



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 05:45 pm GMT

PDB ID : 4U53
Title : Crystal structure of Deoxynivalenol bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.30 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

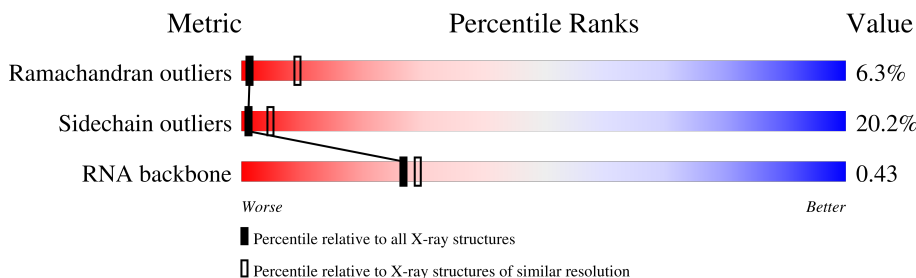
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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	63% (green), 30% (yellow), 7% (orange), 0% (red), 0% (grey)
1	6	1800	62% (green), 33% (yellow), 5% (orange), 0% (red), 0% (grey)
2	S0	251	62% (green), 19% (yellow), 18% (grey), 0% (orange), 0% (red)
2	s0	251	63% (green), 17% (yellow), 18% (grey), 0% (orange), 0% (red)
3	S1	254	60% (green), 21% (yellow), 16% (grey), 0% (orange), 0% (red)
3	s1	254	66% (green), 18% (yellow), 15% (grey), 0% (orange), 0% (red)
4	S2	253	65% (green), 21% (yellow), 14% (grey), 0% (orange), 0% (red)
4	s2	253	62% (green), 23% (yellow), 14% (grey), 0% (orange), 0% (red)









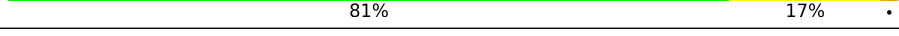

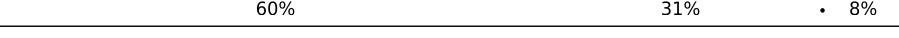
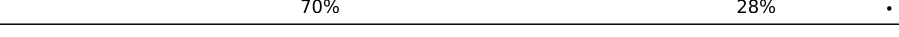

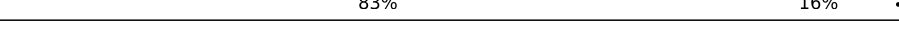


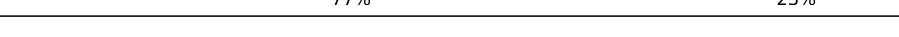

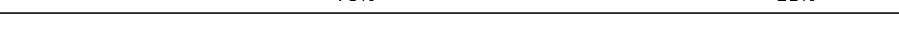






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Mol	Chain	Length	Quality of chain
5	S3	239	72% 20% 7%
5	s3	239	71% 21% 7%
6	S4	260	79% 19%
6	s4	260	80% 18%
7	S5	224	73% 17% 8%
7	s5	224	72% 19% 8%
8	S6	236	78% 18%
8	s6	236	74% 17% 8%
9	S7	189	74% 21% . .
9	s7	189	72% 24% . .
10	S8	200	73% 19% 6%
10	s8	200	77% 16% 6%
11	S9	196	70% 23% 6%
11	s9	196	69% 23% 6%
12	C0	105	72% 18% 9%
12	c0	105	68% 20% 9%
13	C1	155	79% 20%
13	c1	155	75% 18% 6%
14	C2	142	59% 24% 13%
14	c2	142	64% 22% 13%
15	C3	150	78% 20%
15	c3	150	70% 29%
16	C4	136	73% 17% 7%
16	c4	136	67% 26% 6%
17	C5	141	71% 15% 12%

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Mol	Chain	Length	Quality of chain
17	c5	141	 76% 17% . .
18	C6	142	 73% 26% ..
18	c6	142	 74% 25% .
19	C7	136	 67% 16% 5% 12%
19	c7	136	 68% 16% . 14%
20	C8	145	 77% 21% .
20	c8	145	 75% 22% .
21	C9	143	 80% 18% .
21	c9	143	 81% 17% .
22	D0	120	 69% 20% 11%
22	d0	120	 60% 31% . 8%
23	D1	87	 70% 28% .
23	d1	87	 69% 30% .
24	D2	129	 83% 16% .
24	d2	129	 88% 10% .
25	D3	144	 79% 19% .
25	d3	144	 77% 23%
26	D4	134	 82% 17% .
26	d4	134	 78% 21% .
27	D5	107	 38% 25% . 35%
27	d5	107	 54% 10% 36%
28	D6	97	 62% 32% 6%
28	d6	97	 71% 26% .
29	D7	81	 80% 19% .
29	d7	81	 85% 14% .

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Mol	Chain	Length	Quality of chain
30	D8	66	71% 23% 5%
30	d8	66	73% 21% 5%
31	D9	55	80% 16%
31	d9	55	67% 25%
32	E0	60	83% 13%
33	E1	76	51% 34% 8% 7%
33	e1	76	57% 38%
34	SR	318	86% 14%
34	sR	318	85% 15%
35	SM	273	42% 15% 42%
35	sM	273	29% 9% 62%
36	1	3396	50% 35% 8% 7%
36	5	3396	48% 37% 8% 7%
37	3	121	69% 29%
37	7	121	57% 35% 8%
38	4	158	55% 39% 6%
38	8	158	63% 32%
39	L2	253	79% 19%
39	l2	253	77% 22%
40	L3	386	78% 20%
40	l3	386	78% 20%
41	L4	361	76% 20%
41	l4	361	76% 23%
42	L5	296	80% 18%
42	l5	296	78% 19%

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Mol	Chain	Length	Quality of chain
43	L6	175	75% 14% 11%
43	l6	175	75% 14% 10%
44	L7	243	79% 11% 9%
44	l7	243	77% 13% 8%
45	L8	255	70% 21% 9%
45	l8	255	71% 19% 9%
46	L9	191	78% 21% .
46	l9	191	74% 25% .
47	M0	220	75% 20% ..
47	m0	220	75% 20% ..
48	M1	173	72% 22% ..
48	m1	173	71% 25% ..
49	M3	198	80% 17% ..
49	m3	198	76% 21% ..
50	M4	137	80% 19% ..
50	m4	137	82% 18%
51	M5	203	81% 19%
51	m5	203	80% 20%
52	M6	198	83% 16% ..
52	m6	198	78% 20% ...
53	M7	183	78% 22% .
53	m7	183	70% 15% 15%
54	M8	185	87% 13%
54	m8	185	79% 19% .
55	M9	188	83% 17%









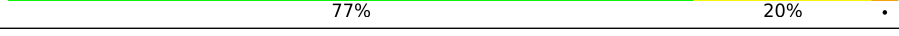

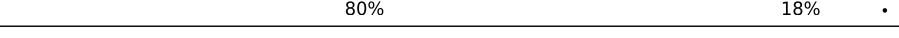
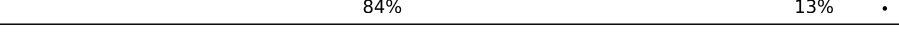

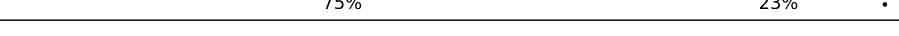


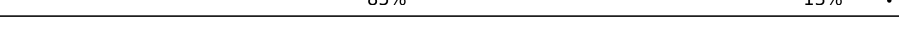

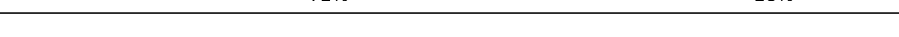






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Mol	Chain	Length	Quality of chain
55	m9	188	84% 16%
56	N0	172	78% 20% .
56	n0	172	78% 22% .
57	N1	159	81% 18% .
57	n1	159	77% 20% .
58	N2	120	68% 15% 17%
58	n2	120	63% 18% 18%
59	N3	136	82% 18%
59	n3	136	88% 12%
60	N4	155	55% 8% . 37%
60	n4	155	70% 15% . 13%
61	N5	141	68% 18% 14%
61	n5	141	63% 22% 15%
62	N6	126	77% 21% .
62	n6	126	79% 21% .
63	N7	135	75% 25%
63	n7	135	76% 23% .
64	N8	148	81% 17% .
64	n8	148	79% 20% .
65	N9	58	79% 19% .
65	n9	58	72% 26% .
66	O0	104	73% 19% . 7%
66	o0	104	79% 17% .
67	O1	112	77% 17% . .
67	o1	112	68% 27% . .

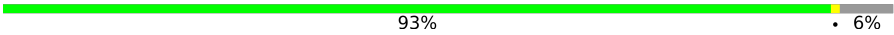

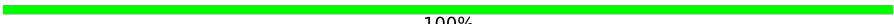

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Mol	Chain	Length	Quality of chain
68	O2	129	 77% 22%
68	o2	129	 76% 20%
69	O3	106	 84% 14%
69	o3	106	 80% 17%
70	O4	119	 74% 18% 6%
70	o4	119	 72% 22% 6%
71	O5	119	 82% 17%
71	o5	119	 78% 21%
72	O6	99	 77% 20%
72	o6	99	 70% 30%
73	O7	87	 80% 18%
73	o7	87	 84% 13%
74	O8	77	 73% 27%
74	o8	77	 75% 23%
75	O9	50	 82% 18%
75	o9	50	 84% 16%
76	Q0	52	 85% 13%
76	q0	52	 69% 29%
77	Q1	25	 72% 28%
77	q1	25	 64% 32%
78	Q2	105	 72% 26%
78	q2	105	 82% 17%
79	Q3	91	 79% 21%
79	q3	91	 79% 20%
80	e0	62	 71% 27%

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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 411183 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
5	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
5	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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	1214	775	230	206	3	0	0	0
13	c1	146	1168	747	221	197	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	L3	386	Total 3075	C 1950	N 584	O 533	S 8	0	0	0
40	l3	386	Total 3075	C 1950	N 584	O 533	S 8	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	L8	233	Total 1804	C 1151	N 323	O 327	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
56	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

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

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

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

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

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

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

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

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

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

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

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

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

- 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 1020	C 647	N 205	O 167	S 1	0	0	0
68	o2	127	Total 1020	C 647	N 205	O 167	S 1	0	0	0

- 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 850	C 540	N 165	O 144	S 1	0	0	0
69	o3	106	Total 850	C 540	N 165	O 144	S 1	0	0	0

- 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 880	C 545	N 179	O 152	S 4	0	0	0
70	o4	112	Total 880	C 545	N 179	O 152	S 4	0	0	0

- 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 969	C 615	N 186	O 167	S 1	0	0	0
71	o5	119	Total 965	C 612	N 185	O 167	S 1	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O	0	0	0
			612	391	115	106			
74	o8	77	Total	C	N	O	0	0	0
			608	388	114	106			

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called Unknown Protein m2.

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

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

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

- Molecule 83 is a protein called Unknown Protein p1.

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

- Molecule 84 is a protein called Unknown Protein p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	123	Total	Mg	0	0
			123	123		
85	S2	1	Total	Mg	0	0
			1	1		
85	S8	1	Total	Mg	0	0
			1	1		
85	C3	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	1	471	Total	Mg	0	0
			471	471		
85	3	14	Total	Mg	0	0
			14	14		
85	4	20	Total	Mg	0	0
			20	20		
85	L2	3	Total	Mg	0	0
			3	3		
85	L3	3	Total	Mg	0	0
			3	3		
85	L4	2	Total	Mg	0	0
			2	2		
85	L5	1	Total	Mg	0	0
			1	1		
85	L7	2	Total	Mg	0	0
			2	2		
85	L8	1	Total	Mg	0	0
			1	1		
85	M0	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	M1	1	Total Mg 1 1	0	0
85	M3	3	Total Mg 3 3	0	0
85	M5	2	Total Mg 2 2	0	0
85	M6	1	Total Mg 1 1	0	0
85	M7	4	Total Mg 4 4	0	0
85	M9	2	Total Mg 2 2	0	0
85	N0	2	Total Mg 2 2	0	0
85	N3	3	Total Mg 3 3	0	0
85	N5	1	Total Mg 1 1	0	0
85	N8	5	Total Mg 5 5	0	0
85	O2	2	Total Mg 2 2	0	0
85	O3	1	Total Mg 1 1	0	0
85	O7	1	Total Mg 1 1	0	0
85	6	147	Total Mg 147 147	0	0
85	s1	1	Total Mg 1 1	0	0
85	s8	2	Total Mg 2 2	0	0
85	s9	1	Total Mg 1 1	0	0
85	c1	1	Total Mg 1 1	0	0
85	c7	1	Total Mg 1 1	0	0
85	c8	2	Total Mg 2 2	0	0
85	d3	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	d6	1	Total 1	Mg 1	0	0
85	sM	2	Total 2	Mg 2	0	0
85	5	496	Total 496	Mg 496	0	0
85	7	18	Total 18	Mg 18	0	0
85	8	15	Total 15	Mg 15	0	0
85	l2	2	Total 2	Mg 2	0	0
85	l3	3	Total 3	Mg 3	0	0
85	l4	1	Total 1	Mg 1	0	0
85	l5	3	Total 3	Mg 3	0	0
85	l7	2	Total 2	Mg 2	0	0
85	l9	1	Total 1	Mg 1	0	0
85	m0	1	Total 1	Mg 1	0	0
85	m1	1	Total 1	Mg 1	0	0
85	m5	2	Total 2	Mg 2	0	0
85	m6	2	Total 2	Mg 2	0	0
85	m7	5	Total 5	Mg 5	0	0
85	n0	2	Total 2	Mg 2	0	0
85	n3	2	Total 2	Mg 2	0	0
85	n6	2	Total 2	Mg 2	0	0
85	n8	2	Total 2	Mg 2	0	0
85	n9	1	Total 1	Mg 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	S6	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	D3	1	7	6	1	0	0
86	D9	1	7	6	1	0	0
86	SR	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	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

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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	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	M9	1	7	6	1	0	0
86	N9	1	7	6	1	0	0
86	O1	1	7	6	1	0	0
86	O3	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	O4	1	7	6	1	0	0
86	O6	1	7	6	1	0	0
86	O7	1	7	6	1	0	0
86	O9	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

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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	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	s8	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
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

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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	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	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	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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	m6	1	7	6	1	0	0
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	n6	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	o7	1	7	6	1	0	0
86	o7	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).

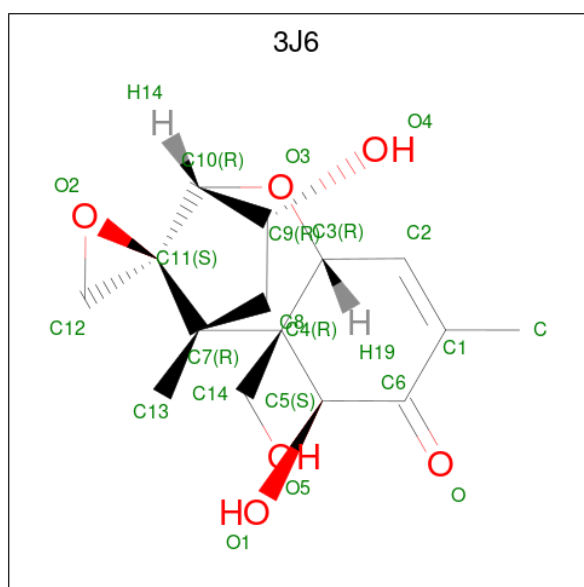
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
87	D6	1	1	1	0	0
87	D7	1	1	1	0	0
87	D9	1	1	1	0	0
87	E1	1	1	1	0	0
87	O7	1	1	1	0	0
87	Q0	1	1	1	0	0
87	Q2	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	Q3	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0	0
			1	1		
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 (3beta,7alpha)-3,7,15-trihydroxy-12,13-epoxytrichothec-9-en-8-one (three-letter code: 3J6) (formula: C₁₅H₂₀O₆).



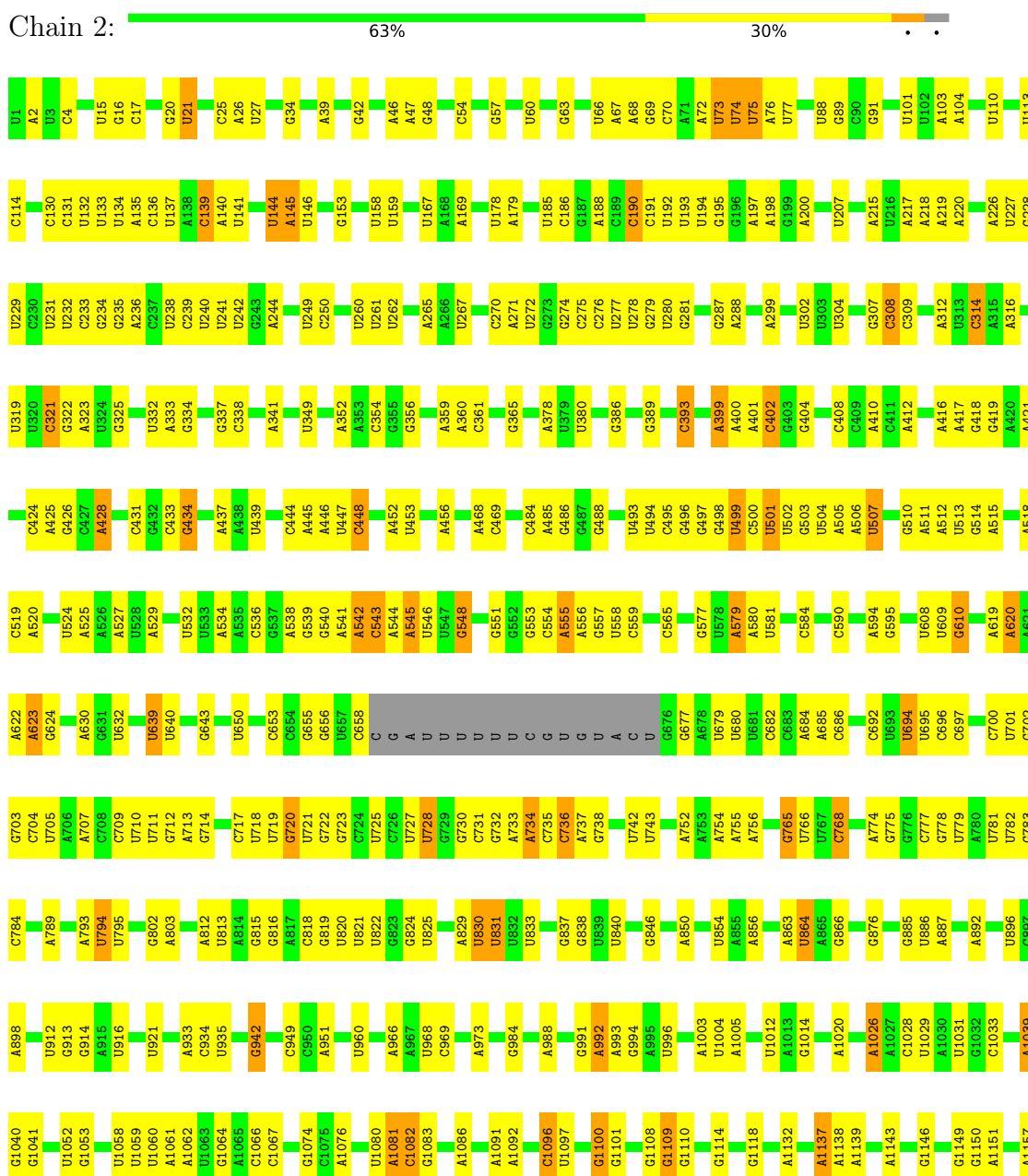
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	C	O	0	0
			21	15	6		
88	5	1	Total	C	O	0	0
			21	15	6		

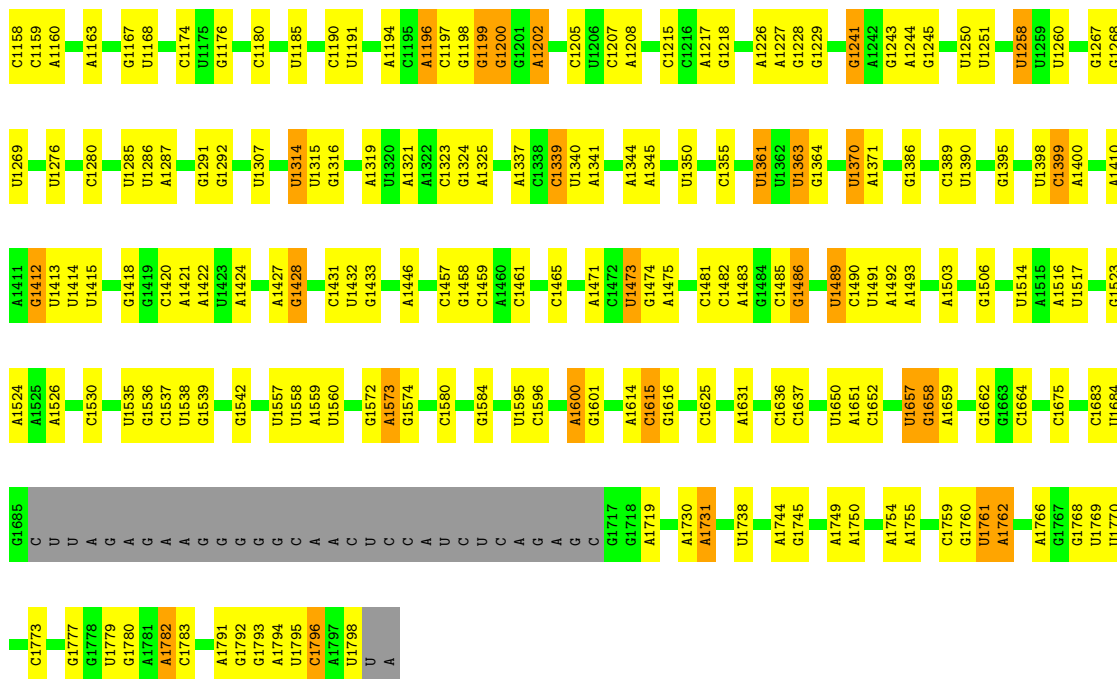
3 Residue-property plots

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.

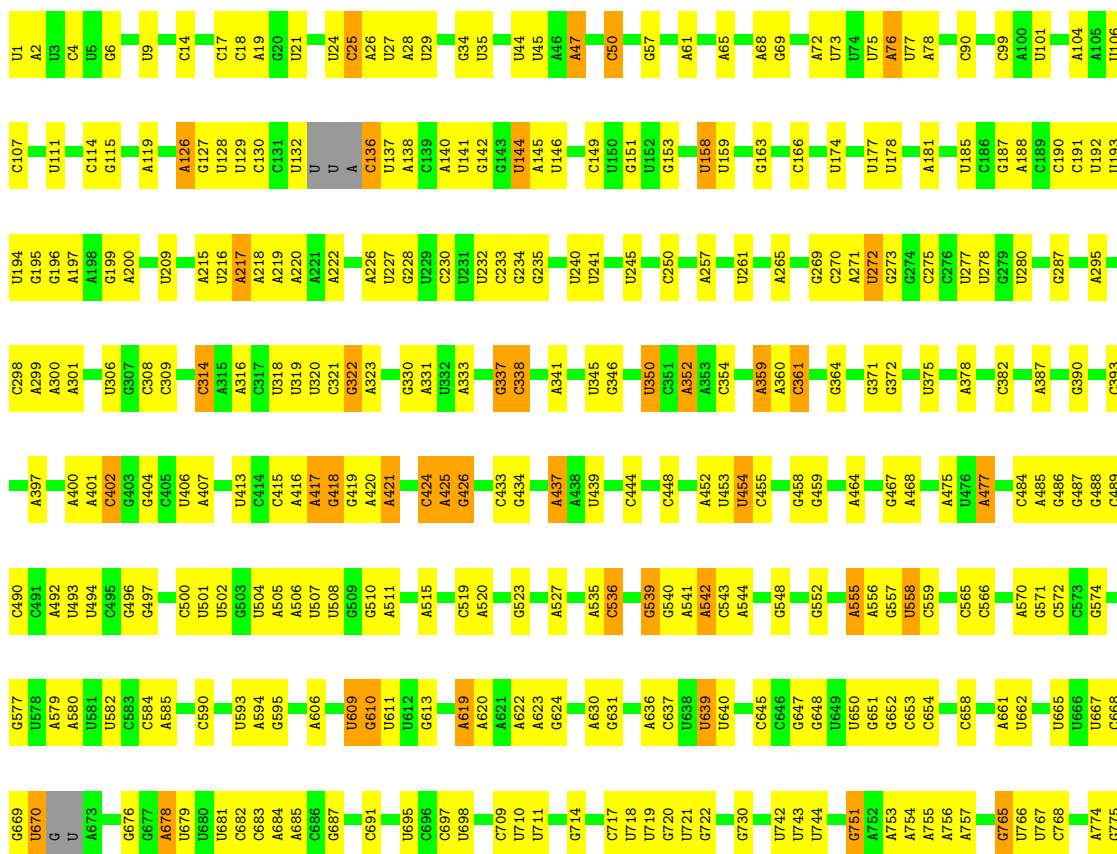
Note EDS failed to run properly.

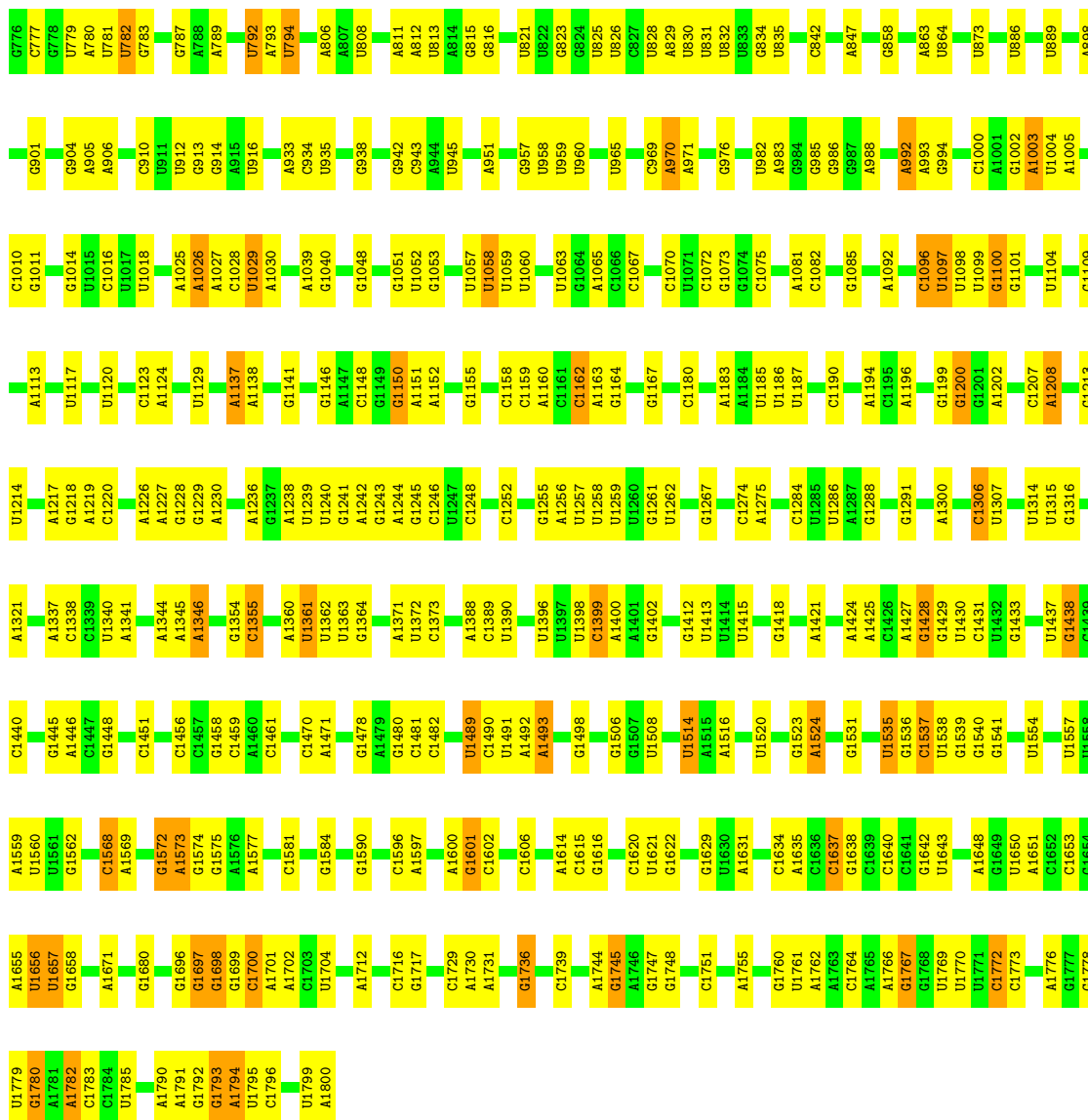
- Molecule 1: 18S ribosomal RNA



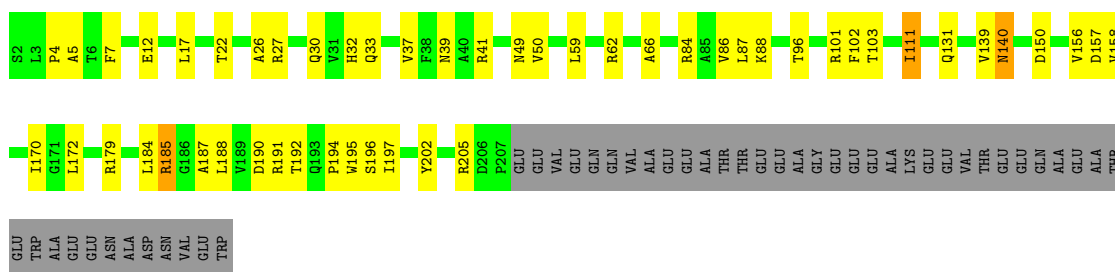


• Molecule 1: 18S ribosomal RNA



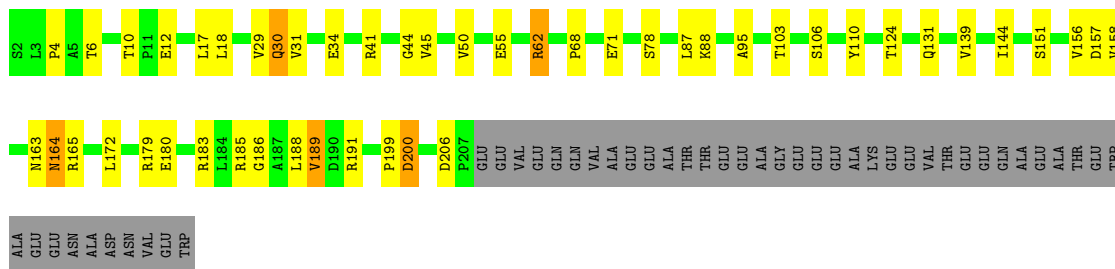


• Molecule 2: 40S ribosomal protein S0-A

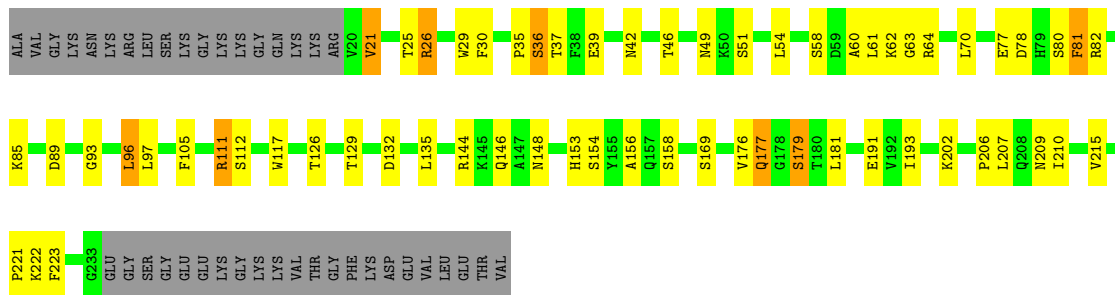


• Molecule 2: 40S ribosomal protein S0-A

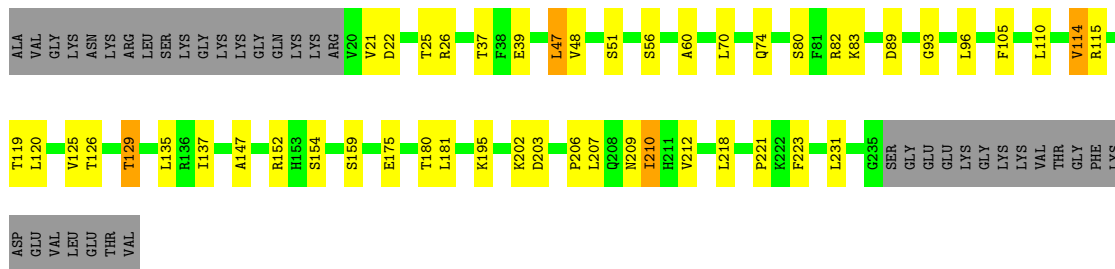




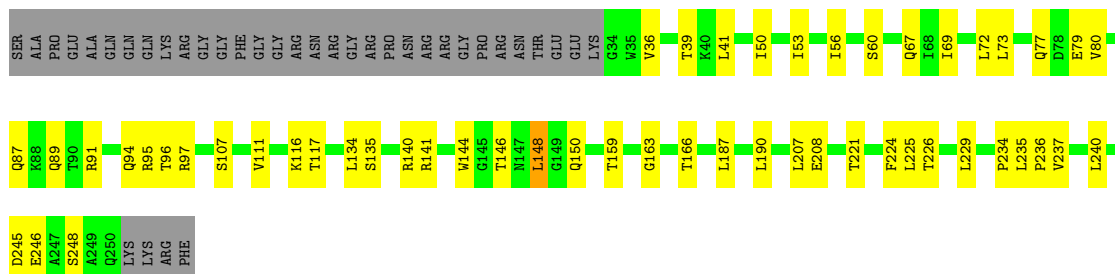
• Molecule 3: 40S ribosomal protein S1-A



• Molecule 3: 40S ribosomal protein S1-A

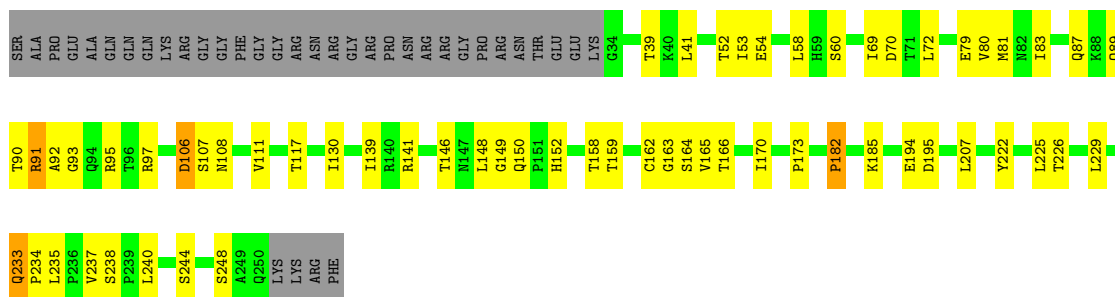


• Molecule 4: 40S ribosomal protein S2



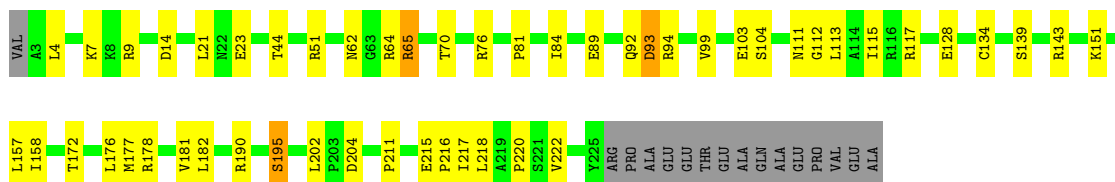
• Molecule 4: 40S ribosomal protein S2

Chain s2:  62% 23% 14%



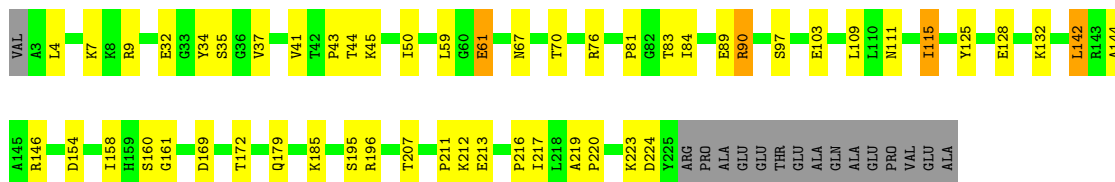
• Molecule 5: 40S ribosomal protein S3

Chain S3:  72% 20% 7%




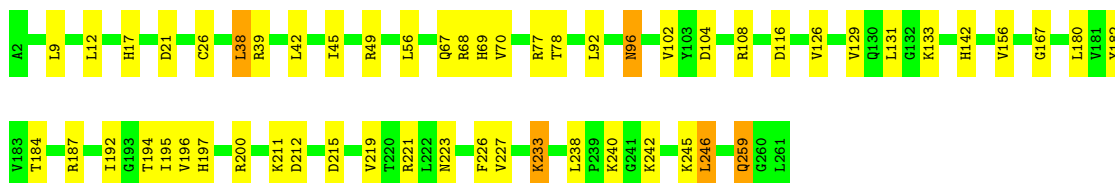
• Molecule 5: 40S ribosomal protein S3

Chain s3:  71% 21% 7%




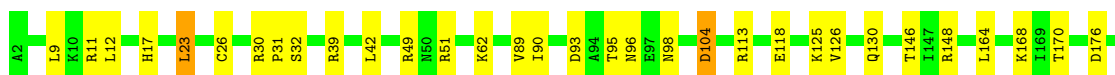
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:  79% 19% 2%



• Molecule 6: 40S ribosomal protein S4-A

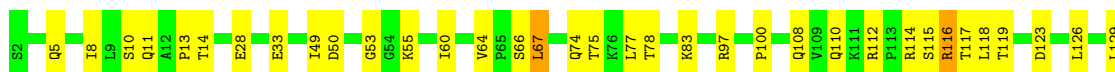
Chain s4:  80% 18% 2%





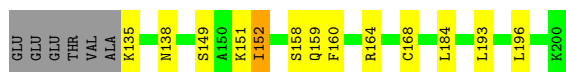
- Molecule 9: 40S ribosomal protein S7-A

Chain s7: 72% 24%



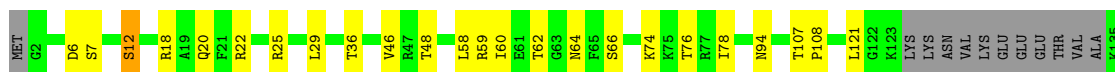
- Molecule 10: 40S ribosomal protein S8-A

Chain S8: 73% 19% 6%



- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 77% 16% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 70% 23% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 69% 23% 6%

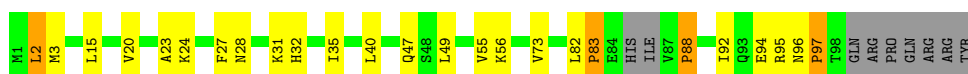




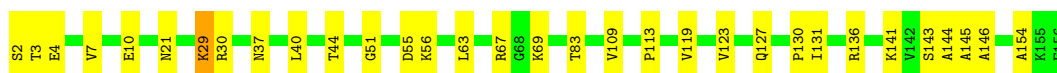
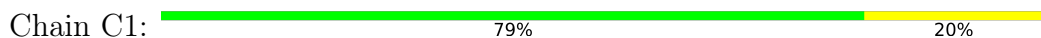
- Molecule 12: 40S ribosomal protein S10-A



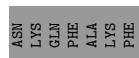
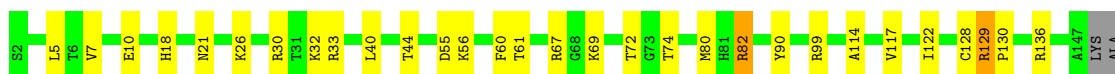
- Molecule 12: 40S ribosomal protein S10-A



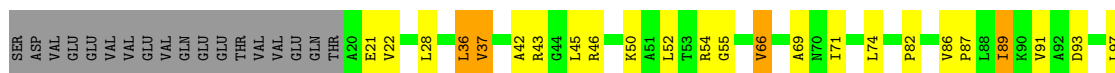
- Molecule 13: 40S ribosomal protein S11-A



- Molecule 13: 40S ribosomal protein S11-A



- Molecule 14: 40S ribosomal protein S12



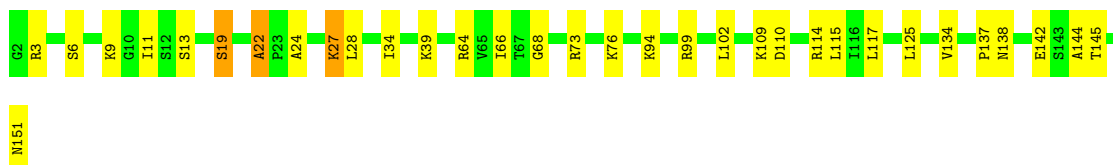
- Molecule 14: 40S ribosomal protein S12





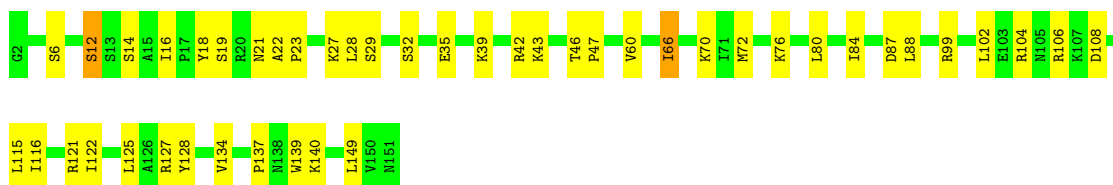
- Molecule 15: 40S ribosomal protein S13

Chain C3: 78% 20%



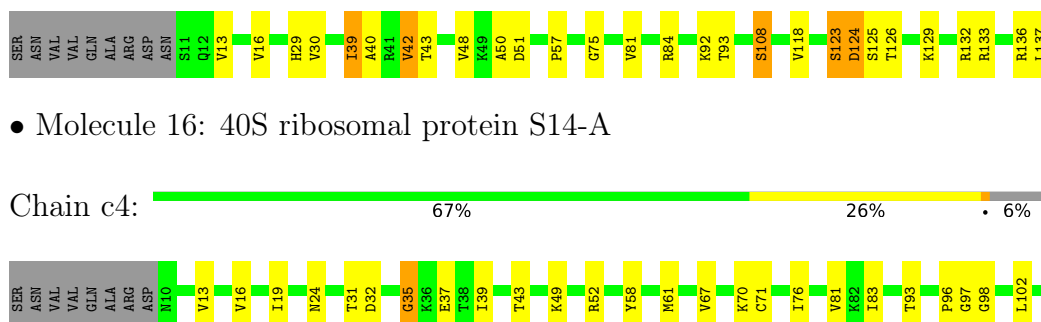
- Molecule 15: 40S ribosomal protein S13

Chain c3: 70% 29%



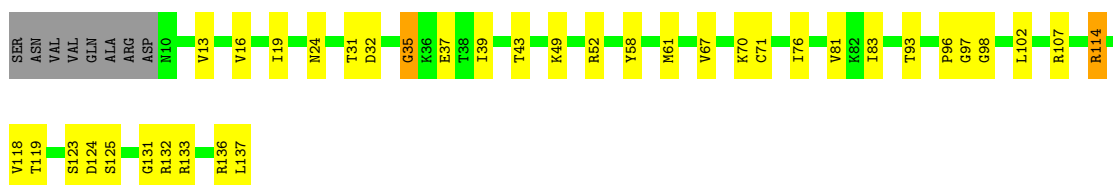
- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 73% 17% 7%



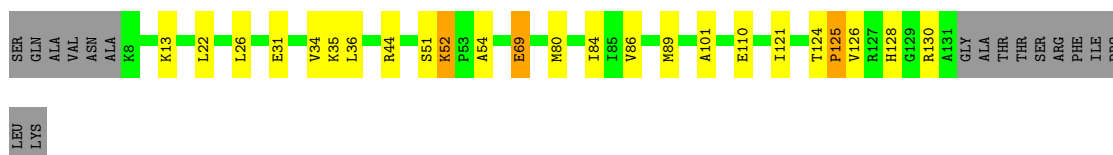
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 67% 26% 6%




- Molecule 17: 40S ribosomal protein S15

Chain C5: 71% 15% 12%



- Molecule 17: 40S ribosomal protein S15

Chain c5:  76% 17%



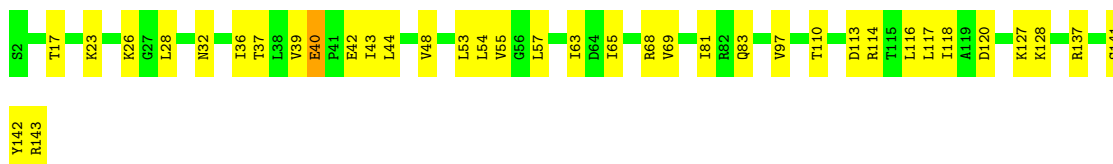
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:  73% 26%



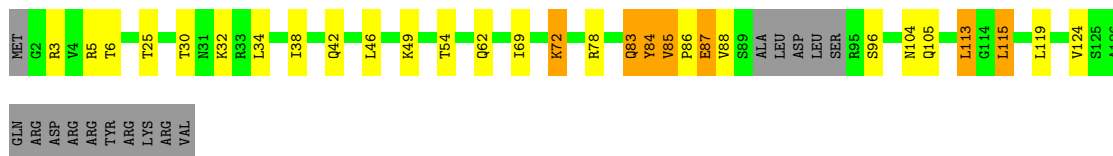
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:  74% 25%



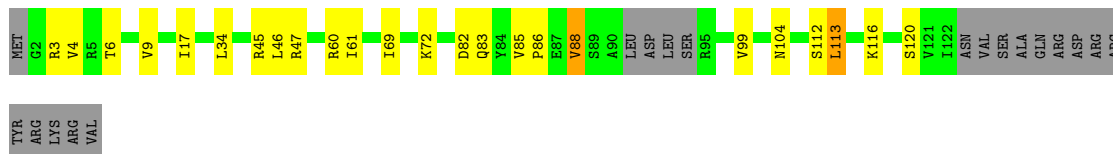
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:  67% 16% 5% 12%




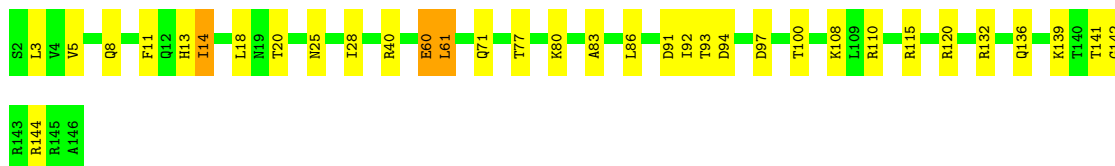
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:  68% 16% 1% 14%



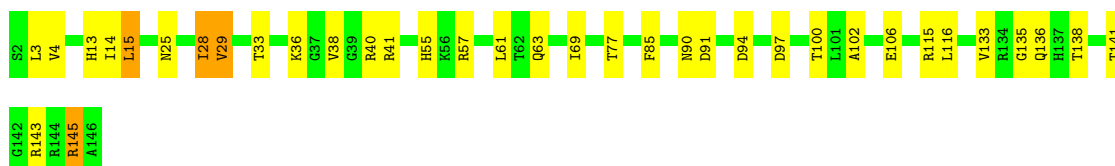
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:  77% 21%



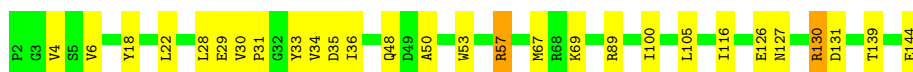
- Molecule 20: 40S ribosomal protein S18-A

Chain c8: 75% 22%



- Molecule 21: 40S ribosomal protein S19-A

Chain C9: 80% 18%



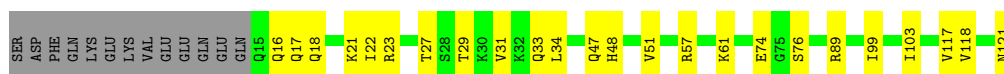
- Molecule 21: 40S ribosomal protein S19-A

Chain c9: 81% 17%



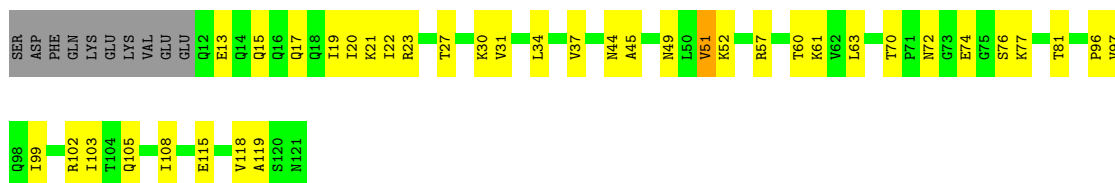
- Molecule 22: 40S ribosomal protein S20

Chain D0: 69% 20% 11%



- Molecule 22: 40S ribosomal protein S20

Chain d0: 60% 31% 8%



- Molecule 23: 40S ribosomal protein S21-A

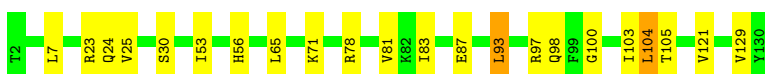
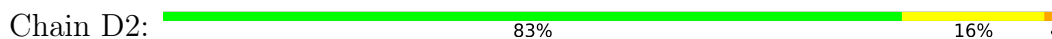
Chain D1: 70% 28%



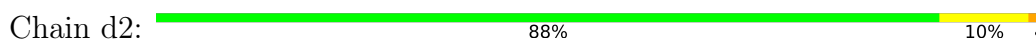
- Molecule 23: 40S ribosomal protein S21-A



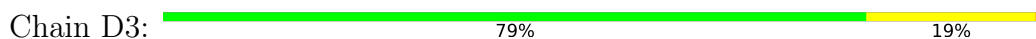
- Molecule 24: 40S ribosomal protein S22-A



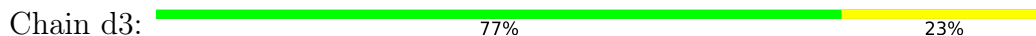
- Molecule 24: 40S ribosomal protein S22-A



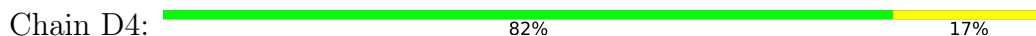
- Molecule 25: 40S ribosomal protein S23-A



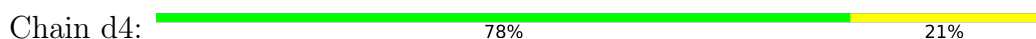
- Molecule 25: 40S ribosomal protein S23-A



- Molecule 26: 40S ribosomal protein S24-A

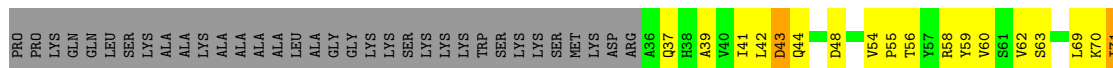
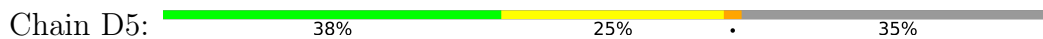


- Molecule 26: 40S ribosomal protein S24-A

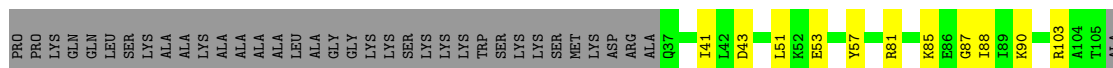




• Molecule 27: 40S ribosomal protein S25-A



• Molecule 27: 40S ribosomal protein S25-A



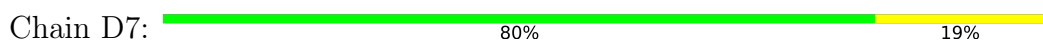
• Molecule 28: 40S ribosomal protein S26-B



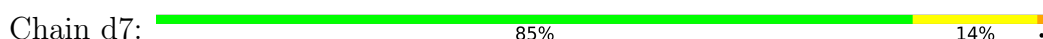
• Molecule 28: 40S ribosomal protein S26-B



• Molecule 29: 40S ribosomal protein S27-A

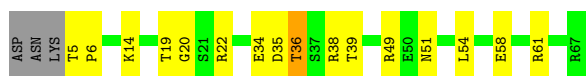


• Molecule 29: 40S ribosomal protein S27-A



- Molecule 30: 40S ribosomal protein S28-A

Chain D8:  71% 23% 5%




- Molecule 30: 40S ribosomal protein S28-A

Chain d8:  73% 21% 5%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9:  80% 16% 4%




- Molecule 31: 40S ribosomal protein S29-A

Chain d9:  67% 25% 8%



- Molecule 32: 40S ribosomal protein S30-A

Chain E0:  83% 13% 4%



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:  51% 34% 8% 7%



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:  57% 38% 5% 2%



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

Chain 1: 50% 35% 8% 7%

G	U	U3	U4	G5	U9	A13	U14	C15	A16	G22	A23	G24	U25	A26	C27	C28	C29	G33	A34	A35	G36	U37	U38	A39	A40	A43	U44	C47	A48	A49	G53	C54	G55	G56	A57	G58	G59	A60	A61	A62	A63	G64	A65	A66	G67	C68	C69	A70	A71	C72	C73	G74																																																																																																																																																																																																																																							
G75	G76	G80	G81	G83	G89	G92	C93	G94	A95	G96	A99	A100	G101	G104	C105	A106	A107	G108	A109	A110	C111	U112	C113	A114	A115	G120	A121	A122	G128	C131	C132	U133	G134	U135	G136	G145	G156	A157	G160	C166	G167	U169	A187	U188	G189	U190	G191																																																																																																																																																																																																																																												
C192	U195	G196	G197	A198	A199	C200	G203	C204	A211	G212	A213	U217	G218	A219	G220	A221	C225	G226	G227	U228	G232	A235	G239	U240	G241	C242	G243	U244	U245	U246	U247	U248	C249	G250	G251	U252	U262	C263	G267	A268	C269	G274	U279	U280	G281	C282	G283																																																																																																																																																																																																																																												
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U	G	U	C	U	C	U	C	C	C	U	U	U	U	U	U	A	G	G	G	G	U	C	U	C	C	C	C	A	U	U	U	U	C	G	G	A	A	U	U	U	U	U	U	U	U	U	U	U	U	U																																																																																																																																																																																																																																									
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U993	U994	U995	U996	U997	U998	U999	U1000
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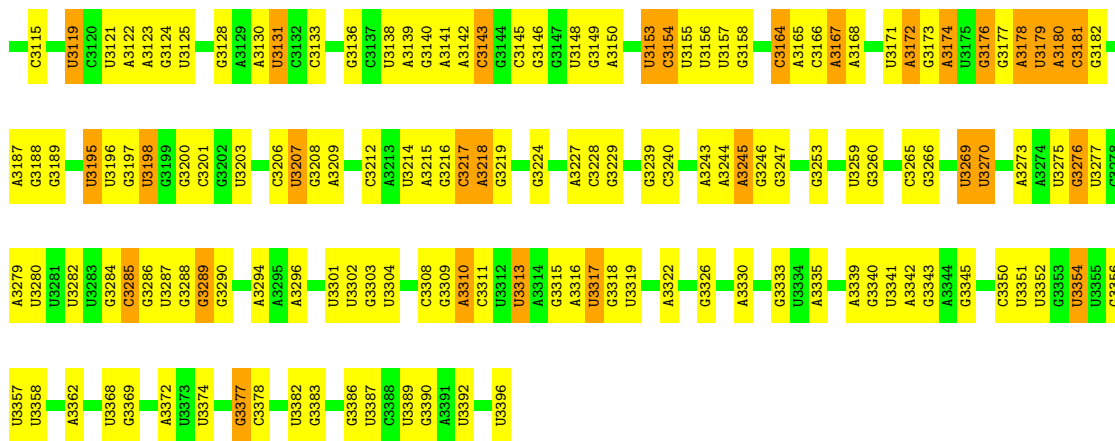
● Molecule 36: 25S ribosomal RNA

Chain 5: 48% 37% 8% 7%

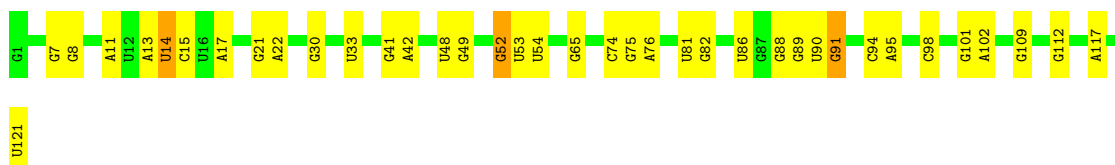
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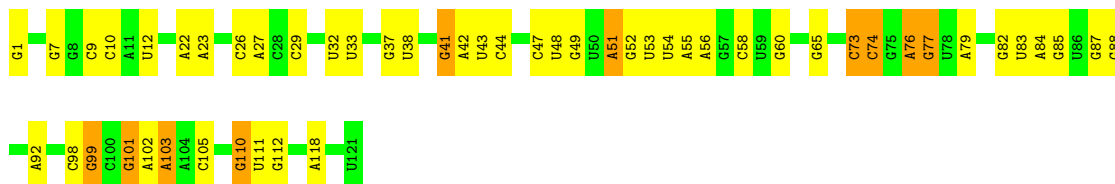
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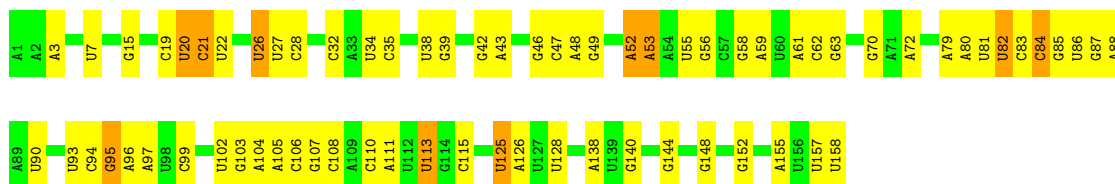
• Molecule 37: 5S ribosomal RNA



