.88	105.80
36	5	2334	U	O5'-P-OP2	-5.21	101.01	105.70
36	1	743	C	C6-N1-C2	5.21	122.38	120.30
36	1	88	A	N1-C6-N6	5.20	121.72	118.60
36	1	1658	G	C8-N9-C4	-5.20	104.32	106.40
37	3	103	A	N1-C6-N6	5.20	121.72	118.60
36	5	665	A	C6-C5-N7	-5.20	128.66	132.30
36	5	986	U	N3-C2-O2	-5.20	118.56	122.20
36	5	3245	A	N1-C6-N6	5.20	121.72	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1331	U	C5-C6-N1	-5.20	120.10	122.70
36	1	2525	G	N9-C4-C5	-5.20	103.32	105.40
36	5	1127	G	OP1-P-OP2	5.20	127.40	119.60
36	5	2186	U	C6-N1-C2	-5.20	117.88	121.00
1	2	1100	G	C4-N9-C1'	5.20	133.26	126.50
36	1	715	A	N7-C8-N9	5.20	116.40	113.80
36	1	1120	A	C5-C6-N6	-5.20	119.54	123.70
36	1	3103	A	C2-N3-C4	-5.20	108.00	110.60
38	8	80	A	N9-C4-C5	5.20	107.88	105.80
40	l3	4	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	2	353	A	N9-C4-C5	-5.20	103.72	105.80
1	2	1086	A	O5'-P-OP2	-5.20	101.02	105.70
36	1	835	G	O4'-C1'-N9	5.20	112.36	108.20
36	1	2190	U	OP2-P-O3'	5.20	116.64	105.20
36	1	3096	C	N3-C4-N4	5.20	121.64	118.00
1	6	564	G	N9-C4-C5	5.20	107.48	105.40
36	5	72	C	N3-C2-O2	-5.20	118.26	121.90
37	7	88	G	C5-C6-O6	5.20	131.72	128.60
36	1	2816	G	N9-C4-C5	-5.20	103.32	105.40
36	1	586	C	N1-C2-O2	-5.20	115.78	118.90
36	1	2799	A	N1-C6-N6	-5.20	115.48	118.60
36	5	32	U	C4-C5-C6	5.20	122.82	119.70
36	5	517	G	C6-C5-N7	-5.20	127.28	130.40
36	5	902	G	C5-C6-O6	-5.20	125.48	128.60
36	5	1302	A	O5'-P-OP1	-5.20	101.03	105.70
36	5	1534	A	N3-C4-C5	-5.20	123.16	126.80
1	2	1644	C	N3-C2-O2	-5.19	118.26	121.90
36	1	2688	U	C6-N1-C1'	-5.19	113.93	121.20
36	5	1170	A	N1-C6-N6	5.19	121.72	118.60
73	O7	65	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	6	106	U	C5-C4-O4	5.19	129.01	125.90
1	6	765	G	O4'-C1'-N9	-5.19	104.05	108.20
1	6	1654	G	C5-C6-O6	-5.19	125.48	128.60
36	5	371	G	C8-N9-C4	5.19	108.48	106.40
36	5	2355	G	C2-N3-C4	-5.19	109.30	111.90
36	5	2723	U	OP1-P-OP2	5.19	127.39	119.60
36	5	3140	G	C5-N7-C8	-5.19	101.70	104.30
36	5	3151	U	N1-C2-N3	-5.19	111.78	114.90
36	1	1149	G	N3-C2-N2	-5.19	116.27	119.90
36	1	2423	U	N1-C2-O2	-5.19	119.17	122.80
36	1	2617	U	C6-N1-C2	-5.19	117.89	121.00
36	1	3362	A	C4-C5-N7	5.19	113.30	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1199	C	N3-C4-C5	-5.19	119.82	121.90
36	5	1407	A	N9-C4-C5	-5.19	103.72	105.80
36	5	2806	U	C5-C6-N1	-5.19	120.11	122.70
1	2	1052	U	N1-C2-O2	5.19	126.43	122.80
1	2	1777	G	N1-C6-O6	5.19	123.01	119.90
1	6	371	G	C8-N9-C1'	-5.19	120.25	127.00
36	1	1201	C	N3-C4-N4	5.19	121.63	118.00
36	1	2126	A	C8-N9-C4	5.19	107.88	105.80
1	6	1660	A	N1-C6-N6	-5.19	115.49	118.60
36	5	1137	C	N3-C4-C5	5.19	123.97	121.90
36	5	3217	C	N3-C4-N4	-5.19	114.37	118.00
1	2	248	U	N3-C2-O2	5.19	125.83	122.20
36	1	1489	A	C8-N9-C4	5.19	107.87	105.80
36	1	2723	U	C2-N3-C4	-5.19	123.89	127.00
36	5	1016	C	O5'-P-OP1	-5.19	101.03	105.70
36	5	1459	C	N1-C2-O2	-5.19	115.79	118.90
36	5	2271	A	N1-C2-N3	-5.19	126.71	129.30
36	5	2727	A	C6-N1-C2	-5.19	115.49	118.60
78	q2	104	LEU	CA-CB-CG	5.19	127.23	115.30
36	1	58	G	N9-C4-C5	-5.18	103.33	105.40
36	1	1592	G	N3-C4-C5	-5.18	126.01	128.60
36	1	2861	U	N1-C2-O2	5.18	126.43	122.80
47	M0	146	ASP	CB-CG-OD1	-5.18	113.63	118.30
36	5	428	A	C8-N9-C4	5.18	107.87	105.80
36	5	1468	A	C8-N9-C4	5.18	107.87	105.80
36	5	2137	U	N1-C2-N3	-5.18	111.79	114.90
36	5	2663	G	C5-C6-O6	-5.18	125.49	128.60
36	1	306	A	O5'-P-OP1	-5.18	101.03	105.70
36	1	658	G	C4-N9-C1'	5.18	133.24	126.50
36	1	1128	U	C5-C6-N1	-5.18	120.11	122.70
36	1	2183	A	N1-C2-N3	5.18	131.89	129.30
1	6	941	A	N1-C6-N6	-5.18	115.49	118.60
36	5	82	C	O5'-P-OP2	-5.18	101.03	105.70
36	5	1689	U	N1-C2-N3	5.18	118.01	114.90
36	5	3191	G	C5-C6-O6	-5.18	125.49	128.60
36	5	3318	G	N3-C4-N9	-5.18	122.89	126.00
36	5	942	U	C4-C5-C6	5.18	122.81	119.70
36	5	947	G	N3-C4-C5	-5.18	126.01	128.60
36	5	1688	U	N1-C2-O2	5.18	126.43	122.80
36	5	2375	G	O4'-C1'-N9	5.18	112.34	108.20
1	2	90	C	N3-C2-O2	-5.18	118.28	121.90
36	1	654	C	C5-C6-N1	-5.18	118.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	900	G	N9-C4-C5	5.18	107.47	105.40
36	1	2531	C	C2-N1-C1'	5.18	124.50	118.80
36	5	30	G	OP1-P-O3'	5.18	116.59	105.20
36	5	1633	C	C6-N1-C2	-5.18	118.23	120.30
36	5	2651	G	OP2-P-O3'	5.18	116.59	105.20
36	5	2964	G	C6-C5-N7	5.18	133.51	130.40
37	7	37	G	N3-C4-N9	5.18	129.11	126.00
37	3	74	C	C6-N1-C2	5.18	122.37	120.30
1	6	1125	A	N1-C6-N6	5.18	121.71	118.60
36	5	2406	C	N3-C2-O2	5.18	125.53	121.90
36	5	2607	G	P-O3'-C3'	5.18	125.91	119.70
1	2	551	G	C8-N9-C4	-5.18	104.33	106.40
1	2	1299	G	N3-C4-C5	-5.18	126.01	128.60
36	1	595	G	N1-C2-N2	-5.18	111.54	116.20
36	1	880	G	C6-C5-N7	5.18	133.51	130.40
36	1	910	G	C2-N3-C4	-5.18	109.31	111.90
36	1	1695	U	C6-N1-C2	5.18	124.11	121.00
36	1	2417	U	C4-C5-C6	5.18	122.81	119.70
36	1	2609	A	C8-N9-C4	5.18	107.87	105.80
1	6	794	U	C5-C6-N1	5.18	125.29	122.70
1	6	1199	G	N3-C4-C5	5.18	131.19	128.60
36	5	497	C	C6-N1-C2	-5.18	118.23	120.30
36	5	658	G	C6-C5-N7	-5.18	127.30	130.40
1	2	1324	G	N1-C2-N2	5.17	120.86	116.20
35	SM	134	ASP	CB-CG-OD2	5.17	122.96	118.30
36	1	1902	G	C8-N9-C4	-5.17	104.33	106.40
36	1	1906	G	C6-C5-N7	-5.17	127.30	130.40
36	1	3362	A	C4-N9-C1'	5.17	135.61	126.30
36	5	95	A	N1-C2-N3	-5.17	126.71	129.30
36	5	756	U	C2-N3-C4	-5.17	123.89	127.00
36	5	2144	A	OP1-P-O3'	5.17	116.58	105.20
36	1	2847	A	C4-C5-N7	5.17	113.29	110.70
36	5	304	G	N1-C6-O6	-5.17	116.80	119.90
36	1	221	A	OP1-P-OP2	5.17	127.36	119.60
36	1	888	A	N1-C6-N6	5.17	121.70	118.60
36	1	1496	C	C2-N1-C1'	5.17	124.49	118.80
36	1	2610	G	C2-N3-C4	-5.17	109.31	111.90
1	6	1698	G	P-O3'-C3'	5.17	125.91	119.70
36	5	801	A	O4'-C1'-N9	-5.17	104.06	108.20
36	5	1803	C	N3-C4-C5	5.17	123.97	121.90
36	5	2618	G	N3-C4-N9	5.17	129.10	126.00
36	1	948	C	C4-C5-C6	5.17	119.98	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1101	G	OP1-P-OP2	5.17	127.35	119.60
36	1	2818	U	O4'-C1'-N1	-5.17	104.06	108.20
1	6	359	A	C6-N1-C2	5.17	121.70	118.60
36	5	1842	A	C8-N9-C4	5.17	107.87	105.80
36	1	392	G	C6-C5-N7	-5.17	127.30	130.40
36	1	2144	A	C5-C6-N6	-5.17	119.57	123.70
36	1	2355	G	C4-C5-C6	5.17	121.90	118.80
36	1	2425	G	C5-C6-N1	5.17	114.08	111.50
1	6	351	C	O5'-P-OP1	-5.17	101.05	105.70
1	6	359	A	C4-N9-C1'	-5.17	117.00	126.30
1	6	565	C	C2-N3-C4	-5.17	117.32	119.90
1	6	1615	C	C3'-C2'-C1'	5.17	105.63	101.50
36	5	1868	G	C4-C5-C6	5.17	121.90	118.80
36	5	2134	G	N1-C2-N2	-5.17	111.55	116.20
36	5	2698	G	N1-C6-O6	5.17	123.00	119.90
36	5	3166	C	C6-N1-C2	-5.17	118.23	120.30
37	7	105	C	N3-C2-O2	-5.17	118.28	121.90
1	2	158	U	P-O3'-C3'	5.17	125.90	119.70
36	1	833	G	N3-C4-N9	5.17	129.10	126.00
36	1	3081	C	C4-C5-C6	5.17	119.98	117.40
1	6	1185	U	N1-C2-O2	5.17	126.42	122.80
38	8	33	A	O5'-P-OP1	-5.17	101.05	105.70
1	2	1085	G	C8-N9-C4	5.16	108.47	106.40
1	2	1218	G	N1-C6-O6	5.16	123.00	119.90
36	1	386	A	N1-C6-N6	5.16	121.70	118.60
36	1	410	U	C5-C4-O4	5.16	129.00	125.90
36	1	655	C	N1-C2-N3	5.16	122.81	119.20
36	1	1899	G	O5'-P-OP1	-5.16	101.05	105.70
1	6	795	U	N1-C2-O2	5.16	126.41	122.80
1	6	1274	C	C2-N3-C4	5.16	122.48	119.90
36	5	373	A	N1-C6-N6	-5.16	115.50	118.60
37	7	28	C	C5-C6-N1	-5.16	118.42	121.00
36	1	2848	G	OP2-P-O3'	5.16	116.55	105.20
1	6	1110	G	N1-C2-N2	-5.16	111.56	116.20
36	5	269	G	C8-N9-C4	5.16	108.46	106.40
36	5	813	G	C6-C5-N7	-5.16	127.30	130.40
36	5	2796	G	OP2-P-O3'	5.16	116.55	105.20
36	5	2964	G	OP1-P-OP2	5.16	127.34	119.60
38	8	100	U	C6-N1-C2	-5.16	117.90	121.00
1	2	1258	U	N1-C2-O2	5.16	126.41	122.80
36	1	363	G	OP1-P-O3'	5.16	116.55	105.20
36	1	1139	G	C5-C6-N1	-5.16	108.92	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1836	C	C2-N1-C1'	5.16	124.47	118.80
36	1	2643	A	N7-C8-N9	-5.16	111.22	113.80
36	1	2836	C	C5-C4-N4	5.16	123.81	120.20
1	6	337	G	C6-C5-N7	-5.16	127.30	130.40
36	1	2537	U	P-O3'-C3'	5.16	125.89	119.70
1	2	403	G	C8-N9-C1'	-5.16	120.30	127.00
36	1	1336	U	N3-C2-O2	-5.16	118.59	122.20
36	1	1367	G	N7-C8-N9	-5.16	110.52	113.10
36	1	2728	G	O4'-C1'-N9	5.16	112.33	108.20
36	5	315	C	N3-C4-C5	5.16	123.96	121.90
36	5	1107	C	C4-C5-C6	5.16	119.98	117.40
36	5	1751	G	N7-C8-N9	-5.16	110.52	113.10
36	5	1792	C	C5-C6-N1	-5.16	118.42	121.00
36	5	2404	A	C8-N9-C1'	-5.16	118.42	127.70
36	1	3302	U	C6-N1-C2	5.15	124.09	121.00
1	6	425	A	OP2-P-O3'	5.15	116.54	105.20
1	6	1340	U	N1-C2-O2	5.15	126.41	122.80
36	5	2777	G	C4-C5-C6	5.15	121.89	118.80
1	2	1176	G	C5-C6-O6	-5.15	125.51	128.60
1	6	147	A	O4'-C1'-N9	5.15	112.32	108.20
1	6	942	G	C8-N9-C4	-5.15	104.34	106.40
36	5	861	C	C5-C6-N1	-5.15	118.42	121.00
36	5	2418	G	N1-C6-O6	5.15	122.99	119.90
1	2	1782	A	C5-C6-N6	5.15	127.82	123.70
36	1	2813	A	N1-C2-N3	5.15	131.88	129.30
38	4	121	U	C5-C4-O4	5.15	128.99	125.90
36	5	7	C	C6-N1-C2	5.15	122.36	120.30
36	5	630	A	C8-N9-C4	5.15	107.86	105.80
69	o3	18	ARG	NE-CZ-NH1	-5.15	117.72	120.30
36	5	3058	U	C2-N1-C1'	5.15	123.88	117.70
36	1	394	G	N3-C4-N9	-5.15	122.91	126.00
36	1	717	C	N1-C2-O2	-5.15	115.81	118.90
36	1	942	U	O5'-P-OP1	5.15	116.88	110.70
38	4	20	U	C5-C6-N1	-5.15	120.13	122.70
1	6	1185	U	N3-C2-O2	-5.15	118.60	122.20
36	5	96	G	O5'-P-OP2	-5.15	101.07	105.70
36	5	1183	C	C2-N3-C4	-5.15	117.33	119.90
36	5	2347	U	C5-C4-O4	-5.15	122.81	125.90
36	1	226	C	N3-C4-N4	5.15	121.60	118.00
38	4	61	A	C5-C6-N1	5.15	120.27	117.70
36	5	3216	G	N3-C4-N9	5.15	129.09	126.00
36	1	916	G	C8-N9-C4	5.14	108.46	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1414	G	N3-C4-N9	5.14	129.09	126.00
36	1	2400	G	C8-N9-C4	5.14	108.46	106.40
36	5	2177	G	C6-C5-N7	-5.14	127.31	130.40
36	5	3028	G	N1-C6-O6	-5.14	116.81	119.90
37	7	56	A	C2-N3-C4	-5.14	108.03	110.60
1	2	53	G	N3-C4-N9	-5.14	122.92	126.00
36	1	651	G	N1-C2-N3	5.14	126.98	123.90
36	1	1404	G	N1-C6-O6	-5.14	116.81	119.90
36	1	1414	G	N9-C4-C5	-5.14	103.34	105.40
36	1	1515	A	C4-C5-C6	5.14	119.57	117.00
36	1	2335	G	C5-C6-N1	5.14	114.07	111.50
1	6	864	U	C6-N1-C1'	-5.14	114.00	121.20
1	6	1745	G	C8-N9-C4	5.14	108.46	106.40
36	5	691	A	OP1-P-O3'	5.14	116.52	105.20
36	5	1408	G	C8-N9-C1'	5.14	133.68	127.00
36	5	1905	G	N9-C4-C5	-5.14	103.34	105.40
36	5	2257	C	C6-N1-C2	-5.14	118.24	120.30
36	5	2572	C	C6-N1-C2	-5.14	118.24	120.30
36	1	51	A	C5-C6-N1	5.14	120.27	117.70
38	8	45	C	N3-C4-C5	-5.14	119.84	121.90
36	1	2127	U	O5'-P-OP1	-5.14	101.08	105.70
36	1	2226	U	N1-C2-N3	5.14	117.98	114.90
38	4	25	G	N1-C2-N3	5.14	126.98	123.90
36	5	370	U	C2-N1-C1'	5.14	123.87	117.70
36	5	813	G	C5-C6-O6	-5.14	125.52	128.60
36	5	1112	A	C6-N1-C2	-5.14	115.52	118.60
36	1	2639	G	C4-N9-C1'	5.14	133.18	126.50
36	1	325	A	C2-N3-C4	5.14	113.17	110.60
36	1	668	G	C8-N9-C4	5.14	108.45	106.40
36	1	880	G	N9-C4-C5	5.14	107.45	105.40
36	1	951	A	C5-C6-N1	-5.14	115.13	117.70
36	1	2846	U	N1-C2-O2	5.14	126.40	122.80
1	6	1	U	N3-C2-O2	-5.14	118.60	122.20
1	6	974	A	C8-N9-C4	5.14	107.86	105.80
36	5	349	A	OP2-P-O3'	5.14	116.50	105.20
36	5	1480	G	C8-N9-C4	5.14	108.45	106.40
1	2	555	A	C8-N9-C4	-5.13	103.75	105.80
36	1	156	G	C5-C6-N1	5.13	114.07	111.50
36	1	846	A	C2-N3-C4	-5.13	108.03	110.60
36	1	1362	G	OP2-P-O3'	5.13	116.50	105.20
36	1	2890	A	OP1-P-OP2	-5.13	111.90	119.60
38	4	40	A	C4-C5-N7	5.13	113.27	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	98	U	N3-C4-O4	5.13	122.99	119.40
1	6	116	U	C4-C5-C6	5.13	122.78	119.70
36	5	61	A	C5-C6-N1	-5.13	115.13	117.70
36	1	2992	U	C5-C4-O4	5.13	128.98	125.90
38	4	37	A	C5-C6-N1	5.13	120.27	117.70
38	4	42	G	N9-C1'-C2'	-5.13	106.35	112.00
36	5	1200	A	N1-C2-N3	5.13	131.87	129.30
1	2	1212	G	C4-C5-N7	5.13	112.85	110.80
36	1	707	U	C5-C4-O4	5.13	128.98	125.90
36	1	773	G	N1-C6-O6	-5.13	116.82	119.90
36	1	924	G	N3-C2-N2	5.13	123.49	119.90
36	1	1121	U	C5-C6-N1	-5.13	120.14	122.70
36	1	1481	A	O5'-P-OP1	5.13	116.86	110.70
1	6	95	G	N1-C6-O6	-5.13	116.82	119.90
36	5	1155	C	C5-C4-N4	-5.13	116.61	120.20
36	5	1528	G	N3-C4-C5	-5.13	126.03	128.60
36	5	1589	A	OP2-P-O3'	5.13	116.49	105.20
36	5	2183	A	N9-C4-C5	-5.13	103.75	105.80
36	5	2889	C	N1-C2-O2	5.13	121.98	118.90
36	1	695	C	C2-N3-C4	-5.13	117.33	119.90
36	1	2945	G	N9-C4-C5	-5.13	103.35	105.40
36	5	98	G	C8-N9-C4	5.13	108.45	106.40
36	1	232	G	N3-C4-C5	-5.13	126.04	128.60
36	1	1389	G	N3-C4-N9	5.13	129.08	126.00
36	1	2209	U	C6-N1-C2	-5.13	117.92	121.00
36	1	2572	C	C6-N1-C1'	-5.13	114.65	120.80
36	5	2864	A	C8-N9-C4	5.13	107.85	105.80
36	1	91	G	OP1-P-O3'	5.13	116.48	105.20
36	1	650	C	OP1-P-OP2	5.13	127.29	119.60
36	1	797	U	OP2-P-O3'	5.13	116.48	105.20
36	1	1314	C	C6-N1-C2	-5.13	118.25	120.30
36	1	1404	G	N3-C2-N2	5.13	123.49	119.90
11	s9	149	ARG	NE-CZ-NH1	5.13	122.86	120.30
36	5	646	A	C2-N3-C4	-5.13	108.04	110.60
36	5	2997	G	C4-C5-N7	5.13	112.85	110.80
36	5	3176	G	N1-C2-N3	5.13	126.98	123.90
1	2	863	A	C5-C6-N6	-5.12	119.60	123.70
1	6	314	C	N1-C2-O2	-5.12	115.83	118.90
1	2	394	C	N1-C2-O2	5.12	121.97	118.90
36	1	1043	C	N3-C4-C5	5.12	123.95	121.90
36	1	1154	A	C4-C5-C6	5.12	119.56	117.00
36	1	1468	A	C2-N3-C4	-5.12	108.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2895	G	C8-N9-C4	5.12	108.45	106.40
1	6	90	C	N3-C2-O2	-5.12	118.31	121.90
36	5	2628	A	N1-C6-N6	-5.12	115.53	118.60
36	5	2836	C	N1-C2-O2	5.12	121.97	118.90
1	2	1108	G	C8-N9-C4	-5.12	104.35	106.40
36	1	803	C	O5'-P-OP1	5.12	116.85	110.70
1	6	43	A	OP1-P-OP2	5.12	127.28	119.60
36	5	1128	U	N1-C2-O2	-5.12	119.22	122.80
36	5	1151	U	N3-C4-C5	-5.12	111.53	114.60
36	5	1888	U	C2-N1-C1'	-5.12	111.55	117.70
36	5	2350	C	O5'-P-OP1	5.12	116.85	110.70
36	5	2646	C	C6-N1-C2	5.12	122.35	120.30
36	1	404	G	C6-C5-N7	-5.12	127.33	130.40
36	1	833	G	N7-C8-N9	-5.12	110.54	113.10
36	1	1635	G	C6-C5-N7	-5.12	127.33	130.40
36	1	2917	G	C5-C6-N1	5.12	114.06	111.50
36	5	3060	C	N3-C4-N4	5.12	121.58	118.00
36	1	363	G	N3-C4-N9	5.12	129.07	126.00
36	1	2645	G	N1-C2-N3	5.12	126.97	123.90
36	1	2699	G	C5-C6-O6	-5.12	125.53	128.60
36	1	2908	G	N1-C2-N3	5.12	126.97	123.90
1	6	364	G	C4-N9-C1'	5.12	133.15	126.50
36	5	345	G	C5-C6-N1	-5.12	108.94	111.50
36	1	1390	A	N9-C4-C5	5.12	107.85	105.80
36	1	1726	C	N3-C4-C5	5.12	123.95	121.90
36	1	2410	U	C2-N1-C1'	-5.12	111.56	117.70
1	6	337	G	O4'-C1'-N9	-5.12	104.11	108.20
1	6	1048	G	C8-N9-C4	5.12	108.45	106.40
36	5	101	G	C8-N9-C4	-5.12	104.35	106.40
36	5	670	C	OP1-P-O3'	5.12	116.45	105.20
36	5	1476	G	N3-C4-N9	-5.12	122.93	126.00
36	5	1549	U	C2-N1-C1'	-5.12	111.56	117.70
36	5	1831	U	C2-N3-C4	5.12	130.07	127.00
37	7	22	A	C4-C5-C6	5.12	119.56	117.00
36	1	345	G	N3-C4-C5	-5.11	126.04	128.60
36	1	851	C	C5-C4-N4	-5.11	116.62	120.20
36	1	1483	G	C5-C6-O6	-5.11	125.53	128.60
36	1	2400	G	OP2-P-O3'	5.11	116.45	105.20
36	1	2986	U	N1-C2-N3	5.11	117.97	114.90
38	4	64	U	C6-N1-C2	-5.11	117.93	121.00
1	6	619	A	C4-C5-C6	-5.11	114.44	117.00
1	6	1596	C	N3-C2-O2	-5.11	118.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	966	U	C6-N1-C2	-5.11	117.93	121.00
36	5	1178	G	C5-N7-C8	-5.11	101.74	104.30
36	5	2190	U	N1-C2-N3	5.11	117.97	114.90
36	5	2314	U	C5-C4-O4	-5.11	122.83	125.90
36	5	2889	C	N3-C4-C5	5.11	123.95	121.90
36	5	2895	G	N1-C2-N2	-5.11	111.60	116.20
36	1	2966	G	N3-C4-N9	5.11	129.07	126.00
36	1	2333	C	C4-C5-C6	5.11	119.96	117.40
36	1	2549	G	C8-N9-C1'	-5.11	120.36	127.00
36	1	2742	C	C6-N1-C2	5.11	122.34	120.30
36	1	2918	G	C8-N9-C1'	-5.11	120.36	127.00
36	5	521	A	C2-N3-C4	-5.11	108.05	110.60
36	5	1080	A	C8-N9-C4	5.11	107.84	105.80
36	5	1495	U	C4-C5-C6	5.11	122.77	119.70
36	5	2354	C	N1-C2-O2	-5.11	115.83	118.90
36	1	54	C	C2-N3-C4	-5.11	117.35	119.90
36	1	1411	C	OP1-P-O3'	5.11	116.44	105.20
36	1	2434	U	C4-C5-C6	5.11	122.77	119.70
36	5	3104	U	O5'-P-OP1	5.11	116.83	110.70
36	1	1911	A	C5-C6-N6	-5.11	119.61	123.70
1	6	317	C	N1-C2-N3	5.11	122.78	119.20
36	5	2193	U	N1-C2-O2	-5.11	119.22	122.80
36	5	2694	A	C6-N1-C2	-5.11	115.54	118.60
36	5	2880	U	C5-C4-O4	5.11	128.96	125.90
36	5	3185	U	C4-C5-C6	5.11	122.77	119.70
36	5	3197	G	N9-C4-C5	5.11	107.44	105.40
36	1	155	G	N3-C4-C5	-5.11	126.05	128.60
36	1	2917	G	N1-C2-N2	5.11	120.79	116.20
38	4	39	G	N9-C4-C5	-5.11	103.36	105.40
1	6	620	A	OP2-P-O3'	5.11	116.43	105.20
36	5	2403	G	N7-C8-N9	5.11	115.65	113.10
36	5	3270	U	C5-C6-N1	-5.11	120.15	122.70
36	1	2295	A	C8-N9-C4	-5.10	103.76	105.80
1	6	371	G	C5-C6-N1	-5.10	108.95	111.50
36	5	2996	U	C2-N1-C1'	5.10	123.82	117.70
37	7	102	A	N9-C4-C5	-5.10	103.76	105.80
78	Q2	70	LEU	CA-CB-CG	5.10	127.04	115.30
1	6	359	A	C8-N9-C1'	5.10	136.88	127.70
1	6	571	G	N9-C4-C5	5.10	107.44	105.40
1	6	1588	G	N1-C6-O6	-5.10	116.84	119.90
36	5	1452	A	N9-C4-C5	-5.10	103.76	105.80
36	5	1608	C	N1-C2-O2	5.10	121.96	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2820	A	N7-C8-N9	5.10	116.35	113.80
1	6	308	C	C5-C6-N1	-5.10	118.45	121.00
36	5	1853	U	N3-C4-O4	-5.10	115.83	119.40
36	5	2607	G	OP2-P-O3'	5.10	116.42	105.20
36	5	2966	G	N3-C4-N9	5.10	129.06	126.00
36	1	158	G	C2-N3-C4	-5.10	109.35	111.90
36	1	1340	G	C6-C5-N7	-5.10	127.34	130.40
36	1	2741	C	N1-C2-O2	5.10	121.96	118.90
36	5	646	A	C5-C6-N6	5.10	127.78	123.70
36	5	2881	C	N3-C4-C5	5.10	123.94	121.90
36	1	914	A	N9-C4-C5	5.10	107.84	105.80
36	1	2300	G	N3-C4-N9	-5.10	122.94	126.00
36	1	2846	U	N3-C4-O4	-5.10	115.83	119.40
38	4	15	G	N7-C8-N9	-5.10	110.55	113.10
38	4	40	A	C5-C6-N6	-5.10	119.62	123.70
1	6	63	G	N1-C6-O6	-5.10	116.84	119.90
36	5	822	G	N3-C4-C5	5.10	131.15	128.60
36	5	2689	A	C6-C5-N7	-5.10	128.73	132.30
36	1	3007	U	O5'-P-OP2	-5.10	101.11	105.70
36	5	2792	A	C6-N1-C2	-5.10	115.54	118.60
36	5	2920	U	N1-C2-N3	5.10	117.96	114.90
38	8	43	A	C6-N1-C2	-5.10	115.54	118.60
36	1	215	G	N3-C4-N9	5.09	129.06	126.00
36	1	699	A	C5-N7-C8	-5.09	101.35	103.90
36	1	943	U	C2-N1-C1'	5.09	123.81	117.70
36	5	2514	U	O5'-P-OP1	-5.09	101.11	105.70
36	5	2836	C	C4-C5-C6	5.09	119.95	117.40
36	1	2381	G	C8-N9-C4	-5.09	104.36	106.40
36	1	3311	C	N3-C4-C5	5.09	123.94	121.90
36	1	1536	G	N1-C6-O6	5.09	122.95	119.90
1	6	812	A	N1-C6-N6	5.09	121.66	118.60
36	5	630	A	C2-N3-C4	-5.09	108.05	110.60
36	5	739	G	N1-C6-O6	-5.09	116.84	119.90
36	5	1198	C	O4'-C1'-N1	5.09	112.27	108.20
36	5	3015	G	N1-C6-O6	5.09	122.95	119.90
38	8	102	U	N1-C2-O2	-5.09	119.23	122.80
36	1	718	G	C6-C5-N7	-5.09	127.35	130.40
36	1	942	U	C4-C5-C6	5.09	122.75	119.70
36	5	221	A	C5-C6-N6	5.09	127.77	123.70
36	5	610	G	C4-C5-N7	-5.09	108.76	110.80
36	5	3181	C	C4-C5-C6	5.09	119.94	117.40
37	7	56	A	N9-C1'-C2'	-5.09	106.40	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	125	U	C2-N1-C1'	5.09	123.81	117.70
1	2	1777	G	C4-C5-N7	5.09	112.83	110.80
36	1	421	G	C5-C6-N1	5.09	114.04	111.50
1	6	606	A	N9-C4-C5	-5.09	103.77	105.80
1	6	1796	C	C2-N3-C4	-5.09	117.36	119.90
36	5	279	U	N1-C2-N3	-5.09	111.85	114.90
36	5	499	G	O5'-P-OP1	-5.09	101.12	105.70
36	5	2194	G	N1-C2-N3	5.09	126.95	123.90
36	1	188	U	N1-C2-N3	5.09	117.95	114.90
36	1	1207	G	C5-C6-O6	-5.09	125.55	128.60
36	1	2197	C	C5-C4-N4	-5.09	116.64	120.20
36	1	2714	G	C8-N9-C1'	5.09	133.61	127.00
36	5	2383	C	N3-C4-N4	5.09	121.56	118.00
36	5	2856	G	C6-C5-N7	-5.09	127.35	130.40
37	7	40	C	C2-N1-C1'	-5.09	113.20	118.80
36	1	332	C	C5-C6-N1	-5.08	118.46	121.00
36	1	2237	C	C6-N1-C2	5.08	122.33	120.30
36	5	1116	G	N3-C4-C5	-5.08	126.06	128.60
36	5	2349	U	OP1-P-O3'	5.08	116.39	105.20
36	1	590	G	C5-C6-O6	-5.08	125.55	128.60
36	1	1891	A	C8-N9-C4	5.08	107.83	105.80
38	4	23	U	C6-N1-C1'	5.08	128.32	121.20
1	6	1058	U	P-O3'-C3'	5.08	125.80	119.70
36	5	2316	G	O5'-P-OP2	-5.08	101.12	105.70
36	5	2761	G	N3-C4-C5	-5.08	126.06	128.60
36	5	3132	C	OP2-P-O3'	5.08	116.38	105.20
36	1	405	U	N3-C2-O2	5.08	125.76	122.20
69	O3	48	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	6	1082	C	C6-N1-C2	-5.08	118.27	120.30
1	6	1127	G	N1-C2-N3	5.08	126.95	123.90
36	5	516	A	N9-C4-C5	-5.08	103.77	105.80
36	5	1362	G	C5-C6-O6	5.08	131.65	128.60
38	8	95	G	N1-C6-O6	-5.08	116.85	119.90
36	5	227	G	N1-C6-O6	5.08	122.95	119.90
1	2	321	C	O4'-C1'-N1	5.08	112.26	108.20
36	1	588	G	C4-C5-N7	-5.08	108.77	110.80
36	1	1141	C	C4-C5-C6	5.08	119.94	117.40
36	1	1418	A	O5'-P-OP2	-5.08	101.13	105.70
1	6	1765	A	C6-C5-N7	5.08	135.85	132.30
36	5	909	G	N1-C6-O6	-5.08	116.85	119.90
36	5	2814	G	N3-C4-N9	5.08	129.05	126.00
36	5	3008	A	C2-N3-C4	-5.08	108.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1403	C	C2-N3-C4	-5.08	117.36	119.90
36	1	2855	U	N3-C4-C5	5.08	117.65	114.60
36	5	653	A	C5-N7-C8	-5.08	101.36	103.90
36	5	681	U	C2-N1-C1'	5.08	123.79	117.70
36	5	1419	A	O4'-C1'-N9	5.08	112.26	108.20
36	1	2123	G	C5-C6-O6	-5.08	125.56	128.60
1	6	1	U	N1-C2-O2	5.08	126.35	122.80
36	5	109	A	O5'-P-OP2	-5.08	101.13	105.70
36	5	2609	A	O5'-P-OP2	-5.08	101.13	105.70
36	5	3227	A	C5-C6-N6	-5.08	119.64	123.70
1	2	499	U	C3'-C2'-C1'	5.07	105.56	101.50
1	2	1170	G	C6-C5-N7	-5.07	127.36	130.40
36	1	41	G	N9-C4-C5	-5.07	103.37	105.40
36	1	725	G	C8-N9-C4	5.07	108.43	106.40
36	1	1307	G	N1-C6-O6	-5.07	116.86	119.90
36	1	1437	C	N1-C2-N3	5.07	122.75	119.20
36	1	2163	C	C4-C5-C6	5.07	119.94	117.40
36	1	2314	U	C4-C5-C6	-5.07	116.66	119.70
36	5	326	U	N1-C2-O2	-5.07	119.25	122.80
36	5	383	G	C2-N3-C4	-5.07	109.36	111.90
36	5	644	G	N1-C6-O6	-5.07	116.86	119.90
36	5	3197	G	N3-C2-N2	-5.07	116.35	119.90
36	1	1349	G	N3-C4-C5	-5.07	126.06	128.60
1	6	272	U	N1-C2-O2	5.07	126.35	122.80
36	5	1158	A	O5'-P-OP2	-5.07	101.14	105.70
36	1	873	C	P-O3'-C3'	5.07	125.78	119.70
36	1	2191	U	C5-C4-O4	5.07	128.94	125.90
36	5	2760	C	C6-N1-C2	5.07	122.33	120.30
36	1	348	A	C8-N9-C4	5.07	107.83	105.80
38	4	50	C	C6-N1-C2	-5.07	118.27	120.30
36	5	1064	A	P-O3'-C3'	5.07	125.78	119.70
36	1	1116	G	N1-C2-N3	5.07	126.94	123.90
36	1	1137	C	C6-N1-C2	5.07	122.33	120.30
36	1	1438	U	N1-C2-N3	5.07	117.94	114.90
36	1	1838	G	N9-C4-C5	-5.07	103.37	105.40
36	1	2945	G	C5-C6-O6	-5.07	125.56	128.60
36	1	3266	G	N9-C4-C5	5.07	107.43	105.40
1	6	619	A	C8-N9-C1'	5.07	136.82	127.70
36	5	427	C	C2-N3-C4	-5.07	117.37	119.90
36	5	1046	A	OP2-P-O3'	5.07	116.35	105.20
36	5	2884	C	N1-C2-O2	-5.07	115.86	118.90
36	5	3227	A	C4-C5-N7	5.07	113.23	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1180	C	N3-C2-O2	-5.07	118.35	121.90
36	1	650	C	C5-C4-N4	-5.07	116.66	120.20
36	1	2363	A	N9-C4-C5	5.07	107.83	105.80
1	6	3	U	C6-N1-C2	5.07	124.04	121.00
13	c1	5	LEU	CA-CB-CG	5.07	126.95	115.30
36	5	432	G	N1-C6-O6	5.07	122.94	119.90
36	5	784	A	C4-C5-N7	5.07	113.23	110.70
36	5	891	G	N1-C6-O6	-5.07	116.86	119.90
36	5	1523	U	C5-C4-O4	5.07	128.94	125.90
36	5	2693	C	C5-C6-N1	-5.07	118.47	121.00
36	5	2843	U	C2-N1-C1'	5.07	123.78	117.70
36	1	781	G	N3-C4-C5	-5.06	126.07	128.60
36	5	660	A	C5-N7-C8	5.06	106.43	103.90
36	5	2882	U	N3-C4-C5	5.06	117.64	114.60
1	2	608	U	N1-C2-N3	5.06	117.94	114.90
36	1	637	C	C6-N1-C1'	-5.06	114.72	120.80
36	5	515	C	C6-N1-C2	5.06	122.33	120.30
36	5	892	U	C2-N1-C1'	-5.06	111.62	117.70
36	5	1200	A	C4-C5-C6	5.06	119.53	117.00
36	5	1530	U	N3-C4-O4	-5.06	115.86	119.40
36	1	2701	U	C5-C4-O4	-5.06	122.86	125.90
36	1	2726	C	OP1-P-O3'	5.06	116.33	105.20
36	5	609	G	N3-C4-N9	-5.06	122.97	126.00
36	5	925	A	C8-N9-C4	5.06	107.82	105.80
36	5	1348	U	O4'-C1'-N1	5.06	112.25	108.20
36	5	1470	U	C6-N1-C2	-5.06	117.96	121.00
36	5	3351	U	C2-N1-C1'	5.06	123.77	117.70
37	7	100	C	C6-N1-C2	5.06	122.32	120.30
1	2	694	U	N3-C2-O2	-5.06	118.66	122.20
36	1	664	U	C5-C6-N1	-5.06	120.17	122.70
36	1	2920	U	C6-N1-C2	5.06	124.03	121.00
36	1	3050	U	N3-C2-O2	-5.06	118.66	122.20
1	6	308	C	C4-C5-C6	5.06	119.93	117.40
36	5	308	A	O5'-P-OP2	-5.06	101.15	105.70
36	5	1048	A	N1-C6-N6	5.06	121.63	118.60
36	5	1408	G	N9-C4-C5	5.06	107.42	105.40
36	5	1533	U	O5'-P-OP1	-5.06	101.15	105.70
36	5	2684	C	C5-C6-N1	-5.06	118.47	121.00
36	1	57	A	C5-C6-N1	-5.06	115.17	117.70
36	1	213	A	N9-C1'-C2'	-5.06	106.44	112.00
1	2	1033	C	N3-C2-O2	-5.05	118.36	121.90
1	2	1324	G	N3-C4-N9	-5.05	122.97	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1153	A	C5-C6-N6	-5.05	119.66	123.70
36	1	1375	G	C5-N7-C8	-5.05	101.77	104.30
36	1	1900	A	C8-N9-C4	5.05	107.82	105.80
36	1	2603	G	N9-C4-C5	-5.05	103.38	105.40
36	1	2733	A	O5'-P-OP2	-5.05	101.15	105.70
1	6	769	A	N1-C6-N6	-5.05	115.57	118.60
36	5	292	U	N3-C4-C5	5.05	117.63	114.60
36	5	906	A	C4-C5-C6	5.05	119.53	117.00
36	5	1113	G	N1-C2-N3	5.05	126.93	123.90
36	1	714	G	N3-C4-N9	5.05	129.03	126.00
36	1	1139	G	C5-C6-O6	5.05	131.63	128.60
36	1	2321	A	N1-C6-N6	-5.05	115.57	118.60
36	1	2879	C	N3-C2-O2	5.05	125.44	121.90
36	5	1166	G	N9-C4-C5	-5.05	103.38	105.40
36	5	2420	C	N1-C2-O2	-5.05	115.87	118.90
36	5	2970	C	N1-C2-O2	5.05	121.93	118.90
36	1	1438	U	N3-C2-O2	-5.05	118.66	122.20
36	1	1770	G	C4-N9-C1'	5.05	133.07	126.50
36	1	2417	U	N1-C2-N3	5.05	117.93	114.90
36	1	3259	U	O4'-C1'-N1	-5.05	104.16	108.20
1	6	1724	U	C2-N1-C1'	-5.05	111.64	117.70
36	5	506	U	C4-C5-C6	5.05	122.73	119.70
36	5	937	G	OP1-P-OP2	5.05	127.18	119.60
36	5	959	C	O4'-C1'-N1	5.05	112.24	108.20
36	5	1189	C	N3-C2-O2	5.05	125.44	121.90
36	5	2696	A	C8-N9-C4	5.05	107.82	105.80
36	5	3343	G	N1-C2-N2	-5.05	111.65	116.20
1	2	728	U	C2-N1-C1'	5.05	123.76	117.70
20	C8	3	LEU	CA-CB-CG	5.05	126.91	115.30
36	1	910	G	C5-C6-N1	-5.05	108.97	111.50
36	1	2349	U	N3-C2-O2	-5.05	118.67	122.20
36	5	215	G	C8-N9-C4	-5.05	104.38	106.40
36	5	942	U	N3-C4-O4	5.05	122.94	119.40
36	5	1153	A	C6-N1-C2	-5.05	115.57	118.60
36	5	1633	C	C2-N1-C1'	5.05	124.35	118.80
36	5	2262	A	C8-N9-C4	5.05	107.82	105.80
36	1	154	U	C5-C6-N1	-5.05	120.18	122.70
36	1	404	G	C8-N9-C4	-5.05	104.38	106.40
36	1	893	C	C5-C6-N1	5.05	123.52	121.00
36	5	753	C	C5-C6-N1	-5.05	118.48	121.00
1	2	1735	U	C5-C6-N1	-5.05	120.18	122.70
36	1	788	C	C2-N1-C1'	-5.05	113.25	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	801	A	C6-N1-C2	5.05	121.63	118.60
36	1	2385	G	N1-C2-N2	5.05	120.74	116.20
36	1	3173	G	C8-N9-C1'	-5.05	120.44	127.00
25	d3	33	LEU	CA-CB-CG	-5.05	103.69	115.30
36	5	57	A	C8-N9-C4	5.05	107.82	105.80
36	5	2403	G	O5'-P-OP1	5.05	116.75	110.70
36	5	3107	U	C6-N1-C2	5.05	124.03	121.00
37	7	47	C	N1-C2-N3	5.05	122.73	119.20
69	o3	7	LEU	CB-CG-CD1	-5.05	102.42	111.00
36	1	108	A	C5-C6-N6	-5.04	119.66	123.70
36	5	1891	A	O5'-P-OP2	-5.04	101.16	105.70
36	5	2662	G	N3-C4-C5	-5.04	126.08	128.60
1	2	447	U	C6-N1-C2	-5.04	117.97	121.00
1	2	934	C	C6-N1-C1'	-5.04	114.75	120.80
1	2	1749	A	N1-C2-N3	5.04	131.82	129.30
36	1	59	G	C4-C5-N7	5.04	112.82	110.80
36	1	188	U	N3-C2-O2	5.04	125.73	122.20
36	1	692	A	N1-C6-N6	5.04	121.63	118.60
36	1	2144	A	C8-N9-C4	5.04	107.82	105.80
1	6	542	A	C4-N9-C1'	5.04	135.38	126.30
1	6	1023	A	C5-C6-N6	-5.04	119.67	123.70
1	6	1652	C	N1-C2-O2	-5.04	115.87	118.90
36	5	403	C	OP2-P-O3'	5.04	116.30	105.20
36	5	2710	C	N1-C2-O2	-5.04	115.87	118.90
36	5	3210	A	N1-C6-N6	-5.04	115.57	118.60
37	7	55	A	O5'-P-OP2	5.04	116.75	110.70
36	1	1130	A	C4-C5-N7	5.04	113.22	110.70
36	1	1205	A	N1-C6-N6	5.04	121.62	118.60
1	6	1748	G	OP2-P-O3'	5.04	116.29	105.20
36	5	1302	A	C8-N9-C4	-5.04	103.78	105.80
36	5	2327	U	C6-N1-C2	5.04	124.02	121.00
36	5	3195	U	C2-N1-C1'	5.04	123.75	117.70
51	m5	197	LEU	CA-CB-CG	-5.04	103.70	115.30
36	1	1164	G	C6-C5-N7	-5.04	127.38	130.40
36	1	1445	U	OP2-P-O3'	5.04	116.29	105.20
36	1	2122	G	N9-C4-C5	5.04	107.42	105.40
71	O5	36	LEU	CA-CB-CG	5.04	126.89	115.30
36	5	2962	U	C5-C6-N1	5.04	125.22	122.70
1	2	514	G	N1-C6-O6	-5.04	116.88	119.90
1	2	1632	C	N3-C2-O2	5.04	125.43	121.90
36	1	1120	A	C6-N1-C2	-5.04	115.58	118.60
36	1	2752	U	N3-C2-O2	-5.04	118.67	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2777	G	N9-C4-C5	5.04	107.42	105.40
36	5	2398	A	N7-C8-N9	-5.04	111.28	113.80
36	5	2404	A	N9-C4-C5	-5.04	103.78	105.80
38	8	55	U	N3-C2-O2	-5.04	118.67	122.20
1	6	362	G	N3-C4-N9	5.04	129.02	126.00
36	1	957	C	O5'-P-OP2	-5.04	101.17	105.70
36	1	1437	C	C6-N1-C2	-5.04	118.29	120.30
36	1	2772	C	N1-C1'-C2'	5.04	120.55	114.00
36	5	2895	G	N1-C2-N3	5.04	126.92	123.90
36	5	3315	G	N1-C2-N3	5.04	126.92	123.90
1	2	973	A	C2-N3-C4	-5.03	108.08	110.60
36	1	602	A	N1-C6-N6	-5.03	115.58	118.60
36	1	2836	C	N3-C2-O2	-5.03	118.38	121.90
1	6	1439	C	C5-C6-N1	5.03	123.52	121.00
36	5	1170	A	C8-N9-C4	5.03	107.81	105.80
36	1	1349	G	N3-C4-N9	5.03	129.02	126.00
36	5	1116	G	C4-N9-C1'	5.03	133.04	126.50
36	5	2345	A	C6-N1-C2	-5.03	115.58	118.60
1	2	1456	C	C6-N1-C2	-5.03	118.29	120.30
36	1	973	A	N1-C2-N3	5.03	131.81	129.30
36	1	2130	G	C8-N9-C4	-5.03	104.39	106.40
36	1	2603	G	O5'-P-OP2	-5.03	101.17	105.70
36	1	2647	A	C8-N9-C4	-5.03	103.79	105.80
36	1	2944	U	C5-C6-N1	5.03	125.22	122.70
36	1	3057	U	N3-C4-O4	-5.03	115.88	119.40
36	1	3325	G	N1-C6-O6	-5.03	116.88	119.90
36	5	216	G	C5-C6-O6	-5.03	125.58	128.60
36	5	1183	C	C5-C6-N1	-5.03	118.48	121.00
36	5	2305	G	C4-C5-C6	5.03	121.82	118.80
36	5	2685	C	N3-C4-C5	5.03	123.91	121.90
36	5	1136	A	N1-C6-N6	5.03	121.62	118.60
36	5	3176	G	N3-C4-C5	-5.03	126.09	128.60
38	8	79	A	O5'-P-OP2	-5.03	101.17	105.70
15	C3	22	ALA	C-N-CA	5.03	143.12	122.00
36	1	722	G	C6-C5-N7	-5.03	127.38	130.40
36	1	3216	G	N1-C6-O6	-5.03	116.88	119.90
47	M0	176	LEU	CA-CB-CG	5.03	126.86	115.30
1	6	1770	U	N1-C2-O2	5.03	126.32	122.80
36	5	218	G	N3-C4-N9	5.03	129.02	126.00
36	5	636	C	N3-C4-C5	5.03	123.91	121.90
36	5	1190	A	N7-C8-N9	5.03	116.31	113.80
36	5	1311	G	C8-N9-C4	5.03	108.41	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2706	G	N1-C2-N2	-5.03	111.68	116.20
36	5	3209	A	C8-N9-C4	-5.03	103.79	105.80
1	2	1291	G	C8-N9-C4	-5.03	104.39	106.40
1	2	1332	C	C6-N1-C2	-5.03	118.29	120.30
36	1	1889	G	N1-C2-N3	-5.03	120.88	123.90
36	1	1926	C	N3-C4-C5	5.03	123.91	121.90
36	1	2140	U	C5-C6-N1	-5.03	120.19	122.70
36	5	69	C	N3-C4-C5	-5.03	119.89	121.90
36	5	960	U	O4'-C1'-N1	-5.03	104.18	108.20
36	5	1590	G	OP2-P-O3'	5.03	116.26	105.20
36	5	2683	U	C2-N1-C1'	5.03	123.73	117.70
36	5	2981	U	C4-C5-C6	5.03	122.72	119.70
36	1	41	G	C5-C6-O6	-5.02	125.59	128.60
36	1	80	G	C5-C6-N1	5.02	114.01	111.50
36	1	1005	G	C5-C6-O6	5.02	131.62	128.60
36	1	1493	G	O4'-C1'-N9	5.02	112.22	108.20
36	1	3307	A	C6-C5-N7	-5.02	128.78	132.30
1	6	965	U	N3-C4-O4	-5.02	115.88	119.40
36	5	112	U	O4'-C1'-N1	5.02	112.22	108.20
36	5	2695	A	N1-C2-N3	5.02	131.81	129.30
36	5	3212	C	N1-C2-O2	-5.02	115.89	118.90
36	5	3271	G	C5-C6-O6	5.02	131.61	128.60
1	2	1622	G	N3-C4-C5	5.02	131.11	128.60
36	1	943	U	N3-C2-O2	-5.02	118.69	122.20
36	1	1495	U	C2-N3-C4	-5.02	123.99	127.00
36	1	2412	G	C4-C5-N7	5.02	112.81	110.80
36	1	3361	G	N1-C2-N2	-5.02	111.68	116.20
36	5	702	C	N3-C4-N4	-5.02	114.48	118.00
36	5	1138	U	C2-N3-C4	-5.02	123.99	127.00
36	5	1556	C	N1-C2-O2	5.02	121.91	118.90
36	5	1819	U	N1-C1'-C2'	-5.02	106.47	112.00
36	5	2943	G	C5-C6-N1	-5.02	108.99	111.50
36	5	3198	U	N1-C2-N3	-5.02	111.89	114.90
36	5	1424	C	C6-N1-C2	5.02	122.31	120.30
36	1	854	G	N1-C2-N3	5.02	126.91	123.90
36	1	1043	C	C6-N1-C2	5.02	122.31	120.30
36	1	1111	U	C5-C4-O4	-5.02	122.89	125.90
36	1	2194	G	C2-N3-C4	-5.02	109.39	111.90
36	1	2982	A	C6-N1-C2	-5.02	115.59	118.60
36	5	96	G	C2-N3-C4	-5.02	109.39	111.90
36	5	222	A	O5'-P-OP1	5.02	116.72	110.70
36	5	933	A	N1-C6-N6	5.02	121.61	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1200	A	P-O3'-C3'	5.02	125.72	119.70
36	5	1805	C	OP1-P-OP2	-5.02	112.07	119.60
36	5	1917	C	OP2-P-O3'	5.02	116.25	105.20
36	5	2136	C	C2-N3-C4	-5.02	117.39	119.90
36	5	2358	A	C8-N9-C4	5.02	107.81	105.80
36	5	2410	U	C2-N3-C4	-5.02	123.99	127.00
36	5	2660	G	OP1-P-OP2	-5.02	112.07	119.60
36	5	3131	U	C6-N1-C1'	-5.02	114.17	121.20
36	1	2973	G	C4-C5-N7	5.02	112.81	110.80
37	3	53	U	N1-C2-O2	-5.02	119.29	122.80
36	5	414	U	N3-C2-O2	5.02	125.71	122.20
36	5	1939	G	C4-N9-C1'	5.02	133.02	126.50
36	5	2836	C	N3-C2-O2	-5.02	118.39	121.90
36	5	2970	C	O5'-P-OP1	-5.02	101.19	105.70
36	5	3095	U	C5-C6-N1	-5.02	120.19	122.70
36	1	1380	G	N1-C6-O6	5.02	122.91	119.90
36	1	1794	G	N1-C6-O6	-5.02	116.89	119.90
36	1	2647	A	C6-N1-C2	-5.02	115.59	118.60
36	1	640	U	N1-C2-O2	-5.01	119.29	122.80
36	1	1838	G	C2-N3-C4	-5.01	109.39	111.90
36	1	2787	G	C5-C6-O6	-5.01	125.59	128.60
36	1	3362	A	C2-N3-C4	-5.01	108.09	110.60
1	6	1354	G	C4-N9-C1'	5.01	133.02	126.50
1	6	1782	A	N1-C6-N6	-5.01	115.59	118.60
36	5	538	G	C5-C6-N1	-5.01	108.99	111.50
36	5	3377	G	N1-C2-N3	-5.01	120.89	123.90
1	2	109	G	N1-C6-O6	5.01	122.91	119.90
36	1	1187	C	C6-N1-C2	5.01	122.31	120.30
36	1	1395	G	OP2-P-O3'	5.01	116.23	105.20
36	1	2887	A	OP2-P-O3'	5.01	116.23	105.20
1	6	1338	C	C6-N1-C2	5.01	122.31	120.30
36	5	682	U	C5-C4-O4	5.01	128.91	125.90
36	5	2385	G	N3-C4-N9	-5.01	122.99	126.00
36	5	2993	G	C5-C6-O6	-5.01	125.59	128.60
1	2	1100	G	N3-C4-C5	-5.01	126.09	128.60
36	1	2758	A	O4'-C1'-N9	5.01	112.21	108.20
1	6	542	A	N7-C8-N9	5.01	116.31	113.80
1	6	587	C	C5-C6-N1	-5.01	118.49	121.00
1	6	1697	G	C2-N3-C4	5.01	114.41	111.90
36	5	878	G	C6-C5-N7	-5.01	127.39	130.40
36	5	1466	G	C5-C6-O6	-5.01	125.59	128.60
36	5	2294	U	C5-C6-N1	-5.01	120.19	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3103	A	OP1-P-OP2	5.01	127.12	119.60
36	5	3326	G	N3-C4-N9	5.01	129.01	126.00
1	2	402	C	C6-N1-C2	5.01	122.30	120.30
36	1	205	C	N3-C4-C5	5.01	123.90	121.90
36	1	935	U	C2-N1-C1'	5.01	123.71	117.70
36	1	1199	C	C5-C6-N1	-5.01	118.50	121.00
36	1	1360	C	C6-N1-C2	5.01	122.30	120.30
36	1	2133	U	N3-C4-C5	5.01	117.61	114.60
1	6	1782	A	N9-C4-C5	5.01	107.80	105.80
36	5	35	A	N9-C4-C5	-5.01	103.80	105.80
36	5	869	G	C8-N9-C4	5.01	108.40	106.40
36	5	960	U	C2-N3-C4	-5.01	123.99	127.00
36	5	1302	A	C5-C6-N1	-5.01	115.19	117.70
36	5	1548	C	N3-C2-O2	5.01	125.41	121.90
36	5	1658	G	OP1-P-OP2	5.01	127.11	119.60
36	5	2831	G	N3-C2-N2	-5.01	116.39	119.90
36	1	910	G	N1-C2-N3	5.01	126.91	123.90
36	1	1689	U	O5'-P-OP1	-5.01	101.19	105.70
36	5	217	U	C2-N3-C4	-5.01	124.00	127.00
36	5	395	A	O5'-P-OP2	-5.01	101.19	105.70
36	5	1914	G	C4-N9-C1'	5.01	133.01	126.50
36	5	3113	A	N7-C8-N9	-5.01	111.30	113.80
36	1	194	U	OP1-P-O3'	5.01	116.22	105.20
36	1	884	A	C2-N3-C4	-5.01	108.10	110.60
36	1	1125	U	C5-C6-N1	-5.01	120.20	122.70
36	1	3266	G	C8-N9-C4	-5.01	104.40	106.40
38	4	41	A	C8-N9-C4	5.01	107.80	105.80
4	s2	229	LEU	CA-CB-CG	5.01	126.81	115.30
36	5	404	G	O5'-P-OP2	-5.01	101.19	105.70
36	5	586	C	N3-C4-C5	5.01	123.90	121.90
36	5	784	A	C6-C5-N7	-5.01	128.80	132.30
36	5	2900	A	OP2-P-O3'	5.01	116.21	105.20
36	5	3001	C	C2-N1-C1'	-5.01	113.29	118.80
37	7	3	U	C5-C6-N1	-5.01	120.20	122.70
38	8	102	U	N3-C4-O4	5.01	122.91	119.40
1	2	1052	U	N3-C2-O2	-5.00	118.70	122.20
36	1	127	G	N1-C6-O6	5.00	122.90	119.90
36	1	2623	G	N1-C6-O6	5.00	122.90	119.90
1	6	1048	G	N9-C4-C5	-5.00	103.40	105.40
36	5	2644	C	OP1-P-OP2	5.00	127.11	119.60
36	5	2693	C	N3-C4-C5	5.00	123.90	121.90
36	5	2728	G	O4'-C1'-N9	5.00	112.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2815	G	N7-C8-N9	-5.00	110.60	113.10
37	7	88	G	C2-N3-C4	-5.00	109.40	111.90
50	m4	106	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	2	1773	C	N3-C2-O2	5.00	125.40	121.90
31	D9	36	LEU	CA-CB-CG	5.00	126.81	115.30
36	1	2632	G	O5'-P-OP2	-5.00	101.20	105.70
36	1	2987	A	C4-N9-C1'	5.00	135.31	126.30
1	6	1227	A	C3'-C2'-C1'	5.00	105.50	101.50
36	5	73	C	C5-C4-N4	-5.00	116.70	120.20
36	5	194	U	C5-C6-N1	-5.00	120.20	122.70
36	1	932	U	N1-C2-O2	-5.00	119.30	122.80
36	1	1434	G	C8-N9-C4	-5.00	104.40	106.40
36	1	1492	G	N1-C2-N2	-5.00	111.70	116.20
36	1	1872	C	N3-C4-N4	-5.00	114.50	118.00
36	1	2412	G	C6-N1-C2	-5.00	122.10	125.10
1	6	1754	A	N1-C6-N6	-5.00	115.60	118.60
36	5	57	A	N1-C2-N3	5.00	131.80	129.30
36	5	928	C	C5-C6-N1	-5.00	118.50	121.00
36	5	2598	G	C6-C5-N7	-5.00	127.40	130.40