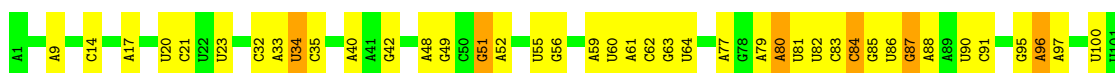
• Molecule 37: 5S ribosomal RNA



• Molecule 38: 5.8S ribosomal RNA



• Molecule 38: 5.8S ribosomal RNA





- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 79% 19%



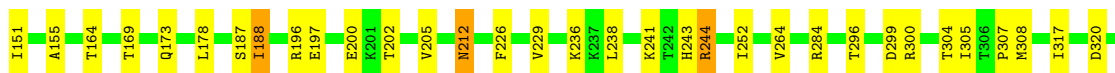
- Molecule 39: 60S ribosomal protein L2-A

Chain l2: 77% 22%



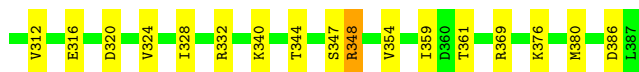
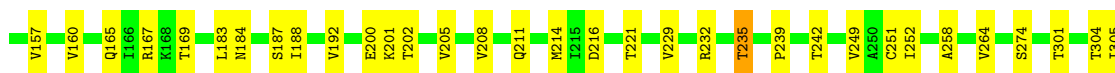
- Molecule 40: 60S ribosomal protein L3

Chain L3: 78% 20%

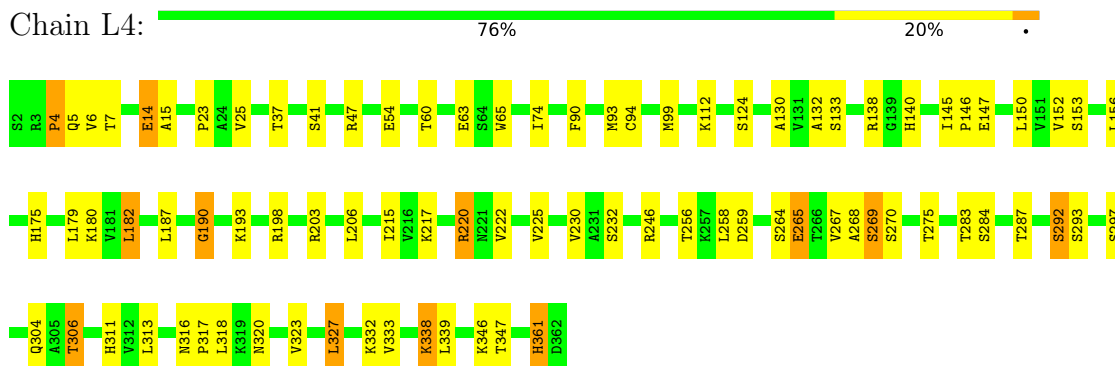


- Molecule 40: 60S ribosomal protein L3

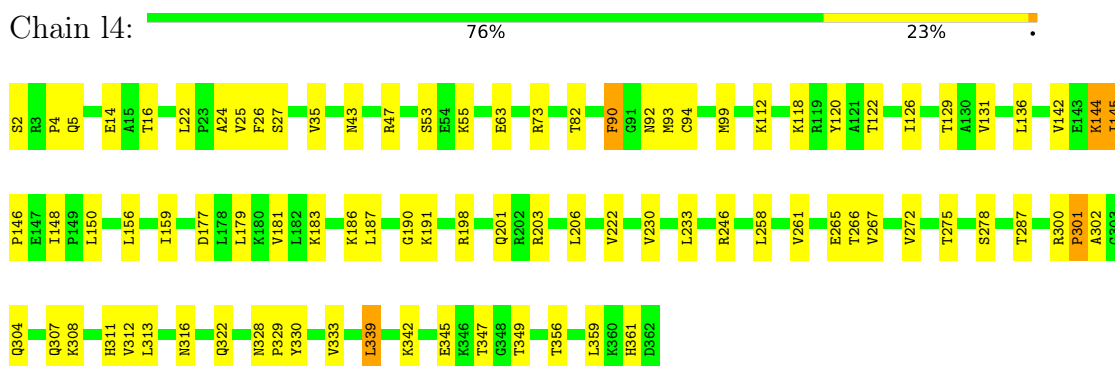
Chain l3: 78% 20%



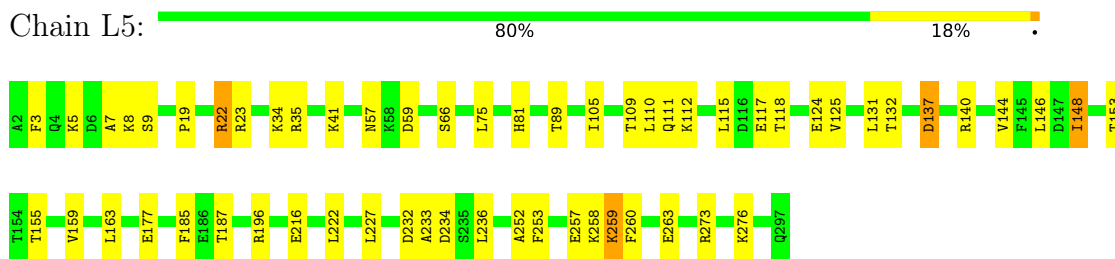
- Molecule 41: 60S ribosomal protein L4-A



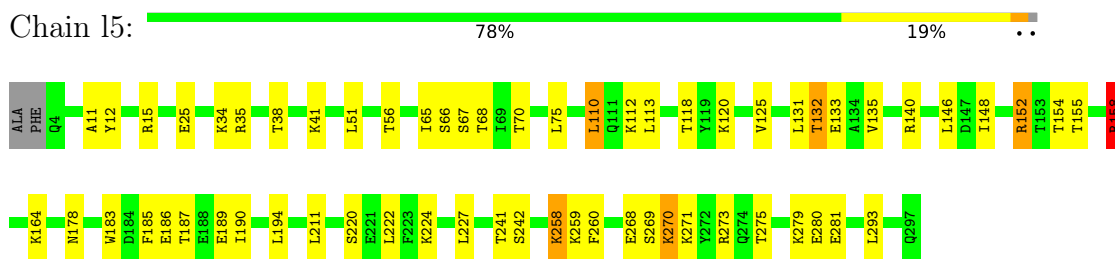
- Molecule 41: 60S ribosomal protein L4-A



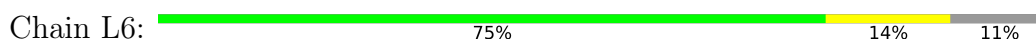
- Molecule 42: 60S ribosomal protein L5



- Molecule 42: 60S ribosomal protein L5



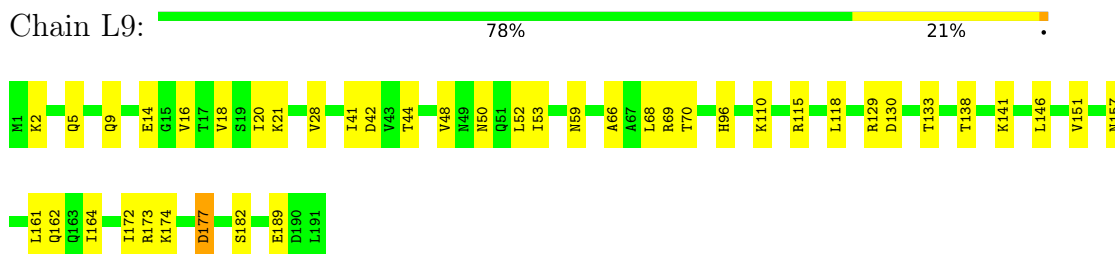
- Molecule 43: 60S ribosomal protein L6-A



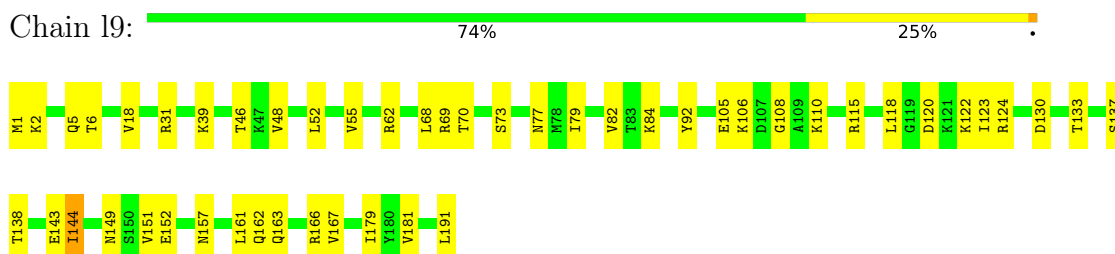
- Molecule 45: 60S ribosomal protein L8-A



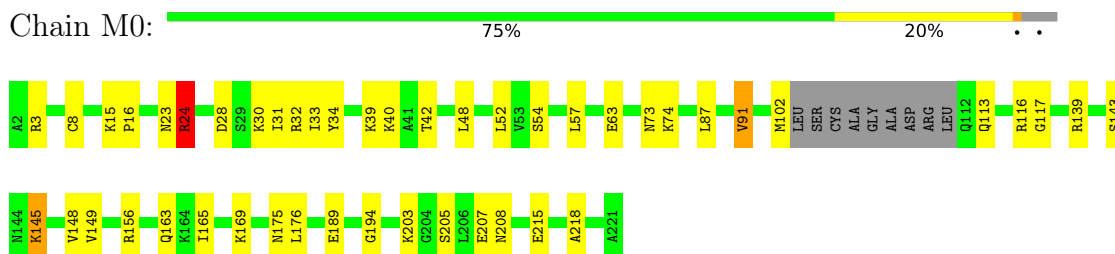
- Molecule 46: 60S ribosomal protein L9-A



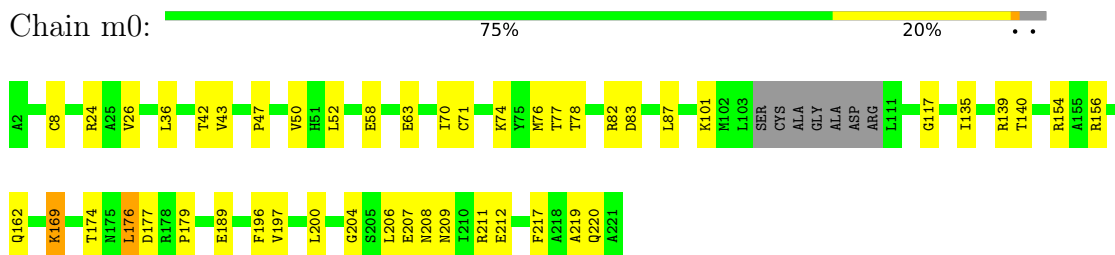
- Molecule 46: 60S ribosomal protein L9-A



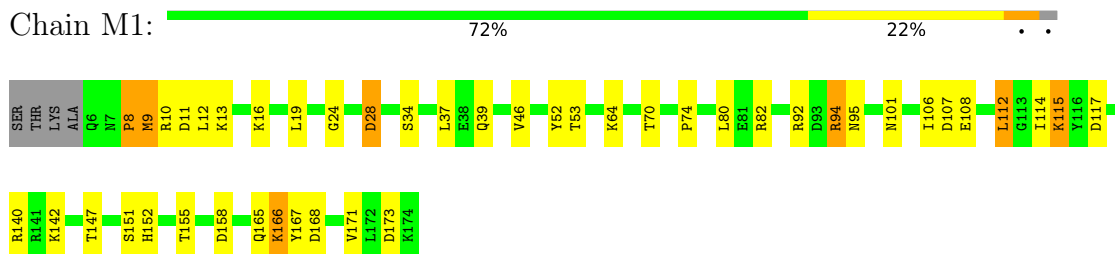
- Molecule 47: 60S ribosomal protein L10



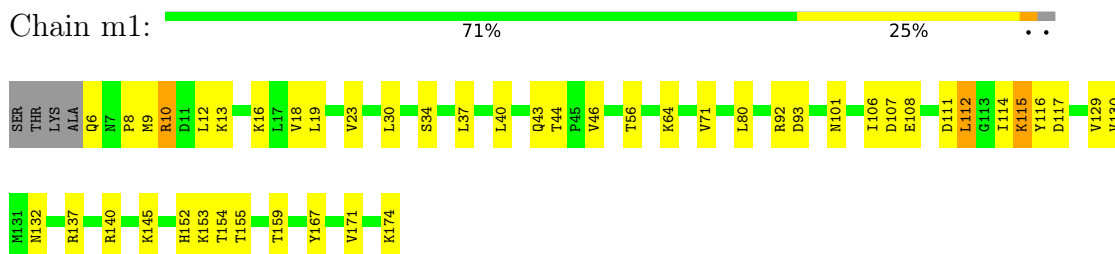
- Molecule 47: 60S ribosomal protein L10



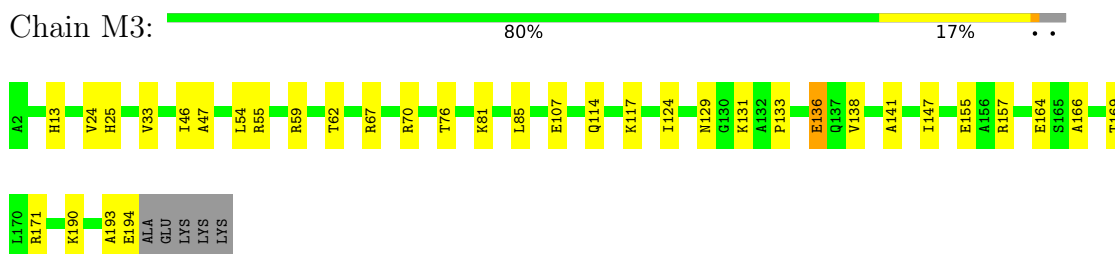
- Molecule 48: 60S ribosomal protein L11-B



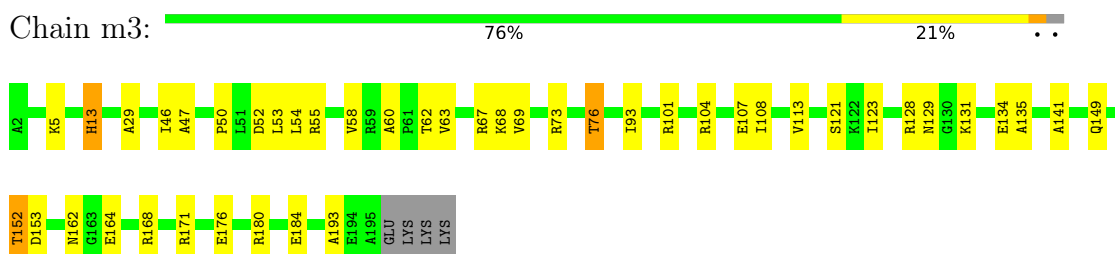
- Molecule 48: 60S ribosomal protein L11-B



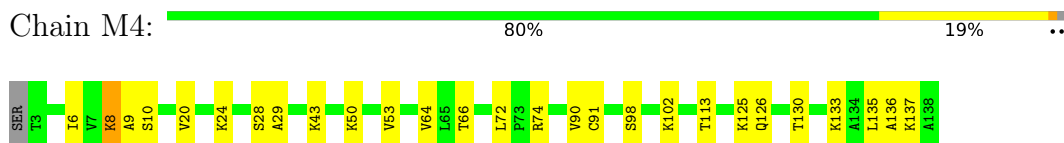
- Molecule 49: 60S ribosomal protein L13-A




- Molecule 49: 60S ribosomal protein L13-A



- Molecule 50: 60S ribosomal protein L14-A




- Molecule 50: 60S ribosomal protein L14-A

Chain m4:  82% 18%




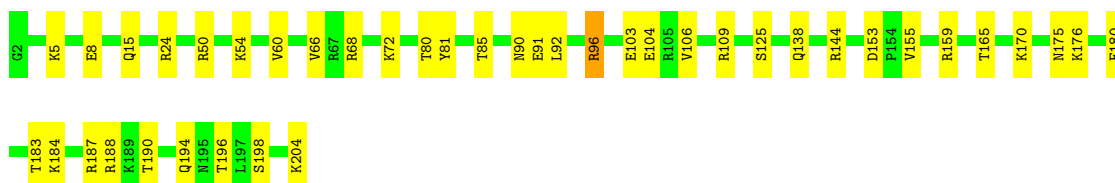
- Molecule 51: 60S ribosomal protein L15-A

Chain M5:  81% 19%




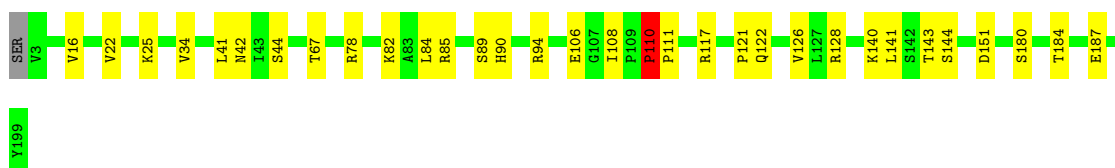
- Molecule 51: 60S ribosomal protein L15-A

Chain m5:  80% 20%




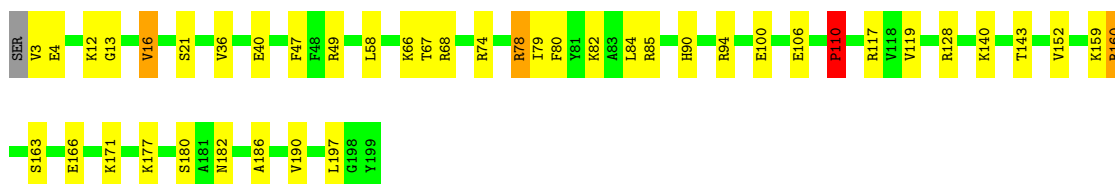
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:  83% 16% ..




- Molecule 52: 60S ribosomal protein L16-A

Chain m6:  78% 20% ...



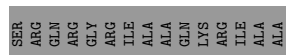
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:  78% 22%



- Molecule 53: 60S ribosomal protein L17-A

Chain m7: 70% 15% 15%



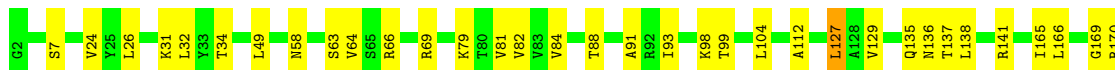
- Molecule 54: 60S ribosomal protein L18-A

Chain M8: 87% 13%



- Molecule 54: 60S ribosomal protein L18-A

Chain m8: 79% 19%



- Molecule 55: 60S ribosomal protein L19-A

Chain M9: 83% 17%

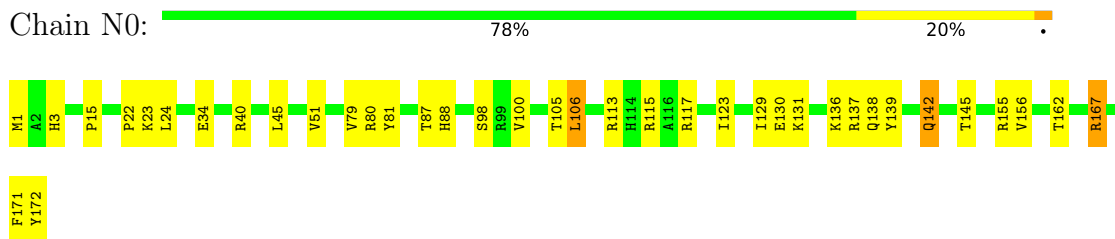


- Molecule 55: 60S ribosomal protein L19-A

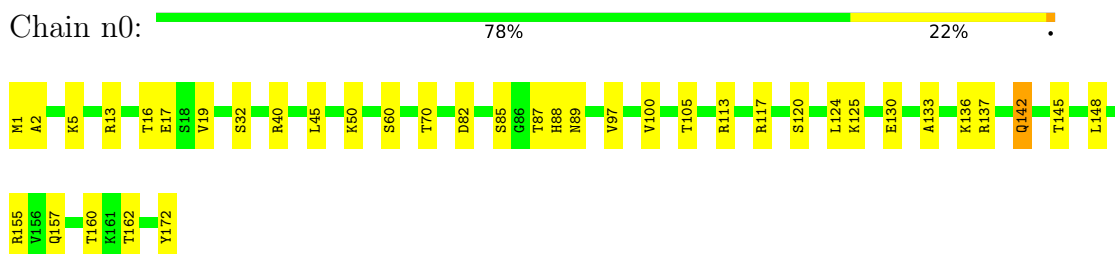
Chain m9: 84% 16%



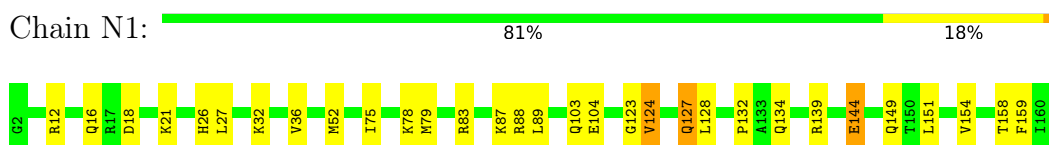
- Molecule 56: 60S ribosomal protein L20-A



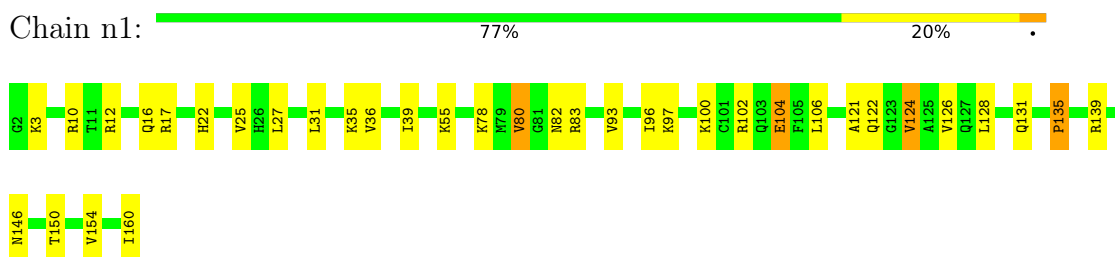
- Molecule 56: 60S ribosomal protein L20-A



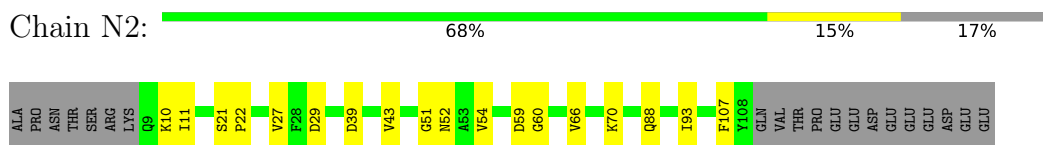
- Molecule 57: 60S ribosomal protein L21-A



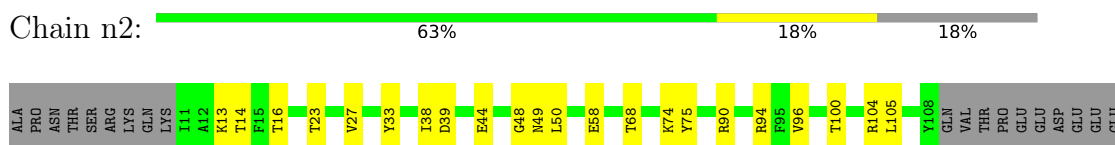
- Molecule 57: 60S ribosomal protein L21-A



- Molecule 58: 60S ribosomal protein L22-A



- Molecule 58: 60S ribosomal protein L22-A



ASP
GLU
GLU

- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 82% 18%



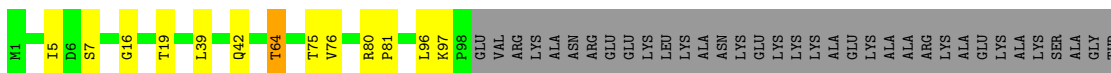
- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 88% 12%



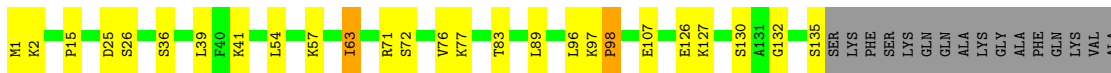
- Molecule 60: 60S ribosomal protein L24-A

Chain N4: 55% 8% 37%

GLN
SER
LYS
PHE
SER
LYS
GLN
GLN
ALA
LYS
GLY
ALA
PHE
GLN
LYS
VAL
ALA
ALA
THR
SER
ARG

- Molecule 60: 60S ribosomal protein L24-A

Chain n4: 70% 15% 13%

ALA
THR
SER
ARG

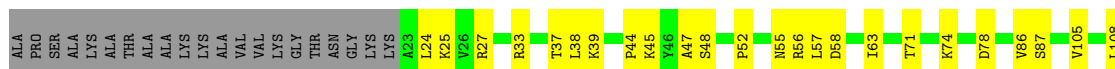
- Molecule 61: 60S ribosomal protein L25

Chain N5: 68% 18% 14%

I139
I142

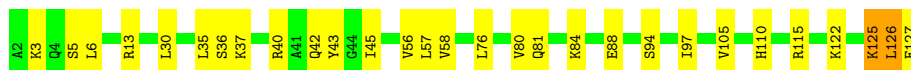
- Molecule 61: 60S ribosomal protein L25

Chain n5: 63% 22% 15%



- Molecule 62: 60S ribosomal protein L26-A

Chain N6: 77% 21%



- Molecule 62: 60S ribosomal protein L26-A

Chain n6: 79% 21%



- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 75% 25%



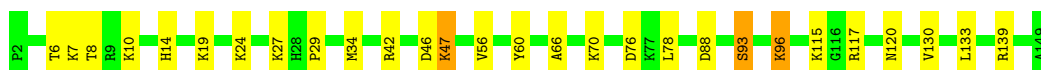
- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 76% 23%



- Molecule 64: 60S ribosomal protein L28

Chain N8: 81% 17%

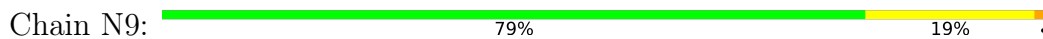


- Molecule 64: 60S ribosomal protein L28

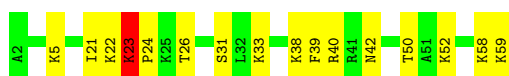
Chain n8: 79% 20%



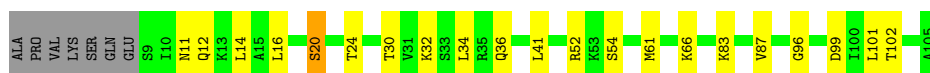
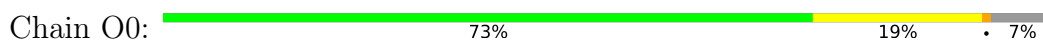
- Molecule 65: 60S ribosomal protein L29



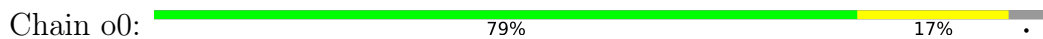
- Molecule 65: 60S ribosomal protein L29



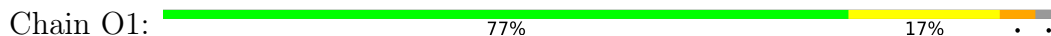
- Molecule 66: 60S ribosomal protein L30



- Molecule 66: 60S ribosomal protein L30



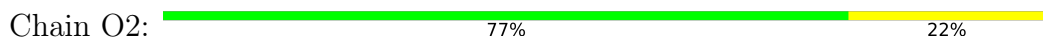
- Molecule 67: 60S ribosomal protein L31-A



- Molecule 67: 60S ribosomal protein L31-A



- Molecule 68: 60S ribosomal protein L32





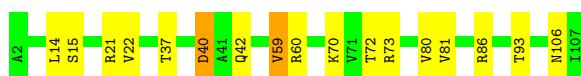
- Molecule 68: 60S ribosomal protein L32

Chain o2: 76% 20%



- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 84% 14%



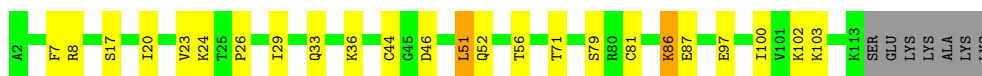
- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 80% 17%



- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 74% 18% 6%



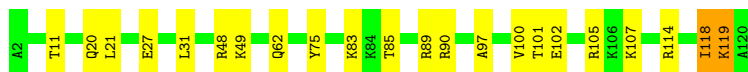
- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 72% 22% 6%



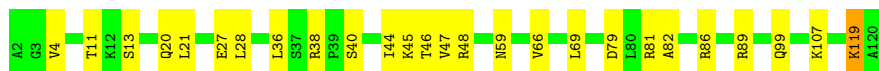
- Molecule 71: 60S ribosomal protein L35-A

Chain O5: 82% 17%

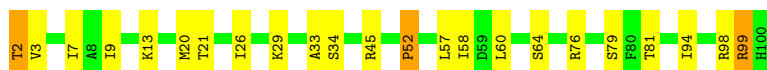
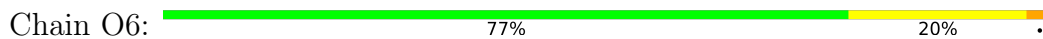


- Molecule 71: 60S ribosomal protein L35-A

Chain o5: 78% 21%



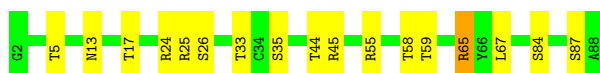
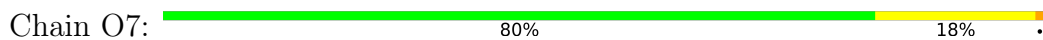
- Molecule 72: 60S ribosomal protein L36-A



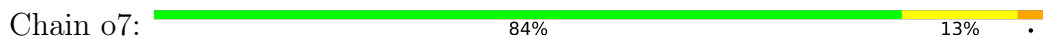
- Molecule 72: 60S ribosomal protein L36-A



- Molecule 73: 60S ribosomal protein L37-A



- Molecule 73: 60S ribosomal protein L37-A



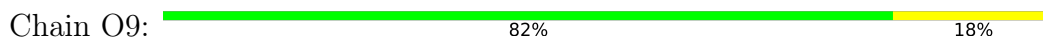
- Molecule 74: 60S ribosomal protein L38



- Molecule 74: 60S ribosomal protein L38

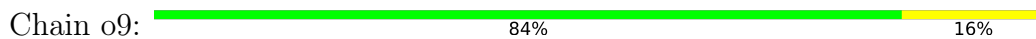


- Molecule 75: 60S ribosomal protein L39

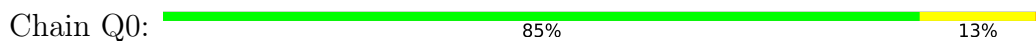




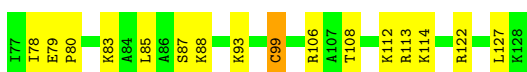
- Molecule 75: 60S ribosomal protein L39



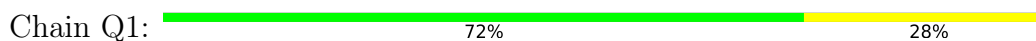
- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



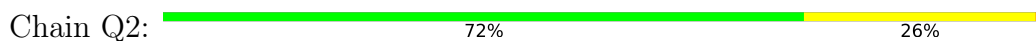
- Molecule 77: 60S ribosomal protein L41-A



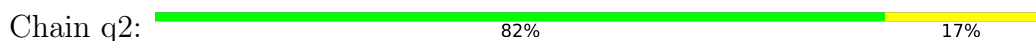
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 78: 60S ribosomal protein L42-A

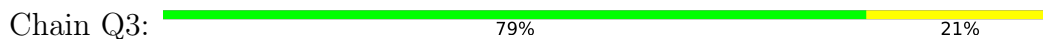


- Molecule 78: 60S ribosomal protein L42-A

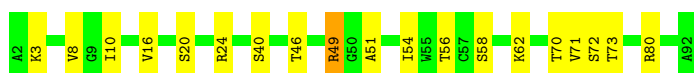
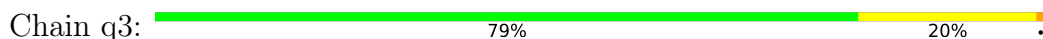




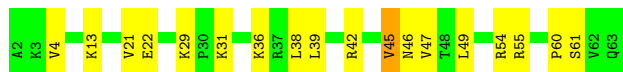
• Molecule 79: 60S ribosomal protein L43-A



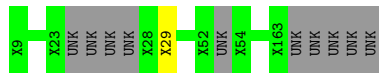
• Molecule 79: 60S ribosomal protein L43-A



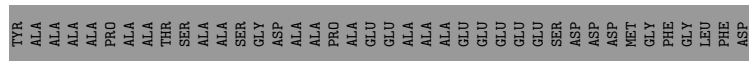
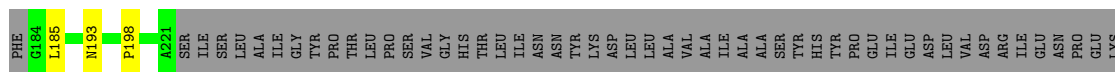
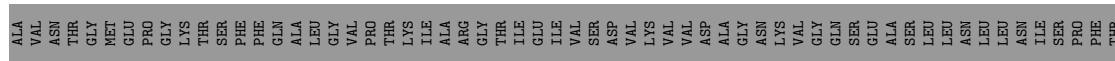
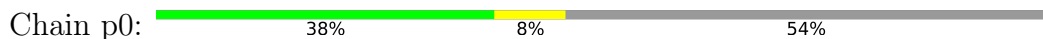
• Molecule 80: 40S ribosomal protein S30-A



• Molecule 81: Unknown Protein m2



• Molecule 82: 60S acidic ribosomal protein P0



• Molecule 83: Unknown Protein p1



There are no outlier residues recorded for this chain.

- Molecule 84: Unknown Protein p2

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	435.84Å 286.77Å 303.77Å 90.00° 99.03° 90.00°	Depositor
Resolution (Å)	49.70 – 3.30	Depositor
% Data completeness (in resolution range)	99.4 (49.70-3.30)	Depositor
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.33Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.202 , 0.255	Depositor
Wilson B-factor (Å ²)	90.1	Xtrriage
Anisotropy	0.099	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	411183	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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, 3J6, ZN, 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	0.74	6/41698 (0.0%)	1.29	289/64972 (0.4%)
1	6	0.88	18/42765 (0.0%)	1.38	477/66634 (0.7%)
2	S0	0.46	0/1617	0.66	0/2215
2	s0	0.48	0/1623	0.69	0/2222
3	S1	0.39	0/1735	0.65	1/2335 (0.0%)
3	s1	0.50	0/1748	0.70	1/2352 (0.0%)
4	S2	0.50	0/1665	0.66	0/2263
4	s2	0.58	0/1665	0.72	0/2263
5	S3	0.50	0/1759	0.66	0/2368
5	s3	0.42	0/1759	0.60	0/2368
6	S4	0.47	0/2109	0.70	1/2839 (0.0%)
6	s4	0.53	0/2109	0.73	0/2839
7	S5	0.40	0/1629	0.59	0/2202
7	s5	0.46	0/1629	0.69	0/2202
8	S6	0.44	0/1823	0.64	0/2439
8	s6	0.55	0/1779	0.70	0/2379
9	S7	0.43	0/1506	0.65	0/2028
9	s7	0.44	0/1516	0.65	0/2043
10	S8	0.54	0/1514	0.71	2/2021 (0.1%)
10	s8	0.60	0/1514	0.74	0/2021
11	S9	0.47	0/1519	0.65	0/2035
11	s9	0.56	0/1519	0.78	1/2035 (0.0%)
12	C0	0.42	0/790	0.64	1/1069 (0.1%)
12	c0	0.37	0/777	0.66	3/1049 (0.3%)
13	C1	0.58	0/1240	0.70	0/1675
13	c1	0.63	0/1194	0.76	0/1610
14	C2	0.38	0/900	0.64	1/1224 (0.1%)
14	c2	0.29	0/900	0.57	0/1224
15	C3	0.47	0/1215	0.68	2/1638 (0.1%)
15	c3	0.54	0/1215	0.71	0/1638
16	C4	0.40	0/901	0.68	0/1217
16	c4	0.52	0/960	0.74	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.46	0/998	0.65	0/1341
17	c5	0.48	0/1060	0.70	1/1426 (0.1%)
18	C6	0.45	0/1125	0.68	1/1510 (0.1%)
18	c6	0.51	0/1131	0.70	0/1518
19	C7	0.44	0/935	0.63	0/1254
19	c7	0.47	0/914	0.69	0/1224
20	C8	0.42	0/1211	0.64	0/1628
20	c8	0.50	0/1211	0.71	1/1628 (0.1%)
21	C9	0.45	0/1130	0.65	1/1517 (0.1%)
21	c9	0.50	0/1130	0.67	1/1517 (0.1%)
22	D0	0.46	0/865	0.65	0/1169
22	d0	0.48	0/892	0.68	0/1205
23	D1	0.46	0/693	0.65	0/935
23	d1	0.52	0/693	0.68	0/935
24	D2	0.50	0/1038	0.75	2/1395 (0.1%)
24	d2	0.61	0/1038	0.76	1/1395 (0.1%)
25	D3	0.61	0/1139	0.75	0/1518
25	d3	0.75	0/1139	0.86	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	0.40	0/571	0.72	0/768
27	d5	0.46	0/566	0.71	0/761
28	D6	0.48	0/782	0.71	0/1047
28	d6	0.65	0/782	0.79	1/1047 (0.1%)
29	D7	0.43	0/620	0.67	0/838
29	d7	0.49	0/620	0.64	0/838
30	D8	0.36	0/499	0.56	0/670
30	d8	0.46	0/499	0.63	0/670
31	D9	0.54	0/452	0.70	1/600 (0.2%)
31	d9	0.48	0/452	0.65	0/600
32	E0	0.48	0/483	0.61	0/643
33	E1	0.43	0/577	0.77	0/770
33	e1	0.39	0/619	0.69	1/822 (0.1%)
34	SR	0.37	0/2494	0.58	0/3393
34	sR	0.42	0/2495	0.59	0/3395
35	SM	0.53	0/1113	0.80	4/1502 (0.3%)
35	sM	0.50	0/683	0.73	1/923 (0.1%)
36	1	1.15	144/75394 (0.2%)	1.64	1754/117545 (1.5%)
36	5	1.19	180/75414 (0.2%)	1.67	1900/117575 (1.6%)
37	3	0.94	1/2883 (0.0%)	1.44	31/4491 (0.7%)
37	7	1.14	3/2883 (0.1%)	1.67	68/4491 (1.5%)
38	4	1.06	2/3746 (0.1%)	1.55	59/5832 (1.0%)
38	8	0.98	1/3746 (0.0%)	1.42	27/5832 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.70	0/1948	0.85	4/2617 (0.2%)
39	l2	0.67	0/1946	0.84	0/2614
40	L3	0.73	0/3146	0.82	1/4228 (0.0%)
40	l3	0.83	2/3146 (0.1%)	0.90	2/4228 (0.0%)
41	L4	0.81	2/2800 (0.1%)	0.91	3/3790 (0.1%)
41	l4	0.72	1/2800 (0.0%)	0.87	0/3790
42	L5	0.57	0/2425	0.71	0/3271
42	l5	0.70	0/2408	0.82	4/3248 (0.1%)
43	L6	0.74	0/1260	0.79	0/1694
43	l6	0.75	0/1269	0.82	1/1705 (0.1%)
44	L7	0.76	0/1821	0.88	2/2451 (0.1%)
44	l7	0.84	0/1828	0.88	4/2461 (0.2%)
45	L8	0.56	0/1836	0.69	0/2481
45	l8	0.51	0/1795	0.64	0/2429
46	L9	0.64	0/1539	0.77	0/2073
46	l9	0.80	0/1539	0.84	0/2073
47	M0	0.77	1/1741 (0.1%)	0.83	1/2335 (0.0%)
47	m0	0.77	1/1758 (0.1%)	0.83	0/2358
48	M1	0.51	0/1374	0.70	0/1842
48	m1	0.67	0/1374	0.85	2/1842 (0.1%)
49	M3	0.75	0/1568	0.84	1/2106 (0.0%)
49	m3	0.68	0/1573	0.80	0/2113
50	M4	0.73	0/1068	0.76	0/1438
50	m4	0.82	0/1074	0.82	1/1446 (0.1%)
51	M5	0.72	0/1757	0.84	0/2354
51	m5	0.66	0/1757	0.80	2/2354 (0.1%)
52	M6	0.82	0/1585	0.85	1/2128 (0.0%)
52	m6	0.98	2/1585 (0.1%)	0.96	2/2128 (0.1%)
53	M7	0.80	1/1443 (0.1%)	0.84	2/1944 (0.1%)
53	m7	0.84	0/1250	0.84	0/1683
54	M8	0.78	0/1465	0.91	1/1965 (0.1%)
54	m8	0.71	0/1465	0.94	5/1965 (0.3%)
55	M9	0.56	0/1538	0.66	0/2050
55	m9	0.62	0/1538	0.72	0/2050
56	N0	0.74	0/1481	0.84	3/1990 (0.2%)
56	n0	0.89	0/1481	0.89	0/1990
57	N1	0.76	0/1300	0.78	0/1743
57	n1	0.83	2/1300 (0.2%)	0.82	1/1743 (0.1%)
58	N2	0.46	0/812	0.63	0/1099
58	n2	0.50	0/794	0.67	0/1076
59	N3	0.69	0/1018	0.83	1/1369 (0.1%)
59	n3	0.81	0/1018	0.87	0/1369
60	N4	0.55	0/712	0.66	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.67	0/1052	0.79	0/1398
61	N5	0.63	0/979	0.77	1/1321 (0.1%)
61	n5	0.67	0/974	0.79	0/1314
62	N6	0.74	0/1004	0.87	1/1341 (0.1%)
62	n6	0.63	0/1004	0.79	0/1341
63	N7	0.54	0/1118	0.70	0/1497
63	n7	0.49	0/1118	0.65	0/1497
64	N8	0.75	0/1204	0.90	0/1612
64	n8	0.77	0/1204	0.87	0/1612
65	N9	0.65	0/473	0.77	1/629 (0.2%)
65	n9	0.79	0/473	0.97	1/629 (0.2%)
66	O0	0.50	0/751	0.66	0/1008
66	o0	0.52	0/775	0.69	0/1040
67	O1	0.63	0/890	0.72	0/1196
67	o1	0.72	0/897	0.84	0/1205
68	O2	0.84	0/1041	0.90	1/1394 (0.1%)
68	o2	0.81	0/1041	0.90	2/1394 (0.1%)
69	O3	0.89	0/868	0.87	1/1168 (0.1%)
69	o3	0.90	0/868	0.90	0/1168
70	O4	0.59	0/890	0.79	1/1189 (0.1%)
70	o4	0.56	0/890	0.76	0/1189
71	O5	0.71	0/978	0.78	0/1301
71	o5	0.56	0/974	0.68	0/1297
72	O6	0.66	0/778	0.76	0/1034
72	o6	0.55	0/777	0.73	0/1033
73	O7	0.75	0/696	0.99	3/923 (0.3%)
73	o7	0.70	0/696	0.86	1/923 (0.1%)
74	O8	0.52	0/618	0.68	0/826
74	o8	0.50	0/614	0.68	0/822
75	O9	0.74	0/443	0.88	0/588
75	o9	0.66	0/443	0.79	0/588
76	Q0	0.69	0/423	0.82	0/562
76	q0	0.94	1/423 (0.2%)	0.92	0/562
77	Q1	0.61	0/234	0.78	0/300
77	q1	0.78	0/234	1.00	0/300
78	Q2	0.88	1/860 (0.1%)	0.90	0/1136
78	q2	0.79	1/860 (0.1%)	0.77	1/1136 (0.1%)
79	Q3	0.71	0/701	0.81	1/934 (0.1%)
79	q3	0.71	0/701	0.80	0/934
80	e0	0.58	0/499	0.74	0/665
82	p0	0.46	0/1092	0.61	0/1474
All	All	0.90	370/430074 (0.1%)	1.30	4696/631364 (0.7%)

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
6	S4	0	1
7	s5	0	1
9	S7	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
25	D3	0	1
27	D5	0	1
28	D6	0	1
33	E1	0	1
39	L2	0	1
39	l2	0	1
40	L3	0	1
43	L6	0	1
43	l6	0	1
44	l7	0	1
45	L8	0	1
46	L9	0	1
48	M1	0	1
52	M6	0	1
52	m6	0	1
54	m8	0	1
56	N0	0	1
56	n0	0	1
59	n3	0	1
64	n8	0	1
65	N9	0	2
67	O1	0	1
72	O6	0	1
81	m2	0	1
All	All	0	36

All (370) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	12.26	2.03	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-11.12	1.29	1.38
36	5	2726	C	N3-C4	-9.57	1.27	1.33
78	q2	17	CYS	CB-SG	9.14	1.97	1.82
36	1	3181	C	N3-C4	-8.78	1.27	1.33
36	5	1152	G	N3-C4	-8.51	1.29	1.35
36	5	2358	A	N9-C4	-8.41	1.32	1.37
36	1	1116	G	N7-C5	-8.32	1.34	1.39
36	1	2875	U	C2-N3	8.29	1.43	1.37
47	m0	8	CYS	CB-SG	-8.05	1.68	1.82
36	1	1164	G	C6-N1	-8.01	1.33	1.39
47	M0	8	CYS	CB-SG	-7.86	1.68	1.82
36	5	951	A	N7-C5	-7.76	1.34	1.39
36	5	2875	U	C2-N3	7.75	1.43	1.37
36	5	1366	A	N3-C4	-7.68	1.30	1.34
36	1	984	G	N7-C5	-7.58	1.34	1.39
36	5	2704	A	N9-C4	-7.53	1.33	1.37
36	5	960	U	N1-C2	7.45	1.45	1.38
36	1	2812	C	N1-C6	-7.45	1.32	1.37
36	5	876	A	N3-C4	-7.36	1.30	1.34
36	5	1874	A	N9-C4	-7.32	1.33	1.37
36	5	2145	A	C6-N1	-7.29	1.30	1.35
36	5	2943	G	C5-C6	-7.27	1.35	1.42
36	5	646	A	C6-N1	-7.22	1.30	1.35
36	5	2943	G	N7-C5	-7.22	1.34	1.39
36	1	952	A	N3-C4	-7.21	1.30	1.34
36	1	2619	G	C5-C4	-7.15	1.33	1.38
36	5	1159	A	N3-C4	-7.15	1.30	1.34
1	6	1653	C	N1-C6	-7.12	1.32	1.37
36	5	3040	A	N9-C4	-7.12	1.33	1.37
36	5	2799	A	C6-N1	-7.11	1.30	1.35
36	5	2626	A	N3-C4	-7.08	1.30	1.34
36	5	523	A	N3-C4	-7.06	1.30	1.34
57	n1	104	GLU	CB-CG	6.89	1.65	1.52
36	5	3008	A	N9-C4	-6.88	1.33	1.37
36	1	1429	G	N9-C8	-6.87	1.33	1.37
36	5	2640	A	N9-C4	-6.87	1.33	1.37
36	1	2820	A	N9-C4	-6.87	1.33	1.37
36	1	3142	A	N9-C4	-6.86	1.33	1.37
41	L4	94	CYS	CB-SG	-6.85	1.70	1.82
36	1	361	A	C6-N1	-6.80	1.30	1.35
36	1	790	U	C2-N3	-6.78	1.33	1.37
36	5	2375	G	C6-N1	-6.73	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	1137	A	N9-C4	-6.73	1.33	1.37
36	5	2644	C	N1-C6	-6.72	1.33	1.37
36	5	999	G	C5-C4	-6.72	1.33	1.38
36	5	1199	C	N1-C6	-6.72	1.33	1.37
36	1	3006	A	N9-C4	-6.72	1.33	1.37
36	1	1432	C	N1-C6	-6.71	1.33	1.37
36	5	2333	C	N1-C6	-6.69	1.33	1.37
36	5	953	G	C5-C4	-6.68	1.33	1.38
36	1	699	A	N9-C4	-6.66	1.33	1.37
36	5	869	G	C6-N1	-6.64	1.34	1.39
1	6	1337	A	N9-C4	-6.61	1.33	1.37
36	1	2213	A	N9-C4	-6.60	1.33	1.37
36	5	3139	A	N3-C4	-6.60	1.30	1.34
36	1	1373	A	N3-C4	-6.59	1.30	1.34
36	5	1301	A	C5-C6	-6.58	1.35	1.41
36	5	2993	G	C5-C4	-6.57	1.33	1.38
36	1	33	G	N7-C5	-6.50	1.35	1.39
1	6	119	A	N9-C4	-6.49	1.33	1.37
36	5	2620	G	N3-C4	-6.49	1.30	1.35
36	1	1116	G	N9-C8	-6.45	1.33	1.37
36	1	2419	A	N9-C4	-6.45	1.33	1.37
36	5	642	U	C2-N3	-6.44	1.33	1.37
36	5	2950	G	C5-C6	-6.44	1.35	1.42
36	5	2804	A	N9-C4	-6.43	1.33	1.37
36	5	1451	C	N1-C6	-6.43	1.33	1.37
36	1	34	A	N9-C4	-6.42	1.33	1.37
36	1	942	U	C4-O4	6.42	1.28	1.23
36	1	2639	G	N7-C5	-6.39	1.35	1.39
36	5	1158	A	C5-C6	-6.37	1.35	1.41
36	1	2714	G	N9-C4	-6.36	1.32	1.38
36	5	519	A	N9-C4	-6.34	1.34	1.37
36	5	1085	A	N9-C4	-6.32	1.34	1.37
36	5	647	A	N9-C8	-6.29	1.32	1.37
36	1	2213	A	N3-C4	-6.27	1.31	1.34
36	5	962	A	C5-C6	-6.27	1.35	1.41
36	5	523	A	N9-C4	-6.22	1.34	1.37
36	1	1143	A	N9-C4	-6.22	1.34	1.37
36	1	1304	A	N9-C4	-6.19	1.34	1.37
36	5	1152	G	C5-C6	-6.18	1.36	1.42
36	5	651	G	N7-C5	-6.17	1.35	1.39
36	5	2814	G	N7-C5	-6.15	1.35	1.39
1	6	337	G	C2-N3	6.14	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	924	G	C5-C4	-6.13	1.34	1.38
36	5	2381	G	N7-C5	-6.13	1.35	1.39
36	5	1139	G	N9-C4	-6.12	1.33	1.38
36	5	2971	A	N9-C4	6.11	1.41	1.37
36	5	3139	A	N9-C4	-6.11	1.34	1.37
36	5	1338	C	N1-C6	-6.09	1.33	1.37
38	8	14	C	N1-C6	-6.09	1.33	1.37
36	5	2879	C	N1-C6	-6.07	1.33	1.37
36	5	691	A	C6-N1	-6.04	1.31	1.35
36	1	2138	A	N7-C5	-6.02	1.35	1.39
36	1	367	A	N9-C4	-6.02	1.34	1.37
36	1	874	U	C2-N3	-6.00	1.33	1.37
36	1	2402	A	C5-C6	-6.00	1.35	1.41
36	5	2942	C	N1-C6	-6.00	1.33	1.37
36	5	1381	A	N9-C4	-5.99	1.34	1.37
36	5	1099	A	C5-C6	-5.99	1.35	1.41
40	l3	251	CYS	CB-SG	-5.98	1.72	1.81
36	5	1081	U	C2-N3	5.98	1.42	1.37
36	5	1048	A	C6-N1	-5.97	1.31	1.35
36	1	2360	C	N1-C6	-5.97	1.33	1.37
36	1	353	G	N7-C5	-5.96	1.35	1.39
36	1	943	U	C2-N3	-5.96	1.33	1.37
36	1	657	A	C5-C6	-5.96	1.35	1.41
36	5	652	G	N3-C4	-5.96	1.31	1.35
36	5	1462	A	N9-C4	-5.96	1.34	1.37
36	1	2409	G	N7-C5	-5.96	1.35	1.39
36	5	2639	G	N7-C5	-5.94	1.35	1.39
36	1	2406	C	N1-C6	-5.94	1.33	1.37
36	5	1332	A	N9-C4	-5.93	1.34	1.37
36	5	1099	A	N7-C5	-5.93	1.35	1.39
36	5	2833	A	C5-C4	-5.93	1.34	1.38
37	7	55	A	C5-C6	-5.92	1.35	1.41
36	1	695	C	N3-C4	-5.91	1.29	1.33
1	6	1744	A	N9-C4	-5.91	1.34	1.37
36	5	1192	C	N1-C2	5.90	1.46	1.40
36	1	3012	A	N9-C4	-5.90	1.34	1.37
36	5	1434	G	N3-C4	-5.90	1.31	1.35
36	1	920	A	C6-N1	-5.89	1.31	1.35
36	1	699	A	N3-C4	-5.89	1.31	1.34
52	m6	40	GLU	CG-CD	5.89	1.60	1.51
76	q0	99	CYS	CB-SG	-5.89	1.72	1.81
41	L4	65	TRP	CB-CG	-5.88	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	962	A	N7-C5	-5.88	1.35	1.39
36	1	1364	C	N1-C6	-5.87	1.33	1.37
36	1	937	G	C5-C6	-5.85	1.36	1.42
36	1	1401	A	C6-N1	-5.84	1.31	1.35
36	1	2396	G	N7-C5	-5.84	1.35	1.39
36	5	3107	U	C2-N3	-5.83	1.33	1.37
36	5	1330	A	C5-C6	-5.82	1.35	1.41
36	5	2872	A	N9-C4	-5.82	1.34	1.37
36	1	338	A	N7-C5	-5.81	1.35	1.39
36	5	345	G	N3-C4	-5.78	1.31	1.35
36	5	2872	A	N7-C5	-5.77	1.35	1.39
36	5	1048	A	N3-C4	-5.77	1.31	1.34
36	1	1452	A	N9-C4	-5.75	1.34	1.37
1	2	1651	A	N9-C4	-5.75	1.34	1.37
36	5	1429	G	N9-C4	-5.75	1.33	1.38
36	1	2748	A	N9-C4	-5.74	1.34	1.37
36	5	1456	A	N9-C4	-5.73	1.34	1.37
36	5	2743	A	N7-C5	-5.70	1.35	1.39
36	5	397	A	N3-C4	-5.69	1.31	1.34
36	5	1390	A	N3-C4	-5.69	1.31	1.34
36	5	1195	A	N9-C4	-5.68	1.34	1.37
36	1	2805	G	C8-N7	-5.67	1.27	1.30
36	5	3091	A	C6-N1	-5.65	1.31	1.35
36	5	2954	U	N3-C4	5.65	1.43	1.38
1	2	1657	U	N1-C2	5.64	1.43	1.38
36	1	2402	A	C5-C4	-5.64	1.34	1.38
36	5	1207	G	C5-C4	-5.64	1.34	1.38
1	6	1137	A	C5-C4	-5.64	1.34	1.38
36	5	2891	U	C2-N3	-5.64	1.33	1.37
37	3	82	G	C6-N1	-5.63	1.35	1.39
36	5	1886	A	N7-C5	-5.63	1.35	1.39
36	1	2986	U	N1-C2	-5.63	1.33	1.38
37	7	118	A	N3-C4	-5.63	1.31	1.34
36	5	1303	A	N9-C4	-5.62	1.34	1.37
36	1	2610	G	C5-C6	-5.61	1.36	1.42
36	5	706	A	N9-C4	-5.61	1.34	1.37
36	5	3086	A	N3-C4	-5.61	1.31	1.34
36	5	2291	A	N9-C4	-5.60	1.34	1.37
36	5	3000	A	N9-C4	-5.60	1.34	1.37
36	5	2809	C	N1-C6	-5.60	1.33	1.37
36	1	2382	G	N1-C2	-5.59	1.33	1.37
36	1	1133	A	N7-C5	-5.59	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2875	U	N3-C4	5.59	1.43	1.38
36	1	1468	A	N9-C4	-5.58	1.34	1.37
36	1	2797	C	N1-C6	-5.58	1.33	1.37
36	5	2876	C	N3-C4	-5.58	1.30	1.33
57	n1	104	GLU	CG-CD	5.55	1.60	1.51
53	M7	138	LYS	CD-CE	5.55	1.65	1.51
1	2	1750	A	N7-C5	-5.54	1.35	1.39
36	1	2762	A	N3-C4	-5.54	1.31	1.34
36	1	1296	C	N3-C4	-5.54	1.30	1.33
36	5	2996	U	N1-C2	5.54	1.43	1.38
36	1	939	U	N1-C2	-5.53	1.33	1.38
36	1	657	A	C5-C4	-5.52	1.34	1.38
36	5	1048	A	C5-C4	-5.52	1.34	1.38
36	1	2404	A	C6-N1	5.50	1.39	1.35
1	6	1745	G	N9-C8	-5.50	1.33	1.37
36	5	2743	A	N9-C8	-5.50	1.33	1.37
36	1	1854	C	N3-C4	-5.50	1.30	1.33
36	1	2726	C	N3-C4	-5.50	1.30	1.33
36	1	2966	G	C5-C4	-5.49	1.34	1.38
36	5	1320	C	N3-C4	-5.49	1.30	1.33
1	2	1730	A	N9-C4	-5.49	1.34	1.37
1	6	163	G	N9-C4	-5.49	1.33	1.38
36	5	866	A	N9-C4	-5.49	1.34	1.37
36	1	1206	G	C2-N3	-5.48	1.28	1.32
36	1	2979	U	C2-N3	-5.48	1.33	1.37
36	5	1117	G	C5-C6	-5.48	1.36	1.42
36	5	3004	C	N1-C2	-5.48	1.34	1.40
36	1	790	U	N3-C4	-5.47	1.33	1.38
36	5	3362	A	N3-C4	-5.47	1.31	1.34
36	1	659	G	C5-C4	-5.47	1.34	1.38
36	5	421	G	C6-N1	-5.46	1.35	1.39
36	5	1048	A	C5-C6	-5.46	1.36	1.41
36	1	1330	A	C5-C6	-5.46	1.36	1.41
36	5	2823	G	N7-C5	-5.45	1.35	1.39
52	m6	80	PHE	CB-CG	-5.45	1.42	1.51
36	1	994	G	C6-N1	-5.45	1.35	1.39
36	5	43	A	C5-C6	-5.44	1.36	1.41
36	5	1115	G	P-O5'	-5.44	1.54	1.59
36	1	925	A	N3-C4	-5.44	1.31	1.34
36	5	657	A	N3-C4	-5.43	1.31	1.34
36	5	2398	A	N3-C4	-5.43	1.31	1.34
36	5	2398	A	C5-C4	-5.43	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	1330	A	N9-C4	-5.43	1.34	1.37
41	14	94	CYS	CB-SG	-5.43	1.73	1.81
36	1	3139	A	N9-C4	-5.42	1.34	1.37
36	1	3180	A	C5-C6	-5.42	1.36	1.41
36	5	2823	G	C5-C6	-5.42	1.36	1.42
36	1	59	G	N7-C5	-5.41	1.36	1.39
36	1	28	C	N1-C6	-5.41	1.33	1.37
36	5	642	U	N1-C2	-5.41	1.33	1.38
36	5	3092	C	N1-C6	-5.40	1.33	1.37
36	1	2725	U	C2-N3	-5.40	1.33	1.37
37	7	56	A	C5-C6	-5.39	1.36	1.41
36	1	957	C	N1-C2	-5.39	1.34	1.40
36	1	627	U	N1-C2	-5.38	1.33	1.38
1	6	630	A	N7-C5	-5.38	1.36	1.39
36	1	1150	A	N9-C4	-5.38	1.34	1.37
36	5	1476	G	N3-C4	-5.38	1.31	1.35
36	1	818	C	N1-C6	-5.38	1.33	1.37
36	5	1587	A	N9-C4	-5.37	1.34	1.37
1	6	1524	A	N9-C4	-5.35	1.34	1.37
36	1	2762	A	N9-C4	-5.34	1.34	1.37
36	5	3382	U	N1-C2	5.34	1.43	1.38
36	1	2169	G	C5-C6	5.34	1.47	1.42
36	1	1167	U	C2-N3	-5.33	1.34	1.37
36	5	2399	A	N9-C4	-5.33	1.34	1.37
36	5	1450	G	C2-N3	-5.33	1.28	1.32
36	1	2924	U	N1-C2	-5.33	1.33	1.38
38	4	52	A	N3-C4	-5.32	1.31	1.34
36	5	367	A	N3-C4	-5.32	1.31	1.34
36	5	952	A	N9-C4	-5.32	1.34	1.37
1	2	334	G	N9-C4	-5.32	1.33	1.38
36	1	1308	A	C6-N1	-5.32	1.31	1.35
36	5	3005	A	N9-C8	-5.32	1.33	1.37
36	1	2363	A	N9-C4	-5.31	1.34	1.37
36	5	1362	G	N9-C8	-5.31	1.34	1.37
36	1	1147	G	N7-C5	-5.30	1.36	1.39
36	5	2280	A	N9-C4	-5.30	1.34	1.37
36	5	923	C	N1-C6	-5.29	1.33	1.37
36	5	3310	A	C6-N1	-5.29	1.31	1.35
36	1	1143	A	N3-C4	-5.29	1.31	1.34
36	1	393	U	C2-N3	-5.28	1.34	1.37
36	1	3306	U	C2-N3	-5.28	1.34	1.37
36	5	343	U	C2-N3	-5.28	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	19	C	N3-C4	-5.28	1.30	1.33
36	1	1002	A	N9-C4	-5.27	1.34	1.37
36	1	1150	A	N3-C4	-5.27	1.31	1.34
36	1	2286	U	C2-N3	-5.27	1.34	1.37
36	1	3306	U	N3-C4	-5.27	1.33	1.38
36	5	691	A	N3-C4	-5.27	1.31	1.34
36	5	2959	C	N1-C6	-5.26	1.33	1.37
36	5	818	C	N1-C6	-5.26	1.33	1.37
36	1	3130	A	N7-C5	-5.25	1.36	1.39
1	6	986	G	N7-C5	-5.25	1.36	1.39
36	1	505	G	N3-C4	-5.25	1.31	1.35
40	13	7	GLU	CG-CD	5.25	1.59	1.51
36	5	953	G	N3-C4	-5.24	1.31	1.35
36	1	1373	A	N9-C4	-5.24	1.34	1.37
36	5	3245	A	N7-C5	-5.24	1.36	1.39
36	5	1115	G	N7-C5	-5.24	1.36	1.39
36	5	1794	G	N9-C8	-5.24	1.34	1.37
36	1	1186	G	N1-C2	-5.23	1.33	1.37
36	5	830	A	C5-C6	-5.23	1.36	1.41
36	1	910	G	N9-C8	-5.23	1.34	1.37
36	5	945	C	N1-C6	-5.22	1.34	1.37
36	5	2799	A	N3-C4	-5.22	1.31	1.34
36	1	2692	A	N7-C5	-5.22	1.36	1.39
36	1	2187	G	N7-C5	-5.21	1.36	1.39
36	1	3006	A	N3-C4	-5.21	1.31	1.34
36	1	2358	A	N3-C4	-5.21	1.31	1.34
36	5	1180	A	N3-C4	-5.21	1.31	1.34
36	5	2283	G	C5-C6	-5.20	1.37	1.42
36	5	2243	A	N3-C4	-5.20	1.31	1.34
36	5	1794	G	N9-C4	-5.20	1.33	1.38
36	5	1868	G	C5-C6	-5.19	1.37	1.42
1	2	992	A	N9-C4	-5.18	1.34	1.37
36	1	936	A	C5-C6	-5.17	1.36	1.41
36	1	1369	A	N9-C4	-5.17	1.34	1.37
36	1	1430	U	N1-C2	-5.17	1.33	1.38
36	5	2950	G	N7-C5	-5.17	1.36	1.39
36	5	367	A	C5-C4	-5.17	1.35	1.38
36	5	1174	G	C5-C4	-5.17	1.34	1.38
36	1	1307	G	N1-C2	-5.17	1.33	1.37
36	1	2640	A	C6-N1	-5.17	1.31	1.35
36	5	1454	A	N9-C4	-5.17	1.34	1.37
36	1	421	G	C5-C4	-5.16	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	657	A	N3-C4	-5.16	1.31	1.34
36	1	657	A	N7-C5	-5.16	1.36	1.39
36	1	803	C	N3-C4	-5.16	1.30	1.33
36	5	1194	G	C5-C4	-5.16	1.34	1.38
36	1	423	A	N7-C5	-5.16	1.36	1.39
36	1	967	A	N3-C4	-5.16	1.31	1.34
36	5	2866	U	N1-C2	5.15	1.43	1.38
36	5	3103	A	N3-C4	-5.15	1.31	1.34
36	1	701	G	N3-C4	-5.14	1.31	1.35
36	5	947	G	N3-C4	-5.14	1.31	1.35
36	1	651	G	N9-C8	-5.14	1.34	1.37
36	1	670	C	N1-C6	-5.14	1.34	1.37
36	1	2394	G	N1-C2	-5.14	1.33	1.37
36	1	1394	A	N9-C4	-5.13	1.34	1.37
36	5	1046	A	N3-C4	-5.13	1.31	1.34
36	5	1195	A	C5-C4	-5.13	1.35	1.38
36	1	1192	C	N1-C2	5.13	1.45	1.40
36	5	3245	A	C5-C6	-5.13	1.36	1.41
36	1	1129	A	N7-C5	-5.13	1.36	1.39
1	6	992	A	C5-C6	-5.13	1.36	1.41
36	5	1116	G	N9-C8	-5.12	1.34	1.37
36	5	647	A	C5-C4	-5.12	1.35	1.38
36	5	3138	U	N1-C2	-5.12	1.33	1.38
36	1	339	C	N3-C4	-5.12	1.30	1.33
36	1	2960	C	N3-C4	-5.12	1.30	1.33
36	1	1392	G	C5-C4	-5.11	1.34	1.38
36	5	45	A	N9-C4	-5.11	1.34	1.37
36	5	3026	G	C5-C6	-5.11	1.37	1.42
36	5	406	G	N3-C4	-5.11	1.31	1.35
36	1	2875	U	N3-C4	5.11	1.43	1.38
36	1	884	A	N9-C4	-5.10	1.34	1.37
1	6	397	A	N9-C4	-5.10	1.34	1.37
36	5	2840	C	N1-C6	-5.09	1.34	1.37
36	1	938	C	C4-C5	-5.09	1.38	1.43
36	5	651	G	N3-C4	-5.09	1.31	1.35
36	5	2419	A	N7-C5	-5.09	1.36	1.39
36	1	2868	U	C2-N3	-5.08	1.34	1.37
36	5	2748	A	C5-C6	-5.08	1.36	1.41
36	5	3178	A	N9-C4	-5.08	1.34	1.37
36	5	3330	A	C5-C4	-5.07	1.35	1.38
36	1	635	G	C5-C6	-5.07	1.37	1.42
36	5	896	A	C5-C4	-5.07	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1370	G	C6-N1	-5.07	1.36	1.39
36	5	3047	U	N3-C4	-5.06	1.33	1.38
36	1	1180	A	N9-C4	-5.06	1.34	1.37
36	5	55	G	N9-C4	-5.06	1.33	1.38
1	6	65	A	C5-C6	-5.06	1.36	1.41
36	5	635	G	C5-C6	-5.06	1.37	1.42
36	5	3032	A	N7-C5	-5.06	1.36	1.39
36	5	2659	G	N7-C5	-5.06	1.36	1.39
36	1	2335	G	C5-C4	-5.05	1.34	1.38
36	5	1193	A	N7-C5	-5.05	1.36	1.39
36	1	1372	C	C2-N3	-5.04	1.31	1.35
36	1	27	C	N1-C6	-5.04	1.34	1.37
1	6	1137	A	N3-C4	-5.04	1.31	1.34
36	1	360	G	N7-C5	-5.04	1.36	1.39
36	5	1309	U	C2-N3	-5.04	1.34	1.37
36	5	2312	A	N3-C4	-5.03	1.31	1.34
36	1	651	G	C5-C4	-5.03	1.34	1.38
36	1	1429	G	C5-C4	-5.03	1.34	1.38
36	5	2857	C	N1-C6	-5.03	1.34	1.37
36	1	2611	U	C2-N3	-5.03	1.34	1.37
1	6	1764	C	N1-C6	-5.03	1.34	1.37
36	5	2138	A	N7-C5	-5.03	1.36	1.39
36	1	2866	U	C4-O4	5.02	1.27	1.23
36	5	981	U	N1-C2	5.02	1.43	1.38
1	6	1027	A	N9-C4	-5.02	1.34	1.37
36	5	1536	G	C2-N3	-5.01	1.28	1.32
36	1	635	G	N7-C5	-5.00	1.36	1.39
36	1	2626	A	N3-C4	-5.00	1.31	1.34
36	1	2644	C	N1-C6	-5.00	1.34	1.37
36	1	2617	U	N3-C4	-5.00	1.33	1.38
36	5	952	A	C5-C6	-5.00	1.36	1.41
36	5	2637	A	N7-C5	-5.00	1.36	1.39
36	5	2899	C	C2-O2	-5.00	1.20	1.24

All (4696) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1116	G	O5'-P-OP1	-18.97	87.94	110.70
36	5	1152	G	C2-N3-C4	-18.00	102.90	111.90
36	5	1152	G	N3-C4-C5	17.23	137.22	128.60
36	5	1152	G	N3-C4-N9	-15.73	116.56	126.00
36	1	1495	U	C5-C6-N1	-15.66	114.87	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	639	G	N1-C6-O6	14.78	128.77	119.90
36	5	2199	G	N1-C6-O6	14.34	128.50	119.90
36	5	1158	A	N1-C6-N6	14.13	127.08	118.60
36	5	424	G	C5-C6-O6	-13.84	120.30	128.60
36	5	1179	A	O5'-P-OP1	-13.82	93.26	105.70
36	1	1838	G	N1-C6-O6	13.28	127.87	119.90
36	5	960	U	N3-C2-O2	-12.66	113.34	122.20
36	5	1152	G	C5-N7-C8	-12.50	98.05	104.30
36	1	282	G	C8-N9-C4	-12.33	101.47	106.40
36	5	2950	G	C4-C5-N7	12.21	115.69	110.80
36	1	435	C	C6-N1-C2	12.21	125.18	120.30
36	5	1306	G	C5-C6-O6	-12.20	121.28	128.60
36	1	790	U	N3-C2-O2	-12.15	113.70	122.20
36	1	1166	G	N1-C6-O6	11.87	127.02	119.90
36	1	2819	A	O5'-P-OP2	-11.72	95.15	105.70
36	5	1200	A	N1-C6-N6	11.64	125.58	118.60
36	1	979	U	N3-C2-O2	-11.47	114.17	122.20
36	5	2726	C	C6-N1-C2	-11.47	115.71	120.30
36	5	1897	G	N1-C6-O6	11.47	126.78	119.90
36	5	3245	A	C2-N3-C4	-11.38	104.91	110.60
1	6	448	C	C6-N1-C2	-11.34	115.76	120.30
36	5	2943	G	N1-C6-O6	11.25	126.65	119.90
36	1	2870	C	C2-N1-C1'	-11.22	106.46	118.80
36	1	2636	A	C8-N9-C4	-11.20	101.32	105.80
36	5	1186	G	O5'-P-OP2	-11.19	95.63	105.70
36	5	426	G	O5'-P-OP2	-11.18	95.64	105.70
36	1	639	G	C5-C6-O6	-11.18	121.89	128.60
36	5	2875	U	C5-C6-N1	11.14	128.27	122.70
36	1	957	C	N1-C2-O2	-11.14	112.22	118.90
36	1	2610	G	N1-C6-O6	11.13	126.58	119.90
36	1	645	A	N1-C6-N6	-11.06	111.96	118.60
36	5	2943	G	C6-C5-N7	-11.06	123.76	130.40
36	1	636	C	N3-C4-C5	11.03	126.31	121.90
36	1	2714	G	N3-C4-C5	11.02	134.11	128.60
36	1	2610	G	C5-C6-O6	-10.99	122.01	128.60
36	1	2868	U	N1-C2-O2	10.94	130.46	122.80
36	5	1152	G	N1-C6-O6	10.93	126.46	119.90
36	5	2893	C	N3-C4-C5	-10.85	117.56	121.90
36	5	2971	A	C2-N3-C4	10.85	116.02	110.60
36	5	3245	A	N7-C8-N9	10.81	119.20	113.80
1	6	1026	A	O5'-P-OP1	-10.76	96.02	105.70
36	5	96	G	O5'-P-OP2	-10.75	96.03	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	17	C	C6-N1-C2	-10.74	116.00	120.30
36	1	369	A	C8-N9-C4	-10.72	101.51	105.80
36	1	1838	G	C6-C5-N7	-10.68	123.99	130.40
36	5	41	G	C4-C5-N7	10.65	115.06	110.80
36	1	2121	G	N1-C6-O6	-10.64	113.52	119.90
36	5	968	G	O5'-P-OP1	-10.64	96.13	105.70
36	1	363	G	C5-C6-O6	-10.62	122.23	128.60
36	5	1150	A	O5'-P-OP2	-10.60	96.16	105.70
36	1	59	G	N1-C6-O6	10.57	126.24	119.90
36	5	2819	A	O5'-P-OP2	-10.57	96.19	105.70
36	5	2375	G	N1-C6-O6	-10.52	113.59	119.90
36	5	3245	A	C5-N7-C8	-10.52	98.64	103.90
36	1	2617	U	C5-C4-O4	10.46	132.18	125.90
36	5	1306	G	N1-C6-O6	10.44	126.16	119.90
36	1	2714	G	N3-C4-N9	-10.44	119.74	126.00
36	5	2950	G	C5-C6-O6	-10.44	122.34	128.60
36	1	2247	G	N1-C6-O6	10.42	126.15	119.90
36	5	966	U	N3-C2-O2	-10.40	114.92	122.20
36	5	960	U	N1-C2-O2	10.39	130.07	122.80
36	5	2872	A	N1-C6-N6	10.38	124.83	118.60
36	1	1495	U	C4-C5-C6	10.38	125.93	119.70
36	5	2899	C	C6-N1-C2	-10.36	116.15	120.30
36	5	2704	A	O5'-P-OP1	-10.34	96.39	105.70
36	5	1481	A	O5'-P-OP2	-10.33	96.41	105.70
36	5	776	U	N3-C2-O2	-10.29	115.00	122.20
36	5	2400	G	N1-C6-O6	10.27	126.06	119.90
36	1	1308	A	O5'-P-OP2	-10.22	96.50	105.70
36	1	885	U	C5-C6-N1	-10.22	117.59	122.70
36	1	2283	G	N1-C6-O6	10.19	126.02	119.90
36	5	2715	A	N9-C4-C5	10.18	109.87	105.80
36	5	1117	G	O5'-P-OP1	-10.14	96.58	105.70
36	5	640	U	N1-C2-O2	-10.13	115.71	122.80
36	5	2954	U	C2-N1-C1'	10.12	129.84	117.70
36	1	70	A	N1-C6-N6	10.07	124.64	118.60
36	5	869	G	N1-C6-O6	-10.07	113.86	119.90
36	5	2726	C	C5-C4-N4	10.04	127.23	120.20
36	5	2943	G	C4-C5-N7	10.03	114.81	110.80
35	SM	135	ALA	N-CA-CB	10.02	124.13	110.10
36	5	2942	C	O5'-P-OP2	-10.02	96.68	105.70
36	5	280	U	O5'-P-OP2	-10.01	96.69	105.70
36	5	776	U	N1-C2-N3	9.98	120.89	114.90
36	1	1166	G	C5-C6-O6	-9.96	122.62	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	652	G	O5'-P-OP2	-9.94	96.76	105.70
36	1	2618	G	N1-C6-O6	-9.93	113.94	119.90
36	5	3181	C	N3-C2-O2	-9.92	114.96	121.90
36	5	2954	U	O4'-C1'-N1	9.89	116.11	108.20
36	1	2846	U	C5-C4-O4	9.88	131.83	125.90
38	8	80	A	C8-N9-C4	-9.88	101.85	105.80
36	5	2350	C	O5'-P-OP2	-9.87	96.82	105.70
36	1	59	G	C5-C6-O6	-9.84	122.70	128.60
36	5	1158	A	C5-C6-N6	-9.83	115.84	123.70
36	5	2822	U	O5'-P-OP1	-9.82	96.86	105.70
36	5	283	G	C4-C5-N7	9.80	114.72	110.80
36	5	2950	G	C6-C5-N7	-9.79	124.53	130.40
36	1	346	C	N1-C2-O2	-9.79	113.03	118.90
36	5	41	G	N1-C6-O6	9.77	125.76	119.90
36	1	979	U	C6-N1-C2	-9.76	115.14	121.00
36	5	1099	A	N1-C6-N6	9.72	124.44	118.60
36	1	3025	C	C6-N1-C2	9.72	124.19	120.30
36	1	2374	C	N3-C2-O2	-9.71	115.10	121.90
36	1	59	G	C6-C5-N7	-9.71	124.57	130.40
36	1	3110	C	C6-N1-C2	-9.71	116.42	120.30
36	5	776	U	C5-C6-N1	-9.71	117.84	122.70
36	1	645	A	N9-C4-C5	9.70	109.68	105.80
36	1	1437	C	C6-N1-C2	-9.68	116.43	120.30
36	1	1838	G	C5-C6-O6	-9.64	122.81	128.60
36	1	2827	U	N1-C2-N3	9.63	120.68	114.90
1	2	553	G	N1-C6-O6	9.61	125.67	119.90
36	5	2715	A	N1-C6-N6	-9.59	112.85	118.60
1	6	163	G	N3-C4-N9	-9.59	120.25	126.00
36	5	420	G	C8-N9-C4	9.56	110.22	106.40
36	5	3245	A	C8-N9-C4	-9.54	101.98	105.80
36	1	648	C	O5'-P-OP1	-9.52	97.13	105.70
36	5	1117	G	C4-C5-N7	9.52	114.61	110.80
36	5	3245	A	C6-C5-N7	-9.52	125.63	132.30
36	1	2726	C	N3-C4-N4	-9.49	111.36	118.00
36	1	3278	C	N1-C2-O2	9.48	124.59	118.90
36	1	347	G	C4-C5-N7	9.47	114.59	110.80
36	1	1116	G	C4-C5-C6	9.45	124.47	118.80
36	1	2764	C	C5-C6-N1	9.44	125.72	121.00
36	5	428	A	N1-C6-N6	9.44	124.27	118.60
36	1	407	A	O5'-P-OP2	-9.44	97.20	105.70
36	1	1179	A	O5'-P-OP1	-9.43	97.22	105.70
36	5	2315	G	O5'-P-OP1	-9.43	97.22	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2643	A	O5'-P-OP1	-9.41	97.23	105.70
36	1	2400	G	C6-C5-N7	-9.40	124.76	130.40
36	1	2643	A	C8-N9-C4	9.38	109.55	105.80
36	1	1403	C	C6-N1-C2	9.36	124.05	120.30
36	1	2639	G	C6-C5-N7	-9.35	124.79	130.40
36	5	1434	G	N9-C4-C5	9.34	109.14	105.40
36	1	651	G	O5'-P-OP2	-9.34	97.29	105.70
36	5	922	U	C5-C6-N1	-9.31	118.04	122.70
36	5	2199	G	C5-C6-O6	-9.30	123.02	128.60
36	5	1152	G	C4-C5-N7	9.29	114.52	110.80
36	5	2186	U	O5'-P-OP2	-9.29	97.34	105.70
36	5	404	G	O5'-P-OP2	-9.28	97.34	105.70
36	1	335	G	C5-C6-O6	-9.28	123.03	128.60
36	5	1006	A	O5'-P-OP2	-9.28	97.35	105.70
36	5	1879	A	N1-C6-N6	9.27	124.17	118.60
36	1	1308	A	C8-N9-C4	-9.27	102.09	105.80
36	1	1296	C	C6-N1-C2	-9.25	116.60	120.30
36	5	343	U	O5'-P-OP1	-9.25	97.38	105.70
36	5	2928	C	C6-N1-C2	-9.24	116.60	120.30
1	2	314	C	O5'-P-OP1	-9.21	97.41	105.70
36	5	1450	G	N1-C6-O6	9.21	125.43	119.90
36	5	41	G	C5-C6-O6	-9.21	123.07	128.60
1	6	1700	C	N1-C2-O2	9.20	124.42	118.90
1	2	1096	C	N1-C2-O2	9.20	124.42	118.90
36	1	638	C	O5'-P-OP2	-9.19	97.43	105.70
36	1	1902	G	C6-C5-N7	-9.19	124.89	130.40
36	1	691	A	O5'-P-OP1	-9.18	97.44	105.70
36	5	2634	U	C5-C4-O4	-9.16	120.41	125.90
36	5	2359	C	C6-N1-C2	9.15	123.96	120.30
36	5	952	A	N1-C6-N6	9.14	124.09	118.60
36	1	609	G	O5'-P-OP2	-9.14	97.48	105.70
36	1	2142	A	C2-N3-C4	9.13	115.17	110.60
73	O7	65	ARG	NE-CZ-NH1	9.12	124.86	120.30
36	1	2808	A	N1-C6-N6	9.11	124.07	118.60
36	5	1181	U	C5-C6-N1	-9.11	118.15	122.70
36	5	1116	G	N3-C4-C5	-9.11	124.05	128.60
36	1	1320	C	C6-N1-C2	-9.10	116.66	120.30
36	5	2794	G	C5-C6-O6	-9.09	123.15	128.60
36	1	3181	C	C5-C4-N4	9.08	126.56	120.20
1	2	1773	C	C6-N1-C2	-9.07	116.67	120.30
36	5	1116	G	C4-C5-C6	9.05	124.23	118.80
36	1	1307	G	N1-C6-O6	-9.05	114.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1837	U	O5'-P-OP1	-9.03	97.58	105.70
36	1	1152	G	O5'-P-OP1	-9.02	97.59	105.70
36	5	559	A	O5'-P-OP2	-9.01	97.59	105.70
36	1	2868	U	N3-C2-O2	-9.00	115.90	122.20
36	5	2950	G	C5-N7-C8	-8.99	99.80	104.30
37	3	90	U	O5'-P-OP2	-8.98	97.62	105.70
38	4	94	C	C6-N1-C2	8.98	123.89	120.30
1	2	73	U	O4'-C1'-N1	8.97	115.38	108.20
36	5	1452	A	N1-C6-N6	8.97	123.98	118.60
36	1	2402	A	C5-C6-N6	-8.97	116.53	123.70
36	5	2295	A	C8-N9-C4	-8.96	102.21	105.80
36	5	2954	U	C6-N1-C1'	-8.95	108.67	121.20
36	1	145	G	N1-C6-O6	8.94	125.26	119.90
36	5	1468	A	N1-C6-N6	8.93	123.95	118.60
36	5	2726	C	N3-C4-N4	-8.92	111.75	118.00
36	5	3143	C	N1-C2-O2	-8.91	113.55	118.90
36	1	1167	U	C5-C6-N1	-8.91	118.24	122.70
36	5	592	A	O5'-P-OP1	-8.91	97.68	105.70
36	5	2283	G	C5-C6-O6	-8.90	123.26	128.60
36	5	1200	A	C5-C6-N6	-8.88	116.59	123.70
36	5	1099	A	C5-C6-N6	-8.88	116.59	123.70
36	5	2290	C	C6-N1-C2	8.88	123.85	120.30
36	5	2199	G	C6-C5-N7	-8.87	125.08	130.40
36	5	1513	G	C8-N9-C4	-8.87	102.85	106.40
36	1	794	U	O5'-P-OP2	-8.86	97.72	105.70
36	5	2283	G	C4-C5-N7	8.86	114.34	110.80
36	1	1196	C	C6-N1-C2	8.85	123.84	120.30
36	5	3245	A	N1-C2-N3	8.85	133.72	129.30
36	5	2398	A	N1-C6-N6	-8.84	113.30	118.60
36	5	3313	U	O5'-P-OP2	-8.83	97.75	105.70
36	1	3217	C	C2-N1-C1'	8.83	128.51	118.80
36	5	2943	G	C5-C6-O6	-8.81	123.31	128.60
36	1	2619	G	O5'-P-OP1	-8.81	97.77	105.70
36	1	960	U	C6-N1-C2	8.80	126.28	121.00
36	5	3099	C	C6-N1-C2	8.80	123.82	120.30
36	5	1117	G	C5-C6-O6	-8.79	123.33	128.60
36	1	1151	U	C6-N1-C2	-8.77	115.73	121.00
36	5	283	G	C5-C6-O6	-8.77	123.34	128.60
36	1	960	U	C5-C6-N1	-8.77	118.32	122.70
36	1	3344	A	N7-C8-N9	8.76	118.18	113.80
36	5	2411	U	C5-C6-N1	-8.76	118.32	122.70
36	1	679	U	O5'-P-OP2	-8.75	97.83	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3092	C	C6-N1-C2	8.74	123.80	120.30
38	8	80	A	N7-C8-N9	8.73	118.17	113.80
36	1	890	C	C6-N1-C2	-8.73	116.81	120.30
36	1	1114	U	C4-C5-C6	-8.72	114.47	119.70
1	2	1291	G	C2-N3-C4	-8.72	107.54	111.90
36	5	1449	A	C4-C5-C6	8.72	121.36	117.00
1	6	1634	C	C2-N1-C1'	8.71	128.39	118.80
1	6	364	G	C5-C6-O6	-8.71	123.37	128.60
37	7	10	C	C2-N1-C1'	8.70	128.37	118.80
36	5	1879	A	C6-C5-N7	-8.69	126.22	132.30
1	2	334	G	N3-C4-C5	8.67	132.94	128.60
1	6	1	U	C2-N1-C1'	8.66	128.10	117.70
1	2	639	U	N3-C2-O2	-8.65	116.14	122.20
36	5	3143	C	N3-C4-C5	-8.65	118.44	121.90
36	1	2247	G	C6-C5-N7	-8.65	125.21	130.40
1	6	29	U	C5-C4-O4	8.65	131.09	125.90
1	6	631	G	O5'-P-OP2	-8.64	97.92	105.70
36	1	984	G	N3-C4-C5	-8.64	124.28	128.60
36	5	2715	A	C8-N9-C4	-8.64	102.34	105.80
36	1	27	C	O5'-P-OP1	-8.64	97.93	105.70
36	5	1428	A	O5'-P-OP2	-8.63	97.93	105.70
36	1	3181	C	N3-C4-N4	-8.63	111.96	118.00
38	4	103	G	N3-C4-C5	-8.62	124.29	128.60
36	5	2283	G	O5'-P-OP2	-8.61	97.95	105.70
36	5	2996	U	N1-C2-O2	8.61	128.83	122.80
36	5	361	A	N1-C6-N6	-8.61	113.44	118.60
36	1	1156	C	N3-C2-O2	-8.60	115.88	121.90
36	5	3245	A	N1-C6-N6	8.60	123.76	118.60
36	5	2732	G	O5'-P-OP2	-8.59	97.97	105.70
36	5	1897	G	C5-C6-O6	-8.59	123.45	128.60
36	1	639	G	C6-C5-N7	-8.59	125.25	130.40
36	5	1390	A	N9-C4-C5	8.58	109.23	105.80
36	1	1151	U	O5'-P-OP2	8.57	120.99	110.70
36	1	1362	G	C8-N9-C4	8.56	109.83	106.40
1	6	858	G	O4'-C1'-N9	8.56	115.05	108.20
48	m1	112	LEU	CA-CB-CG	8.56	134.98	115.30
36	1	3265	C	C6-N1-C2	8.54	123.72	120.30
36	1	1381	A	O5'-P-OP1	-8.54	98.02	105.70
1	6	542	A	O4'-C1'-N9	8.53	115.02	108.20
36	5	2726	C	N3-C2-O2	-8.53	115.93	121.90
36	1	917	A	O5'-P-OP2	-8.53	98.03	105.70
36	5	1127	G	N1-C6-O6	-8.52	114.79	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	907	G	N9-C4-C5	-8.52	101.99	105.40
36	5	1316	C	N3-C4-N4	8.51	123.96	118.00
36	1	645	A	C8-N9-C4	-8.50	102.40	105.80
36	5	1079	A	N1-C6-N6	-8.50	113.50	118.60
36	1	1116	G	C6-C5-N7	-8.50	125.30	130.40
36	1	2379	U	N1-C2-O2	-8.49	116.86	122.80
36	5	1075	A	C8-N9-C4	8.49	109.20	105.80
36	5	2715	A	C5-C6-N6	8.48	130.49	123.70
36	1	797	U	O5'-P-OP1	-8.47	98.07	105.70
36	5	966	U	N1-C2-O2	8.47	128.73	122.80
36	1	1902	G	C4-C5-N7	8.46	114.19	110.80
36	1	1367	G	O5'-P-OP1	-8.46	98.09	105.70
36	5	651	G	C8-N9-C4	-8.46	103.02	106.40
36	1	2714	G	C2-N3-C4	-8.46	107.67	111.90
36	5	1158	A	C6-C5-N7	-8.46	126.38	132.30
1	6	426	G	O5'-P-OP2	-8.45	98.09	105.70
36	5	424	G	N1-C6-O6	8.45	124.97	119.90
36	5	1316	C	N3-C4-C5	-8.44	118.52	121.90
36	1	2400	G	N1-C6-O6	8.44	124.97	119.90
36	5	2818	U	O5'-P-OP1	-8.44	98.11	105.70
36	1	919	U	O5'-P-OP2	-8.44	98.11	105.70
36	1	1729	A	O5'-P-OP2	-8.43	98.11	105.70
36	1	2889	C	N1-C2-O2	8.43	123.96	118.90
1	6	1700	C	C2-N1-C1'	8.43	128.07	118.80
36	5	1379	G	C8-N9-C4	8.43	109.77	106.40
36	5	939	U	O5'-P-OP2	-8.42	98.12	105.70
36	5	2866	U	N3-C2-O2	-8.42	116.31	122.20
36	1	1838	G	N9-C4-C5	-8.41	102.03	105.40
36	5	2572	C	N1-C2-O2	8.41	123.95	118.90
36	1	1495	U	C2-N1-C1'	-8.41	107.61	117.70
36	5	2246	G	O5'-P-OP2	8.40	120.79	110.70
36	1	655	C	N1-C2-O2	-8.40	113.86	118.90
36	1	939	U	N1-C2-O2	-8.40	116.92	122.80
36	5	923	C	C6-N1-C2	8.40	123.66	120.30
36	5	1450	G	N3-C2-N2	-8.39	114.03	119.90
36	5	2358	A	C8-N9-C4	8.39	109.16	105.80
36	1	1343	A	O5'-P-OP2	-8.39	98.15	105.70
36	1	984	G	C8-N9-C4	-8.38	103.05	106.40
36	1	274	G	N1-C6-O6	8.37	124.92	119.90
36	1	421	G	C2-N3-C4	8.37	116.08	111.90
36	1	24	G	C2-N3-C4	-8.36	107.72	111.90
37	7	101	G	N1-C6-O6	8.36	124.91	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	639	U	N1-C2-O2	8.35	128.65	122.80
36	1	406	G	O4'-C1'-N9	8.34	114.87	108.20
36	5	424	G	C4-C5-N7	8.33	114.13	110.80
36	5	1868	G	C6-C5-N7	-8.33	125.40	130.40
37	7	37	G	N9-C4-C5	-8.33	102.07	105.40
36	1	1902	G	N1-C6-O6	8.32	124.89	119.90
36	5	3154	C	N1-C2-O2	8.31	123.89	118.90
36	5	1306	G	C4-C5-N7	8.31	114.12	110.80
36	1	2827	U	C5-C4-O4	8.30	130.88	125.90
36	1	421	G	C5-C6-N1	8.30	115.65	111.50
36	5	1049	C	C6-N1-C2	-8.30	116.98	120.30
36	1	1414	G	N1-C6-O6	8.29	124.87	119.90
36	1	386	A	N1-C6-N6	8.28	123.57	118.60
36	5	2893	C	C6-N1-C2	-8.28	116.99	120.30
36	5	666	A	N1-C6-N6	-8.27	113.64	118.60
36	1	1114	U	C5-C6-N1	8.26	126.83	122.70
36	1	3260	G	N1-C6-O6	8.26	124.85	119.90
36	5	2944	U	C5-C6-N1	8.25	126.83	122.70
1	6	119	A	C2-N3-C4	-8.25	106.47	110.60
36	1	3134	A	O5'-P-OP2	-8.25	98.28	105.70
36	5	2176	U	N3-C2-O2	-8.24	116.43	122.20
38	4	32	C	N3-C4-C5	8.24	125.20	121.90
36	1	2726	C	N3-C2-O2	-8.23	116.14	121.90
36	5	1493	G	O5'-P-OP1	-8.23	98.29	105.70
36	1	1148	G	C5-C6-O6	-8.23	123.67	128.60
36	1	1484	U	P-O3'-C3'	8.23	129.57	119.70
36	1	925	A	C6-N1-C2	-8.22	113.67	118.60
36	1	3362	A	O4'-C1'-N9	8.22	114.78	108.20
36	5	2287	C	C6-N1-C2	-8.22	117.01	120.30
36	1	2572	C	C2-N1-C1'	8.22	127.84	118.80
37	3	95	A	N1-C6-N6	8.22	123.53	118.60
1	6	1025	A	N1-C6-N6	8.22	123.53	118.60
36	1	716	A	N1-C6-N6	8.21	123.53	118.60
36	5	1307	G	P-O3'-C3'	8.21	129.56	119.70
36	1	1192	C	N1-C2-O2	8.21	123.83	118.90
36	5	1884	A	N1-C6-N6	8.21	123.53	118.60
36	1	2431	C	O5'-P-OP2	-8.21	98.31	105.70
36	5	3244	A	O5'-P-OP2	-8.20	98.32	105.70
37	7	9	C	C6-N1-C2	8.20	123.58	120.30
36	5	640	U	N3-C4-O4	8.20	125.14	119.40
36	5	2145	A	C8-N9-C4	-8.20	102.52	105.80
36	5	1153	A	N1-C6-N6	8.20	123.52	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1323	G	C5-C6-O6	-8.20	123.68	128.60
36	5	1114	U	OP2-P-O3'	8.19	123.22	105.20
36	1	1365	G	N3-C4-C5	-8.18	124.51	128.60
36	1	107	A	N1-C6-N6	8.18	123.51	118.60
36	5	1370	G	N3-C4-C5	-8.17	124.52	128.60
36	5	2572	C	C2-N1-C1'	8.16	127.78	118.80
1	6	364	G	N3-C4-N9	8.16	130.90	126.00
36	5	2290	C	O5'-P-OP2	-8.16	98.36	105.70
37	7	87	G	N1-C6-O6	8.15	124.79	119.90
36	5	3181	C	C6-N1-C2	-8.14	117.04	120.30
36	5	1158	A	N9-C4-C5	-8.14	102.55	105.80
73	O7	65	ARG	NE-CZ-NH2	-8.13	116.23	120.30
36	1	2392	C	C6-N1-C2	8.13	123.55	120.30
36	1	640	U	N1-C2-O2	-8.13	117.11	122.80
36	1	3210	A	N1-C6-N6	-8.13	113.72	118.60
36	1	2812	C	C6-N1-C2	8.12	123.55	120.30
36	1	1128	U	N3-C4-O4	-8.12	113.72	119.40
36	5	1362	G	C8-N9-C4	8.12	109.65	106.40
36	5	881	C	C5-C6-N1	8.11	125.05	121.00
36	5	907	G	N3-C4-N9	8.11	130.86	126.00
36	1	1308	A	N7-C8-N9	8.10	117.85	113.80
36	1	218	G	O5'-P-OP2	-8.09	98.42	105.70
36	5	1301	A	N1-C6-N6	8.09	123.45	118.60
36	1	2871	G	O5'-P-OP2	-8.08	98.43	105.70
36	5	651	G	N3-C4-C5	-8.08	124.56	128.60
36	5	2872	A	C4-C5-N7	8.08	114.74	110.70
36	5	2375	G	C5-C6-O6	8.07	133.44	128.60
36	1	2636	A	N7-C8-N9	8.07	117.83	113.80
36	1	1320	C	N3-C4-C5	-8.06	118.67	121.90
1	6	1000	C	C2-N1-C1'	8.06	127.67	118.80
1	6	453	U	N3-C2-O2	-8.06	116.56	122.20
36	5	2872	A	C5-C6-N6	-8.06	117.25	123.70
36	5	2634	U	C2-N3-C4	-8.05	122.17	127.00
44	17	229	PHE	CB-CG-CD1	8.05	126.44	120.80
36	5	651	G	C4-C5-C6	8.04	123.63	118.80
37	7	37	G	C5-C6-O6	-8.04	123.77	128.60
36	5	806	A	O5'-P-OP1	-8.04	98.46	105.70
1	6	889	U	O5'-P-OP1	-8.03	98.47	105.70
1	6	65	A	N1-C6-N6	8.03	123.42	118.60
36	1	2617	U	C5-C6-N1	-8.03	118.69	122.70
36	1	2618	G	C8-N9-C4	-8.03	103.19	106.40
36	5	1366	A	N9-C4-C5	8.01	109.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2603	G	C4-C5-N7	7.99	114.00	110.80
36	1	2617	U	N1-C2-N3	7.98	119.69	114.90
1	6	14	C	C6-N1-C2	-7.98	117.11	120.30
36	5	1392	G	C8-N9-C4	7.98	109.59	106.40
36	1	2846	U	N3-C2-O2	-7.97	116.62	122.20
36	5	2899	C	C2-N1-C1'	7.96	127.56	118.80
1	6	858	G	C4-N9-C1'	7.96	136.85	126.50
36	1	1495	U	N1-C2-O2	-7.95	117.23	122.80
37	7	87	G	C5-C6-O6	-7.95	123.83	128.60
36	1	363	G	N1-C6-O6	7.95	124.67	119.90
36	1	2355	G	N1-C6-O6	7.95	124.67	119.90
36	1	2870	C	C6-N1-C1'	7.94	130.33	120.80
36	5	913	A	C8-N9-C4	-7.94	102.62	105.80
36	1	2197	C	C6-N1-C2	7.92	123.47	120.30
36	1	979	U	C2-N1-C1'	7.92	127.20	117.70
1	2	402	C	C6-N1-C2	7.91	123.47	120.30
36	1	2572	C	N1-C2-O2	7.91	123.65	118.90
36	5	2699	G	C8-N9-C4	7.91	109.56	106.40
38	8	96	A	C8-N9-C4	7.91	108.96	105.80
36	5	1161	G	C5-C6-N1	7.90	115.45	111.50
36	5	1399	A	N1-C6-N6	7.90	123.34	118.60
36	5	1292	C	C6-N1-C2	7.90	123.46	120.30
36	1	2247	G	C5-C6-O6	-7.90	123.86	128.60
36	1	1192	C	C2-N1-C1'	7.90	127.49	118.80
36	1	1495	U	N1-C2-N3	7.90	119.64	114.90
36	5	38	U	O5'-P-OP2	-7.90	98.59	105.70
36	5	1321	G	N1-C6-O6	7.90	124.64	119.90
36	5	2331	C	N3-C4-C5	-7.89	118.74	121.90
36	1	1858	A	C2-N3-C4	7.89	114.54	110.60
36	5	2295	A	C5-C6-N1	7.89	121.64	117.70
36	5	2524	A	O4'-C1'-N9	7.88	114.51	108.20
36	5	776	U	C4-C5-C6	7.88	124.43	119.70
36	5	2332	A	C8-N9-C4	7.87	108.95	105.80
36	1	716	A	N9-C4-C5	-7.86	102.65	105.80
36	5	1437	C	C6-N1-C2	-7.86	117.16	120.30
36	1	1099	A	N1-C6-N6	7.86	123.32	118.60
36	5	3181	C	C2-N1-C1'	7.86	127.45	118.80
36	1	426	G	N3-C4-C5	-7.86	124.67	128.60
1	2	1600	A	N1-C6-N6	7.85	123.31	118.60
37	3	8	G	N1-C6-O6	-7.85	115.19	119.90
36	1	1157	G	N1-C2-N3	7.85	128.61	123.90
36	1	1389	G	C4-C5-N7	7.84	113.94	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2395	G	O5'-P-OP2	-7.84	98.64	105.70
36	5	610	G	N1-C6-O6	-7.84	115.19	119.90
36	5	708	G	C8-N9-C4	-7.84	103.26	106.40
36	5	1868	G	C4-C5-N7	7.84	113.94	110.80
38	8	114	G	O5'-P-OP1	-7.84	98.64	105.70
36	5	437	G	N3-C4-N9	-7.84	121.30	126.00
36	1	703	G	N3-C4-N9	-7.83	121.30	126.00
36	1	2356	A	N1-C6-N6	7.83	123.30	118.60
36	1	70	A	C6-C5-N7	-7.83	126.82	132.30
36	1	347	G	C5-N7-C8	-7.83	100.39	104.30
36	5	3218	A	N1-C6-N6	7.83	123.30	118.60
1	2	1363	U	N1-C2-O2	7.82	128.28	122.80
36	1	1154	A	C8-N9-C4	-7.82	102.67	105.80
36	1	2283	G	C5-C6-O6	-7.81	123.91	128.60
36	5	907	G	O5'-P-OP1	-7.81	98.67	105.70
36	5	1317	A	C2-N3-C4	7.81	114.50	110.60
36	1	2679	A	C2-N3-C4	-7.80	106.70	110.60
36	5	2820	A	C8-N9-C4	-7.80	102.68	105.80
36	1	2692	A	N1-C6-N6	7.80	123.28	118.60
36	1	65	A	P-O3'-C3'	7.80	129.06	119.70
36	1	3277	U	N3-C2-O2	-7.80	116.74	122.20
36	5	650	C	C2-N1-C1'	-7.79	110.23	118.80
36	5	2938	G	C2-N3-C4	7.79	115.79	111.90
1	2	553	G	C6-C5-N7	-7.78	125.73	130.40
36	1	1852	G	N1-C6-O6	7.78	124.57	119.90
36	1	2679	A	O4'-C1'-N9	7.78	114.42	108.20
38	8	109	A	C5-C6-N1	7.78	121.59	117.70
1	2	1745	G	N3-C4-N9	7.77	130.66	126.00
36	1	1148	G	N1-C6-O6	7.77	124.56	119.90
1	6	957	G	N1-C6-O6	7.77	124.56	119.90
36	5	1592	G	C5-C6-N1	-7.77	107.61	111.50
36	5	1192	C	N1-C2-O2	7.77	123.56	118.90
36	5	1434	G	N3-C4-N9	-7.77	121.34	126.00
1	2	1657	U	O4'-C1'-N1	7.76	114.41	108.20
36	1	2279	A	N9-C4-C5	-7.76	102.70	105.80
36	5	2893	C	N3-C4-N4	7.76	123.43	118.00
36	5	2935	U	O5'-P-OP2	-7.76	98.72	105.70
36	5	880	G	C8-N9-C4	7.76	109.50	106.40
36	1	2314	U	C5-C4-O4	-7.75	121.25	125.90
36	5	647	A	C4-C5-C6	7.75	120.88	117.00
36	1	145	G	C6-C5-N7	-7.75	125.75	130.40
36	1	2887	A	N1-C6-N6	7.75	123.25	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1902	G	N1-C6-O6	7.75	124.55	119.90
36	1	27	C	C6-N1-C2	-7.74	117.20	120.30
36	1	1902	G	C5-C6-O6	-7.74	123.95	128.60
36	5	2354	C	N1-C2-O2	-7.74	114.25	118.90
36	5	2994	A	C8-N9-C4	-7.74	102.70	105.80
36	5	2699	G	C5-C6-O6	-7.74	123.96	128.60
36	1	2409	G	N3-C4-C5	-7.73	124.73	128.60
1	6	144	U	N3-C2-O2	-7.73	116.79	122.20
36	1	790	U	N1-C2-N3	7.73	119.54	114.90
36	5	964	G	C8-N9-C4	-7.73	103.31	106.40
37	3	91	G	C6-C5-N7	-7.73	125.76	130.40
36	1	2642	A	C5-C6-N1	-7.73	113.84	117.70
36	5	2988	C	C5-C6-N1	-7.73	117.14	121.00
36	1	300	G	O5'-P-OP1	-7.72	98.75	105.70
1	6	1793	G	N1-C6-O6	-7.71	115.27	119.90
36	1	2408	U	O5'-P-OP1	-7.70	98.77	105.70
36	1	282	G	N9-C4-C5	7.70	108.48	105.40
1	6	1629	G	O5'-P-OP2	-7.70	98.77	105.70
36	5	1152	G	C8-N9-C1'	7.70	137.01	127.00
36	1	2889	C	N3-C2-O2	-7.70	116.51	121.90
36	1	2827	U	C5-C6-N1	-7.69	118.85	122.70
36	1	1002	A	C8-N9-C4	7.68	108.87	105.80
36	5	922	U	C2-N3-C4	-7.68	122.39	127.00
36	5	974	G	N3-C4-C5	-7.68	124.76	128.60
36	5	1367	G	N1-C6-O6	7.68	124.51	119.90
36	5	2419	A	C8-N9-C4	-7.67	102.73	105.80
36	5	3245	A	C4-C5-N7	7.67	114.54	110.70
44	17	232	ARG	NE-CZ-NH1	-7.67	116.46	120.30
1	6	1011	G	O5'-P-OP2	-7.67	98.80	105.70
36	5	2995	A	O5'-P-OP2	-7.67	98.80	105.70
36	5	2848	G	N1-C6-O6	7.66	124.50	119.90
36	1	3181	C	C6-N1-C2	-7.66	117.23	120.30
36	5	960	U	OP2-P-O3'	7.66	122.05	105.20
36	5	3090	U	O5'-P-OP1	-7.66	98.81	105.70
36	1	925	A	C5-C6-N6	-7.66	117.58	123.70
36	5	1323	G	C4-C5-N7	7.66	113.86	110.80
36	5	2928	C	N3-C4-N4	7.65	123.36	118.00
36	5	966	U	C6-N1-C2	-7.65	116.41	121.00
36	1	2617	U	C4-C5-C6	7.65	124.29	119.70
36	1	1335	C	C6-N1-C2	7.65	123.36	120.30
36	1	355	A	C2-N3-C4	-7.64	106.78	110.60
1	2	1560	U	N3-C2-O2	-7.64	116.85	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1491	A	O5'-P-OP1	-7.64	98.82	105.70
42	15	152	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	6	1637	C	C2-N1-C1'	7.64	127.20	118.80
36	5	1200	A	C6-C5-N7	-7.63	126.95	132.30
36	1	2624	G	N7-C8-N9	7.63	116.91	113.10
1	2	91	G	N1-C6-O6	7.62	124.47	119.90
36	5	41	G	C5-N7-C8	-7.62	100.49	104.30
36	1	2730	G	N1-C6-O6	7.62	124.47	119.90
36	5	907	G	C8-N9-C4	7.62	109.45	106.40
36	5	2372	A	P-O3'-C3'	7.61	128.83	119.70
1	2	334	G	C8-N9-C4	7.61	109.44	106.40
36	5	2881	C	C6-N1-C2	7.60	123.34	120.30
36	5	1117	G	N1-C6-O6	7.60	124.46	119.90
36	1	586	C	N3-C2-O2	7.60	127.22	121.90
1	2	1100	G	C6-C5-N7	-7.60	125.84	130.40
36	1	53	G	C5-C6-O6	7.60	133.16	128.60
1	6	630	A	N1-C6-N6	7.59	123.16	118.60
36	5	2410	U	N1-C2-O2	-7.59	117.48	122.80
36	1	49	A	N1-C6-N6	7.59	123.16	118.60
36	1	220	G	N1-C6-O6	7.59	124.45	119.90
36	5	877	C	N3-C4-C5	7.59	124.94	121.90
36	1	1049	C	O5'-P-OP1	-7.59	98.87	105.70
36	5	2413	A	C2-N3-C4	-7.59	106.81	110.60
36	5	651	G	C6-C5-N7	-7.58	125.85	130.40
38	4	38	U	N3-C2-O2	-7.58	116.89	122.20
36	5	909	G	C5-C6-O6	7.58	133.15	128.60
36	5	1370	G	N3-C4-N9	7.58	130.55	126.00
36	1	343	U	O5'-P-OP2	-7.57	98.88	105.70
36	5	3377	G	C5-C6-O6	-7.57	124.06	128.60
36	5	591	G	C8-N9-C4	7.57	109.43	106.40
36	5	929	A	O5'-P-OP2	-7.56	98.89	105.70
36	1	1437	C	C2-N1-C1'	7.56	127.11	118.80
36	5	2412	G	N1-C2-N2	-7.56	109.40	116.20
36	1	49	A	C8-N9-C4	7.56	108.82	105.80
1	2	1745	G	C5-C6-O6	-7.55	124.07	128.60
36	1	1001	G	N1-C6-O6	7.55	124.43	119.90
36	1	2730	G	C5-C6-N1	-7.55	107.72	111.50
36	5	800	G	C8-N9-C4	7.55	109.42	106.40
36	5	1886	A	N1-C2-N3	-7.55	125.52	129.30
1	6	1537	C	C6-N1-C1'	7.55	129.86	120.80
37	7	101	G	C6-C5-N7	-7.55	125.87	130.40
36	1	947	G	C2-N3-C4	-7.54	108.13	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2610	G	C4-C5-N7	7.54	113.81	110.80
1	6	1634	C	C6-N1-C2	-7.54	117.29	120.30
36	5	3140	G	C4-C5-N7	7.54	113.81	110.80
36	5	1912	U	C6-N1-C2	7.53	125.52	121.00
1	6	1614	A	C2-N3-C4	-7.53	106.84	110.60
36	1	2815	G	N9-C4-C5	-7.53	102.39	105.40
1	6	453	U	C2-N1-C1'	7.52	126.73	117.70
36	5	3115	C	C6-N1-C2	-7.52	117.29	120.30
36	1	2779	A	C8-N9-C4	7.51	108.81	105.80
36	5	2234	G	N9-C4-C5	-7.51	102.40	105.40
36	5	1142	G	C8-N9-C4	-7.51	103.40	106.40
36	5	2627	C	C6-N1-C2	-7.51	117.30	120.30
36	1	2304	C	C6-N1-C2	-7.50	117.30	120.30
1	2	934	C	C2-N1-C1'	7.50	127.05	118.80
36	1	2639	G	N3-C4-N9	7.49	130.50	126.00
36	1	2764	C	C6-N1-C2	-7.49	117.30	120.30
1	2	1039	A	O4'-C1'-N9	7.49	114.19	108.20
36	5	907	G	N3-C2-N2	7.49	125.14	119.90
1	6	782	U	N1-C2-O2	7.49	128.04	122.80
1	6	1773	C	N3-C4-C5	-7.49	118.91	121.90
36	5	3181	C	N1-C2-O2	7.49	123.39	118.90
36	1	678	G	N3-C2-N2	-7.48	114.66	119.90
37	7	105	C	N1-C2-O2	7.48	123.39	118.90
36	1	3344	A	C5-N7-C8	-7.48	100.16	103.90
15	C3	22	ALA	C-N-CD	-7.48	104.15	120.60
36	5	3335	A	N1-C6-N6	7.48	123.09	118.60
1	2	1759	C	C6-N1-C2	7.47	123.29	120.30
1	6	25	C	N1-C2-O2	-7.47	114.42	118.90
36	5	2272	G	O4'-C1'-N9	7.47	114.18	108.20
1	2	453	U	C2-N1-C1'	7.47	126.67	117.70
36	1	289	A	N1-C6-N6	7.46	123.08	118.60
36	1	1835	A	O5'-P-OP1	-7.46	98.98	105.70
36	5	2353	G	C5-C6-O6	-7.46	124.12	128.60
36	1	1158	A	N1-C6-N6	7.45	123.07	118.60
36	1	1848	G	O5'-P-OP1	-7.45	99.00	105.70
36	5	1481	A	C8-N9-C4	-7.45	102.82	105.80
36	1	1151	U	N3-C4-C5	-7.45	110.13	114.60
36	1	681	U	N3-C4-O4	7.45	124.61	119.40
1	6	765	G	C8-N9-C4	7.45	109.38	106.40
36	1	2247	G	C4-C5-N7	7.44	113.78	110.80
36	5	3382	U	N3-C2-O2	-7.44	116.99	122.20
36	1	636	C	C2-N3-C4	-7.43	116.18	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2729	U	O5'-P-OP1	-7.43	99.01	105.70
36	5	1710	C	C6-N1-C2	7.43	123.27	120.30
36	5	977	C	N3-C2-O2	-7.43	116.70	121.90
36	1	578	A	N1-C6-N6	7.43	123.06	118.60
36	1	2610	G	C6-C5-N7	-7.42	125.95	130.40
36	5	2877	G	N3-C4-N9	7.42	130.46	126.00
36	5	2849	C	N1-C2-O2	-7.42	114.45	118.90
36	1	676	G	C4-N9-C1'	7.42	136.14	126.50
36	1	2831	G	N1-C6-O6	7.42	124.35	119.90
36	5	3166	C	N1-C2-O2	7.41	123.34	118.90
36	1	2796	G	C8-N9-C4	-7.41	103.44	106.40
36	5	373	A	C8-N9-C4	7.40	108.76	105.80
36	5	2297	U	C2-N1-C1'	-7.40	108.82	117.70
36	5	1215	U	N1-C2-O2	-7.40	117.62	122.80
1	2	1200	G	N1-C6-O6	7.40	124.34	119.90
36	1	1279	C	C6-N1-C2	-7.39	117.34	120.30
36	5	2121	G	N3-C4-N9	7.39	130.44	126.00
36	5	3382	U	N1-C2-O2	7.39	127.97	122.80
36	5	2121	G	N9-C4-C5	-7.39	102.44	105.40
36	1	716	A	C8-N9-C4	7.39	108.75	105.80
36	5	933	A	C6-N1-C2	-7.38	114.17	118.60
36	5	804	C	N3-C4-N4	7.38	123.17	118.00
36	1	1495	U	C2-N3-C4	-7.38	122.57	127.00
36	1	2356	A	N9-C4-C5	-7.38	102.85	105.80
1	6	558	U	N1-C2-O2	7.37	127.96	122.80
36	1	2777	G	N9-C4-C5	7.37	108.35	105.40
36	5	996	A	O5'-P-OP2	-7.37	99.07	105.70
36	1	1055	A	O5'-P-OP1	-7.37	99.07	105.70
36	1	2795	U	O5'-P-OP1	-7.36	99.07	105.70
36	1	1150	A	O5'-P-OP2	-7.36	99.08	105.70
36	1	96	G	C2-N3-C4	-7.35	108.22	111.90
36	5	951	A	C8-N9-C4	-7.35	102.86	105.80
36	1	1116	G	N3-C4-C5	-7.35	124.93	128.60
36	5	2411	U	C2-N3-C4	-7.35	122.59	127.00
36	5	2620	G	N9-C4-C5	7.35	108.34	105.40
36	1	1114	U	OP2-P-O3'	7.34	121.36	105.20
36	1	645	A	C6-N1-C2	-7.34	114.19	118.60
36	5	1215	U	N3-C2-O2	7.34	127.34	122.20
36	1	2996	U	C2-N1-C1'	7.34	126.51	117.70
1	6	107	C	C6-N1-C2	7.34	123.23	120.30
36	5	2872	A	C5-N7-C8	-7.34	100.23	103.90
1	6	1793	G	C6-C5-N7	7.33	134.80	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	96	G	N1-C6-O6	7.33	124.30	119.90
36	1	394	G	N9-C4-C5	7.33	108.33	105.40
36	1	1365	G	N3-C4-N9	7.33	130.40	126.00
36	5	650	C	N1-C2-O2	-7.32	114.51	118.90
36	1	935	U	N3-C2-O2	-7.32	117.08	122.20
36	1	1128	U	N3-C4-C5	7.31	118.99	114.60
36	5	2421	U	N1-C2-N3	7.31	119.29	114.90
36	5	881	C	C4-C5-C6	-7.31	113.75	117.40
36	1	3187	A	O5'-P-OP2	-7.31	99.12	105.70
36	1	1317	A	O5'-P-OP2	-7.30	99.13	105.70
36	5	1192	C	N3-C2-O2	-7.30	116.79	121.90
36	1	640	U	N3-C2-O2	7.30	127.31	122.20
36	5	216	G	O5'-P-OP1	-7.30	99.13	105.70
36	5	2913	C	N1-C2-O2	-7.30	114.52	118.90
36	5	2983	C	O5'-P-OP1	-7.30	99.13	105.70
36	5	3362	A	O4'-C1'-N9	7.30	114.04	108.20
36	1	347	G	C5-C6-O6	-7.29	124.22	128.60
36	5	2278	C	C4-C5-C6	-7.29	113.75	117.40
36	5	1390	A	N1-C6-N6	-7.29	114.23	118.60
36	1	639	G	C4-C5-N7	7.29	113.72	110.80
36	5	2198	A	O5'-P-OP2	-7.29	99.14	105.70
38	4	28	C	C6-N1-C2	-7.28	117.39	120.30
36	1	1307	G	P-O3'-C3'	7.28	128.44	119.70
36	5	1306	G	C6-C5-N7	-7.28	126.03	130.40
36	5	437	G	C8-N9-C4	-7.28	103.49	106.40
36	5	3154	C	C2-N1-C1'	7.28	126.81	118.80
36	1	3344	A	C8-N9-C4	-7.28	102.89	105.80
1	6	1306	C	C6-N1-C2	-7.27	117.39	120.30
36	1	57	A	C2-N3-C4	-7.27	106.96	110.60
1	6	194	U	C2-N1-C1'	7.27	126.42	117.70
36	5	1846	C	C5-C6-N1	-7.27	117.37	121.00
36	1	919	U	O5'-P-OP1	7.26	119.42	110.70
36	5	3002	C	C6-N1-C2	7.26	123.21	120.30
36	1	2964	G	N9-C4-C5	7.26	108.31	105.40
36	5	2376	G	C6-C5-N7	-7.26	126.04	130.40
36	5	2967	A	O5'-P-OP1	7.26	119.41	110.70
36	1	347	G	N1-C6-O6	7.26	124.25	119.90
1	6	1634	C	N1-C2-O2	7.26	123.25	118.90
36	5	2322	C	C6-N1-C2	-7.26	117.40	120.30
36	5	2737	C	O5'-P-OP2	-7.26	99.17	105.70
36	1	3209	A	N1-C6-N6	7.25	122.95	118.60
36	5	2234	G	C8-N9-C4	7.25	109.30	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	611	A	N1-C6-N6	7.25	122.95	118.60
36	5	2891	U	C5-C6-N1	-7.25	119.08	122.70
36	5	3154	C	C6-N1-C2	-7.25	117.40	120.30
36	1	2405	C	N3-C4-C5	-7.25	119.00	121.90
36	1	2730	G	C2-N3-C4	-7.24	108.28	111.90
36	5	437	G	N9-C4-C5	7.24	108.30	105.40
36	1	1919	G	C8-N9-C4	-7.24	103.50	106.40
36	1	2590	A	N1-C6-N6	-7.24	114.26	118.60
36	1	2870	C	C6-N1-C2	7.24	123.19	120.30
36	5	3004	C	C6-N1-C2	7.24	123.19	120.30
36	5	2375	G	N9-C4-C5	7.24	108.30	105.40
36	5	2950	G	N1-C6-O6	7.24	124.24	119.90
36	1	1820	U	P-O3'-C3'	7.23	128.38	119.70
36	1	649	A	C8-N9-C4	7.22	108.69	105.80
36	5	3285	C	C2-N1-C1'	7.22	126.75	118.80
36	1	1506	A	N1-C6-N6	-7.22	114.27	118.60
1	6	577	G	C6-C5-N7	-7.22	126.07	130.40
36	1	1389	G	N9-C4-C5	-7.22	102.51	105.40
36	1	1905	G	OP2-P-O3'	7.22	121.08	105.20
36	5	1370	G	N1-C2-N2	-7.22	109.70	116.20
36	5	2801	A	N1-C6-N6	-7.22	114.27	118.60
36	5	55	G	N3-C4-C5	7.21	132.21	128.60
1	6	901	G	C4-C5-N7	7.21	113.68	110.80
1	2	287	G	O4'-C1'-N9	7.21	113.97	108.20
36	1	2978	U	O4'-C1'-N1	7.21	113.97	108.20
36	1	350	C	C2-N1-C1'	7.21	126.73	118.80
36	5	3133	C	C6-N1-C2	-7.21	117.42	120.30
36	1	3306	U	N3-C4-O4	-7.20	114.36	119.40
36	5	612	U	O5'-P-OP1	-7.20	99.22	105.70
1	2	15	U	C6-N1-C2	-7.20	116.68	121.00
1	6	453	U	N1-C2-O2	7.20	127.84	122.80
36	5	1155	C	C5-C6-N1	7.20	124.60	121.00
36	5	1390	A	C8-N9-C4	-7.20	102.92	105.80
36	5	715	A	C5-C6-N1	7.20	121.30	117.70
36	1	76	G	N1-C6-O6	7.20	124.22	119.90
36	5	1506	A	C8-N9-C4	-7.20	102.92	105.80
36	1	2702	A	C8-N9-C4	-7.19	102.92	105.80
36	5	817	A	N1-C6-N6	7.19	122.92	118.60
1	2	831	U	C5-C6-N1	7.19	126.30	122.70
36	5	2880	U	N1-C2-N3	7.19	119.21	114.90
1	6	1085	G	N1-C6-O6	-7.19	115.59	119.90
1	6	1748	G	C8-N9-C4	7.19	109.28	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3218	A	C4-C5-N7	7.19	114.29	110.70
36	1	640	U	N3-C4-O4	7.19	124.43	119.40
36	5	2359	C	C5-C6-N1	-7.19	117.41	121.00
36	1	793	C	C6-N1-C2	-7.18	117.43	120.30
38	4	53	A	C2-N3-C4	7.18	114.19	110.60
38	4	84	C	C6-N1-C2	7.18	123.17	120.30
36	1	1450	G	C4-C5-N7	7.17	113.67	110.80
36	5	2130	G	O5'-P-OP2	-7.17	99.24	105.70
36	1	960	U	C2-N1-C1'	-7.17	109.09	117.70
36	5	1012	G	C4-N9-C1'	-7.17	117.18	126.50
36	5	1183	C	C6-N1-C2	7.17	123.17	120.30
1	2	1100	G	C4-N9-C1'	7.17	135.82	126.50
36	5	86	G	C5-C6-O6	-7.17	124.30	128.60
1	2	1241	G	O4'-C1'-N9	7.16	113.93	108.20
37	3	101	G	C8-N9-C4	7.16	109.27	106.40
1	6	782	U	N3-C2-O2	-7.16	117.19	122.20
36	1	2382	G	N1-C2-N2	-7.16	109.76	116.20
1	6	29	U	N3-C2-O2	-7.16	117.19	122.20
36	1	5	G	C8-N9-C4	-7.16	103.54	106.40
12	C0	88	PRO	N-CA-CB	7.16	111.89	103.30
1	6	364	G	C8-N9-C1'	-7.15	117.70	127.00
36	1	925	A	N1-C6-N6	7.15	122.89	118.60
36	5	803	C	C6-N1-C2	-7.15	117.44	120.30
36	1	2726	C	C5-C4-N4	7.14	125.20	120.20
1	2	542	A	O4'-C1'-N9	7.14	113.91	108.20
1	6	452	A	N1-C6-N6	7.14	122.88	118.60
36	5	830	A	C5-C6-N6	-7.14	117.99	123.70
36	5	3050	U	C5-C4-O4	7.14	130.18	125.90
38	4	26	U	C6-N1-C2	-7.13	116.72	121.00
36	5	3197	G	N3-C4-N9	-7.13	121.72	126.00
36	1	1408	G	C6-C5-N7	-7.13	126.12	130.40
36	5	2381	G	C6-C5-N7	-7.13	126.12	130.40
36	5	2980	U	N3-C2-O2	-7.13	117.21	122.20
36	5	1129	A	O5'-P-OP2	-7.13	99.28	105.70
1	6	1029	U	C2-N1-C1'	-7.13	109.14	117.70
10	S8	29	LEU	CA-CB-CG	7.13	131.69	115.30
36	5	1152	G	N3-C2-N2	-7.13	114.91	119.90
36	5	3136	G	C2-N3-C4	-7.13	108.34	111.90
36	5	3339	A	N1-C6-N6	7.13	122.88	118.60
36	1	2923	U	O5'-P-OP1	-7.12	99.29	105.70
1	6	1581	C	N3-C4-C5	7.12	124.75	121.90
36	1	2884	C	N3-C4-C5	7.12	124.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2205	U	O4'-C1'-N1	7.12	113.89	108.20
36	1	211	A	N1-C2-N3	7.12	132.86	129.30
1	6	1745	G	C8-N9-C1'	-7.11	117.75	127.00
36	1	1838	G	C4-C5-N7	7.11	113.64	110.80
1	6	163	G	N3-C4-C5	7.11	132.15	128.60
36	1	1001	G	N9-C4-C5	-7.10	102.56	105.40
36	1	3344	A	O4'-C1'-N9	7.10	113.88	108.20
36	1	2760	C	N3-C4-C5	-7.10	119.06	121.90
1	6	1180	C	C6-N1-C2	-7.10	117.46	120.30
36	5	2917	G	C5-C6-O6	-7.10	124.34	128.60
36	5	1116	G	C4-N9-C1'	7.09	135.72	126.50
36	5	283	G	C6-C5-N7	-7.09	126.15	130.40
36	5	428	A	C5-C6-N6	-7.09	118.03	123.70
36	5	2131	A	N1-C6-N6	7.09	122.85	118.60
36	1	2936	A	O5'-P-OP1	-7.09	99.32	105.70
1	6	17	C	N3-C2-O2	-7.09	116.94	121.90
36	5	2381	G	N1-C6-O6	7.09	124.15	119.90
1	2	1731	A	N1-C6-N6	7.08	122.85	118.60