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	38	THR	Peptide
19	C7	85	VAL	Peptide
25	D3	78	LYS	Peptide
27	D5	94	LYS	Peptide
27	D5	96	SER	Peptide
33	E1	138	ARG	Peptide
39	L2	142	ASP	Peptide
39	L2	19	HIS	Peptide
41	L4	129	THR	Peptide
45	L8	74	THR	Peptide
48	M1	8	PRO	Peptide
52	M6	110	PRO	Peptide
56	N0	1	MET	Peptide
65	N9	20	GLY	Peptide
72	O6	78	GLY	Peptide
75	O9	33	ASN	Peptide
9	S7	131	PHE	Peptide

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Mol	Chain	Res	Type	Group
10	S8	147	ALA	Peptide
18	c6	41	PRO	Peptide
19	c7	87	GLU	Peptide
22	d0	70	THR	Peptide
40	l3	234	GLY	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
81	m2	29	UNK	Peptide
50	m4	10	SER	Peptide
52	m6	110	PRO	Peptide
56	n0	133	ALA	Peptide
56	n0	170	THR	Peptide
56	n0	3	HIS	Peptide
64	n8	66	ALA	Peptide
69	o3	105	SER	Peptide
5	s3	203	PRO	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide
11	s9	89	ASP	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	140 (69%)	38 (19%)	26 (13%)	0	1
2	s0	204/251 (81%)	148 (72%)	33 (16%)	23 (11%)	0	2
3	S1	212/254 (84%)	149 (70%)	39 (18%)	24 (11%)	0	2
3	s1	214/254 (84%)	173 (81%)	32 (15%)	9 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	S2	215/253 (85%)	175 (81%)	27 (13%)	13 (6%)	1	12
4	s2	215/253 (85%)	176 (82%)	26 (12%)	13 (6%)	1	12
5	S3	221/239 (92%)	177 (80%)	30 (14%)	14 (6%)	1	10
5	s3	221/239 (92%)	168 (76%)	35 (16%)	18 (8%)	1	5
6	S4	258/260 (99%)	206 (80%)	42 (16%)	10 (4%)	3	22
6	s4	258/260 (99%)	212 (82%)	26 (10%)	20 (8%)	1	6
7	S5	204/224 (91%)	158 (78%)	30 (15%)	16 (8%)	1	6
7	s5	204/224 (91%)	144 (71%)	45 (22%)	15 (7%)	1	7
8	S6	224/236 (95%)	194 (87%)	18 (8%)	12 (5%)	2	14
8	s6	216/236 (92%)	189 (88%)	17 (8%)	10 (5%)	2	18
9	S7	182/189 (96%)	142 (78%)	25 (14%)	15 (8%)	1	5
9	s7	184/189 (97%)	144 (78%)	23 (12%)	17 (9%)	1	3
10	S8	184/200 (92%)	155 (84%)	19 (10%)	10 (5%)	2	14
10	s8	184/200 (92%)	158 (86%)	18 (10%)	8 (4%)	2	20
11	S9	183/196 (93%)	135 (74%)	36 (20%)	12 (7%)	1	9
11	s9	183/196 (93%)	149 (81%)	25 (14%)	9 (5%)	2	17
12	C0	94/105 (90%)	66 (70%)	20 (21%)	8 (8%)	1	4
12	c0	92/105 (88%)	64 (70%)	12 (13%)	16 (17%)	0	0
13	C1	153/155 (99%)	124 (81%)	18 (12%)	11 (7%)	1	7
13	c1	144/155 (93%)	118 (82%)	17 (12%)	9 (6%)	1	10
14	C2	122/142 (86%)	71 (58%)	32 (26%)	19 (16%)	0	1
14	c2	122/142 (86%)	69 (57%)	31 (25%)	22 (18%)	0	0
15	C3	148/150 (99%)	119 (80%)	21 (14%)	8 (5%)	2	14
15	c3	148/150 (99%)	110 (74%)	27 (18%)	11 (7%)	1	7
16	C4	125/136 (92%)	87 (70%)	24 (19%)	14 (11%)	0	2
16	c4	126/136 (93%)	95 (75%)	16 (13%)	15 (12%)	0	2
17	C5	122/141 (86%)	86 (70%)	26 (21%)	10 (8%)	1	5
17	c5	133/141 (94%)	88 (66%)	25 (19%)	20 (15%)	0	1
18	C6	139/142 (98%)	114 (82%)	14 (10%)	11 (8%)	1	6
18	c6	140/142 (99%)	113 (81%)	21 (15%)	6 (4%)	2	20
19	C7	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	c7	113/136 (83%)	89 (79%)	15 (13%)	9 (8%)	1	6
20	C8	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	5
20	c8	143/145 (99%)	112 (78%)	20 (14%)	11 (8%)	1	6
21	C9	141/143 (99%)	109 (77%)	23 (16%)	9 (6%)	1	10
21	c9	141/143 (99%)	117 (83%)	17 (12%)	7 (5%)	2	16
22	D0	105/120 (88%)	78 (74%)	23 (22%)	4 (4%)	3	22
22	d0	108/120 (90%)	82 (76%)	19 (18%)	7 (6%)	1	10
23	D1	85/87 (98%)	59 (69%)	19 (22%)	7 (8%)	1	5
23	d1	85/87 (98%)	65 (76%)	13 (15%)	7 (8%)	1	5
24	D2	127/129 (98%)	106 (84%)	16 (13%)	5 (4%)	3	22
24	d2	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	19	58
25	D3	142/144 (99%)	108 (76%)	20 (14%)	14 (10%)	0	3
25	d3	142/144 (99%)	121 (85%)	16 (11%)	5 (4%)	3	24
26	D4	132/134 (98%)	108 (82%)	14 (11%)	10 (8%)	1	7
26	d4	132/134 (98%)	101 (76%)	17 (13%)	14 (11%)	0	2
27	D5	68/107 (64%)	46 (68%)	12 (18%)	10 (15%)	0	1
27	d5	67/107 (63%)	50 (75%)	13 (19%)	4 (6%)	1	12
28	D6	95/97 (98%)	55 (58%)	21 (22%)	19 (20%)	0	0
28	d6	95/97 (98%)	69 (73%)	19 (20%)	7 (7%)	1	7
29	D7	79/81 (98%)	59 (75%)	17 (22%)	3 (4%)	3	22
29	d7	79/81 (98%)	58 (73%)	14 (18%)	7 (9%)	1	4
30	D8	61/66 (92%)	46 (75%)	12 (20%)	3 (5%)	2	17
30	d8	61/66 (92%)	44 (72%)	15 (25%)	2 (3%)	4	25
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	1	12
31	d9	51/55 (93%)	38 (74%)	8 (16%)	5 (10%)	0	3
32	E0	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	1	4
33	E1	69/76 (91%)	32 (46%)	17 (25%)	20 (29%)	0	0
33	e1	74/76 (97%)	39 (53%)	17 (23%)	18 (24%)	0	0
34	SR	316/318 (99%)	265 (84%)	43 (14%)	8 (2%)	5	32
34	sR	316/318 (99%)	263 (83%)	40 (13%)	13 (4%)	3	21
35	SM	155/273 (57%)	105 (68%)	32 (21%)	18 (12%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	sM	98/273 (36%)	60 (61%)	21 (21%)	17 (17%)	0	0
39	L2	250/253 (99%)	222 (89%)	21 (8%)	7 (3%)	5	29
39	l2	250/253 (99%)	205 (82%)	27 (11%)	18 (7%)	1	7
40	L3	384/386 (100%)	316 (82%)	52 (14%)	16 (4%)	3	20
40	l3	384/386 (100%)	334 (87%)	32 (8%)	18 (5%)	2	17
41	L4	359/361 (99%)	299 (83%)	38 (11%)	22 (6%)	1	12
41	l4	359/361 (99%)	299 (83%)	37 (10%)	23 (6%)	1	10
42	L5	294/296 (99%)	243 (83%)	35 (12%)	16 (5%)	2	14
42	l5	292/296 (99%)	255 (87%)	28 (10%)	9 (3%)	4	26
43	L6	152/175 (87%)	142 (93%)	8 (5%)	2 (1%)	12	47
43	l6	153/175 (87%)	136 (89%)	13 (8%)	4 (3%)	5	31
44	L7	220/243 (90%)	189 (86%)	22 (10%)	9 (4%)	3	21
44	l7	221/243 (91%)	190 (86%)	25 (11%)	6 (3%)	5	30
45	L8	231/255 (91%)	182 (79%)	34 (15%)	15 (6%)	1	10
45	l8	229/255 (90%)	180 (79%)	32 (14%)	17 (7%)	1	7
46	L9	189/191 (99%)	158 (84%)	20 (11%)	11 (6%)	1	13
46	l9	189/191 (99%)	166 (88%)	18 (10%)	5 (3%)	5	31
47	M0	207/220 (94%)	177 (86%)	21 (10%)	9 (4%)	2	20
47	m0	209/220 (95%)	160 (77%)	31 (15%)	18 (9%)	1	4
48	M1	167/173 (96%)	127 (76%)	23 (14%)	17 (10%)	0	3
48	m1	167/173 (96%)	136 (81%)	21 (13%)	10 (6%)	1	12
49	M3	191/198 (96%)	156 (82%)	28 (15%)	7 (4%)	3	22
49	m3	192/198 (97%)	153 (80%)	23 (12%)	16 (8%)	1	5
50	M4	134/137 (98%)	118 (88%)	10 (8%)	6 (4%)	2	18
50	m4	135/137 (98%)	119 (88%)	13 (10%)	3 (2%)	6	35
51	M5	201/203 (99%)	178 (89%)	20 (10%)	3 (2%)	10	44
51	m5	201/203 (99%)	171 (85%)	24 (12%)	6 (3%)	4	28
52	M6	195/198 (98%)	174 (89%)	17 (9%)	4 (2%)	7	37
52	m6	195/198 (98%)	170 (87%)	19 (10%)	6 (3%)	4	26
53	M7	181/183 (99%)	151 (83%)	23 (13%)	7 (4%)	3	22
53	m7	153/183 (84%)	135 (88%)	16 (10%)	2 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	M8	183/185 (99%)	153 (84%)	22 (12%)	8 (4%)	2	19
54	m8	183/185 (99%)	152 (83%)	25 (14%)	6 (3%)	4	25
55	M9	186/188 (99%)	162 (87%)	22 (12%)	2 (1%)	14	51
55	m9	186/188 (99%)	159 (86%)	24 (13%)	3 (2%)	9	43
56	N0	170/172 (99%)	149 (88%)	15 (9%)	6 (4%)	3	24
56	n0	170/172 (99%)	153 (90%)	13 (8%)	4 (2%)	6	34
57	N1	157/159 (99%)	136 (87%)	18 (12%)	3 (2%)	8	39
57	n1	157/159 (99%)	137 (87%)	15 (10%)	5 (3%)	4	26
58	N2	98/120 (82%)	82 (84%)	11 (11%)	5 (5%)	2	15
58	n2	96/120 (80%)	79 (82%)	13 (14%)	4 (4%)	3	20
59	N3	134/136 (98%)	119 (89%)	12 (9%)	3 (2%)	6	35
59	n3	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	6	35
60	N4	96/155 (62%)	73 (76%)	14 (15%)	9 (9%)	0	3
60	n4	133/155 (86%)	106 (80%)	15 (11%)	12 (9%)	1	4
61	N5	119/141 (84%)	105 (88%)	12 (10%)	2 (2%)	9	42
61	n5	118/141 (84%)	92 (78%)	15 (13%)	11 (9%)	0	3
62	N6	124/126 (98%)	113 (91%)	9 (7%)	2 (2%)	9	43
62	n6	124/126 (98%)	107 (86%)	12 (10%)	5 (4%)	3	21
63	N7	133/135 (98%)	112 (84%)	16 (12%)	5 (4%)	3	22
63	n7	133/135 (98%)	109 (82%)	13 (10%)	11 (8%)	1	5
64	N8	146/148 (99%)	118 (81%)	21 (14%)	7 (5%)	2	17
64	n8	146/148 (99%)	119 (82%)	21 (14%)	6 (4%)	3	21
65	N9	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	3	23
65	n9	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0	2
66	O0	95/104 (91%)	83 (87%)	9 (10%)	3 (3%)	4	26
66	o0	98/104 (94%)	84 (86%)	14 (14%)	0	100	100
67	O1	107/112 (96%)	96 (90%)	5 (5%)	6 (6%)	2	14
67	o1	107/112 (96%)	93 (87%)	9 (8%)	5 (5%)	2	17
68	O2	125/129 (97%)	111 (89%)	10 (8%)	4 (3%)	4	26
68	o2	125/129 (97%)	100 (80%)	18 (14%)	7 (6%)	2	14
69	O3	104/106 (98%)	90 (86%)	10 (10%)	4 (4%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	o3	104/106 (98%)	92 (88%)	10 (10%)	2 (2%)	8	39
70	O4	110/120 (92%)	88 (80%)	18 (16%)	4 (4%)	3	23
70	o4	110/120 (92%)	97 (88%)	10 (9%)	3 (3%)	5	30
71	O5	117/119 (98%)	100 (86%)	11 (9%)	6 (5%)	2	15
71	o5	117/119 (98%)	97 (83%)	17 (14%)	3 (3%)	5	31
72	O6	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	7
72	o6	97/99 (98%)	84 (87%)	9 (9%)	4 (4%)	3	21
73	O7	85/87 (98%)	70 (82%)	13 (15%)	2 (2%)	6	34
73	o7	85/87 (98%)	65 (76%)	17 (20%)	3 (4%)	3	24
74	O8	75/77 (97%)	59 (79%)	12 (16%)	4 (5%)	2	15
74	o8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	2	15
75	O9	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
75	o9	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	7	37
76	Q0	50/52 (96%)	46 (92%)	1 (2%)	3 (6%)	1	12
76	q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	21
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
78	Q2	103/105 (98%)	82 (80%)	15 (15%)	6 (6%)	1	13
78	q2	103/105 (98%)	90 (87%)	9 (9%)	4 (4%)	3	22
79	Q3	89/91 (98%)	76 (85%)	9 (10%)	4 (4%)	2	18
79	q3	89/91 (98%)	77 (86%)	11 (12%)	1 (1%)	14	51
80	e0	60/62 (97%)	42 (70%)	11 (18%)	7 (12%)	0	2
82	p0	139/311 (45%)	117 (84%)	15 (11%)	7 (5%)	2	16
All	All	22333/24143 (92%)	18126 (81%)	2889 (13%)	1318 (6%)	1	12