36	1	1864	A	C8-N9-C4	7.08	108.63	105.80
54	m8	127	LEU	CA-CB-CG	7.08	131.59	115.30
36	1	3218	A	N1-C6-N6	7.08	122.85	118.60
36	1	59	G	C4-C5-N7	7.08	113.63	110.80
36	5	1317	A	N1-C2-N3	-7.08	125.76	129.30
36	1	1149	G	N1-C6-O6	7.07	124.14	119.90
36	5	1449	A	N1-C2-N3	7.07	132.83	129.30
36	5	3214	U	N3-C2-O2	-7.07	117.25	122.20
36	1	2402	A	C5-C6-N1	7.06	121.23	117.70
36	1	803	C	O5'-P-OP1	7.06	119.18	110.70
36	5	2800	G	N3-C2-N2	-7.05	114.96	119.90
36	5	2927	C	N1-C2-O2	-7.05	114.67	118.90
36	5	2142	A	C5-C6-N1	7.05	121.23	117.70
36	1	339	C	N3-C4-N4	-7.05	113.07	118.00
36	1	2986	U	N1-C2-O2	-7.05	117.87	122.80
36	1	2374	C	C2-N1-C1'	7.05	126.55	118.80
36	5	3153	U	N1-C2-O2	7.05	127.73	122.80
36	1	2381	G	N3-C4-C5	-7.04	125.08	128.60
36	5	2811	A	N1-C6-N6	-7.04	114.37	118.60
36	1	1316	C	N3-C4-N4	7.04	122.93	118.00
36	1	1445	U	N1-C2-O2	-7.04	117.87	122.80
36	5	923	C	C5-C4-N4	-7.04	115.27	120.20
36	5	2848	G	C6-C5-N7	-7.04	126.18	130.40
36	5	2864	A	C8-N9-C4	7.04	108.61	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	337	G	C4-N9-C1'	7.03	135.64	126.50
36	5	55	G	O5'-P-OP2	-7.03	99.37	105.70
36	5	2899	C	N1-C2-N3	7.03	124.12	119.20
1	2	551	G	C8-N9-C4	-7.03	103.59	106.40
36	1	663	C	C6-N1-C2	7.03	123.11	120.30
36	1	1793	C	O5'-P-OP1	-7.03	99.37	105.70
1	6	639	U	C2-N1-C1'	7.03	126.14	117.70
36	5	2693	C	C6-N1-C2	7.03	123.11	120.30
1	6	779	U	O4'-C1'-N1	7.03	113.82	108.20
37	7	99	G	N1-C6-O6	-7.03	115.69	119.90
36	1	1389	G	C5-C6-O6	-7.02	124.39	128.60
36	1	874	U	O5'-P-OP1	-7.02	99.38	105.70
36	1	191	U	N1-C2-N3	7.02	119.11	114.90
36	5	2349	U	OP1-P-O3'	7.02	120.64	105.20
1	2	577	G	C4-C5-N7	7.02	113.61	110.80
36	1	2406	C	N3-C4-N4	7.01	122.91	118.00
36	5	3026	G	N1-C6-O6	7.01	124.11	119.90
36	1	3362	A	N7-C8-N9	7.01	117.31	113.80
36	1	1450	G	C5-C6-O6	-7.01	124.39	128.60
36	5	2980	U	C6-N1-C2	-7.01	116.80	121.00
36	1	1174	G	N3-C4-N9	7.00	130.20	126.00
36	5	2201	G	N3-C4-C5	-7.00	125.10	128.60
36	1	1007	U	C6-N1-C2	7.00	125.20	121.00
36	1	2996	U	C6-N1-C1'	-7.00	111.40	121.20
36	1	964	G	N3-C2-N2	-7.00	115.00	119.90
36	1	2325	G	C8-N9-C4	-7.00	103.60	106.40
36	5	1115	G	C4-N9-C1'	7.00	135.60	126.50
36	5	2850	G	C5-C6-O6	-7.00	124.40	128.60
36	1	2639	G	C4-N9-C1'	7.00	135.59	126.50
1	6	1361	U	C2-N1-C1'	7.00	126.09	117.70
37	3	117	A	N1-C6-N6	6.99	122.80	118.60
1	6	322	G	N1-C6-O6	6.99	124.10	119.90
36	1	979	U	N1-C2-O2	6.99	127.69	122.80
36	1	1144	U	C5-C6-N1	-6.99	119.20	122.70
36	1	1173	U	C5-C6-N1	-6.99	119.20	122.70
36	5	1300	G	N1-C6-O6	6.99	124.09	119.90
36	5	2317	A	O5'-P-OP2	-6.99	99.41	105.70
36	5	2872	A	C6-C5-N7	-6.99	127.41	132.30
36	1	1174	G	C8-N9-C1'	-6.99	117.92	127.00
37	7	98	C	O5'-P-OP2	-6.99	99.41	105.70
36	5	2920	U	N1-C2-N3	6.99	119.09	114.90
36	1	2356	A	C5-C6-N6	-6.98	118.11	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2388	U	N3-C2-O2	6.98	127.09	122.20
36	5	2403	G	O5'-P-OP2	-6.98	99.42	105.70
36	1	2870	C	N3-C4-C5	6.98	124.69	121.90
1	6	1596	C	N3-C2-O2	-6.98	117.02	121.90
36	5	877	C	C5-C4-N4	-6.98	115.32	120.20
36	5	2956	A	C8-N9-C4	-6.98	103.01	105.80
36	5	2868	U	C5-C6-N1	6.98	126.19	122.70
36	1	2169	G	N1-C6-O6	-6.97	115.72	119.90
36	5	2817	A	C2-N3-C4	6.97	114.09	110.60
36	1	925	A	N1-C2-N3	6.97	132.79	129.30
36	1	2853	A	N1-C6-N6	6.97	122.78	118.60
1	6	609	U	N3-C4-O4	-6.97	114.52	119.40
36	5	617	G	N9-C4-C5	-6.97	102.61	105.40
36	5	1099	A	C6-C5-N7	-6.97	127.42	132.30
36	5	3112	G	C4-C5-N7	6.97	113.59	110.80
1	2	334	G	C2-N3-C4	-6.97	108.42	111.90
36	5	1116	G	C5-C6-N1	-6.96	108.02	111.50
36	1	24	G	N1-C2-N2	-6.96	109.93	116.20
36	5	2376	G	N1-C6-O6	6.96	124.08	119.90
1	2	623	A	O5'-P-OP1	-6.96	99.44	105.70
36	1	1048	A	N1-C2-N3	-6.96	125.82	129.30
1	6	364	G	N1-C6-O6	6.96	124.07	119.90
1	6	1396	U	C6-N1-C2	-6.96	116.83	121.00
36	5	43	A	O4'-C1'-N9	6.96	113.77	108.20
36	1	802	C	O5'-P-OP2	6.96	119.05	110.70
36	5	2699	G	N1-C6-O6	6.96	124.07	119.90
36	5	2880	U	C6-N1-C2	-6.95	116.83	121.00
36	5	942	U	N3-C4-C5	-6.94	110.43	114.60
36	1	957	C	N3-C2-O2	6.94	126.76	121.90
1	6	571	G	N9-C4-C5	6.94	108.18	105.40
36	1	220	G	C4-C5-N7	6.94	113.58	110.80
36	1	1442	U	N3-C2-O2	6.94	127.06	122.20
36	1	3344	A	C2-N3-C4	-6.94	107.13	110.60
36	5	57	A	N1-C6-N6	6.94	122.76	118.60
36	5	3098	G	O5'-P-OP2	-6.94	99.46	105.70
1	6	577	G	N7-C8-N9	6.94	116.57	113.10
37	7	53	U	O5'-P-OP2	-6.93	99.46	105.70
1	6	163	G	N3-C2-N2	-6.93	115.05	119.90
36	5	1591	G	C5-C6-O6	-6.93	124.44	128.60
1	2	1600	A	C5-C6-N1	-6.93	114.23	117.70
36	1	3046	A	C2-N3-C4	-6.93	107.14	110.60
1	6	1637	C	N1-C2-O2	6.93	123.06	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1143	A	C2-N3-C4	-6.93	107.14	110.60
36	5	1507	G	C6-C5-N7	-6.93	126.24	130.40
36	5	2400	G	C6-C5-N7	-6.92	126.25	130.40
36	5	3270	U	O5'-P-OP1	-6.92	99.47	105.70
36	5	1126	G	C5-C6-N1	-6.92	108.04	111.50
36	1	788	C	C6-N1-C2	6.92	123.07	120.30
36	5	776	U	C2-N3-C4	-6.92	122.85	127.00
36	5	1161	G	C2-N3-C4	6.92	115.36	111.90
36	5	1301	A	C4-C5-N7	6.92	114.16	110.70
37	7	56	A	N1-C6-N6	6.92	122.75	118.60
36	1	3265	C	C2-N1-C1'	-6.92	111.19	118.80
36	5	1164	G	O5'-P-OP2	-6.92	99.47	105.70
36	5	1323	G	N1-C6-O6	6.92	124.05	119.90
36	1	2636	A	N9-C4-C5	6.92	108.57	105.80
36	5	1152	G	N1-C2-N3	6.91	128.05	123.90
36	1	804	C	OP1-P-O3'	6.91	120.39	105.20
36	1	2279	A	N1-C6-N6	6.91	122.74	118.60
36	1	3087	A	C4-C5-C6	6.91	120.45	117.00
38	4	32	C	C2-N1-C1'	-6.91	111.20	118.80
36	5	2867	C	N3-C4-C5	-6.91	119.14	121.90
36	5	2283	G	N1-C6-O6	6.90	124.04	119.90
36	1	3217	C	C6-N1-C1'	-6.90	112.52	120.80
36	1	958	C	N3-C4-C5	6.90	124.66	121.90
36	1	2808	A	C6-C5-N7	-6.90	127.47	132.30
36	1	3006	A	C2-N3-C4	-6.90	107.15	110.60
36	5	406	G	O4'-C1'-N9	6.90	113.72	108.20
1	6	467	G	N3-C4-N9	6.90	130.14	126.00
36	1	2298	U	O4'-C1'-N1	6.90	113.72	108.20
1	2	507	U	N1-C2-O2	6.89	127.62	122.80
36	1	2121	G	N3-C2-N2	6.89	124.72	119.90
1	2	768	C	C6-N1-C2	-6.89	117.54	120.30
36	1	361	A	N1-C6-N6	-6.89	114.47	118.60
36	1	363	G	O5'-P-OP1	-6.89	99.50	105.70
37	7	47	C	C2-N3-C4	-6.89	116.46	119.90
36	1	933	A	O5'-P-OP2	-6.89	99.50	105.70
36	5	638	C	O5'-P-OP2	6.89	118.96	110.70
36	1	1405	U	N3-C4-C5	6.88	118.73	114.60
36	5	2968	G	C8-N9-C1'	-6.88	118.05	127.00
36	5	1506	A	N9-C4-C5	6.88	108.55	105.80
36	5	1846	C	C6-N1-C2	6.88	123.05	120.30
36	5	952	A	N9-C4-C5	-6.88	103.05	105.80
36	5	2112	U	C6-N1-C2	-6.88	116.87	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2409	G	O5'-P-OP2	-6.88	99.51	105.70
36	5	2572	C	N3-C2-O2	-6.88	117.08	121.90
36	1	580	C	O5'-P-OP1	-6.88	99.51	105.70
36	5	428	A	N9-C4-C5	-6.88	103.05	105.80
36	1	2853	A	C5-C6-N6	-6.88	118.20	123.70
36	5	1844	C	C6-N1-C2	-6.88	117.55	120.30
36	1	2802	A	OP2-P-O3'	6.87	120.32	105.20
36	5	2849	C	N3-C2-O2	6.87	126.71	121.90
36	1	2356	A	C8-N9-C4	6.87	108.55	105.80
1	6	257	A	N1-C6-N6	6.87	122.72	118.60
1	2	448	C	C6-N1-C2	-6.87	117.55	120.30
36	1	857	G	C5-C6-N1	-6.87	108.07	111.50
36	1	2364	G	C5-C6-O6	-6.87	124.48	128.60
36	5	2194	G	C2-N3-C4	-6.87	108.47	111.90
37	7	12	U	C5-C4-O4	-6.86	121.78	125.90
36	5	2583	C	C6-N1-C2	-6.86	117.56	120.30
36	5	584	G	C8-N9-C4	-6.86	103.66	106.40
36	5	1379	G	N9-C4-C5	-6.86	102.66	105.40
36	1	646	A	C2-N3-C4	-6.86	107.17	110.60
36	5	1496	C	C5-C6-N1	6.86	124.43	121.00
37	7	10	C	C6-N1-C1'	-6.86	112.57	120.80
1	6	1058	U	OP1-P-O3'	6.86	120.28	105.20
65	n9	23	LYS	C-N-CD	6.86	142.80	128.40
36	1	24	G	N9-C4-C5	-6.85	102.66	105.40
36	5	919	U	C2-N3-C4	-6.85	122.89	127.00
36	5	1695	U	N3-C2-O2	-6.85	117.40	122.20
36	5	2726	C	N1-C2-N3	6.85	124.00	119.20
1	6	1767	G	C8-N9-C4	6.85	109.14	106.40
36	5	2866	U	N1-C2-O2	6.85	127.59	122.80
36	5	784	A	N1-C6-N6	6.85	122.71	118.60
36	5	216	G	N1-C6-O6	6.85	124.01	119.90
36	1	2644	C	C5-C6-N1	-6.84	117.58	121.00
36	5	3050	U	C6-N1-C2	-6.84	116.89	121.00
36	5	1158	A	C4-C5-N7	6.84	114.12	110.70
36	1	938	C	C6-N1-C2	-6.84	117.56	120.30
36	5	816	A	C8-N9-C4	-6.83	103.07	105.80
1	2	553	G	C5-C6-N1	-6.83	108.08	111.50
1	2	554	C	N1-C2-O2	6.83	123.00	118.90
36	1	1428	A	N1-C6-N6	6.83	122.70	118.60
36	5	952	A	C5-C6-N6	-6.83	118.23	123.70
36	5	1317	A	C5-C6-N6	-6.83	118.23	123.70
36	5	1085	A	C2-N3-C4	-6.83	107.19	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3197	G	N3-C2-N2	-6.83	115.12	119.90
37	7	79	A	N1-C6-N6	6.83	122.70	118.60
1	6	777	C	C6-N1-C2	-6.83	117.57	120.30
38	4	113	U	C5-C4-O4	6.83	130.00	125.90
36	5	2608	G	OP2-P-O3'	6.82	120.21	105.20
36	1	1124	U	N3-C4-C5	6.82	118.69	114.60
36	5	2950	G	N3-C4-N9	6.82	130.09	126.00
36	1	1447	G	N1-C6-O6	-6.82	115.81	119.90
36	1	2618	G	N9-C4-C5	6.82	108.13	105.40
36	5	3218	A	C5-N7-C8	-6.82	100.49	103.90
36	1	2815	G	C8-N9-C4	6.82	109.13	106.40
36	1	1313	G	C6-C5-N7	-6.81	126.31	130.40
36	5	822	G	N1-C6-O6	6.81	123.99	119.90
36	5	1160	C	N3-C4-C5	-6.81	119.17	121.90
36	1	1307	G	C5-C6-O6	6.81	132.69	128.60
1	6	982	U	C6-N1-C2	6.81	125.08	121.00
36	1	1114	U	O5'-P-OP2	-6.81	99.57	105.70
36	5	91	G	C6-C5-N7	-6.81	126.31	130.40
37	7	37	G	N1-C6-O6	6.81	123.98	119.90
36	1	569	A	C8-N9-C4	6.81	108.52	105.80
1	2	543	C	N3-C2-O2	-6.80	117.14	121.90
36	5	2827	U	N1-C2-O2	6.80	127.56	122.80
36	5	2804	A	C8-N9-C4	6.80	108.52	105.80
36	5	3343	G	N1-C2-N2	-6.80	110.08	116.20
36	1	1054	A	O5'-P-OP2	-6.80	99.58	105.70
36	1	1161	G	O5'-P-OP2	-6.80	99.58	105.70
36	5	2353	G	N1-C6-O6	6.80	123.98	119.90
36	5	2400	G	C5-C6-O6	-6.80	124.52	128.60
36	1	2624	G	C5-N7-C8	-6.80	100.90	104.30
36	5	420	G	N7-C8-N9	-6.80	109.70	113.10
36	5	1368	U	N3-C2-O2	6.80	126.96	122.20
1	2	1432	U	C6-N1-C2	6.79	125.08	121.00
36	5	1591	G	O5'-P-OP1	-6.79	99.59	105.70
36	5	2400	G	OP2-P-O3'	6.79	120.14	105.20
36	5	880	G	N7-C8-N9	-6.79	109.71	113.10
1	2	1363	U	N3-C2-O2	-6.79	117.45	122.20
36	1	1300	G	N3-C4-N9	6.79	130.07	126.00
36	1	721	G	C4-C5-N7	6.78	113.51	110.80
36	1	585	A	C8-N9-C4	6.78	108.51	105.80
36	1	3212	C	C6-N1-C2	6.78	123.01	120.30
36	5	1592	G	C5-C6-O6	6.78	132.67	128.60
36	1	1200	A	C5-N7-C8	6.78	107.29	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2241	U	C5-C4-O4	6.78	129.97	125.90
36	5	2377	G	C8-N9-C4	6.78	109.11	106.40
36	5	3028	G	N1-C2-N2	-6.78	110.10	116.20
36	1	802	C	C6-N1-C2	-6.78	117.59	120.30
36	1	925	A	C6-C5-N7	-6.78	127.56	132.30
36	5	610	G	C4-C5-N7	-6.78	108.09	110.80
36	1	2273	G	N7-C8-N9	-6.77	109.71	113.10
36	5	942	U	N3-C4-O4	6.77	124.14	119.40
36	1	873	C	N1-C2-O2	-6.77	114.84	118.90
36	1	960	U	C2-N3-C4	-6.77	122.94	127.00
36	1	2618	G	C5-C6-N1	6.77	114.89	111.50
36	5	2924	U	O5 ¹ -P-OP1	-6.77	99.60	105.70
36	1	331	G	N3-C2-N2	-6.77	115.16	119.90
36	1	1381	A	O5 ¹ -P-OP2	6.77	118.82	110.70
1	2	507	U	C2-N1-C1'	6.77	125.82	117.70
36	5	298	U	C5-C6-N1	6.77	126.08	122.70
37	7	41	G	N1-C6-O6	6.77	123.96	119.90
36	1	1459	C	N1-C2-O2	-6.76	114.84	118.90
36	1	2856	G	C8-N9-C4	6.76	109.11	106.40
36	1	3217	C	N1-C2-O2	6.76	122.96	118.90
36	5	3154	C	N3-C2-O2	-6.76	117.17	121.90
36	1	1858	A	C8-N9-C4	-6.76	103.10	105.80
36	1	369	A	N7-C8-N9	6.75	117.18	113.80
36	5	3217	C	C2-N1-C1'	-6.75	111.37	118.80
36	5	2923	U	N1-C2-N3	6.75	118.95	114.90
36	5	869	G	C5-C6-N1	6.75	114.88	111.50
36	5	2333	C	C6-N1-C2	6.75	123.00	120.30
36	1	2846	U	N3-C4-O4	-6.75	114.67	119.40
36	1	2300	G	C8-N9-C4	-6.75	103.70	106.40
36	5	55	G	C8-N9-C4	6.75	109.10	106.40
36	5	195	U	O5 ¹ -P-OP2	-6.74	99.63	105.70
36	5	1316	C	N1-C2-O2	-6.74	114.86	118.90
36	1	33	G	N1-C6-O6	6.74	123.94	119.90
36	1	1136	A	C5-C6-N6	-6.74	118.31	123.70
36	5	1475	A	O5 ¹ -P-OP1	6.74	118.78	110.70
36	5	2881	C	N3-C2-O2	6.74	126.62	121.90
36	5	2295	A	C2-N3-C4	6.74	113.97	110.60
1	2	590	C	C6-N1-C2	-6.73	117.61	120.30
36	1	3260	G	C5-C6-O6	-6.73	124.56	128.60
36	1	1125	U	O5 ¹ -P-OP1	-6.73	99.64	105.70
24	d2	93	LEU	CA-CB-CG	6.73	130.78	115.30
36	1	29	C	C6-N1-C2	6.73	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1103	A	P-O3'-C3'	6.72	127.77	119.70
36	1	3278	C	C2-N1-C1'	6.72	126.20	118.80
1	2	1110	G	C8-N9-C4	6.72	109.09	106.40
1	6	1002	G	C6-C5-N7	-6.72	126.37	130.40
36	5	952	A	C4-C5-N7	6.72	114.06	110.70
36	5	1127	G	N3-C4-C5	-6.72	125.24	128.60
36	5	2893	C	N1-C2-O2	-6.72	114.87	118.90
36	1	626	U	O5'-P-OP1	-6.72	99.65	105.70
36	5	1362	G	N7-C8-N9	-6.72	109.74	113.10
36	1	1149	G	C4-C5-C6	6.71	122.83	118.80
36	5	2860	U	N3-C4-O4	-6.71	114.70	119.40
36	1	435	C	C2-N1-C1'	-6.71	111.42	118.80
1	6	1048	G	C4-C5-N7	6.71	113.48	110.80
36	5	1331	U	C5-C6-N1	-6.71	119.34	122.70
36	1	91	G	C8-N9-C4	6.71	109.08	106.40
36	1	377	A	N1-C6-N6	6.71	122.63	118.60
36	1	2915	U	N1-C2-O2	-6.71	118.10	122.80
36	1	664	U	C6-N1-C2	6.71	125.02	121.00
1	2	1658	G	C6-C5-N7	-6.71	126.38	130.40
1	2	1291	G	N3-C4-C5	6.70	131.95	128.60
36	1	699	A	C2-N3-C4	-6.70	107.25	110.60
36	1	716	A	O5'-P-OP1	-6.70	99.67	105.70
36	1	2381	G	C4-N9-C1'	6.70	135.21	126.50
36	1	2273	G	C8-N9-C4	6.70	109.08	106.40
36	5	1589	A	N1-C6-N6	6.70	122.62	118.60
37	7	92	A	N1-C6-N6	6.70	122.62	118.60
36	1	304	G	C4-C5-N7	-6.70	108.12	110.80
36	5	523	A	N1-C6-N6	-6.70	114.58	118.60
36	5	1305	U	N3-C4-O4	6.70	124.09	119.40
36	1	2121	G	C5-C6-O6	6.70	132.62	128.60
36	5	2419	A	N7-C8-N9	6.70	117.15	113.80
25	d3	132	LEU	CA-CB-CG	-6.69	99.90	115.30
1	6	407	A	N1-C2-N3	-6.69	125.95	129.30
36	5	952	A	C8-N9-C4	6.69	108.48	105.80
37	7	37	G	C4-C5-N7	6.69	113.48	110.80
1	6	1096	C	C6-N1-C2	6.69	122.98	120.30
36	1	1151	U	C5-C6-N1	6.69	126.04	122.70
36	5	1329	U	C2-N3-C4	-6.69	122.99	127.00
36	1	1366	A	C8-N9-C4	-6.69	103.13	105.80
1	2	1580	C	C6-N1-C2	6.68	122.97	120.30
1	6	1697	G	N3-C4-C5	-6.68	125.26	128.60
36	5	1157	G	OP2-P-O3'	6.68	119.91	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	15	110	LEU	CA-CB-CG	6.68	130.68	115.30
35	SM	134	ASP	CB-CA-C	-6.68	97.03	110.40
1	6	420	A	N1-C6-N6	6.68	122.61	118.60
36	5	2117	A	N9-C4-C5	6.68	108.47	105.80
36	1	2400	G	C2-N3-C4	-6.68	108.56	111.90
36	1	3278	C	N3-C2-O2	-6.68	117.22	121.90
36	1	937	G	C8-N9-C4	6.68	109.07	106.40
1	6	1470	C	C6-N1-C2	-6.68	117.63	120.30
36	5	1116	G	C4-C5-N7	-6.68	108.13	110.80
36	1	2884	C	C6-N1-C2	6.68	122.97	120.30
36	1	3256	G	N1-C6-O6	6.68	123.91	119.90
36	1	1408	G	N1-C6-O6	6.67	123.91	119.90
36	5	1161	G	C5-C6-O6	-6.67	124.60	128.60
36	5	2249	G	O5'-P-OP2	-6.67	99.69	105.70
36	1	2827	U	N3-C4-O4	-6.67	114.73	119.40
36	5	1301	A	C5-N7-C8	-6.67	100.57	103.90
36	1	72	C	C6-N1-C2	6.66	122.97	120.30
36	1	675	C	N3-C4-N4	6.66	122.66	118.00
36	5	3112	G	C5-C6-O6	-6.66	124.60	128.60
1	2	1745	G	N9-C4-C5	-6.66	102.73	105.40
36	1	347	G	C6-C5-N7	-6.66	126.40	130.40
36	5	914	A	N1-C6-N6	6.66	122.60	118.60
36	1	2727	A	N1-C6-N6	-6.66	114.60	118.60
36	5	2572	C	C6-N1-C2	-6.66	117.64	120.30
36	5	2631	U	OP1-P-O3'	6.66	119.85	105.20
36	5	966	U	O5'-P-OP2	-6.66	99.71	105.70
36	1	2375	G	N1-C6-O6	-6.66	115.91	119.90
36	1	24	G	C8-N9-C4	6.65	109.06	106.40
1	6	858	G	C8-N9-C1'	-6.65	118.35	127.00
36	5	610	G	C5-C6-O6	6.65	132.59	128.60
36	1	2400	G	C4-C5-N7	6.65	113.46	110.80
38	4	140	G	C8-N9-C4	-6.65	103.74	106.40
1	6	1634	C	C5-C6-N1	6.65	124.33	121.00
1	6	1640	C	N1-C2-O2	6.65	122.89	118.90
36	5	617	G	C4-C5-N7	6.65	113.46	110.80
36	5	830	A	N1-C6-N6	6.65	122.59	118.60
36	5	938	C	C5-C4-N4	-6.65	115.55	120.20
1	6	1120	U	N3-C2-O2	-6.65	117.55	122.20
36	5	2875	U	C2-N1-C1'	6.65	125.68	117.70
37	7	105	C	N3-C4-C5	-6.65	119.24	121.90
36	1	790	U	C6-N1-C2	-6.65	117.01	121.00
36	1	2237	C	C6-N1-C2	6.64	122.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1000	C	N3-C2-O2	-6.64	117.25	121.90
1	2	1241	G	C4-N9-C1'	6.64	135.13	126.50
1	2	1761	U	C6-N1-C2	-6.64	117.01	121.00
36	5	417	A	OP2-P-O3'	6.64	119.82	105.20
36	5	3335	A	N9-C4-C5	-6.64	103.14	105.80
36	1	3218	A	C5-C6-N6	-6.64	118.39	123.70
36	1	213	A	N1-C6-N6	6.63	122.58	118.60
36	5	1865	A	C2-N3-C4	-6.63	107.28	110.60
51	m5	96	ARG	NE-CZ-NH1	6.63	123.62	120.30
36	5	2692	A	O5'-P-OP1	-6.63	99.73	105.70
36	1	3208	G	C4-N9-C1'	-6.63	117.88	126.50
36	5	911	C	N1-C2-O2	-6.63	114.92	118.90
36	5	2620	G	C5-C6-O6	6.63	132.58	128.60
36	5	644	G	C5-C6-O6	6.63	132.57	128.60
36	1	1151	U	N1-C2-O2	-6.62	118.16	122.80
36	5	2875	U	C2-N3-C4	6.62	130.97	127.00
1	2	577	G	C5-N7-C8	-6.62	100.99	104.30
36	5	2727	A	O5'-P-OP2	-6.62	99.74	105.70
36	1	1103	A	O5'-P-OP2	6.62	118.64	110.70
36	1	2392	C	N3-C4-C5	6.62	124.55	121.90
36	5	1181	U	C4-C5-C6	6.62	123.67	119.70
36	5	1438	U	N3-C2-O2	-6.62	117.57	122.20
36	5	2932	U	O5'-P-OP1	-6.62	99.74	105.70
1	6	421	A	N1-C6-N6	6.62	122.57	118.60
36	5	869	G	O5'-P-OP2	-6.62	99.75	105.70
36	5	1902	G	C6-C5-N7	-6.62	126.43	130.40
36	5	3245	A	C5-C6-N1	-6.61	114.39	117.70
36	5	784	A	C5-C6-N6	-6.61	118.41	123.70
36	5	816	A	N9-C4-C5	6.61	108.44	105.80
36	5	1101	G	C6-C5-N7	-6.61	126.43	130.40
36	1	1514	G	C4-N9-C1'	6.61	135.09	126.50
36	5	2870	C	N3-C4-C5	6.61	124.54	121.90
36	5	283	G	C5-N7-C8	-6.61	101.00	104.30
36	5	641	C	N3-C4-C5	6.61	124.54	121.90
36	5	1889	G	N3-C4-N9	6.61	129.96	126.00
1	6	44	U	N1-C2-O2	-6.60	118.18	122.80
36	1	1192	C	C5-C6-N1	6.60	124.30	121.00
54	M8	138	LEU	CA-CB-CG	6.60	130.48	115.30
1	2	831	U	C6-N1-C2	-6.59	117.04	121.00
36	1	2391	G	N9-C4-C5	6.59	108.04	105.40
38	8	20	U	N1-C2-O2	-6.59	118.18	122.80
36	1	2639	G	C8-N9-C1'	-6.59	118.43	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3217	C	N3-C2-O2	-6.59	117.29	121.90
36	1	307	A	O5'-P-OP2	-6.59	99.77	105.70
56	N0	40	ARG	NE-CZ-NH2	6.59	123.59	120.30
40	l3	4	ARG	NE-CZ-NH1	6.59	123.59	120.30
36	1	1190	A	C6-C5-N7	-6.58	127.69	132.30
36	1	2972	G	C8-N9-C4	-6.58	103.77	106.40
1	6	1440	C	C6-N1-C2	-6.58	117.67	120.30
36	5	370	U	C2-N1-C1'	6.58	125.60	117.70
36	5	640	U	N3-C2-O2	6.58	126.81	122.20
36	1	2306	C	N1-C2-O2	6.58	122.85	118.90
36	1	2692	A	C6-C5-N7	-6.58	127.69	132.30
35	sM	167	PRO	N-CA-CB	6.58	111.20	103.30
36	5	1716	U	C5-C6-N1	6.58	125.99	122.70
1	2	74	U	O4'-C1'-N1	6.58	113.46	108.20
36	1	1878	G	C8-N9-C4	-6.58	103.77	106.40
36	1	2144	A	O4'-C1'-N9	6.58	113.46	108.20
44	L7	83	LEU	CA-CB-CG	6.58	130.43	115.30
36	1	2836	C	C5-C4-N4	6.58	124.80	120.20
36	5	1710	C	N3-C4-C5	6.58	124.53	121.90
36	5	2114	C	C6-N1-C2	-6.58	117.67	120.30
1	2	1658	G	C4-C5-N7	6.57	113.43	110.80
36	1	672	A	C8-N9-C4	6.57	108.43	105.80
36	1	2869	U	C2-N1-C1'	6.57	125.59	117.70
70	O4	51	LEU	CA-CB-CG	6.57	130.42	115.30
36	5	1366	A	C8-N9-C4	-6.57	103.17	105.80
36	1	1468	A	C2-N3-C4	-6.57	107.31	110.60
36	1	435	C	C5-C6-N1	-6.57	117.72	121.00
36	5	628	A	N1-C6-N6	-6.57	114.66	118.60
36	5	2416	U	C5-C6-N1	6.57	125.98	122.70
36	5	2948	C	N3-C4-C5	6.57	124.53	121.90
36	5	2713	U	C5-C4-O4	-6.57	121.96	125.90
36	1	858	A	O5'-P-OP2	-6.56	99.79	105.70
36	1	1437	C	N3-C2-O2	-6.56	117.31	121.90
36	1	350	C	N1-C2-O2	6.56	122.84	118.90
36	1	2714	G	C5-N7-C8	-6.56	101.02	104.30
36	1	3101	G	N1-C6-O6	-6.56	115.96	119.90
36	1	2124	G	N1-C6-O6	6.56	123.84	119.90
36	1	2182	A	C8-N9-C4	-6.56	103.18	105.80
1	6	151	G	N3-C2-N2	-6.56	115.31	119.90
36	1	1378	U	C5-C4-O4	-6.56	121.97	125.90
1	2	1096	C	C2-N1-C1'	6.56	126.01	118.80
36	1	298	U	N1-C2-O2	6.56	127.39	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	232	G	N3-C4-C5	-6.55	125.32	128.60
36	5	2303	A	C8-N9-C4	6.55	108.42	105.80
1	6	1537	C	C6-N1-C2	-6.55	117.68	120.30
36	5	908	G	C5-C6-O6	-6.55	124.67	128.60
36	1	589	A	O5'-P-OP1	-6.55	99.80	105.70
36	5	1902	G	C5-C6-O6	-6.55	124.67	128.60
36	5	827	A	N1-C6-N6	-6.55	114.67	118.60
36	5	1099	A	C4-C5-N7	6.55	113.97	110.70
36	5	1846	C	C2-N3-C4	-6.55	116.63	119.90
36	5	1370	G	N1-C6-O6	-6.54	115.97	119.90
36	1	942	U	N3-C4-O4	6.54	123.98	119.40
36	1	2183	A	C5-C6-N6	-6.54	118.47	123.70
36	5	816	A	O5'-P-OP2	-6.54	99.81	105.70
1	6	18	C	C6-N1-C2	-6.54	117.68	120.30
36	5	3362	A	N7-C8-N9	6.54	117.07	113.80
1	6	1029	U	C5-C4-O4	6.54	129.82	125.90
1	6	1700	C	C6-N1-C1'	-6.54	112.95	120.80
1	6	1744	A	C8-N9-C4	6.54	108.42	105.80
36	1	1154	A	C4-C5-C6	6.54	120.27	117.00
36	1	1556	C	C2-N1-C1'	6.53	125.99	118.80
36	5	1149	G	C5-C6-O6	-6.53	124.68	128.60
36	5	2941	A	O4'-C1'-N9	-6.53	102.97	108.20
41	L4	182	LEU	CA-CB-CG	6.53	130.32	115.30
36	1	353	G	C6-C5-N7	-6.53	126.48	130.40
36	5	3303	G	O5'-P-OP2	-6.53	99.82	105.70
36	5	2310	U	N3-C2-O2	-6.53	117.63	122.20
36	5	2552	C	N1-C2-O2	6.53	122.82	118.90
36	1	2376	G	C5-N7-C8	-6.53	101.04	104.30
36	1	2603	G	C6-C5-N7	-6.53	126.48	130.40
36	5	2375	G	C4-C5-N7	-6.53	108.19	110.80
1	2	1389	C	C2-N1-C1'	6.52	125.98	118.80
36	1	1124	U	OP1-P-O3'	6.52	119.55	105.20
36	1	1741	A	C2-N3-C4	-6.52	107.34	110.60
36	1	2617	U	N3-C2-O2	-6.52	117.64	122.20
36	1	3179	U	O5'-P-OP1	-6.52	99.83	105.70
36	5	2392	C	N3-C4-C5	6.52	124.51	121.90
1	2	1196	A	P-O3'-C3'	6.51	127.52	119.70
1	6	364	G	N9-C4-C5	-6.51	102.79	105.40
36	1	432	G	C5-C6-N1	-6.51	108.24	111.50
51	m5	96	ARG	NE-CZ-NH2	-6.51	117.04	120.30
36	1	938	C	C5-C6-N1	6.51	124.26	121.00
36	1	1003	A	N1-C6-N6	6.51	122.51	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	C4-N9-C1'	-6.51	118.04	126.50
1	2	1761	U	P-O3'-C3'	6.51	127.51	119.70
36	1	24	G	C8-N9-C1'	-6.51	118.54	127.00
36	1	1156	C	C2-N1-C1'	6.51	125.96	118.80
36	1	1884	A	O5'-P-OP2	-6.51	99.84	105.70
36	1	298	U	C2-N1-C1'	6.51	125.51	117.70
36	1	895	A	O5'-P-OP1	-6.51	99.84	105.70
1	2	1595	U	N3-C4-O4	6.50	123.95	119.40
36	5	102	C	C5-C4-N4	-6.50	115.65	120.20
36	5	1152	G	C5-C6-O6	-6.50	124.70	128.60
36	5	1396	C	OP2-P-O3'	6.50	119.51	105.20
73	o7	65	ARG	NE-CZ-NH1	6.50	123.55	120.30
36	1	729	C	C6-N1-C2	-6.50	117.70	120.30
36	5	911	C	C2-N3-C4	-6.50	116.65	119.90
36	5	2314	U	N1-C2-O2	-6.50	118.25	122.80
36	5	3377	G	N1-C6-O6	6.50	123.80	119.90
36	1	639	G	N9-C4-C5	-6.50	102.80	105.40
36	1	704	U	N3-C4-O4	6.50	123.95	119.40
36	1	1001	G	C6-C5-N7	-6.50	126.50	130.40
36	1	2121	G	N3-C4-C5	-6.50	125.35	128.60
35	SM	167	PRO	N-CA-CB	6.50	111.09	103.30
1	6	1137	A	C8-N9-C4	6.50	108.40	105.80
36	1	2306	C	C2-N1-C1'	6.49	125.94	118.80
36	5	1894	U	C5-C6-N1	-6.49	119.45	122.70
36	1	1391	C	C4-C5-C6	6.49	120.65	117.40
36	5	1536	G	N1-C6-O6	6.49	123.80	119.90
36	5	3026	G	C5-C6-O6	-6.49	124.70	128.60
1	2	1761	U	N3-C2-O2	-6.49	117.66	122.20
36	1	428	A	C4-C5-C6	-6.49	113.75	117.00
36	5	2419	A	C6-C5-N7	-6.49	127.76	132.30
36	1	33	G	O5'-P-OP1	-6.49	99.86	105.70
36	5	2696	A	C5-N7-C8	-6.49	100.66	103.90
37	7	51	A	C8-N9-C4	-6.49	103.20	105.80
36	1	1713	G	N3-C4-C5	6.49	131.84	128.60
1	6	1000	C	C6-N1-C2	-6.49	117.71	120.30
36	1	2423	U	O5'-P-OP2	-6.48	99.87	105.70
36	1	2612	U	C5-C6-N1	-6.48	119.46	122.70
1	6	1568	C	P-O3'-C3'	6.48	127.48	119.70
36	5	283	G	O4'-C1'-N9	-6.48	103.01	108.20
36	5	2351	U	N1-C2-N3	6.48	118.79	114.90
36	1	979	U	O4'-C1'-N1	6.48	113.38	108.20
36	5	1181	U	C5-C4-O4	6.48	129.79	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1445	U	N3-C2-O2	6.48	126.73	122.20
36	1	3215	A	N1-C6-N6	6.48	122.49	118.60
1	6	1340	U	N3-C2-O2	-6.48	117.66	122.20
36	5	694	C	N3-C2-O2	-6.48	117.36	121.90
36	5	1177	G	C6-N1-C2	-6.48	121.21	125.10
36	5	360	G	C8-N9-C4	-6.48	103.81	106.40
36	5	2199	G	N3-C2-N2	-6.48	115.37	119.90
36	1	2818	U	C5-C6-N1	6.48	125.94	122.70
1	6	858	G	C6-C5-N7	-6.48	126.51	130.40
36	1	145	G	C5-C6-O6	-6.47	124.72	128.60
36	1	3214	U	N3-C2-O2	-6.47	117.67	122.20
1	6	1421	A	C8-N9-C4	6.47	108.39	105.80
12	c0	83	PRO	N-CA-CB	6.47	111.07	103.30
36	5	983	A	C6-N1-C2	-6.47	114.72	118.60
36	5	578	A	N1-C6-N6	6.47	122.48	118.60
37	7	105	C	N3-C2-O2	-6.47	117.37	121.90
1	2	1744	A	O5'-P-OP1	-6.47	99.88	105.70
36	1	2403	G	N1-C6-O6	6.47	123.78	119.90
1	6	1657	U	N1-C2-O2	6.47	127.33	122.80
37	7	83	U	C5-C6-N1	-6.47	119.47	122.70
38	4	20	U	C5-C6-N1	-6.47	119.47	122.70
1	6	1780	G	C4-C5-N7	6.47	113.39	110.80
36	5	424	G	C5-C6-N1	6.46	114.73	111.50
36	1	1206	G	O5'-P-OP2	-6.46	99.88	105.70
36	5	1080	A	N7-C8-N9	-6.46	110.57	113.80
36	5	2616	C	O5'-P-OP2	6.46	118.45	110.70
1	6	1029	U	C6-N1-C1'	6.46	130.24	121.20
36	5	1303	A	N1-C2-N3	-6.46	126.07	129.30
36	5	1476	G	C5-C6-O6	6.46	132.47	128.60
36	5	2929	C	C2-N3-C4	-6.46	116.67	119.90
36	5	939	U	O5'-P-OP1	6.46	118.45	110.70
36	5	3172	A	N1-C2-N3	6.46	132.53	129.30
36	1	1433	A	N9-C4-C5	6.45	108.38	105.80
36	1	2383	C	C5-C4-N4	-6.45	115.68	120.20
36	5	649	A	C5-C6-N6	-6.45	118.54	123.70
36	5	2435	G	N9-C4-C5	-6.45	102.82	105.40
36	1	1807	G	N3-C4-C5	-6.45	125.37	128.60
36	1	1886	A	O5'-P-OP2	-6.45	99.89	105.70
36	1	2968	G	N1-C6-O6	6.45	123.77	119.90
36	1	596	C	N3-C2-O2	-6.45	117.39	121.90
1	6	17	C	N1-C2-O2	6.45	122.77	118.90
1	6	298	C	N3-C2-O2	6.45	126.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	758	C	C2-N1-C1'	-6.45	111.71	118.80
36	5	2143	A	C2-N3-C4	6.45	113.82	110.60
36	1	2637	A	O5'-P-OP1	-6.44	99.90	105.70
36	1	1336	U	N1-C2-N3	6.44	118.76	114.90
1	6	1650	U	N3-C4-O4	6.44	123.91	119.40
36	5	2245	C	C6-N1-C2	-6.44	117.72	120.30
1	2	410	A	O5'-P-OP1	-6.43	99.91	105.70
1	2	507	U	N3-C2-O2	-6.43	117.70	122.20
36	1	3025	C	C5-C6-N1	-6.43	117.78	121.00
36	5	1110	U	N1-C2-O2	6.43	127.30	122.80
36	1	2942	C	O5'-P-OP1	6.43	118.42	110.70
1	2	1363	U	C2-N1-C1'	6.43	125.42	117.70
36	5	3362	A	C8-N9-C4	-6.43	103.23	105.80
36	1	145	G	C4-C5-N7	6.43	113.37	110.80
36	1	858	A	C4-C5-C6	6.43	120.22	117.00
36	5	358	G	C5-C6-O6	-6.43	124.75	128.60
36	5	2321	A	OP2-P-O3'	6.43	119.34	105.20
36	5	3195	U	OP1-P-O3'	6.43	119.34	105.20
1	2	54	C	C6-N1-C2	-6.42	117.73	120.30
36	5	2334	U	O5'-P-OP2	-6.42	99.92	105.70
36	5	3131	U	C6-N1-C2	6.42	124.85	121.00
1	2	554	C	C2-N1-C1'	6.42	125.86	118.80
36	1	2283	G	N3-C2-N2	-6.42	115.41	119.90
36	5	102	C	N3-C4-N4	6.42	122.49	118.00
1	6	19	A	C8-N9-C4	6.42	108.37	105.80
37	7	37	G	C8-N9-C4	6.42	108.97	106.40
68	o2	44	ARG	NE-CZ-NH1	-6.42	117.09	120.30
36	5	2710	C	N1-C2-O2	-6.41	115.05	118.90
36	1	92	G	N3-C4-C5	-6.41	125.39	128.60
36	1	1869	C	O5'-P-OP2	-6.41	99.93	105.70
36	1	2159	U	C6-N1-C2	6.41	124.85	121.00
41	L4	327	LEU	CA-CB-CG	6.41	130.04	115.30
36	5	1481	A	N7-C8-N9	6.41	117.01	113.80
36	1	2243	A	O5'-P-OP2	-6.41	99.93	105.70
36	5	813	G	C5-C6-O6	-6.41	124.76	128.60
36	5	999	G	N7-C8-N9	-6.41	109.90	113.10
36	5	1321	G	C6-C5-N7	-6.41	126.56	130.40
36	5	2606	G	OP1-P-O3'	6.41	119.29	105.20
36	5	2968	G	C4-N9-C1'	6.41	134.83	126.50
1	6	387	A	C2-N3-C4	6.40	113.80	110.60
36	5	2821	C	N1-C2-O2	-6.40	115.06	118.90
36	1	709	A	C8-N9-C4	6.40	108.36	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1082	U	C2-N1-C1'	6.40	125.38	117.70
38	4	27	U	C5-C6-N1	6.40	125.90	122.70
36	5	3269	U	P-O3'-C3'	6.40	127.38	119.70
38	8	9	A	N1-C6-N6	6.40	122.44	118.60
36	1	131	C	C6-N1-C2	-6.40	117.74	120.30
36	1	423	A	N9-C4-C5	6.40	108.36	105.80
36	1	3175	U	N3-C2-O2	-6.40	117.72	122.20
1	6	1614	A	O4'-C1'-N9	6.40	113.32	108.20
36	5	2211	U	N3-C2-O2	-6.40	117.72	122.20
36	5	2874	G	C5-C6-O6	6.40	132.44	128.60
36	5	1126	G	C2-N3-C4	-6.39	108.70	111.90
53	M7	138	LYS	CD-CE-NZ	6.39	126.40	111.70
1	6	415	C	N3-C2-O2	-6.39	117.42	121.90
36	5	1661	G	N1-C6-O6	6.39	123.73	119.90
1	6	901	G	C5-C6-O6	-6.39	124.77	128.60
36	5	1470	U	C2-N1-C1'	6.39	125.37	117.70
36	5	2167	A	C8-N9-C4	-6.39	103.25	105.80
36	5	2644	C	O5'-P-OP1	-6.39	99.95	105.70
36	5	2852	C	C6-N1-C2	6.39	122.86	120.30
36	1	1103	A	OP1-P-O3'	6.39	119.25	105.20
36	5	1716	U	C2-N1-C1'	6.39	125.36	117.70
36	5	3140	G	O5'-P-OP1	-6.39	99.95	105.70
36	1	3104	U	C5-C6-N1	-6.38	119.51	122.70
36	5	971	G	C4-C5-N7	-6.38	108.25	110.80
36	5	1897	G	C4-C5-N7	6.38	113.35	110.80
36	1	345	G	N3-C4-C5	-6.38	125.41	128.60
36	1	2924	U	C2-N1-C1'	-6.38	110.04	117.70
1	2	453	U	N3-C2-O2	-6.38	117.73	122.20
36	1	3143	C	N1-C2-O2	-6.38	115.07	118.90
1	6	1785	U	N3-C2-O2	-6.38	117.73	122.20
36	1	627	U	N3-C2-O2	6.38	126.67	122.20
37	3	33	U	N3-C2-O2	-6.38	117.73	122.20
36	5	2978	U	N3-C2-O2	-6.38	117.73	122.20
36	1	2755	C	N3-C2-O2	6.38	126.36	121.90
25	d3	45	GLY	N-CA-C	-6.38	97.16	113.10
36	5	51	A	N1-C6-N6	6.38	122.43	118.60
36	5	3182	G	OP1-P-OP2	-6.37	110.04	119.60
36	1	1269	U	C2-N1-C1'	6.37	125.35	117.70
1	2	830	U	N3-C2-O2	-6.37	117.74	122.20
36	1	857	G	N3-C4-N9	-6.37	122.18	126.00
36	5	2928	C	C2-N1-C1'	6.37	125.81	118.80
36	5	2395	G	O5'-P-OP1	6.37	118.34	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	75	U	N1-C2-O2	6.37	127.26	122.80
1	6	1117	U	N3-C4-C5	-6.37	110.78	114.60
36	5	3285	C	N1-C2-O2	6.37	122.72	118.90
36	1	350	C	C6-N1-C1'	-6.36	113.17	120.80
36	1	1475	A	C8-N9-C4	6.36	108.35	105.80
36	5	2772	C	P-O3'-C3'	6.36	127.34	119.70
1	6	1793	G	C4-C5-N7	-6.36	108.25	110.80
36	5	994	G	C5-C6-N1	6.36	114.68	111.50
1	2	380	U	N3-C2-O2	-6.36	117.75	122.20
36	1	1405	U	C2-N3-C4	-6.36	123.19	127.00
36	1	2924	U	C6-N1-C2	6.36	124.81	121.00
36	5	2613	U	O5'-P-OP1	-6.36	99.98	105.70
1	2	577	G	N1-C6-O6	6.36	123.71	119.90
36	1	895	A	C6-C5-N7	-6.36	127.85	132.30
36	1	2182	A	N7-C8-N9	6.36	116.98	113.80
1	6	1747	G	O5'-P-OP1	6.36	118.33	110.70
36	1	324	A	C8-N9-C4	-6.35	103.26	105.80
36	1	790	U	C5-C4-O4	6.35	129.71	125.90
38	4	88	A	N9-C4-C5	-6.35	103.26	105.80
36	5	1452	A	C4-C5-N7	6.35	113.88	110.70
36	5	2750	U	O5'-P-OP1	6.35	118.33	110.70
36	1	1488	G	N1-C6-O6	6.35	123.71	119.90
1	2	334	G	N3-C4-N9	-6.35	122.19	126.00
36	1	2700	G	N1-C6-O6	6.35	123.71	119.90
1	2	1198	G	C8-N9-C4	-6.35	103.86	106.40
36	1	685	G	N1-C6-O6	6.35	123.71	119.90
36	1	2314	U	N3-C2-O2	6.35	126.64	122.20
38	4	103	G	C8-N9-C4	-6.35	103.86	106.40
36	5	2117	A	C5-C6-N6	6.35	128.78	123.70
36	5	3041	U	C4-C5-C6	-6.35	115.89	119.70
36	5	1016	C	O5'-P-OP1	-6.35	99.99	105.70
36	5	2598	G	N1-C6-O6	6.35	123.71	119.90
1	2	334	G	C4-N9-C1'	-6.34	118.25	126.50
36	1	2692	A	C8-N9-C4	-6.34	103.26	105.80
36	5	1403	C	N3-C4-N4	6.34	122.44	118.00
36	5	1589	A	C5-C6-N6	-6.34	118.62	123.70
36	1	70	A	N7-C8-N9	6.34	116.97	113.80
1	6	858	G	N7-C8-N9	6.34	116.27	113.10
36	5	1335	C	N3-C2-O2	6.34	126.34	121.90
36	5	1368	U	O5'-P-OP1	-6.34	99.99	105.70
36	5	1909	A	C8-N9-C4	6.34	108.34	105.80
36	1	70	A	C5-N7-C8	-6.34	100.73	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3266	G	N9-C4-C5	6.34	107.94	105.40
36	1	2952	G	N1-C6-O6	6.34	123.70	119.90
36	5	776	U	C5-C4-O4	6.34	129.70	125.90
36	5	1049	C	C5-C6-N1	6.34	124.17	121.00
36	5	1152	G	N7-C8-N9	6.34	116.27	113.10
36	1	3181	C	N3-C2-O2	-6.34	117.46	121.90
1	6	402	C	N3-C4-C5	6.33	124.43	121.90
36	5	2124	G	C8-N9-C4	6.33	108.93	106.40
36	1	1043	C	N3-C4-C5	6.33	124.43	121.90
38	4	46	G	N1-C6-O6	-6.33	116.10	119.90
1	2	1082	C	C2-N1-C1'	6.33	125.76	118.80
36	1	820	A	C8-N9-C4	-6.33	103.27	105.80
36	1	1330	A	N1-C6-N6	6.33	122.40	118.60
36	5	1392	G	N7-C8-N9	-6.33	109.94	113.10
36	1	1514	G	C6-C5-N7	-6.33	126.61	130.40
36	1	3266	G	C8-N9-C4	-6.32	103.87	106.40
36	5	2139	A	N1-C2-N3	6.32	132.46	129.30
36	5	3004	C	N3-C2-O2	6.32	126.33	121.90
1	2	42	G	N1-C6-O6	-6.32	116.11	119.90
36	1	1943	C	C6-N1-C2	-6.32	117.77	120.30
1	2	244	A	N1-C6-N6	6.32	122.39	118.60
36	1	286	U	N3-C2-O2	-6.32	117.78	122.20
36	1	423	A	C8-N9-C4	-6.32	103.27	105.80
36	5	994	G	N3-C4-N9	6.32	129.79	126.00
36	1	1822	C	C6-N1-C2	-6.32	117.77	120.30
36	1	2887	A	C4-C5-N7	6.32	113.86	110.70
1	6	1745	G	N1-C6-O6	6.32	123.69	119.90
36	5	1053	A	N1-C6-N6	-6.32	114.81	118.60
36	5	1366	A	N1-C6-N6	-6.32	114.81	118.60
36	5	3028	G	N3-C2-N2	6.32	124.32	119.90
36	1	670	C	C4-C5-C6	6.31	120.56	117.40
36	5	998	A	OP2-P-O3'	6.31	119.09	105.20
38	8	56	G	N1-C6-O6	6.31	123.69	119.90
36	1	3074	G	N1-C6-O6	6.31	123.69	119.90
36	1	60	A	N1-C6-N6	6.31	122.39	118.60
36	5	943	U	N1-C2-N3	6.31	118.69	114.90
36	5	1080	A	C8-N9-C4	6.31	108.32	105.80
36	5	1101	G	C8-N9-C1'	-6.31	118.80	127.00
36	5	2944	U	O5'-P-OP1	-6.31	100.02	105.70
36	5	3164	C	O4'-C1'-N1	6.31	113.24	108.20
38	8	84	C	C6-N1-C2	-6.30	117.78	120.30
36	1	1858	A	N3-C4-C5	-6.30	122.39	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2620	G	C8-N9-C4	6.30	108.92	106.40
36	5	2646	C	C6-N1-C2	6.30	122.82	120.30
36	1	646	A	C5-C6-N1	-6.30	114.55	117.70
36	1	649	A	N7-C8-N9	-6.30	110.65	113.80
36	5	921	A	OP2-P-O3'	6.30	119.05	105.20
36	5	610	G	N9-C4-C5	6.29	107.92	105.40
36	1	716	A	C4-C5-N7	6.29	113.85	110.70
38	4	103	G	C4-N9-C1'	6.29	134.68	126.50
36	5	1788	C	O5'-P-OP2	-6.29	100.04	105.70
36	5	2651	G	C8-N9-C4	6.29	108.92	106.40
36	1	635	G	C5-C6-O6	-6.29	124.83	128.60
36	1	1116	G	C4-N9-C1'	6.29	134.68	126.50
36	5	3311	C	C6-N1-C2	-6.29	117.78	120.30
36	5	428	A	C8-N9-C4	6.29	108.32	105.80
36	1	76	G	C6-C5-N7	-6.29	126.63	130.40
36	1	2344	U	C5-C6-N1	-6.29	119.56	122.70
36	1	2407	C	C6-N1-C2	6.29	122.82	120.30
36	1	2594	C	O5'-P-OP2	-6.29	100.04	105.70
36	1	2777	G	C5-C6-O6	6.29	132.37	128.60
36	5	584	G	N9-C4-C5	6.29	107.92	105.40
36	5	1200	A	C4-C5-C6	6.29	120.14	117.00
36	5	3075	G	C5-C6-N1	-6.29	108.36	111.50
36	5	1710	C	C5-C6-N1	-6.29	117.86	121.00
1	2	91	G	C5-C6-O6	-6.29	124.83	128.60
36	1	770	G	O4'-C1'-N9	6.28	113.23	108.20
36	5	911	C	C5-C6-N1	-6.28	117.86	121.00
36	5	923	C	C6-N1-C1'	-6.28	113.26	120.80
36	5	1148	G	C5-C6-O6	-6.28	124.83	128.60
36	5	57	A	C5-C6-N6	-6.28	118.67	123.70
36	1	2343	C	N3-C4-C5	6.28	124.41	121.90
38	4	56	G	O5'-P-OP2	-6.28	100.05	105.70
1	6	813	U	C2-N1-C1'	6.28	125.24	117.70
36	5	906	A	C8-N9-C4	-6.28	103.29	105.80
36	5	1110	U	C4-C5-C6	-6.28	115.93	119.70
36	5	2950	G	N9-C4-C5	-6.28	102.89	105.40
36	1	3206	C	C2-N1-C1'	-6.28	111.89	118.80
36	5	1450	G	N1-C2-N2	6.28	121.85	116.20
36	1	1157	G	C2-N3-C4	-6.28	108.76	111.90
36	1	2572	C	N3-C2-O2	-6.28	117.51	121.90
36	5	2277	C	C6-N1-C2	6.28	122.81	120.30
20	c8	15	LEU	CA-CB-CG	6.27	129.73	115.30
36	1	2692	A	C5-C6-N6	-6.27	118.68	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	608	U	C5-C4-O4	6.27	129.66	125.90
1	2	1762	A	O5'-P-OP1	-6.27	100.06	105.70
36	1	2872	A	C5-C6-N6	-6.27	118.69	123.70
36	1	3180	A	C5-C6-N6	-6.27	118.69	123.70
36	1	3206	C	C6-N1-C1'	6.27	128.32	120.80
1	6	65	A	N9-C4-C5	-6.27	103.29	105.80
36	5	922	U	C6-N1-C2	6.27	124.76	121.00
36	5	1152	G	O5'-P-OP1	-6.27	100.06	105.70
36	1	2968	G	N3-C2-N2	-6.27	115.51	119.90
1	6	1150	G	C2-N3-C4	-6.26	108.77	111.90
36	5	1421	G	C5-C6-N1	-6.26	108.37	111.50
36	5	2943	G	N9-C4-C5	-6.26	102.89	105.40
36	1	1300	G	N9-C4-C5	-6.26	102.89	105.40
1	2	1761	U	C5-C4-O4	6.26	129.66	125.90
36	5	1879	A	C5-N7-C8	-6.26	100.77	103.90
36	5	2757	U	O5'-P-OP1	-6.26	100.06	105.70
38	4	22	U	C5-C6-N1	-6.26	119.57	122.70
36	1	1144	U	C2-N3-C4	-6.26	123.25	127.00
36	5	91	G	N1-C6-O6	6.26	123.65	119.90
36	1	101	G	OP2-P-O3'	6.25	118.96	105.20
36	1	362	U	C6-N1-C2	6.25	124.75	121.00
36	1	901	G	N1-C6-O6	6.25	123.65	119.90
36	1	2283	G	N3-C4-C5	6.25	131.73	128.60
1	6	21	U	C5-C4-O4	-6.25	122.15	125.90
1	6	111	U	C6-N1-C2	-6.25	117.25	121.00
36	5	361	A	C4-C5-N7	-6.25	107.57	110.70
36	5	640	U	C6-N1-C2	-6.25	117.25	121.00
36	1	1838	G	N3-C4-N9	6.25	129.75	126.00
36	1	2621	G	N3-C2-N2	-6.25	115.53	119.90
36	1	1190	A	C4-N9-C1'	6.25	137.54	126.30
1	2	542	A	N7-C8-N9	6.25	116.92	113.80
1	2	453	U	N1-C2-O2	6.24	127.17	122.80
36	1	586	C	N1-C2-O2	-6.24	115.15	118.90
36	5	1154	A	C2-N3-C4	6.24	113.72	110.60
36	5	3049	A	C8-N9-C4	6.24	108.30	105.80
37	7	9	C	C2-N1-C1'	-6.24	111.93	118.80
36	5	2283	G	C5-N7-C8	-6.24	101.18	104.30
36	5	3043	C	C6-N1-C2	6.24	122.80	120.30
36	1	1846	C	N1-C2-O2	-6.24	115.16	118.90
36	1	2957	G	N3-C2-N2	-6.24	115.53	119.90
36	5	2275	A	O5'-P-OP1	-6.24	100.08	105.70
36	5	2715	A	OP2-P-O3'	6.24	118.93	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1306	G	N1-C6-O6	6.24	123.64	119.90
36	5	1126	G	C6-C5-N7	-6.24	126.66	130.40
36	5	2717	U	C5-C6-N1	-6.24	119.58	122.70
1	2	307	G	C8-N9-C1'	-6.24	118.89	127.00
36	5	2710	C	N3-C2-O2	6.24	126.27	121.90
1	6	539	G	C8-N9-C4	-6.24	103.91	106.40
36	5	1552	G	N1-C6-O6	6.24	123.64	119.90
36	5	3276	G	O5'-P-OP1	-6.24	100.09	105.70
36	1	925	A	C8-N9-C4	-6.23	103.31	105.80
36	5	1336	U	C5-C6-N1	6.23	125.82	122.70
36	5	2354	C	N3-C2-O2	6.23	126.26	121.90
36	5	969	C	C5-C6-N1	-6.23	117.88	121.00
36	5	2797	C	N3-C4-C5	-6.23	119.41	121.90
36	5	2812	C	C6-N1-C2	-6.23	117.81	120.30
36	1	1514	G	C8-N9-C1'	-6.23	118.90	127.00
36	1	3310	A	C8-N9-C4	6.23	108.29	105.80
36	5	2610	G	N1-C6-O6	6.23	123.64	119.90
36	5	3000	A	C2-N3-C4	-6.23	107.48	110.60
36	5	2164	A	C4-C5-C6	6.23	120.11	117.00
36	5	3392	U	N3-C2-O2	-6.23	117.84	122.20
1	2	308	C	C2-N1-C1'	-6.23	111.95	118.80
36	5	1591	G	N1-C6-O6	6.23	123.64	119.90
36	1	1487	G	N9-C4-C5	6.22	107.89	105.40
36	1	2827	U	C6-N1-C1'	6.22	129.91	121.20
36	1	2935	U	N3-C4-C5	-6.22	110.87	114.60
36	5	1162	U	OP1-P-OP2	6.22	128.94	119.60
36	5	1914	G	N1-C6-O6	-6.22	116.17	119.90
37	3	98	C	C5-C6-N1	-6.22	117.89	121.00
36	5	3215	A	C5-C6-N1	-6.22	114.59	117.70
36	5	2176	U	N1-C2-N3	6.22	118.63	114.90
36	1	655	C	N3-C4-C5	-6.22	119.41	121.90
1	6	1541	G	C8-N9-C4	-6.22	103.91	106.40
36	5	806	A	N3-C4-N9	-6.22	122.42	127.40
37	7	55	A	N1-C6-N6	6.22	122.33	118.60
36	1	1159	A	O4'-C1'-N9	6.22	113.17	108.20
36	1	1313	G	C4-C5-N7	6.22	113.29	110.80
1	6	1779	U	O5'-P-OP2	-6.22	100.11	105.70
36	5	1475	A	O5'-P-OP2	-6.22	100.11	105.70
1	2	447	U	C6-N1-C2	-6.21	117.27	121.00
1	2	1428	G	O5'-P-OP1	-6.21	100.11	105.70
1	2	794	U	P-O3'-C3'	6.21	127.15	119.70
1	6	1778	G	C5-N7-C8	-6.21	101.19	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1119	C	OP2-P-O3'	6.21	118.87	105.20
36	5	1907	C	O5'-P-OP2	-6.21	100.11	105.70
36	5	2879	C	O5'-P-OP2	-6.21	100.11	105.70
36	5	3166	C	C2-N1-C1'	6.21	125.63	118.80
36	5	2161	G	N9-C4-C5	6.21	107.88	105.40
1	2	579	A	O4'-C1'-N9	6.21	113.17	108.20
1	6	1514	U	C5-C4-O4	6.21	129.62	125.90
36	5	3143	C	N3-C4-N4	6.21	122.35	118.00
36	1	942	U	OP1-P-OP2	-6.21	110.29	119.60
1	6	1651	A	N1-C6-N6	6.21	122.32	118.60
1	2	728	U	C2-N1-C1'	6.21	125.15	117.70
36	5	2631	U	O5'-P-OP2	-6.21	100.11	105.70
36	1	393	U	C5-C4-O4	6.20	129.62	125.90
37	3	91	G	N1-C6-O6	6.20	123.62	119.90
36	5	2334	U	N3-C2-O2	-6.20	117.86	122.20
36	1	2381	G	N3-C4-N9	6.20	129.72	126.00
36	1	2835	U	C5-C6-N1	-6.20	119.60	122.70
36	5	398	A	O5'-P-OP2	-6.20	100.12	105.70
36	1	645	A	C5-C6-N1	6.20	120.80	117.70
36	1	1838	G	C8-N9-C1'	-6.20	118.94	127.00
36	1	2924	U	N1-C2-O2	-6.20	118.46	122.80
36	5	2346	C	N1-C2-O2	-6.20	115.18	118.90
36	1	2300	G	C6-C5-N7	-6.20	126.68	130.40
36	1	888	A	N1-C6-N6	6.20	122.32	118.60
38	4	107	G	N1-C6-O6	-6.20	116.18	119.90
1	2	1291	G	N3-C4-N9	-6.19	122.28	126.00
36	5	960	U	C5-C4-O4	6.19	129.62	125.90
1	2	74	U	O5'-P-OP1	-6.19	100.13	105.70
1	2	1100	G	N1-C6-O6	6.19	123.62	119.90
38	4	42	G	N9-C4-C5	-6.19	102.92	105.40
36	5	2878	G	C5-C6-O6	-6.19	124.88	128.60
36	1	2300	G	N7-C8-N9	6.19	116.19	113.10
36	5	599	C	N1-C2-O2	-6.19	115.19	118.90
36	1	2910	A	C2-N3-C4	-6.19	107.51	110.60
36	1	3209	A	N9-C4-C5	-6.19	103.32	105.80
36	1	650	C	OP2-P-O3'	6.19	118.81	105.20
36	5	514	G	C5-C6-O6	-6.19	124.89	128.60
36	1	334	A	C8-N9-C4	-6.18	103.33	105.80
36	1	335	G	C4-C5-N7	6.18	113.27	110.80
36	1	3256	G	C5-C6-O6	-6.18	124.89	128.60
36	5	890	C	O5'-P-OP2	-6.18	100.13	105.70
1	6	1785	U	N1-C2-N3	6.18	118.61	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1343	A	O5'-P-OP2	-6.18	100.14	105.70
36	1	96	G	N3-C4-C5	6.18	131.69	128.60
36	1	394	G	C8-N9-C4	-6.18	103.93	106.40
36	1	627	U	N1-C2-O2	-6.18	118.47	122.80
36	5	585	A	O5'-P-OP2	-6.18	100.14	105.70
37	7	56	A	C2-N3-C4	-6.18	107.51	110.60
36	1	1556	C	N1-C2-O2	6.18	122.61	118.90
31	D9	36	LEU	CA-CB-CG	6.18	129.50	115.30
36	5	3343	G	N3-C2-N2	6.17	124.22	119.90
36	5	2951	G	O5'-P-OP1	-6.17	100.14	105.70
36	5	2790	A	O5'-P-OP2	-6.17	100.15	105.70
1	2	1241	G	C6-C5-N7	-6.17	126.70	130.40
1	6	1123	C	C5-C4-N4	-6.17	115.88	120.20
36	1	1182	A	O5'-P-OP1	-6.17	100.15	105.70
36	1	2354	C	N1-C2-O2	-6.17	115.20	118.90
52	M6	141	LEU	CB-CG-CD2	-6.17	100.52	111.00
1	6	364	G	C8-N9-C4	6.17	108.87	106.40
36	5	2824	G	C5-C6-O6	-6.17	124.90	128.60
36	5	2993	G	C5-C6-N1	6.17	114.58	111.50
38	8	34	U	N1-C2-N3	6.17	118.60	114.90
1	2	17	C	C6-N1-C2	-6.17	117.83	120.30
36	1	721	G	C6-C5-N7	-6.17	126.70	130.40
1	6	158	U	P-O3'-C3'	6.17	127.10	119.70
1	6	1729	C	C6-N1-C2	6.17	122.77	120.30
36	1	1077	U	C5-C6-N1	-6.16	119.62	122.70
36	5	2629	U	N3-C2-O2	6.16	126.52	122.20
36	1	1099	A	C5-C6-N6	-6.16	118.77	123.70
1	6	1152	A	N9-C4-C5	-6.16	103.33	105.80
36	1	2339	C	O5'-P-OP2	-6.16	100.16	105.70
36	5	1452	A	N9-C4-C5	-6.16	103.34	105.80
36	5	2700	G	C5-C6-O6	-6.16	124.90	128.60
36	1	304	G	N9-C4-C5	6.16	107.86	105.40
37	7	77	G	N9-C4-C5	-6.16	102.94	105.40
36	1	2827	U	C2-N1-C1'	-6.16	110.31	117.70
36	5	650	C	C5-C6-N1	-6.16	117.92	121.00
36	1	3004	C	N3-C4-C5	6.15	124.36	121.90
36	1	640	U	C5-C6-N1	6.15	125.78	122.70
1	6	957	G	N3-C2-N2	-6.15	115.59	119.90
36	5	2400	G	N9-C4-C5	-6.15	102.94	105.40
36	1	1795	U	O5'-P-OP1	-6.15	100.17	105.70
36	1	439	C	N1-C2-O2	6.15	122.59	118.90
36	1	2764	C	C2-N1-C1'	6.15	125.56	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2887	A	C6-C5-N7	-6.15	128.00	132.30
1	6	371	G	C6-C5-N7	-6.15	126.71	130.40
36	1	2257	C	O4'-C1'-N1	6.15	113.12	108.20
36	5	283	G	N9-C4-C5	-6.14	102.94	105.40
36	1	345	G	N3-C4-N9	6.14	129.69	126.00
36	1	1450	G	N1-C6-O6	6.14	123.58	119.90
36	5	1885	U	C6-N1-C2	6.14	124.69	121.00
36	1	1156	C	C2-N3-C4	-6.14	116.83	119.90
36	1	829	U	N1-C2-O2	6.14	127.10	122.80
36	1	2971	A	C2-N3-C4	6.14	113.67	110.60
36	5	323	A	C8-N9-C4	-6.14	103.34	105.80
36	5	1449	A	C6-C5-N7	-6.14	128.00	132.30
1	2	1773	C	N3-C4-C5	-6.14	119.44	121.90
36	5	335	G	O5'-P-OP2	6.14	118.07	110.70
36	5	651	G	C4-N9-C1'	6.14	134.48	126.50
36	5	874	U	O5'-P-OP1	-6.14	100.18	105.70
36	5	1879	A	C4-C5-C6	6.14	120.07	117.00
36	1	1897	G	N1-C6-O6	6.13	123.58	119.90
36	5	1158	A	C2-N3-C4	-6.13	107.53	110.60
1	2	694	U	N1-C2-O2	6.13	127.09	122.80
37	3	95	A	C6-C5-N7	-6.13	128.01	132.30
36	5	1878	G	C4-N9-C1'	6.13	134.47	126.50
1	2	694	U	C2-N1-C1'	6.13	125.06	117.70
1	6	448	C	N3-C4-C5	-6.13	119.45	121.90
1	2	802	G	C8-N9-C4	-6.13	103.95	106.40
36	5	967	A	N1-C6-N6	-6.12	114.92	118.60
36	5	1468	A	N9-C4-C5	-6.12	103.35	105.80
36	5	2730	G	C5-C6-O6	-6.12	124.92	128.60
1	2	1370	U	P-O3'-C3'	6.12	127.05	119.70
36	1	2924	U	C5-C6-N1	-6.12	119.64	122.70
1	6	1600	A	O4'-C1'-N9	6.12	113.10	108.20
36	5	973	A	N1-C6-N6	6.12	122.27	118.60
36	5	1868	G	N9-C4-C5	-6.12	102.95	105.40
36	5	2278	C	N1-C2-O2	6.12	122.57	118.90
1	6	938	G	N1-C6-O6	6.12	123.57	119.90
36	5	1804	A	C8-N9-C4	6.12	108.25	105.80
36	1	2967	A	N1-C6-N6	6.12	122.27	118.60
54	m8	166	LEU	CA-CB-CG	6.12	129.37	115.30
36	5	3033	A	C2-N3-C4	-6.12	107.54	110.60
1	2	942	G	N1-C6-O6	-6.12	116.23	119.90
36	5	227	G	O5'-P-OP2	-6.12	100.20	105.70
36	5	952	A	O5'-P-OP2	-6.12	100.20	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2383	C	N1-C2-O2	-6.12	115.23	118.90
36	1	1133	A	O5'-P-OP2	-6.11	100.20	105.70
36	5	1163	A	N9-C4-C5	6.11	108.25	105.80
1	6	1389	C	N1-C2-O2	6.11	122.57	118.90
1	2	1100	G	C8-N9-C1'	-6.11	119.06	127.00
36	1	2920	U	N1-C2-O2	-6.11	118.52	122.80
36	5	2199	G	C4-C5-C6	6.11	122.47	118.80
38	8	77	A	C8-N9-C4	6.11	108.24	105.80
1	6	1200	G	N3-C4-N9	-6.11	122.33	126.00
1	6	1389	C	C2-N1-C1'	6.11	125.52	118.80
1	6	1778	G	N7-C8-N9	6.11	116.16	113.10
38	8	34	U	N3-C2-O2	-6.11	117.92	122.20
1	2	825	U	C5-C6-N1	6.11	125.75	122.70
36	1	1185	C	C6-N1-C2	6.11	122.74	120.30
36	1	2151	C	C6-N1-C2	6.11	122.74	120.30
37	3	33	U	N1-C2-O2	6.11	127.07	122.80
1	6	542	A	N1-C2-N3	6.11	132.35	129.30
1	6	864	U	N3-C2-O2	-6.11	117.93	122.20
36	5	2860	U	C6-N1-C2	6.11	124.66	121.00
36	1	960	U	N3-C4-C5	6.10	118.26	114.60
36	5	2730	G	N1-C6-O6	6.10	123.56	119.90
36	1	1434	G	N1-C6-O6	6.10	123.56	119.90
1	6	126	A	C8-N9-C4	6.10	108.24	105.80
1	2	610	G	C8-N9-C1'	-6.10	119.07	127.00
36	1	706	A	C8-N9-C4	6.10	108.24	105.80
36	1	800	G	C5-C6-O6	-6.10	124.94	128.60
36	1	304	G	N3-C2-N2	-6.10	115.63	119.90
36	1	1190	A	N1-C6-N6	6.10	122.26	118.60
36	5	1118	C	N3-C4-C5	6.10	124.34	121.90
36	5	2278	C	N3-C4-C5	6.10	124.34	121.90
1	2	543	C	N1-C2-O2	6.09	122.56	118.90
1	6	406	U	C4-C5-C6	6.09	123.36	119.70
36	1	2959	C	N1-C2-O2	-6.09	115.25	118.90
36	1	3101	G	C6-C5-N7	6.09	134.05	130.40
36	1	893	C	C5-C6-N1	6.09	124.05	121.00
36	5	813	G	N1-C6-O6	6.09	123.55	119.90
36	5	2128	C	C6-N1-C2	-6.09	117.86	120.30
36	1	1442	U	C5-C4-O4	-6.09	122.25	125.90
36	1	76	G	C8-N9-C4	-6.09	103.97	106.40
36	1	3092	C	C5-C6-N1	-6.09	117.96	121.00
1	2	1600	A	N9-C4-C5	-6.08	103.37	105.80
36	1	596	C	C6-N1-C2	-6.08	117.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2187	G	C6-C5-N7	-6.08	126.75	130.40
36	1	2406	C	C5-C4-N4	-6.08	115.94	120.20
36	5	359	U	OP2-P-O3'	6.08	118.58	105.20
36	5	2114	C	C5-C6-N1	6.08	124.04	121.00
36	5	3200	G	N1-C6-O6	6.08	123.55	119.90
36	5	3343	G	N3-C4-N9	6.08	129.65	126.00
36	1	580	C	N1-C2-O2	-6.08	115.25	118.90
1	6	1745	G	N9-C4-C5	-6.08	102.97	105.40
36	5	35	A	O5'-P-OP2	-6.08	100.23	105.70
36	5	1012	G	N3-C4-C5	6.08	131.64	128.60
36	1	937	G	C5-C6-O6	-6.08	124.95	128.60
36	1	2183	A	C5-C6-N1	6.08	120.74	117.70
36	5	582	G	C5-C6-O6	6.08	132.25	128.60
36	5	1791	C	C6-N1-C2	-6.08	117.87	120.30
1	2	620	A	C8-N9-C4	-6.08	103.37	105.80
36	1	2658	G	O5'-P-OP2	-6.08	100.23	105.70
36	1	2732	G	N1-C6-O6	6.08	123.55	119.90
1	6	402	C	C6-N1-C2	6.08	122.73	120.30
36	1	2917	G	O5'-P-OP2	-6.07	100.23	105.70
36	5	1548	C	N1-C2-O2	-6.07	115.26	118.90
36	5	2698	G	N1-C6-O6	6.07	123.54	119.90
36	1	922	U	N1-C2-O2	6.07	127.05	122.80
1	6	577	G	C4-C5-N7	6.07	113.23	110.80
36	1	2402	A	N1-C6-N6	6.07	122.24	118.60
36	1	2625	C	N1-C2-O2	-6.07	115.26	118.90
37	7	74	C	N1-C2-O2	-6.07	115.26	118.90
50	m4	72	LEU	CA-CB-CG	6.07	129.26	115.30
36	5	391	A	C8-N9-C4	6.07	108.23	105.80
36	5	425	G	O5'-P-OP1	6.07	117.98	110.70
36	1	2223	A	C8-N9-C4	-6.07	103.37	105.80
1	6	19	A	N1-C6-N6	6.07	122.24	118.60
36	5	1885	U	C5-C6-N1	-6.07	119.67	122.70
36	5	2215	A	C8-N9-C4	6.07	108.23	105.80
36	5	3195	U	P-O3'-C3'	6.07	126.98	119.70
36	1	369	A	C2-N3-C4	6.06	113.63	110.60
36	1	1386	A	C6-N1-C2	-6.06	114.96	118.60
1	6	1637	C	C6-N1-C1'	-6.06	113.53	120.80
36	5	1060	U	C5-C6-N1	-6.06	119.67	122.70
10	S8	8	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	6	610	G	C8-N9-C1'	-6.06	119.13	127.00
36	5	958	C	N3-C4-C5	6.06	124.32	121.90
36	5	2161	G	C4-C5-N7	-6.06	108.38	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2743	A	C4-C5-C6	6.06	120.03	117.00
36	1	105	C	C6-N1-C2	6.06	122.72	120.30
36	1	3362	A	C5-N7-C8	-6.05	100.87	103.90
36	5	2199	G	C5-C6-N1	-6.05	108.47	111.50
36	5	2996	U	N3-C2-O2	-6.05	117.96	122.20
1	2	325	G	N3-C4-C5	6.05	131.63	128.60
1	2	1399	C	C5-C6-N1	6.05	124.03	121.00
36	1	2209	U	C5-C6-N1	6.05	125.72	122.70
36	5	1323	G	C6-C5-N7	-6.05	126.77	130.40
36	5	1900	A	N1-C6-N6	6.05	122.23	118.60
36	5	3301	U	C6-N1-C2	6.05	124.63	121.00
36	5	3382	U	C2-N1-C1'	6.05	124.96	117.70
36	1	1320	C	C2-N1-C1'	6.05	125.45	118.80
1	6	1	U	N1-C2-O2	6.05	127.03	122.80
1	2	1389	C	N1-C2-O2	6.04	122.53	118.90
36	5	1476	G	N1-C6-O6	-6.04	116.27	119.90
1	6	1025	A	C6-C5-N7	-6.04	128.07	132.30
36	5	1116	G	N1-C2-N3	6.04	127.53	123.90
37	7	58	C	O5'-P-OP2	-6.04	100.26	105.70
38	8	32	C	C6-N1-C2	6.04	122.72	120.30
36	1	678	G	N1-C2-N2	6.04	121.63	116.20
36	1	2814	G	O5'-P-OP2	6.04	117.95	110.70
36	1	3089	C	C6-N1-C2	-6.04	117.89	120.30
36	5	1306	G	C5-N7-C8	-6.04	101.28	104.30
36	1	706	A	N1-C6-N6	6.04	122.22	118.60
36	1	2812	C	C5-C6-N1	-6.04	117.98	121.00
1	6	1642	G	C5-C6-O6	-6.04	124.98	128.60
36	5	1554	U	C2-N1-C1'	6.04	124.94	117.70
37	3	8	G	C5-C6-O6	6.03	132.22	128.60
36	1	859	G	C8-N9-C1'	-6.03	119.16	127.00
36	1	1192	C	C2-N3-C4	6.03	122.92	119.90
36	1	282	G	N7-C8-N9	6.03	116.11	113.10
36	1	2983	C	O5'-P-OP1	-6.03	100.27	105.70
36	5	1403	C	N1-C2-O2	-6.03	115.28	118.90
1	2	421	A	N1-C6-N6	6.03	122.22	118.60
36	1	398	A	C5-C6-N6	-6.03	118.88	123.70
36	1	1154	A	N9-C4-C5	6.03	108.21	105.80
36	5	2993	G	C5-C6-O6	-6.03	124.98	128.60
36	5	3335	A	C5-C6-N6	-6.03	118.88	123.70
36	1	340	C	N1-C2-O2	6.03	122.52	118.90
36	5	1496	C	C2-N1-C1'	6.03	125.43	118.80
37	7	73	C	C6-N1-C2	-6.03	117.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1431	G	N1-C6-O6	-6.02	116.29	119.90
1	6	577	G	C8-N9-C4	-6.02	103.99	106.40
36	5	1879	A	C4-C5-N7	6.02	113.71	110.70
36	5	2980	U	N1-C2-N3	6.02	118.52	114.90
48	m1	152	HIS	N-CA-C	-6.02	94.74	111.00
36	1	2400	G	N9-C4-C5	-6.02	102.99	105.40
36	1	2639	G	C4-C5-C6	6.02	122.41	118.80
1	6	65	A	C2-N3-C4	-6.02	107.59	110.60
36	5	21	G	N3-C4-N9	-6.02	122.39	126.00
36	5	881	C	N1-C2-O2	6.02	122.51	118.90
36	5	666	A	N9-C4-C5	6.02	108.21	105.80
1	2	1749	A	C8-N9-C4	6.02	108.21	105.80
1	6	1537	C	N1-C2-O2	-6.02	115.29	118.90
36	5	787	G	N1-C6-O6	6.02	123.51	119.90
36	5	1166	G	O5'-P-OP1	-6.02	100.28	105.70
36	5	2823	G	N1-C6-O6	6.02	123.51	119.90
36	5	2978	U	O4'-C1'-N1	6.02	113.02	108.20
36	1	3214	U	N1-C2-O2	6.02	127.01	122.80
36	5	1301	A	C6-C5-N7	-6.01	128.09	132.30
36	1	70	A	C5-C6-N6	-6.01	118.89	123.70
1	6	957	G	C5-C6-N1	-6.01	108.50	111.50
1	6	1634	C	N3-C2-O2	-6.01	117.69	121.90
1	2	321	C	C6-N1-C2	-6.01	117.90	120.30
36	1	3054	U	C5-C6-N1	-6.01	119.70	122.70
36	1	690	A	N1-C6-N6	-6.01	115.00	118.60
38	4	15	G	N3-C2-N2	6.01	124.11	119.90
36	5	80	G	C5-C6-O6	-6.01	125.00	128.60
36	5	1192	C	C4-C5-C6	6.01	120.40	117.40
36	5	1662	G	C6-C5-N7	-6.01	126.80	130.40
38	4	84	C	C5-C6-N1	-6.00	118.00	121.00
36	1	426	G	C4-N9-C1'	6.00	134.31	126.50
38	4	108	C	C6-N1-C2	-6.00	117.90	120.30
36	1	369	A	O5'-P-OP2	-6.00	100.30	105.70
36	1	1885	U	C4-C5-C6	6.00	123.30	119.70
36	5	2687	G	O5'-P-OP2	-6.00	100.30	105.70
36	1	220	G	C5-C6-O6	-6.00	125.00	128.60
36	1	2315	G	C8-N9-C4	-6.00	104.00	106.40
36	5	647	A	C8-N9-C1'	-6.00	116.91	127.70
36	5	961	C	N1-C2-O2	6.00	122.50	118.90
36	5	2727	A	C8-N9-C4	-6.00	103.40	105.80
36	5	420	G	N1-C6-O6	6.00	123.50	119.90
37	7	77	G	C5-C6-O6	-5.99	125.00	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1657	U	C4-C5-C6	5.99	123.30	119.70
1	2	307	G	N3-C4-N9	5.99	129.59	126.00
36	1	1783	U	C5-C4-O4	5.99	129.49	125.90
1	6	47	A	N1-C6-N6	5.99	122.19	118.60
36	5	824	C	C6-N1-C2	-5.99	117.90	120.30
36	5	2811	A	C5-C6-N1	5.99	120.69	117.70
36	5	951	A	N7-C8-N9	5.99	116.79	113.80
36	1	695	C	N3-C4-N4	-5.99	113.81	118.00
1	6	257	A	N9-C4-C5	-5.99	103.41	105.80
36	5	1152	G	C6-C5-N7	-5.99	126.81	130.40
36	1	2306	C	C6-N1-C1'	-5.98	113.62	120.80
65	N9	20	GLY	N-CA-C	5.98	128.06	113.10
36	5	2117	A	N1-C6-N6	-5.98	115.01	118.60
36	5	2314	U	N3-C2-O2	5.98	126.39	122.20
36	1	2866	U	N3-C2-O2	-5.98	118.01	122.20
1	6	1729	C	N3-C4-C5	5.98	124.29	121.90
36	5	84	U	C6-N1-C2	5.98	124.59	121.00
36	5	1239	C	C2-N1-C1'	5.98	125.38	118.80
36	1	69	C	N3-C4-C5	-5.98	119.51	121.90
1	6	421	A	N9-C4-C5	-5.98	103.41	105.80
36	5	2305	G	C8-N9-C4	-5.98	104.01	106.40
36	5	2333	C	C5-C4-N4	-5.98	116.01	120.20
36	5	2659	G	C6-C5-N7	-5.98	126.81	130.40
36	1	3319	U	P-O3'-C3'	5.98	126.87	119.70
36	5	110	G	C8-N9-C4	5.98	108.79	106.40
36	1	2376	G	C5-C6-N1	5.98	114.49	111.50
36	1	645	A	C4-C5-N7	-5.97	107.71	110.70
36	1	959	C	N3-C4-C5	5.97	124.29	121.90
36	1	1306	G	C5-C6-O6	-5.97	125.02	128.60
36	1	2374	C	N1-C2-O2	5.97	122.48	118.90
36	5	420	G	N9-C4-C5	-5.97	103.01	105.40
36	5	3188	G	N1-C6-O6	-5.97	116.32	119.90
36	5	1667	A	N9-C4-C5	-5.97	103.41	105.80
36	5	2882	U	O5'-P-OP2	-5.97	100.33	105.70
36	1	1403	C	N3-C2-O2	5.97	126.08	121.90
36	1	676	G	C6-C5-N7	-5.97	126.82	130.40
36	1	1408	G	N3-C4-N9	5.97	129.58	126.00
1	6	245	U	N3-C2-O2	-5.97	118.02	122.20
36	5	1900	A	C5-C6-N6	-5.97	118.93	123.70
36	1	2777	G	C4-C5-N7	-5.96	108.41	110.80
36	5	1101	G	N3-C2-N2	5.96	124.07	119.90
36	5	1879	A	C5-C6-N1	-5.96	114.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2273	G	C4-N9-C1'	-5.96	118.75	126.50
36	5	21	G	N3-C4-C5	5.96	131.58	128.60
36	5	1452	A	C5-C6-N6	-5.96	118.93	123.70
36	5	652	G	C6-C5-N7	-5.96	126.82	130.40
36	5	1667	A	N1-C6-N6	5.96	122.18	118.60
36	5	3105	U	N1-C2-N3	5.96	118.48	114.90
36	5	673	U	N1-C2-O2	-5.96	118.63	122.80
36	5	1448	U	C6-N1-C2	5.96	124.58	121.00
36	1	75	G	C6-C5-N7	-5.96	126.83	130.40
36	1	2526	C	C5-C6-N1	5.96	123.98	121.00
36	5	934	G	C2-N3-C4	5.96	114.88	111.90
36	5	2796	G	C5-C6-O6	5.96	132.18	128.60
36	5	2832	C	C6-N1-C2	5.96	122.68	120.30
36	1	2795	U	OP1-P-OP2	5.96	128.53	119.60
1	6	209	U	C2-N1-C1'	-5.96	110.55	117.70
36	5	2345	A	C8-N9-C4	5.96	108.18	105.80
36	1	988	U	C5-C6-N1	-5.96	119.72	122.70
36	1	2376	G	N7-C8-N9	5.96	116.08	113.10
36	5	24	G	C8-N9-C4	5.96	108.78	106.40
1	6	477	A	N1-C6-N6	5.95	122.17	118.60
36	5	1541	G	C4-C5-N7	5.95	113.18	110.80
36	1	2355	G	C6-C5-N7	-5.95	126.83	130.40
36	1	2374	C	C6-N1-C2	-5.95	117.92	120.30
36	5	2350	C	O5'-P-OP1	5.95	117.84	110.70
36	5	1331	U	C2-N3-C4	-5.95	123.43	127.00
36	5	1631	C	C6-N1-C2	-5.95	117.92	120.30
36	5	2984	C	C2-N3-C4	-5.95	116.92	119.90
36	5	646	A	C2-N3-C4	-5.95	107.63	110.60
36	5	2205	U	C5-C6-N1	5.95	125.67	122.70
36	5	2620	G	N3-C4-N9	-5.95	122.43	126.00
36	1	388	G	N3-C2-N2	-5.95	115.74	119.90
36	1	1450	G	C5-N7-C8	-5.95	101.33	104.30
36	1	2646	C	N3-C4-C5	5.95	124.28	121.90
1	6	1782	A	C8-N9-C4	-5.95	103.42	105.80
36	5	2971	A	N1-C2-N3	-5.95	126.33	129.30
36	1	1174	G	C4-N9-C1'	5.94	134.23	126.50
36	1	1416	C	N3-C4-N4	-5.94	113.84	118.00
36	1	1643	A	C8-N9-C4	5.94	108.18	105.80
36	1	1902	G	C5-N7-C8	-5.94	101.33	104.30
36	5	716	A	N9-C4-C5	-5.94	103.42	105.80
36	5	2397	A	C8-N9-C4	5.94	108.18	105.80
36	1	25	U	O5'-P-OP2	5.94	117.83	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1308	A	C2-N3-C4	-5.94	107.63	110.60
36	1	2983	C	C5-C4-N4	5.94	124.36	120.20
1	6	1778	G	C8-N9-C4	-5.94	104.02	106.40
36	5	1153	A	C5-C6-N6	-5.94	118.95	123.70
36	5	2409	G	C8-N9-C4	-5.94	104.02	106.40
36	1	836	A	N1-C6-N6	-5.94	115.03	118.60
36	1	1838	G	C4-C5-C6	5.94	122.36	118.80
36	5	2376	G	C5-N7-C8	-5.94	101.33	104.30
36	5	2310	U	O5'-P-OP2	-5.94	100.36	105.70
36	1	961	C	C4-C5-C6	5.94	120.37	117.40
36	1	2419	A	OP1-P-OP2	-5.94	110.69	119.60
36	1	3268	A	N1-C2-N3	5.94	132.27	129.30
36	5	644	G	C4-C5-C6	5.94	122.36	118.80
36	5	891	G	C8-N9-C4	-5.94	104.03	106.40
36	5	2416	U	C6-N1-C2	-5.94	117.44	121.00
1	2	1489	U	N3-C2-O2	-5.94	118.05	122.20
36	1	203	G	C8-N9-C4	5.94	108.78	106.40
36	1	1334	U	N3-C4-O4	5.94	123.56	119.40
36	5	1153	A	C6-C5-N7	-5.94	128.15	132.30
36	1	644	G	C8-N9-C4	-5.93	104.03	106.40
36	1	917	A	N1-C6-N6	-5.93	115.04	118.60
38	8	61	A	O5'-P-OP1	-5.93	100.36	105.70
36	1	1392	G	O4'-C1'-N9	5.93	112.94	108.20
1	6	1773	C	N3-C4-N4	5.93	122.15	118.00
36	5	871	U	N1-C2-N3	5.93	118.46	114.90
36	5	1842	A	OP2-P-O3'	5.93	118.25	105.20
36	1	2904	U	O5'-P-OP1	5.93	117.82	110.70
36	5	3206	C	C6-N1-C2	-5.93	117.93	120.30
1	6	309	C	N3-C2-O2	5.93	126.05	121.90
1	2	794	U	N1-C2-O2	5.93	126.95	122.80
36	1	2114	C	O5'-P-OP2	-5.93	100.37	105.70
1	2	554	C	C6-N1-C1'	-5.92	113.69	120.80
36	1	1864	A	N7-C8-N9	-5.92	110.84	113.80
36	1	2169	G	C4-C5-N7	-5.92	108.43	110.80
36	1	2803	A	O5'-P-OP1	-5.92	100.37	105.70
36	5	2765	C	C5-C6-N1	5.92	123.96	121.00
36	5	3064	U	N1-C2-N3	5.92	118.45	114.90
1	2	380	U	C2-N1-C1'	5.92	124.81	117.70
36	1	637	C	P-O3'-C3'	5.92	126.81	119.70
36	1	953	G	OP1-P-O3'	5.92	118.23	105.20
1	6	1535	U	C5-C6-N1	-5.92	119.74	122.70
36	5	712	G	N1-C6-O6	5.92	123.45	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	406	G	N1-C6-O6	-5.92	116.35	119.90
36	5	2626	A	N1-C2-N3	5.92	132.26	129.30
36	1	3051	U	C5-C6-N1	5.92	125.66	122.70
36	5	881	C	C2-N3-C4	5.92	122.86	119.90
36	5	41	G	C6-C5-N7	-5.92	126.85	130.40
36	5	437	G	C8-N9-C1'	5.92	134.69	127.00
36	5	1178	G	C6-C5-N7	-5.92	126.85	130.40
36	5	2353	G	N9-C4-C5	-5.92	103.03	105.40
36	1	951	A	C5-C6-N1	-5.92	114.74	117.70
36	5	2715	A	C4-C5-N7	-5.92	107.74	110.70
36	1	2372	A	C5-C6-N6	-5.91	118.97	123.70
36	5	994	G	C2-N3-C4	5.91	114.86	111.90
36	5	2871	G	O5'-P-OP2	-5.91	100.38	105.70
36	5	2951	G	N3-C4-N9	5.91	129.55	126.00
36	1	885	U	C6-N1-C2	5.91	124.55	121.00
36	1	1167	U	C2-N1-C1'	-5.91	110.61	117.70
36	1	3362	A	C6-C5-N7	-5.91	128.16	132.30
36	5	2737	C	N1-C2-O2	-5.91	115.35	118.90
36	1	804	C	N3-C2-O2	-5.91	117.76	121.90
36	1	3180	A	C4-C5-N7	5.91	113.65	110.70
1	6	382	C	N1-C2-O2	-5.91	115.35	118.90
36	1	27	C	N3-C4-C5	-5.91	119.54	121.90
1	2	1432	U	C5-C6-N1	-5.91	119.75	122.70
1	6	1412	G	C8-N9-C1'	5.91	134.68	127.00
36	5	3020	U	N1-C2-O2	-5.91	118.67	122.80
36	5	55	G	N1-C6-O6	5.90	123.44	119.90
36	5	857	G	N3-C2-N2	-5.90	115.77	119.90
36	5	2145	A	C4-C5-C6	5.90	119.95	117.00
36	1	39	A	C5-C6-N6	-5.90	118.98	123.70
36	1	650	C	N1-C2-O2	-5.90	115.36	118.90
36	1	2279	A	C5-C6-N6	-5.90	118.98	123.70
36	1	3264	G	C8-N9-C4	5.90	108.76	106.40
36	5	2761	G	C6-N1-C2	-5.90	121.56	125.10
1	2	1081	A	N1-C6-N6	-5.90	115.06	118.60
36	1	281	G	C2-N3-C4	5.90	114.85	111.90
36	1	1424	C	O5'-P-OP1	-5.90	100.39	105.70
36	1	1279	C	C5-C6-N1	5.90	123.95	121.00
36	1	2337	C	C6-N1-C2	-5.90	117.94	120.30
36	1	3266	G	N3-C4-N9	-5.90	122.46	126.00
1	6	992	A	C4-C5-N7	5.90	113.65	110.70
36	1	757	C	N3-C2-O2	5.90	126.03	121.90
36	5	650	C	C6-N1-C2	5.90	122.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2865	U	N1-C2-N3	-5.90	111.36	114.90
1	6	1736	G	C8-N9-C4	-5.89	104.04	106.40
36	5	1116	G	OP2-P-O3'	5.89	118.17	105.20
36	5	1897	G	N3-C2-N2	-5.89	115.77	119.90
36	5	2288	G	O5'-P-OP2	-5.89	100.39	105.70
36	5	3362	A	C5-N7-C8	-5.89	100.95	103.90
36	1	512	U	C6-N1-C2	5.89	124.53	121.00
36	1	908	G	O4'-C1'-N9	-5.89	103.49	108.20
36	1	2624	G	N1-C6-O6	5.89	123.44	119.90
1	6	1274	C	C6-N1-C2	-5.89	117.94	120.30
36	5	1127	G	C2-N3-C4	5.89	114.85	111.90
36	5	1404	G	N3-C2-N2	5.89	124.03	119.90
36	5	2643	A	N9-C4-C5	-5.89	103.44	105.80
36	1	1487	G	N3-C2-N2	-5.89	115.78	119.90
36	1	2305	G	C5-C6-O6	-5.89	125.07	128.60
36	1	2335	G	N7-C8-N9	-5.89	110.16	113.10
1	6	577	G	N1-C6-O6	5.89	123.43	119.90
1	6	1152	A	N1-C6-N6	5.89	122.13	118.60
36	5	1407	A	O5'-P-OP2	-5.89	100.40	105.70
36	5	1434	G	C8-N9-C1'	5.89	134.66	127.00
36	5	1613	A	O4'-C1'-N9	5.89	112.91	108.20
1	2	1600	A	C2-N3-C4	-5.89	107.66	110.60
36	1	61	A	N1-C6-N6	5.89	122.13	118.60
36	1	585	A	N7-C8-N9	-5.89	110.86	113.80
38	4	140	G	N9-C4-C5	5.89	107.75	105.40
36	1	433	A	N1-C6-N6	5.88	122.13	118.60
36	1	1144	U	N1-C2-O2	-5.88	118.68	122.80
36	5	938	C	C4-C5-C6	-5.88	114.46	117.40
36	5	1056	U	C5-C6-N1	5.88	125.64	122.70
36	5	2404	A	N7-C8-N9	5.88	116.74	113.80
36	1	92	G	N3-C4-N9	5.88	129.53	126.00
36	1	968	G	C5-C6-N1	5.88	114.44	111.50
36	1	2585	G	N3-C4-C5	-5.88	125.66	128.60
36	5	650	C	N3-C4-N4	-5.88	113.88	118.00
36	5	1001	G	N1-C6-O6	-5.88	116.37	119.90
36	5	1329	U	C5-C4-O4	-5.88	122.37	125.90
36	1	1465	A	C8-N9-C4	5.88	108.15	105.80
36	5	2398	A	N7-C8-N9	-5.88	110.86	113.80
36	1	797	U	OP2-P-O3'	5.88	118.13	105.20
36	1	1116	G	C8-N9-C4	-5.88	104.05	106.40
1	6	577	G	C5-N7-C8	-5.88	101.36	104.30
36	5	2820	A	C2-N3-C4	5.88	113.54	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2848	G	C5-C6-O6	-5.88	125.07	128.60
21	C9	57	ARG	NE-CZ-NH1	5.88	123.24	120.30
36	1	932	U	C5-C4-O4	-5.88	122.38	125.90
36	5	1060	U	C2-N3-C4	-5.88	123.47	127.00
1	2	1324	G	N3-C2-N2	-5.87	115.79	119.90
24	D2	93	LEU	CA-CB-CG	5.87	128.81	115.30
36	1	1346	G	N1-C6-O6	5.87	123.42	119.90
36	1	1349	G	C2-N3-C4	5.87	114.84	111.90
36	1	2138	A	C4-C5-C6	5.87	119.94	117.00
36	1	2184	U	C5-C6-N1	5.87	125.64	122.70
36	1	2345	A	N1-C6-N6	5.87	122.12	118.60
36	5	2112	U	C5-C6-N1	5.87	125.64	122.70
1	2	434	G	O5'-P-OP2	-5.87	100.42	105.70
36	1	289	A	N9-C4-C5	-5.87	103.45	105.80
36	5	295	A	C2-N3-C4	-5.87	107.67	110.60
36	5	1868	G	N1-C6-O6	5.87	123.42	119.90
36	5	2811	A	C6-N1-C2	-5.87	115.08	118.60
36	5	2898	G	O4'-C1'-N9	-5.87	103.51	108.20
36	1	394	G	C5-C6-O6	5.86	132.12	128.60
36	1	2381	G	C6-C5-N7	-5.86	126.88	130.40
1	6	1187	U	C6-N1-C2	-5.86	117.48	121.00
36	5	1599	G	C8-N9-C4	5.86	108.75	106.40
36	5	1869	C	C6-N1-C2	5.86	122.65	120.30
36	1	1409	G	N1-C6-O6	-5.86	116.38	119.90
1	2	1280	C	N3-C4-C5	-5.86	119.56	121.90
36	1	994	G	N1-C2-N2	-5.86	110.92	116.20
1	6	151	G	N3-C4-N9	-5.86	122.48	126.00
1	6	539	G	N7-C8-N9	5.86	116.03	113.10
1	6	542	A	P-O3'-C3'	5.86	126.73	119.70
36	5	1496	C	O5'-P-OP1	5.86	117.73	110.70
36	5	1938	U	C6-N1-C2	5.86	124.52	121.00
36	1	2700	G	C6-C5-N7	-5.86	126.89	130.40
36	5	936	A	P-O3'-C3'	5.86	126.73	119.70
36	1	2376	G	C8-N9-C4	-5.86	104.06	106.40
36	5	1119	C	OP1-P-O3'	-5.86	92.31	105.20
36	5	2740	A	C8-N9-C4	-5.86	103.46	105.80
1	6	337	G	C8-N9-C1'	-5.86	119.39	127.00
36	5	101	G	O4'-C1'-N9	5.86	112.89	108.20
36	1	1435	A	O5'-P-OP2	5.85	117.72	110.70
1	6	1396	U	C5-C6-N1	5.85	125.63	122.70
36	5	907	G	N1-C2-N2	-5.85	110.93	116.20
36	5	1412	G	C8-N9-C4	-5.85	104.06	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1434	G	C8-N9-C4	-5.85	104.06	106.40
36	5	3209	A	O4'-C1'-N9	5.85	112.88	108.20
36	1	2872	A	N1-C6-N6	5.85	122.11	118.60
36	1	2983	C	C4-C5-C6	5.85	120.33	117.40
37	3	52	G	O5'-P-OP2	-5.85	100.43	105.70
1	6	337	G	C6-C5-N7	-5.85	126.89	130.40
1	6	352	A	N1-C6-N6	-5.85	115.09	118.60
36	5	514	G	N1-C6-O6	5.85	123.41	119.90
36	5	938	C	N3-C4-C5	5.85	124.24	121.90
36	1	2961	G	N1-C6-O6	5.85	123.41	119.90
36	5	99	A	C8-N9-C4	5.85	108.14	105.80
36	5	2809	C	C6-N1-C2	5.85	122.64	120.30
37	7	41	G	C8-N9-C4	5.85	108.74	106.40
36	1	676	G	C8-N9-C4	-5.85	104.06	106.40
36	1	3362	A	N1-C6-N6	5.85	122.11	118.60
36	5	410	U	C5-C6-N1	5.85	125.62	122.70
37	7	84	A	O5'-P-OP1	-5.85	100.44	105.70
1	6	29	U	N1-C2-N3	5.85	118.41	114.90
36	5	2308	C	O5'-P-OP2	-5.85	100.44	105.70
36	1	262	U	N3-C2-O2	5.84	126.29	122.20
36	1	2281	A	C8-N9-C4	5.84	108.14	105.80
36	5	1115	G	C6-C5-N7	-5.84	126.89	130.40
36	5	1450	G	C5-C6-O6	-5.84	125.09	128.60
1	6	306	U	C2-N3-C4	-5.84	123.49	127.00
36	5	1163	A	N1-C6-N6	-5.84	115.09	118.60
1	2	448	C	N3-C4-C5	-5.84	119.56	121.90
36	1	369	A	N3-C4-C5	-5.84	122.71	126.80
36	1	787	G	O5'-P-OP2	-5.84	100.44	105.70
36	1	838	G	C8-N9-C4	5.84	108.74	106.40
36	1	1207	G	N1-C6-O6	5.84	123.40	119.90
36	1	1449	A	C2-N3-C4	5.84	113.52	110.60
1	6	194	U	N1-C2-O2	5.84	126.89	122.80
36	5	338	A	OP2-P-O3'	5.84	118.05	105.20
36	5	780	A	N1-C6-N6	5.84	122.11	118.60
36	5	2938	G	N9-C4-C5	5.84	107.74	105.40
36	1	1389	G	N3-C4-N9	5.84	129.50	126.00
1	6	934	C	N3-C2-O2	-5.84	117.81	121.90
36	5	1333	C	C6-N1-C2	-5.84	117.96	120.30
37	3	82	G	N1-C2-N2	-5.84	110.95	116.20
36	1	2634	U	C5-C4-O4	-5.84	122.40	125.90
36	1	3092	C	C2-N3-C4	-5.84	116.98	119.90
36	5	365	A	N9-C4-C5	-5.84	103.47	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	413	U	C5-C6-N1	-5.84	119.78	122.70
36	5	2784	G	C8-N9-C4	-5.84	104.06	106.40
36	5	2914	G	N3-C4-C5	-5.84	125.68	128.60
36	1	2808	A	C4-C5-C6	5.83	119.92	117.00
36	5	1931	U	C2-N1-C1'	-5.83	110.70	117.70
37	7	76	A	O4'-C1'-N9	5.83	112.87	108.20
36	1	916	G	N1-C6-O6	-5.83	116.40	119.90
36	1	1386	A	C5-C6-N6	-5.83	119.03	123.70
36	1	1911	A	N1-C6-N6	5.83	122.10	118.60
1	6	1560	U	N3-C2-O2	-5.83	118.12	122.20
36	5	1500	G	C8-N9-C4	5.83	108.73	106.40
36	5	2412	G	N3-C2-N2	5.83	123.98	119.90
36	1	3101	G	C5-C6-N1	5.83	114.42	111.50
36	1	359	U	N3-C4-C5	-5.83	111.10	114.60
36	1	2351	U	O5'-P-OP2	5.83	117.69	110.70
36	1	2963	C	C4-C5-C6	5.83	120.31	117.40
36	1	2969	A	C2-N3-C4	-5.83	107.69	110.60
36	1	3184	A	N1-C6-N6	5.83	122.10	118.60
1	6	1002	G	C4-C5-N7	5.83	113.13	110.80
1	6	1520	U	N3-C2-O2	5.83	126.28	122.20
36	1	958	C	C2-N3-C4	-5.83	116.99	119.90
36	5	1897	G	C5-N7-C8	-5.83	101.39	104.30
36	5	1368	U	N1-C2-O2	-5.83	118.72	122.80
36	5	2420	C	N1-C2-O2	-5.83	115.41	118.90
36	5	2942	C	N3-C4-N4	5.83	122.08	118.00
1	2	399	A	N1-C6-N6	-5.82	115.11	118.60
36	1	22	G	N1-C6-O6	-5.82	116.41	119.90
36	1	1076	C	N1-C2-O2	5.82	122.39	118.90
1	6	864	U	C2-N1-C1'	5.82	124.69	117.70
36	5	341	G	N3-C4-N9	-5.82	122.51	126.00
36	5	638	C	O5'-P-OP1	-5.82	100.46	105.70
36	5	913	A	N9-C4-C5	5.82	108.13	105.80
36	5	999	G	C8-N9-C4	5.82	108.73	106.40
36	5	2864	A	N9-C4-C5	-5.82	103.47	105.80
36	5	3322	A	N1-C6-N6	5.82	122.09	118.60
38	4	53	A	N1-C6-N6	-5.82	115.11	118.60
1	6	209	U	N3-C2-O2	5.82	126.27	122.20
36	5	2112	U	C2-N1-C1'	5.82	124.68	117.70
36	5	2885	C	C2-N3-C4	-5.82	116.99	119.90
1	2	1412	G	C4-N9-C1'	-5.82	118.94	126.50
36	1	895	A	N1-C6-N6	5.82	122.09	118.60
36	5	567	G	N3-C4-N9	5.82	129.49	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1302	A	C2-N3-C4	5.82	113.51	110.60
36	5	3167	A	C8-N9-C4	-5.82	103.47	105.80
36	1	76	G	C4-C5-C6	5.82	122.29	118.80
36	1	2378	C	C5-C4-N4	-5.82	116.13	120.20
36	5	2803	A	O5'-P-OP1	-5.82	100.47	105.70
37	7	10	C	N3-C4-N4	5.81	122.07	118.00
36	1	2884	C	C5-C4-N4	-5.81	116.13	120.20
36	5	961	C	N3-C2-O2	-5.81	117.83	121.90
36	5	1160	C	C2-N1-C1'	-5.81	112.41	118.80
36	5	1869	C	N3-C4-C5	5.81	124.22	121.90
36	5	2211	U	N1-C2-N3	5.81	118.39	114.90
36	5	2403	G	O5'-P-OP1	5.81	117.67	110.70
36	5	2640	A	C8-N9-C4	5.81	108.12	105.80
1	2	734	A	P-O3'-C3'	5.81	126.67	119.70
36	1	2884	C	C4-C5-C6	-5.81	114.50	117.40
36	5	59	G	N1-C6-O6	-5.81	116.42	119.90
36	5	3195	U	N1-C2-O2	5.81	126.87	122.80
36	5	1911	A	N1-C6-N6	5.81	122.08	118.60
36	5	2316	G	C4-C5-N7	-5.81	108.48	110.80
36	1	432	G	N1-C6-O6	5.81	123.38	119.90
36	1	925	A	C5-N7-C8	-5.81	101.00	103.90
1	6	1640	C	C2-N1-C1'	5.81	125.19	118.80
36	1	678	G	O5'-P-OP1	-5.80	100.48	105.70
36	1	1420	C	C6-N1-C2	-5.80	117.98	120.30
1	6	858	G	C4-C5-N7	5.80	113.12	110.80
36	5	1854	C	C6-N1-C2	-5.80	117.98	120.30
36	1	1316	C	N3-C4-C5	-5.80	119.58	121.90
36	1	2300	G	C4-C5-C6	5.80	122.28	118.80
36	5	283	G	N1-C6-O6	5.80	123.38	119.90
36	5	1894	U	C2-N1-C1'	-5.80	110.74	117.70
36	5	3124	G	N9-C4-C5	5.80	107.72	105.40
36	1	430	U	N3-C2-O2	-5.80	118.14	122.20
36	1	1112	A	O5'-P-OP2	-5.80	100.48	105.70
36	1	3135	U	C5-C6-N1	-5.80	119.80	122.70
1	6	1	U	N3-C2-O2	-5.80	118.14	122.20
36	1	1837	U	N1-C2-O2	-5.80	118.74	122.80
36	1	715	A	O4'-C1'-N9	5.80	112.84	108.20
36	1	2730	G	C6-C5-N7	-5.80	126.92	130.40
1	6	1745	G	N3-C4-N9	5.79	129.48	126.00
1	2	356	G	N1-C6-O6	5.79	123.38	119.90
36	1	907	G	C5-N7-C8	5.79	107.20	104.30
62	N6	76	LEU	CA-CB-CG	5.79	128.63	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	453	U	C6-N1-C2	-5.79	117.52	121.00
36	5	2923	U	C6-N1-C2	-5.79	117.52	121.00
38	8	88	A	C8-N9-C4	5.79	108.12	105.80
36	5	639	G	N1-C6-O6	5.79	123.38	119.90
1	2	1118	G	N1-C6-O6	5.79	123.37	119.90
36	1	1136	A	C5-C6-N1	5.79	120.59	117.70
36	5	1300	G	C5-C6-O6	-5.79	125.13	128.60
36	5	2278	C	C5-C6-N1	5.79	123.89	121.00
1	2	75	U	N3-C2-O2	-5.79	118.15	122.20
36	1	1192	C	C6-N1-C1'	-5.79	113.85	120.80
36	5	1375	G	O5'-P-OP2	-5.79	100.49	105.70
36	5	2552	C	N3-C2-O2	-5.79	117.85	121.90
36	1	2572	C	C6-N1-C1'	-5.79	113.86	120.80
36	1	608	A	N1-C6-N6	5.79	122.07	118.60
36	1	1330	A	C2-N3-C4	-5.79	107.71	110.60
36	1	2865	U	N3-C4-C5	5.79	118.07	114.60
36	1	2899	C	C2-N3-C4	-5.79	117.01	119.90
38	4	113	U	N1-C2-N3	5.79	118.37	114.90
1	6	982	U	C5-C6-N1	-5.79	119.81	122.70
36	5	960	U	N3-C4-O4	-5.79	115.35	119.40
36	5	2389	C	O5'-P-OP1	-5.79	100.49	105.70
36	5	2659	G	N1-C6-O6	5.79	123.37	119.90
36	1	1506	A	C5-C6-N6	5.78	128.33	123.70
36	5	1499	C	N3-C2-O2	5.78	125.95	121.90
36	5	1813	A	C8-N9-C4	-5.78	103.49	105.80
1	2	545	A	OP1-P-O3'	5.78	117.92	105.20
36	1	2406	C	N3-C2-O2	5.78	125.95	121.90
36	1	2590	A	N9-C4-C5	5.78	108.11	105.80
1	2	1745	G	C5-C6-N1	5.78	114.39	111.50
1	2	1779	U	C2-N1-C1'	-5.78	110.76	117.70