All (1318) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	32	HIS
2	S0	66	ALA
2	S0	68	PRO
2	S0	111	ILE
2	S0	158	VAL

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Mol	Chain	Res	Type
2	S0	191	ARG
3	S1	36	SER
3	S1	37	THR
3	S1	49	ASN
3	S1	58	SER
3	S1	63	GLY
3	S1	132	ASP
3	S1	148	ASN
3	S1	154	SER
3	S1	158	SER
3	S1	221	PRO
4	S2	48	GLY
4	S2	107	SER
4	S2	148	LEU
5	S3	31	GLU
5	S3	62	ASN
5	S3	65	ARG
5	S3	93	ASP
5	S3	211	PRO
5	S3	220	PRO
6	S4	242	LYS
7	S5	26	ALA
7	S5	35	GLN
7	S5	39	GLU
7	S5	51	VAL
7	S5	58	LEU
7	S5	101	GLY
8	S6	173	PRO
8	S6	174	LYS
9	S7	31	SER
9	S7	32	PRO
9	S7	64	VAL
9	S7	111	LYS
9	S7	131	PHE
9	S7	132	PRO
11	S9	134	ILE
11	S9	150	LEU
11	S9	164	PHE
12	C0	54	TYR
12	C0	61	TRP
12	C0	87	VAL
12	C0	88	PRO

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Mol	Chain	Res	Type
13	C1	29	LYS
13	C1	144	ALA
14	C2	21	GLU
14	C2	93	ASP
14	C2	126	TRP
14	C2	131	ASP
15	C3	19	SER
15	C3	22	ALA
15	C3	27	LYS
15	C3	68	GLY
15	C3	138	ASN
16	C4	92	LYS
16	C4	124	ASP
16	C4	126	THR
17	C5	22	LEU
17	C5	54	ALA
17	C5	125	PRO
17	C5	126	VAL
18	C6	39	VAL
18	C6	41	PRO
18	C6	59	LYS
18	C6	138	PHE
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	124	VAL
20	C8	14	ILE
20	C8	60	GLU
20	C8	91	ASP
20	C8	92	ILE
20	C8	144	ARG
21	C9	31	PRO
21	C9	53	TRP
23	D1	2	GLU
23	D1	4	ASP
24	D2	83	ILE
25	D3	3	LYS
25	D3	70	LYS
25	D3	128	SER
25	D3	138	GLU
25	D3	144	ARG
26	D4	5	VAL

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Mol	Chain	Res	Type
26	D4	36	SER
27	D5	37	GLN
27	D5	39	ALA
27	D5	44	GLN
27	D5	71	ILE
27	D5	97	LYS
28	D6	11	ASN
28	D6	45	VAL
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
29	D7	38	PRO
29	D7	62	ILE
31	D9	8	PHE
32	E0	13	LYS
32	E0	47	VAL
33	E1	87	THR
33	E1	102	VAL
33	E1	103	LEU
33	E1	106	TYR
33	E1	110	ALA
33	E1	138	ARG
34	SR	160	GLU
34	SR	161	LYS
34	SR	318	ALA
35	SM	87	THR
35	SM	140	ASP
35	SM	154	TYR
35	SM	166	VAL
35	SM	167	PRO
39	L2	17	THR
39	L2	234	LYS
40	L3	4	ARG
40	L3	5	LYS
40	L3	140	ASP
40	L3	173	GLN
40	L3	188	ILE
40	L3	348	ARG
40	L3	385	LYS
41	L4	90	PHE
41	L4	143	GLU

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Mol	Chain	Res	Type
41	L4	146	PRO
41	L4	220	ARG
41	L4	291	ASN
41	L4	304	GLN
41	L4	311	HIS
41	L4	320	ASN
41	L4	338	LYS
42	L5	59	ASP
42	L5	215	ASP
42	L5	223	PHE
42	L5	233	ALA
42	L5	234	ASP
42	L5	258	LYS
43	L6	98	VAL
44	L7	24	GLU
45	L8	25	PRO
45	L8	115	ALA
45	L8	116	VAL
46	L9	50	ASN
46	L9	62	ARG
46	L9	190	ASP
47	M0	145	LYS
47	M0	219	ALA
48	M1	8	PRO
48	M1	9	MET
48	M1	11	ASP
48	M1	94	ARG
48	M1	95	ASN
48	M1	165	GLN
48	M1	173	ASP
49	M3	47	ALA
49	M3	76	THR
49	M3	129	ASN
49	M3	166	ALA
50	M4	8	LYS
50	M4	9	ALA
50	M4	29	ALA
52	M6	90	HIS
52	M6	111	PRO
52	M6	173	ALA
53	M7	3	ARG
53	M7	157	VAL

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Mol	Chain	Res	Type
54	M8	41	ASP
56	N0	138	GLN
56	N0	167	ARG
58	N2	50	LEU
58	N2	51	GLY
60	N4	81	PRO
62	N6	84	LYS
63	N7	35	SER
63	N7	128	GLN
64	N8	76	ASP
66	O0	100	ILE
67	O1	5	LYS
67	O1	83	GLU
68	O2	126	LEU
71	O5	39	PRO
71	O5	92	LEU
72	O6	27	SER
72	O6	33	ALA
72	O6	34	SER
73	O7	12	HIS
76	Q0	78	ILE
78	Q2	100	LYS
79	Q3	58	SER
2	s0	4	PRO
2	s0	8	ASP
2	s0	49	ASN
2	s0	65	ALA
2	s0	164	ASN
2	s0	186	GLY
2	s0	189	VAL
2	s0	206	ASP
3	s1	206	PRO
3	s1	223	PHE
4	s2	92	ALA
4	s2	106	ASP
5	s3	115	ILE
5	s3	211	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	12	LEU
6	s4	104	ASP
6	s4	118	GLU

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Mol	Chain	Res	Type
6	s4	163	ASP
6	s4	164	LEU
6	s4	195	ILE
6	s4	196	VAL
7	s5	28	PRO
7	s5	39	GLU
7	s5	43	PHE
7	s5	184	PHE
7	s5	204	GLY
8	s6	68	LEU
8	s6	70	PRO
8	s6	122	GLU
8	s6	153	VAL
8	s6	173	PRO
8	s6	174	LYS
9	s7	30	SER
9	s7	64	VAL
9	s7	67	LEU
9	s7	116	ARG
9	s7	131	PHE
10	s8	101	ILE
11	s9	121	SER
12	c0	2	LEU
12	c0	82	LEU
12	c0	83	PRO
12	c0	88	PRO
12	c0	92	ILE
12	c0	94	GLU
12	c0	97	PRO
13	c1	114	ALA
13	c1	133	LYS
14	c2	82	PRO
14	c2	131	ASP
15	c3	60	VAL
15	c3	66	ILE
15	c3	137	PRO
15	c3	139	TRP
15	c3	140	LYS
16	c4	98	GLY
16	c4	126	THR
16	c4	132	ARG
17	c5	11	VAL

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Mol	Chain	Res	Type
17	c5	17	TYR
17	c5	51	SER
17	c5	52	LYS
17	c5	125	PRO
18	c6	42	GLU
18	c6	116	LEU
19	c7	67	ARG
19	c7	88	VAL
19	c7	104	ASN
20	c8	60	GLU
20	c8	91	ASP
20	c8	92	ILE
20	c8	135	GLY
22	d0	15	GLN
22	d0	49	ASN
22	d0	51	VAL
22	d0	97	VAL
22	d0	118	VAL
23	d1	4	ASP
23	d1	44	ARG
25	d3	138	GLU
26	d4	30	PRO
26	d4	32	ARG
26	d4	52	LYS
26	d4	54	ALA
26	d4	121	THR
26	d4	123	LYS
27	d5	85	LYS
28	d6	47	ALA
28	d6	63	ALA
29	d7	38	PRO
29	d7	60	SER
31	d9	6	VAL
31	d9	16	LYS
80	e0	60	PRO
33	e1	79	LYS
33	e1	83	LYS
33	e1	84	VAL
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	102	VAL

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Mol	Chain	Res	Type
33	e1	103	LEU
33	e1	106	TYR
34	sR	4	ASN
34	sR	149	ASP
34	sR	160	GLU
34	sR	163	ASP
34	sR	165	ASP
34	sR	282	SER
35	sM	48	ARG
35	sM	63	ASP
39	l2	24	GLN
39	l2	56	ALA
39	l2	238	ILE
40	l3	3	HIS
40	l3	140	ASP
40	l3	142	ALA
40	l3	235	THR
40	l3	302	LYS
40	l3	347	SER
41	l4	4	PRO
41	l4	15	ALA
41	l4	24	ALA
41	l4	301	PRO
41	l4	339	LEU
41	l4	345	GLU
41	l4	353	ALA
42	l5	178	ASN
42	l5	260	PHE
43	l6	98	VAL
45	l8	25	PRO
45	l8	26	LEU
45	l8	34	PHE
45	l8	48	ARG
45	l8	240	ASN
46	l9	167	VAL
47	m0	3	ARG
47	m0	82	ARG
47	m0	215	GLU
47	m0	219	ALA
48	m1	8	PRO
48	m1	9	MET
48	m1	10	ARG

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Mol	Chain	Res	Type
48	m1	108	GLU
48	m1	111	ASP
49	m3	47	ALA
49	m3	134	GLU
49	m3	140	SER
49	m3	150	PRO
49	m3	152	THR
50	m4	136	ALA
51	m5	76	PRO
51	m5	81	TYR
51	m5	91	GLU
51	m5	184	LYS
52	m6	4	GLU
52	m6	110	PRO
53	m7	3	ARG
55	m9	36	ASN
56	n0	2	ALA
57	n1	122	GLN
57	n1	136	ARG
57	n1	148	PRO
58	n2	50	LEU
59	n3	42	SER
60	n4	71	ARG
60	n4	76	VAL
61	n5	25	LYS
61	n5	44	PRO
62	n6	83	ASP
63	n7	16	GLY
63	n7	102	GLU
63	n7	105	SER
63	n7	129	TRP
64	n8	47	LYS
64	n8	76	ASP
65	n9	7	HIS
65	n9	21	ILE
65	n9	23	LYS
65	n9	39	PHE
67	o1	5	LYS
68	o2	4	LEU
68	o2	5	PRO
68	o2	6	HIS
68	o2	27	ARG

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Mol	Chain	Res	Type
69	o3	88	ASN
72	o6	33	ALA
72	o6	64	SER
73	o7	67	LEU
73	o7	84	SER
73	o7	85	LYS
78	q2	104	LEU
82	p0	93	LEU
82	p0	198	PRO
2	S0	5	ALA
2	S0	39	ASN
2	S0	49	ASN
2	S0	95	ALA
2	S0	139	VAL
2	S0	185	ARG
2	S0	190	ASP
2	S0	195	TRP
3	S1	51	SER
3	S1	54	LEU
3	S1	62	LYS
3	S1	177	GLN
3	S1	179	SER
3	S1	201	THR
3	S1	206	PRO
3	S1	213	ARG
4	S2	47	ALA
4	S2	91	ARG
5	S3	64	ARG
5	S3	164	VAL
5	S3	218	LEU
6	S4	3	ARG
6	S4	12	LEU
6	S4	95	THR
6	S4	104	ASP
7	S5	63	GLN
7	S5	64	VAL
7	S5	81	ARG
7	S5	150	GLY
7	S5	153	GLY
8	S6	20	ASP
8	S6	122	GLU
8	S6	152	ASP

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Mol	Chain	Res	Type
8	S6	165	GLY
9	S7	98	ILE
9	S7	186	PRO
10	S8	40	ALA
10	S8	52	ASN
11	S9	31	ALA
11	S9	82	ARG
11	S9	98	ALA
11	S9	163	PRO
12	C0	64	TYR
12	C0	94	GLU
13	C1	6	THR
13	C1	30	ARG
13	C1	113	PRO
13	C1	145	ALA
13	C1	154	ALA
14	C2	75	VAL
14	C2	91	VAL
16	C4	39	ILE
16	C4	42	VAL
16	C4	51	ASP
18	C6	97	VAL
18	C6	113	ASP
19	C7	41	ILE
19	C7	72	LYS
19	C7	87	GLU
20	C8	79	TYR
20	C8	87	ASN
21	C9	12	GLN
21	C9	39	THR
21	C9	69	LYS
23	D1	28	ASP
23	D1	43	GLY
25	D3	78	LYS
25	D3	97	ASP
25	D3	114	LYS
25	D3	137	LYS
26	D4	4	ALA
26	D4	33	ALA
27	D5	43	ASP
27	D5	69	LEU
28	D6	9	GLY

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Mol	Chain	Res	Type
28	D6	18	VAL
28	D6	32	LYS
28	D6	63	ALA
28	D6	65	PRO
29	D7	63	LEU
30	D8	36	THR
31	D9	11	PRO
33	E1	84	VAL
33	E1	85	TYR
33	E1	90	LYS
33	E1	98	VAL
33	E1	105	TYR
33	E1	127	GLY
34	SR	51	ASP
35	SM	86	ASN
35	SM	111	GLY
35	SM	139	GLU
39	L2	47	GLN
39	L2	250	GLN
41	L4	15	ALA
41	L4	190	GLY
41	L4	268	ALA
41	L4	317	PRO
42	L5	6	ASP
42	L5	57	ASN
42	L5	188	GLU
42	L5	259	LYS
44	L7	26	VAL
44	L7	91	GLY
44	L7	191	VAL
45	L8	36	ILE
45	L8	39	ALA
45	L8	80	TYR
45	L8	85	ASN
45	L8	156	ASP
47	M0	25	ALA
47	M0	117	GLY
47	M0	207	GLU
48	M1	24	GLY
48	M1	65	ILE
48	M1	114	ILE
48	M1	152	HIS

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Mol	Chain	Res	Type
48	M1	167	TYR
49	M3	141	ALA
49	M3	193	ALA
51	M5	81	TYR
53	M7	160	ALA
53	M7	161	ALA
53	M7	164	LYS
54	M8	99	THR
54	M8	183	GLY
57	N1	159	PHE
58	N2	11	ILE
58	N2	20	SER
60	N4	86	SER
64	N8	96	LYS
66	O0	70	PHE
67	O1	6	ASP
68	O2	27	ARG
68	O2	29	ALA
70	O4	47	CYS
71	O5	118	ILE
72	O6	3	VAL
72	O6	28	TYR
78	Q2	15	LYS
2	s0	44	GLY
2	s0	66	ALA
2	s0	95	ALA
2	s0	158	VAL
2	s0	162	CYS
2	s0	185	ARG
3	s1	93	GLY
3	s1	106	THR
3	s1	154	SER
3	s1	232	HIS
4	s2	149	GLY
4	s2	150	GLN
4	s2	163	GLY
5	s3	90	ARG
5	s3	179	GLN
5	s3	195	SER
6	s4	117	GLU
6	s4	135	GLY
6	s4	205	PHE

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Mol	Chain	Res	Type
6	s4	245	LYS
7	s5	54	LYS
7	s5	60	ASP
7	s5	81	ARG
8	s6	154	ARG
9	s7	8	ILE
9	s7	106	SER
9	s7	155	ASP
10	s8	122	GLY
10	s8	136	SER
11	s9	167	ALA
12	c0	30	ALA
12	c0	32	HIS
13	c1	28	SER
13	c1	55	ASP
13	c1	128	CYS
14	c2	26	ASP
14	c2	89	ILE
14	c2	118	ALA
14	c2	119	SER
15	c3	18	TYR
15	c3	29	SER
15	c3	87	ASP
15	c3	108	ASP
16	c4	37	GLU
16	c4	131	GLY
17	c5	22	LEU
17	c5	69	GLU
17	c5	132	GLY
17	c5	136	SER
19	c7	37	GLU
19	c7	99	VAL
19	c7	116	LYS
20	c8	61	LEU
20	c8	145	ARG
21	c9	26	GLY
21	c9	29	GLU
21	c9	33	TYR
21	c9	34	VAL
21	c9	51	GLU
21	c9	66	TYR
23	d1	6	GLY

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Mol	Chain	Res	Type
25	d3	128	SER
26	d4	33	ALA
26	d4	35	VAL
26	d4	49	LYS
26	d4	50	ALA
26	d4	53	ASP
28	d6	8	ASN
28	d6	13	LYS
29	d7	63	LEU
31	d9	7	TRP
80	e0	49	LEU
80	e0	51	ASN
33	e1	85	TYR
33	e1	100	LEU
33	e1	110	ALA
34	sR	186	PHE
34	sR	271	VAL
35	sM	42	ALA
35	sM	50	ASN
35	sM	66	ALA
35	sM	84	LYS
35	sM	122	GLU
35	sM	167	PRO
35	sM	172	VAL
39	l2	172	GLY
39	l2	215	ASN
39	l2	240	ALA
40	l3	23	ALA
40	l3	129	ALA
40	l3	200	GLU
40	l3	386	ASP
41	l4	90	PHE
41	l4	311	HIS
41	l4	342	LYS
44	l7	158	LYS
45	l8	121	SER
45	l8	122	LYS
45	l8	133	LYS
45	l8	202	GLU
45	l8	203	VAL
45	l8	237	ILE
46	l9	144	ILE

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Mol	Chain	Res	Type
47	m0	25	ALA
47	m0	27	PRO
47	m0	117	GLY
47	m0	194	GLY
47	m0	207	GLU
48	m1	94	ARG
48	m1	95	ASN
48	m1	114	ILE
49	m3	76	THR
49	m3	133	PRO
50	m4	135	LEU
51	m5	183	THR
52	m6	13	GLY
52	m6	16	VAL
53	m7	67	ILE
54	m8	84	VAL
54	m8	99	THR
58	n2	91	ASP
60	n4	25	ASP
60	n4	26	SER
60	n4	63	ILE
60	n4	95	SER
60	n4	98	PRO
61	n5	24	LEU
61	n5	47	ALA
61	n5	48	SER
62	n6	84	LYS
64	n8	12	ARG
64	n8	84	GLU
64	n8	120	ASN
65	n9	25	LYS
67	o1	45	GLY
68	o2	127	ALA
70	o4	79	SER
71	o5	82	ALA
72	o6	98	ARG
74	o8	18	ALA
74	o8	19	ASP
78	q2	14	GLY
78	q2	78	LYS
79	q3	51	ALA
82	p0	68	SER

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Mol	Chain	Res	Type
82	p0	102	SER
2	S0	30	GLN
2	S0	94	GLY
2	S0	187	ALA
2	S0	192	THR
4	S2	36	VAL
4	S2	150	GLN
5	S3	44	THR
5	S3	216	PRO
6	S4	26	CYS
7	S5	43	PHE
8	S6	69	LEU
8	S6	89	ASP
8	S6	138	ALA
8	S6	148	SER
8	S6	149	LYS
8	S6	150	GLU
9	S7	29	ASN
9	S7	85	PHE
9	S7	116	ARG
10	S8	22	ARG
10	S8	120	THR
11	S9	16	LYS
11	S9	147	MET
12	C0	60	SER
13	C1	51	GLY
13	C1	55	ASP
13	C1	146	ALA
14	C2	25	GLU
14	C2	66	VAL
14	C2	69	ALA
14	C2	87	PRO
14	C2	89	ILE
14	C2	106	ILE
14	C2	107	ASP
16	C4	50	ALA
16	C4	108	SER
16	C4	109	GLY
16	C4	125	SER
17	C5	53	PRO
17	C5	80	MET
19	C7	42	GLN

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Mol	Chain	Res	Type
19	C7	83	GLN
19	C7	113	LEU
19	C7	115	LEU
20	C8	7	GLU
20	C8	61	LEU
20	C8	80	LYS
20	C8	134	ARG
23	D1	10	GLU
24	D2	31	SER
24	D2	57	ARG
25	D3	20	ARG
25	D3	41	SER
25	D3	131	SER
26	D4	6	THR
26	D4	99	LYS
27	D5	38	HIS
27	D5	56	THR
28	D6	36	ILE
28	D6	46	GLU
28	D6	75	VAL
30	D8	35	ASP
32	E0	51	ASN
33	E1	83	LYS
33	E1	94	LYS
33	E1	111	GLU
35	SM	52	PRO
35	SM	64	LYS
35	SM	88	ARG
35	SM	89	ARG
35	SM	173	GLU
35	SM	174	LEU
39	L2	130	SER
39	L2	251	LYS
40	L3	155	ALA
40	L3	351	LEU
40	L3	378	ALA
42	L5	7	ALA
42	L5	178	ASN
42	L5	213	ASP
42	L5	253	PHE
42	L5	260	PHE
44	L7	25	GLN

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Mol	Chain	Res	Type
45	L8	157	VAL
45	L8	161	GLU
45	L8	196	ALA
46	L9	40	HIS
46	L9	110	LYS
46	L9	120	ASP
47	M0	16	PRO
48	M1	115	LYS
50	M4	10	SER
54	M8	167	SER
56	N0	2	ALA
56	N0	142	GLN
57	N1	124	VAL
59	N3	134	GLY
60	N4	97	LYS
64	N8	78	LEU
66	O0	96	GLY
67	O1	60	TRP
69	O3	59	VAL
69	O3	88	ASN
70	O4	77	GLY
74	O8	33	LYS
74	O8	74	LYS
78	Q2	94	GLY
79	Q3	7	LYS
79	Q3	51	ALA
2	s0	10	THR
2	s0	68	PRO
2	s0	167	LYS
2	s0	183	ARG
3	s1	26	ARG
3	s1	63	GLY
4	s2	236	PRO
4	s2	238	SER
5	s3	61	GLU
5	s3	76	ARG
5	s3	93	ASP
5	s3	216	PRO
5	s3	219	ALA
6	s4	11	ARG
6	s4	47	PHE
6	s4	168	LYS

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Mol	Chain	Res	Type
6	s4	213	SER
7	s5	36	ALA
7	s5	45	LYS
9	s7	10	SER
9	s7	74	GLN
9	s7	111	LYS
9	s7	133	THR
9	s7	176	LEU
10	s8	100	ALA
11	s9	65	LYS
11	s9	118	LEU
12	c0	24	LYS
12	c0	95	ARG
13	c1	7	VAL
13	c1	8	GLN
14	c2	58	LEU
14	c2	87	PRO
14	c2	93	ASP
14	c2	101	ALA
14	c2	106	ILE
14	c2	108	ARG
16	c4	11	SER
16	c4	12	GLN
16	c4	50	ALA
16	c4	51	ASP
17	c5	7	ALA
17	c5	68	PRO
18	c6	113	ASP
19	c7	68	GLY
20	c8	3	LEU
20	c8	55	HIS
22	d0	17	GLN
22	d0	96	PRO
23	d1	10	GLU
23	d1	42	GLU
24	d2	68	ARG
25	d3	89	ASN
26	d4	58	PHE
27	d5	87	GLY
28	d6	35	ALA
28	d6	62	TYR
31	d9	47	ALA

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Mol	Chain	Res	Type
33	e1	81	LYS
33	e1	111	GLU
33	e1	127	GLY
33	e1	146	SER
35	sM	64	LYS
35	sM	67	GLY
39	l2	14	SER
39	l2	160	SER
40	l3	4	ARG
40	l3	244	ARG
40	l3	385	LYS
41	l4	157	GLU
41	l4	277	PRO
41	l4	302	ALA
41	l4	305	ALA
42	l5	92	LEU
42	l5	258	LYS
44	l7	32	ALA
44	l7	91	GLY
44	l7	191	VAL
45	l8	39	ALA
45	l8	43	LYS
45	l8	118	GLU
45	l8	123	GLN
46	l9	122	LYS
47	m0	76	MET
47	m0	145	LYS
47	m0	220	GLN
49	m3	50	PRO
49	m3	62	THR
49	m3	135	ALA
49	m3	142	ALA
54	m8	167	SER
57	n1	146	ASN
58	n2	52	ASN
58	n2	104	ARG
59	n3	124	ASP
61	n5	40	LEU
61	n5	55	ASN
61	n5	64	GLU
62	n6	125	LYS
63	n7	125	GLY

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Mol	Chain	Res	Type
63	n7	128	GLN
65	n9	31	SER
70	o4	47	CYS
71	o5	119	LYS
75	o9	44	TRP
82	p0	47	GLY
2	S0	64	ILE
2	S0	103	THR
2	S0	194	PRO
3	S1	209	ASN
4	S2	106	ASP
4	S2	135	SER
4	S2	235	LEU
4	S2	248	SER
5	S3	112	GLY
5	S3	196	ARG
5	S3	217	ILE
6	S4	39	ARG
6	S4	165	ALA
7	S5	49	GLU
7	S5	54	LYS
7	S5	127	GLN
9	S7	112	ARG
10	S8	10	LYS
10	S8	59	ARG
10	S8	106	ALA
10	S8	149	SER
10	S8	152	ILE
14	C2	112	ALA
15	C3	17	PRO
16	C4	18	ARG
16	C4	114	ARG
17	C5	51	SER
17	C5	52	LYS
18	C6	33	GLY
21	C9	38	LYS
24	D2	78	ARG
25	D3	40	SER
28	D6	64	LEU
33	E1	118	ARG
33	E1	137	ASP
34	SR	105	GLY

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Mol	Chain	Res	Type
35	SM	53	ARG
39	L2	143	GLU
40	L3	66	LYS
40	L3	174	LYS
40	L3	386	ASP
41	L4	14	GLU
41	L4	232	SER
41	L4	269	SER
41	L4	318	LEU
42	L5	137	ASP
44	L7	204	PRO
46	L9	2	LYS
46	L9	189	GLU
48	M1	108	GLU
48	M1	117	ASP
49	M3	136	GLU
51	M5	94	TYR
52	M6	16	VAL
53	M7	84	PRO
54	M8	162	ALA
55	M9	3	ASN
56	N0	129	ILE
57	N1	125	ALA
58	N2	52	ASN
60	N4	63	ILE
60	N4	77	LYS
60	N4	87	LEU
61	N5	108	LEU
62	N6	126	LEU
63	N7	102	GLU
63	N7	103	GLN
64	N8	15	VAL
64	N8	47	LYS
67	O1	82	GLU
68	O2	13	HIS
70	O4	48	GLY
71	O5	97	ALA
71	O5	119	LYS
73	O7	86	ALA
76	Q0	80	PRO
78	Q2	8	ARG
78	Q2	34	SER

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Mol	Chain	Res	Type
78	Q2	96	GLU
2	s0	5	ALA
2	s0	103	THR
4	s2	83	ILE
4	s2	107	SER
4	s2	235	LEU
5	s3	4	LEU
5	s3	45	LYS
5	s3	196	ARG
6	s4	30	ARG
6	s4	90	ILE
7	s5	56	ALA
8	s6	152	ASP
10	s8	56	ARG
11	s9	164	PHE
12	c0	31	LYS
14	c2	22	VAL
14	c2	45	LEU
14	c2	54	ARG
16	c4	35	GLY
16	c4	97	GLY
17	c5	6	ASN
17	c5	14	THR
17	c5	109	PRO
17	c5	127	ARG
17	c5	130	ARG
17	c5	131	ALA
20	c8	14	ILE
23	d1	43	GLY
25	d3	70	LYS
25	d3	109	ARG
26	d4	3	ASP
26	d4	36	SER
28	d6	61	GLU
29	d7	61	THR
29	d7	62	ILE
30	d8	33	LEU
30	d8	57	MET
80	e0	11	ALA
33	e1	129	GLY
34	sR	161	LYS
34	sR	168	THR

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Mol	Chain	Res	Type
35	sM	43	ASP
35	sM	46	LYS
35	sM	121	LYS
39	l2	70	ARG
39	l2	80	GLU
39	l2	125	ALA
39	l2	133	TYR
39	l2	194	ASN
39	l2	234	LYS
39	l2	247	ARG
39	l2	249	SER
40	l3	187	SER
40	l3	247	ARG
41	l4	145	ILE
42	l5	279	LYS
42	l5	294	ALA
43	l6	10	TYR
43	l6	173	MET
47	m0	77	THR
47	m0	83	ASP
47	m0	176	LEU
47	m0	214	PRO
49	m3	60	ALA
50	m4	78	THR
51	m5	98	LEU
54	m8	147	ARG
55	m9	155	LEU
56	n0	154	HIS
60	n4	74	LYS
60	n4	77	LYS
61	n5	38	LEU
61	n5	58	ASP
61	n5	97	LYS
62	n6	126	LEU
63	n7	6	LYS
63	n7	103	GLN
63	n7	104	PRO
64	n8	78	LEU
67	o1	83	GLU
71	o5	40	SER
76	q0	78	ILE
78	q2	74	CYS

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Mol	Chain	Res	Type
82	p0	33	VAL
2	S0	27	ARG
2	S0	65	ALA
3	S1	23	PRO
3	S1	131	ASP
4	S2	39	THR
6	S4	195	ILE
7	S5	154	ALA
10	S8	9	HIS
11	S9	60	LEU
11	S9	168	ARG
14	C2	22	VAL
14	C2	82	PRO
14	C2	108	ARG
14	C2	119	SER
15	C3	3	ARG
15	C3	137	PRO
16	C4	24	ASN
16	C4	75	GLY
17	C5	69	GLU
18	C6	32	ASN
19	C7	84	TYR
20	C8	25	ASN
21	C9	29	GLU
22	D0	17	GLN
22	D0	59	PRO
23	D1	46	ILE
23	D1	81	ASN
25	D3	112	LYS
26	D4	34	ASN
26	D4	51	GLU
27	D5	54	VAL
28	D6	8	ASN
28	D6	47	ALA
32	E0	14	VAL
32	E0	60	PRO
33	E1	93	HIS
33	E1	100	LEU
35	SM	12	VAL
40	L3	289	ASP
40	L3	317	ILE
41	L4	140	HIS

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Mol	Chain	Res	Type
41	L4	305	ALA
44	L7	163	LEU
44	L7	178	ILE
44	L7	188	ILE
45	L8	122	LYS
45	L8	136	LEU
46	L9	42	ASP
47	M0	24	ARG
47	M0	211	ARG
48	M1	39	GLN
48	M1	64	LYS
50	M4	6	ILE
51	M5	187	ARG
55	M9	53	LYS
59	N3	131	SER
60	N4	96	LEU
64	N8	24	LYS
64	N8	70	LYS
67	O1	7	VAL
69	O3	76	GLY
69	O3	94	PHE
70	O4	33	GLN
76	Q0	79	GLU
2	s0	30	GLN
4	s2	182	PRO
7	s5	29	ILE
7	s5	35	GLN
7	s5	82	PHE
8	s6	165	GLY
9	s7	34	LEU
9	s7	112	ARG
10	s8	78	ILE
10	s8	94	ASN
11	s9	134	ILE
11	s9	147	MET
12	c0	3	MET
12	c0	35	ILE
14	c2	21	GLU
14	c2	40	GLY
14	c2	66	VAL
14	c2	81	ASP
14	c2	91	VAL