12	c0	97	PRO	N-CA-CB	5.78	110.24	103.30
36	5	867	G	N1-C6-O6	5.78	123.37	119.90
36	5	2865	U	C4-C5-C6	-5.78	116.23	119.70
36	5	3087	A	N9-C4-C5	5.78	108.11	105.80
36	5	2420	C	N3-C2-O2	5.78	125.94	121.90
36	5	1373	A	N1-C6-N6	5.78	122.07	118.60
36	1	1592	G	C5-C6-N1	-5.78	108.61	111.50
36	5	914	A	O5'-P-OP2	-5.78	100.50	105.70
36	5	1496	C	O5'-P-OP2	-5.78	100.50	105.70
36	5	2957	G	O4'-C1'-N9	-5.78	103.58	108.20
36	5	3092	C	C6-N1-C2	5.78	122.61	120.30
36	1	1190	A	C8-N9-C1'	-5.77	117.31	127.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2603	G	N9-C4-C5	-5.77	103.09	105.40
1	2	501	U	OP1-P-O3'	5.77	117.90	105.20
21	c9	57	ARG	NE-CZ-NH1	5.77	123.19	120.30
38	8	51	G	C8-N9-C4	-5.77	104.09	106.40
36	1	2870	C	N3-C2-O2	5.77	125.94	121.90
1	6	542	A	N1-C6-N6	-5.77	115.14	118.60
36	1	410	U	C5-C6-N1	5.77	125.58	122.70
36	1	651	G	O5'-P-OP1	5.77	117.62	110.70
36	5	221	A	C8-N9-C4	5.77	108.11	105.80
36	5	834	U	C2-N1-C1'	-5.76	110.78	117.70
36	5	2943	G	C8-N9-C1'	-5.76	119.51	127.00
1	2	75	U	C2-N1-C1'	5.76	124.62	117.70
36	1	3016	A	N1-C6-N6	5.76	122.06	118.60
36	5	1507	G	N7-C8-N9	5.76	115.98	113.10
36	1	110	G	N9-C1'-C2'	-5.76	105.66	112.00
36	1	1400	G	N3-C4-C5	-5.76	125.72	128.60
36	1	2183	A	C6-N1-C2	-5.76	115.14	118.60
36	5	942	U	C6-N1-C2	-5.76	117.54	121.00
1	2	1114	G	N3-C4-N9	5.76	129.46	126.00
1	6	1537	C	C2-N1-C1'	-5.76	112.47	118.80
36	1	1419	A	O5'-P-OP1	5.76	117.61	110.70
36	1	2178	A	N1-C6-N6	-5.76	115.15	118.60
36	1	2875	U	N3-C2-O2	5.76	126.23	122.20
36	1	2697	A	N1-C6-N6	-5.75	115.15	118.60
36	5	906	A	OP1-P-O3'	5.75	117.86	105.20
1	2	1600	A	C6-C5-N7	-5.75	128.27	132.30
36	1	706	A	N9-C4-C5	-5.75	103.50	105.80
36	1	1445	U	C2-N1-C1'	-5.75	110.80	117.70
36	5	2875	U	N3-C4-O4	5.75	123.43	119.40
36	1	676	G	C8-N9-C1'	-5.75	119.52	127.00
36	1	1907	C	N3-C4-C5	-5.75	119.60	121.90
36	1	2398	A	C8-N9-C4	5.75	108.10	105.80
36	1	2639	G	N3-C4-C5	-5.75	125.72	128.60
36	5	1115	G	C8-N9-C1'	-5.75	119.52	127.00
36	5	3145	C	C5-C6-N1	-5.75	118.12	121.00
1	6	1739	C	N1-C2-O2	-5.75	115.45	118.90
36	5	1910	A	OP2-P-O3'	5.75	117.85	105.20
36	1	578	A	C5-C6-N6	-5.75	119.10	123.70
36	1	3110	C	C5-C6-N1	5.75	123.87	121.00
36	5	82	C	N3-C4-C5	-5.75	119.60	121.90
36	1	156	G	C5-C6-O6	-5.75	125.15	128.60
36	1	401	U	N1-C2-O2	5.75	126.82	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2590	A	C8-N9-C4	-5.75	103.50	105.80
1	6	298	C	N1-C2-O2	-5.75	115.45	118.90
1	6	1745	G	C6-C5-N7	-5.75	126.95	130.40
36	5	639	G	C5-C6-N1	-5.75	108.63	111.50
36	5	2820	A	N7-C8-N9	5.75	116.67	113.80
36	1	948	C	O5'-P-OP1	5.75	117.59	110.70
36	5	2905	U	C2-N3-C4	-5.74	123.55	127.00
36	5	3052	G	C8-N9-C4	-5.74	104.10	106.40
36	5	3287	U	N3-C2-O2	-5.74	118.18	122.20
1	2	103	A	N1-C6-N6	5.74	122.04	118.60
36	1	55	G	N1-C6-O6	5.74	123.34	119.90
36	1	637	C	C6-N1-C2	5.74	122.60	120.30
36	1	1466	G	N3-C4-N9	5.74	129.44	126.00
1	6	1029	U	N3-C4-O4	-5.74	115.38	119.40
1	6	1745	G	C5-C6-O6	-5.74	125.16	128.60
36	5	41	G	N9-C4-C5	-5.74	103.10	105.40
36	5	2643	A	N1-C6-N6	5.74	122.04	118.60
1	2	720	G	OP1-P-O3'	5.74	117.82	105.20
36	1	432	G	C6-C5-N7	-5.74	126.96	130.40
36	1	3018	C	N1-C2-O2	-5.74	115.46	118.90
36	5	3197	G	N3-C4-C5	5.74	131.47	128.60
37	7	47	C	C5-C6-N1	-5.74	118.13	121.00
36	1	2904	U	O5'-P-OP2	-5.74	100.54	105.70
38	4	26	U	N3-C2-O2	-5.73	118.19	122.20
1	6	610	G	C4-N9-C1'	5.73	133.96	126.50
36	5	909	G	N1-C6-O6	-5.73	116.46	119.90
36	1	682	U	N1-C2-O2	5.73	126.81	122.80
36	1	2760	C	C6-N1-C2	-5.73	118.01	120.30
1	6	418	G	C4-C5-N7	5.73	113.09	110.80
36	5	3141	A	O5'-P-OP1	-5.73	100.54	105.70
36	5	3201	C	C6-N1-C2	-5.73	118.01	120.30
36	5	3335	A	C4-C5-N7	5.73	113.57	110.70
1	2	1664	C	O5'-P-OP2	-5.73	100.54	105.70
36	1	345	G	N1-C2-N2	-5.73	111.04	116.20
36	1	1175	C	C6-N1-C2	5.73	122.59	120.30
36	1	1662	G	N1-C6-O6	5.73	123.34	119.90
36	5	1848	G	OP1-P-OP2	5.73	128.20	119.60
36	5	2340	U	C5-C4-O4	-5.73	122.46	125.90
36	1	70	A	C4-C5-N7	5.73	113.56	110.70
36	1	1492	G	N3-C4-N9	5.73	129.44	126.00
36	1	3087	A	N1-C2-N3	5.73	132.16	129.30
1	6	1058	U	P-O3'-C3'	5.73	126.57	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2333	C	C5-C6-N1	-5.73	118.14	121.00
36	5	2716	U	C6-N1-C2	-5.73	117.56	121.00
1	6	558	U	C2-N1-C1'	5.73	124.57	117.70
1	6	1700	C	N3-C2-O2	-5.73	117.89	121.90
15	C3	22	ALA	C-N-CA	5.72	146.05	122.00
36	1	2142	A	N3-C4-C5	-5.72	122.79	126.80
36	1	2617	U	N3-C4-O4	-5.72	115.39	119.40
36	5	2638	C	O5'-P-OP2	-5.72	100.55	105.70
36	5	2915	U	C5-C4-O4	-5.72	122.47	125.90
54	m8	174	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	2	1291	G	N1-C2-N3	5.72	127.33	123.90
1	2	499	U	C2-N1-C1'	5.72	124.56	117.70
36	1	883	A	C6-N1-C2	-5.72	115.17	118.60
36	1	1713	G	N3-C4-N9	-5.72	122.57	126.00
36	1	2148	U	N3-C2-O2	5.72	126.20	122.20
36	5	215	G	N3-C4-C5	-5.72	125.74	128.60
36	1	908	G	N3-C2-N2	-5.72	115.90	119.90
1	2	610	G	C4-N9-C1'	5.72	133.93	126.50
36	1	1389	G	N1-C6-O6	5.72	123.33	119.90
1	6	1751	C	C2-N1-C1'	-5.72	112.51	118.80
36	5	1794	G	C8-N9-C4	5.72	108.69	106.40
36	1	220	G	C6-C5-N7	-5.71	126.97	130.40
36	1	2187	G	C8-N9-C4	-5.71	104.11	106.40
36	1	2298	U	N3-C4-O4	-5.71	115.40	119.40
36	5	942	U	N1-C2-O2	-5.71	118.80	122.80
37	7	105	C	C2-N1-C1'	5.71	125.09	118.80
36	5	1889	G	C5-C6-O6	-5.71	125.17	128.60
36	5	2707	C	N3-C4-C5	5.71	124.19	121.90
36	5	2954	U	N3-C4-O4	5.71	123.40	119.40
36	1	536	U	O5'-P-OP1	-5.71	100.56	105.70
36	1	1535	A	N1-C6-N6	5.71	122.03	118.60
36	1	1713	G	C4-N9-C1'	-5.71	119.08	126.50
36	1	1855	U	O5'-P-OP1	-5.71	100.56	105.70
36	1	2306	C	N3-C2-O2	-5.71	117.90	121.90
1	6	1772	C	C6-N1-C2	-5.71	118.02	120.30
36	5	1239	C	C5-C6-N1	5.71	123.86	121.00
36	1	2194	G	N1-C6-O6	5.71	123.33	119.90
36	1	3081	C	C5-C6-N1	-5.71	118.14	121.00
1	6	163	G	C8-N9-C4	-5.71	104.12	106.40
36	5	121	A	N1-C6-N6	5.71	122.03	118.60
1	2	1782	A	C8-N9-C4	-5.71	103.52	105.80
1	6	331	A	C8-N9-C4	5.71	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	378	A	N1-C2-N3	-5.71	126.45	129.30
36	5	1541	G	N9-C4-C5	-5.71	103.12	105.40
36	5	394	G	C4-C5-N7	-5.71	108.52	110.80
36	5	397	A	N9-C4-C5	5.71	108.08	105.80
36	5	2951	G	C8-N9-C1'	-5.71	119.58	127.00
37	7	83	U	C2-N1-C1'	-5.71	110.85	117.70
36	1	644	G	C5-C6-N1	-5.70	108.65	111.50
36	1	3344	A	C6-C5-N7	-5.70	128.31	132.30
36	5	3374	U	N3-C4-C5	5.70	118.02	114.60
36	1	1329	U	C2-N1-C1'	5.70	124.54	117.70
36	5	873	C	C4-C5-C6	5.70	120.25	117.40
36	1	388	G	C8-N9-C4	-5.70	104.12	106.40
36	1	2314	U	N1-C2-N3	-5.70	111.48	114.90
1	6	314	C	C6-N1-C2	-5.70	118.02	120.30
36	5	2757	U	N1-C2-O2	-5.70	118.81	122.80
36	1	2828	G	C4-N9-C1'	5.70	133.91	126.50
36	1	3242	G	C8-N9-C4	5.70	108.68	106.40
36	5	1897	G	C6-C5-N7	-5.70	126.98	130.40
36	1	191	U	OP2-P-O3'	5.70	117.73	105.20
36	1	228	U	C5-C6-N1	-5.70	119.85	122.70
36	1	1349	G	N3-C4-C5	-5.70	125.75	128.60
1	6	1539	G	O4'-C1'-N9	-5.70	103.64	108.20
36	5	2874	G	O5'-P-OP2	-5.70	100.57	105.70
36	1	2964	G	C4-C5-N7	-5.70	108.52	110.80
1	6	901	G	N1-C6-O6	5.70	123.32	119.90
36	5	859	G	N3-C4-N9	5.70	129.42	126.00
36	5	1473	G	C8-N9-C4	5.70	108.68	106.40
36	5	2830	G	N1-C2-N3	5.70	127.32	123.90
36	5	966	U	C2-N1-C1'	5.69	124.53	117.70
1	2	1658	G	N9-C4-C5	-5.69	103.12	105.40
36	1	1149	G	N3-C2-N2	-5.69	115.92	119.90
36	5	953	G	OP1-P-O3'	5.69	117.72	105.20
1	2	969	C	C6-N1-C2	5.69	122.58	120.30
36	1	988	U	C6-N1-C2	5.69	124.42	121.00
1	6	593	U	C6-N1-C2	-5.69	117.58	121.00
11	s9	149	ARG	NE-CZ-NH1	5.69	123.14	120.30
36	5	665	A	N1-C6-N6	5.69	122.01	118.60
36	5	2230	C	C6-N1-C2	5.69	122.58	120.30
36	5	2868	U	C2-N3-C4	5.69	130.41	127.00
36	5	2943	G	C4-N9-C1'	5.69	133.90	126.50
36	1	1932	A	N1-C6-N6	5.69	122.01	118.60
36	1	2325	G	N7-C8-N9	5.69	115.94	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1698	G	C5-C6-O6	5.69	132.01	128.60
59	N3	87	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	6	1572	G	C8-N9-C4	-5.69	104.12	106.40
36	5	2821	C	C2-N3-C4	-5.69	117.06	119.90
36	1	191	U	C6-N1-C2	-5.69	117.59	121.00
36	1	690	A	N9-C4-C5	5.69	108.08	105.80
36	1	2828	G	N3-C2-N2	5.68	123.88	119.90
37	3	14	U	C6-N1-C2	5.68	124.41	121.00
36	5	2806	U	C5-C6-N1	-5.68	119.86	122.70
38	8	64	U	N3-C2-O2	-5.68	118.22	122.20
36	1	1148	G	C8-N9-C4	5.68	108.67	106.40
36	1	2514	U	O5'-P-OP1	-5.68	100.59	105.70
36	1	2662	G	N3-C4-C5	5.68	131.44	128.60
36	1	2944	U	N3-C2-O2	-5.68	118.22	122.20
36	5	2231	C	O4'-C1'-N1	5.68	112.75	108.20
14	C2	103	LEU	CA-CB-CG	5.68	128.37	115.30
1	6	1568	C	C6-N1-C2	-5.68	118.03	120.30
36	5	3089	C	C5-C6-N1	5.68	123.84	121.00
1	2	968	U	C5-C6-N1	-5.68	119.86	122.70
36	1	1329	U	N3-C2-O2	-5.68	118.22	122.20
36	5	2915	U	N3-C2-O2	5.68	126.18	122.20
36	1	3177	G	N1-C6-O6	5.68	123.31	119.90
36	5	1360	C	N1-C2-O2	-5.68	115.49	118.90
1	2	1292	G	N1-C6-O6	-5.68	116.49	119.90
36	1	232	G	N3-C4-N9	5.68	129.41	126.00
36	1	945	C	C6-N1-C2	5.68	122.57	120.30
36	1	1001	G	C5-C6-O6	-5.68	125.19	128.60
36	1	2607	G	N3-C2-N2	5.68	123.87	119.90
38	4	103	G	N3-C4-N9	5.68	129.41	126.00
36	5	207	U	N3-C2-O2	5.68	126.17	122.20
36	5	1294	A	N1-C6-N6	-5.68	115.19	118.60
36	1	895	A	C2-N3-C4	-5.67	107.76	110.60
36	5	768	C	C6-N1-C2	-5.67	118.03	120.30
36	5	2105	G	N1-C6-O6	5.67	123.30	119.90
36	1	934	G	C4-N9-C1'	5.67	133.87	126.50
36	1	1335	C	C5-C6-N1	-5.67	118.16	121.00
1	6	1656	U	O5'-P-OP2	-5.67	100.60	105.70
36	5	1303	A	C8-N9-C4	5.67	108.07	105.80
36	1	2381	G	C4-C5-C6	5.67	122.20	118.80
1	6	144	U	C2-N1-C1'	5.67	124.50	117.70
36	5	961	C	C2-N1-C1'	5.67	125.04	118.80
36	5	1099	A	C5-N7-C8	-5.67	101.06	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2981	U	N3-C2-O2	-5.67	118.23	122.20
36	1	1206	G	C5-C6-N1	-5.67	108.67	111.50
36	5	2992	U	C5-C4-O4	-5.67	122.50	125.90
38	8	33	A	C8-N9-C4	5.67	108.07	105.80
52	m6	78	ARG	NE-CZ-NH2	-5.67	117.47	120.30
36	5	1079	A	C5-C6-N6	5.67	128.23	123.70
36	5	635	G	C4-C5-N7	5.67	113.07	110.80
40	l3	216	ASP	CB-CG-OD1	5.67	123.40	118.30
1	6	794	U	C2-N1-C1'	5.66	124.50	117.70
36	1	362	U	O5'-P-OP1	-5.66	100.60	105.70
36	1	790	U	N1-C2-O2	5.66	126.76	122.80
36	5	196	G	N9-C4-C5	-5.66	103.14	105.40
36	1	24	G	N1-C2-N3	5.66	127.30	123.90
36	1	1466	G	C8-N9-C1'	-5.66	119.64	127.00
36	1	2915	U	N3-C2-O2	5.66	126.16	122.20
1	6	104	A	O5'-P-OP2	-5.66	100.61	105.70
36	5	2388	U	C5-C4-O4	-5.66	122.50	125.90
36	5	2402	A	O4'-C1'-N9	5.66	112.73	108.20
36	5	2865	U	C2-N3-C4	5.66	130.40	127.00
36	1	670	C	N3-C4-C5	-5.66	119.64	121.90
36	1	1452	A	C8-N9-C4	5.66	108.06	105.80
36	5	2286	U	N1-C2-N3	5.66	118.30	114.90
36	5	2355	G	C4-C5-N7	5.66	113.06	110.80
36	5	2105	G	C5-C6-O6	-5.66	125.21	128.60
36	1	1346	G	N3-C2-N2	-5.66	115.94	119.90
36	1	1868	G	N3-C4-C5	-5.66	125.77	128.60
36	1	3143	C	N3-C2-O2	5.66	125.86	121.90
37	3	94	C	C6-N1-C2	5.66	122.56	120.30
1	6	1671	A	N1-C2-N3	5.66	132.13	129.30
36	5	922	U	N3-C4-C5	5.66	117.99	114.60
36	5	2632	G	O5'-P-OP1	-5.66	100.61	105.70
1	6	1614	A	N1-C6-N6	5.65	121.99	118.60
36	5	1476	G	N3-C4-N9	-5.65	122.61	126.00
36	5	2938	G	C4-C5-N7	-5.65	108.54	110.80
1	2	542	A	C4-N9-C1'	5.65	136.47	126.30
36	1	1520	G	C2-N3-C4	5.65	114.73	111.90
1	6	1730	A	C4-C5-C6	5.65	119.83	117.00
36	5	278	U	O5'-P-OP2	-5.65	100.61	105.70
36	5	1939	G	N3-C4-N9	5.65	129.39	126.00
36	5	3245	A	C4-C5-C6	5.65	119.83	117.00
36	1	2191	U	C5-C4-O4	5.65	129.29	125.90
1	6	1793	G	C5-C6-O6	5.65	131.99	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	639	G	C4-C5-C6	5.65	122.19	118.80
36	5	798	G	O5'-P-OP1	-5.65	100.61	105.70
36	5	2938	G	C6-C5-N7	5.65	133.79	130.40
36	5	3178	A	O5'-P-OP2	5.65	117.48	110.70
36	5	720	A	N1-C6-N6	5.65	121.99	118.60
36	5	1665	C	N1-C2-O2	5.65	122.29	118.90
36	1	1099	A	C6-C5-N7	-5.65	128.35	132.30
36	1	2815	G	C2-N3-C4	-5.65	109.08	111.90
36	5	2400	G	C4-C5-N7	5.65	113.06	110.80
36	5	3330	A	C6-N1-C2	-5.65	115.21	118.60
36	1	2148	U	C6-N1-C2	5.65	124.39	121.00
36	1	2284	C	C6-N1-C2	-5.64	118.04	120.30
36	1	2325	G	C5-C6-O6	-5.64	125.21	128.60
1	6	765	G	O4'-C1'-N9	-5.64	103.68	108.20
36	5	3042	U	N1-C2-O2	-5.64	118.85	122.80
36	5	3050	U	N1-C2-N3	5.64	118.29	114.90
36	1	619	A	C8-N9-C4	5.64	108.06	105.80
36	1	1330	A	N3-C4-C5	5.64	130.75	126.80
1	6	965	U	N1-C2-O2	5.64	126.75	122.80
36	5	2930	A	O4'-C1'-N9	5.64	112.71	108.20
36	5	3087	A	N1-C6-N6	-5.64	115.22	118.60
36	1	859	G	N9-C4-C5	-5.64	103.14	105.40
36	5	3150	A	C5-C6-N1	-5.64	114.88	117.70
1	2	1100	G	C4-C5-C6	5.64	122.18	118.80
36	5	644	G	N3-C4-C5	-5.64	125.78	128.60
36	5	2145	A	N7-C8-N9	5.64	116.62	113.80
36	5	3105	U	C6-N1-C1'	5.64	129.09	121.20
36	5	3119	U	O5'-P-OP2	-5.64	100.62	105.70
36	5	3330	A	N9-C4-C5	5.64	108.06	105.80
36	1	2836	C	N3-C2-O2	-5.64	117.95	121.90
36	1	2868	U	C2-N1-C1'	5.64	124.47	117.70
1	6	1	U	C6-N1-C1'	-5.64	113.31	121.20
36	5	684	G	O5'-P-OP2	-5.64	100.63	105.70
36	5	2917	G	C6-C5-N7	-5.64	127.02	130.40
1	2	1422	A	C8-N9-C4	5.64	108.06	105.80
36	5	403	C	C6-N1-C2	-5.64	118.05	120.30
36	5	662	U	N1-C2-N3	5.64	118.28	114.90
36	1	2325	G	C4-C5-N7	5.63	113.05	110.80
36	1	2976	A	C6-N1-C2	-5.63	115.22	118.60
36	5	1116	G	C8-N9-C4	-5.63	104.15	106.40
36	5	1135	A	C8-N9-C4	-5.63	103.55	105.80
36	5	2796	G	O5'-P-OP2	-5.63	100.63	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2824	G	N1-C6-O6	5.63	123.28	119.90
36	5	1126	G	N1-C6-O6	5.63	123.28	119.90
36	5	2931	C	C5-C4-N4	-5.63	116.26	120.20
36	1	653	A	O5'-P-OP2	-5.63	100.63	105.70
36	5	2833	A	C8-N9-C4	5.63	108.05	105.80
36	1	3116	G	N3-C4-C5	-5.63	125.78	128.60
36	1	929	A	OP1-P-O3'	5.63	117.58	105.20
36	1	2815	G	N1-C6-O6	5.63	123.28	119.90
1	6	372	G	N3-C4-N9	5.63	129.38	126.00
36	1	2796	G	N7-C8-N9	5.63	115.91	113.10
36	5	754	G	N1-C6-O6	-5.63	116.52	119.90
36	5	1323	G	C5-N7-C8	-5.63	101.49	104.30
36	5	1448	U	C5-C6-N1	-5.63	119.89	122.70
36	5	2370	G	N3-C2-N2	-5.63	115.96	119.90
36	5	2719	U	C2-N1-C1'	-5.63	110.95	117.70
36	5	361	A	C6-C5-N7	5.62	136.24	132.30
36	5	1307	G	C2'-C3'-O3'	5.62	122.70	113.70
36	1	63	A	C8-N9-C4	-5.62	103.55	105.80
36	1	398	A	C2-N3-C4	5.62	113.41	110.60
36	5	1851	G	N1-C6-O6	5.62	123.27	119.90
36	5	2125	A	C8-N9-C4	-5.62	103.55	105.80
1	2	1176	G	C6-C5-N7	-5.62	127.03	130.40
1	2	1314	U	O4'-C1'-N1	5.62	112.70	108.20
36	1	946	U	N3-C4-O4	5.62	123.33	119.40
36	5	341	G	N3-C4-C5	5.62	131.41	128.60
36	5	968	G	OP1-P-OP2	5.62	128.03	119.60
36	1	2946	A	N1-C6-N6	5.62	121.97	118.60
36	1	3055	U	C5-C4-O4	-5.62	122.53	125.90
1	6	194	U	N3-C2-O2	-5.62	118.27	122.20
1	6	29	U	C6-N1-C2	-5.62	117.63	121.00
36	5	1081	U	N3-C2-O2	5.62	126.13	122.20
36	5	1520	G	N3-C4-C5	-5.62	125.79	128.60
36	5	2988	C	C2-N3-C4	-5.62	117.09	119.90
36	1	1520	G	C5-N7-C8	5.62	107.11	104.30
36	1	2372	A	N1-C6-N6	5.62	121.97	118.60
36	1	2643	A	O5'-P-OP2	5.62	117.44	110.70
1	6	295	A	C8-N9-C4	5.62	108.05	105.80
1	6	433	C	C5-C4-N4	-5.62	116.27	120.20
36	5	582	G	N1-C6-O6	-5.62	116.53	119.90
36	1	2138	A	C6-C5-N7	-5.61	128.37	132.30
36	5	1495	U	C2-N1-C1'	5.61	124.44	117.70
36	5	1548	C	C6-N1-C2	-5.61	118.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2682	C	N1-C1'-C2'	-5.61	105.83	112.00
1	2	1339	C	P-O3'-C3'	5.61	126.43	119.70
36	1	390	G	N1-C6-O6	-5.61	116.53	119.90
1	6	424	C	C6-N1-C1'	-5.61	114.07	120.80
36	5	835	G	N3-C2-N2	5.61	123.83	119.90
36	5	1315	U	N3-C4-O4	5.61	123.33	119.40
36	1	2777	G	C8-N9-C4	-5.61	104.16	106.40
36	5	1170	A	C8-N9-C4	5.61	108.04	105.80
36	5	1302	A	O5'-P-OP2	5.61	117.43	110.70
36	5	2699	G	N9-C4-C5	-5.61	103.16	105.40
36	1	1488	G	N3-C2-N2	-5.61	115.97	119.90
36	1	2702	A	N9-C4-C5	5.61	108.04	105.80
36	1	2846	U	N1-C2-N3	5.61	118.26	114.90
1	6	21	U	N3-C4-O4	5.61	123.33	119.40
36	5	1881	A	N1-C6-N6	5.61	121.97	118.60
36	5	2887	A	OP2-P-O3'	5.61	117.53	105.20
36	1	860	G	N1-C6-O6	5.61	123.26	119.90
36	1	2233	A	N1-C6-N6	-5.61	115.24	118.60
36	1	2302	G	N3-C4-C5	-5.61	125.80	128.60
36	1	2986	U	C5-C6-N1	-5.61	119.90	122.70
36	1	3277	U	N1-C2-O2	5.61	126.72	122.80
1	6	337	G	N3-C2-N2	5.61	123.82	119.90
1	6	352	A	OP2-P-O3'	5.61	117.53	105.20
36	5	1101	G	N9-C4-C5	-5.61	103.16	105.40
36	5	1330	A	N1-C6-N6	5.61	121.96	118.60
36	5	1483	G	O4'-C1'-N9	5.61	112.68	108.20
36	1	1514	G	C4-C5-C6	5.60	122.16	118.80
36	1	1724	U	O5'-P-OP1	5.60	117.42	110.70
36	1	2607	G	N3-C4-N9	5.60	129.36	126.00
36	1	2808	A	N9-C4-C5	-5.60	103.56	105.80
1	2	144	U	N1-C2-N3	5.60	118.26	114.90
36	1	2814	G	O5'-P-OP1	-5.60	100.66	105.70
1	6	535	A	N1-C6-N6	5.60	121.96	118.60
1	6	992	A	C5-C6-N6	-5.60	119.22	123.70
1	6	1027	A	C2-N3-C4	-5.60	107.80	110.60
36	5	2201	G	C2-N3-C4	5.60	114.70	111.90
36	5	2738	A	O5'-P-OP2	-5.60	100.66	105.70
36	5	2927	C	OP2-P-O3'	5.60	117.53	105.20
1	2	608	U	N3-C2-O2	-5.60	118.28	122.20
36	1	694	C	O5'-P-OP2	-5.60	100.66	105.70
36	5	871	U	C5-C4-O4	5.60	129.26	125.90
36	5	1460	A	C8-N9-C4	-5.60	103.56	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2359	C	C2-N3-C4	-5.60	117.10	119.90
36	5	3050	U	N3-C2-O2	-5.60	118.28	122.20
36	5	3362	A	C2-N3-C4	-5.60	107.80	110.60
37	7	26	C	C4-C5-C6	5.60	120.20	117.40
36	1	1124	U	N3-C4-O4	-5.60	115.48	119.40
1	6	99	C	C6-N1-C2	-5.60	118.06	120.30
36	5	2954	U	N1-C2-O2	5.60	126.72	122.80
36	5	3078	U	C2-N1-C1'	5.60	124.42	117.70
36	1	651	G	C5-N7-C8	5.60	107.10	104.30
36	1	2383	C	N3-C4-C5	5.60	124.14	121.90
36	5	362	U	C5-C6-N1	5.60	125.50	122.70
36	5	649	A	O5'-P-OP2	-5.60	100.66	105.70
36	5	1379	G	C2-N3-C4	-5.60	109.10	111.90
36	5	2774	C	N3-C4-C5	-5.60	119.66	121.90
36	1	1367	G	N1-C6-O6	5.59	123.26	119.90
36	1	1885	U	C5-C6-N1	-5.59	119.90	122.70
36	1	2624	G	C8-N9-C4	-5.59	104.16	106.40
36	5	1391	C	N3-C4-C5	-5.59	119.66	121.90
36	1	49	A	N9-C4-C5	-5.59	103.56	105.80
36	1	1154	A	N1-C2-N3	5.59	132.10	129.30
36	1	1932	A	C5-C6-N6	-5.59	119.22	123.70
36	5	2376	G	N1-C2-N3	5.59	127.26	123.90
36	1	790	U	N3-C4-O4	-5.59	115.49	119.40
36	1	1150	A	C8-N9-C4	5.59	108.04	105.80
36	1	2112	U	P-O3'-C3'	5.59	126.41	119.70
36	1	2279	A	C8-N9-C4	5.59	108.04	105.80
36	1	2827	U	C2-N3-C4	-5.59	123.64	127.00
1	6	101	U	N1-C2-O2	5.59	126.71	122.80
36	5	1001	G	O5'-P-OP2	5.59	117.41	110.70
1	2	1176	G	N1-C6-O6	5.59	123.25	119.90
36	1	395	A	O5'-P-OP2	-5.59	100.67	105.70
36	1	1136	A	C6-N1-C2	-5.59	115.25	118.60
36	1	1168	U	C5-C4-O4	5.59	129.25	125.90
36	1	1713	G	C6-C5-N7	5.59	133.75	130.40
36	1	2550	U	N3-C2-O2	-5.59	118.29	122.20
36	5	41	G	N3-C4-C5	5.59	131.39	128.60
36	5	694	C	N1-C2-N3	5.59	123.11	119.20
36	5	3110	C	N3-C4-C5	5.59	124.14	121.90
36	5	3177	G	C8-N9-C4	5.59	108.64	106.40
38	4	21	C	C6-N1-C2	5.59	122.53	120.30
36	1	95	A	C8-N9-C4	5.59	108.03	105.80
36	1	2957	G	N9-C4-C5	5.59	107.64	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1338	C	N3-C4-N4	5.59	121.91	118.00
36	1	1332	A	OP2-P-O3'	5.58	117.49	105.20
1	6	1562	G	N1-C6-O6	5.58	123.25	119.90
1	6	1793	G	C4-N9-C1'	-5.58	119.24	126.50
36	5	3317	U	N3-C2-O2	-5.58	118.29	122.20
36	1	802	C	N1-C2-O2	-5.58	115.55	118.90
36	1	2278	C	N1-C2-O2	5.58	122.25	118.90
38	4	88	A	C4-C5-N7	5.58	113.49	110.70
1	6	571	G	C8-N9-C4	-5.58	104.17	106.40
36	5	507	U	N3-C4-O4	5.58	123.31	119.40
36	1	2356	A	C4-C5-N7	5.58	113.49	110.70
36	1	2826	U	C5-C4-O4	-5.58	122.55	125.90
1	6	1655	A	N1-C6-N6	5.58	121.95	118.60
36	5	2201	G	N3-C4-N9	5.58	129.35	126.00
1	6	425	A	OP2-P-O3'	5.58	117.48	105.20
36	1	2403	G	C6-C5-N7	-5.58	127.05	130.40
1	6	29	U	N3-C4-C5	-5.58	111.25	114.60
36	5	2329	C	O5'-P-OP2	-5.58	100.68	105.70
36	5	2336	U	N3-C2-O2	-5.58	118.30	122.20
36	5	3043	C	N3-C4-C5	5.58	124.13	121.90
36	1	577	C	N1-C2-O2	-5.58	115.55	118.90
36	1	1396	C	C6-N1-C2	5.58	122.53	120.30
1	2	1109	G	C8-N9-C4	-5.58	104.17	106.40
36	1	703	G	N3-C4-C5	5.58	131.39	128.60
36	1	1134	G	N3-C4-C5	-5.58	125.81	128.60
36	1	3039	C	C6-N1-C2	-5.58	118.07	120.30
36	5	2315	G	C5-C6-O6	5.58	131.94	128.60
36	5	2915	U	C6-N1-C2	5.58	124.34	121.00
54	m8	104	LEU	CA-CB-CG	5.58	128.12	115.30
36	5	859	G	N3-C4-C5	-5.57	125.81	128.60
36	5	2358	A	C2-N3-C4	-5.57	107.81	110.60
36	5	3140	G	C5-C6-O6	-5.57	125.26	128.60
36	5	799	G	C8-N9-C4	5.57	108.63	106.40
1	2	1258	U	C2-N1-C1'	5.57	124.39	117.70
36	1	1097	G	P-O3'-C3'	5.57	126.38	119.70
1	6	418	G	O5'-P-OP1	-5.57	100.69	105.70
36	5	1316	C	C5-C6-N1	5.57	123.78	121.00
78	q2	17	CYS	CA-CB-SG	5.57	124.03	114.00
36	5	2723	U	O5'-P-OP2	-5.57	100.69	105.70
36	1	1829	G	N9-C4-C5	5.57	107.63	105.40
36	1	3038	U	N3-C2-O2	5.57	126.10	122.20
36	5	1176	C	N1-C2-O2	-5.57	115.56	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1898	G	O4'-C1'-N9	5.57	112.65	108.20
1	2	15	U	C5-C6-N1	5.57	125.48	122.70
1	2	1174	C	N1-C2-O2	5.57	122.24	118.90
36	1	903	U	N3-C4-C5	-5.57	111.26	114.60
36	1	1842	A	N1-C6-N6	-5.57	115.26	118.60
36	5	2531	C	C2-N1-C1'	5.57	124.92	118.80
1	2	608	U	N1-C2-N3	5.56	118.24	114.90
37	3	48	U	C2-N1-C1'	5.56	124.38	117.70
36	5	1127	G	C8-N9-C4	-5.56	104.17	106.40
36	5	2327	U	C5-C6-N1	-5.56	119.92	122.70
36	5	2708	C	N3-C4-C5	5.56	124.12	121.90
36	1	2702	A	C5-C6-N6	5.56	128.15	123.70
1	6	65	A	C4-C5-N7	5.56	113.48	110.70
1	2	632	U	N3-C4-O4	-5.56	115.51	119.40
36	1	672	A	N1-C6-N6	5.56	121.94	118.60
36	1	808	A	C8-N9-C4	5.56	108.02	105.80
36	5	920	A	OP1-P-OP2	-5.56	111.26	119.60
36	5	2951	G	N3-C4-C5	-5.56	125.82	128.60
37	3	89	G	C8-N9-C4	5.56	108.62	106.40
1	6	144	U	N1-C2-O2	5.56	126.69	122.80
36	5	365	A	O5'-P-OP1	-5.56	100.70	105.70
36	5	1489	A	C4-C5-C6	5.56	119.78	117.00
36	5	3044	G	C8-N9-C4	-5.56	104.18	106.40
36	1	356	C	N1-C2-O2	-5.56	115.57	118.90
1	6	350	U	C5-C6-N1	-5.56	119.92	122.70
36	5	1316	C	N3-C2-O2	5.56	125.79	121.90
36	5	2205	U	C2-N1-C1'	5.56	124.37	117.70
1	2	380	U	N1-C2-O2	5.55	126.69	122.80
1	2	765	G	O4'-C1'-N9	-5.55	103.76	108.20
36	5	612	U	O5'-P-OP2	5.55	117.36	110.70
36	5	1040	A	N1-C6-N6	-5.55	115.27	118.60
36	5	1665	C	N3-C2-O2	-5.55	118.01	121.90
36	5	2404	A	N1-C6-N6	5.55	121.93	118.60
36	5	3317	U	P-O3'-C3'	5.55	126.37	119.70
36	5	1012	G	C8-N9-C1'	5.55	134.22	127.00
37	3	89	G	N3-C4-N9	5.55	129.33	126.00
1	6	1152	A	C5-C6-N6	-5.55	119.26	123.70
36	5	207	U	C5-C4-O4	-5.55	122.57	125.90
36	5	1126	G	C4-C5-C6	5.55	122.13	118.80
36	5	2866	U	C6-N1-C2	-5.55	117.67	121.00
36	1	285	A	N1-C2-N3	5.55	132.07	129.30
36	1	941	G	C8-N9-C4	-5.55	104.18	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2964	G	O4'-C1'-N9	5.55	112.64	108.20
1	6	1745	G	C8-N9-C4	5.55	108.62	106.40
36	5	358	G	N1-C6-O6	5.55	123.23	119.90
36	5	2659	G	C5-C6-O6	-5.55	125.27	128.60
54	m8	166	LEU	CB-CG-CD1	-5.55	101.56	111.00
36	1	1339	C	C2-N3-C4	-5.55	117.13	119.90
36	1	1369	A	C8-N9-C4	-5.55	103.58	105.80
36	1	2808	A	O4'-C1'-N9	-5.55	103.76	108.20
36	1	942	U	N3-C4-C5	-5.55	111.27	114.60
36	1	1906	G	C6-C5-N7	-5.55	127.07	130.40
36	5	2295	A	N9-C4-C5	5.55	108.02	105.80
36	1	641	C	C5-C6-N1	5.54	123.77	121.00
36	1	1506	A	N9-C4-C5	5.54	108.02	105.80
36	1	517	G	C5-C6-O6	5.54	131.93	128.60
36	1	837	A	N1-C6-N6	5.54	121.93	118.60
1	6	402	C	C5-C6-N1	-5.54	118.23	121.00
36	5	2112	U	P-O3'-C3'	5.54	126.35	119.70
36	1	611	A	C4-C5-N7	5.54	113.47	110.70
36	1	937	G	N9-C4-C5	-5.54	103.18	105.40
36	1	945	C	N3-C4-C5	5.54	124.12	121.90
36	1	1129	A	N1-C6-N6	5.54	121.92	118.60
36	1	1330	A	C8-N9-C4	5.54	108.02	105.80
36	1	1351	U	N3-C2-O2	-5.54	118.32	122.20
36	1	1450	G	N9-C4-C5	-5.54	103.18	105.40
36	1	2823	G	C4-C5-N7	-5.54	108.58	110.80
36	5	869	G	N3-C2-N2	5.54	123.78	119.90
36	5	1939	G	C6-C5-N7	-5.54	127.08	130.40
36	1	1200	A	N7-C8-N9	-5.54	111.03	113.80
36	5	429	U	C5-C6-N1	-5.54	119.93	122.70
36	1	3242	G	O4'-C1'-N9	-5.54	103.77	108.20
1	6	813	U	C6-N1-C1'	-5.54	113.45	121.20
36	5	2845	A	N7-C8-N9	5.54	116.57	113.80
1	2	48	G	OP2-P-O3'	5.54	117.38	105.20
36	1	716	A	C5-C6-N6	-5.54	119.27	123.70
36	1	959	C	C2-N3-C4	-5.54	117.13	119.90
1	6	555	A	C8-N9-C4	-5.54	103.59	105.80
36	5	1403	C	C5-C4-N4	-5.54	116.33	120.20
1	2	16	G	N3-C4-C5	-5.53	125.83	128.60
36	1	830	A	C8-N9-C4	-5.53	103.59	105.80
36	1	3208	G	C8-N9-C4	5.53	108.61	106.40
36	1	984	G	C6-N1-C2	-5.53	121.78	125.10
36	5	3032	A	C8-N9-C4	-5.53	103.59	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2901	G	C6-C5-N7	-5.53	127.08	130.40
36	5	1101	G	C4-N9-C1'	5.53	133.69	126.50
36	5	514	G	C4-C5-N7	5.53	113.01	110.80
36	5	634	C	OP2-P-O3'	5.53	117.36	105.20
36	1	91	G	N9-C4-C5	-5.53	103.19	105.40
36	1	1157	G	OP2-P-O3'	5.53	117.36	105.20
36	1	2748	A	C2-N3-C4	-5.53	107.84	110.60
1	6	1389	C	N3-C2-O2	-5.53	118.03	121.90
36	5	523	A	O5'-P-OP2	-5.53	100.73	105.70
36	5	3176	G	C4-C5-N7	-5.53	108.59	110.80
36	1	195	U	N3-C2-O2	-5.53	118.33	122.20
36	1	269	G	N3-C4-N9	-5.53	122.69	126.00
1	6	647	G	N3-C4-N9	-5.53	122.68	126.00
1	6	1337	A	C8-N9-C4	5.53	108.01	105.80
36	5	817	A	C6-C5-N7	-5.53	128.43	132.30
36	5	967	A	N9-C4-C5	5.53	108.01	105.80
36	5	2248	C	OP1-P-O3'	5.53	117.36	105.20
36	5	3215	A	C2-N3-C4	-5.53	107.84	110.60
36	5	1131	G	C5-C6-N1	-5.52	108.74	111.50
36	5	1428	A	N1-C6-N6	-5.52	115.29	118.60
36	1	829	U	C2-N1-C1'	5.52	124.33	117.70
36	1	1331	U	N3-C2-O2	-5.52	118.33	122.20
36	1	2273	G	N3-C4-C5	5.52	131.36	128.60
36	5	1190	A	C8-N9-C4	-5.52	103.59	105.80
36	5	1319	G	N3-C4-C5	-5.52	125.84	128.60
36	1	1115	G	OP1-P-O3'	5.52	117.34	105.20
12	c0	88	PRO	N-CA-CB	5.52	109.92	103.30
36	1	901	G	C8-N9-C4	5.52	108.61	106.40
36	1	947	G	C5-C6-N1	-5.52	108.74	111.50
36	1	48	A	O4'-C1'-N9	5.52	112.61	108.20
36	1	220	G	C5-N7-C8	-5.52	101.54	104.30
36	1	1124	U	C4-C5-C6	-5.52	116.39	119.70
36	1	1190	A	C4-C5-C6	5.52	119.76	117.00
36	1	1796	G	N3-C4-C5	-5.52	125.84	128.60
36	1	2805	G	N9-C4-C5	-5.52	103.19	105.40
36	5	75	G	C5-C6-O6	-5.52	125.29	128.60
36	5	784	A	N9-C4-C5	-5.52	103.59	105.80
36	5	1534	A	N3-C4-C5	-5.52	122.94	126.80
36	1	1389	G	C6-C5-N7	-5.52	127.09	130.40
1	6	426	G	C4-N9-C1'	5.52	133.67	126.50
1	6	639	U	N3-C2-O2	-5.52	118.34	122.20
1	2	88	U	N3-C2-O2	-5.51	118.34	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	641	C	C4-C5-C6	-5.51	114.64	117.40
36	1	1399	A	O5'-P-OP1	5.51	117.32	110.70
36	1	2555	G	N3-C4-N9	-5.51	122.69	126.00
1	6	1097	U	P-O3'-C3'	5.51	126.32	119.70
36	5	959	C	N3-C4-C5	-5.51	119.69	121.90
36	5	1900	A	C4-C5-N7	5.51	113.46	110.70
36	5	2245	C	N3-C2-O2	-5.51	118.04	121.90
1	6	338	C	C5-C6-N1	5.51	123.76	121.00
36	5	1208	U	N3-C2-O2	-5.51	118.34	122.20
36	5	2531	C	N1-C2-O2	5.51	122.21	118.90
1	2	1560	U	C5-C4-O4	5.51	129.21	125.90
36	1	2371	G	OP1-P-O3'	5.51	117.32	105.20
36	1	2430	A	C8-N9-C4	-5.51	103.60	105.80
1	6	1614	A	N1-C2-N3	5.51	132.06	129.30
36	5	1193	A	N1-C6-N6	5.51	121.91	118.60
36	5	1398	U	C5-C4-O4	5.51	129.21	125.90
36	5	2874	G	C5-C6-N1	-5.51	108.74	111.50
28	d6	10	ARG	NE-CZ-NH1	-5.51	117.55	120.30
36	5	3309	G	C4-N9-C1'	5.51	133.66	126.50
1	2	734	A	OP1-P-O3'	5.51	117.32	105.20
36	5	868	C	C6-N1-C2	5.51	122.50	120.30
36	5	1390	A	C5-C6-N6	5.51	128.11	123.70
1	2	15	U	C2-N1-C1'	5.51	124.31	117.70
1	2	349	U	C5-C6-N1	-5.51	119.95	122.70
36	1	2278	C	N3-C4-N4	-5.51	114.14	118.00
36	5	40	A	O5'-P-OP1	-5.51	100.74	105.70
36	5	1101	G	N1-C2-N2	-5.51	111.24	116.20
36	1	2858	U	OP2-P-O3'	5.50	117.31	105.20
3	s1	47	LEU	CA-CB-CG	5.50	127.96	115.30
36	5	2914	G	N3-C4-N9	5.50	129.30	126.00
36	1	432	G	N9-C4-C5	-5.50	103.20	105.40
36	1	859	G	N3-C4-N9	5.50	129.30	126.00
36	1	1164	G	C4-N9-C1'	5.50	133.65	126.50
36	1	1346	G	O5'-P-OP2	-5.50	100.75	105.70
36	5	1012	G	C8-N9-C4	5.50	108.60	106.40
36	5	1064	A	N1-C6-N6	5.50	121.90	118.60
36	5	2634	U	N1-C2-N3	5.50	118.20	114.90
1	2	934	C	C6-N1-C1'	-5.50	114.20	120.80
36	1	919	U	N3-C4-C5	5.50	117.90	114.60
36	1	1175	C	C5-C6-N1	-5.50	118.25	121.00
36	5	2887	A	C4-C5-C6	5.50	119.75	117.00
36	5	3000	A	C8-N9-C4	5.50	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3131	U	N3-C4-O4	-5.50	115.55	119.40
1	2	1412	G	C8-N9-C1'	5.50	134.15	127.00
36	1	289	A	C5-C6-N6	-5.50	119.30	123.70
36	1	804	C	C2-N3-C4	-5.50	117.15	119.90
36	1	968	G	C6-N1-C2	-5.50	121.80	125.10
36	1	2121	G	N1-C2-N2	-5.50	111.25	116.20
36	1	2513	U	OP1-P-O3'	5.50	117.30	105.20
36	1	3214	U	C2-N1-C1'	5.50	124.30	117.70
1	6	119	A	N3-C4-C5	5.50	130.65	126.80
1	6	424	C	C2-N1-C1'	5.50	124.85	118.80
36	5	648	C	O5'-P-OP1	-5.50	100.75	105.70
36	5	2334	U	N1-C2-N3	5.50	118.20	114.90
36	5	2683	U	N1-C2-O2	5.50	126.65	122.80
36	1	25	U	N1-C2-O2	-5.50	118.95	122.80
36	1	919	U	N1-C2-O2	5.50	126.65	122.80
36	1	1303	A	N9-C4-C5	-5.50	103.60	105.80
36	1	2153	U	C6-N1-C2	-5.50	117.70	121.00
1	6	1100	G	N3-C4-C5	-5.50	125.85	128.60
1	6	1355	C	C6-N1-C2	-5.50	118.10	120.30
36	5	669	U	N3-C2-O2	-5.50	118.35	122.20
36	5	981	U	C6-N1-C2	-5.50	117.70	121.00
36	5	3203	U	O5'-P-OP1	-5.50	100.75	105.70
36	5	3339	A	N9-C4-C5	-5.50	103.60	105.80
36	1	340	C	C2-N1-C1'	5.50	124.84	118.80
36	1	947	G	C6-C5-N7	-5.50	127.10	130.40
36	1	2733	A	O5'-P-OP1	5.50	117.29	110.70
1	6	609	U	C5-C6-N1	-5.50	119.95	122.70
1	2	421	A	N9-C4-C5	-5.49	103.60	105.80
36	1	796	U	N1-C2-O2	-5.49	118.95	122.80
36	1	1428	A	C2-N3-C4	-5.49	107.85	110.60
36	5	1450	G	C5-N7-C8	-5.49	101.55	104.30
36	5	2295	A	C6-N1-C2	-5.49	115.30	118.60
1	6	1117	U	C6-N1-C2	-5.49	117.70	121.00
1	6	1306	C	C5-C6-N1	5.49	123.75	121.00
36	5	1931	U	N3-C4-O4	-5.49	115.56	119.40
1	6	523	G	C8-N9-C4	5.49	108.60	106.40
1	6	1100	G	N3-C4-N9	5.49	129.29	126.00
36	5	2199	G	C8-N9-C1'	-5.49	119.86	127.00
1	2	1202	A	C8-N9-C4	-5.49	103.61	105.80
36	1	704	U	O5'-P-OP2	-5.49	100.76	105.70
36	1	2336	U	C6-N1-C2	5.49	124.29	121.00
36	5	2374	C	N1-C2-O2	-5.49	115.61	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	41	G	C8-N9-C1'	-5.49	119.87	127.00
36	1	2391	G	C4-C5-N7	-5.49	108.61	110.80
36	1	2901	G	N1-C6-O6	5.49	123.19	119.90
1	6	1025	A	C8-N9-C4	5.49	108.00	105.80
1	6	1025	A	N9-C4-C5	-5.49	103.61	105.80
1	2	1033	C	N3-C2-O2	-5.49	118.06	121.90
38	4	82	U	N1-C2-O2	-5.49	118.96	122.80
1	6	337	G	C4-C5-C6	5.49	122.09	118.80
36	5	2372	A	C4-C5-C6	5.49	119.74	117.00
1	2	942	G	C8-N9-C4	-5.48	104.21	106.40
36	1	939	U	N3-C2-O2	5.48	126.04	122.20
1	6	536	C	C5-C6-N1	5.48	123.74	121.00
1	6	1456	C	C4-C5-C6	5.48	120.14	117.40
1	2	378	A	N1-C6-N6	5.48	121.89	118.60
36	1	2402	A	O5'-P-OP2	-5.48	100.77	105.70
56	N0	167	ARG	N-CA-C	-5.48	96.20	111.00
36	5	170	G	C4-N9-C1'	5.48	133.62	126.50
36	5	2246	G	O5'-P-OP1	-5.48	100.77	105.70
36	5	2800	G	N3-C4-N9	-5.48	122.71	126.00
1	2	720	G	P-O3'-C3'	5.48	126.28	119.70
36	1	2812	C	OP1-P-O3'	5.48	117.25	105.20
1	6	1680	G	C5-C6-N1	5.48	114.24	111.50
36	1	2552	C	O4'-C1'-N1	5.48	112.58	108.20
36	1	2639	G	N1-C6-O6	5.48	123.19	119.90
36	5	1881	A	C5-C6-N6	-5.48	119.32	123.70
1	6	163	G	C5-N7-C8	-5.48	101.56	104.30
36	5	1124	U	N3-C4-O4	-5.48	115.57	119.40
36	5	2290	C	C5-C6-N1	-5.48	118.26	121.00
36	1	1514	G	N3-C4-N9	5.47	129.28	126.00
36	1	3024	A	O5'-P-OP1	-5.47	100.77	105.70
1	6	163	G	N9-C4-C5	5.47	107.59	105.40
1	6	1412	G	C4-N9-C1'	-5.47	119.38	126.50
36	5	518	G	C5-C6-O6	-5.47	125.31	128.60
36	5	1294	A	O4'-C1'-N9	5.47	112.58	108.20
1	2	145	A	C8-N9-C4	-5.47	103.61	105.80
36	1	967	A	N1-C2-N3	5.47	132.04	129.30
36	1	1389	G	N3-C2-N2	5.47	123.73	119.90
36	1	2836	C	C4-C5-C6	5.47	120.14	117.40
36	1	3266	G	N3-C2-N2	-5.47	116.07	119.90
1	6	639	U	N1-C2-O2	5.47	126.63	122.80
1	6	1162	C	C6-N1-C2	-5.47	118.11	120.30
36	5	1468	A	C4-C5-N7	5.47	113.44	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1528	G	N3-C4-C5	-5.47	125.86	128.60
36	5	2875	U	N1-C2-N3	-5.47	111.62	114.90
36	5	2877	G	N3-C2-N2	5.47	123.73	119.90
36	5	2962	U	N1-C2-O2	-5.47	118.97	122.80
36	5	3140	G	N1-C6-O6	5.47	123.18	119.90
36	1	63	A	N9-C4-C5	5.47	107.99	105.80
36	1	1425	U	C5-C4-O4	5.47	129.18	125.90
36	1	2937	G	C8-N9-C4	5.47	108.59	106.40
36	1	2948	C	N3-C4-C5	5.47	124.09	121.90
1	6	354	C	C5-C6-N1	5.47	123.73	121.00
36	1	2369	G	N3-C4-N9	5.47	129.28	126.00
37	3	8	G	C4-C5-N7	-5.47	108.61	110.80
1	6	1085	G	C5-C6-O6	5.47	131.88	128.60
1	6	1776	A	N1-C6-N6	5.47	121.88	118.60
36	5	585	A	C2-N3-C4	-5.47	107.87	110.60
36	5	980	A	N1-C6-N6	-5.47	115.32	118.60
37	7	88	G	N1-C6-O6	-5.47	116.62	119.90
38	8	87	G	N3-C4-N9	5.47	129.28	126.00
1	2	1137	A	C8-N9-C4	5.47	107.99	105.80
36	1	72	C	C2-N1-C1'	-5.47	112.79	118.80
36	1	994	G	N1-C6-O6	-5.47	116.62	119.90
36	1	2516	U	N1-C2-N3	5.47	118.18	114.90
1	6	1346	A	O4'-C1'-N9	5.47	112.57	108.20
36	5	2719	U	C5-C6-N1	-5.47	119.97	122.70
1	2	608	U	N3-C4-O4	-5.46	115.57	119.40
1	2	1026	A	O5'-P-OP1	-5.46	100.78	105.70
36	1	107	A	C4-C5-N7	5.46	113.43	110.70
36	1	335	G	N1-C6-O6	5.46	123.18	119.90
36	1	2145	A	C8-N9-C4	-5.46	103.61	105.80
1	6	318	U	O5'-P-OP2	-5.46	100.78	105.70
1	6	1361	U	N1-C2-O2	5.46	126.63	122.80
36	1	279	U	OP1-P-O3'	5.46	117.22	105.20
1	6	1640	C	C6-N1-C1'	-5.46	114.24	120.80
36	5	3372	A	C8-N9-C4	-5.46	103.61	105.80
36	1	701	G	N1-C6-O6	5.46	123.18	119.90
1	6	1697	G	N3-C4-N9	5.46	129.28	126.00
36	5	106	A	C8-N9-C4	5.46	107.98	105.80
36	5	665	A	C5-C6-N6	-5.46	119.33	123.70
36	5	969	C	OP1-P-O3'	5.46	117.21	105.20
36	5	2552	C	C2-N1-C1'	5.46	124.81	118.80
36	1	329	U	C6-N1-C2	-5.46	117.72	121.00
36	1	659	G	OP2-P-O3'	5.46	117.21	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	121	A	C8-N9-C4	5.46	107.98	105.80
36	5	906	A	N9-C4-C5	5.46	107.98	105.80
36	5	2376	G	C5-C6-O6	-5.46	125.32	128.60
36	1	2642	A	C6-N1-C2	5.46	121.88	118.60
36	1	2984	C	C5-C4-N4	5.46	124.02	120.20
36	5	994	G	OP1-P-O3'	5.46	117.21	105.20
1	2	89	G	N3-C4-C5	5.46	131.33	128.60
1	2	794	U	N3-C2-O2	-5.46	118.38	122.20
1	6	687	G	N3-C4-N9	-5.46	122.73	126.00
1	6	1698	G	N1-C6-O6	-5.46	116.63	119.90
36	5	677	A	C8-N9-C4	-5.46	103.62	105.80
36	1	642	U	C6-N1-C2	-5.46	117.73	121.00
36	1	2636	A	C5-N7-C8	-5.46	101.17	103.90
36	1	2175	U	C5-C4-O4	5.45	129.17	125.90
1	6	1562	G	C5-C6-O6	-5.45	125.33	128.60
36	5	969	C	C2-N3-C4	-5.45	117.17	119.90
36	1	619	A	N9-C4-C5	-5.45	103.62	105.80
36	1	1351	U	N1-C2-O2	5.45	126.61	122.80
36	5	1138	U	C5-C4-O4	-5.45	122.63	125.90
36	5	1301	A	N9-C4-C5	-5.45	103.62	105.80
1	2	1280	C	C6-N1-C2	-5.45	118.12	120.30
36	1	200	C	N1-C2-O2	5.45	122.17	118.90
36	1	642	U	N1-C2-N3	5.45	118.17	114.90
36	1	925	A	N7-C8-N9	5.45	116.52	113.80
36	1	1586	G	N3-C4-C5	-5.45	125.88	128.60
36	1	2616	C	O5'-P-OP1	-5.45	100.80	105.70
1	6	65	A	C6-C5-N7	-5.45	128.49	132.30
36	5	652	G	N3-C4-C5	-5.45	125.88	128.60
38	8	20	U	N1-C2-N3	5.45	118.17	114.90
36	1	433	A	C5-C6-N6	-5.45	119.34	123.70
36	5	105	C	C6-N1-C2	5.45	122.48	120.30
36	5	3143	C	C6-N1-C2	-5.45	118.12	120.30
1	2	312	A	C8-N9-C4	-5.45	103.62	105.80
36	1	651	G	N3-C4-N9	5.45	129.27	126.00
36	1	2871	G	C5-N7-C8	-5.45	101.58	104.30
1	6	613	G	N3-C4-C5	-5.45	125.88	128.60
1	2	1324	G	N1-C2-N2	5.44	121.10	116.20
1	6	1698	G	P-O3'-C3'	5.44	126.23	119.70
36	5	283	G	C8-N9-C1'	-5.44	119.92	127.00
36	5	1003	A	C2-N3-C4	-5.44	107.88	110.60
36	5	2273	G	C8-N9-C1'	5.44	134.08	127.00
36	5	2643	A	C5-C6-N6	-5.44	119.34	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	99	G	N1-C2-N2	-5.44	111.30	116.20
36	1	701	G	C4-C5-C6	5.44	122.06	118.80
36	1	1201	C	N3-C4-C5	-5.44	119.72	121.90
38	4	47	C	C5-C6-N1	-5.44	118.28	121.00
36	5	510	G	C5-C6-O6	5.44	131.87	128.60
36	5	1155	C	C2-N1-C1'	5.44	124.79	118.80
36	5	1657	C	N1-C2-O2	5.44	122.17	118.90
1	2	992	A	N3-C4-C5	5.44	130.61	126.80
36	1	353	G	C5-C6-O6	-5.44	125.34	128.60
36	1	873	C	C2-N1-C1'	-5.44	112.82	118.80
36	1	2325	G	N1-C6-O6	5.44	123.17	119.90
1	6	1648	A	C8-N9-C4	5.44	107.98	105.80
36	5	1463	U	N1-C2-O2	-5.44	118.99	122.80
36	5	2249	G	N3-C4-C5	-5.44	125.88	128.60
36	5	2633	U	C5-C6-N1	-5.44	119.98	122.70
36	5	3180	A	N1-C2-N3	5.44	132.02	129.30
36	1	2406	C	OP1-P-OP2	5.44	127.76	119.60
37	3	101	G	N9-C4-C5	-5.44	103.22	105.40
1	6	1573	A	P-O3'-C3'	5.44	126.23	119.70
36	1	2181	C	N3-C4-C5	5.44	124.08	121.90
36	1	2775	U	N1-C2-N3	5.44	118.16	114.90
36	1	3002	C	N3-C4-C5	5.44	124.08	121.90
36	5	3045	G	N1-C6-O6	5.44	123.16	119.90
36	1	55	G	N9-C4-C5	-5.44	103.23	105.40
36	1	2815	G	C4-C5-N7	5.44	112.97	110.80
36	1	3103	A	C2-N3-C4	-5.44	107.88	110.60
37	3	15	C	C6-N1-C2	5.44	122.47	120.30
36	5	2376	G	C4-C5-N7	5.44	112.97	110.80
36	5	2867	C	N1-C2-O2	-5.44	115.64	118.90
36	1	188	U	N3-C4-C5	-5.43	111.34	114.60
36	1	1434	G	C6-C5-N7	-5.43	127.14	130.40
36	1	2409	G	C8-N9-C4	-5.43	104.23	106.40
1	6	1514	U	N3-C4-O4	-5.43	115.60	119.40
36	5	1072	G	O5'-P-OP2	-5.43	100.81	105.70
36	5	2306	C	OP2-P-O3'	5.43	117.16	105.20
36	5	2419	A	C5-N7-C8	-5.43	101.18	103.90
36	5	2421	U	C4-C5-C6	5.43	122.96	119.70
36	5	3150	A	C2-N3-C4	-5.43	107.88	110.60
36	5	3218	A	P-O3'-C3'	5.43	126.22	119.70
36	5	3240	C	N1-C2-O2	5.43	122.16	118.90
1	2	830	U	N1-C2-O2	5.43	126.60	122.80
36	1	661	G	C5-C6-O6	5.43	131.86	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1206	G	N9-C4-C5	5.43	107.57	105.40
36	1	1795	U	N3-C4-C5	5.43	117.86	114.60
1	6	308	C	C5-C6-N1	-5.43	118.28	121.00
36	5	1370	G	N3-C2-N2	5.43	123.70	119.90
36	5	3011	A	N1-C6-N6	-5.43	115.34	118.60
1	2	21	U	C5-C6-N1	5.43	125.42	122.70
36	1	1151	U	N1-C2-N3	5.43	118.16	114.90
36	1	2679	A	N1-C2-N3	5.43	132.01	129.30
36	1	2944	U	N1-C2-O2	5.43	126.60	122.80
36	5	1117	G	N9-C4-C5	-5.43	103.23	105.40
36	1	933	A	C4-C5-C6	5.43	119.72	117.00
36	1	2808	A	C8-N9-C1'	-5.43	117.93	127.70
36	5	2928	C	C5-C6-N1	5.43	123.71	121.00
38	8	55	U	C6-N1-C2	-5.43	117.74	121.00
36	1	718	G	N3-C4-C5	5.43	131.31	128.60
36	1	2643	A	N9-C4-C5	-5.43	103.63	105.80
1	2	543	C	C6-N1-C2	-5.43	118.13	120.30
36	1	682	U	N3-C2-O2	-5.43	118.40	122.20
36	1	1344	G	OP2-P-O3'	5.43	117.14	105.20
36	1	1447	G	C5-C6-O6	5.43	131.86	128.60
36	1	2381	G	C8-N9-C1'	-5.43	119.95	127.00
36	5	2211	U	C4-C5-C6	5.43	122.96	119.70
36	5	2704	A	OP2-P-O3'	5.43	117.14	105.20
36	5	2899	C	N3-C4-N4	5.43	121.80	118.00
36	5	3362	A	N1-C2-N3	5.43	132.01	129.30
36	1	2101	C	P-O3'-C3'	5.42	126.21	119.70
36	1	3265	C	N3-C4-C5	5.42	124.07	121.90
38	4	113	U	C5-C6-N1	-5.42	119.99	122.70
36	5	1043	C	O5'-P-OP1	5.42	117.21	110.70
36	5	1119	C	C2-N3-C4	-5.42	117.19	119.90
36	5	2372	A	N3-C4-C5	-5.42	123.00	126.80
36	5	2891	U	N3-C4-O4	-5.42	115.60	119.40
37	7	74	C	N3-C2-O2	5.42	125.70	121.90
36	5	1178	G	C5-N7-C8	-5.42	101.59	104.30
36	1	1154	A	N3-C4-C5	-5.42	123.01	126.80
36	1	1307	G	C2'-C3'-O3'	5.42	122.38	113.70
36	1	2186	U	C5-C4-O4	5.42	129.15	125.90
69	O3	73	ARG	NE-CZ-NH1	-5.42	117.59	120.30
36	5	2987	A	C6-N1-C2	5.42	121.85	118.60
36	5	3154	C	C5-C6-N1	5.42	123.71	121.00
36	1	1868	G	C8-N9-C4	-5.42	104.23	106.40
36	1	346	C	N3-C2-O2	5.42	125.69	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	809	G	N1-C6-O6	5.42	123.15	119.90
36	1	2551	U	C2-N1-C1'	5.42	124.20	117.70
36	1	2984	C	N1-C2-N3	5.42	122.99	119.20
36	1	3221	C	O5'-P-OP1	-5.42	100.82	105.70
36	5	3018	C	O5'-P-OP2	-5.42	100.82	105.70
36	1	107	A	C5-C6-N6	-5.42	119.37	123.70
36	1	2952	G	C5-C6-O6	-5.42	125.35	128.60
38	4	7	U	N1-C2-N3	5.42	118.15	114.90
1	6	35	U	N1-C2-N3	5.42	118.15	114.90
1	6	552	G	C5-C6-O6	-5.42	125.35	128.60
1	6	1643	U	N1-C2-N3	5.42	118.15	114.90
37	7	1	G	C4-N9-C1'	5.42	133.54	126.50
36	1	2886	U	N3-C2-O2	5.41	125.99	122.20
38	4	3	A	C2-N3-C4	5.41	113.31	110.60
36	5	112	U	C2-N1-C1'	5.41	124.20	117.70
36	5	1149	G	C2-N3-C4	5.41	114.61	111.90
36	5	1839	A	O5'-P-OP1	-5.41	100.83	105.70
37	7	76	A	N1-C6-N6	-5.41	115.35	118.60
1	2	393	C	C6-N1-C2	5.41	122.47	120.30
36	1	2846	U	C6-N1-C2	-5.41	117.75	121.00
36	5	2195	C	C5-C4-N4	-5.41	116.41	120.20
36	5	2794	G	C5-C6-N1	5.41	114.21	111.50
36	1	3276	G	N3-C4-C5	5.41	131.31	128.60
1	6	1129	U	C5-C4-O4	5.41	129.15	125.90
1	6	1791	A	N1-C6-N6	5.41	121.85	118.60
36	5	644	G	C4-N9-C1'	5.41	133.53	126.50
36	5	3153	U	N3-C2-O2	-5.41	118.41	122.20
37	7	92	A	C5-C6-N6	-5.41	119.37	123.70
37	7	110	G	N3-C4-C5	5.41	131.31	128.60
36	1	669	U	C5-C6-N1	-5.41	120.00	122.70
36	1	2361	A	N1-C2-N3	5.41	132.00	129.30
1	6	584	C	C6-N1-C2	-5.41	118.14	120.30
36	5	837	A	C8-N9-C4	-5.41	103.64	105.80
1	2	1081	A	C6-C5-N7	5.41	136.08	132.30
36	1	1331	U	C2-N1-C1'	5.41	124.19	117.70
36	1	2572	C	C6-N1-C2	-5.41	118.14	120.30
36	1	2618	G	O5'-P-OP2	-5.41	100.83	105.70
36	5	2121	G	O5'-P-OP2	-5.41	100.83	105.70
36	1	1320	C	C4-C5-C6	5.40	120.10	117.40
36	5	2851	A	N9-C4-C5	5.40	107.96	105.80
36	5	2992	U	N3-C4-O4	5.40	123.18	119.40
1	2	973	A	O5'-P-OP1	5.40	117.18	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	573	C	N3-C4-C5	5.40	124.06	121.90
36	5	1884	A	O5'-P-OP2	-5.40	100.84	105.70
36	1	282	G	P-O3'-C3'	5.40	126.18	119.70
36	1	2550	U	N1-C2-N3	5.40	118.14	114.90
36	1	2887	A	C5-C6-N6	-5.40	119.38	123.70
1	6	1634	C	C6-N1-C1'	-5.40	114.32	120.80
36	5	2857	C	OP2-P-O3'	5.40	117.08	105.20
36	1	428	A	N1-C6-N6	-5.40	115.36	118.60
36	1	2939	G	C4-C5-N7	-5.40	108.64	110.80
1	6	1000	C	O4'-C1'-N1	5.40	112.52	108.20
36	5	3218	A	C6-C5-N7	-5.40	128.52	132.30
36	1	53	G	N1-C6-O6	-5.40	116.66	119.90
36	1	2644	C	C4-C5-C6	5.40	120.10	117.40
36	5	403	C	N3-C4-N4	5.40	121.78	118.00
1	2	1675	C	C5-C6-N1	-5.39	118.30	121.00
36	1	634	C	C6-N1-C2	5.39	122.46	120.30
36	1	2382	G	N3-C2-N2	5.39	123.68	119.90
36	1	2398	A	N7-C8-N9	-5.39	111.10	113.80
36	5	816	A	N1-C6-N6	-5.39	115.36	118.60
36	1	2185	G	C5-C6-N1	-5.39	108.80	111.50
41	L4	190	GLY	N-CA-C	5.39	126.58	113.10
36	5	364	G	C4-C5-N7	5.39	112.96	110.80
38	8	100	U	C2-N1-C1'	5.39	124.17	117.70
36	5	352	A	O5'-P-OP1	-5.39	100.85	105.70
36	5	414	U	N1-C2-O2	-5.39	119.03	122.80
36	5	873	C	C6-N1-C2	-5.39	118.14	120.30
36	5	1381	A	C2-N3-C4	-5.39	107.90	110.60
36	5	2748	A	N1-C6-N6	5.39	121.83	118.60
36	5	3005	A	OP1-P-OP2	5.39	127.69	119.60
36	1	584	G	N9-C4-C5	5.39	107.56	105.40
36	1	1514	G	N1-C2-N2	-5.39	111.35	116.20
1	6	455	C	N1-C2-O2	-5.39	115.67	118.90
1	6	951	A	C8-N9-C4	5.39	107.96	105.80
1	6	1697	G	C2-N3-C4	5.39	114.59	111.90
36	5	879	U	C5-C4-O4	-5.39	122.67	125.90
36	5	2249	G	C8-N9-C4	-5.39	104.24	106.40
36	5	2993	G	C6-N1-C2	-5.39	121.87	125.10
36	5	3214	U	C5-C4-O4	5.39	129.13	125.90
36	5	3285	C	C6-N1-C1'	-5.39	114.33	120.80
36	1	2126	A	C4-C5-C6	-5.39	114.31	117.00
36	1	3079	U	N1-C2-N3	5.39	118.13	114.90
37	3	91	G	C4-C5-N7	5.39	112.95	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	588	G	C8-N9-C4	-5.39	104.25	106.40
38	4	42	G	C8-N9-C4	5.39	108.56	106.40
36	5	1116	G	C5-C6-O6	5.39	131.83	128.60
36	5	1730	G	C8-N9-C4	5.39	108.55	106.40
36	5	3131	U	N3-C4-C5	5.39	117.83	114.60
1	6	300	A	O5'-P-OP1	-5.38	100.85	105.70
1	6	965	U	N3-C4-C5	5.38	117.83	114.60
36	5	1046	A	O5'-P-OP1	-5.38	100.85	105.70
36	5	1365	G	N1-C2-N3	5.38	127.13	123.90
36	5	1429	G	C8-N9-C4	5.38	108.55	106.40
36	5	1454	A	C8-N9-C4	5.38	107.95	105.80
36	5	2346	C	N3-C2-O2	5.38	125.67	121.90
36	5	3123	A	C8-N9-C4	5.38	107.95	105.80
36	5	2211	U	C5-C4-O4	5.38	129.13	125.90
36	5	2728	G	O5'-P-OP2	-5.38	100.86	105.70
36	5	2943	G	C5-N7-C8	-5.38	101.61	104.30
36	1	587	U	OP2-P-O3'	5.38	117.04	105.20
36	1	1905	G	N3-C4-N9	-5.38	122.77	126.00
37	3	88	G	C8-N9-C4	-5.38	104.25	106.40
36	5	834	U	C6-N1-C2	5.38	124.23	121.00
36	5	2514	U	C5-C6-N1	5.38	125.39	122.70
36	5	3055	U	O5'-P-OP2	-5.38	100.86	105.70
36	1	937	G	O5'-P-OP1	-5.38	100.86	105.70
36	5	2868	U	N1-C2-O2	5.38	126.57	122.80
1	2	389	G	C5-C6-O6	-5.38	125.37	128.60
36	1	688	G	N3-C4-C5	-5.38	125.91	128.60
38	4	95	G	C4-N9-C1'	-5.38	119.51	126.50
36	5	1884	A	C5-C6-N6	-5.38	119.40	123.70
36	5	2411	U	C6-N1-C2	5.38	124.23	121.00
36	5	2818	U	P-O3'-C3'	5.38	126.16	119.70
36	5	3115	C	N1-C2-N3	5.38	122.96	119.20
36	5	3177	G	N9-C4-C5	-5.38	103.25	105.40
1	2	551	G	N7-C8-N9	5.38	115.79	113.10
36	1	221	A	N1-C6-N6	-5.38	115.37	118.60
36	1	1001	G	C8-N9-C1'	-5.38	120.01	127.00
36	1	1408	G	C5-C6-O6	-5.38	125.37	128.60
38	4	20	U	C2-N3-C4	-5.38	123.77	127.00
36	5	1003	A	N1-C2-N3	5.38	131.99	129.30
36	5	2934	A	N1-C2-N3	-5.38	126.61	129.30
1	2	1324	G	N9-C4-C5	5.38	107.55	105.40
36	1	2358	A	N1-C6-N6	5.38	121.83	118.60
36	5	804	C	C6-N1-C2	-5.38	118.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1289	G	N1-C6-O6	-5.38	116.67	119.90
36	5	3040	A	N7-C8-N9	-5.38	111.11	113.80
36	1	2369	G	C5-C6-O6	-5.37	125.38	128.60
36	5	2818	U	C5'-C4'-O4'	-5.37	102.65	109.10
36	1	611	A	C5-C6-N6	-5.37	119.40	123.70
36	1	3174	A	N1-C6-N6	5.37	121.82	118.60
36	5	206	G	C5-C6-N1	5.37	114.19	111.50
36	5	2286	U	C6-N1-C2	-5.37	117.78	121.00
36	5	2860	U	C5-C4-O4	5.37	129.12	125.90
36	5	3115	C	N1-C2-O2	-5.37	115.68	118.90
36	5	916	G	OP1-P-O3'	5.37	117.02	105.20
36	5	3061	G	C5-C6-O6	-5.37	125.38	128.60
1	2	1307	U	N3-C2-O2	-5.37	118.44	122.20
36	1	345	G	C4-N9-C1'	5.37	133.48	126.50
36	1	347	G	N7-C8-N9	5.37	115.78	113.10
36	1	1311	G	N9-C4-C5	-5.37	103.25	105.40
36	1	1364	C	OP2-P-O3'	5.37	117.01	105.20
36	5	196	G	C5-C6-O6	-5.37	125.38	128.60
36	5	640	U	C5-C6-N1	5.37	125.39	122.70
36	5	801	A	N1-C2-N3	5.37	131.98	129.30
36	5	1301	A	C5-C6-N6	-5.37	119.41	123.70
36	5	1433	A	C8-N9-C4	-5.37	103.65	105.80
36	5	2693	C	N3-C4-C5	5.37	124.05	121.90
36	1	2352	A	O5'-P-OP2	-5.37	100.87	105.70
1	6	417	A	C8-N9-C4	-5.37	103.65	105.80
36	1	361	A	C4-C5-C6	-5.37	114.32	117.00
36	1	1408	G	C4-C5-C6	5.37	122.02	118.80
36	5	1310	G	N1-C6-O6	-5.37	116.68	119.90
36	5	2700	G	C5-C6-N1	5.37	114.18	111.50
1	2	1190	C	C6-N1-C2	5.36	122.44	120.30
1	2	1323	C	N3-C2-O2	-5.36	118.14	121.90
36	1	984	G	C6-C5-N7	-5.36	127.18	130.40
36	1	1447	G	C4-C5-N7	-5.36	108.66	110.80
36	1	3046	A	O5'-P-OP1	-5.36	100.87	105.70
1	6	1600	A	N1-C6-N6	5.36	121.82	118.60
36	5	2514	U	O5'-P-OP1	-5.36	100.87	105.70
36	1	1108	U	C6-N1-C2	5.36	124.22	121.00
36	5	2392	C	C2-N1-C1'	-5.36	112.90	118.80
36	5	2412	G	N3-C4-N9	5.36	129.22	126.00
36	5	2623	G	N3-C2-N2	5.36	123.65	119.90
36	1	2113	A	N1-C6-N6	5.36	121.82	118.60
1	6	994	G	C6-C5-N7	-5.36	127.18	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1399	C	C6-N1-C2	-5.36	118.16	120.30
36	5	3040	A	C8-N9-C4	5.36	107.94	105.80
36	1	211	A	C6-N1-C2	-5.36	115.39	118.60
36	1	899	U	N3-C2-O2	-5.36	118.45	122.20
36	1	2190	U	OP2-P-O3'	5.36	116.99	105.20
36	1	2966	G	N3-C4-C5	-5.36	125.92	128.60
1	6	477	A	N9-C4-C5	-5.36	103.66	105.80
1	6	1141	G	O5'-P-OP1	-5.36	100.88	105.70
1	6	1361	U	C6-N1-C1'	-5.36	113.70	121.20
1	6	1614	A	C6-C5-N7	-5.36	128.55	132.30
36	5	2642	A	C5-C6-N6	5.36	127.99	123.70
36	1	315	C	C2-N1-C1'	5.36	124.69	118.80
36	1	1331	U	N1-C2-O2	5.36	126.55	122.80
36	1	2126	A	C8-N9-C4	5.36	107.94	105.80
36	5	437	G	N1-C2-N2	5.36	121.02	116.20
36	5	3289	G	N9-C1'-C2'	-5.36	106.11	112.00
1	2	1199	G	C8-N9-C1'	-5.35	120.04	127.00
36	1	315	C	C5-C6-N1	5.35	123.68	121.00
36	1	576	C	N1-C2-O2	-5.35	115.69	118.90
36	1	657	A	O5'-P-OP2	5.35	117.12	110.70
36	1	1784	G	N3-C4-N9	-5.35	122.79	126.00
36	5	1896	A	O5'-P-OP1	-5.35	100.88	105.70
18	C6	40	GLU	C-N-CD	-5.35	108.82	120.60
36	1	47	C	C6-N1-C2	5.35	122.44	120.30
36	1	757	C	N1-C2-O2	-5.35	115.69	118.90
36	1	3275	U	OP1-P-O3'	5.35	116.97	105.20
36	5	110	G	N7-C8-N9	-5.35	110.42	113.10
36	5	420	G	C5-C6-O6	-5.35	125.39	128.60
36	5	959	C	O4'-C1'-N1	5.35	112.48	108.20
36	5	3022	G	O4'-C1'-N9	5.35	112.48	108.20
36	1	1387	G	C5-C6-O6	5.35	131.81	128.60
36	1	2292	U	C2-N1-C1'	5.35	124.12	117.70
36	5	222	A	O5'-P-OP1	5.35	117.12	110.70
36	5	1469	C	O5'-P-OP2	-5.35	100.88	105.70
36	1	35	A	N1-C6-N6	5.35	121.81	118.60
36	1	676	G	C4-C5-C6	5.35	122.01	118.80
36	1	2283	G	C2-N3-C4	-5.35	109.23	111.90
36	1	2391	G	N3-C2-N2	-5.35	116.16	119.90
36	1	2400	G	OP2-P-O3'	5.35	116.97	105.20
36	5	609	G	N3-C2-N2	-5.35	116.16	119.90
36	5	1152	G	C5-C6-N1	-5.35	108.83	111.50
1	2	1386	G	C8-N9-C4	5.35	108.54	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1405	U	C5-C6-N1	-5.35	120.03	122.70
1	6	1003	A	C8-N9-C4	5.35	107.94	105.80
36	5	1547	G	N3-C4-C5	5.35	131.27	128.60
36	5	3315	G	N1-C2-N3	5.35	127.11	123.90
36	1	655	C	C4-C5-C6	5.35	120.07	117.40
36	1	1114	U	N1-C2-N3	-5.35	111.69	114.90
1	6	90	C	N3-C2-O2	-5.35	118.16	121.90
1	2	334	G	N7-C8-N9	-5.34	110.43	113.10
24	D2	104	LEU	CA-CB-CG	5.34	127.59	115.30
36	1	1177	G	C8-N9-C4	-5.34	104.26	106.40
36	1	1429	G	N3-C4-N9	5.34	129.21	126.00
36	1	2692	A	N7-C8-N9	5.34	116.47	113.80
37	7	79	A	N9-C4-C5	-5.34	103.66	105.80
1	2	70	C	C6-N1-C2	5.34	122.44	120.30
36	1	936	A	N1-C6-N6	5.34	121.81	118.60
36	5	1149	G	N1-C6-O6	5.34	123.11	119.90
36	5	3041	U	N3-C2-O2	5.34	125.94	122.20
1	2	16	G	N3-C4-N9	5.34	129.21	126.00
1	2	1114	G	C6-C5-N7	-5.34	127.19	130.40
36	1	1168	U	N3-C2-O2	-5.34	118.46	122.20
36	1	2306	C	O4'-C1'-N1	-5.34	103.93	108.20
38	4	144	G	N3-C2-N2	-5.34	116.16	119.90
1	6	106	U	C5-C4-O4	5.34	129.10	125.90
1	6	418	G	C5-C6-O6	-5.34	125.39	128.60
36	5	83	U	N3-C2-O2	-5.34	118.46	122.20
36	5	358	G	C8-N9-C4	5.34	108.54	106.40
36	5	2377	G	C6-C5-N7	5.34	133.60	130.40
36	5	2645	G	C8-N9-C4	5.34	108.54	106.40
1	2	144	U	N3-C2-O2	-5.34	118.46	122.20
36	5	429	U	C6-N1-C2	5.34	124.20	121.00
36	5	1327	C	C6-N1-C2	5.34	122.44	120.30
36	5	2799	A	N9-C4-C5	5.34	107.94	105.80
1	6	631	G	C5-C6-O6	-5.34	125.40	128.60
36	1	910	G	C4-C5-C6	5.34	122.00	118.80
36	1	979	U	N1-C2-N3	5.34	118.10	114.90
36	1	3142	A	C5-N7-C8	-5.34	101.23	103.90
79	Q3	29	LEU	CA-CB-CG	-5.34	103.03	115.30
1	6	782	U	C2-N1-C1'	5.34	124.10	117.70
16	c4	35	GLY	N-CA-C	5.34	126.44	113.10
36	5	2193	U	N3-C2-O2	5.34	125.94	122.20
36	1	420	G	O4'-C1'-N9	5.33	112.47	108.20
36	1	820	A	C6-N1-C2	-5.33	115.40	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	871	U	C6-N1-C1'	5.33	128.67	121.20
36	5	2171	G	N1-C6-O6	-5.33	116.70	119.90
36	1	2403	G	OP1-P-O3'	5.33	116.93	105.20
36	5	1489	A	N3-C4-C5	-5.33	123.07	126.80
36	5	2853	A	C4-C5-C6	-5.33	114.33	117.00
36	5	3309	G	C8-N9-C1'	-5.33	120.06	127.00
36	1	339	C	C2-N3-C4	-5.33	117.23	119.90
36	1	432	G	C2-N3-C4	-5.33	109.23	111.90
36	1	645	A	N3-C4-C5	-5.33	123.07	126.80
36	1	803	C	N3-C4-C5	5.33	124.03	121.90
36	1	933	A	N3-C4-C5	-5.33	123.07	126.80
36	1	1313	G	N1-C6-O6	5.33	123.10	119.90
36	1	1448	U	OP2-P-O3'	5.33	116.93	105.20
36	1	2296	A	C2-N3-C4	-5.33	107.94	110.60
36	1	2372	A	OP1-P-O3'	5.33	116.93	105.20
36	5	1169	A	O5'-P-OP2	-5.33	100.90	105.70
36	5	3048	A	O5'-P-OP2	-5.33	100.90	105.70
36	5	227	G	C8-N9-C4	5.33	108.53	106.40
36	5	793	C	N3-C4-N4	5.33	121.73	118.00
36	5	994	G	N3-C2-N2	5.33	123.63	119.90
36	1	369	A	N9-C4-C5	5.33	107.93	105.80
36	1	1296	C	N3-C2-O2	-5.33	118.17	121.90
1	6	1601	G	N1-C6-O6	-5.33	116.70	119.90
36	5	298	U	C6-N1-C2	-5.33	117.80	121.00
36	5	3207	U	N3-C4-C5	-5.33	111.40	114.60
36	1	1269	U	N1-C2-O2	5.33	126.53	122.80
36	1	1844	C	O5'-P-OP1	-5.33	100.91	105.70
36	5	2694	A	N1-C6-N6	-5.33	115.40	118.60
1	2	190	C	O4'-C1'-N1	5.33	112.46	108.20
36	1	944	C	OP2-P-O3'	5.33	116.92	105.20
36	1	2283	G	C5-N7-C8	-5.33	101.64	104.30
36	1	2639	G	C5-C6-O6	-5.33	125.41	128.60
36	1	2831	G	C5-C6-O6	-5.33	125.40	128.60
36	1	3311	C	OP1-P-OP2	5.33	127.59	119.60
1	6	695	U	C2-N1-C1'	5.33	124.09	117.70
36	1	596	C	N1-C2-O2	5.32	122.09	118.90
36	1	1501	U	C6-N1-C2	5.32	124.19	121.00
36	1	2808	A	C4-N9-C1'	5.32	135.88	126.30
36	1	2850	G	N3-C4-N9	5.32	129.19	126.00
36	1	2966	G	N3-C4-N9	5.32	129.19	126.00
1	6	458	G	C8-N9-C4	-5.32	104.27	106.40
36	5	307	A	N1-C6-N6	-5.32	115.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	770	G	N1-C6-O6	-5.32	116.71	119.90
36	5	855	U	OP2-P-O3'	5.32	116.91	105.20
36	5	1110	U	C5-C6-N1	5.32	125.36	122.70
36	1	393	U	N3-C4-O4	-5.32	115.68	119.40
36	1	857	G	N9-C4-C5	5.32	107.53	105.40
36	1	1385	C	C2-N1-C1'	-5.32	112.95	118.80
36	1	2255	A	C8-N9-C4	5.32	107.93	105.80
38	4	94	C	C6-N1-C1'	-5.32	114.42	120.80
36	5	1413	G	N3-C4-N9	5.32	129.19	126.00
36	5	2142	A	C2-N3-C4	5.32	113.26	110.60
36	5	2689	A	O4'-C1'-N9	5.32	112.46	108.20
36	1	866	A	C8-N9-C4	5.32	107.93	105.80
36	1	1300	G	C8-N9-C1'	-5.32	120.09	127.00
36	1	2202	C	C6-N1-C2	-5.32	118.17	120.30
36	5	1420	C	N1-C2-O2	-5.32	115.71	118.90
36	1	3362	A	C8-N9-C4	-5.32	103.67	105.80
73	O7	5	THR	C-N-CD	5.32	139.57	128.40
1	6	678	A	P-O3'-C3'	5.32	126.08	119.70
36	5	510	G	N3-C2-N2	5.32	123.62	119.90
36	5	2370	G	N1-C2-N3	5.32	127.09	123.90
1	2	308	C	N1-C2-O2	-5.31	115.71	118.90
36	1	2870	C	N3-C4-N4	-5.31	114.28	118.00
1	6	609	U	C5-C4-O4	5.31	129.09	125.90
36	5	2971	A	N3-C4-N9	5.31	131.65	127.40
36	1	911	C	C2-N3-C4	-5.31	117.24	119.90
36	5	1012	G	N3-C4-N9	-5.31	122.81	126.00
36	5	2953	U	O5'-P-OP2	5.31	117.08	110.70
36	5	673	U	C5-C6-N1	-5.31	120.04	122.70
36	5	1886	A	O5'-P-OP2	-5.31	100.92	105.70
1	2	949	C	C6-N1-C2	-5.31	118.18	120.30
36	1	2330	C	C5-C4-N4	-5.31	116.48	120.20
36	1	2758	A	N7-C8-N9	-5.31	111.15	113.80
53	M7	3	ARG	NE-CZ-NH2	-5.31	117.64	120.30
36	5	1155	C	O5'-P-OP1	-5.31	100.92	105.70
36	5	2372	A	C8-N9-C4	-5.31	103.68	105.80
36	5	2823	G	C6-C5-N7	-5.31	127.21	130.40
1	2	728	U	N1-C2-O2	5.31	126.52	122.80
36	1	927	C	N3-C4-N4	5.31	121.72	118.00
36	1	1897	G	C6-C5-N7	-5.31	127.22	130.40
1	6	1148	C	OP2-P-O3'	5.31	116.88	105.20
36	5	1113	G	C5-C6-N1	-5.31	108.85	111.50
36	5	1374	G	N1-C2-N2	-5.31	111.42	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1437	C	N3-C2-O2	-5.31	118.19	121.90
36	5	1943	C	C6-N1-C2	-5.31	118.18	120.30
36	5	2965	U	C5-C4-O4	-5.31	122.72	125.90
37	7	48	U	C4-C5-C6	5.31	122.88	119.70
36	1	357	A	C6-N1-C2	-5.31	115.42	118.60
1	6	585	A	C8-N9-C4	5.31	107.92	105.80
36	5	519	A	N1-C6-N6	5.31	121.78	118.60
36	1	1807	G	C8-N9-C4	-5.30	104.28	106.40
36	5	1480	G	O4'-C1'-N9	5.30	112.44	108.20
39	L2	25	GLY	N-CA-C	-5.30	99.84	113.10
36	5	746	A	OP2-P-O3'	5.30	116.87	105.20
36	1	2783	U	C5-C6-N1	5.30	125.35	122.70
1	6	9	U	O5'-P-OP1	-5.30	100.93	105.70
36	5	610	G	C8-N9-C4	-5.30	104.28	106.40
36	5	2135	U	O5'-P-OP2	-5.30	100.93	105.70
36	5	2629	U	C5-C4-O4	-5.30	122.72	125.90
36	1	956	U	N3-C4-C5	-5.30	111.42	114.60
36	1	2293	C	N3-C4-N4	5.30	121.71	118.00
36	1	2369	G	N3-C4-C5	-5.30	125.95	128.60
37	7	77	G	N1-C6-O6	5.30	123.08	119.90
1	2	412	A	N1-C6-N6	5.30	121.78	118.60
1	2	499	U	C5-C4-O4	-5.30	122.72	125.90
36	1	27	C	OP1-P-OP2	5.30	127.55	119.60
36	1	1082	U	N1-C2-O2	5.30	126.51	122.80
36	1	3181	C	N1-C2-N3	5.30	122.91	119.20
36	5	1116	G	C8-N9-C1'	-5.30	120.11	127.00
36	5	2572	C	C6-N1-C1'	-5.30	114.44	120.80
1	2	103	A	C5-C6-N6	-5.30	119.46	123.70
1	2	1014	G	C8-N9-C4	-5.30	104.28	106.40
36	1	645	A	N1-C2-N3	5.30	131.95	129.30
36	1	1646	G	N3-C4-C5	5.30	131.25	128.60
36	1	1669	C	C6-N1-C2	5.30	122.42	120.30
36	5	994	G	N3-C4-C5	-5.30	125.95	128.60
36	5	2419	A	N1-C6-N6	5.30	121.78	118.60
36	5	2643	A	C4-C5-N7	5.30	113.35	110.70
36	5	2965	U	N1-C2-O2	-5.30	119.09	122.80
36	5	3174	A	N7-C8-N9	5.30	116.45	113.80
36	1	410	U	C6-N1-C2	-5.29	117.82	121.00
36	1	717	C	C6-N1-C2	-5.29	118.18	120.30
36	1	1604	G	C4-N9-C1'	5.29	133.38	126.50
36	5	1127	G	C5-C6-N1	5.29	114.15	111.50
36	5	1200	A	N3-C4-N9	5.29	131.64	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2622	C	N3-C4-C5	-5.29	119.78	121.90
1	2	864	U	N3-C2-O2	-5.29	118.50	122.20
36	1	1296	C	N1-C2-N3	5.29	122.91	119.20
36	1	2781	U	N1-C2-O2	-5.29	119.09	122.80
38	4	7	U	OP2-P-O3'	5.29	116.84	105.20
47	M0	24	ARG	NE-CZ-NH1	5.29	122.95	120.30
36	5	195	U	N3-C2-O2	-5.29	118.50	122.20
36	1	1419	A	C5'-C4'-O4'	5.29	115.45	109.10
36	1	2523	A	N1-C6-N6	5.29	121.78	118.60
36	1	2723	U	N1-C2-O2	-5.29	119.10	122.80
1	6	1614	A	C5-C6-N1	-5.29	115.05	117.70
36	5	2277	C	N1-C2-O2	5.29	122.08	118.90
36	1	128	G	C6-C5-N7	-5.29	127.23	130.40
36	1	2754	G	C8-N9-C4	5.29	108.52	106.40
36	5	3049	A	N7-C8-N9	-5.29	111.16	113.80
36	1	1154	A	C6-N1-C2	-5.29	115.43	118.60
36	1	1724	U	O5'-P-OP2	-5.29	100.94	105.70
36	1	2612	U	C2-N3-C4	-5.29	123.83	127.00
36	1	2982	A	C4-C5-C6	5.29	119.64	117.00
1	6	272	U	P-O3'-C3'	5.29	126.05	119.70
1	6	619	A	C4-N9-C1'	-5.29	116.78	126.30
36	5	55	G	C2-N3-C4	-5.29	109.26	111.90
36	5	1466	G	C5-C6-O6	-5.29	125.43	128.60
36	5	2112	U	N3-C2-O2	-5.29	118.50	122.20
36	5	2871	G	N3-C4-N9	5.29	129.17	126.00
36	1	1849	C	N3-C4-N4	5.29	121.70	118.00
1	6	1412	G	N3-C4-N9	-5.29	122.83	126.00
36	5	1158	A	O5'-P-OP1	5.29	117.04	110.70
36	5	1367	G	C5-C6-N1	-5.29	108.86	111.50
36	5	2823	G	C4-C5-N7	5.29	112.92	110.80
36	1	979	U	C5-C6-N1	5.29	125.34	122.70
36	1	1305	U	N1-C2-N3	5.29	118.07	114.90
36	1	2948	C	C6-N1-C2	5.29	122.41	120.30
36	5	1716	U	C6-N1-C2	-5.29	117.83	121.00
36	5	3006	A	C2-N3-C4	-5.29	107.96	110.60
36	5	421	G	N3-C4-C5	-5.28	125.96	128.60
36	5	2523	A	N1-C6-N6	-5.28	115.43	118.60
36	1	858	A	C8-N9-C4	-5.28	103.69	105.80
38	4	99	C	C6-N1-C2	5.28	122.41	120.30
1	6	943	C	C2-N1-C1'	-5.28	112.99	118.80
36	5	2145	A	N9-C4-C5	5.28	107.91	105.80
36	5	2355	G	N1-C6-O6	5.28	123.07	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	110	G	N3-C4-N9	-5.28	122.83	126.00
37	3	86	U	N3-C4-C5	5.28	117.77	114.60
36	5	417	A	C8-N9-C4	5.28	107.91	105.80
36	5	2300	G	C4-C5-N7	5.28	112.91	110.80
36	5	3046	A	C5-C6-N1	5.28	120.34	117.70
36	5	3308	C	C4-C5-C6	5.28	120.04	117.40
36	1	228	U	O5'-P-OP1	-5.28	100.95	105.70
36	1	2643	A	N7-C8-N9	-5.28	111.16	113.80
36	1	2857	C	OP2-P-O3'	5.28	116.81	105.20
36	1	2984	C	N1-C2-O2	-5.28	115.73	118.90
36	1	956	U	C5-C4-O4	5.28	129.07	125.90
36	1	2361	A	N1-C6-N6	-5.28	115.43	118.60
36	1	3121	U	OP1-P-O3'	5.28	116.81	105.20
1	6	1029	U	N1-C2-N3	5.28	118.07	114.90
36	5	1606	U	C5-C6-N1	-5.28	120.06	122.70
36	5	2800	G	N3-C4-C5	5.28	131.24	128.60
36	5	3041	U	N3-C4-C5	5.28	117.77	114.60
1	2	1132	A	C5-C6-N6	-5.28	119.48	123.70
36	1	2405	C	N3-C4-N4	5.28	121.69	118.00
38	4	125	U	N1-C2-O2	5.28	126.49	122.80
36	5	1117	G	C5-N7-C8	-5.28	101.66	104.30
36	1	968	G	N3-C4-C5	-5.27	125.96	128.60
36	1	1453	A	C8-N9-C4	-5.27	103.69	105.80
56	N0	106	LEU	CA-CB-CG	5.27	127.43	115.30
36	5	645	A	C8-N9-C4	-5.27	103.69	105.80
36	5	1365	G	C6-C5-N7	-5.27	127.24	130.40
36	5	2342	U	C5-C6-N1	-5.27	120.06	122.70
36	5	3140	G	C6-C5-N7	-5.27	127.24	130.40
1	2	447	U	N3-C4-O4	5.27	123.09	119.40
36	5	3317	U	C6-N1-C2	-5.27	117.84	121.00
36	1	820	A	N7-C8-N9	5.27	116.44	113.80
36	1	1308	A	C5-C6-N1	-5.27	115.06	117.70
36	1	970	A	C8-N9-C4	-5.27	103.69	105.80
36	1	2821	C	OP1-P-OP2	5.27	127.50	119.60
36	5	1188	U	N1-C2-N3	5.27	118.06	114.90
36	5	2843	U	N3-C2-O2	-5.27	118.51	122.20
36	1	44	U	C5-C4-O4	5.27	129.06	125.90
36	1	1164	G	C5-C6-O6	5.27	131.76	128.60
36	1	1330	A	N9-C4-C5	-5.27	103.69	105.80
36	5	878	G	N3-C2-N2	5.27	123.59	119.90
36	5	1196	C	C6-N1-C2	5.27	122.41	120.30
36	5	1412	G	N7-C8-N9	5.27	115.73	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2618	G	N3-C4-C5	-5.27	125.97	128.60
36	5	2642	A	N1-C6-N6	-5.27	115.44	118.60
36	1	1377	G	C5-C6-O6	-5.27	125.44	128.60
36	5	808	A	N9-C4-C5	5.27	107.91	105.80
36	5	1327	C	N3-C4-C5	5.27	124.01	121.90
36	5	2366	C	C2-N3-C4	5.27	122.53	119.90
36	1	659	G	C4-C5-N7	5.26	112.91	110.80
36	1	930	U	N1-C2-O2	-5.26	119.11	122.80
37	3	30	G	C8-N9-C4	-5.26	104.29	106.40
36	5	869	G	N1-C2-N2	-5.26	111.46	116.20
36	5	1101	G	N3-C4-N9	5.26	129.16	126.00
36	1	3120	C	N1-C2-O2	5.26	122.06	118.90
1	6	426	G	N3-C4-C5	-5.26	125.97	128.60
36	5	2616	C	N3-C2-O2	5.26	125.58	121.90
36	5	3387	U	N3-C2-O2	-5.26	118.52	122.20
1	2	428	A	N9-C4-C5	5.26	107.91	105.80
36	1	267	G	N1-C6-O6	5.26	123.06	119.90
36	1	925	A	C4-C5-C6	5.26	119.63	117.00
36	1	1164	G	C8-N9-C1'	-5.26	120.16	127.00
1	6	361	C	OP1-P-OP2	-5.26	111.71	119.60
1	6	1267	G	C8-N9-C4	5.26	108.50	106.40
36	5	644	G	C8-N9-C4	-5.26	104.30	106.40
36	1	1141	C	C4-C5-C6	5.26	120.03	117.40
36	1	2842	U	N1-C2-O2	5.26	126.48	122.80
36	1	2980	U	C6-N1-C2	-5.26	117.84	121.00
37	3	48	U	C5-C4-O4	-5.26	122.74	125.90
1	6	552	G	N9-C4-C5	-5.26	103.30	105.40
1	6	1508	U	C6-N1-C2	5.26	124.16	121.00
36	5	29	C	C6-N1-C2	5.26	122.40	120.30
36	5	661	G	N3-C2-N2	5.26	123.58	119.90
36	5	984	G	N3-C4-N9	5.26	129.16	126.00
36	5	1895	A	C5-N7-C8	-5.26	101.27	103.90
36	5	2938	G	N1-C6-O6	-5.26	116.74	119.90
1	2	501	U	P-O3'-C3'	5.26	126.01	119.70
1	2	694	U	N3-C2-O2	-5.26	118.52	122.20
36	1	2604	U	C5-C6-N1	-5.26	120.07	122.70
36	5	2300	G	N1-C2-N2	-5.26	111.47	116.20
36	1	9	U	C2-N1-C1'	-5.26	111.39	117.70
36	1	346	C	C5-C6-N1	-5.26	118.37	121.00
36	1	401	U	N3-C2-O2	-5.26	118.52	122.20
36	1	765	C	N3-C2-O2	-5.26	118.22	121.90
36	5	1128	U	C2-N3-C4	-5.26	123.85	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	73	C	C5-C6-N1	5.26	123.63	121.00
36	1	2177	G	C5-C6-N1	5.25	114.13	111.50
1	6	467	G	N3-C4-C5	-5.25	125.97	128.60
1	2	1473	U	C5-C4-O4	5.25	129.05	125.90
36	1	107	A	C6-C5-N7	-5.25	128.62	132.30
36	1	199	A	N1-C6-N6	5.25	121.75	118.60
36	1	1212	A	N9-C4-C5	-5.25	103.70	105.80
36	1	1434	G	C5-N7-C8	-5.25	101.67	104.30
36	5	1144	U	O5'-P-OP1	-5.25	100.97	105.70
36	5	2143	A	OP1-P-O3'	5.25	116.76	105.20
36	5	2621	G	N3-C4-C5	5.25	131.23	128.60
36	5	3149	G	O5'-P-OP1	5.25	117.00	110.70
1	2	15	U	N3-C2-O2	-5.25	118.52	122.20
1	2	1662	G	N1-C6-O6	-5.25	116.75	119.90
36	1	24	G	C6-C5-N7	-5.25	127.25	130.40
36	1	2344	U	C6-N1-C2	5.25	124.15	121.00
36	1	2800	G	N1-C2-N2	-5.25	111.47	116.20
36	5	575	G	C2-N3-C4	5.25	114.53	111.90
36	5	1413	G	N3-C4-C5	-5.25	125.97	128.60
36	5	1476	G	N3-C4-C5	5.25	131.23	128.60
36	5	1561	G	O4'-C1'-N9	5.25	112.40	108.20
1	2	548	G	N3-C4-N9	5.25	129.15	126.00
36	1	2953	U	N3-C4-O4	5.25	123.08	119.40
1	6	1745	G	C4-N9-C1'	5.25	133.32	126.50
36	5	37	U	OP2-P-O3'	5.25	116.75	105.20
36	5	2372	A	OP2-P-O3'	5.25	116.75	105.20
36	1	274	G	C5-C6-O6	-5.25	125.45	128.60
36	1	1043	C	C6-N1-C2	5.25	122.40	120.30
36	1	1484	U	C5-C6-N1	5.25	125.32	122.70
36	1	2382	G	C2-N3-C4	-5.25	109.28	111.90
36	1	3036	G	N3-C4-C5	-5.25	125.97	128.60
1	6	1744	A	N9-C4-C5	-5.25	103.70	105.80
36	5	293	C	C6-N1-C2	5.25	122.40	120.30
36	5	2117	A	C8-N9-C4	-5.25	103.70	105.80
36	5	2902	A	N1-C6-N6	5.25	121.75	118.60
36	1	1076	C	C6-N1-C1'	-5.25	114.50	120.80
36	5	417	A	N7-C8-N9	-5.25	111.18	113.80
36	5	653	A	O5'-P-OP1	-5.25	100.98	105.70
36	5	1329	U	P-O3'-C3'	5.25	126.00	119.70
37	7	29	C	C6-N1-C2	5.25	122.40	120.30
1	6	76	A	OP1-P-O3'	5.25	116.74	105.20
36	1	282	G	C2'-C3'-O3'	5.24	122.09	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	368	G	C6-C5-N7	-5.24	127.25	130.40
36	1	714	G	N1-C6-O6	5.24	123.05	119.90
36	1	1521	G	O5'-P-OP1	-5.24	100.98	105.70
1	6	1200	G	N3-C4-C5	5.24	131.22	128.60
36	5	644	G	C4-C5-N7	-5.24	108.70	110.80
36	5	1049	C	C2-N1-C1'	5.24	124.57	118.80
36	5	1380	G	O5'-P-OP2	-5.24	100.98	105.70
36	5	2891	U	N3-C4-C5	5.24	117.75	114.60
36	5	3044	G	N7-C8-N9	5.24	115.72	113.10
36	5	3091	A	N1-C6-N6	-5.24	115.45	118.60
36	1	1303	A	N1-C6-N6	5.24	121.75	118.60
36	1	3310	A	N9-C4-C5	-5.24	103.70	105.80
36	5	1939	G	N3-C2-N2	5.24	123.57	119.90
36	1	2874	G	C5-C6-N1	-5.24	108.88	111.50
1	6	1027	A	N1-C6-N6	5.24	121.74	118.60
36	5	767	U	O4'-C1'-N1	5.24	112.39	108.20
36	5	1043	C	N3-C2-O2	-5.24	118.23	121.90
36	5	2935	U	C5-C4-O4	-5.24	122.75	125.90
36	1	936	A	C5-C6-N6	-5.24	119.51	123.70
36	1	2526	C	C6-N1-C2	-5.24	118.20	120.30
36	1	2818	U	C4-C5-C6	-5.24	116.56	119.70
36	5	592	A	C8-N9-C4	5.24	107.90	105.80
36	5	960	U	OP1-P-O3'	-5.24	93.67	105.20
36	5	2757	U	N3-C4-O4	5.24	123.07	119.40
36	1	426	G	N3-C4-N9	5.24	129.14	126.00
39	L2	128	ARG	NE-CZ-NH1	-5.24	117.68	120.30
36	5	3146	G	N9-C4-C5	-5.24	103.31	105.40
36	1	39	A	N1-C6-N6	5.24	121.74	118.60
36	1	1137	C	C6-N1-C2	5.24	122.39	120.30
36	1	1414	G	N3-C4-C5	5.24	131.22	128.60
36	1	1431	G	C5-C6-O6	5.24	131.74	128.60
36	1	2187	G	N1-C6-O6	5.24	123.04	119.90
36	1	2418	G	OP2-P-O3'	5.24	116.72	105.20
1	6	217	A	P-O3'-C3'	5.24	125.98	119.70
36	5	411	U	C5-C6-N1	-5.24	120.08	122.70
36	5	1064	A	O4'-C1'-N9	-5.24	104.01	108.20
36	5	2823	G	C5-C6-O6	-5.24	125.46	128.60
36	1	298	U	C6-N1-C1'	-5.23	113.87	121.20
44	L7	163	LEU	CA-CB-CG	-5.23	103.26	115.30
36	1	588	G	N9-C4-C5	5.23	107.49	105.40
36	1	984	G	C2-N3-C4	5.23	114.52	111.90
36	1	2924	U	N3-C2-O2	5.23	125.86	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2989	U	C5-C4-O4	-5.23	122.76	125.90
36	1	3267	A	N1-C6-N6	-5.23	115.46	118.60
1	6	1606	C	N1-C2-O2	5.23	122.04	118.90
36	5	1468	A	C5-C6-N6	-5.23	119.51	123.70
36	5	2523	A	N9-C4-C5	5.23	107.89	105.80
36	5	2880	U	N3-C2-O2	-5.23	118.54	122.20
36	5	2951	G	C4-N9-C1'	5.23	133.30	126.50
36	5	3354	U	C2-N1-C1'	5.23	123.98	117.70
36	1	70	A	C4-C5-C6	5.23	119.61	117.00
36	1	788	C	C2-N1-C1'	-5.23	113.05	118.80
36	1	907	G	N3-C4-N9	5.23	129.14	126.00
36	1	2361	A	C2-N3-C4	-5.23	107.98	110.60
1	6	397	A	C2-N3-C4	-5.23	107.98	110.60
36	5	379	C	C6-N1-C2	-5.23	118.21	120.30
36	5	1848	G	O5'-P-OP2	-5.23	100.99	105.70
36	5	3296	A	N1-C6-N6	5.23	121.74	118.60
36	1	635	G	C4-C5-N7	5.23	112.89	110.80
36	1	2619	G	OP1-P-O3'	5.23	116.70	105.20
38	4	39	G	O5'-P-OP1	-5.23	100.99	105.70
36	5	1507	G	C8-N9-C4	-5.23	104.31	106.40
36	5	2353	G	C6-C5-N7	-5.23	127.26	130.40
36	1	1200	A	C4-C5-C6	5.23	119.61	117.00
36	1	3006	A	N1-C2-N3	5.23	131.91	129.30
38	4	61	A	OP2-P-O3'	5.23	116.70	105.20
36	5	1154	A	N1-C6-N6	-5.23	115.46	118.60
36	5	2820	A	OP2-P-O3'	5.23	116.70	105.20
36	5	2879	C	N3-C2-O2	5.23	125.56	121.90
36	5	3326	G	N3-C4-N9	5.23	129.14	126.00
37	7	82	G	C6-C5-N7	-5.23	127.26	130.40
1	2	378	A	C5-C6-N6	-5.23	119.52	123.70
1	6	364	G	C4-N9-C1'	5.23	133.29	126.50
1	6	901	G	N9-C4-C5	-5.23	103.31	105.40
36	5	1701	C	C6-N1-C2	-5.23	118.21	120.30
36	5	3119	U	N1-C2-O2	-5.23	119.14	122.80
1	2	555	A	C8-N9-C4	-5.22	103.71	105.80
36	1	2169	G	C6-C5-N7	5.22	133.53	130.40
36	1	2397	A	O5'-P-OP2	-5.22	101.00	105.70
1	6	359	A	C4-N9-C1'	-5.22	116.89	126.30
1	6	1337	A	N3-C4-C5	5.22	130.46	126.80
36	5	927	C	C6-N1-C2	-5.22	118.21	120.30
36	5	1308	A	OP1-P-OP2	-5.22	111.76	119.60
37	7	85	G	OP2-P-O3'	5.22	116.69	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1365	G	C4-N9-C1'	5.22	133.29	126.50
36	1	2756	C	N3-C4-N4	5.22	121.66	118.00
36	1	2816	G	C5-C6-O6	-5.22	125.47	128.60
36	1	3098	G	C4-C5-N7	5.22	112.89	110.80
36	5	2877	G	C8-N9-C1'	-5.22	120.21	127.00
36	1	1206	G	C4-C5-N7	-5.22	108.71	110.80
36	1	2996	U	N1-C2-O2	5.22	126.45	122.80
40	L3	4	ARG	NE-CZ-NH2	-5.22	117.69	120.30
37	7	41	G	N9-C4-C5	-5.22	103.31	105.40
1	2	1241	G	C4-C5-N7	5.22	112.89	110.80
36	1	2406	C	N1-C2-O2	-5.22	115.77	118.90
36	1	2671	A	C4-C5-C6	-5.22	114.39	117.00
1	6	163	G	C2-N3-C4	-5.22	109.29	111.90
1	6	1361	U	C5-C6-N1	5.22	125.31	122.70
36	5	3322	A	C6-C5-N7	-5.22	128.65	132.30
1	6	970	A	N1-C6-N6	5.22	121.73	118.60
1	6	1438	G	N3-C4-N9	5.22	129.13	126.00
36	5	2916	U	O5'-P-OP2	5.22	116.96	110.70
36	5	3026	G	C8-N9-C4	5.22	108.49	106.40
1	2	354	C	N3-C4-C5	-5.22	119.81	121.90
1	2	1215	C	C6-N1-C2	-5.22	118.21	120.30
36	1	1114	U	N1-C2-O2	5.22	126.45	122.80
36	1	2887	A	C5-N7-C8	-5.22	101.29	103.90
38	4	88	A	C5-C6-N6	-5.22	119.53	123.70
1	6	1537	C	O4'-C1'-N1	5.22	112.37	108.20
36	5	916	G	P-O3'-C3'	5.22	125.96	119.70
36	5	2154	U	C6-N1-C2	-5.22	117.87	121.00
36	5	2234	G	N1-C6-O6	5.22	123.03	119.90
36	1	1151	U	N3-C4-O4	5.21	123.05	119.40
1	6	128	U	N1-C2-O2	-5.21	119.15	122.80
1	6	1637	C	N3-C2-O2	-5.21	118.25	121.90
1	6	1780	G	N9-C4-C5	-5.21	103.31	105.40
1	6	1793	G	C8-N9-C1'	5.21	133.78	127.00
36	5	908	G	N1-C6-O6	5.21	123.03	119.90
36	5	1476	G	C6-C5-N7	5.21	133.53	130.40
36	5	2953	U	N3-C4-O4	5.21	123.05	119.40
36	5	2978	U	C5-C6-N1	-5.21	120.09	122.70
1	2	1339	C	C3'-C2'-C1'	5.21	105.67	101.50
36	1	245	U	N3-C2-O2	-5.21	118.55	122.20
36	5	376	G	N3-C4-C5	-5.21	125.99	128.60
1	2	1041	G	C8-N9-C4	-5.21	104.31	106.40