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Mol	Chain	Res	Type
14	c2	115	VAL
15	c3	22	ALA
16	c4	114	ARG
16	c4	122	PRO
16	c4	124	ASP
17	c5	50	THR
17	c5	135	THR
20	c8	7	GLU
20	c8	19	ASN
23	d1	41	GLU
27	d5	38	HIS
27	d5	104	ALA
80	e0	47	VAL
80	e0	54	ARG
33	e1	124	PRO
34	sR	66	HIS
34	sR	277	GLU
35	sM	168	GLU
39	l2	142	ASP
41	l4	120	TYR
41	l4	195	ARG
41	l4	233	LEU
44	l7	157	ASN
45	l8	69	LEU
45	l8	112	GLU
46	l9	21	LYS
47	m0	47	PRO
48	m1	117	ASP
49	m3	141	ALA
49	m3	153	ASP
54	m8	43	PRO
54	m8	112	ALA
55	m9	183	ALA
56	n0	129	ILE
56	n0	139	TYR
60	n4	72	SER
60	n4	83	THR
62	n6	92	GLY
63	n7	56	LYS
63	n7	127	ASN
67	o1	7	VAL
67	o1	82	GLU

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Mol	Chain	Res	Type
68	o2	8	LYS
69	o3	59	VAL
70	o4	48	GLY
72	o6	97	SER
74	o8	17	ARG
2	S0	28	ASN
3	S1	182	ALA
3	S1	210	ILE
4	S2	175	GLY
9	S7	15	GLU
9	S7	84	LYS
17	C5	66	ALA
18	C6	40	GLU
21	C9	118	PRO
21	C9	119	LYS
22	D0	55	PRO
26	D4	104	SER
33	E1	148	TYR
34	SR	163	ASP
34	SR	194	GLY
41	L4	233	LEU
43	L6	6	ALA
45	L8	253	SER
46	L9	59	ASN
50	M4	28	SER
53	M7	97	ASN
54	M8	133	LYS
59	N3	82	ALA
60	N4	76	VAL
65	N9	25	LYS
71	O5	90	ARG
72	O6	11	LEU
72	O6	21	THR
74	O8	70	PRO
3	s1	178	GLY
4	s2	234	PRO
5	s3	43	PRO
6	s4	93	ASP
6	s4	95	THR
6	s4	260	GLY
7	s5	100	ASN
10	s8	62	THR

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Mol	Chain	Res	Type
11	s9	110	GLN
12	c0	23	ALA
12	c0	96	ASN
13	c1	24	LYS
17	c5	126	VAL
18	c6	4	VAL
21	c9	103	LYS
29	d7	41	LEU
29	d7	75	GLU
35	sM	47	ALA
40	l3	297	SER
41	l4	5	GLN
41	l4	14	GLU
41	l4	71	VAL
41	l4	190	GLY
42	l5	125	VAL
42	l5	215	ASP
42	l5	270	LYS
43	l6	172	HIS
44	l7	178	ILE
47	m0	169	LYS
49	m3	162	ASN
52	m6	111	PRO
57	n1	127	GLN
59	n3	16	GLY
60	n4	64	THR
68	o2	124	GLY
76	q0	80	PRO
9	S7	73	VAL
11	S9	162	SER
18	C6	56	GLY
24	D2	77	PRO
31	D9	6	VAL
34	SR	15	GLY
35	SM	20	LEU
35	SM	172	VAL
41	L4	4	PRO
63	N7	36	HIS
2	s0	139	VAL
13	c1	129	ARG
18	c6	40	GLU
19	c7	38	ILE

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Mol	Chain	Res	Type
34	sR	194	GLY
39	l2	13	GLY
82	p0	197	PHE
2	S0	31	VAL
3	S1	93	GLY
12	C0	35	ILE
13	C1	7	VAL
14	C2	115	VAL
18	C6	29	ILE
26	D4	35	VAL
30	D8	20	GLY
40	L3	96	PRO
46	L9	164	ILE
54	M8	132	PRO
56	N0	61	ILE
65	N9	21	ILE
5	s3	33	GLY
5	s3	163	PRO
15	c3	65	VAL
18	c6	97	VAL
41	l4	25	VAL
46	l9	108	GLY
48	m1	45	PRO
52	m6	190	VAL
6	S4	233	LYS
22	D0	106	ILE
28	D6	59	TYR
47	M0	91	VAL
2	s0	97	PRO
4	s2	151	PRO
8	s6	69	LEU
9	s7	73	VAL
40	l3	141	GLY
74	o8	35	GLY
28	D6	97	PRO
41	L4	272	VAL
45	L8	190	VAL
54	M8	84	VAL
60	N4	80	ARG
61	N5	26	VAL
11	s9	165	GLY
14	c2	63	VAL

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Mol	Chain	Res	Type
16	c4	96	PRO
31	d9	11	PRO
40	l3	185	GLY
49	m3	93	ILE
74	O8	37	PRO
79	Q3	90	VAL
9	s7	32	PRO
19	c7	117	LEU
80	e0	27	PRO
35	sM	51	ARG

5.3.2 Protein sidechains [i](#)

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%)	134 (82%)	30 (18%)	1 8
2	s0	165/209 (79%)	137 (83%)	28 (17%)	2 10
3	S1	191/223 (86%)	147 (77%)	44 (23%)	1 3
3	s1	192/223 (86%)	154 (80%)	38 (20%)	1 7
4	S2	176/204 (86%)	140 (80%)	36 (20%)	1 6
4	s2	176/204 (86%)	127 (72%)	49 (28%)	0 1
5	S3	182/194 (94%)	149 (82%)	33 (18%)	1 8
5	s3	182/194 (94%)	144 (79%)	38 (21%)	1 6
6	S4	221/221 (100%)	177 (80%)	44 (20%)	1 6
6	s4	221/221 (100%)	179 (81%)	42 (19%)	1 8
7	S5	173/190 (91%)	145 (84%)	28 (16%)	2 11
7	s5	173/190 (91%)	140 (81%)	33 (19%)	1 8
8	S6	188/201 (94%)	152 (81%)	36 (19%)	1 8
8	s6	187/201 (93%)	158 (84%)	29 (16%)	2 12
9	S7	165/169 (98%)	135 (82%)	30 (18%)	1 8
9	s7	165/169 (98%)	131 (79%)	34 (21%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	S8	150/161 (93%)	123 (82%)	27 (18%)	1	9
10	s8	150/161 (93%)	125 (83%)	25 (17%)	2	10
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	3
11	s9	158/165 (96%)	121 (77%)	37 (23%)	1	3
12	C0	77/98 (79%)	62 (80%)	15 (20%)	1	7
12	c0	73/98 (74%)	61 (84%)	12 (16%)	2	11
13	C1	129/136 (95%)	108 (84%)	21 (16%)	2	11
13	c1	129/136 (95%)	105 (81%)	24 (19%)	1	8
14	C2	88/118 (75%)	70 (80%)	18 (20%)	1	6
14	c2	88/118 (75%)	68 (77%)	20 (23%)	1	4
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	6
15	c3	127/127 (100%)	104 (82%)	23 (18%)	1	8
16	C4	81/104 (78%)	63 (78%)	18 (22%)	1	4
16	c4	97/104 (93%)	72 (74%)	25 (26%)	0	2
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1	6
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	9
18	C6	117/118 (99%)	96 (82%)	21 (18%)	2	9
18	c6	118/118 (100%)	96 (81%)	22 (19%)	1	8
19	C7	94/124 (76%)	74 (79%)	20 (21%)	1	5
19	c7	92/124 (74%)	71 (77%)	21 (23%)	1	4
20	C8	128/128 (100%)	92 (72%)	36 (28%)	0	1
20	c8	128/128 (100%)	99 (77%)	29 (23%)	1	4
21	C9	115/115 (100%)	89 (77%)	26 (23%)	1	4
21	c9	115/115 (100%)	95 (83%)	20 (17%)	2	10
22	D0	100/113 (88%)	83 (83%)	17 (17%)	2	10
22	d0	103/113 (91%)	74 (72%)	29 (28%)	0	1
23	D1	74/74 (100%)	57 (77%)	17 (23%)	1	3
23	d1	74/74 (100%)	53 (72%)	21 (28%)	0	1
24	D2	110/110 (100%)	86 (78%)	24 (22%)	1	5
24	d2	110/110 (100%)	92 (84%)	18 (16%)	2	11
25	D3	119/119 (100%)	103 (87%)	16 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	d3	119/119 (100%)	98 (82%)	21 (18%)	2	9
26	D4	112/112 (100%)	101 (90%)	11 (10%)	8	31
26	d4	112/112 (100%)	90 (80%)	22 (20%)	1	7
27	D5	61/88 (69%)	42 (69%)	19 (31%)	0	0
27	d5	61/88 (69%)	49 (80%)	12 (20%)	1	7
28	D6	83/83 (100%)	63 (76%)	20 (24%)	0	3
28	d6	83/83 (100%)	67 (81%)	16 (19%)	1	8
29	D7	70/70 (100%)	61 (87%)	9 (13%)	4	19
29	d7	70/70 (100%)	58 (83%)	12 (17%)	2	10
30	D8	56/59 (95%)	40 (71%)	16 (29%)	0	1
30	d8	56/59 (95%)	43 (77%)	13 (23%)	1	3
31	D9	47/48 (98%)	35 (74%)	12 (26%)	0	2
31	d9	47/48 (98%)	38 (81%)	9 (19%)	1	8
32	E0	51/51 (100%)	44 (86%)	7 (14%)	3	17
33	E1	62/66 (94%)	47 (76%)	15 (24%)	0	2
33	e1	66/66 (100%)	49 (74%)	17 (26%)	0	2
34	SR	260/261 (100%)	225 (86%)	35 (14%)	4	18
34	sR	260/261 (100%)	229 (88%)	31 (12%)	5	22
35	SM	97/228 (42%)	75 (77%)	22 (23%)	1	4
35	sM	54/228 (24%)	44 (82%)	10 (18%)	1	8
39	L2	193/195 (99%)	150 (78%)	43 (22%)	1	4
39	l2	192/195 (98%)	157 (82%)	35 (18%)	1	8
40	L3	319/322 (99%)	254 (80%)	65 (20%)	1	6
40	l3	320/322 (99%)	249 (78%)	71 (22%)	1	4
41	L4	288/288 (100%)	235 (82%)	53 (18%)	1	8
41	l4	288/288 (100%)	227 (79%)	61 (21%)	1	5
42	L5	244/244 (100%)	203 (83%)	41 (17%)	2	10
42	l5	243/244 (100%)	200 (82%)	43 (18%)	2	9
43	L6	134/152 (88%)	110 (82%)	24 (18%)	2	9
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	10
44	L7	186/204 (91%)	161 (87%)	25 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	l7	187/204 (92%)	160 (86%)	27 (14%)	3	15
45	L8	187/207 (90%)	154 (82%)	33 (18%)	2	9
45	l8	177/207 (86%)	148 (84%)	29 (16%)	2	11
46	L9	171/171 (100%)	139 (81%)	32 (19%)	1	8
46	l9	171/171 (100%)	125 (73%)	46 (27%)	0	2
47	M0	177/186 (95%)	143 (81%)	34 (19%)	1	8
47	m0	179/186 (96%)	152 (85%)	27 (15%)	3	14
48	M1	147/150 (98%)	116 (79%)	31 (21%)	1	6
48	m1	147/150 (98%)	113 (77%)	34 (23%)	1	3
49	M3	154/158 (98%)	123 (80%)	31 (20%)	1	6
49	m3	154/158 (98%)	127 (82%)	27 (18%)	2	9
50	M4	107/108 (99%)	87 (81%)	20 (19%)	1	8
50	m4	108/108 (100%)	83 (77%)	25 (23%)	1	3
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	10
51	m5	175/175 (100%)	144 (82%)	31 (18%)	2	9
52	M6	160/161 (99%)	139 (87%)	21 (13%)	4	19
52	m6	160/161 (99%)	125 (78%)	35 (22%)	1	5
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	4
53	m7	125/145 (86%)	94 (75%)	31 (25%)	0	2
54	M8	150/150 (100%)	129 (86%)	21 (14%)	3	16
54	m8	150/150 (100%)	118 (79%)	32 (21%)	1	5
55	M9	153/153 (100%)	128 (84%)	25 (16%)	2	11
55	m9	153/153 (100%)	127 (83%)	26 (17%)	2	10
56	N0	156/156 (100%)	126 (81%)	30 (19%)	1	8
56	n0	156/156 (100%)	120 (77%)	36 (23%)	1	3
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1	4
57	n1	136/136 (100%)	105 (77%)	31 (23%)	1	4
58	N2	87/106 (82%)	66 (76%)	21 (24%)	0	3
58	n2	85/106 (80%)	71 (84%)	14 (16%)	2	10
59	N3	104/104 (100%)	81 (78%)	23 (22%)	1	4
59	n3	104/104 (100%)	88 (85%)	16 (15%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	N4	57/129 (44%)	51 (90%)	6 (10%)	7	28
60	n4	100/129 (78%)	80 (80%)	20 (20%)	1	6
61	N5	104/117 (89%)	79 (76%)	25 (24%)	0	3
61	n5	104/117 (89%)	89 (86%)	15 (14%)	3	15
62	N6	109/109 (100%)	89 (82%)	20 (18%)	1	8
62	n6	109/109 (100%)	89 (82%)	20 (18%)	1	8
63	N7	115/115 (100%)	90 (78%)	25 (22%)	1	5
63	n7	115/115 (100%)	86 (75%)	29 (25%)	0	2
64	N8	118/118 (100%)	98 (83%)	20 (17%)	2	10
64	n8	118/118 (100%)	93 (79%)	25 (21%)	1	5
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1	5
65	n9	46/46 (100%)	32 (70%)	14 (30%)	0	0
66	O0	81/87 (93%)	70 (86%)	11 (14%)	3	17
66	o0	84/87 (97%)	65 (77%)	19 (23%)	1	4
67	O1	92/96 (96%)	76 (83%)	16 (17%)	2	10
67	o1	94/96 (98%)	66 (70%)	28 (30%)	0	1
68	O2	109/110 (99%)	89 (82%)	20 (18%)	1	8
68	o2	109/110 (99%)	88 (81%)	21 (19%)	1	8
69	O3	90/90 (100%)	74 (82%)	16 (18%)	2	9
69	o3	90/90 (100%)	78 (87%)	12 (13%)	4	18
70	O4	95/102 (93%)	81 (85%)	14 (15%)	3	14
70	o4	95/102 (93%)	78 (82%)	17 (18%)	2	9
71	O5	104/104 (100%)	85 (82%)	19 (18%)	1	8
71	o5	103/104 (99%)	77 (75%)	26 (25%)	0	2
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1	6
72	o6	80/81 (99%)	57 (71%)	23 (29%)	0	1
73	O7	70/70 (100%)	53 (76%)	17 (24%)	0	2
73	o7	70/70 (100%)	62 (89%)	8 (11%)	5	24
74	O8	68/68 (100%)	46 (68%)	22 (32%)	0	0
74	o8	67/68 (98%)	53 (79%)	14 (21%)	1	6
75	O9	45/45 (100%)	37 (82%)	8 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	o9	45/45 (100%)	34 (76%)	11 (24%)	0	2
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	2	10
76	q0	47/47 (100%)	34 (72%)	13 (28%)	0	1
77	Q1	23/23 (100%)	17 (74%)	6 (26%)	0	2
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	67 (74%)	23 (26%)	0	2
78	q2	90/90 (100%)	68 (76%)	22 (24%)	0	2
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1	6
79	q3	71/71 (100%)	59 (83%)	12 (17%)	2	10
80	e0	53/53 (100%)	43 (81%)	10 (19%)	1	8
82	p0	105/253 (42%)	86 (82%)	19 (18%)	1	8
All	All	18727/20241 (92%)	15053 (80%)	3674 (20%)	1	7

All (3674) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	6	THR
2	S0	7	PHE
2	S0	10	THR
2	S0	16	LEU
2	S0	32	HIS
2	S0	50	VAL
2	S0	52	LYS
2	S0	57	LEU
2	S0	59	LEU
2	S0	62	ARG
2	S0	72	ASP
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	98	ILE
2	S0	101	ARG
2	S0	110	TYR
2	S0	111	ILE
2	S0	119	ARG
2	S0	128	SER
2	S0	157	ASP

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Mol	Chain	Res	Type
2	S0	162	CYS
2	S0	165	ARG
2	S0	169	SER
2	S0	170	ILE
2	S0	172	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	200	ASP
3	S1	21	VAL
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	33	LYS
3	S1	39	GLU
3	S1	46	THR
3	S1	55	LYS
3	S1	61	LEU
3	S1	65	VAL
3	S1	70	LEU
3	S1	77	GLU
3	S1	78	ASP
3	S1	81	PHE
3	S1	85	LYS
3	S1	89	ASP
3	S1	91	VAL
3	S1	96	LEU
3	S1	97	LEU
3	S1	104	ASP
3	S1	105	PHE
3	S1	110	LEU
3	S1	111	ARG
3	S1	115	ARG
3	S1	117	TRP
3	S1	135	LEU
3	S1	144	ARG
3	S1	169	SER
3	S1	170	GLU
3	S1	173	THR
3	S1	177	GLN
3	S1	181	LEU
3	S1	183	GLN
3	S1	184	LEU

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Mol	Chain	Res	Type
3	S1	204	ILE
3	S1	206	PRO
3	S1	212	VAL
3	S1	215	VAL
3	S1	218	LEU
3	S1	219	LYS
3	S1	222	LYS
3	S1	223	PHE
3	S1	225	VAL
3	S1	232	HIS
4	S2	39	THR
4	S2	41	LEU
4	S2	50	ILE
4	S2	53	ILE
4	S2	54	GLU
4	S2	69	ILE
4	S2	73	LEU
4	S2	77	GLN
4	S2	87	GLN
4	S2	89	GLN
4	S2	91	ARG
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	111	VAL
4	S2	113	LEU
4	S2	117	THR
4	S2	134	LEU
4	S2	137	ILE
4	S2	140	ARG
4	S2	148	LEU
4	S2	150	GLN
4	S2	159	THR
4	S2	166	THR
4	S2	186	LYS
4	S2	187	LEU
4	S2	207	LEU
4	S2	208	GLU
4	S2	221	THR
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR

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Mol	Chain	Res	Type
4	S2	229	LEU
4	S2	240	LEU
4	S2	242	ILE
4	S2	245	ASP
5	S3	4	LEU
5	S3	5	ILE
5	S3	7	LYS
5	S3	21	LEU
5	S3	23	GLU
5	S3	37	VAL
5	S3	46	THR
5	S3	65	ARG
5	S3	67	ASN
5	S3	76	ARG
5	S3	84	ILE
5	S3	92	GLN
5	S3	93	ASP
5	S3	94	ARG
5	S3	103	GLU
5	S3	105	MET
5	S3	110	LEU
5	S3	113	LEU
5	S3	117	ARG
5	S3	128	GLU
5	S3	143	ARG
5	S3	146	ARG
5	S3	151	LYS
5	S3	158	ILE
5	S3	166	ASP
5	S3	172	THR
5	S3	178	ARG
5	S3	186	VAL
5	S3	189	MET
5	S3	190	ARG
5	S3	197	THR
5	S3	207	THR
5	S3	223	LYS
6	S4	7	LYS
6	S4	9	LEU
6	S4	11	ARG
6	S4	12	LEU
6	S4	38	LEU

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Mol	Chain	Res	Type
6	S4	45	ILE
6	S4	49	ARG
6	S4	54	TYR
6	S4	56	LEU
6	S4	62	LYS
6	S4	68	ARG
6	S4	70	VAL
6	S4	77	ARG
6	S4	81	THR
6	S4	92	LEU
6	S4	95	THR
6	S4	108	ARG
6	S4	113	ARG
6	S4	117	GLU
6	S4	126	VAL
6	S4	128	LYS
6	S4	129	VAL
6	S4	131	LEU
6	S4	133	LYS
6	S4	155	LYS
6	S4	160	VAL
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	211	LYS
6	S4	215	ASP
6	S4	221	ARG
6	S4	226	PHE
6	S4	227	VAL
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	247	SER
6	S4	248	ILE
6	S4	258	GLN
6	S4	259	GLN
7	S5	24	VAL
7	S5	25	LEU
7	S5	32	GLU

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Mol	Chain	Res	Type
7	S5	38	THR
7	S5	43	PHE
7	S5	45	LYS
7	S5	46	TRP
7	S5	48	PHE
7	S5	53	VAL
7	S5	65	ARG
7	S5	76	ARG
7	S5	79	ASN
7	S5	89	ILE
7	S5	90	ILE
7	S5	93	LEU
7	S5	95	ASN
7	S5	109	LYS
7	S5	112	ARG
7	S5	122	ASN
7	S5	131	GLN
7	S5	147	THR
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	186	ASN
7	S5	194	LEU
7	S5	203	LYS
7	S5	225	ARG
8	S6	5	ILE
8	S6	7	TYR
8	S6	13	GLN
8	S6	19	ASP
8	S6	25	ARG
8	S6	45	PHE
8	S6	51	LYS
8	S6	56	ASN
8	S6	58	LYS
8	S6	65	GLN
8	S6	78	THR
8	S6	79	LYS
8	S6	83	CYS
8	S6	98	ARG
8	S6	108	VAL
8	S6	120	GLU
8	S6	125	THR

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Mol	Chain	Res	Type
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	131	LYS
8	S6	132	ARG
8	S6	133	LEU
8	S6	143	LYS
8	S6	151	ASP
8	S6	154	ARG
8	S6	155	ASP
8	S6	169	TYR
8	S6	170	THR
8	S6	175	ILE
8	S6	177	ARG
8	S6	193	LEU
8	S6	211	LEU
8	S6	212	LEU
8	S6	214	LYS
8	S6	223	LYS
9	S7	16	LEU
9	S7	28	GLU
9	S7	37	GLU
9	S7	38	LEU
9	S7	46	ILE
9	S7	50	ASP
9	S7	67	LEU
9	S7	70	PHE
9	S7	71	HIS
9	S7	75	THR
9	S7	77	LEU
9	S7	85	PHE
9	S7	87	ASP
9	S7	90	VAL
9	S7	97	ARG
9	S7	104	ARG
9	S7	109	VAL
9	S7	110	GLN
9	S7	114	ARG
9	S7	116	ARG
9	S7	119	THR
9	S7	126	LEU
9	S7	130	VAL

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Mol	Chain	Res	Type
9	S7	144	VAL
9	S7	147	ASN
9	S7	154	LEU
9	S7	162	ILE
9	S7	164	TYR
9	S7	166	LEU
9	S7	185	ILE
10	S8	6	ASP
10	S8	7	SER
10	S8	8	ARG
10	S8	10	LYS
10	S8	17	LYS
10	S8	20	GLN
10	S8	21	PHE
10	S8	22	ARG
10	S8	29	LEU
10	S8	36	THR
10	S8	38	ILE
10	S8	46	VAL
10	S8	56	ARG
10	S8	58	LEU
10	S8	60	ILE
10	S8	82	VAL
10	S8	107	THR
10	S8	135	LYS
10	S8	138	ASN
10	S8	140	GLU
10	S8	149	SER
10	S8	151	LYS
10	S8	152	ILE
10	S8	164	ARG
10	S8	184	LEU
10	S8	193	LEU
10	S8	196	LEU
11	S9	3	ARG
11	S9	14	THR
11	S9	20	GLU
11	S9	28	LEU
11	S9	30	LEU
11	S9	36	LEU
11	S9	39	LYS
11	S9	40	LYS

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Mol	Chain	Res	Type
11	S9	46	SER
11	S9	48	GLN
11	S9	54	ARG
11	S9	57	ARG
11	S9	64	GLU
11	S9	78	ARG
11	S9	82	ARG
11	S9	83	VAL
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	97	LEU
11	S9	99	LEU
11	S9	110	GLN
11	S9	118	LEU
11	S9	121	SER
11	S9	130	THR
11	S9	134	ILE
11	S9	138	LYS
11	S9	149	ARG
11	S9	151	ASP
11	S9	155	HIS
11	S9	157	ASP
11	S9	161	THR
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	180	LYS
11	S9	182	GLU
12	C0	7	ASP
12	C0	8	ARG
12	C0	20	VAL
12	C0	28	ASN
12	C0	32	HIS
12	C0	33	GLU
12	C0	46	LEU
12	C0	49	LEU
12	C0	55	VAL
12	C0	56	LYS
12	C0	71	GLU
12	C0	76	LEU
12	C0	78	GLU

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Mol	Chain	Res	Type
12	C0	81	ASN
12	C0	82	LEU
13	C1	4	GLU
13	C1	7	VAL
13	C1	8	GLN
13	C1	21	ASN
13	C1	29	LYS
13	C1	40	LEU
13	C1	44	THR
13	C1	54	ILE
13	C1	56	LYS
13	C1	67	ARG
13	C1	69	LYS
13	C1	74	THR
13	C1	76	VAL
13	C1	79	LYS
13	C1	83	THR
13	C1	87	ARG
13	C1	94	ILE
13	C1	109	VAL
13	C1	123	VAL
13	C1	131	ILE
13	C1	140	VAL
14	C2	25	GLU
14	C2	28	LEU
14	C2	33	ARG
14	C2	41	LEU
14	C2	43	ARG
14	C2	46	ARG
14	C2	61	VAL
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
14	C2	139	HIS
14	C2	140	PHE
15	C3	3	ARG

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Mol	Chain	Res	Type
15	C3	4	MET
15	C3	6	SER
15	C3	9	LYS
15	C3	19	SER
15	C3	21	ASN
15	C3	27	LYS
15	C3	34	ILE
15	C3	39	LYS
15	C3	46	THR
15	C3	61	THR
15	C3	64	ARG
15	C3	66	ILE
15	C3	73	ARG
15	C3	76	LYS
15	C3	83	GLU
15	C3	88	LEU
15	C3	99	ARG
15	C3	102	LEU
15	C3	105	ASN
15	C3	115	LEU
15	C3	125	LEU
15	C3	141	TYR
15	C3	142	GLU
15	C3	149	LEU
15	C3	151	ASN
16	C4	16	VAL
16	C4	20	TYR
16	C4	29	HIS
16	C4	30	VAL
16	C4	31	THR
16	C4	42	VAL
16	C4	76	ILE
16	C4	81	VAL
16	C4	92	LYS
16	C4	99	GLN
16	C4	107	ARG
16	C4	114	ARG
16	C4	115	ILE
16	C4	118	VAL
16	C4	123	SER
16	C4	132	ARG
16	C4	136	ARG

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Mol	Chain	Res	Type
16	C4	137	LEU
17	C5	20	VAL
17	C5	22	LEU
17	C5	31	GLU
17	C5	34	VAL
17	C5	35	LYS
17	C5	36	LEU
17	C5	40	ARG
17	C5	43	ARG
17	C5	44	ARG
17	C5	47	ARG
17	C5	52	LYS
17	C5	60	LEU
17	C5	69	GLU
17	C5	80	MET
17	C5	84	ILE
17	C5	89	MET
17	C5	94	VAL
17	C5	100	LYS
17	C5	106	GLU
17	C5	110	GLU
17	C5	121	ILE
18	C6	4	VAL
18	C6	14	LYS
18	C6	17	THR
18	C6	19	VAL
18	C6	26	LYS
18	C6	28	LEU
18	C6	29	ILE
18	C6	39	VAL
18	C6	47	LYS
18	C6	53	LEU
18	C6	54	LEU
18	C6	66	ARG
18	C6	68	ARG
18	C6	69	VAL
18	C6	98	ASP
18	C6	106	LYS
18	C6	116	LEU
18	C6	121	SER
18	C6	136	SER
18	C6	137	ARG

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Mol	Chain	Res	Type
18	C6	143	ARG
19	C7	5	ARG
19	C7	6	THR
19	C7	19	ARG
19	C7	29	GLN
19	C7	34	LEU
19	C7	38	ILE
19	C7	40	THR
19	C7	41	ILE
19	C7	43	SER
19	C7	54	THR
19	C7	55	THR
19	C7	69	ILE
19	C7	72	LYS
19	C7	76	GLU
19	C7	83	GLN
19	C7	84	TYR
19	C7	88	VAL
19	C7	105	GLN
19	C7	113	LEU
19	C7	115	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	6	GLN
20	C8	8	GLN
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	17	LEU
20	C8	20	THR
20	C8	22	VAL
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	32	LEU
20	C8	34	THR
20	C8	40	ARG
20	C8	46	VAL
20	C8	53	ASP
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	77	THR
20	C8	80	LYS
20	C8	103	ASN
20	C8	108	LYS
20	C8	119	ILE
20	C8	120	ARG
20	C8	131	LEU
20	C8	132	ARG
20	C8	136	GLN
20	C8	138	THR
20	C8	140	THR
20	C8	141	THR
20	C8	143	ARG
21	C9	4	VAL
21	C9	6	VAL
21	C9	12	GLN
21	C9	13	ASP
21	C9	18	TYR
21	C9	22	LEU
21	C9	28	LEU
21	C9	30	VAL
21	C9	33	TYR
21	C9	34	VAL
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	39	THR
21	C9	43	ASN
21	C9	57	ARG
21	C9	67	MET
21	C9	94	ILE
21	C9	103	LYS
21	C9	111	ILE
21	C9	117	SER
21	C9	130	ARG
21	C9	131	ASP
21	C9	133	ASP
21	C9	134	ARG
21	C9	139	THR
22	D0	15	GLN

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Mol	Chain	Res	Type
22	D0	21	LYS
22	D0	22	ILE
22	D0	23	ARG
22	D0	27	THR
22	D0	31	VAL
22	D0	42	VAL
22	D0	43	LYS
22	D0	47	GLN
22	D0	50	LEU
22	D0	57	ARG
22	D0	58	LEU
22	D0	72	ASN
22	D0	74	GLU
22	D0	85	ARG
22	D0	89	ARG
22	D0	103	ILE
23	D1	2	GLU
23	D1	3	ASN
23	D1	5	LYS
23	D1	8	LEU
23	D1	9	VAL
23	D1	11	LEU
23	D1	18	SER
23	D1	24	ILE
23	D1	25	LYS
23	D1	32	VAL
23	D1	36	VAL
23	D1	52	THR
23	D1	65	SER
23	D1	68	SER
23	D1	69	LEU
23	D1	78	LEU
23	D1	80	LYS
24	D2	2	THR
24	D2	4	SER
24	D2	22	LYS
24	D2	24	GLN
24	D2	25	VAL
24	D2	27	ILE
24	D2	29	PRO
24	D2	31	SER
24	D2	49	GLU

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Mol	Chain	Res	Type
24	D2	53	ILE
24	D2	65	LEU
24	D2	71	LYS
24	D2	76	SER
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	121	VAL
24	D2	125	ILE
24	D2	126	LEU
24	D2	129	VAL
25	D3	7	ARG
25	D3	19	ARG
25	D3	28	ASN
25	D3	40	SER
25	D3	56	LYS
25	D3	59	ILE
25	D3	73	ARG
25	D3	84	THR
25	D3	97	ASP
25	D3	100	ASP
25	D3	107	PHE
25	D3	110	LYS
25	D3	114	LYS
25	D3	127	VAL
25	D3	138	GLU
25	D3	144	ARG
26	D4	32	ARG
26	D4	34	ASN
26	D4	51	GLU
26	D4	57	VAL
26	D4	74	LEU
26	D4	96	LEU
26	D4	100	VAL
26	D4	102	LYS
26	D4	107	GLN
26	D4	124	ARG
26	D4	128	LYS

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Mol	Chain	Res	Type
27	D5	37	GLN
27	D5	42	LEU
27	D5	48	ASP
27	D5	49	ARG
27	D5	58	ARG
27	D5	59	TYR
27	D5	60	VAL
27	D5	63	SER
27	D5	68	ARG
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	93	SER
27	D5	95	HIS
27	D5	100	ILE
27	D5	102	THR
28	D6	7	SER
28	D6	30	ILE
28	D6	36	ILE
28	D6	38	ARG
28	D6	44	ILE
28	D6	45	VAL
28	D6	46	GLU
28	D6	53	LEU
28	D6	61	GLU
28	D6	64	LEU
28	D6	67	THR
28	D6	68	TYR
28	D6	70	LYS
28	D6	77	CYS
28	D6	79	ILE
28	D6	82	ARG
28	D6	83	ILE
28	D6	85	ARG
28	D6	88	SER
28	D6	90	GLU
29	D7	3	LEU
29	D7	20	LYS
29	D7	29	ARG

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Mol	Chain	Res	Type
29	D7	30	SER
29	D7	41	LEU
29	D7	55	THR
29	D7	62	ILE
29	D7	65	THR
29	D7	72	LYS
30	D8	5	THR
30	D8	8	THR
30	D8	13	ILE
30	D8	14	LYS
30	D8	19	THR
30	D8	31	GLU
30	D8	32	PHE
30	D8	38	ARG
30	D8	39	THR
30	D8	40	ILE
30	D8	49	ARG
30	D8	54	LEU
30	D8	57	MET
30	D8	58	GLU
30	D8	64	ARG
30	D8	65	ARG
31	D9	5	ASN
31	D9	7	TRP
31	D9	9	SER
31	D9	10	HIS
31	D9	12	ARG
31	D9	19	ARG
31	D9	21	CYS
31	D9	22	ARG
31	D9	23	VAL
31	D9	28	THR
31	D9	36	LEU
31	D9	40	ARG
32	E0	3	LYS
32	E0	20	LYS
32	E0	22	GLU
32	E0	28	LYS
32	E0	39	LEU
32	E0	42	ARG
32	E0	47	VAL
33	E1	83	LYS

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Mol	Chain	Res	Type
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
33	E1	106	TYR
33	E1	107	LYS
33	E1	108	VAL
33	E1	109	ASP
33	E1	115	THR
33	E1	118	ARG
33	E1	126	CYS
33	E1	139	LEU
33	E1	146	SER
33	E1	150	VAL
34	SR	10	ARG
34	SR	21	THR
34	SR	52	GLN
34	SR	58	VAL
34	SR	59	ARG
34	SR	60	SER
34	SR	72	THR
34	SR	76	ASP
34	SR	82	SER
34	SR	94	VAL
34	SR	117	LYS
34	SR	126	SER
34	SR	136	ILE
34	SR	141	LEU
34	SR	143	THR
34	SR	144	LEU
34	SR	149	ASP
34	SR	153	GLN
34	SR	165	ASP
34	SR	184	ASN
34	SR	191	ASP
34	SR	196	ASN
34	SR	207	ASP
34	SR	211	ILE
34	SR	213	SER
34	SR	232	TYR
34	SR	234	LEU
34	SR	238	ASP

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Mol	Chain	Res	Type
34	SR	248	ASN
34	SR	266	ASP
34	SR	268	GLN
34	SR	277	GLU
34	SR	300	THR
34	SR	316	MET
34	SR	317	THR
35	SM	23	LYS
35	SM	28	SER
35	SM	34	LYS
35	SM	46	LYS
35	SM	48	ARG
35	SM	51	ARG
35	SM	61	ILE
35	SM	68	ARG
35	SM	69	ARG
35	SM	70	ASN
35	SM	72	ARG
35	SM	75	ASP
35	SM	77	THR
35	SM	84	LYS
35	SM	89	ARG
35	SM	91	THR
35	SM	96	ARG
35	SM	100	THR
35	SM	102	THR
35	SM	117	LEU
35	SM	121	LYS
35	SM	130	GLU
39	L2	17	THR
39	L2	18	SER
39	L2	19	HIS
39	L2	23	ARG
39	L2	28	LYS
39	L2	31	THR
39	L2	32	LEU
39	L2	36	GLU
39	L2	44	ILE
39	L2	45	VAL
39	L2	48	ILE
39	L2	49	VAL
39	L2	52	SER

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Mol	Chain	Res	Type
39	L2	70	ARG
39	L2	71	LEU
39	L2	74	GLU
39	L2	95	SER
39	L2	96	LEU
39	L2	101	VAL
39	L2	104	LEU
39	L2	109	GLU
39	L2	112	ILE
39	L2	116	VAL
39	L2	118	GLU
39	L2	137	ILE
39	L2	142	ASP
39	L2	157	VAL
39	L2	165	VAL
39	L2	168	VAL
39	L2	169	ILE
39	L2	175	VAL
39	L2	179	LEU
39	L2	180	LEU
39	L2	190	ARG
39	L2	197	PRO
39	L2	202	VAL
39	L2	205	ASN
39	L2	207	VAL
39	L2	225	ILE
39	L2	226	SER
39	L2	227	ARG
39	L2	230	VAL
39	L2	245	LEU
40	L3	3	HIS
40	L3	7	GLU
40	L3	10	ARG
40	L3	17	LEU
40	L3	19	ARG
40	L3	25	ILE
40	L3	30	LYS
40	L3	37	ARG
40	L3	39	LYS
40	L3	44	THR
40	L3	47	LEU
40	L3	55	THR

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Mol	Chain	Res	Type
40	L3	56	ILE
40	L3	67	PHE
40	L3	70	ARG
40	L3	73	VAL
40	L3	79	VAL
40	L3	81	THR
40	L3	84	VAL
40	L3	85	VAL
40	L3	97	ARG
40	L3	100	ARG
40	L3	103	THR
40	L3	114	VAL
40	L3	120	LYS
40	L3	134	SER
40	L3	139	GLN
40	L3	148	LEU
40	L3	150	ARG
40	L3	157	VAL
40	L3	160	VAL
40	L3	167	ARG
40	L3	169	THR
40	L3	178	LEU
40	L3	183	LEU
40	L3	187	SER
40	L3	188	ILE
40	L3	192	VAL
40	L3	196	ARG
40	L3	205	VAL
40	L3	210	GLU
40	L3	212	ASN
40	L3	213	GLU
40	L3	232	ARG
40	L3	235	THR
40	L3	238	LEU
40	L3	241	LYS
40	L3	244	ARG
40	L3	266	ARG
40	L3	277	SER
40	L3	284	ARG
40	L3	287	LYS
40	L3	296	THR
40	L3	300	ARG

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Mol	Chain	Res	Type
40	L3	305	ILE
40	L3	308	MET
40	L3	320	ASP
40	L3	332	ARG
40	L3	337	THR
40	L3	338	LEU
40	L3	349	LYS
40	L3	352	GLU
40	L3	355	SER
40	L3	364	LYS
40	L3	386	ASP
41	L4	3	ARG
41	L4	25	VAL
41	L4	27	SER
41	L4	54	GLU
41	L4	60	THR
41	L4	69	ARG
41	L4	73	ARG
41	L4	74	ILE
41	L4	93	MET
41	L4	99	MET
41	L4	112	LYS
41	L4	120	TYR
41	L4	134	LEU
41	L4	138	ARG
41	L4	142	VAL
41	L4	147	GLU
41	L4	150	LEU
41	L4	152	VAL
41	L4	156	LEU
41	L4	158	SER
41	L4	170	LYS
41	L4	176	SER
41	L4	179	LEU
41	L4	186	LYS
41	L4	187	LEU
41	L4	193	LYS
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	206	LEU
41	L4	211	GLU

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Mol	Chain	Res	Type
41	L4	220	ARG
41	L4	222	VAL
41	L4	226	GLU
41	L4	230	VAL
41	L4	246	ARG
41	L4	258	LEU
41	L4	259	ASP
41	L4	267	VAL
41	L4	270	SER
41	L4	278	SER
41	L4	284	SER
41	L4	287	THR
41	L4	288	ARG
41	L4	292	SER
41	L4	306	THR
41	L4	307	GLN
41	L4	311	HIS
41	L4	323	VAL
41	L4	327	LEU
41	L4	333	VAL
41	L4	338	LYS
41	L4	346	LYS
42	L5	5	LYS
42	L5	9	SER
42	L5	22	ARG
42	L5	23	ARG
42	L5	35	ARG
42	L5	41	LYS
42	L5	66	SER
42	L5	69	ILE
42	L5	75	LEU
42	L5	92	LEU
42	L5	93	THR
42	L5	105	ILE
42	L5	112	LYS
42	L5	115	LEU
42	L5	117	GLU
42	L5	118	THR
42	L5	122	VAL
42	L5	131	LEU
42	L5	140	ARG
42	L5	146	LEU

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Mol	Chain	Res	Type
42	L5	151	GLN
42	L5	152	ARG
42	L5	173	VAL
42	L5	177	GLU
42	L5	185	PHE
42	L5	187	THR
42	L5	197	SER
42	L5	203	HIS
42	L5	205	SER
42	L5	206	GLN
42	L5	216	GLU
42	L5	222	LEU
42	L5	227	LEU
42	L5	234	ASP
42	L5	241	THR
42	L5	242	SER
42	L5	259	LYS
42	L5	261	THR
42	L5	263	GLU
42	L5	290	ILE
42	L5	293	LEU
43	L6	2	SER
43	L6	5	LYS
43	L6	15	VAL
43	L6	21	THR
43	L6	28	GLN
43	L6	31	ARG
43	L6	35	VAL
43	L6	52	VAL
43	L6	62	THR
43	L6	64	LEU
43	L6	70	LYS
43	L6	76	LEU
43	L6	78	ARG
43	L6	79	VAL
43	L6	84	VAL
43	L6	89	THR
43	L6	90	LYS
43	L6	98	VAL
43	L6	136	GLU
43	L6	146	ILE
43	L6	152	THR

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Mol	Chain	Res	Type
43	L6	155	LEU
43	L6	160	SER
43	L6	170	LYS
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	43	ILE
44	L7	47	ARG
44	L7	60	ARG
44	L7	78	GLU
44	L7	82	LYS
44	L7	83	LEU
44	L7	92	ILE
44	L7	93	ASN
44	L7	101	LYS
44	L7	110	ARG
44	L7	118	LYS
44	L7	124	LEU
44	L7	128	LYS
44	L7	141	TYR
44	L7	158	LYS
44	L7	164	SER
44	L7	179	LEU
44	L7	182	ASP
44	L7	184	LEU
44	L7	189	ILE
44	L7	204	PRO
44	L7	239	LEU
45	L8	26	LEU
45	L8	41	GLN
45	L8	43	LYS
45	L8	50	VAL
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	84	ARG
45	L8	92	LYS
45	L8	98	ARG
45	L8	101	THR
45	L8	118	GLU
45	L8	132	VAL
45	L8	136	LEU

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Mol	Chain	Res	Type
45	L8	144	GLU
45	L8	150	LEU
45	L8	156	ASP
45	L8	169	LEU
45	L8	173	MET
45	L8	180	VAL
45	L8	181	LYS
45	L8	185	ARG
45	L8	189	LEU
45	L8	194	THR
45	L8	206	GLU
45	L8	211	LEU
45	L8	214	LEU
45	L8	216	SER
45	L8	218	ILE
45	L8	221	ASN
45	L8	224	ASP
45	L8	241	LYS
45	L8	248	LYS
46	L9	4	ILE
46	L9	6	THR
46	L9	14	GLU
46	L9	18	VAL
46	L9	19	SER
46	L9	22	SER
46	L9	33	THR
46	L9	41	ILE
46	L9	48	VAL
46	L9	49	ASN
46	L9	52	LEU
46	L9	55	VAL
46	L9	62	ARG
46	L9	65	VAL
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	73	SER
46	L9	78	MET
46	L9	82	VAL
46	L9	118	LEU
46	L9	132	VAL
46	L9	133	THR

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Mol	Chain	Res	Type
46	L9	135	GLU
46	L9	138	THR
46	L9	139	ASN
46	L9	151	VAL
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	177	ASP
46	L9	189	GLU
47	M0	12	GLN
47	M0	24	ARG
47	M0	26	VAL
47	M0	30	LYS
47	M0	32	ARG
47	M0	35	ASP
47	M0	36	LEU
47	M0	39	LYS
47	M0	40	LYS
47	M0	48	LEU
47	M0	52	LEU
47	M0	54	SER
47	M0	57	LEU
47	M0	63	GLU
47	M0	87	LEU
47	M0	102	MET
47	M0	130	ASP
47	M0	133	GLN
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	166	ILE
47	M0	175	ASN
47	M0	176	LEU
47	M0	177	ASP
47	M0	178	ARG
47	M0	185	ARG
47	M0	190	VAL
47	M0	203	LYS

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Mol	Chain	Res	Type
47	M0	205	SER
48	M1	10	ARG
48	M1	12	LEU
48	M1	16	LYS
48	M1	25	GLU
48	M1	39	GLN
48	M1	44	THR
48	M1	52	TYR
48	M1	53	THR
48	M1	56	THR
48	M1	65	ILE
48	M1	71	VAL
48	M1	80	LEU
48	M1	82	ARG
48	M1	85	LYS
48	M1	92	ARG
48	M1	94	ARG
48	M1	95	ASN
48	M1	101	ASN
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	115	LYS
48	M1	127	PHE
48	M1	137	ARG
48	M1	138	VAL
48	M1	140	ARG
48	M1	148	VAL
48	M1	155	THR
48	M1	166	LYS
48	M1	171	VAL
48	M1	173	ASP
49	M3	20	GLU
49	M3	33	VAL
49	M3	35	ARG
49	M3	41	THR
49	M3	54	LEU
49	M3	55	ARG
49	M3	57	VAL
49	M3	58	VAL
49	M3	59	ARG
49	M3	70	ARG

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Mol	Chain	Res	Type
49	M3	76	THR
49	M3	85	LEU
49	M3	101	ARG
49	M3	108	ILE
49	M3	113	VAL
49	M3	114	GLN
49	M3	115	ARG
49	M3	117	LYS
49	M3	121	SER
49	M3	124	ILE
49	M3	131	LYS
49	M3	134	GLU
49	M3	136	GLU
49	M3	137	GLN
49	M3	140	SER
49	M3	164	GLU
49	M3	168	ARG
49	M3	174	ARG
49	M3	180	ARG
49	M3	182	ILE
49	M3	190	LYS
50	M4	3	THR
50	M4	8	LYS
50	M4	15	VAL
50	M4	25	LYS
50	M4	38	ILE
50	M4	39	ILE
50	M4	42	LYS
50	M4	53	VAL
50	M4	64	VAL
50	M4	66	THR
50	M4	90	VAL
50	M4	91	CYS
50	M4	93	LYS
50	M4	98	SER
50	M4	102	LYS
50	M4	106	ARG
50	M4	107	GLU
50	M4	113	THR
50	M4	125	LYS
50	M4	135	LEU
51	M5	20	ARG

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Mol	Chain	Res	Type
51	M5	22	LEU
51	M5	38	ARG
51	M5	43	THR
51	M5	49	ARG
51	M5	50	ARG
51	M5	66	VAL
51	M5	68	ARG
51	M5	75	VAL
51	M5	77	LYS
51	M5	80	THR
51	M5	97	SER
51	M5	104	GLU
51	M5	106	VAL
51	M5	109	ARG
51	M5	113	LEU
51	M5	117	ASN
51	M5	133	ILE
51	M5	138	GLN
51	M5	151	ILE
51	M5	153	ASP
51	M5	155	VAL
51	M5	159	ARG
51	M5	167	THR
51	M5	170	LYS
51	M5	175	ASN
51	M5	183	THR
51	M5	184	LYS
51	M5	188	ARG
51	M5	190	THR
52	M6	27	LEU
52	M6	34	VAL
52	M6	36	VAL
52	M6	51	LYS
52	M6	58	LEU
52	M6	68	ARG
52	M6	78	ARG
52	M6	79	ILE
52	M6	84	LEU
52	M6	94	ARG
52	M6	106	GLU
52	M6	116	LYS
52	M6	117	ARG

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Mol	Chain	Res	Type
52	M6	124	LEU
52	M6	126	VAL
52	M6	128	ARG
52	M6	143	THR
52	M6	160	ARG
52	M6	170	LYS
52	M6	184	THR
52	M6	190	VAL
53	M7	3	ARG
53	M7	7	THR
53	M7	9	THR
53	M7	10	ASN
53	M7	14	SER
53	M7	20	SER
53	M7	23	ARG
53	M7	32	THR
53	M7	36	ILE
53	M7	41	LEU
53	M7	52	LEU
53	M7	67	ILE
53	M7	69	ARG
53	M7	78	VAL
53	M7	79	THR
53	M7	107	LEU
53	M7	112	LEU
53	M7	114	VAL
53	M7	118	GLN
53	M7	119	VAL
53	M7	126	ARG
53	M7	127	ARG
53	M7	136	ILE
53	M7	138	LYS
53	M7	144	SER
53	M7	153	LYS
53	M7	157	VAL
53	M7	168	LEU
53	M7	173	ARG
53	M7	180	LYS
53	M7	181	ARG
54	M8	3	ILE
54	M8	17	THR
54	M8	24	VAL

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Mol	Chain	Res	Type
54	M8	26	LEU
54	M8	32	LEU
54	M8	34	THR
54	M8	41	ASP
54	M8	63	SER
54	M8	69	ARG
54	M8	86	THR
54	M8	100	THR
54	M8	132	PRO
54	M8	135	GLN
54	M8	138	LEU
54	M8	139	ILE
54	M8	141	ARG
54	M8	147	ARG
54	M8	168	THR
54	M8	171	LYS
54	M8	180	ARG
54	M8	182	LYS
55	M9	5	ARG
55	M9	29	THR
55	M9	30	SER
55	M9	41	ILE
55	M9	44	LEU
55	M9	49	THR
55	M9	51	VAL
55	M9	55	VAL
55	M9	70	LYS
55	M9	71	ARG
55	M9	74	ARG
55	M9	81	ARG
55	M9	99	LEU
55	M9	103	ARG
55	M9	104	ARG
55	M9	110	ARG
55	M9	115	ILE
55	M9	116	ASP
55	M9	134	HIS
55	M9	160	GLU
55	M9	164	LEU
55	M9	165	LYS
55	M9	176	ARG
55	M9	180	LYS

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Mol	Chain	Res	Type
55	M9	182	ASP
56	N0	1	MET
56	N0	17	GLU
56	N0	21	GLU
56	N0	47	LYS
56	N0	50	LYS
56	N0	51	VAL
56	N0	57	GLU
56	N0	79	VAL
56	N0	80	ARG
56	N0	81	TYR
56	N0	85	SER
56	N0	87	THR
56	N0	105	THR
56	N0	106	LEU
56	N0	115	ARG
56	N0	117	ARG
56	N0	120	SER
56	N0	122	HIS
56	N0	130	GLU
56	N0	132	THR
56	N0	137	ARG
56	N0	142	GLN
56	N0	145	THR
56	N0	155	ARG
56	N0	156	VAL
56	N0	157	GLN
56	N0	160	THR
56	N0	167	ARG
56	N0	169	SER
56	N0	171	PHE
57	N1	12	ARG
57	N1	25	VAL
57	N1	26	HIS
57	N1	27	LEU
57	N1	32	LYS
57	N1	38	ASP
57	N1	39	ILE
57	N1	50	LYS
57	N1	52	MET
57	N1	68	THR
57	N1	78	LYS

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Mol	Chain	Res	Type
57	N1	79	MET
57	N1	80	VAL
57	N1	83	ARG
57	N1	88	ARG
57	N1	89	LEU
57	N1	102	ARG
57	N1	104	GLU
57	N1	106	LEU
57	N1	122	GLN
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	136	ARG
57	N1	139	ARG
57	N1	141	VAL
57	N1	143	THR
57	N1	144	GLU
57	N1	149	GLN
57	N1	160	ILE
58	N2	10	LYS
58	N2	16	THR
58	N2	29	ASP
58	N2	32	SER
58	N2	38	ILE
58	N2	39	ASP
58	N2	43	VAL
58	N2	49	ASN
58	N2	52	ASN
58	N2	54	VAL
58	N2	55	THR
58	N2	62	VAL
58	N2	66	VAL
58	N2	70	LYS
58	N2	72	SER
58	N2	87	ASN
58	N2	88	GLN
58	N2	92	TRP
58	N2	93	ILE
58	N2	98	THR
58	N2	100	THR
59	N3	9	THR
59	N3	13	ILE

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Mol	Chain	Res	Type
59	N3	14	SER
59	N3	19	VAL
59	N3	24	ASN
59	N3	25	CYS
59	N3	32	ARG
59	N3	46	LEU
59	N3	66	LYS
59	N3	69	LEU
59	N3	73	VAL
59	N3	74	MET
59	N3	79	VAL
59	N3	83	LYS
59	N3	87	ARG
59	N3	102	ILE
59	N3	104	ASN
59	N3	106	LYS
59	N3	115	THR
59	N3	125	LEU
59	N3	128	ARG
59	N3	135	VAL
59	N3	137	VAL
60	N4	7	SER
60	N4	19	THR
60	N4	39	LEU
60	N4	45	ASN
60	N4	54	LEU
60	N4	64	THR
61	N5	26	VAL
61	N5	27	ARG
61	N5	28	THR
61	N5	34	LEU
61	N5	38	LEU
61	N5	45	LYS
61	N5	57	LEU
61	N5	63	ILE
61	N5	73	MET
61	N5	74	LYS
61	N5	81	ILE
61	N5	86	VAL
61	N5	92	LYS
61	N5	96	LYS
61	N5	102	LEU

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Mol	Chain	Res	Type
61	N5	108	LEU
61	N5	109	LYS
61	N5	110	VAL
61	N5	112	THR
61	N5	115	ARG
61	N5	125	ARG
61	N5	127	THR
61	N5	135	ILE
61	N5	139	ILE
61	N5	142	ILE
62	N6	13	ARG
62	N6	36	SER
62	N6	37	LYS
62	N6	38	GLU
62	N6	40	ARG
62	N6	42	GLN
62	N6	45	ILE
62	N6	51	ARG
62	N6	56	VAL
62	N6	57	LEU
62	N6	60	ARG
62	N6	67	GLU
62	N6	74	TYR
62	N6	80	VAL
62	N6	89	LYS
62	N6	94	SER
62	N6	105	VAL
62	N6	115	ARG
62	N6	125	LYS
62	N6	126	LEU
63	N7	14	VAL
63	N7	15	ARG
63	N7	21	LYS
63	N7	24	VAL
63	N7	25	ILE
63	N7	33	SER
63	N7	46	ILE
63	N7	52	LYS
63	N7	54	THR
63	N7	57	HIS
63	N7	64	LYS
63	N7	72	ILE

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Mol	Chain	Res	Type
63	N7	80	LEU
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	87	LEU
63	N7	90	GLU
63	N7	99	GLU
63	N7	102	GLU
63	N7	103	GLN
63	N7	109	GLU
63	N7	126	LYS
63	N7	134	LEU
63	N7	135	ARG
64	N8	6	THR
64	N8	7	LYS
64	N8	8	THR
64	N8	10	LYS
64	N8	26	ARG
64	N8	34	MET
64	N8	42	ARG
64	N8	46	ASP
64	N8	47	LYS
64	N8	56	VAL
64	N8	60	TYR
64	N8	67	HIS
64	N8	78	LEU
64	N8	85	ASP
64	N8	88	ASP
64	N8	92	LYS
64	N8	115	LYS
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
65	N9	3	LYS
65	N9	13	THR
65	N9	18	ARG
65	N9	22	LYS
65	N9	25	LYS
65	N9	33	LYS
65	N9	39	PHE
65	N9	41	ARG
65	N9	50	THR

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Mol	Chain	Res	Type
65	N9	59	LYS
66	O0	16	LEU
66	O0	20	SER
66	O0	28	LYS
66	O0	40	LYS
66	O0	54	SER
66	O0	79	THR
66	O0	83	LYS
66	O0	99	ASP
66	O0	100	ILE
66	O0	101	LEU
66	O0	103	THR
67	O1	8	VAL
67	O1	9	THR
67	O1	13	THR
67	O1	16	LEU
67	O1	26	LYS
67	O1	31	ARG
67	O1	64	VAL
67	O1	68	GLU
67	O1	79	ARG
67	O1	84	ASP
67	O1	86	LYS
67	O1	91	SER
67	O1	94	GLU
67	O1	106	THR
67	O1	107	VAL
67	O1	110	GLU
68	O2	4	LEU
68	O2	10	VAL
68	O2	15	LYS
68	O2	19	ARG
68	O2	33	ARG
68	O2	34	LYS
68	O2	41	VAL
68	O2	54	LYS
68	O2	55	ILE
68	O2	61	LYS
68	O2	62	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	83	GLU

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Mol	Chain	Res	Type
68	O2	89	THR
68	O2	91	THR
68	O2	106	VAL
68	O2	109	LEU
68	O2	120	THR
68	O2	128	LEU
69	O3	15	SER
69	O3	28	SER
69	O3	31	LYS
69	O3	33	GLU
69	O3	37	THR
69	O3	48	ARG
69	O3	49	ILE
69	O3	54	ARG
69	O3	65	ARG
69	O3	70	LYS
69	O3	73	ARG
69	O3	80	VAL
69	O3	90	PRO
69	O3	93	THR
69	O3	98	VAL
69	O3	106	ASN
70	O4	5	VAL
70	O4	20	ILE
70	O4	21	LYS
70	O4	29	ILE
70	O4	51	LEU
70	O4	56	THR
70	O4	58	ARG
70	O4	65	VAL
70	O4	71	THR
70	O4	86	LYS
70	O4	88	ARG
70	O4	102	LYS
70	O4	104	VAL
70	O4	105	VAL
71	O5	4	VAL
71	O5	20	GLN
71	O5	27	GLU
71	O5	43	LYS
71	O5	47	VAL
71	O5	48	ARG

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Mol	Chain	Res	Type
71	O5	49	LYS
71	O5	71	LYS
71	O5	76	GLN
71	O5	86	ARG
71	O5	89	ARG
71	O5	90	ARG
71	O5	94	LYS
71	O5	101	THR
71	O5	102	GLU
71	O5	105	ARG
71	O5	107	LYS
71	O5	118	ILE
71	O5	119	LYS
72	O6	11	LEU
72	O6	21	THR
72	O6	26	ILE
72	O6	28	TYR
72	O6	34	SER
72	O6	36	ARG
72	O6	45	ARG
72	O6	52	PRO
72	O6	57	LEU
72	O6	58	ILE
72	O6	66	GLU
72	O6	68	ARG
72	O6	70	ARG
72	O6	71	LYS
72	O6	76	ARG
72	O6	81	THR
72	O6	88	GLU
73	O7	5	THR
73	O7	17	THR
73	O7	19	CYS
73	O7	21	ARG
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	36	SER
73	O7	44	THR
73	O7	55	ARG
73	O7	58	THR
73	O7	59	THR

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Mol	Chain	Res	Type
73	O7	64	MET
73	O7	65	ARG
73	O7	67	LEU
73	O7	80	THR
73	O7	82	SER
74	O8	5	ILE
74	O8	17	ARG
74	O8	22	THR
74	O8	24	THR
74	O8	25	VAL
74	O8	29	LYS
74	O8	31	LEU
74	O8	32	ASN
74	O8	41	THR
74	O8	45	VAL
74	O8	46	ARG
74	O8	52	TYR
74	O8	53	THR
74	O8	55	VAL
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	68	SER
74	O8	69	LEU
74	O8	72	THR
74	O8	77	ARG
74	O8	78	LEU
75	O9	4	GLN
75	O9	5	LYS
75	O9	21	ARG
75	O9	23	LEU
75	O9	25	GLN
75	O9	29	LEU
75	O9	36	ARG
75	O9	45	ARG
76	Q0	78	ILE
76	Q0	85	LEU
76	Q0	88	LYS
76	Q0	97	ARG
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	126	LYS

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Mol	Chain	Res	Type
76	Q0	127	LEU
77	Q1	6	ARG
77	Q1	9	ARG
77	Q1	10	THR
77	Q1	11	ARG
77	Q1	13	LEU
77	Q1	23	ARG
78	Q2	3	ASN
78	Q2	8	ARG
78	Q2	26	THR
78	Q2	28	TYR
78	Q2	29	LYS
78	Q2	45	ARG
78	Q2	48	SER
78	Q2	54	THR
78	Q2	60	LYS
78	Q2	70	LEU
78	Q2	71	ARG
78	Q2	78	LYS
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	87	ARG
78	Q2	88	CYS
78	Q2	89	LYS
78	Q2	92	GLU
78	Q2	93	LEU
78	Q2	100	LYS
78	Q2	104	LEU
78	Q2	105	GLN
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	24	ARG
79	Q3	25	GLN
79	Q3	31	ILE
79	Q3	33	GLN
79	Q3	45	LYS
79	Q3	49	ARG
79	Q3	59	CYS
79	Q3	60	CYS
79	Q3	70	THR
79	Q3	71	VAL

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Mol	Chain	Res	Type
79	Q3	82	THR
79	Q3	90	VAL
79	Q3	91	GLU
2	s0	9	LEU
2	s0	10	THR
2	s0	12	GLU
2	s0	24	LEU
2	s0	29	VAL
2	s0	30	GLN
2	s0	50	VAL
2	s0	55	GLU
2	s0	57	LEU
2	s0	59	LEU
2	s0	83	GLN
2	s0	87	LEU
2	s0	96	THR
2	s0	101	ARG
2	s0	106	SER
2	s0	111	ILE
2	s0	124	THR
2	s0	144	ILE
2	s0	154	GLU
2	s0	162	CYS
2	s0	172	LEU
2	s0	179	ARG
2	s0	180	GLU
2	s0	183	ARG
2	s0	185	ARG
2	s0	188	LEU
2	s0	189	VAL
2	s0	198	MET
3	s1	21	VAL
3	s1	25	THR
3	s1	36	SER
3	s1	37	THR
3	s1	47	LEU
3	s1	51	SER
3	s1	55	LYS
3	s1	62	LYS
3	s1	64	ARG
3	s1	70	LEU
3	s1	73	LEU

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Mol	Chain	Res	Type
3	s1	81	PHE
3	s1	82	ARG
3	s1	96	LEU
3	s1	97	LEU
3	s1	105	PHE
3	s1	110	LEU
3	s1	120	LEU
3	s1	125	VAL
3	s1	126	THR
3	s1	127	VAL
3	s1	129	THR
3	s1	148	ASN
3	s1	154	SER
3	s1	169	SER
3	s1	173	THR
3	s1	175	GLU
3	s1	180	THR
3	s1	181	LEU
3	s1	184	LEU
3	s1	185	THR
3	s1	193	ILE
3	s1	202	LYS
3	s1	205	PHE
3	s1	212	VAL
3	s1	223	PHE
3	s1	231	LEU
3	s1	232	HIS
4	s2	41	LEU
4	s2	50	ILE
4	s2	52	THR
4	s2	53	ILE
4	s2	55	GLU
4	s2	58	LEU
4	s2	60	SER
4	s2	61	LEU
4	s2	69	ILE
4	s2	72	LEU
4	s2	73	LEU
4	s2	77	GLN
4	s2	80	VAL
4	s2	81	MET
4	s2	83	ILE

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Mol	Chain	Res	Type
4	s2	84	LYS
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	94	GLN
4	s2	95	ARG
4	s2	96	THR
4	s2	97	ARG
4	s2	111	VAL
4	s2	117	THR
4	s2	130	ILE
4	s2	137	ILE
4	s2	139	ILE
4	s2	141	ARG
4	s2	148	LEU
4	s2	153	SER
4	s2	158	THR
4	s2	166	THR
4	s2	170	ILE
4	s2	181	SER
4	s2	194	GLU
4	s2	205	ARG
4	s2	207	LEU
4	s2	210	THR
4	s2	221	THR
4	s2	222	TYR
4	s2	226	THR
4	s2	229	LEU
4	s2	232	GLU
4	s2	233	GLN
4	s2	238	SER
4	s2	245	ASP
4	s2	248	SER
5	s3	4	LEU
5	s3	9	ARG
5	s3	14	ASP
5	s3	21	LEU
5	s3	29	LEU
5	s3	32	GLU
5	s3	34	TYR
5	s3	37	VAL

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Mol	Chain	Res	Type
5	s3	39	VAL
5	s3	44	THR
5	s3	46	THR
5	s3	61	GLU
5	s3	69	LEU
5	s3	70	THR
5	s3	84	ILE
5	s3	90	ARG
5	s3	93	ASP
5	s3	105	MET
5	s3	116	ARG
5	s3	127	MET
5	s3	128	GLU
5	s3	132	LYS
5	s3	139	SER
5	s3	143	ARG
5	s3	146	ARG
5	s3	148	LYS
5	s3	158	ILE
5	s3	159	HIS
5	s3	164	VAL
5	s3	168	ILE
5	s3	172	THR
5	s3	176	LEU
5	s3	189	MET
5	s3	204	ASP
5	s3	212	LYS
5	s3	213	GLU
5	s3	223	LYS
5	s3	224	ASP
6	s4	6	LYS
6	s4	7	LYS
6	s4	12	LEU
6	s4	16	HIS
6	s4	23	LEU
6	s4	30	ARG
6	s4	38	LEU
6	s4	39	ARG
6	s4	41	SER
6	s4	42	LEU
6	s4	45	ILE
6	s4	49	ARG

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Mol	Chain	Res	Type
6	s4	51	ARG
6	s4	70	VAL
6	s4	78	THR
6	s4	89	VAL
6	s4	95	THR
6	s4	98	ASN
6	s4	104	ASP
6	s4	108	ARG
6	s4	116	ASP
6	s4	123	LEU
6	s4	126	VAL
6	s4	128	LYS
6	s4	130	GLN
6	s4	131	LEU
6	s4	146	THR
6	s4	147	ILE
6	s4	148	ARG
6	s4	156	VAL
6	s4	164	LEU
6	s4	170	THR
6	s4	176	ASP
6	s4	180	LEU
6	s4	181	VAL
6	s4	182	TYR
6	s4	184	THR
6	s4	210	ILE
6	s4	214	LEU
6	s4	221	ARG
6	s4	222	LEU
6	s4	246	LEU
7	s5	23	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU
7	s5	38	THR
7	s5	41	LYS
7	s5	45	LYS
7	s5	63	GLN
7	s5	64	VAL
7	s5	68	ILE
7	s5	76	ARG
7	s5	83	ARG

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Mol	Chain	Res	Type
7	s5	86	GLN
7	s5	89	ILE
7	s5	93	LEU
7	s5	100	ASN
7	s5	102	ARG
7	s5	119	ASP
7	s5	122	ASN
7	s5	125	THR
7	s5	128	ASN
7	s5	143	ARG
7	s5	147	THR
7	s5	148	ARG
7	s5	157	ARG
7	s5	162	VAL
7	s5	170	GLN
7	s5	194	LEU
7	s5	203	LYS
7	s5	208	SER
7	s5	216	GLU
7	s5	219	ARG
7	s5	225	ARG
8	s6	17	GLU
8	s6	21	GLU
8	s6	34	GLN
8	s6	64	LYS
8	s6	67	VAL
8	s6	76	LEU
8	s6	81	VAL
8	s6	93	LYS
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU
8	s6	111	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	137	ARG
8	s6	143	LYS
8	s6	153	VAL

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Mol	Chain	Res	Type
8	s6	154	ARG
8	s6	169	TYR
8	s6	177	ARG
8	s6	180	THR
8	s6	182	GLN
8	s6	191	ARG
8	s6	193	LEU
8	s6	215	ARG
9	s7	9	LEU
9	s7	11	GLN
9	s7	15	GLU
9	s7	18	LEU
9	s7	24	PHE
9	s7	28	GLU
9	s7	33	GLU
9	s7	39	ARG
9	s7	50	ASP
9	s7	51	VAL
9	s7	60	ILE
9	s7	67	LEU
9	s7	74	GLN
9	s7	75	THR
9	s7	77	LEU
9	s7	79	ARG
9	s7	80	GLU
9	s7	81	LEU
9	s7	86	GLN
9	s7	87	ASP
9	s7	97	ARG
9	s7	101	LYS
9	s7	112	ARG
9	s7	114	ARG
9	s7	115	SER
9	s7	116	ARG
9	s7	118	LEU
9	s7	123	ASP
9	s7	134	GLU
9	s7	143	LEU
9	s7	144	VAL
9	s7	166	LEU
9	s7	176	LEU
9	s7	185	ILE

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Mol	Chain	Res	Type
10	s8	7	SER
10	s8	20	GLN
10	s8	22	ARG
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	49	ARG
10	s8	54	LYS
10	s8	58	LEU
10	s8	59	ARG
10	s8	61	GLU
10	s8	62	THR
10	s8	74	LYS
10	s8	76	THR
10	s8	77	ARG
10	s8	93	THR
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	158	SER
10	s8	161	SER
10	s8	183	ILE
11	s9	3	ARG
11	s9	7	THR
11	s9	9	SER
11	s9	16	LYS
11	s9	17	ARG
11	s9	21	SER
11	s9	28	LEU
11	s9	37	LYS
11	s9	46	SER
11	s9	49	LEU
11	s9	54	ARG
11	s9	77	ILE
11	s9	78	ARG
11	s9	81	VAL
11	s9	87	SER
11	s9	93	LEU
11	s9	94	ASP

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Mol	Chain	Res	Type
11	s9	96	VAL
11	s9	99	LEU
11	s9	105	LEU
11	s9	109	LEU
11	s9	111	THR
11	s9	113	VAL
11	s9	115	LYS
11	s9	120	LYS
11	s9	126	ARG
11	s9	130	THR
11	s9	132	ARG
11	s9	134	ILE
11	s9	150	LEU
11	s9	161	THR
11	s9	162	SER
11	s9	168	ARG
11	s9	172	VAL
11	s9	180	LYS
11	s9	182	GLU
11	s9	184	SER
12	c0	2	LEU
12	c0	5	LYS
12	c0	15	LEU
12	c0	20	VAL
12	c0	27	PHE
12	c0	28	ASN
12	c0	33	GLU
12	c0	43	ILE
12	c0	47	GLN
12	c0	48	SER
12	c0	55	VAL
12	c0	57	THR
13	c1	2	SER
13	c1	5	LEU
13	c1	10	GLU
13	c1	21	ASN
13	c1	26	LYS
13	c1	30	ARG
13	c1	31	THR
13	c1	32	LYS
13	c1	33	ARG
13	c1	40	LEU

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Mol	Chain	Res	Type
13	c1	44	THR
13	c1	46	LYS
13	c1	52	SER
13	c1	56	LYS
13	c1	60	PHE
13	c1	67	ARG
13	c1	71	LEU
13	c1	76	VAL
13	c1	78	THR
13	c1	79	LYS
13	c1	80	MET
13	c1	109	VAL
13	c1	123	VAL
13	c1	129	ARG
14	c2	30	VAL
14	c2	36	LEU
14	c2	37	VAL
14	c2	43	ARG
14	c2	58	LEU
14	c2	59	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	66	VAL
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	89	ILE
14	c2	103	LEU
14	c2	121	VAL
14	c2	125	ASN
14	c2	132	GLU
14	c2	138	GLU
14	c2	140	PHE
15	c3	6	SER
15	c3	12	SER
15	c3	16	ILE
15	c3	21	ASN
15	c3	25	TRP
15	c3	27	LYS
15	c3	28	LEU
15	c3	29	SER

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Mol	Chain	Res	Type
15	c3	39	LYS
15	c3	48	SER
15	c3	66	ILE
15	c3	67	THR
15	c3	70	LYS
15	c3	76	LYS
15	c3	80	LEU
15	c3	87	ASP
15	c3	93	LYS
15	c3	102	LEU
15	c3	104	ARG
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	138	ASN
16	c4	16	VAL
16	c4	20	TYR
16	c4	24	ASN
16	c4	26	THR
16	c4	28	VAL
16	c4	43	THR
16	c4	49	LYS
16	c4	51	ASP
16	c4	62	LEU
16	c4	79	VAL
16	c4	84	ARG
16	c4	92	LYS
16	c4	93	THR
16	c4	102	LEU
16	c4	107	ARG
16	c4	114	ARG
16	c4	119	THR
16	c4	123	SER
16	c4	124	ASP
16	c4	126	THR
16	c4	127	ARG
16	c4	129	LYS
16	c4	132	ARG
16	c4	133	ARG
16	c4	136	ARG
17	c5	12	PHE
17	c5	24	LYS

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Mol	Chain	Res	Type
17	c5	27	GLU
17	c5	28	MET
17	c5	29	SER
17	c5	34	VAL
17	c5	36	LEU
17	c5	40	ARG
17	c5	49	MET
17	c5	52	LYS
17	c5	69	GLU
17	c5	71	GLU
17	c5	97	TYR
17	c5	102	PHE
17	c5	107	ILE
17	c5	121	ILE
17	c5	124	THR
17	c5	127	ARG
18	c6	12	LYS
18	c6	17	THR
18	c6	23	LYS
18	c6	26	LYS
18	c6	28	LEU
18	c6	37	THR
18	c6	39	VAL
18	c6	40	GLU
18	c6	43	ILE
18	c6	53	LEU
18	c6	57	LEU
18	c6	58	ASP
18	c6	63	ILE
18	c6	68	ARG
18	c6	69	VAL
18	c6	83	GLN
18	c6	94	GLN
18	c6	107	LYS
18	c6	110	THR
18	c6	114	ARG
18	c6	137	ARG
18	c6	143	ARG
19	c7	3	ARG
19	c7	4	VAL
19	c7	6	THR
19	c7	25	THR

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Mol	Chain	Res	Type
19	c7	27	ASP
19	c7	29	GLN
19	c7	34	LEU
19	c7	38	ILE
19	c7	46	LEU
19	c7	47	ARG
19	c7	55	THR
19	c7	62	GLN
19	c7	67	ARG
19	c7	69	ILE
19	c7	72	LYS
19	c7	85	VAL
19	c7	88	VAL
19	c7	106	THR
19	c7	108	ASP
19	c7	110	VAL
19	c7	113	LEU
20	c8	3	LEU
20	c8	4	VAL
20	c8	6	GLN
20	c8	25	ASN
20	c8	27	LYS
20	c8	28	ILE
20	c8	29	VAL
20	c8	33	THR
20	c8	38	VAL
20	c8	40	ARG
20	c8	54	LEU
20	c8	57	ARG
20	c8	61	LEU
20	c8	62	THR
20	c8	63	GLN
20	c8	68	ARG
20	c8	74	GLN
20	c8	77	THR
20	c8	85	PHE
20	c8	94	ASP
20	c8	100	THR
20	c8	105	VAL
20	c8	116	LEU
20	c8	119	ILE
20	c8	120	ARG

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Mol	Chain	Res	Type
20	c8	131	LEU
20	c8	133	VAL
20	c8	138	THR
20	c8	141	THR
21	c9	27	LYS
21	c9	28	LEU
21	c9	29	GLU
21	c9	37	VAL
21	c9	41	SER
21	c9	57	ARG
21	c9	68	ARG
21	c9	70	GLN
21	c9	71	VAL
21	c9	86	ARG
21	c9	88	VAL
21	c9	89	ARG
21	c9	111	ILE
21	c9	123	ARG
21	c9	132	LEU
21	c9	139	THR
21	c9	140	LEU
21	c9	141	GLU
21	c9	142	GLU
21	c9	143	ASP
22	d0	13	GLU
22	d0	16	GLN
22	d0	22	ILE
22	d0	24	ILE
22	d0	27	THR
22	d0	31	VAL
22	d0	34	LEU
22	d0	44	ASN
22	d0	46	GLU
22	d0	47	GLN
22	d0	51	VAL
22	d0	57	ARG
22	d0	61	LYS
22	d0	63	LEU
22	d0	70	THR
22	d0	72	ASN
22	d0	74	GLU
22	d0	76	SER

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Mol	Chain	Res	Type
22	d0	88	LYS
22	d0	98	GLN
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	105	GLN
22	d0	107	THR
22	d0	108	ILE
22	d0	114	VAL
22	d0	115	GLU
22	d0	121	ASN
23	d1	1	MET
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	17	CYS
23	d1	18	SER
23	d1	31	SER
23	d1	32	VAL
23	d1	34	ILE
23	d1	38	LYS
23	d1	41	GLU
23	d1	50	TYR
23	d1	52	THR
23	d1	62	ARG
23	d1	74	GLN
23	d1	78	LEU
23	d1	81	ASN
23	d1	85	TYR
24	d2	6	VAL
24	d2	7	LEU
24	d2	25	VAL
24	d2	26	LEU
24	d2	27	ILE
24	d2	33	VAL
24	d2	56	HIS
24	d2	65	LEU
24	d2	70	ASN
24	d2	86	ILE

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Mol	Chain	Res	Type
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	104	LEU
24	d2	117	ARG
24	d2	125	ILE
24	d2	128	PHE
24	d2	129	VAL
25	d3	9	LEU
25	d3	14	LYS
25	d3	16	ARG
25	d3	17	VAL
25	d3	19	ARG
25	d3	27	ASN
25	d3	29	TYR
25	d3	33	LEU
25	d3	52	ILE
25	d3	73	ARG
25	d3	75	GLN
25	d3	83	VAL
25	d3	84	THR
25	d3	94	ASN
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	109	ARG
25	d3	125	VAL
25	d3	133	LEU
25	d3	138	GLU
26	d4	2	SER
26	d4	8	ARG
26	d4	12	VAL
26	d4	21	LYS
26	d4	26	ASP
26	d4	43	LYS
26	d4	44	LEU
26	d4	47	VAL
26	d4	49	LYS
26	d4	51	GLU
26	d4	55	VAL
26	d4	62	THR
26	d4	77	ASN

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Mol	Chain	Res	Type
26	d4	88	THR
26	d4	92	VAL
26	d4	105	ARG
26	d4	107	GLN
26	d4	114	ARG
26	d4	121	THR
26	d4	128	LYS
26	d4	132	ARG
26	d4	133	ASN
27	d5	41	ILE
27	d5	42	LEU
27	d5	43	ASP
27	d5	46	LYS
27	d5	57	TYR
27	d5	60	VAL
27	d5	63	SER
27	d5	68	ARG
27	d5	81	ARG
27	d5	88	ILE
27	d5	92	ILE
27	d5	93	SER
28	d6	5	ARG
28	d6	10	ARG
28	d6	18	VAL
28	d6	26	CYS
28	d6	28	LYS
28	d6	38	ARG
28	d6	41	ILE
28	d6	43	ASN
28	d6	46	GLU
28	d6	51	ARG
28	d6	53	LEU
28	d6	55	GLU
28	d6	76	SER
28	d6	82	ARG
28	d6	89	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	5	GLN
29	d7	14	SER
29	d7	26	GLN
29	d7	36	LYS

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Mol	Chain	Res	Type
29	d7	43	ILE
29	d7	45	THR
29	d7	46	VAL
29	d7	48	SER
29	d7	56	CYS
29	d7	72	LYS
29	d7	77	THR
30	d8	5	THR
30	d8	13	ILE
30	d8	16	LEU
30	d8	19	THR
30	d8	22	ARG
30	d8	26	THR
30	d8	30	VAL
30	d8	32	PHE
30	d8	33	LEU
30	d8	54	LEU
30	d8	64	ARG
30	d8	65	ARG
30	d8	66	LEU
31	d9	10	HIS
31	d9	12	ARG
31	d9	21	CYS
31	d9	28	THR
31	d9	30	LEU
31	d9	36	LEU
31	d9	40	ARG
31	d9	42	CYS
31	d9	54	LYS
80	e0	14	VAL
80	e0	21	VAL
80	e0	22	GLU
80	e0	24	THR
80	e0	29	LYS
80	e0	44	PHE
80	e0	45	VAL
80	e0	46	ASN
80	e0	49	LEU
80	e0	56	MET
33	e1	78	LYS
33	e1	80	ARG
33	e1	87	THR

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Mol	Chain	Res	Type
33	e1	89	LYS
33	e1	90	LYS
33	e1	96	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	109	ASP
33	e1	113	LYS
33	e1	119	ARG
33	e1	120	GLU
33	e1	135	HIS
33	e1	147	VAL
33	e1	148	TYR
33	e1	151	ASN
34	sR	10	ARG
34	sR	29	GLN
34	sR	32	LEU
34	sR	58	VAL
34	sR	65	SER
34	sR	66	HIS
34	sR	70	ASP
34	sR	76	ASP
34	sR	96	THR
34	sR	104	VAL
34	sR	106	HIS
34	sR	123	ILE
34	sR	131	ILE
34	sR	145	LEU
34	sR	149	ASP
34	sR	176	LYS
34	sR	178	VAL
34	sR	184	ASN
34	sR	207	ASP
34	sR	222	LEU
34	sR	228	LYS
34	sR	232	TYR
34	sR	242	SER
34	sR	258	THR
34	sR	270	LEU
34	sR	275	ARG
34	sR	286	GLU
34	sR	300	THR

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Mol	Chain	Res	Type
34	sR	309	VAL
34	sR	310	ILE
34	sR	319	ASN
35	sM	27	LYS
35	sM	41	SER
35	sM	43	ASP
35	sM	45	SER
35	sM	55	SER
35	sM	61	ILE
35	sM	68	ARG
35	sM	74	LYS
35	sM	75	ASP
35	sM	77	THR
39	l2	23	ARG
39	l2	32	LEU
39	l2	41	ILE
39	l2	44	ILE
39	l2	45	VAL
39	l2	46	LYS
39	l2	48	ILE
39	l2	49	VAL
39	l2	62	VAL
39	l2	70	ARG
39	l2	74	GLU
39	l2	82	VAL
39	l2	96	LEU
39	l2	97	ASN
39	l2	101	VAL
39	l2	114	SER
39	l2	116	VAL
39	l2	119	LYS
39	l2	134	VAL
39	l2	137	ILE
39	l2	142	ASP
39	l2	147	ARG
39	l2	155	LYS
39	l2	157	VAL
39	l2	161	ASP
39	l2	169	ILE
39	l2	177	LYS
39	l2	188	LYS
39	l2	193	ARG

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Mol	Chain	Res	Type
39	12	200	ARG
39	12	227	ARG
39	12	230	VAL
39	12	243	THR
39	12	246	LEU
39	12	250	GLN
40	13	5	LYS
40	13	7	GLU
40	13	10	ARG
40	13	17	LEU
40	13	19	ARG
40	13	28	ARG
40	13	37	ARG
40	13	44	THR
40	13	47	LEU
40	13	50	LYS
40	13	55	THR
40	13	56	ILE
40	13	69	LYS
40	13	70	ARG
40	13	73	VAL
40	13	81	THR
40	13	85	VAL
40	13	103	THR
40	13	111	SER
40	13	114	VAL
40	13	125	SER
40	13	139	GLN
40	13	140	ASP
40	13	145	GLU
40	13	146	ARG
40	13	150	ARG
40	13	160	VAL
40	13	167	ARG
40	13	169	THR
40	13	178	LEU
40	13	183	LEU
40	13	188	ILE
40	13	191	LYS
40	13	196	ARG
40	13	202	THR
40	13	205	VAL

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Mol	Chain	Res	Type
40	13	211	GLN
40	13	212	ASN
40	13	213	GLU
40	13	221	THR
40	13	232	ARG
40	13	238	LEU
40	13	244	ARG
40	13	248	LYS
40	13	252	ILE
40	13	266	ARG
40	13	274	SER
40	13	276	THR
40	13	282	ILE
40	13	284	ARG
40	13	287	LYS
40	13	297	SER
40	13	302	LYS
40	13	304	THR
40	13	308	MET
40	13	319	ASN
40	13	323	MET
40	13	324	VAL
40	13	328	ILE
40	13	332	ARG
40	13	336	VAL
40	13	338	LEU
40	13	339	ARG
40	13	340	LYS
40	13	347	SER
40	13	354	VAL
40	13	359	ILE
40	13	363	SER
40	13	364	LYS
40	13	382	THR
40	13	384	LYS
41	14	6	VAL
41	14	14	GLU
41	14	42	VAL
41	14	47	ARG
41	14	64	SER
41	14	67	THR
41	14	75	PRO

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Mol	Chain	Res	Type
41	14	93	MET
41	14	99	MET
41	14	114	ASN
41	14	118	LYS
41	14	133	SER
41	14	136	LEU
41	14	138	ARG
41	14	144	LYS
41	14	145	ILE
41	14	150	LEU
41	14	152	VAL
41	14	156	LEU
41	14	158	SER
41	14	160	GLN
41	14	163	LYS
41	14	172	VAL
41	14	177	ASP
41	14	179	LEU
41	14	180	LYS
41	14	183	LYS
41	14	186	LYS
41	14	187	LEU
41	14	195	ARG
41	14	200	THR
41	14	203	ARG
41	14	206	LEU
41	14	222	VAL
41	14	229	ASN
41	14	230	VAL
41	14	244	LEU
41	14	246	ARG
41	14	256	THR
41	14	258	LEU
41	14	265	GLU
41	14	276	LEU
41	14	283	THR
41	14	292	SER
41	14	299	ILE
41	14	300	ARG
41	14	301	PRO
41	14	306	THR
41	14	307	GLN

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Mol	Chain	Res	Type
41	14	319	LYS
41	14	322	GLN
41	14	327	LEU
41	14	338	LYS
41	14	341	SER
41	14	342	LYS
41	14	345	GLU
41	14	347	THR
41	14	356	THR
41	14	357	GLU
41	14	358	THR
41	14	359	LEU
42	15	5	LYS
42	15	6	ASP
42	15	10	SER
42	15	13	SER
42	15	27	LYS
42	15	34	LYS
42	15	45	ASN
42	15	51	LEU
42	15	65	ILE
42	15	66	SER
42	15	68	THR
42	15	70	THR
42	15	75	LEU
42	15	81	HIS
42	15	84	PRO
42	15	89	THR
42	15	110	LEU
42	15	112	LYS
42	15	118	THR
42	15	120	LYS
42	15	128	GLU
42	15	140	ARG
42	15	144	VAL
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	183	TRP

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Mol	Chain	Res	Type
42	15	185	PHE
42	15	187	THR
42	15	194	LEU
42	15	211	LEU
42	15	214	ASP
42	15	234	ASP
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS
42	15	264	GLN
42	15	268	GLU
42	15	277	LEU
42	15	282	ARG
43	16	2	SER
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	52	VAL
43	16	64	LEU
43	16	65	ILE
43	16	76	LEU
43	16	78	ARG
43	16	79	VAL
43	16	84	VAL
43	16	89	THR
43	16	93	VAL
43	16	98	VAL
43	16	108	LYS
43	16	131	LYS
43	16	152	THR
43	16	155	LEU
43	16	170	LYS
43	16	173	MET
44	17	26	VAL
44	17	41	ARG
44	17	45	LEU
44	17	46	GLU
44	17	60	ARG
44	17	77	VAL

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Mol	Chain	Res	Type
44	17	83	LEU
44	17	93	ASN
44	17	98	LYS
44	17	101	LYS
44	17	121	LYS
44	17	124	LEU
44	17	130	ILE
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	184	LEU
44	17	196	LYS
44	17	219	LYS
44	17	229	PHE
44	17	234	GLU
44	17	239	LEU
44	17	244	ASN
45	18	26	LEU
45	18	41	GLN
45	18	47	SER
45	18	49	TYR
45	18	50	VAL
45	18	63	LYS
45	18	68	ARG
45	18	71	VAL
45	18	74	THR
45	18	79	GLN
45	18	89	GLU
45	18	90	THR
45	18	95	ASN
45	18	109	LEU
45	18	136	LEU
45	18	146	LYS
45	18	149	LYS
45	18	160	ILE
45	18	163	VAL
45	18	164	VAL
45	18	172	LYS

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Mol	Chain	Res	Type
45	18	191	ASN
45	18	197	VAL
45	18	214	LEU
45	18	217	THR
45	18	224	ASP
45	18	241	LYS
45	18	245	LYS
45	18	248	LYS
46	19	1	MET
46	19	5	GLN
46	19	16	VAL
46	19	17	THR
46	19	18	VAL
46	19	20	ILE
46	19	23	ARG
46	19	28	VAL
46	19	31	ARG
46	19	33	THR
46	19	39	LYS
46	19	41	ILE
46	19	44	THR
46	19	46	THR
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	77	ASN
46	19	80	THR
46	19	82	VAL
46	19	90	MET
46	19	92	TYR
46	19	105	GLU
46	19	106	LYS
46	19	107	ASP
46	19	118	LEU
46	19	124	ARG
46	19	129	ARG
46	19	132	VAL
46	19	133	THR

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Mol	Chain	Res	Type
46	l9	138	THR
46	l9	143	GLU
46	l9	144	ILE
46	l9	151	VAL
46	l9	157	ASN
46	l9	161	LEU
46	l9	162	GLN
46	l9	166	ARG
46	l9	170	LYS
46	l9	173	ARG
46	l9	177	ASP
46	l9	188	THR
47	m0	3	ARG
47	m0	24	ARG
47	m0	29	SER
47	m0	36	LEU
47	m0	39	LYS
47	m0	42	THR
47	m0	48	LEU
47	m0	52	LEU
47	m0	58	GLU
47	m0	63	GLU
47	m0	71	CYS
47	m0	74	LYS
47	m0	78	THR
47	m0	87	LEU
47	m0	143	SER
47	m0	144	ASN
47	m0	154	ARG
47	m0	162	GLN
47	m0	169	LYS
47	m0	176	LEU
47	m0	177	ASP
47	m0	189	GLU
47	m0	193	ASP
47	m0	200	LEU
47	m0	206	LEU
47	m0	211	ARG
47	m0	212	GLU
48	m1	6	GLN
48	m1	10	ARG
48	m1	12	LEU

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Mol	Chain	Res	Type
48	m1	13	LYS
48	m1	18	VAL
48	m1	23	VAL
48	m1	30	LEU
48	m1	35	LYS
48	m1	41	SER
48	m1	44	THR
48	m1	46	VAL
48	m1	47	GLN
48	m1	54	VAL
48	m1	55	ARG
48	m1	56	THR
48	m1	65	ILE
48	m1	80	LEU
48	m1	82	ARG
48	m1	92	ARG
48	m1	94	ARG
48	m1	106	ILE
48	m1	107	ASP
48	m1	112	LEU
48	m1	114	ILE
48	m1	119	SER
48	m1	122	ILE
48	m1	140	ARG
48	m1	142	LYS
48	m1	152	HIS
48	m1	153	LYS
48	m1	154	THR
48	m1	159	THR
48	m1	161	SER
48	m1	166	LYS
49	m3	52	ASP
49	m3	53	LEU
49	m3	54	LEU
49	m3	58	VAL
49	m3	62	THR
49	m3	67	ARG
49	m3	68	LYS
49	m3	73	ARG
49	m3	76	THR
49	m3	80	VAL
49	m3	107	GLU

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Mol	Chain	Res	Type
49	m3	118	GLU
49	m3	122	LYS
49	m3	123	ILE
49	m3	124	ILE
49	m3	131	LYS
49	m3	138	VAL
49	m3	147	ILE
49	m3	149	GLN
49	m3	152	THR
49	m3	153	ASP
49	m3	154	VAL
49	m3	157	ARG
49	m3	164	GLU
49	m3	168	ARG
49	m3	171	ARG
49	m3	184	GLU
50	m4	3	THR
50	m4	4	ASP
50	m4	5	SER
50	m4	6	ILE
50	m4	8	LYS
50	m4	15	VAL
50	m4	16	GLU
50	m4	23	ILE
50	m4	31	LYS
50	m4	37	GLU
50	m4	41	GLN
50	m4	42	LYS
50	m4	50	LYS
50	m4	53	VAL
50	m4	60	LEU
50	m4	63	VAL
50	m4	64	VAL
50	m4	80	THR
50	m4	98	SER
50	m4	109	ARG
50	m4	113	THR
50	m4	119	GLN
50	m4	124	ARG
50	m4	128	ARG
50	m4	135	LEU
51	m5	5	LYS

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Mol	Chain	Res	Type
51	m5	10	LEU
51	m5	15	GLN
51	m5	22	LEU
51	m5	44	ARG
51	m5	50	ARG
51	m5	66	VAL
51	m5	67	ARG
51	m5	73	ARG
51	m5	76	PRO
51	m5	80	THR
51	m5	83	LYS
51	m5	92	LEU
51	m5	96	ARG
51	m5	98	LEU
51	m5	105	ARG
51	m5	106	VAL
51	m5	135	VAL
51	m5	138	GLN
51	m5	153	ASP
51	m5	159	ARG
51	m5	165	THR
51	m5	171	SER
51	m5	176	LYS
51	m5	178	HIS
51	m5	188	ARG
51	m5	190	THR
51	m5	194	GLN
51	m5	196	THR
51	m5	198	SER
51	m5	204	LYS
52	m6	3	VAL
52	m6	4	GLU
52	m6	12	LYS
52	m6	22	VAL
52	m6	34	VAL
52	m6	36	VAL
52	m6	40	GLU
52	m6	41	LEU
52	m6	46	GLU
52	m6	66	LYS
52	m6	67	THR
52	m6	74	ARG

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Mol	Chain	Res	Type
52	m6	78	ARG
52	m6	84	LEU
52	m6	100	GLU
52	m6	103	LYS
52	m6	106	GLU
52	m6	108	ILE
52	m6	110	PRO
52	m6	115	LYS
52	m6	116	LYS
52	m6	117	ARG
52	m6	124	LEU
52	m6	128	ARG
52	m6	129	LEU
52	m6	134	LYS
52	m6	143	THR
52	m6	152	VAL
52	m6	170	LYS
52	m6	171	LYS
52	m6	175	THR
52	m6	182	ASN
52	m6	190	VAL
52	m6	192	LYS
52	m6	197	LEU
53	m7	3	ARG
53	m7	7	THR
53	m7	9	THR
53	m7	13	LYS
53	m7	24	VAL
53	m7	29	THR
53	m7	32	THR
53	m7	42	THR
53	m7	56	ARG
53	m7	61	ARG
53	m7	69	ARG
53	m7	70	THR
53	m7	78	VAL
53	m7	79	THR
53	m7	89	LYS
53	m7	103	GLU
53	m7	105	LYS
53	m7	107	LEU
53	m7	112	LEU

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Mol	Chain	Res	Type
53	m7	119	VAL
53	m7	120	ASN
53	m7	121	GLN
53	m7	127	ARG
53	m7	128	ARG
53	m7	131	ARG
53	m7	136	ILE
53	m7	142	SER
53	m7	144	SER
53	m7	148	LEU
53	m7	153	LYS
53	m7	155	GLU
54	m8	7	SER
54	m8	12	ARG
54	m8	17	THR
54	m8	21	SER
54	m8	24	VAL
54	m8	26	LEU
54	m8	31	LYS
54	m8	32	LEU
54	m8	34	THR
54	m8	39	ARG
54	m8	41	ASP
54	m8	49	LEU
54	m8	57	ILE
54	m8	63	SER
54	m8	64	VAL
54	m8	66	ARG
54	m8	69	ARG
54	m8	80	THR
54	m8	81	VAL
54	m8	86	THR
54	m8	93	ILE
54	m8	113	LYS
54	m8	127	LEU
54	m8	135	GLN
54	m8	136	ASN
54	m8	138	LEU
54	m8	146	SER
54	m8	147	ARG
54	m8	161	LYS
54	m8	166	LEU

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Mol	Chain	Res	Type
54	m8	178	ARG
54	m8	179	ARG
55	m9	7	GLN
55	m9	9	ARG
55	m9	10	LEU
55	m9	14	VAL
55	m9	17	VAL
55	m9	29	THR
55	m9	36	ASN
55	m9	43	LYS
55	m9	52	LYS
55	m9	57	VAL
55	m9	59	SER
55	m9	63	THR
55	m9	74	ARG
55	m9	88	ARG
55	m9	99	LEU
55	m9	127	SER
55	m9	128	LYS
55	m9	139	VAL
55	m9	152	GLU
55	m9	153	LYS
55	m9	156	ASN
55	m9	164	LEU
55	m9	165	LYS
55	m9	167	ARG
55	m9	173	ARG
55	m9	177	VAL
56	n0	8	GLN
56	n0	13	ARG
56	n0	16	THR
56	n0	18	SER
56	n0	23	LYS
56	n0	45	LEU
56	n0	52	LYS
56	n0	70	THR
56	n0	73	LYS
56	n0	74	ASN
56	n0	80	ARG
56	n0	81	TYR
56	n0	82	ASP
56	n0	87	THR

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Mol	Chain	Res	Type
56	n0	92	LYS
56	n0	97	VAL
56	n0	99	ARG
56	n0	100	VAL
56	n0	104	GLU
56	n0	105	THR
56	n0	115	ARG
56	n0	117	ARG
56	n0	125	LYS
56	n0	130	GLU
56	n0	137	ARG
56	n0	145	THR
56	n0	148	LEU
56	n0	150	PHE
56	n0	153	PRO
56	n0	155	ARG
56	n0	157	GLN
56	n0	160	THR
56	n0	161	LYS
56	n0	162	THR
56	n0	167	ARG
56	n0	172	TYR
57	n1	9	SER
57	n1	12	ARG
57	n1	17	ARG
57	n1	21	LYS
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	32	LYS
57	n1	38	ASP
57	n1	52	MET
57	n1	68	THR
57	n1	80	VAL
57	n1	83	ARG
57	n1	86	GLU
57	n1	92	ARG
57	n1	93	VAL
57	n1	96	ILE
57	n1	97	LYS
57	n1	102	ARG
57	n1	104	GLU

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Mol	Chain	Res	Type
57	n1	118	GLU
57	n1	124	VAL
57	n1	126	VAL
57	n1	128	LEU
57	n1	130	ARG
57	n1	131	GLN
57	n1	139	ARG
57	n1	143	THR
57	n1	150	THR
57	n1	158	THR
57	n1	160	ILE
58	n2	13	LYS
58	n2	16	THR
58	n2	17	VAL
58	n2	27	VAL
58	n2	37	LEU
58	n2	43	VAL
58	n2	47	VAL
58	n2	50	LEU
58	n2	63	VAL
58	n2	66	VAL
58	n2	68	THR
58	n2	75	TYR
58	n2	90	ARG
58	n2	96	VAL
59	n3	7	GLN
59	n3	13	ILE
59	n3	40	LYS
59	n3	45	ARG
59	n3	48	ARG
59	n3	66	LYS
59	n3	69	LEU
59	n3	70	ARG
59	n3	71	LYS
59	n3	74	MET
59	n3	77	ILE
59	n3	88	ARG
59	n3	102	ILE
59	n3	115	THR
59	n3	131	SER
59	n3	135	VAL
60	n4	1	MET

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Mol	Chain	Res	Type
60	n4	5	ILE
60	n4	19	THR
60	n4	39	LEU
60	n4	54	LEU
60	n4	57	LYS
60	n4	58	HIS
60	n4	63	ILE
60	n4	82	ILE
60	n4	89	LEU
60	n4	96	LEU
60	n4	97	LYS
60	n4	98	PRO
60	n4	100	VAL
60	n4	104	ASN
60	n4	116	LYS
60	n4	119	GLU
60	n4	126	GLU
60	n4	127	LYS
60	n4	134	GLN
61	n5	24	LEU
61	n5	27	ARG
61	n5	33	ARG
61	n5	37	THR
61	n5	48	SER
61	n5	56	ARG
61	n5	57	LEU
61	n5	65	GLN
61	n5	71	THR
61	n5	86	VAL
61	n5	102	LEU
61	n5	115	ARG
61	n5	117	ASN
61	n5	124	VAL
61	n5	135	ILE
62	n6	10	SER
62	n6	12	ARG
62	n6	13	ARG
62	n6	14	LYS
62	n6	17	LYS
62	n6	32	SER
62	n6	37	LYS
62	n6	45	ILE

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Mol	Chain	Res	Type
62	n6	50	ILE
62	n6	51	ARG
62	n6	56	VAL
62	n6	57	LEU
62	n6	66	GLN
62	n6	74	TYR
62	n6	76	LEU
62	n6	90	VAL
62	n6	94	SER
62	n6	97	ILE
62	n6	113	LYS
62	n6	120	GLN
63	n7	3	LYS
63	n7	14	VAL
63	n7	15	ARG
63	n7	17	ARG
63	n7	24	VAL
63	n7	28	PRO
63	n7	33	SER
63	n7	34	LYS
63	n7	46	ILE
63	n7	47	GLU
63	n7	52	LYS
63	n7	72	ILE
63	n7	73	LYS
63	n7	75	VAL
63	n7	77	TYR
63	n7	81	LEU
63	n7	83	THR
63	n7	86	THR
63	n7	93	LYS
63	n7	95	VAL
63	n7	97	SER
63	n7	98	THR
63	n7	100	THR
63	n7	102	GLU
63	n7	103	GLN
63	n7	105	SER
63	n7	126	LYS
63	n7	134	LEU
63	n7	135	ARG
64	n8	3	SER

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Mol	Chain	Res	Type
64	n8	6	THR
64	n8	8	THR
64	n8	10	LYS
64	n8	15	VAL
64	n8	22	ILE
64	n8	24	LYS
64	n8	25	HIS
64	n8	26	ARG
64	n8	27	LYS
64	n8	34	MET
64	n8	42	ARG
64	n8	47	LYS
64	n8	60	TYR
64	n8	73	LEU
64	n8	78	LEU
64	n8	81	LEU
64	n8	88	ASP
64	n8	91	LEU
64	n8	98	THR
64	n8	123	VAL
64	n8	124	ILE
64	n8	128	ARG
64	n8	132	LYS
64	n8	133	LEU
65	n9	3	LYS
65	n9	12	GLN
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	27	TYR
65	n9	38	LYS
65	n9	40	ARG
65	n9	54	LEU
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	12	GLN
66	o0	17	VAL
66	o0	19	LYS

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Mol	Chain	Res	Type
66	o0	40	LYS
66	o0	44	ILE
66	o0	48	THR
66	o0	50	VAL
66	o0	52	ARG
66	o0	56	LEU
66	o0	61	MET
66	o0	68	TYR
66	o0	74	ASN
66	o0	76	GLU
66	o0	83	LYS
66	o0	86	ARG
66	o0	87	VAL
66	o0	99	ASP
66	o0	101	LEU
67	o1	6	ASP
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	28	ARG
67	o1	31	ARG
67	o1	34	LYS
67	o1	35	GLU
67	o1	44	MET
67	o1	46	THR
67	o1	51	LEU
67	o1	64	VAL
67	o1	68	GLU
67	o1	73	LEU
67	o1	76	SER
67	o1	83	GLU
67	o1	84	ASP
67	o1	89	LEU
67	o1	91	SER
67	o1	93	VAL
67	o1	97	LEU
67	o1	100	SER
67	o1	102	LYS
67	o1	106	THR
67	o1	107	VAL
67	o1	110	GLU

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Mol	Chain	Res	Type
67	o1	112	ASP
68	o2	8	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	44	ARG
68	o2	51	SER
68	o2	54	LYS
68	o2	61	LYS
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	84	THR
68	o2	87	MET
68	o2	91	THR
68	o2	95	GLU
68	o2	113	LYS
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	14	LEU
69	o3	15	SER
69	o3	31	LYS
69	o3	37	THR
69	o3	70	LYS
69	o3	74	THR
69	o3	81	VAL
69	o3	84	THR
69	o3	86	ARG
69	o3	92	LYS
69	o3	93	THR
70	o4	5	VAL
70	o4	17	SER
70	o4	19	LYS
70	o4	20	ILE
70	o4	21	LYS
70	o4	22	VAL
70	o4	23	VAL
70	o4	25	THR

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Mol	Chain	Res	Type
70	o4	30	LEU
70	o4	31	ARG
70	o4	46	ASP
70	o4	57	LEU
70	o4	58	ARG
70	o4	71	THR
70	o4	87	GLU
70	o4	98	GLN
70	o4	104	VAL
71	o5	4	VAL
71	o5	11	THR
71	o5	20	GLN
71	o5	27	GLU
71	o5	30	GLU
71	o5	31	LEU
71	o5	36	LEU
71	o5	37	SER
71	o5	38	ARG
71	o5	45	LYS
71	o5	46	THR
71	o5	47	VAL
71	o5	49	LYS
71	o5	62	GLN
71	o5	68	GLN
71	o5	69	LEU
71	o5	79	ASP
71	o5	81	ARG
71	o5	85	THR
71	o5	89	ARG
71	o5	90	ARG
71	o5	100	VAL
71	o5	101	THR
71	o5	107	LYS
71	o5	108	GLN
71	o5	113	GLN
72	o6	3	VAL
72	o6	7	ILE
72	o6	9	ILE
72	o6	21	THR
72	o6	26	ILE
72	o6	29	LYS
72	o6	35	ASN

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Mol	Chain	Res	Type
72	o6	36	ARG
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	60	LEU
72	o6	67	LYS
72	o6	68	ARG
72	o6	74	LYS
72	o6	76	ARG
72	o6	79	SER
72	o6	81	THR
72	o6	87	VAL
72	o6	88	GLU
72	o6	90	MET
72	o6	94	ILE
72	o6	98	ARG
73	o7	17	THR
73	o7	33	THR
73	o7	36	SER
73	o7	44	THR
73	o7	54	LYS
73	o7	65	ARG
73	o7	68	LYS
73	o7	80	THR
74	o8	8	ILE
74	o8	12	LEU
74	o8	14	LEU
74	o8	15	THR
74	o8	17	ARG
74	o8	19	ASP
74	o8	20	VAL
74	o8	24	THR
74	o8	41	THR
74	o8	50	SER
74	o8	53	THR
74	o8	64	LYS
74	o8	65	LEU
74	o8	72	THR
75	o9	4	GLN
75	o9	6	SER
75	o9	15	LYS
75	o9	17	LYS

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Mol	Chain	Res	Type
75	o9	21	ARG
75	o9	27	ILE
75	o9	34	THR
75	o9	45	ARG
75	o9	46	ARG
75	o9	47	THR
75	o9	48	LYS
76	q0	78	ILE
76	q0	79	GLU
76	q0	80	PRO
76	q0	85	LEU
76	q0	88	LYS
76	q0	91	CYS
76	q0	97	ARG
76	q0	106	ARG
76	q0	108	THR
76	q0	112	LYS
76	q0	113	ARG
76	q0	126	LYS
76	q0	127	LEU
77	q1	4	LYS
77	q1	6	ARG
77	q1	10	THR
77	q1	11	ARG
77	q1	13	LEU
77	q1	14	LYS
77	q1	18	ARG
77	q1	21	ARG
77	q1	23	ARG
78	q2	6	LYS
78	q2	7	THR
78	q2	8	ARG
78	q2	13	LYS
78	q2	16	THR
78	q2	35	LEU
78	q2	41	ARG
78	q2	44	ASP
78	q2	45	ARG
78	q2	46	LYS
78	q2	47	GLN
78	q2	61	LYS
78	q2	71	ARG

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Mol	Chain	Res	Type
78	q2	78	LYS
78	q2	79	THR
78	q2	80	ARG
78	q2	83	LEU
78	q2	84	THR
78	q2	93	LEU
78	q2	100	LYS
78	q2	104	LEU
78	q2	105	GLN
79	q3	3	LYS
79	q3	8	VAL
79	q3	33	GLN
79	q3	40	SER
79	q3	42	CYS
79	q3	48	LYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	58	SER
79	q3	70	THR
79	q3	90	VAL
82	p0	4	ILE
82	p0	5	ARG
82	p0	7	LYS
82	p0	17	GLU
82	p0	30	VAL
82	p0	44	GLU
82	p0	48	ARG
82	p0	51	VAL
82	p0	67	LEU
82	p0	70	LEU
82	p0	72	ASP
82	p0	74	GLU
82	p0	76	LEU
82	p0	80	VAL
82	p0	93	LEU
82	p0	97	LYS
82	p0	104	ARG
82	p0	185	LEU
82	p0	192	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
2	S0	163	ASN
3	S1	157	GLN
3	S1	177	GLN
3	S1	232	HIS
4	S2	89	GLN
8	S6	34	GLN
10	S8	138	ASN
11	S9	110	GLN
18	C6	83	GLN
19	C7	105	GLN
21	C9	70	GLN
22	D0	17	GLN
23	D1	74	GLN
25	D3	79	ASN
34	SR	153	GLN
34	SR	159	ASN
34	SR	198	ASN
39	L2	83	HIS
41	L4	311	HIS
42	L5	40	HIS
45	L8	38	GLN
46	L9	37	ASN
51	M5	194	GLN
59	N3	98	ASN
59	N3	104	ASN
65	N9	45	HIS
68	O2	88	HIS
75	O9	32	ASN
78	Q2	82	GLN
3	s1	208	GLN
3	s1	209	ASN
3	s1	211	HIS
9	s7	11	GLN
9	s7	71	HIS
11	s9	124	HIS
11	s9	133	HIS
17	c5	114	HIS
21	c9	64	HIS
23	d1	3	ASN
24	d2	113	HIS
26	d4	22	GLN
29	d7	42	ASN
33	e1	93	HIS

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Mol	Chain	Res	Type
34	sR	182	ASN
35	sM	71	ASN
39	l2	233	GLN
42	l5	57	ASN
42	l5	81	HIS
44	l7	64	GLN
46	l9	49	ASN
46	l9	51	GLN
47	m0	55	ASN
47	m0	144	ASN
47	m0	175	ASN
52	m6	31	GLN
55	m9	7	GLN
59	n3	132	ASN
64	n8	25	HIS
64	n8	44	ASN
64	n8	49	HIS
76	q0	119	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	487 (27%)	58 (3%)
1	6	1793/1800 (99%)	477 (26%)	48 (2%)
36	1	3145/3396 (92%)	709 (22%)	82 (2%)
36	5	3146/3396 (92%)	741 (23%)	85 (2%)
37	3	120/121 (99%)	21 (17%)	1 (0%)
37	7	120/121 (99%)	20 (16%)	1 (0%)
38	4	157/158 (99%)	41 (26%)	2 (1%)
38	8	157/158 (99%)	34 (21%)	2 (1%)
All	All	10385/10950 (94%)	2530 (24%)	279 (2%)

All (2530) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	27	U

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Mol	Chain	Res	Type
1	2	34	G
1	2	40	A
1	2	41	A
1	2	42	G
1	2	45	U
1	2	46	A
1	2	47	A
1	2	57	G
1	2	59	C
1	2	60	U
1	2	63	G
1	2	66	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	104	A
1	2	114	C
1	2	116	U
1	2	121	U
1	2	127	G
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	149	C
1	2	153	G
1	2	158	U
1	2	159	U
1	2	169	A

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Mol	Chain	Res	Type
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	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	236	A
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	250	C
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	273	G
1	2	275	C

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Mol	Chain	Res	Type
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	284	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	309	C
1	2	314	C
1	2	316	A
1	2	317	C
1	2	319	U
1	2	321	C
1	2	322	G
1	2	337	G
1	2	338	C
1	2	351	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	363	G
1	2	381	C
1	2	387	A
1	2	390	G
1	2	397	A
1	2	399	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
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	437	A

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Mol	Chain	Res	Type
1	2	439	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	450	U
1	2	454	U
1	2	468	A
1	2	484	C
1	2	485	A
1	2	488	G
1	2	489	C
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	519	C
1	2	527	A
1	2	532	U
1	2	534	A
1	2	537	G
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A

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Mol	Chain	Res	Type
1	2	543	C
1	2	544	A
1	2	546	U
1	2	548	G
1	2	555	A
1	2	556	A
1	2	558	U
1	2	559	C
1	2	565	C
1	2	579	A
1	2	580	A
1	2	583	C
1	2	594	A
1	2	595	G
1	2	609	U
1	2	610	G
1	2	619	A
1	2	620	A
1	2	621	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	630	A
1	2	639	U
1	2	649	U
1	2	650	U
1	2	653	C
1	2	654	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	692	C
1	2	694	U
1	2	695	U

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Mol	Chain	Res	Type
1	2	696	C
1	2	697	C
1	2	700	C
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	743	U
1	2	745	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G

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Mol	Chain	Res	Type
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	793	A
1	2	794	U
1	2	795	U
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G
1	2	830	U
1	2	831	U
1	2	832	U
1	2	836	U
1	2	841	U
1	2	844	A
1	2	846	G
1	2	848	C
1	2	856	A
1	2	860	U
1	2	862	A
1	2	863	A
1	2	864	U
1	2	886	U
1	2	898	A
1	2	911	U
1	2	912	U
1	2	913	G
1	2	914	G
1	2	916	U
1	2	921	U
1	2	933	A
1	2	935	U

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Mol	Chain	Res	Type
1	2	942	G
1	2	944	A
1	2	951	A
1	2	960	U
1	2	961	U
1	2	966	A
1	2	991	G
1	2	992	A
1	2	993	A
1	2	996	U
1	2	999	U
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1025	A
1	2	1026	A
1	2	1028	C
1	2	1039	A
1	2	1040	G
1	2	1043	A
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1064	G
1	2	1074	G
1	2	1075	C
1	2	1080	U
1	2	1081	A
1	2	1082	C
1	2	1086	A
1	2	1087	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1109	G
1	2	1138	A
1	2	1143	A

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Mol	Chain	Res	Type
1	2	1150	G
1	2	1151	A
1	2	1155	G
1	2	1157	A
1	2	1158	C
1	2	1159	C
1	2	1160	A
1	2	1167	G
1	2	1176	G
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	1217	A
1	2	1218	G
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1244	A
1	2	1245	G
1	2	1251	U
1	2	1257	U
1	2	1258	U
1	2	1262	U
1	2	1268	G
1	2	1285	U
1	2	1286	U
1	2	1301	U
1	2	1314	U
1	2	1315	U
1	2	1320	U
1	2	1321	A
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A

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Mol	Chain	Res	Type
1	2	1345	A
1	2	1346	A
1	2	1355	C
1	2	1361	U
1	2	1363	U
1	2	1364	G
1	2	1368	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1378	U
1	2	1379	C
1	2	1384	A
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1412	G
1	2	1413	U
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1432	U
1	2	1435	G
1	2	1446	A
1	2	1447	C
1	2	1448	G
1	2	1457	C
1	2	1459	C
1	2	1461	C
1	2	1462	G
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1478	G
1	2	1482	C
1	2	1483	A
1	2	1486	G
1	2	1488	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A

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Mol	Chain	Res	Type
1	2	1493	A
1	2	1503	A
1	2	1506	G
1	2	1510	U
1	2	1514	U
1	2	1515	A
1	2	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1526	A
1	2	1533	C
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1539	G
1	2	1540	G
1	2	1542	G
1	2	1557	U
1	2	1559	A
1	2	1563	C
1	2	1569	A
1	2	1573	A
1	2	1574	G
1	2	1584	G
1	2	1591	C
1	2	1592	A
1	2	1600	A
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1624	C
1	2	1627	U
1	2	1631	A
1	2	1653	C
1	2	1657	U
1	2	1658	G
1	2	1682	U
1	2	1683	C
1	2	1684	U

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Mol	Chain	Res	Type
1	2	1685	G
1	2	1729	C
1	2	1755	A
1	2	1756	A
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1770	U
1	2	1772	C
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1790	A
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
1	2	1798	U
36	1	26	A
36	1	40	A
36	1	49	A
36	1	59	G
36	1	60	A
36	1	61	A
36	1	65	A
36	1	66	A
36	1	73	C
36	1	74	G
36	1	75	G
36	1	76	G
36	1	83	U
36	1	85	A
36	1	92	G
36	1	93	C
36	1	94	G
36	1	99	A
36	1	106	A
36	1	109	A
36	1	110	G
36	1	111	C
36	1	116	A

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Mol	Chain	Res	Type
36	1	117	U
36	1	120	G
36	1	121	A
36	1	122	A
36	1	133	U
36	1	136	G
36	1	140	C
36	1	156	G
36	1	157	A
36	1	160	G
36	1	165	A
36	1	166	C
36	1	170	G
36	1	173	G
36	1	187	A
36	1	190	U
36	1	191	U
36	1	210	U
36	1	213	A
36	1	218	G
36	1	219	A
36	1	239	G
36	1	240	U
36	1	243	G
36	1	245	U
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	253	A
36	1	267	G
36	1	269	G
36	1	282	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	299	G
36	1	315	C
36	1	323	A
36	1	326	U
36	1	329	U

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Mol	Chain	Res	Type
36	1	339	C
36	1	349	A
36	1	350	C
36	1	351	A
36	1	376	G
36	1	390	G
36	1	398	A
36	1	399	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	414	U
36	1	421	G
36	1	422	A
36	1	438	A
36	1	439	C
36	1	440	A
36	1	495	G
36	1	498	A
36	1	507	U
36	1	520	U
36	1	521	A
36	1	531	G
36	1	535	G
36	1	541	U
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	557	A
36	1	558	U
36	1	559	A
36	1	560	G
36	1	578	A
36	1	579	G
36	1	588	G
36	1	592	A
36	1	600	G
36	1	604	G

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Mol	Chain	Res	Type
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	637	C
36	1	638	C
36	1	639	G
36	1	643	U
36	1	648	C
36	1	649	A
36	1	658	G
36	1	660	A
36	1	661	G
36	1	677	A
36	1	679	U
36	1	681	U
36	1	691	A
36	1	699	A
36	1	705	A
36	1	709	A
36	1	712	G
36	1	714	G
36	1	715	A
36	1	716	A
36	1	719	U
36	1	762	U
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	786	A
36	1	798	G
36	1	803	C

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Mol	Chain	Res	Type
36	1	806	A
36	1	807	A
36	1	817	A
36	1	830	A
36	1	849	C
36	1	861	C
36	1	874	U
36	1	875	G
36	1	878	G
36	1	879	U
36	1	890	C
36	1	896	A
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	923	C
36	1	924	G
36	1	937	G
36	1	944	C
36	1	953	G
36	1	959	C
36	1	960	U
36	1	962	A
36	1	963	G
36	1	978	G
36	1	979	U
36	1	981	U
36	1	982	C
36	1	993	G
36	1	994	G
36	1	1000	C
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1014	U
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1021	G

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Mol	Chain	Res	Type
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1037	C
36	1	1042	U
36	1	1046	A
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1064	A
36	1	1065	A
36	1	1068	C
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	1113	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	1177	G
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1185	C
36	1	1191	U
36	1	1192	C
36	1	1193	A

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Mol	Chain	Res	Type
36	1	1196	C
36	1	1201	C
36	1	1209	G
36	1	1213	G
36	1	1216	C
36	1	1217	A
36	1	1221	A
36	1	1222	G
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1235	U
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1242	G
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1251	A
36	1	1254	C
36	1	1258	U
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	1286	A
36	1	1287	A
36	1	1307	G
36	1	1308	A
36	1	1309	U

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Mol	Chain	Res	Type
36	1	1313	G
36	1	1320	C
36	1	1330	A
36	1	1331	U
36	1	1332	A
36	1	1345	G
36	1	1348	U
36	1	1349	G
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1363	A
36	1	1386	A
36	1	1387	G
36	1	1399	A
36	1	1400	G
36	1	1405	U
36	1	1406	A
36	1	1417	G
36	1	1418	A
36	1	1419	A
36	1	1425	U
36	1	1428	A
36	1	1429	G
36	1	1433	A
36	1	1434	G
36	1	1437	C
36	1	1443	G
36	1	1446	A
36	1	1450	G
36	1	1452	A
36	1	1455	U
36	1	1467	A
36	1	1481	A
36	1	1482	A
36	1	1502	C
36	1	1506	A
36	1	1508	C
36	1	1511	U

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Mol	Chain	Res	Type
36	1	1527	C
36	1	1549	U
36	1	1555	U
36	1	1556	C
36	1	1557	A
36	1	1560	G
36	1	1561	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1571	A
36	1	1572	U
36	1	1576	G
36	1	1578	C
36	1	1579	C
36	1	1580	A
36	1	1581	C
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1596	C
36	1	1605	A
36	1	1607	U
36	1	1608	C
36	1	1620	U
36	1	1621	A
36	1	1624	G
36	1	1629	U
36	1	1639	C
36	1	1640	G
36	1	1642	A
36	1	1643	A
36	1	1645	U
36	1	1657	C
36	1	1658	G
36	1	1683	A

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Mol	Chain	Res	Type
36	1	1684	U
36	1	1688	U
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1725	C
36	1	1736	G
36	1	1741	A
36	1	1742	U
36	1	1750	A
36	1	1751	G
36	1	1761	C
36	1	1762	C
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1770	G
36	1	1775	G
36	1	1776	G
36	1	1780	G
36	1	1782	U
36	1	1797	A
36	1	1801	U
36	1	1809	A
36	1	1810	A
36	1	1812	G
36	1	1813	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	1835	A
36	1	1839	A
36	1	1841	A
36	1	1842	A
36	1	1845	G
36	1	1846	C
36	1	1847	A
36	1	1849	C

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Mol	Chain	Res	Type
36	1	1850	A
36	1	1855	U
36	1	1857	C
36	1	1866	C
36	1	1871	U
36	1	1877	U
36	1	1879	A
36	1	1880	U
36	1	1901	A
36	1	1906	G
36	1	1931	U
36	1	1932	A
36	1	1935	G
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	1954	G
36	1	2097	U
36	1	2101	C
36	1	2102	U
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2114	C
36	1	2121	G
36	1	2122	G
36	1	2131	A
36	1	2134	G
36	1	2140	U
36	1	2144	A
36	1	2158	A
36	1	2164	A
36	1	2169	G
36	1	2170	U
36	1	2205	U
36	1	2206	G
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2223	A
36	1	2225	U
36	1	2229	A

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Mol	Chain	Res	Type
36	1	2244	A
36	1	2245	C
36	1	2246	G
36	1	2249	G
36	1	2250	G
36	1	2252	A
36	1	2254	U
36	1	2255	A
36	1	2256	A
36	1	2265	C
36	1	2272	G
36	1	2273	G
36	1	2280	A
36	1	2281	A
36	1	2282	U
36	1	2283	G
36	1	2301	U
36	1	2307	G
36	1	2309	A
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2317	A
36	1	2318	U
36	1	2330	C
36	1	2334	U
36	1	2336	U
36	1	2352	A
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2392	C
36	1	2393	G
36	1	2394	G
36	1	2397	A
36	1	2402	A
36	1	2403	G
36	1	2411	U
36	1	2416	U

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Mol	Chain	Res	Type
36	1	2418	G
36	1	2419	A
36	1	2425	G
36	1	2427	U
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	2522	G
36	1	2523	A
36	1	2532	U
36	1	2533	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2544	U
36	1	2547	A
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2561	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2581	U
36	1	2585	G
36	1	2593	A
36	1	2602	G
36	1	2606	G

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Mol	Chain	Res	Type
36	1	2607	G
36	1	2614	G
36	1	2623	G
36	1	2637	A
36	1	2652	U
36	1	2653	C
36	1	2656	A
36	1	2672	G
36	1	2674	A
36	1	2675	C
36	1	2676	A
36	1	2677	G
36	1	2681	U
36	1	2685	C
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	2714	G
36	1	2719	U
36	1	2720	G
36	1	2728	G
36	1	2729	U
36	1	2752	U
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	2800	G
36	1	2801	A
36	1	2802	A
36	1	2803	A
36	1	2810	C
36	1	2815	G

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Mol	Chain	Res	Type
36	1	2817	A
36	1	2818	U
36	1	2821	C
36	1	2829	U
36	1	2834	G
36	1	2839	G
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2849	C
36	1	2853	A
36	1	2855	U
36	1	2860	U
36	1	2863	G
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2876	C
36	1	2886	U
36	1	2887	A
36	1	2889	C
36	1	2893	C
36	1	2896	A
36	1	2897	A
36	1	2898	G
36	1	2899	C
36	1	2910	A
36	1	2923	U
36	1	2925	C
36	1	2928	C
36	1	2935	U
36	1	2936	A
36	1	2942	C
36	1	2947	G
36	1	2954	U
36	1	2955	U
36	1	2971	A
36	1	2979	U
36	1	2990	G
36	1	2997	G
36	1	3012	A
36	1	3030	G

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Mol	Chain	Res	Type
36	1	3034	C
36	1	3040	A
36	1	3055	U
36	1	3056	U
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3086	A
36	1	3087	A
36	1	3092	C
36	1	3113	A
36	1	3119	U
36	1	3122	A
36	1	3127	A
36	1	3130	A
36	1	3131	U
36	1	3139	A
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3164	C
36	1	3165	A
36	1	3167	A
36	1	3168	A
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3186	A
36	1	3187	A
36	1	3196	U
36	1	3197	G

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Mol	Chain	Res	Type
36	1	3198	U
36	1	3207	U
36	1	3210	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3227	A
36	1	3228	C
36	1	3229	G
36	1	3235	C
36	1	3244	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3265	C
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	3287	U
36	1	3289	G
36	1	3293	U
36	1	3294	A
36	1	3304	U
36	1	3309	G
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3330	A
36	1	3335	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3348	G

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Mol	Chain	Res	Type
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	3369	G
36	1	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
37	3	7	G
37	3	13	A
37	3	14	U
37	3	18	C
37	3	21	G
37	3	22	A
37	3	23	A
37	3	42	A
37	3	45	A
37	3	54	U
37	3	57	G
37	3	59	U
37	3	65	G
37	3	74	C
37	3	76	A
37	3	83	U
37	3	84	A
37	3	91	G
37	3	101	G
37	3	102	A
37	3	112	G
38	4	2	A
38	4	26	U
38	4	34	U
38	4	35	C
38	4	47	C
38	4	48	A
38	4	49	G

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Mol	Chain	Res	Type
38	4	50	C
38	4	51	G
38	4	52	A
38	4	59	A
38	4	62	C
38	4	63	G
38	4	69	U
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	93	U
38	4	95	G
38	4	104	A
38	4	105	A
38	4	106	C
38	4	110	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	155	A
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	42	G
1	6	47	A

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Mol	Chain	Res	Type
1	6	50	C
1	6	57	G
1	6	60	U
1	6	65	A
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	78	A
1	6	99	C
1	6	104	A
1	6	114	C
1	6	126	A
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	146	U
1	6	158	U
1	6	159	U
1	6	166	C
1	6	177	U
1	6	178	U
1	6	181	A
1	6	185	U
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	195	G
1	6	197	A
1	6	198	A

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Mol	Chain	Res	Type
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	222	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	235	G
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	260	U
1	6	261	U
1	6	265	A
1	6	266	A
1	6	271	A
1	6	272	U
1	6	273	G
1	6	275	C
1	6	276	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	299	A
1	6	301	A
1	6	308	C
1	6	314	C
1	6	316	A
1	6	320	U
1	6	321	C
1	6	322	G
1	6	337	G
1	6	338	C

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Mol	Chain	Res	Type
1	6	346	G
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	417	A
1	6	418	G
1	6	419	G
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	445	A
1	6	446	A
1	6	447	U
1	6	448	C
1	6	454	U
1	6	468	A
1	6	477	A
1	6	484	C
1	6	485	A
1	6	486	G
1	6	487	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	504	U

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Mol	Chain	Res	Type
1	6	505	A
1	6	506	A
1	6	507	U
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	515	A
1	6	519	C
1	6	527	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	557	G
1	6	558	U
1	6	559	C
1	6	565	C
1	6	570	A
1	6	574	G
1	6	577	G
1	6	578	U
1	6	579	A
1	6	580	A
1	6	582	U
1	6	585	A
1	6	594	A
1	6	595	G
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	634	G
1	6	639	U
1	6	648	G
1	6	650	U
1	6	651	G

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Mol	Chain	Res	Type
1	6	652	G
1	6	653	C
1	6	658	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	669	G
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	680	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C
1	6	695	U
1	6	697	C
1	6	698	U
1	6	709	C
1	6	710	U
1	6	711	U
1	6	714	G
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	723	G
1	6	730	G
1	6	740	A
1	6	743	U
1	6	751	G
1	6	753	A
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G

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Mol	Chain	Res	Type
1	6	774	A
1	6	775	G
1	6	777	C
1	6	779	U
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G
1	6	789	A
1	6	792	U
1	6	793	A
1	6	794	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	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	856	A
1	6	858	G
1	6	859	A
1	6	862	A
1	6	863	A
1	6	873	U
1	6	885	G
1	6	898	A
1	6	906	A
1	6	912	U
1	6	913	G
1	6	914	G

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Mol	Chain	Res	Type
1	6	916	U
1	6	928	U
1	6	933	A
1	6	935	U
1	6	940	A
1	6	942	G
1	6	951	A
1	6	959	U
1	6	960	U
1	6	969	C
1	6	970	A
1	6	971	A
1	6	987	G
1	6	992	A
1	6	993	A
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1008	G
1	6	1018	U
1	6	1021	C
1	6	1026	A
1	6	1028	C
1	6	1039	A
1	6	1040	G
1	6	1041	G
1	6	1052	U
1	6	1053	G
1	6	1056	U
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1071	U
1	6	1073	G
1	6	1076	A
1	6	1081	A
1	6	1082	C
1	6	1091	A
1	6	1092	A
1	6	1096	C
1	6	1097	U

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Mol	Chain	Res	Type
1	6	1098	U
1	6	1100	G
1	6	1101	G
1	6	1109	G
1	6	1111	G
1	6	1137	A
1	6	1138	A
1	6	1139	A
1	6	1146	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	1190	C
1	6	1194	A
1	6	1196	A
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1204	A
1	6	1217	A
1	6	1218	G
1	6	1220	C
1	6	1225	U
1	6	1227	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1231	U
1	6	1236	A
1	6	1239	U
1	6	1240	U
1	6	1241	G
1	6	1242	A
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1249	U

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Mol	Chain	Res	Type
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1259	U
1	6	1262	U
1	6	1269	U
1	6	1284	C
1	6	1286	U
1	6	1288	G
1	6	1291	G
1	6	1306	C
1	6	1307	U
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1338	C
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	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	1383	G
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1413	U
1	6	1414	U
1	6	1415	U
1	6	1424	A
1	6	1427	A

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Mol	Chain	Res	Type
1	6	1428	G
1	6	1430	U
1	6	1433	G
1	6	1435	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	1480	G
1	6	1481	C
1	6	1482	C
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1517	U
1	6	1523	G
1	6	1524	A
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1553	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1573	A
1	6	1574	G
1	6	1575	G
1	6	1576	A

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Mol	Chain	Res	Type
1	6	1577	A
1	6	1582	U
1	6	1584	G
1	6	1590	G
1	6	1601	G
1	6	1607	G
1	6	1615	C
1	6	1616	G
1	6	1618	C
1	6	1619	C
1	6	1620	C
1	6	1621	U
1	6	1622	G
1	6	1634	C
1	6	1637	C
1	6	1638	G
1	6	1657	U
1	6	1658	G
1	6	1678	A
1	6	1680	G
1	6	1696	G
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1710	U
1	6	1712	A
1	6	1716	C
1	6	1717	G
1	6	1731	A
1	6	1736	G
1	6	1742	U
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A

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Mol	Chain	Res	Type
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	9	U
36	5	15	C
36	5	16	A
36	5	26	A
36	5	40	A
36	5	44	U
36	5	49	A
36	5	60	A
36	5	65	A
36	5	66	A
36	5	76	G
36	5	92	G
36	5	96	G
36	5	99	A
36	5	109	A
36	5	110	G
36	5	113	C
36	5	116	A
36	5	117	U
36	5	120	G
36	5	121	A
36	5	122	A
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	156	G
36	5	157	A
36	5	160	G
36	5	161	G
36	5	165	A
36	5	166	C
36	5	170	G
36	5	171	G
36	5	172	G

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Mol	Chain	Res	Type
36	5	173	G
36	5	174	C
36	5	179	C
36	5	180	C
36	5	181	U
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	221	A
36	5	227	G
36	5	231	G
36	5	235	A
36	5	236	G
36	5	237	G
36	5	239	G
36	5	240	U
36	5	241	G
36	5	244	G
36	5	246	U
36	5	247	C
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	263	C
36	5	269	G
36	5	270	U
36	5	271	C
36	5	284	A
36	5	286	U
36	5	295	A
36	5	305	U
36	5	321	C

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Mol	Chain	Res	Type
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	379	C
36	5	382	U
36	5	390	G
36	5	391	A
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	404	G
36	5	421	G
36	5	422	A
36	5	425	G
36	5	437	G
36	5	438	A
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	521	A
36	5	532	A
36	5	535	G
36	5	542	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	551	A
36	5	552	G
36	5	553	U
36	5	555	U
36	5	557	A

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Mol	Chain	Res	Type
36	5	558	U
36	5	559	A
36	5	560	G
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	705	A
36	5	712	G
36	5	715	A
36	5	716	A
36	5	719	U
36	5	725	G
36	5	726	G
36	5	727	G
36	5	736	A
36	5	747	A
36	5	748	U
36	5	758	C
36	5	766	U
36	5	767	U
36	5	768	C
36	5	772	U
36	5	776	U
36	5	777	U
36	5	781	G
36	5	785	G

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Mol	Chain	Res	Type
36	5	786	A
36	5	806	A
36	5	817	A
36	5	826	G
36	5	830	A
36	5	851	C
36	5	854	G
36	5	861	C
36	5	865	U
36	5	871	U
36	5	874	U
36	5	879	U
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	938	C
36	5	944	C
36	5	948	C
36	5	953	G
36	5	959	C
36	5	960	U
36	5	961	C
36	5	964	G
36	5	979	U
36	5	983	A
36	5	993	G
36	5	994	G
36	5	997	A
36	5	1000	C
36	5	1001	G
36	5	1002	A
36	5	1010	G

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Mol	Chain	Res	Type
36	5	1013	G
36	5	1015	U
36	5	1017	C
36	5	1019	G
36	5	1021	G
36	5	1022	U
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1027	A
36	5	1028	U
36	5	1029	G
36	5	1035	G
36	5	1041	U
36	5	1047	A
36	5	1049	C
36	5	1052	U
36	5	1063	G
36	5	1064	A
36	5	1065	A
36	5	1066	G
36	5	1071	U
36	5	1072	G
36	5	1079	A
36	5	1081	U
36	5	1082	U
36	5	1088	U
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1112	A
36	5	1115	G
36	5	1117	G
36	5	1131	G
36	5	1144	U
36	5	1152	G
36	5	1153	A

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Mol	Chain	Res	Type
36	5	1159	A
36	5	1178	G
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1190	A
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1201	C
36	5	1205	A
36	5	1209	G
36	5	1212	A
36	5	1222	G
36	5	1223	A
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	1245	A
36	5	1246	G
36	5	1252	A
36	5	1258	U
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1281	G
36	5	1285	G
36	5	1292	C
36	5	1305	U
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1313	G
36	5	1314	C
36	5	1324	U
36	5	1330	A

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Mol	Chain	Res	Type
36	5	1331	U
36	5	1332	A
36	5	1348	U
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1370	G
36	5	1372	C
36	5	1380	G
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1398	U
36	5	1399	A
36	5	1400	G
36	5	1406	A
36	5	1417	G
36	5	1418	A
36	5	1419	A
36	5	1428	A
36	5	1431	G
36	5	1432	C
36	5	1433	A
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1455	U
36	5	1477	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	1527	C
36	5	1533	U
36	5	1536	G

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Mol	Chain	Res	Type
36	5	1539	A
36	5	1549	U
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1564	U
36	5	1565	G
36	5	1566	A
36	5	1567	U
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1573	G
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1580	A
36	5	1581	C
36	5	1583	A
36	5	1589	A
36	5	1600	U
36	5	1619	A
36	5	1620	U
36	5	1629	U
36	5	1633	C
36	5	1637	A
36	5	1639	C
36	5	1642	A
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1657	C
36	5	1664	G
36	5	1683	A
36	5	1687	U

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Mol	Chain	Res	Type
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	1741	A
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	1769	G
36	5	1770	G
36	5	1780	G
36	5	1781	C
36	5	1793	C
36	5	1795	U
36	5	1797	A
36	5	1810	A
36	5	1812	G
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1819	U
36	5	1820	U
36	5	1821	U
36	5	1839	A
36	5	1840	U
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1849	C
36	5	1850	A
36	5	1851	G
36	5	1866	C
36	5	1875	G

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Mol	Chain	Res	Type
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1886	A
36	5	1893	A
36	5	1895	A
36	5	1901	A
36	5	1906	G
36	5	1908	A
36	5	1918	C
36	5	1932	A
36	5	1935	G
36	5	1947	G
36	5	2094	C
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	2134	G
36	5	2140	U
36	5	2144	A
36	5	2158	A
36	5	2169	G
36	5	2176	U
36	5	2187	G
36	5	2188	A
36	5	2192	C
36	5	2198	A
36	5	2201	G
36	5	2205	U
36	5	2206	G
36	5	2209	U
36	5	2210	G
36	5	2213	A
36	5	2222	A
36	5	2223	A
36	5	2225	U
36	5	2234	G

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Mol	Chain	Res	Type
36	5	2244	A
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	2270	A
36	5	2273	G
36	5	2279	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	2368	A
36	5	2371	G
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2386	A
36	5	2392	C
36	5	2393	G
36	5	2397	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2410	U
36	5	2411	U
36	5	2418	G
36	5	2435	G
36	5	2436	U
36	5	2437	G
36	5	2440	G
36	5	2441	A

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Mol	Chain	Res	Type
36	5	2443	A
36	5	2444	C
36	5	2504	U
36	5	2505	U
36	5	2506	U
36	5	2507	C
36	5	2508	U
36	5	2509	U
36	5	2510	U
36	5	2511	A
36	5	2512	C
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	2531	C
36	5	2535	A
36	5	2536	A
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2549	G
36	5	2552	C
36	5	2555	G
36	5	2558	U
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2573	G
36	5	2574	G
36	5	2585	G
36	5	2587	U
36	5	2589	G

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Mol	Chain	Res	Type
36	5	2593	A
36	5	2594	C
36	5	2596	U
36	5	2598	G
36	5	2606	G
36	5	2607	G
36	5	2608	G
36	5	2614	G
36	5	2615	G
36	5	2619	G
36	5	2647	A
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	2683	U
36	5	2689	A
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2705	A
36	5	2714	G
36	5	2719	U
36	5	2727	A
36	5	2728	G
36	5	2729	U
36	5	2740	A
36	5	2742	C
36	5	2752	U
36	5	2753	G
36	5	2755	C
36	5	2762	A
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2781	U
36	5	2783	U
36	5	2796	G

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Mol	Chain	Res	Type
36	5	2797	C
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2802	A
36	5	2810	C
36	5	2814	G
36	5	2816	G
36	5	2817	A
36	5	2818	U
36	5	2819	A
36	5	2820	A
36	5	2821	C
36	5	2828	G
36	5	2829	U
36	5	2837	A
36	5	2838	A
36	5	2839	G
36	5	2843	U
36	5	2845	A
36	5	2847	A
36	5	2849	C
36	5	2853	A
36	5	2863	G
36	5	2865	U
36	5	2871	G
36	5	2872	A
36	5	2875	U
36	5	2877	G
36	5	2880	U
36	5	2881	C
36	5	2887	A
36	5	2889	C
36	5	2896	A
36	5	2897	A
36	5	2898	G
36	5	2899	C
36	5	2912	G
36	5	2914	G
36	5	2921	U
36	5	2922	G
36	5	2923	U

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Mol	Chain	Res	Type
36	5	2924	U
36	5	2928	C
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2944	U
36	5	2947	G
36	5	2954	U
36	5	2956	A
36	5	2957	G
36	5	2967	A
36	5	2971	A
36	5	2972	G
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2992	U
36	5	2993	G
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3028	G
36	5	3030	G
36	5	3034	C
36	5	3049	A
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3092	C
36	5	3119	U
36	5	3122	A
36	5	3123	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3150	A
36	5	3153	U
36	5	3155	U

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Mol	Chain	Res	Type
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3164	C
36	5	3165	A
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3178	A
36	5	3179	U
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3198	U
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3227	A
36	5	3228	C
36	5	3229	G
36	5	3238	G
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3265	C
36	5	3266	G
36	5	3268	A
36	5	3269	U
36	5	3270	U
36	5	3273	A
36	5	3274	A
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3279	A

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Mol	Chain	Res	Type
36	5	3282	U
36	5	3284	G
36	5	3285	C
36	5	3286	G
36	5	3287	U
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3313	U
36	5	3316	A
36	5	3317	U
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	3378	C
36	5	3382	U
36	5	3385	U
36	5	3386	G
36	5	3389	U
36	5	3390	G
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	27	A
37	7	38	U
37	7	50	U
37	7	54	U
37	7	55	A
37	7	60	G

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Mol	Chain	Res	Type
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	95	A
37	7	99	G
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	34	U
38	8	35	C
38	8	48	A
38	8	59	A
38	8	62	C
38	8	63	G
38	8	69	U
38	8	77	A
38	8	78	G
38	8	79	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	90	U
38	8	95	G
38	8	96	A
38	8	97	A
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	138	A
38	8	148	G

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Mol	Chain	Res	Type
38	8	152	G
38	8	156	U
38	8	157	U
38	8	158	U

All (279) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	73	U
1	2	74	U
1	2	103	A
1	2	114	C
1	2	126	A
1	2	130	C
1	2	131	C
1	2	136	C
1	2	139	C
1	2	144	U
1	2	158	U
1	2	217	A
1	2	218	A
1	2	240	U
1	2	265	A
1	2	278	U
1	2	280	U
1	2	321	C
1	2	400	A
1	2	417	A
1	2	484	C
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	510	G
1	2	512	A
1	2	555	A
1	2	558	U
1	2	685	A
1	2	704	C
1	2	720	G

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Mol	Chain	Res	Type
1	2	721	U
1	2	734	A
1	2	755	A
1	2	794	U
1	2	829	A
1	2	913	G
1	2	1058	U
1	2	1081	A
1	2	1157	A
1	2	1196	A
1	2	1207	C
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1339	C
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1489	U
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1657	U
1	2	1761	U
36	1	43	A
36	1	65	A
36	1	169	U
36	1	239	G
36	1	282	G
36	1	374	A
36	1	397	A
36	1	547	G
36	1	588	G
36	1	594	U
36	1	637	C
36	1	715	A
36	1	763	G
36	1	816	A
36	1	873	C
36	1	916	G
36	1	981	U
36	1	993	G

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Mol	Chain	Res	Type
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
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	1507	G
36	1	1554	U
36	1	1556	C
36	1	1562	C
36	1	1607	U
36	1	1716	U
36	1	1724	U
36	1	1751	G
36	1	1815	U
36	1	1820	U
36	1	1846	C
36	1	1858	A
36	1	1931	U
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2249	G
36	1	2372	A
36	1	2374	C
36	1	2418	G
36	1	2513	U
36	1	2522	G
36	1	2537	U
36	1	2538	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2677	G

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Mol	Chain	Res	Type
36	1	2704	A
36	1	2728	G
36	1	2772	C
36	1	2801	A
36	1	2818	U
36	1	2896	A
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3139	A
36	1	3195	U
36	1	3196	U
36	1	3207	U
36	1	3228	C
36	1	3245	A
36	1	3269	U
36	1	3316	A
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
37	3	13	A
38	4	85	G
38	4	125	U
1	6	25	C
1	6	66	U
1	6	76	A
1	6	114	C
1	6	136	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	345	U
1	6	400	A
1	6	417	A
1	6	512	A
1	6	542	A
1	6	557	G

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Mol	Chain	Res	Type
1	6	651	G
1	6	664	U
1	6	667	U
1	6	678	A
1	6	697	C
1	6	717	C
1	6	720	G
1	6	755	A
1	6	829	A
1	6	834	G
1	6	913	G
1	6	1051	G
1	6	1058	U
1	6	1097	U
1	6	1227	A
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	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	169	U
36	5	210	U
36	5	238	A
36	5	285	A
36	5	588	G
36	5	594	U
36	5	735	A
36	5	765	C
36	5	767	U
36	5	873	C

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Mol	Chain	Res	Type
36	5	896	A
36	5	908	G
36	5	916	G
36	5	937	G
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1160	C
36	5	1181	U
36	5	1192	C
36	5	1222	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	1481	A
36	5	1514	G
36	5	1554	U
36	5	1560	G
36	5	1572	U
36	5	1716	U
36	5	1724	U
36	5	1792	C
36	5	1816	A
36	5	1819	U
36	5	1841	A
36	5	1858	A
36	5	1878	G
36	5	1879	A
36	5	2093	A
36	5	2101	C
36	5	2112	U
36	5	2121	G
36	5	2204	C
36	5	2209	U

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Mol	Chain	Res	Type
36	5	2255	A
36	5	2257	C
36	5	2372	A
36	5	2374	C
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2539	C
36	5	2586	G
36	5	2593	A
36	5	2682	C
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2818	U
36	5	2876	C
36	5	2896	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	3269	U
36	5	3275	U
36	5	3289	G
36	5	3317	U
36	5	3340	G
36	5	3341	U
36	5	3357	U
37	7	49	G
38	8	89	A
38	8	111	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2555 ligands modelled in this entry, 1424 are monoatomic - leaving 1131 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	1	4188	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	5	4175	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4048	-	0,6,6	-	-	-	-	-
86	OHX	5	4056	-	0,6,6	-	-	-	-	-
86	OHX	5	4067	-	0,6,6	-	-	-	-	-
86	OHX	6	2152	-	0,6,6	-	-	-	-	-
86	OHX	1	4108	-	0,6,6	-	-	-	-	-
86	OHX	5	3907	-	0,6,6	-	-	-	-	-
86	OHX	6	2198	-	0,6,6	-	-	-	-	-
86	OHX	6	2144	-	0,6,6	-	-	-	-	-
86	OHX	5	3980	-	0,6,6	-	-	-	-	-
86	OHX	6	2120	-	0,6,6	-	-	-	-	-
86	OHX	5	3994	-	0,6,6	-	-	-	-	-
86	OHX	2	2108	-	0,6,6	-	-	-	-	-
86	OHX	5	4027	-	0,6,6	-	-	-	-	-
86	OHX	5	4090	-	0,6,6	-	-	-	-	-
86	OHX	1	4009	-	0,6,6	-	-	-	-	-
86	OHX	4	221	-	0,6,6	-	-	-	-	-
86	OHX	1	4076	-	0,6,6	-	-	-	-	-
86	OHX	5	4039	-	0,6,6	-	-	-	-	-
86	OHX	2	2134	-	0,6,6	-	-	-	-	-
86	OHX	4	237	-	0,6,6	-	-	-	-	-
86	OHX	3	216	-	0,6,6	-	-	-	-	-
86	OHX	6	2084	-	0,6,6	-	-	-	-	-
86	OHX	2	2132	-	0,6,6	-	-	-	-	-
86	OHX	6	2155	-	0,6,6	-	-	-	-	-
86	OHX	5	4183	-	0,6,6	-	-	-	-	-
86	OHX	5	4226	-	0,6,6	-	-	-	-	-
86	OHX	2	2115	-	0,6,6	-	-	-	-	-
86	OHX	m4	201	-	0,6,6	-	-	-	-	-
86	OHX	2	2073	-	0,6,6	-	-	-	-	-
86	OHX	1	4148	-	0,6,6	-	-	-	-	-
86	OHX	1	4171	-	0,6,6	-	-	-	-	-
86	OHX	5	4077	-	0,6,6	-	-	-	-	-
86	OHX	1	4125	-	0,6,6	-	-	-	-	-
86	OHX	5	4132	-	0,6,6	-	-	-	-	-
86	OHX	1	3963	-	0,6,6	-	-	-	-	-
86	OHX	5	3919	-	0,6,6	-	-	-	-	-
86	OHX	1	4121	-	0,6,6	-	-	-	-	-
86	OHX	5	4160	-	0,6,6	-	-	-	-	-
86	OHX	5	4162	-	0,6,6	-	-	-	-	-
86	OHX	6	2136	-	0,6,6	-	-	-	-	-
86	OHX	7	226	-	0,6,6	-	-	-	-	-
86	OHX	2	2101	-	0,6,6	-	-	-	-	-
86	OHX	2	2158	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4032	-	0,6,6	-	-	-	-	-
86	OHX	1	4158	-	0,6,6	-	-	-	-	-
86	OHX	5	3905	-	0,6,6	-	-	-	-	-
86	OHX	5	3968	-	0,6,6	-	-	-	-	-
86	OHX	6	2053	-	0,6,6	-	-	-	-	-
86	OHX	1	3989	-	0,6,6	-	-	-	-	-
86	OHX	1	4092	-	0,6,6	-	-	-	-	-
86	OHX	2	2162	-	0,6,6	-	-	-	-	-
86	OHX	5	4055	-	0,6,6	-	-	-	-	-
86	OHX	1	3883	-	0,6,6	-	-	-	-	-
86	OHX	6	2061	-	0,6,6	-	-	-	-	-
86	OHX	1	3997	-	0,6,6	-	-	-	-	-
86	OHX	1	4170	-	0,6,6	-	-	-	-	-
86	OHX	6	2150	-	0,6,6	-	-	-	-	-
86	OHX	5	4151	-	0,6,6	-	-	-	-	-
86	OHX	2	2156	-	0,6,6	-	-	-	-	-
86	OHX	5	3989	-	0,6,6	-	-	-	-	-
86	OHX	5	4097	-	0,6,6	-	-	-	-	-
86	OHX	5	4174	-	0,6,6	-	-	-	-	-
86	OHX	6	2190	-	0,6,6	-	-	-	-	-
86	OHX	1	4046	-	0,6,6	-	-	-	-	-
86	OHX	1	3951	-	0,6,6	-	-	-	-	-
86	OHX	6	2076	-	0,6,6	-	-	-	-	-
86	OHX	6	2165	-	0,6,6	-	-	-	-	-
86	OHX	2	2096	-	0,6,6	-	-	-	-	-
86	OHX	5	4208	-	0,6,6	-	-	-	-	-
86	OHX	5	4093	-	0,6,6	-	-	-	-	-
86	OHX	6	2072	-	0,6,6	-	-	-	-	-
86	OHX	5	4154	-	0,6,6	-	-	-	-	-
86	OHX	5	4195	-	0,6,6	-	-	-	-	-
86	OHX	5	4170	-	0,6,6	-	-	-	-	-
86	OHX	1	4192	-	0,6,6	-	-	-	-	-
86	OHX	2	2072	-	0,6,6	-	-	-	-	-
86	OHX	7	218	-	0,6,6	-	-	-	-	-
86	OHX	1	3878	-	0,6,6	-	-	-	-	-
86	OHX	1	3956	-	0,6,6	-	-	-	-	-
86	OHX	5	3928	-	0,6,6	-	-	-	-	-
86	OHX	2	2161	-	0,6,6	-	-	-	-	-
86	OHX	6	2157	-	0,6,6	-	-	-	-	-
86	OHX	1	4180	-	0,6,6	-	-	-	-	-
86	OHX	5	3938	-	0,6,6	-	-	-	-	-
86	OHX	1	4152	-	0,6,6	-	-	-	-	-
86	OHX	5	4197	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2178	-	0,6,6	-	-	-	-	-
86	OHX	6	2186	-	0,6,6	-	-	-	-	-
86	OHX	5	4221	-	0,6,6	-	-	-	-	-
86	OHX	S8	301	-	0,6,6	-	-	-	-	-
86	OHX	1	3932	-	0,6,6	-	-	-	-	-
86	OHX	6	2126	-	0,6,6	-	-	-	-	-
86	OHX	1	4179	-	0,6,6	-	-	-	-	-
86	OHX	1	4115	-	0,6,6	-	-	-	-	-
86	OHX	2	2179	-	0,6,6	-	-	-	-	-
86	OHX	5	4171	-	0,6,6	-	-	-	-	-
86	OHX	1	3947	-	0,6,6	-	-	-	-	-
86	OHX	5	4001	-	0,6,6	-	-	-	-	-
86	OHX	2	2030	-	0,6,6	-	-	-	-	-
86	OHX	1	3868	-	0,6,6	-	-	-	-	-
86	OHX	M5	303	-	0,6,6	-	-	-	-	-
86	OHX	6	2181	-	0,6,6	-	-	-	-	-
86	OHX	5	4232	-	0,6,6	-	-	-	-	-
86	OHX	1	3904	-	0,6,6	-	-	-	-	-
86	OHX	1	4069	-	0,6,6	-	-	-	-	-
86	OHX	1	4130	-	0,6,6	-	-	-	-	-
86	OHX	5	3988	-	0,6,6	-	-	-	-	-
86	OHX	2	2024	-	0,6,6	-	-	-	-	-
86	OHX	1	4060	-	0,6,6	-	-	-	-	-
86	OHX	2	2133	-	0,6,6	-	-	-	-	-
86	OHX	1	3898	-	0,6,6	-	-	-	-	-
86	OHX	1	3973	-	0,6,6	-	-	-	-	-
86	OHX	1	4001	-	0,6,6	-	-	-	-	-
86	OHX	2	2168	-	0,6,6	-	-	-	-	-
86	OHX	1	4010	-	0,6,6	-	-	-	-	-
86	OHX	1	4164	-	0,6,6	-	-	-	-	-
86	OHX	1	4173	-	0,6,6	-	-	-	-	-
86	OHX	6	2148	-	0,6,6	-	-	-	-	-
86	OHX	6	2149	-	0,6,6	-	-	-	-	-
86	OHX	5	4046	-	0,6,6	-	-	-	-	-
86	OHX	5	4141	-	0,6,6	-	-	-	-	-
86	OHX	6	2180	-	0,6,6	-	-	-	-	-
86	OHX	5	4130	-	0,6,6	-	-	-	-	-
86	OHX	1	3867	-	0,6,6	-	-	-	-	-
86	OHX	1	3887	-	0,6,6	-	-	-	-	-
86	OHX	5	3973	-	0,6,6	-	-	-	-	-
86	OHX	5	4010	-	0,6,6	-	-	-	-	-
86	OHX	5	4030	-	0,6,6	-	-	-	-	-
86	OHX	5	3943	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	6	2045	-	0,6,6	-	-	-		
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	N1	201	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	n3	204	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	5	3898	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	m7	206	-	0,6,6	-	-	-		
86	OHX	O7	105	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	n9	102	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	14	402	-	0,6,6	-	-	-		
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	7	227	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	n5	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2142	-	0,6,6	-	-	-	-	-
86	OHX	5	3974	-	0,6,6	-	-	-	-	-
86	OHX	5	4060	-	0,6,6	-	-	-	-	-
86	OHX	2	2114	-	0,6,6	-	-	-	-	-
86	OHX	1	4204	-	0,6,6	-	-	-	-	-
86	OHX	2	2050	-	0,6,6	-	-	-	-	-
86	OHX	3	218	-	0,6,6	-	-	-	-	-
86	OHX	6	2177	-	0,6,6	-	-	-	-	-
86	OHX	1	3965	-	0,6,6	-	-	-	-	-
86	OHX	2	2043	-	0,6,6	-	-	-	-	-
86	OHX	1	3937	-	0,6,6	-	-	-	-	-
86	OHX	2	2054	-	0,6,6	-	-	-	-	-
86	OHX	6	2187	-	0,6,6	-	-	-	-	-
86	OHX	6	2051	-	0,6,6	-	-	-	-	-
86	OHX	2	2091	-	0,6,6	-	-	-	-	-
86	OHX	1	4064	-	0,6,6	-	-	-	-	-
86	OHX	2	2087	-	0,6,6	-	-	-	-	-
86	OHX	1	4084	-	0,6,6	-	-	-	-	-
86	OHX	1	3912	-	0,6,6	-	-	-	-	-
86	OHX	1	3924	-	0,6,6	-	-	-	-	-
86	OHX	1	4198	-	0,6,6	-	-	-	-	-
86	OHX	2	2130	-	0,6,6	-	-	-	-	-
86	OHX	6	2066	-	0,6,6	-	-	-	-	-
86	OHX	5	4011	-	0,6,6	-	-	-	-	-
86	OHX	2	2092	-	0,6,6	-	-	-	-	-
86	OHX	1	3984	-	0,6,6	-	-	-	-	-
86	OHX	1	3890	-	0,6,6	-	-	-	-	-
86	OHX	5	3901	-	0,6,6	-	-	-	-	-
86	OHX	1	3886	-	0,6,6	-	-	-	-	-
86	OHX	5	4064	-	0,6,6	-	-	-	-	-
86	OHX	5	4075	-	0,6,6	-	-	-	-	-
86	OHX	5	4158	-	0,6,6	-	-	-	-	-
86	OHX	1	4150	-	0,6,6	-	-	-	-	-
86	OHX	m0	302	-	0,6,6	-	-	-	-	-
86	OHX	5	3899	-	0,6,6	-	-	-	-	-
86	OHX	5	3902	-	0,6,6	-	-	-	-	-
86	OHX	1	4000	-	0,6,6	-	-	-	-	-
86	OHX	6	2093	-	0,6,6	-	-	-	-	-
86	OHX	s9	201	-	0,6,6	-	-	-	-	-
86	OHX	5	3985	-	0,6,6	-	-	-	-	-
86	OHX	3	214	-	0,6,6	-	-	-	-	-
86	OHX	5	3997	-	0,6,6	-	-	-	-	-
86	OHX	1	4119	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	15	302	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	5	4233	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	L3	402	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	O7	106	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4180	-	0,6,6	-	-	-	-	-
86	OHX	1	4185	-	0,6,6	-	-	-	-	-
86	OHX	5	3963	-	0,6,6	-	-	-	-	-
86	OHX	5	4123	-	0,6,6	-	-	-	-	-
86	OHX	8	223	-	0,6,6	-	-	-	-	-
86	OHX	5	3959	-	0,6,6	-	-	-	-	-
86	OHX	o3	202	-	0,6,6	-	-	-	-	-
86	OHX	5	4121	-	0,6,6	-	-	-	-	-
86	OHX	1	3880	-	0,6,6	-	-	-	-	-
86	OHX	m1	201	-	0,6,6	-	-	-	-	-
86	OHX	5	4079	-	0,6,6	-	-	-	-	-
86	OHX	4	223	-	0,6,6	-	-	-	-	-
86	OHX	6	2108	-	0,6,6	-	-	-	-	-
86	OHX	1	4167	-	0,6,6	-	-	-	-	-
86	OHX	5	4230	-	0,6,6	-	-	-	-	-
86	OHX	5	3957	-	0,6,6	-	-	-	-	-
86	OHX	1	3949	-	0,6,6	-	-	-	-	-
86	OHX	1	4074	-	0,6,6	-	-	-	-	-
86	OHX	2	2041	-	0,6,6	-	-	-	-	-
86	OHX	6	2073	-	0,6,6	-	-	-	-	-
86	OHX	5	4116	-	0,6,6	-	-	-	-	-
86	OHX	5	4216	-	0,6,6	-	-	-	-	-
86	OHX	5	4143	-	0,6,6	-	-	-	-	-
86	OHX	5	4246	-	0,6,6	-	-	-	-	-
86	OHX	C3	201	-	0,6,6	-	-	-	-	-
86	OHX	5	4188	-	0,6,6	-	-	-	-	-
86	OHX	5	4177	-	0,6,6	-	-	-	-	-
86	OHX	1	4133	-	0,6,6	-	-	-	-	-
86	OHX	1	4065	-	0,6,6	-	-	-	-	-
86	OHX	5	4087	-	0,6,6	-	-	-	-	-
86	OHX	5	4145	-	0,6,6	-	-	-	-	-
86	OHX	1	4054	-	0,6,6	-	-	-	-	-
86	OHX	1	3933	-	0,6,6	-	-	-	-	-
86	OHX	4	233	-	0,6,6	-	-	-	-	-
86	OHX	5	4181	-	0,6,6	-	-	-	-	-
86	OHX	1	4194	-	0,6,6	-	-	-	-	-
86	OHX	5	4238	-	0,6,6	-	-	-	-	-
86	OHX	1	4176	-	0,6,6	-	-	-	-	-
86	OHX	5	4091	-	0,6,6	-	-	-	-	-
86	OHX	6	2046	-	0,6,6	-	-	-	-	-
86	OHX	2	2150	-	0,6,6	-	-	-	-	-
86	OHX	6	2101	-	0,6,6	-	-	-	-	-
86	OHX	1	4016	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2180	-	0,6,6	-	-	-	-	-
86	OHX	2	2062	-	0,6,6	-	-	-	-	-
86	OHX	1	4020	-	0,6,6	-	-	-	-	-
86	OHX	m5	304	-	0,6,6	-	-	-	-	-
86	OHX	1	4070	-	0,6,6	-	-	-	-	-
86	OHX	6	2131	-	0,6,6	-	-	-	-	-
86	OHX	2	2181	-	0,6,6	-	-	-	-	-
86	OHX	2	2033	-	0,6,6	-	-	-	-	-
86	OHX	3	225	-	0,6,6	-	-	-	-	-
86	OHX	1	4019	-	0,6,6	-	-	-	-	-
86	OHX	2	2178	-	0,6,6	-	-	-	-	-
86	OHX	5	4156	-	0,6,6	-	-	-	-	-
86	OHX	5	4049	-	0,6,6	-	-	-	-	-
86	OHX	1	4109	-	0,6,6	-	-	-	-	-
86	OHX	2	2157	-	0,6,6	-	-	-	-	-
86	OHX	5	3934	-	0,6,6	-	-	-	-	-
86	OHX	8	215	-	0,6,6	-	-	-	-	-
86	OHX	2	2148	-	0,6,6	-	-	-	-	-
86	OHX	2	2149	-	0,6,6	-	-	-	-	-
86	OHX	1	3931	-	0,6,6	-	-	-	-	-
86	OHX	5	4138	-	0,6,6	-	-	-	-	-
86	OHX	1	4140	-	0,6,6	-	-	-	-	-
86	OHX	6	2074	-	0,6,6	-	-	-	-	-
86	OHX	5	4140	-	0,6,6	-	-	-	-	-
86	OHX	1	4058	-	0,6,6	-	-	-	-	-
86	OHX	2	2069	-	0,6,6	-	-	-	-	-
86	OHX	1	3914	-	0,6,6	-	-	-	-	-
86	OHX	1	3998	-	0,6,6	-	-	-	-	-
86	OHX	6	2048	-	0,6,6	-	-	-	-	-
86	OHX	5	3904	-	0,6,6	-	-	-	-	-
86	OHX	2	2106	-	0,6,6	-	-	-	-	-
86	OHX	2	2147	-	0,6,6	-	-	-	-	-
86	OHX	2	2049	-	0,6,6	-	-	-	-	-
86	OHX	1	4086	-	0,6,6	-	-	-	-	-
86	OHX	1	4168	-	0,6,6	-	-	-	-	-
86	OHX	6	2068	-	0,6,6	-	-	-	-	-
86	OHX	1	3897	-	0,6,6	-	-	-	-	-
86	OHX	5	3911	-	0,6,6	-	-	-	-	-
86	OHX	5	4173	-	0,6,6	-	-	-	-	-
86	OHX	1	4156	-	0,6,6	-	-	-	-	-
86	OHX	5	4228	-	0,6,6	-	-	-	-	-
86	OHX	5	4131	-	0,6,6	-	-	-	-	-
86	OHX	1	4165	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	13	403	-	0,6,6	-	-	-		
86	OHX	1	4200	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	5	4194	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3987	-	0,6,6	-	-	-	-	-
86	OHX	5	4119	-	0,6,6	-	-	-	-	-
86	OHX	1	3869	-	0,6,6	-	-	-	-	-
86	OHX	M7	206	-	0,6,6	-	-	-	-	-
86	OHX	5	4125	-	0,6,6	-	-	-	-	-
86	OHX	6	2166	-	0,6,6	-	-	-	-	-
86	OHX	1	3920	-	0,6,6	-	-	-	-	-
86	OHX	2	2042	-	0,6,6	-	-	-	-	-
86	OHX	5	4179	-	0,6,6	-	-	-	-	-
86	OHX	1	3999	-	0,6,6	-	-	-	-	-
86	OHX	5	4069	-	0,6,6	-	-	-	-	-
86	OHX	5	3940	-	0,6,6	-	-	-	-	-
86	OHX	2	2034	-	0,6,6	-	-	-	-	-
86	OHX	1	4066	-	0,6,6	-	-	-	-	-
86	OHX	5	4201	-	0,6,6	-	-	-	-	-
86	OHX	6	2176	-	0,6,6	-	-	-	-	-
86	OHX	2	2146	-	0,6,6	-	-	-	-	-
86	OHX	1	3960	-	0,6,6	-	-	-	-	-
86	OHX	2	2070	-	0,6,6	-	-	-	-	-
86	OHX	2	2124	-	0,6,6	-	-	-	-	-
86	OHX	5	3920	-	0,6,6	-	-	-	-	-
86	OHX	5	4086	-	0,6,6	-	-	-	-	-
86	OHX	1	3969	-	0,6,6	-	-	-	-	-
86	OHX	1	3957	-	0,6,6	-	-	-	-	-
86	OHX	SR	401	-	0,6,6	-	-	-	-	-
86	OHX	5	4042	-	0,6,6	-	-	-	-	-
86	OHX	5	4066	-	0,6,6	-	-	-	-	-
86	OHX	5	3960	-	0,6,6	-	-	-	-	-
86	OHX	8	229	-	0,6,6	-	-	-	-	-
86	OHX	1	4107	-	0,6,6	-	-	-	-	-
86	OHX	1	4199	-	0,6,6	-	-	-	-	-
86	OHX	6	2146	-	0,6,6	-	-	-	-	-
86	OHX	5	3941	-	0,6,6	-	-	-	-	-
86	OHX	6	2123	-	0,6,6	-	-	-	-	-
86	OHX	5	4041	-	0,6,6	-	-	-	-	-
86	OHX	3	224	-	0,6,6	-	-	-	-	-
86	OHX	5	4095	-	0,6,6	-	-	-	-	-
86	OHX	6	2167	-	0,6,6	-	-	-	-	-
86	OHX	2	2105	-	0,6,6	-	-	-	-	-
86	OHX	5	3916	-	0,6,6	-	-	-	-	-
86	OHX	5	4104	-	0,6,6	-	-	-	-	-
86	OHX	1	4028	-	0,6,6	-	-	-	-	-
86	OHX	1	4112	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	1	4209	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2043	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	7	228	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	8	214	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	1	4211	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	13	404	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	o2	201	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	M8	201	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	q1	102	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	4	238	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	1	4210	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	m0	301	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	O3	201	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	14	403	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	5	4218	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	5	4178	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	d4	202	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	s8	304	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	Q2	503	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
86	OHX	15	303	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	1	4197	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	M7	207	-	0,6,6	-	-	-		
88	3KF	1	4212	85	25,25,25	0.85	0	30,39,39	0.93	1 (3%)
86	OHX	n3	203	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	1	4208	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	1	4117	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
88	3KF	5	4248	85	25,25,25	0.60	0	30,39,39	0.98	2 (6%)
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	7	225	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	6	2044	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		
86	OHX	15	304	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	1	4161	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	5	3897	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	L4	402	-	0,6,6	-	-	-		
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	M9	202	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	4	222	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	m6	204	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4081	-	0,6,6	-	-	-	-	-
86	OHX	5	3993	-	0,6,6	-	-	-	-	-
86	OHX	5	4103	-	0,6,6	-	-	-	-	-
86	OHX	5	4105	-	0,6,6	-	-	-	-	-
86	OHX	5	4134	-	0,6,6	-	-	-	-	-
86	OHX	6	2112	-	0,6,6	-	-	-	-	-
86	OHX	1	3925	-	0,6,6	-	-	-	-	-
86	OHX	5	3976	-	0,6,6	-	-	-	-	-
86	OHX	5	4169	-	0,6,6	-	-	-	-	-
86	OHX	2	2165	-	0,6,6	-	-	-	-	-
86	OHX	5	4115	-	0,6,6	-	-	-	-	-
86	OHX	5	4235	-	0,6,6	-	-	-	-	-
86	OHX	19	202	-	0,6,6	-	-	-	-	-
86	OHX	6	2116	-	0,6,6	-	-	-	-	-
86	OHX	1	4011	-	0,6,6	-	-	-	-	-
86	OHX	5	4211	-	0,6,6	-	-	-	-	-
86	OHX	6	2141	-	0,6,6	-	-	-	-	-
86	OHX	sR	401	-	0,6,6	-	-	-	-	-
86	OHX	6	2171	-	0,6,6	-	-	-	-	-
86	OHX	5	4025	-	0,6,6	-	-	-	-	-
86	OHX	5	4061	-	0,6,6	-	-	-	-	-
86	OHX	5	3970	-	0,6,6	-	-	-	-	-
86	OHX	5	4192	-	0,6,6	-	-	-	-	-
86	OHX	5	4223	-	0,6,6	-	-	-	-	-
86	OHX	1	4116	-	0,6,6	-	-	-	-	-
86	OHX	5	4012	-	0,6,6	-	-	-	-	-
86	OHX	5	4243	-	0,6,6	-	-	-	-	-
86	OHX	2	2163	-	0,6,6	-	-	-	-	-
86	OHX	2	2125	-	0,6,6	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	3KF	5	4248	85	-	-	0/4/4/4
88	3KF	1	4212	85	-	-	0/4/4/4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4212	3KF	O3-C11-C12	-2.66	103.48	109.01
88	5	4248	3KF	C5-C4-C13	2.26	122.00	119.22
88	5	4248	3KF	O4-C10-C11	-2.09	105.53	110.35

There are no chirality outliers.

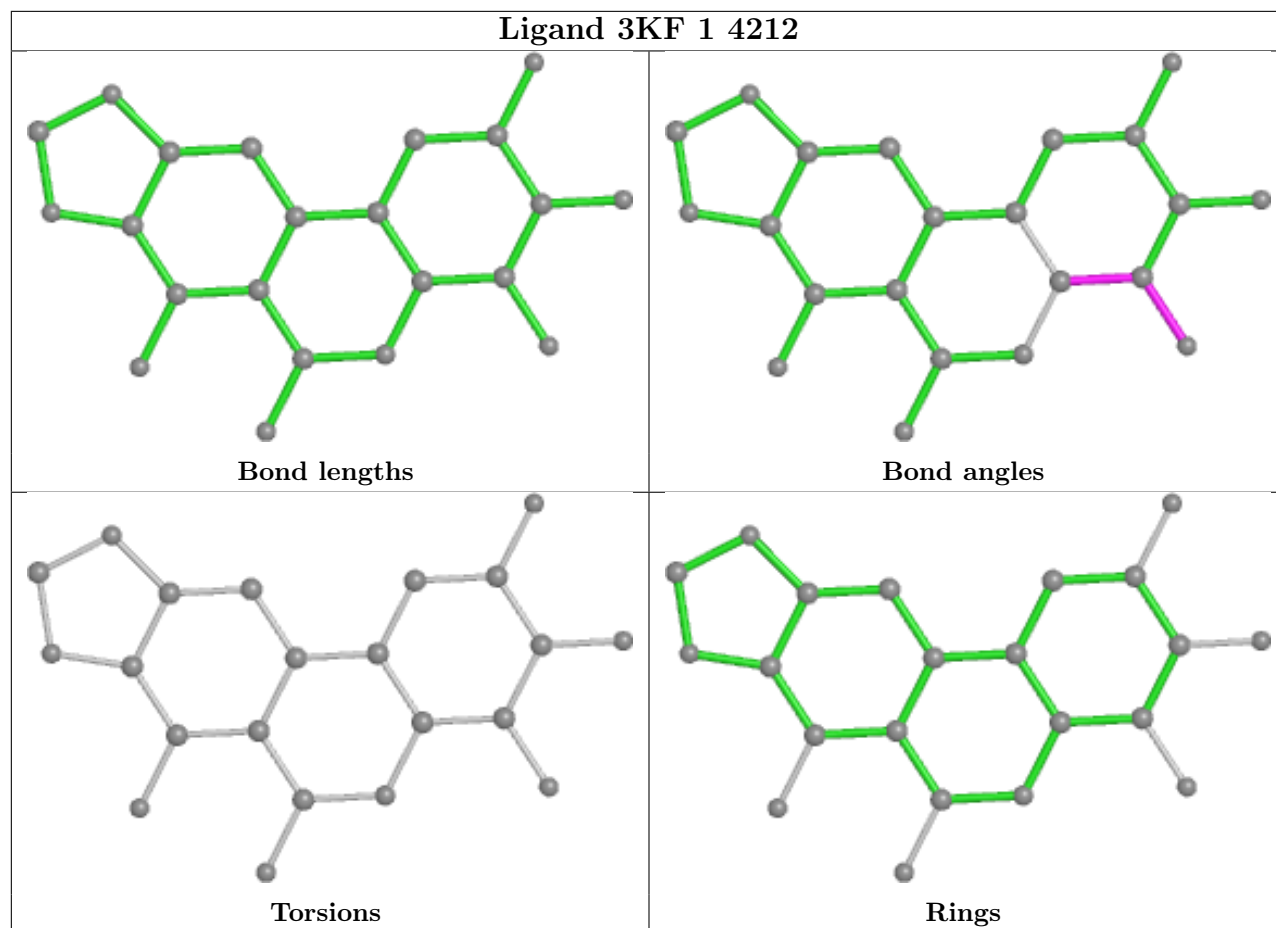
There are no torsion outliers.

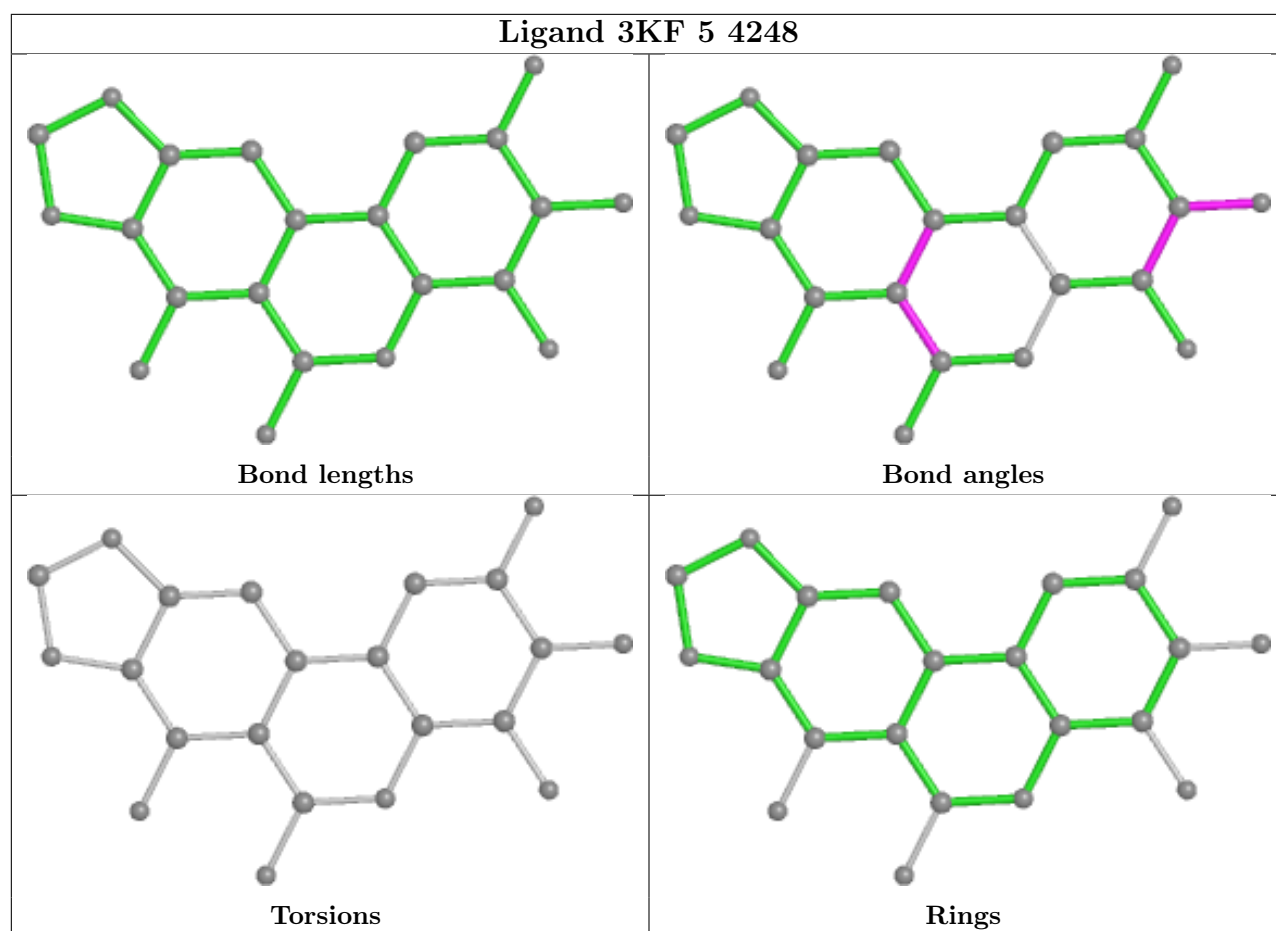
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2162	OHX	0	1
86	5	3939	OHX	0	1

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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.