1	2	1241	G	C8-N9-C1'	-5.21	120.22	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2376	G	N3-C4-C5	-5.21	125.99	128.60
36	1	2618	G	N3-C4-C5	-5.21	125.99	128.60
36	1	3088	G	N3-C2-N2	-5.21	116.25	119.90
1	6	1643	U	C2-N3-C4	-5.21	123.87	127.00
36	5	830	A	C4-C5-N7	5.21	113.31	110.70
36	5	1834	U	N3-C4-C5	-5.21	111.47	114.60
36	5	2794	G	N9-C4-C5	-5.21	103.31	105.40
1	2	1777	G	C6-C5-N7	-5.21	127.27	130.40
36	1	1519	G	C8-N9-C4	5.21	108.48	106.40
1	6	1600	A	N9-C1'-C2'	5.21	120.77	114.00
36	5	340	C	N3-C4-N4	-5.21	114.35	118.00
36	5	424	G	N9-C4-C5	-5.21	103.32	105.40
36	5	922	U	N3-C4-O4	-5.21	115.75	119.40
36	5	1468	A	C6-C5-N7	-5.21	128.65	132.30
36	1	1403	C	C2-N1-C1'	-5.21	113.07	118.80
36	1	2805	G	N1-C6-O6	5.21	123.03	119.90
38	4	94	C	C5-C4-N4	-5.21	116.55	120.20
1	6	18	C	C5-C6-N1	5.21	123.60	121.00
1	6	858	G	C5-N7-C8	-5.21	101.70	104.30
36	5	803	C	N1-C2-O2	-5.21	115.78	118.90
36	5	1003	A	C8-N9-C4	5.21	107.88	105.80
1	2	1560	U	C6-N1-C2	-5.21	117.88	121.00
36	1	688	G	C5-C6-O6	-5.21	125.48	128.60
36	1	908	G	N1-C2-N2	5.21	120.89	116.20
36	1	2692	A	C4-C5-N7	5.21	113.30	110.70
38	4	115	C	C6-N1-C2	5.21	122.38	120.30
1	6	14	C	N1-C2-O2	-5.21	115.78	118.90
36	5	80	G	N1-C6-O6	5.21	123.02	119.90
36	5	977	C	N1-C2-O2	5.21	122.02	118.90
36	5	1911	A	O5'-P-OP2	-5.21	101.02	105.70
1	2	866	G	N3-C4-C5	5.20	131.20	128.60
36	1	1156	C	C4-C5-C6	5.20	120.00	117.40
36	5	1874	A	C8-N9-C4	5.20	107.88	105.80
36	5	2965	U	N3-C2-O2	5.20	125.84	122.20
36	5	3317	U	C5-C4-O4	5.20	129.02	125.90
1	2	1558	U	C2-N1-C1'	5.20	123.94	117.70
36	1	556	U	N3-C2-O2	5.20	125.84	122.20
36	1	1204	A	O5'-P-OP1	-5.20	101.02	105.70
36	5	1008	U	C5-C6-N1	-5.20	120.10	122.70
36	1	1369	A	O5'-P-OP1	-5.20	101.02	105.70
36	5	798	G	N1-C6-O6	5.20	123.02	119.90
36	5	2697	A	C5-C6-N6	-5.20	119.54	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1096	C	N3-C2-O2	-5.20	118.26	121.90
36	1	590	G	C5-C6-O6	-5.20	125.48	128.60
36	1	1045	C	OP2-P-O3'	5.20	116.64	105.20
36	1	2232	A	O5'-P-OP2	-5.20	101.02	105.70
36	1	2400	G	C5-C6-N1	-5.20	108.90	111.50
36	1	2647	A	C6-N1-C2	-5.20	115.48	118.60
36	5	564	G	C4-C5-N7	-5.20	108.72	110.80
36	5	1772	U	N3-C2-O2	-5.20	118.56	122.20
36	5	2848	G	C4-C5-C6	5.20	121.92	118.80
37	7	43	U	C5-C6-N1	-5.20	120.10	122.70
1	2	307	G	N9-C4-C5	-5.20	103.32	105.40
36	1	970	A	C5-N7-C8	-5.20	101.30	103.90
1	6	590	C	C6-N1-C2	-5.20	118.22	120.30
36	5	128	G	N3-C4-N9	5.20	129.12	126.00
36	5	1139	G	C5-C6-O6	-5.20	125.48	128.60
36	5	1870	C	N1-C2-O2	-5.20	115.78	118.90
1	2	866	G	C4-C5-N7	5.20	112.88	110.80
36	1	404	G	C5-C6-N1	-5.20	108.90	111.50
36	1	1139	G	C5-C6-O6	5.20	131.72	128.60
36	5	567	G	N1-C2-N2	-5.20	111.52	116.20
36	5	641	C	C6-N1-C2	5.20	122.38	120.30
36	5	1321	G	C5-C6-N1	-5.20	108.90	111.50
38	4	32	C	N3-C2-O2	5.19	125.54	121.90
36	5	1164	G	OP1-P-OP2	5.19	127.39	119.60
36	5	1695	U	N1-C2-N3	5.19	118.02	114.90
36	1	326	U	O5'-P-OP2	-5.19	101.03	105.70
36	1	1386	A	N1-C6-N6	5.19	121.72	118.60
36	1	1428	A	N1-C2-N3	5.19	131.90	129.30
36	1	2307	G	OP2-P-O3'	5.19	116.62	105.20
1	6	558	U	N3-C2-O2	-5.19	118.56	122.20
36	5	221	A	N7-C8-N9	-5.19	111.20	113.80
36	5	1408	G	OP2-P-O3'	5.19	116.62	105.20
36	5	2299	A	C5-C6-N1	-5.19	115.10	117.70
36	5	2338	C	N3-C4-C5	-5.19	119.82	121.90
36	5	2692	A	N1-C6-N6	-5.19	115.48	118.60
36	5	3302	U	C2-N1-C1'	-5.19	111.47	117.70
1	2	1307	U	C2-N1-C1'	5.19	123.93	117.70
36	1	35	A	O5'-P-OP2	-5.19	101.03	105.70
36	1	636	C	C5-C6-N1	-5.19	118.40	121.00
36	1	967	A	C2-N3-C4	-5.19	108.00	110.60
36	5	1300	G	C6-C5-N7	-5.19	127.29	130.40
36	5	2112	U	OP2-P-O3'	5.19	116.62	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2865	U	C5-C6-N1	5.19	125.30	122.70
43	16	30	LEU	CA-CB-CG	5.19	127.24	115.30
36	1	274	G	C6-C5-N7	-5.19	127.29	130.40
36	1	573	C	C6-N1-C2	5.19	122.38	120.30
36	1	984	G	C4-C5-C6	5.19	121.91	118.80
1	6	209	U	N1-C2-O2	-5.19	119.17	122.80
1	6	976	G	C4-C5-N7	5.19	112.88	110.80
36	1	993	G	C5-C6-N1	5.19	114.09	111.50
36	1	1140	G	N3-C2-N2	5.19	123.53	119.90
36	5	934	G	N3-C4-C5	-5.19	126.01	128.60
36	5	2248	C	N1-C2-O2	-5.19	115.79	118.90
36	5	2814	G	C6-C5-N7	-5.19	127.29	130.40
36	1	1330	A	C4-C5-N7	5.19	113.29	110.70
1	6	437	A	N1-C6-N6	-5.19	115.49	118.60
37	7	42	A	O5'-P-OP2	5.19	116.92	110.70
57	n1	106	LEU	CA-CB-CG	-5.19	103.37	115.30
1	6	19	A	N9-C4-C5	-5.18	103.73	105.80
1	6	558	U	P-O3'-C3'	5.18	125.92	119.70
1	2	1650	U	C6-N1-C2	5.18	124.11	121.00
35	SM	134	ASP	CB-CG-OD2	5.18	122.96	118.30
36	1	400	G	C8-N9-C4	-5.18	104.33	106.40
1	6	28	A	OP1-P-O3'	5.18	116.60	105.20
1	6	390	G	OP1-P-OP2	5.18	127.38	119.60
36	5	3128	G	OP2-P-O3'	5.18	116.60	105.20
36	1	1127	G	C5-C6-O6	-5.18	125.49	128.60
37	3	8	G	C6-C5-N7	5.18	133.51	130.40
36	5	382	U	N1-C2-N3	5.18	118.01	114.90
36	5	1085	A	O5'-P-OP1	-5.18	101.04	105.70
36	5	3216	G	C8-N9-C4	5.18	108.47	106.40
1	2	386	G	OP1-P-O3'	5.18	116.59	105.20
36	1	1165	A	C8-N9-C4	5.18	107.87	105.80
36	1	2537	U	P-O3'-C3'	5.18	125.92	119.70
36	1	3210	A	C5-C6-N1	5.18	120.29	117.70
36	5	650	C	C6-N1-C1'	5.18	127.02	120.80
36	5	2618	G	N3-C4-N9	5.18	129.11	126.00
36	5	1305	U	C6-N1-C1'	-5.18	113.95	121.20
36	5	1846	C	P-O3'-C3'	-5.18	113.49	119.70
36	1	590	G	N9-C4-C5	-5.18	103.33	105.40
36	1	1047	A	O5'-P-OP2	-5.18	101.04	105.70
36	1	1175	C	C2-N3-C4	-5.18	117.31	119.90
1	6	413	U	N1-C2-N3	5.18	118.01	114.90
36	5	1520	G	C5-C6-O6	-5.18	125.49	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2128	C	O5'-P-OP2	-5.18	101.04	105.70
36	5	2337	C	N1-C2-O2	5.18	122.01	118.90
36	1	1129	A	N9-C4-C5	-5.17	103.73	105.80
36	1	1414	G	C4-C5-N7	5.17	112.87	110.80
36	1	1501	U	C2-N1-C1'	-5.17	111.49	117.70
1	6	1657	U	N3-C2-O2	-5.17	118.58	122.20
36	5	2950	G	N7-C8-N9	5.17	115.69	113.10
38	8	80	A	N3-C4-C5	-5.17	123.18	126.80
38	8	113	U	N3-C2-O2	-5.17	118.58	122.20
36	5	976	U	C6-N1-C2	-5.17	117.90	121.00
1	2	323	A	O5'-P-OP2	-5.17	101.05	105.70
36	5	1520	G	C6-C5-N7	-5.17	127.30	130.40
36	5	1727	G	N1-C6-O6	-5.17	116.80	119.90
1	2	139	C	P-O3'-C3'	5.17	125.91	119.70
36	1	1468	A	C8-N9-C4	5.17	107.87	105.80
36	1	1904	C	OP2-P-O3'	5.17	116.57	105.20
36	1	2292	U	N1-C2-O2	5.17	126.42	122.80
36	1	3373	U	C6-N1-C2	5.17	124.10	121.00
1	6	107	C	C5-C6-N1	-5.17	118.42	121.00
36	5	720	A	C4-C5-N7	5.17	113.28	110.70
36	5	1210	U	N3-C4-O4	-5.17	115.78	119.40
36	5	1329	U	C6-N1-C1'	-5.17	113.96	121.20
36	5	1889	G	N3-C4-C5	-5.17	126.02	128.60
36	1	2310	U	O5'-P-OP1	-5.17	101.05	105.70
36	1	3298	C	C6-N1-C2	5.17	122.37	120.30
1	6	593	U	C5-C4-O4	5.17	129.00	125.90
36	5	407	A	C4-N9-C1'	5.17	135.60	126.30
36	5	960	U	N1-C1'-C2'	5.17	120.72	114.00
36	5	2871	G	N3-C4-C5	-5.17	126.02	128.60
36	5	2909	U	N1-C2-O2	-5.17	119.18	122.80
36	1	217	U	OP1-P-OP2	5.17	127.35	119.60
36	1	1545	A	N7-C8-N9	5.17	116.38	113.80
36	1	2624	G	C4-C5-N7	5.17	112.87	110.80
1	6	1650	U	N3-C2-O2	5.17	125.82	122.20
36	5	815	G	C4-N9-C1'	5.17	133.22	126.50
36	5	1336	U	O5'-P-OP2	-5.17	101.05	105.70
36	5	1438	U	C6-N1-C2	-5.17	117.90	121.00
36	5	2850	G	N1-C6-O6	5.17	123.00	119.90
36	5	3086	A	C2-N3-C4	-5.17	108.02	110.60
3	S1	96	LEU	CA-CB-CG	5.17	127.18	115.30
36	1	105	C	C5-C4-N4	-5.17	116.58	120.20
36	1	1201	C	N3-C4-N4	5.17	121.61	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1495	U	C6-N1-C1'	5.17	128.43	121.20
36	1	2760	C	N1-C2-O2	-5.17	115.80	118.90
1	2	1205	C	C6-N1-C2	5.16	122.37	120.30
36	1	55	G	C8-N9-C4	5.16	108.47	106.40
36	1	903	U	C4-C5-C6	5.16	122.80	119.70
36	1	2283	G	C4-C5-N7	5.16	112.87	110.80
36	5	423	A	OP2-P-O3'	5.16	116.56	105.20
36	5	630	A	C2-N3-C4	-5.16	108.02	110.60
36	5	1449	A	C6-N1-C2	-5.16	115.50	118.60
36	5	2917	G	N1-C6-O6	5.16	123.00	119.90
36	1	1295	G	N1-C6-O6	-5.16	116.80	119.90
36	1	2378	C	C6-N1-C2	5.16	122.36	120.30
36	5	1842	A	O5'-P-OP2	-5.16	101.05	105.70
36	1	2974	U	N1-C2-N3	5.16	118.00	114.90
49	M3	85	LEU	CA-CB-CG	5.16	127.17	115.30
1	6	1124	A	C8-N9-C4	5.16	107.86	105.80
1	6	1186	U	N3-C2-O2	-5.16	118.59	122.20
36	5	424	G	C6-C5-N7	-5.16	127.30	130.40
36	5	2165	G	N3-C2-N2	5.16	123.51	119.90
36	5	2887	A	N1-C6-N6	5.16	121.70	118.60
36	1	2305	G	C6-N1-C2	-5.16	122.00	125.10
1	6	1014	G	C5-C6-O6	5.16	131.70	128.60
36	5	1149	G	N3-C4-N9	5.16	129.09	126.00
36	5	1154	A	C5-C6-N1	5.16	120.28	117.70
36	5	2685	C	C6-N1-C2	5.16	122.36	120.30
36	5	3179	U	C5-C6-N1	5.16	125.28	122.70
36	1	2124	G	C5-C6-O6	-5.16	125.51	128.60
36	5	2772	C	OP2-P-O3'	5.16	116.55	105.20
36	5	3005	A	N1-C6-N6	5.16	121.69	118.60
36	1	225	C	C5-C6-N1	-5.16	118.42	121.00
36	1	2884	C	N3-C2-O2	5.16	125.51	121.90
36	1	3043	C	N1-C2-O2	5.16	121.99	118.90
36	5	411	U	C4-C5-C6	5.16	122.79	119.70
36	5	673	U	N1-C2-N3	5.16	117.99	114.90
36	5	1463	U	N3-C2-O2	5.16	125.81	122.20
36	5	2598	G	C6-C5-N7	-5.16	127.31	130.40
36	1	120	G	C2-N3-C4	-5.15	109.32	111.90
36	1	1187	C	C6-N1-C2	5.15	122.36	120.30
36	1	1724	U	N3-C2-O2	5.15	125.81	122.20
36	1	2368	A	OP2-P-O3'	5.15	116.54	105.20
36	5	2397	A	OP1-P-O3'	5.15	116.54	105.20
36	1	1429	G	N3-C4-C5	-5.15	126.02	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2360	C	C6-N1-C2	5.15	122.36	120.30
36	1	2376	G	C6-N1-C2	-5.15	122.01	125.10
36	1	3278	C	C5-C6-N1	5.15	123.58	121.00
36	5	391	A	N7-C8-N9	-5.15	111.22	113.80
36	5	800	G	O4'-C1'-N9	-5.15	104.08	108.20
36	5	1434	G	N1-C2-N2	5.15	120.84	116.20
36	5	3086	A	C5-C6-N1	-5.15	115.12	117.70
36	5	3212	C	N1-C2-O2	-5.15	115.81	118.90
37	7	44	C	OP2-P-O3'	5.15	116.53	105.20
1	2	1361	U	C2-N1-C1'	5.15	123.88	117.70
36	1	922	U	C2-N1-C1'	5.15	123.88	117.70
36	1	1064	A	C8-N9-C4	5.15	107.86	105.80
36	1	2868	U	C5-C6-N1	5.15	125.28	122.70
36	1	3297	U	N1-C2-O2	-5.15	119.19	122.80
1	6	318	U	N1-C2-O2	-5.15	119.19	122.80
1	6	337	G	N3-C4-N9	5.15	129.09	126.00
1	6	1164	G	C8-N9-C4	5.15	108.46	106.40
36	5	1495	U	C5-C6-N1	5.15	125.28	122.70
36	5	2202	C	N1-C2-O2	-5.15	115.81	118.90
36	5	2333	C	C2-N3-C4	-5.15	117.33	119.90
36	5	2996	U	O5'-P-OP2	-5.15	101.06	105.70
36	1	2314	U	C4-C5-C6	-5.15	116.61	119.70
38	4	61	A	N1-C6-N6	-5.15	115.51	118.60
39	L2	176	ASP	CB-CG-OD1	-5.15	113.67	118.30
36	5	880	G	C4-N9-C1'	-5.15	119.81	126.50
36	5	2290	C	N3-C4-C5	5.15	123.96	121.90
36	1	803	C	C4-C5-C6	-5.15	114.83	117.40
36	1	1300	G	C6-C5-N7	-5.15	127.31	130.40
36	1	2344	U	C2-N1-C1'	-5.15	111.52	117.70
36	1	2372	A	C8-N9-C4	-5.15	103.74	105.80
1	6	1000	C	C6-N1-C1'	-5.15	114.62	120.80
36	5	1190	A	C4-N9-C1'	5.15	135.57	126.30
36	5	2359	C	N3-C4-C5	5.15	123.96	121.90
36	5	2763	U	C5-C4-O4	-5.15	122.81	125.90
36	5	3266	G	N9-C4-C5	5.15	107.46	105.40
36	1	833	G	N3-C4-N9	-5.15	122.91	126.00
36	5	652	G	C6-N1-C2	-5.15	122.01	125.10
36	5	1118	C	O5'-P-OP2	-5.15	101.07	105.70
36	5	1554	U	N1-C2-O2	5.15	126.40	122.80
36	5	2340	U	C5-C6-N1	5.15	125.27	122.70
36	5	3174	A	C8-N9-C4	-5.15	103.74	105.80
36	1	1428	A	C6-C5-N7	-5.14	128.70	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	390	G	N3-C4-C5	-5.14	126.03	128.60
36	5	1012	G	C6-C5-N7	5.14	133.49	130.40
36	5	1307	G	C4-C5-N7	5.14	112.86	110.80
36	5	2331	C	N3-C4-N4	5.14	121.60	118.00
1	2	1662	G	C5-C6-N1	5.14	114.07	111.50
6	S4	246	LEU	CA-CB-CG	5.14	127.13	115.30
36	1	698	U	N1-C2-N3	5.14	117.99	114.90
36	1	1171	G	N9-C4-C5	5.14	107.46	105.40
36	1	1310	G	N1-C2-N2	-5.14	111.57	116.20
36	1	2522	G	C4-N9-C1'	5.14	133.19	126.50
36	1	2791	G	C8-N9-C4	-5.14	104.34	106.40
17	c5	36	LEU	CA-CB-CG	5.14	127.13	115.30
36	1	386	A	C6-C5-N7	-5.14	128.70	132.30
36	5	1176	C	N3-C2-O2	5.14	125.50	121.90
36	5	3105	U	C2-N1-C1'	-5.14	111.53	117.70
36	1	344	A	OP2-P-O3'	5.14	116.51	105.20
36	1	802	C	N3-C4-N4	5.14	121.60	118.00
36	1	2409	G	N3-C4-N9	5.14	129.08	126.00
36	1	2828	G	C5-C6-O6	5.14	131.68	128.60
36	5	935	U	C5-C4-O4	-5.14	122.82	125.90
36	5	1174	G	O5'-P-OP1	-5.14	101.07	105.70
36	5	1417	G	C5-C6-N1	5.14	114.07	111.50
36	5	2572	C	C5-C6-N1	5.14	123.57	121.00
36	5	2794	G	C4-C5-N7	5.14	112.86	110.80
36	1	1163	A	OP1-P-OP2	5.14	127.31	119.60
68	O2	66	LEU	CB-CG-CD2	-5.14	102.27	111.00
36	1	428	A	C6-C5-N7	5.14	135.90	132.30
36	1	1164	G	N1-C6-O6	-5.14	116.82	119.90
36	1	2875	U	C5-C6-N1	5.14	125.27	122.70
1	6	572	C	O5'-P-OP2	5.14	116.86	110.70
1	6	1535	U	N3-C4-O4	-5.14	115.81	119.40
36	5	3070	A	N1-C6-N6	5.14	121.68	118.60
36	5	3368	U	C2-N1-C1'	-5.14	111.54	117.70
1	2	1096	C	C6-N1-C1'	-5.13	114.64	120.80
36	1	1712	G	C5-C6-O6	-5.13	125.52	128.60
36	5	1434	G	C6-C5-N7	5.13	133.48	130.40
36	5	1597	C	N3-C4-N4	5.13	121.59	118.00
36	1	2887	A	OP2-P-O3'	5.13	116.49	105.20
36	1	2996	U	N1-C2-N3	-5.13	111.82	114.90
36	5	776	U	N3-C4-O4	-5.13	115.81	119.40
36	5	3005	A	N3-C4-N9	5.13	131.51	127.40
1	6	751	G	C5-C6-O6	-5.13	125.52	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	682	U	N3-C4-O4	-5.13	115.81	119.40
36	5	1054	A	C8-N9-C4	5.13	107.85	105.80
36	5	1300	G	C4-C5-N7	5.13	112.85	110.80
36	5	2286	U	N3-C2-O2	-5.13	118.61	122.20
36	5	2626	A	O5'-P-OP2	5.13	116.86	110.70
36	1	661	G	O5'-P-OP1	-5.13	101.08	105.70
36	1	931	C	N3-C2-O2	-5.13	118.31	121.90
1	6	29	U	C4-C5-C6	5.13	122.78	119.70
36	5	280	U	O5'-P-OP1	5.13	116.86	110.70
36	1	1515	A	N1-C6-N6	5.13	121.68	118.60
36	1	2121	G	C4-C5-N7	-5.13	108.75	110.80
36	1	2988	C	N1-C2-O2	-5.13	115.82	118.90
36	5	34	A	OP2-P-O3'	5.13	116.48	105.20
36	5	1506	A	N1-C6-N6	-5.13	115.52	118.60
1	2	1745	G	C4-C5-N7	5.13	112.85	110.80
36	1	269	G	C8-N9-C1'	5.13	133.66	127.00
36	1	1373	A	C5-N7-C8	-5.13	101.34	103.90
36	5	2435	G	C8-N9-C4	5.13	108.45	106.40
36	5	2627	C	N1-C2-N3	5.13	122.79	119.20
1	2	110	U	C5-C6-N1	5.12	125.26	122.70
36	1	1186	G	N3-C4-N9	5.12	129.07	126.00
36	1	1852	G	C6-C5-N7	-5.12	127.33	130.40
36	1	2917	G	C2-N3-C4	5.12	114.46	111.90
36	1	2917	G	C4-C5-N7	-5.12	108.75	110.80
36	5	216	G	C5-C6-O6	-5.12	125.53	128.60
1	2	1731	A	N9-C4-C5	-5.12	103.75	105.80
36	1	27	C	N1-C2-O2	-5.12	115.83	118.90
36	1	1518	U	N3-C2-O2	-5.12	118.61	122.20
1	6	323	A	C8-N9-C4	-5.12	103.75	105.80
1	6	421	A	C8-N9-C4	5.12	107.85	105.80
36	5	202	G	N9-C4-C5	-5.12	103.35	105.40
44	17	232	ARG	NE-CZ-NH2	5.12	122.86	120.30
36	1	1174	G	N3-C4-C5	-5.12	126.04	128.60
36	1	2541	U	P-O3'-C3'	5.12	125.84	119.70
36	1	2938	G	OP1-P-OP2	5.12	127.28	119.60
36	5	1153	A	OP2-P-O3'	5.12	116.47	105.20
36	5	1215	U	N3-C4-O4	5.12	122.98	119.40
36	5	2305	G	N7-C8-N9	5.12	115.66	113.10
36	5	2524	A	N9-C1'-C2'	5.12	120.66	114.00
36	5	2801	A	C6-N1-C2	-5.12	115.53	118.60
36	5	3099	C	C5-C6-N1	-5.12	118.44	121.00
38	4	125	U	C2-N1-C1'	5.12	123.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1025	A	C4-C5-C6	5.12	119.56	117.00
1	2	1269	U	C2-N1-C1'	5.12	123.84	117.70
36	1	2292	U	N3-C2-O2	-5.12	118.62	122.20
1	6	1	U	C5-C6-N1	5.12	125.26	122.70
1	6	454	U	C5-C6-N1	-5.12	120.14	122.70
36	5	673	U	C2-N1-C1'	-5.12	111.56	117.70
36	5	706	A	C8-N9-C4	5.12	107.85	105.80
36	5	920	A	O5'-P-OP1	5.12	116.84	110.70
36	5	1413	G	N1-C2-N3	5.12	126.97	123.90
36	5	791	A	N1-C6-N6	5.12	121.67	118.60
36	5	1520	G	C4-N9-C1'	5.12	133.15	126.50
36	1	1905	G	N3-C4-C5	5.12	131.16	128.60
36	5	1178	G	N7-C8-N9	5.12	115.66	113.10
36	5	1196	C	N1-C2-O2	5.12	121.97	118.90
36	5	2984	C	C5-C6-N1	-5.12	118.44	121.00
36	1	199	A	O4'-C1'-N9	5.11	112.29	108.20
36	1	1439	U	N1-C2-N3	5.11	117.97	114.90
36	1	1742	U	C5-C4-O4	-5.11	122.83	125.90
36	1	2174	G	N7-C8-N9	5.11	115.66	113.10
36	1	2273	G	C4-N9-C1'	-5.11	119.85	126.50
36	1	3012	A	C2-N3-C4	-5.11	108.04	110.60
39	L2	191	LEU	CA-CB-CG	-5.11	103.54	115.30
1	6	1412	G	C6-C5-N7	5.11	133.47	130.40
1	6	1489	U	C2-N1-C1'	5.11	123.83	117.70
36	5	530	G	C8-N9-C4	-5.11	104.36	106.40
36	5	640	U	N3-C4-C5	-5.11	111.53	114.60
36	5	2735	U	C5-C6-N1	5.11	125.26	122.70
36	5	667	C	N1-C2-O2	5.11	121.97	118.90
36	5	2194	G	N1-C2-N3	5.11	126.97	123.90
36	1	61	A	N9-C4-C5	-5.11	103.76	105.80
36	1	1311	G	C8-N9-C4	5.11	108.44	106.40
36	1	1545	A	C8-N9-C4	-5.11	103.76	105.80
38	4	15	G	N9-C4-C5	-5.11	103.36	105.40
1	6	257	A	C5-C6-N6	-5.11	119.61	123.70
36	5	971	G	N3-C2-N2	-5.11	116.32	119.90
68	o2	4	LEU	C-N-CA	-5.11	100.54	122.00
36	1	1149	G	C5-C6-N1	-5.11	108.94	111.50
36	1	1375	G	O5'-P-OP2	-5.11	101.10	105.70
36	1	2610	G	N9-C4-C5	-5.11	103.36	105.40
61	N5	34	LEU	CA-CB-CG	5.11	127.05	115.30
36	5	99	A	N7-C8-N9	-5.11	111.25	113.80
36	5	3095	U	OP1-P-O3'	5.11	116.44	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1916	U	C5-C6-N1	-5.11	120.15	122.70
36	1	2723	U	N3-C2-O2	5.11	125.78	122.20
36	5	867	G	C5-C6-N1	-5.11	108.95	111.50
36	5	1186	G	O5'-P-OP1	5.11	116.83	110.70
36	5	1381	A	OP1-P-O3'	5.11	116.44	105.20
36	5	2881	C	C2-N1-C1'	-5.11	113.18	118.80
1	6	371	G	C4-N9-C1'	5.11	133.14	126.50
1	6	413	U	C6-N1-C2	-5.11	117.94	121.00
1	6	1493	A	N1-C6-N6	5.11	121.66	118.60
36	5	576	C	N3-C4-C5	5.11	123.94	121.90
36	5	1433	A	N1-C6-N6	-5.11	115.54	118.60
1	2	529	A	N1-C6-N6	5.10	121.66	118.60
1	2	736	C	C5-C6-N1	5.10	123.55	121.00
36	1	1835	A	C6-N1-C2	5.10	121.66	118.60
36	1	2402	A	C6-N1-C2	-5.10	115.54	118.60
36	5	1317	A	C4-C5-N7	5.10	113.25	110.70
36	5	1541	G	C5-C6-O6	-5.10	125.54	128.60
36	5	2271	A	N1-C6-N6	-5.10	115.54	118.60
36	5	2937	G	N1-C6-O6	5.10	122.96	119.90
36	1	637	C	N1-C2-O2	5.10	121.96	118.90
36	1	809	G	C5-C6-O6	-5.10	125.54	128.60
36	1	579	G	O5'-P-OP1	5.10	116.82	110.70
1	6	1187	U	C5-C6-N1	5.10	125.25	122.70
36	5	1215	U	C5-C4-O4	-5.10	122.84	125.90
36	5	2145	A	C4-N9-C1'	5.10	135.48	126.30
1	2	408	C	N1-C2-O2	-5.10	115.84	118.90
36	1	1107	C	C6-N1-C2	5.10	122.34	120.30
36	1	1547	G	C5-N7-C8	5.10	106.85	104.30
36	1	2760	C	C4-C5-C6	5.10	119.95	117.40
38	4	113	U	C4-C5-C6	5.10	122.76	119.70
1	6	1152	A	C8-N9-C4	5.10	107.84	105.80
36	5	1590	G	N1-C6-O6	-5.10	116.84	119.90
36	5	3198	U	OP1-P-OP2	5.10	127.25	119.60
36	5	3287	U	C6-N1-C2	-5.10	117.94	121.00
36	5	649	A	N1-C2-N3	-5.10	126.75	129.30
36	5	1140	G	OP1-P-O3'	5.10	116.41	105.20
36	5	1534	A	C2-N3-C4	5.10	113.15	110.60
36	5	2797	C	N1-C2-O2	-5.10	115.84	118.90
36	5	3335	A	C6-C5-N7	-5.10	128.73	132.30
44	17	229	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	2	1241	G	N7-C8-N9	5.09	115.65	113.10
36	1	859	G	C8-N9-C4	5.09	108.44	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2249	G	N9-C1'-C2'	-5.09	106.40	112.00
1	6	1480	G	C4-C5-N7	5.09	112.84	110.80
36	5	3004	C	C4-C5-C6	-5.09	114.85	117.40
36	5	2199	G	C4-N9-C1'	5.09	133.12	126.50
36	5	2392	C	N1-C2-O2	-5.09	115.84	118.90
1	2	802	G	N3-C4-C5	-5.09	126.05	128.60
36	1	927	C	C5-C4-N4	-5.09	116.64	120.20
36	1	1849	C	C5-C4-N4	-5.09	116.64	120.20
36	1	2614	G	C5-N7-C8	5.09	106.84	104.30
36	1	2835	U	C6-N1-C2	5.09	124.06	121.00
1	6	337	G	N3-C4-C5	-5.09	126.06	128.60
36	5	1452	A	C6-C5-N7	-5.09	128.74	132.30
37	7	103	A	C5-C6-N1	5.09	120.25	117.70
1	2	885	G	N1-C6-O6	5.09	122.95	119.90
36	1	922	U	C6-N1-C1'	-5.09	114.08	121.20
36	1	2325	G	C5-N7-C8	-5.09	101.76	104.30
36	1	2832	C	OP1-P-OP2	5.09	127.23	119.60
36	1	3101	G	C2-N3-C4	5.09	114.44	111.90
37	3	81	U	C5-C6-N1	-5.09	120.16	122.70
1	6	136	C	C2-N1-C1'	5.09	124.40	118.80
1	6	1412	G	N9-C4-C5	5.09	107.44	105.40
36	5	1178	G	C4-C5-N7	5.09	112.84	110.80
36	5	2830	G	C4-C5-C6	5.09	121.85	118.80
36	5	3330	A	N1-C6-N6	-5.09	115.55	118.60
36	1	298	U	N3-C2-O2	-5.09	118.64	122.20
36	1	1349	G	N3-C4-N9	5.09	129.05	126.00
37	7	105	C	C2-N3-C4	5.09	122.44	119.90
1	2	553	G	C4-C5-C6	5.09	121.85	118.80
1	2	1659	A	N7-C8-N9	5.09	116.34	113.80
36	1	304	G	C6-N1-C2	-5.09	122.05	125.10
36	1	398	A	O5'-P-OP2	-5.09	101.12	105.70
36	1	1664	G	C8-N9-C4	-5.09	104.37	106.40
1	6	571	G	N1-C6-O6	-5.09	116.85	119.90
1	6	636	A	OP1-P-OP2	-5.09	111.97	119.60
36	5	1115	G	OP1-P-OP2	-5.09	111.97	119.60
36	5	1891	A	N1-C6-N6	5.08	121.65	118.60
1	2	1596	C	N3-C2-O2	-5.08	118.34	121.90
36	1	711	A	OP2-P-O3'	5.08	116.38	105.20
36	1	1217	A	OP2-P-O3'	5.08	116.38	105.20
38	4	88	A	C8-N9-C4	5.08	107.83	105.80
1	6	1478	G	C4-N9-C1'	5.08	133.11	126.50
36	5	845	G	N9-C4-C5	-5.08	103.37	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	971	G	C5-N7-C8	5.08	106.84	104.30
36	5	1914	G	C5-C6-O6	5.08	131.65	128.60
36	5	2865	U	N1-C2-O2	5.08	126.36	122.80
1	2	456	A	N1-C6-N6	-5.08	115.55	118.60
36	1	590	G	N3-C4-N9	5.08	129.05	126.00
36	1	1480	G	N1-C6-O6	5.08	122.95	119.90
36	1	1829	G	N1-C2-N3	-5.08	120.85	123.90
36	1	2828	G	C8-N9-C1'	-5.08	120.39	127.00
36	5	651	G	N7-C8-N9	5.08	115.64	113.10
36	5	1142	G	N3-C4-C5	-5.08	126.06	128.60
36	5	2905	U	C5-C6-N1	-5.08	120.16	122.70
36	1	33	G	C4-C5-C6	5.08	121.85	118.80
36	1	269	G	C6-C5-N7	5.08	133.45	130.40
36	1	1433	A	N1-C6-N6	-5.08	115.55	118.60
36	1	1820	U	OP2-P-O3'	5.08	116.38	105.20
1	6	1458	G	C4-N9-C1'	5.08	133.10	126.50
36	5	202	G	N1-C6-O6	5.08	122.95	119.90
36	5	321	C	N1-C2-O2	5.08	121.95	118.90
36	5	647	A	N1-C2-N3	5.08	131.84	129.30
36	5	779	G	C5-C6-O6	-5.08	125.55	128.60
36	5	2231	C	C2-N1-C1'	5.08	124.39	118.80
38	8	91	C	C6-N1-C2	-5.08	118.27	120.30
52	m6	68	ARG	NE-CZ-NH2	5.08	122.84	120.30
36	1	3029	A	C8-N9-C4	-5.08	103.77	105.80
36	5	1177	G	N3-C4-C5	-5.08	126.06	128.60
36	5	1513	G	N7-C8-N9	5.08	115.64	113.10
36	5	2188	A	O5'-P-OP1	-5.08	101.13	105.70
1	2	542	A	C5-N7-C8	-5.08	101.36	103.90
36	1	1001	G	C4-C5-N7	5.08	112.83	110.80
36	1	1484	U	C6-N1-C2	-5.08	117.95	121.00
36	1	1850	A	C4-C5-N7	5.08	113.24	110.70
36	1	2208	A	OP2-P-O3'	5.08	116.37	105.20
36	1	3268	A	C4-C5-C6	5.08	119.54	117.00
37	3	75	G	O5'-P-OP1	-5.08	101.13	105.70
36	5	824	C	N3-C2-O2	-5.08	118.35	121.90
36	5	998	A	N1-C2-N3	5.08	131.84	129.30
36	5	1317	A	C5-C6-N1	5.08	120.24	117.70
36	5	1335	C	N1-C2-O2	-5.08	115.86	118.90
36	5	2908	G	C8-N9-C4	-5.08	104.37	106.40
1	2	1539	G	N7-C8-N9	5.07	115.64	113.10
36	1	989	A	C8-N9-C4	5.07	107.83	105.80
36	1	2355	G	C5-C6-O6	-5.07	125.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1117	U	N1-C2-N3	5.07	117.94	114.90
36	5	155	G	OP1-P-O3'	5.07	116.36	105.20
36	5	283	G	C4-N9-C1'	5.07	133.10	126.50
36	5	1202	A	N1-C2-N3	5.07	131.84	129.30
36	5	2330	C	OP2-P-O3'	5.07	116.36	105.20
36	5	2801	A	C5-C6-N1	5.07	120.24	117.70
36	5	3313	U	OP1-P-OP2	5.07	127.21	119.60
37	7	55	A	C4-C5-N7	5.07	113.24	110.70
36	1	212	G	O4'-C1'-N9	5.07	112.26	108.20
36	1	658	G	C8-N9-C1'	-5.07	120.41	127.00
36	1	2899	C	C2-N1-C1'	5.07	124.38	118.80
1	2	581	U	C2-N1-C1'	5.07	123.78	117.70
36	1	414	U	O5'-P-OP2	-5.07	101.14	105.70
36	1	1108	U	N3-C4-C5	5.07	117.64	114.60
36	1	1362	G	N7-C8-N9	-5.07	110.56	113.10
36	5	2831	G	N3-C4-C5	-5.07	126.06	128.60
36	5	3214	U	N1-C2-N3	5.07	117.94	114.90
36	1	33	G	C5-C6-N1	-5.07	108.97	111.50
36	1	893	C	C6-N1-C2	-5.07	118.27	120.30
36	1	1836	C	N1-C2-O2	5.07	121.94	118.90
36	1	3209	A	C5-C6-N6	-5.07	119.64	123.70
38	4	110	C	N1-C2-O2	-5.07	115.86	118.90
36	1	104	G	OP2-P-O3'	5.07	116.35	105.20
36	1	907	G	O4'-C1'-N9	5.07	112.25	108.20
36	1	1187	C	N3-C4-C5	5.07	123.93	121.90
36	1	2585	G	C2-N3-C4	5.07	114.43	111.90
36	1	2697	A	N9-C4-C5	5.07	107.83	105.80
1	6	794	U	C5-C6-N1	5.07	125.23	122.70
36	5	817	A	OP2-P-O3'	5.07	116.35	105.20
36	5	1878	G	C8-N9-C1'	-5.07	120.41	127.00
36	5	2920	U	C2-N3-C4	-5.07	123.96	127.00
36	1	262	U	N1-C2-O2	-5.07	119.25	122.80
36	1	1476	G	C5-C6-O6	5.07	131.64	128.60
36	1	1496	C	C6-N1-C2	-5.07	118.27	120.30
36	1	2357	A	C8-N9-C4	-5.07	103.77	105.80
36	1	2389	C	N3-C4-C5	5.07	123.93	121.90
36	1	3180	A	N1-C6-N6	5.07	121.64	118.60
1	6	163	G	C8-N9-C1'	5.06	133.58	127.00
36	1	500	C	C6-N1-C2	-5.06	118.28	120.30
36	1	1167	U	C5-C4-O4	5.06	128.94	125.90
36	1	1431	G	N3-C4-C5	-5.06	126.07	128.60
36	1	3010	U	C6-N1-C2	-5.06	117.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	611	U	C2-N1-C1'	5.06	123.78	117.70
36	5	683	U	N3-C4-C5	-5.06	111.56	114.60
36	5	1837	U	N1-C2-O2	-5.06	119.26	122.80
36	5	2968	G	N1-C2-N3	5.06	126.94	123.90
36	5	3309	G	O4'-C1'-N9	5.06	112.25	108.20
36	1	1850	A	C5-N7-C8	-5.06	101.37	103.90
36	1	2599	U	C5-C6-N1	5.06	125.23	122.70
36	1	2814	G	OP1-P-O3'	5.06	116.33	105.20
1	6	1596	C	N3-C4-N4	-5.06	114.46	118.00
36	1	80	G	C5-C6-N1	5.06	114.03	111.50
36	1	885	U	N3-C4-O4	-5.06	115.86	119.40
36	1	2983	C	C5-C6-N1	-5.06	118.47	121.00
1	6	695	U	C5-C6-N1	5.06	125.23	122.70
1	6	1600	A	C4-C5-N7	5.06	113.23	110.70
1	6	1704	U	C2-N1-C1'	5.06	123.77	117.70
36	5	2651	G	N3-C4-C5	5.06	131.13	128.60
42	15	158	ARG	NE-CZ-NH2	-5.06	117.77	120.30
36	1	649	A	N1-C6-N6	-5.06	115.56	118.60
36	1	856	G	N1-C6-O6	5.06	122.93	119.90
36	1	900	G	C4-C5-N7	-5.06	108.78	110.80
1	6	106	U	C6-N1-C1'	5.06	128.28	121.20
1	6	459	G	C8-N9-C4	-5.06	104.38	106.40
1	6	1794	A	N1-C6-N6	-5.06	115.56	118.60
36	5	543	C	C6-N1-C2	-5.06	118.28	120.30
36	5	919	U	C5-C4-O4	-5.06	122.87	125.90
36	5	1342	C	C5-C6-N1	-5.06	118.47	121.00
36	5	1352	A	P-O3'-C3'	5.06	125.77	119.70
36	5	1665	C	N3-C4-C5	5.06	123.92	121.90
36	5	2353	G	C8-N9-C4	5.06	108.42	106.40
36	5	808	A	C8-N9-C4	-5.06	103.78	105.80
36	5	3212	C	C2-N1-C1'	-5.06	113.24	118.80
36	1	1207	G	N9-C4-C5	-5.05	103.38	105.40
36	1	2871	G	C5-C6-O6	-5.05	125.57	128.60
1	6	1761	U	N3-C2-O2	-5.05	118.66	122.20
36	5	1210	U	C5-C4-O4	5.05	128.93	125.90
36	5	2204	C	P-O3'-C3'	5.05	125.77	119.70
36	5	2923	U	N3-C2-O2	-5.05	118.66	122.20
36	1	2336	U	C5-C6-N1	-5.05	120.17	122.70
1	6	1016	C	N3-C2-O2	5.05	125.44	121.90
36	5	1166	G	C5-C6-O6	-5.05	125.57	128.60
36	5	2130	G	N3-C4-N9	-5.05	122.97	126.00
1	2	447	U	N3-C4-C5	-5.05	111.57	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1486	G	C5-N7-C8	-5.05	101.77	104.30
1	2	1573	A	P-O3'-C3'	5.05	125.76	119.70
36	1	1430	U	N3-C2-O2	5.05	125.74	122.20
38	4	28	C	OP2-P-O3'	5.05	116.31	105.20
33	e1	100	LEU	CA-CB-CG	5.05	126.92	115.30
36	5	1442	U	OP1-P-O3'	5.05	116.31	105.20
36	5	2804	A	C5-C6-N6	5.05	127.74	123.70
36	5	2968	G	N3-C4-N9	5.05	129.03	126.00
36	5	3287	U	N1-C2-O2	5.05	126.34	122.80
37	7	92	A	N9-C4-C5	-5.05	103.78	105.80
36	1	939	U	O5'-P-OP2	-5.05	101.16	105.70
36	1	1397	C	C2-N1-C1'	-5.05	113.25	118.80
36	1	1450	G	O5'-P-OP1	-5.05	101.16	105.70
36	1	2617	U	O5'-P-OP1	5.05	116.76	110.70
37	3	117	A	N9-C4-C5	-5.05	103.78	105.80
36	5	352	A	N1-C6-N6	5.05	121.63	118.60
36	5	2689	A	N1-C2-N3	5.05	131.82	129.30
36	5	2699	G	N7-C8-N9	-5.05	110.58	113.10
36	5	2717	U	C2-N1-C1'	-5.05	111.64	117.70
36	5	3125	U	OP1-P-O3'	5.05	116.31	105.20
36	5	3392	U	N1-C2-N3	5.05	117.93	114.90
36	1	1303	A	C8-N9-C4	5.05	107.82	105.80
36	1	1414	G	C5-C6-O6	-5.05	125.57	128.60
36	5	23	A	C8-N9-C4	5.05	107.82	105.80
38	4	72	A	N1-C6-N6	5.05	121.63	118.60
36	5	806	A	N1-C6-N6	-5.05	115.57	118.60
36	5	2360	C	OP2-P-O3'	5.05	116.30	105.20
36	5	2556	C	N3-C2-O2	-5.05	118.37	121.90
36	5	3383	G	N1-C6-O6	5.05	122.93	119.90
36	1	709	A	N7-C8-N9	-5.04	111.28	113.80
36	5	705	A	OP1-P-OP2	-5.04	112.03	119.60
37	7	84	A	OP1-P-O3'	5.04	116.30	105.20
36	1	192	C	C6-N1-C2	-5.04	118.28	120.30
36	1	1475	A	N7-C8-N9	-5.04	111.28	113.80
36	1	1724	U	N1-C2-O2	-5.04	119.27	122.80
36	1	2177	G	N3-C4-N9	5.04	129.03	126.00
36	1	3278	C	C2-N3-C4	5.04	122.42	119.90
1	6	337	G	N1-C2-N2	-5.04	111.66	116.20
1	6	792	U	C6-N1-C2	-5.04	117.97	121.00
1	6	938	G	C6-C5-N7	-5.04	127.37	130.40
1	6	1748	G	N7-C8-N9	-5.04	110.58	113.10
36	5	938	C	OP1-P-O3'	5.04	116.30	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2792	A	C8-N9-C4	-5.04	103.78	105.80
36	1	2851	A	C8-N9-C4	5.04	107.82	105.80
36	1	2964	G	N3-C4-N9	-5.04	122.97	126.00
36	1	3056	U	N1-C2-O2	-5.04	119.27	122.80
36	1	3278	C	C6-N1-C2	-5.04	118.28	120.30
1	6	1498	G	C6-C5-N7	-5.04	127.38	130.40
36	5	579	G	N3-C4-N9	-5.04	122.98	126.00
36	5	1116	G	N9-C4-C5	5.04	107.42	105.40
36	5	1667	A	C4-C5-N7	5.04	113.22	110.70
36	5	1844	C	C2-N1-C1'	5.04	124.35	118.80
36	5	2616	C	OP2-P-O3'	5.04	116.29	105.20
36	1	227	G	C5-C6-O6	-5.04	125.58	128.60
36	5	1493	G	O4'-C1'-N9	5.04	112.23	108.20
36	1	60	A	N9-C4-C5	-5.04	103.78	105.80
36	1	324	A	OP1-P-O3'	5.04	116.29	105.20
36	1	420	G	O5'-P-OP2	-5.04	101.17	105.70
36	1	1513	G	N3-C4-C5	-5.04	126.08	128.60
36	1	1556	C	N3-C2-O2	-5.04	118.37	121.90
36	1	2651	G	O5'-P-OP1	-5.04	101.17	105.70
1	6	1568	C	C2-N1-C1'	5.04	124.34	118.80
36	5	1261	G	O4'-C1'-N9	5.04	112.23	108.20
36	5	1547	G	C8-N9-C4	5.04	108.42	106.40
36	5	1939	G	C4-N9-C1'	5.04	133.05	126.50
36	5	2599	U	C5-C6-N1	-5.04	120.18	122.70
36	1	221	A	N9-C4-C5	5.04	107.81	105.80
1	6	1602	C	N3-C2-O2	-5.04	118.37	121.90
36	1	107	A	N9-C4-C5	-5.04	103.79	105.80
36	1	2874	G	O5'-P-OP1	5.04	116.74	110.70
1	6	406	U	C5-C6-N1	-5.04	120.18	122.70
36	5	2139	A	C2-N3-C4	-5.04	108.08	110.60
37	7	32	U	OP1-P-O3'	5.04	116.28	105.20
38	8	17	A	C2-N3-C4	-5.04	108.08	110.60
1	2	378	A	C4-C5-N7	5.03	113.22	110.70
36	1	188	U	C6-N1-C2	-5.03	117.98	121.00
36	5	1877	U	C6-N1-C2	5.03	124.02	121.00
36	5	2381	G	C4-C5-C6	5.03	121.82	118.80
36	5	2701	U	O5'-P-OP1	-5.03	101.17	105.70
38	8	40	A	C8-N9-C4	-5.03	103.79	105.80
36	1	292	U	N1-C2-O2	-5.03	119.28	122.80
36	1	2293	C	C6-N1-C2	-5.03	118.29	120.30
1	2	378	A	N9-C4-C5	-5.03	103.79	105.80
1	2	1796	C	C4-C5-C6	5.03	119.92	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	713	U	C5-C6-N1	-5.03	120.19	122.70
36	1	881	C	N1-C2-O2	5.03	121.92	118.90
36	1	934	G	C8-N9-C1'	-5.03	120.46	127.00
36	5	510	G	N1-C6-O6	-5.03	116.88	119.90
36	5	806	A	N9-C4-C5	5.03	107.81	105.80
36	5	2136	C	C6-N1-C2	5.03	122.31	120.30
1	2	42	G	C5-C6-O6	5.03	131.62	128.60
36	1	2697	A	C5-C6-N6	5.03	127.72	123.70
36	1	3101	G	C4-C5-C6	-5.03	115.78	118.80
36	5	666	A	O5'-P-OP1	-5.03	101.17	105.70
36	1	1439	U	C6-N1-C2	-5.03	117.98	121.00
36	1	1790	G	O5'-P-OP1	-5.03	101.17	105.70
1	6	1137	A	O5'-P-OP1	5.03	116.73	110.70
36	5	980	A	C5-C6-N1	5.03	120.21	117.70
36	5	1398	U	C6-N1-C1'	5.03	128.24	121.20
36	5	218	G	N1-C6-O6	-5.03	116.88	119.90
36	5	1159	A	O5'-P-OP2	-5.03	101.18	105.70
36	5	2339	C	O4'-C1'-N1	-5.03	104.18	108.20
36	5	2830	G	C4-N9-C1'	5.03	133.03	126.50
36	5	3208	G	N1-C6-O6	5.03	122.92	119.90
36	5	3326	G	N1-C2-N2	-5.03	111.68	116.20
1	2	1012	U	C2-N3-C4	5.02	130.01	127.00
36	1	352	A	O4'-C1'-N9	5.02	112.22	108.20
1	6	45	U	N3-C4-O4	-5.02	115.88	119.40
36	5	1338	C	C5-C4-N4	-5.02	116.68	120.20
36	5	2676	A	C8-N9-C4	-5.02	103.79	105.80
1	2	1432	U	C2-N1-C1'	-5.02	111.67	117.70
36	1	1168	U	N3-C4-O4	-5.02	115.89	119.40
36	1	1378	U	C6-N1-C1'	-5.02	114.17	121.20
36	1	3293	U	N3-C2-O2	5.02	125.72	122.20
1	6	794	U	N1-C2-O2	5.02	126.31	122.80
36	5	646	A	N1-C6-N6	-5.02	115.59	118.60
36	5	1939	G	C8-N9-C1'	-5.02	120.47	127.00
36	5	2375	G	C6-C5-N7	5.02	133.41	130.40
1	2	1651	A	C5-C6-N1	-5.02	115.19	117.70
36	1	24	G	C5-C6-N1	-5.02	108.99	111.50
36	1	3109	G	C2-N3-C4	5.02	114.41	111.90
1	2	1615	C	C6-N1-C2	-5.02	118.29	120.30
36	1	1164	G	C4-C5-C6	5.02	121.81	118.80
36	1	1483	G	O4'-C1'-N9	5.02	112.21	108.20
36	1	3248	C	C5-C6-N1	5.02	123.51	121.00
1	6	670	U	N1-C2-O2	5.02	126.31	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2698	G	C5-C6-O6	-5.02	125.59	128.60
42	15	15	ARG	NE-CZ-NH1	-5.02	117.79	120.30
36	1	1402	C	N3-C4-C5	5.02	123.91	121.90
36	1	3196	U	O4'-C1'-N1	5.02	112.21	108.20
36	5	873	C	P-O3'-C3'	5.02	125.72	119.70
36	5	919	U	C5-C6-N1	-5.02	120.19	122.70
36	5	2968	G	O4'-C1'-N9	-5.02	104.19	108.20
36	5	2988	C	N3-C4-N4	-5.02	114.49	118.00
36	1	1000	C	C6-N1-C1'	-5.01	114.78	120.80
36	1	1318	A	O4'-C1'-N9	-5.01	104.19	108.20
36	1	2521	U	C5-C6-N1	-5.01	120.19	122.70
36	1	2806	U	O5'-P-OP2	-5.01	101.19	105.70
36	1	3295	A	O4'-C1'-N9	5.01	112.21	108.20
1	6	375	U	C2-N1-C1'	-5.01	111.68	117.70
1	6	382	C	N3-C2-O2	5.01	125.41	121.90
1	6	1704	U	C5-C6-N1	5.01	125.21	122.70
36	5	834	U	N3-C4-O4	-5.01	115.89	119.40
36	5	1405	U	N1-C2-N3	5.01	117.91	114.90
36	5	2607	G	N1-C6-O6	-5.01	116.89	119.90
36	1	2223	A	N7-C8-N9	5.01	116.31	113.80
36	5	2218	G	C8-N9-C4	5.01	108.41	106.40
36	5	3176	G	N3-C4-C5	-5.01	126.09	128.60
36	1	60	A	C5-C6-N6	-5.01	119.69	123.70
1	6	751	G	O5'-P-OP1	-5.01	101.19	105.70
1	6	1428	G	C8-N9-C4	-5.01	104.39	106.40
36	5	504	A	N1-C2-N3	-5.01	126.79	129.30
36	5	2617	U	N3-C4-C5	-5.01	111.59	114.60
36	5	2626	A	O5'-P-OP1	-5.01	101.19	105.70
36	5	2707	C	C6-N1-C2	5.01	122.31	120.30
1	2	1659	A	C8-N9-C4	-5.01	103.80	105.80
36	1	1146	C	C5-C6-N1	5.01	123.50	121.00
36	1	3375	A	O5'-P-OP2	-5.01	101.19	105.70
1	6	687	G	N3-C4-C5	5.01	131.10	128.60
1	6	1208	A	O4'-C1'-N9	5.01	112.21	108.20
36	5	2761	G	C5-C6-N1	5.01	114.00	111.50
36	5	2989	U	N1-C2-N3	5.01	117.91	114.90
36	5	2992	U	C6-N1-C1'	-5.01	114.19	121.20
36	5	3097	C	C5-C6-N1	5.01	123.50	121.00
36	1	2400	G	P-O3'-C3'	5.01	125.71	119.70
36	1	3329	U	C6-N1-C2	-5.01	118.00	121.00
36	1	964	G	N1-C2-N2	5.01	120.71	116.20
36	5	6	A	C8-N9-C4	5.01	107.80	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	681	U	C5-C4-O4	-5.01	122.90	125.90
36	1	2944	U	O5'-P-OP1	-5.00	101.20	105.70
38	4	42	G	C2-N3-C4	-5.00	109.40	111.90
1	6	1003	A	O5'-P-OP2	5.00	116.71	110.70
1	6	1421	A	N1-C6-N6	5.00	121.60	118.60
36	5	779	G	N1-C6-O6	5.00	122.90	119.90
36	5	1339	C	C6-N1-C2	-5.00	118.30	120.30
1	2	101	U	C5-C6-N1	-5.00	120.20	122.70
1	2	548	G	N3-C4-C5	-5.00	126.10	128.60
36	1	2748	A	C8-N9-C4	5.00	107.80	105.80
1	6	50	C	N3-C4-C5	-5.00	119.90	121.90
36	5	71	A	O5'-P-OP1	-5.00	101.20	105.70
36	5	370	U	C6-N1-C1'	-5.00	114.19	121.20
36	5	521	A	C2-N3-C4	-5.00	108.10	110.60
36	5	716	A	N1-C6-N6	5.00	121.60	118.60
36	5	2163	C	N3-C2-O2	-5.00	118.40	121.90
36	5	2879	C	N1-C2-O2	-5.00	115.90	118.90
36	1	53	G	C4-C5-N7	-5.00	108.80	110.80
36	1	873	C	C6-N1-C1'	5.00	126.80	120.80
36	1	1329	U	C6-N1-C2	-5.00	118.00	121.00
36	1	1829	G	C2-N3-C4	5.00	114.40	111.90
36	1	2524	A	O4'-C1'-N9	5.00	112.20	108.20
36	1	3140	G	N3-C4-N9	5.00	129.00	126.00
1	6	1030	A	O4'-C1'-N9	-5.00	104.20	108.20
36	5	106	A	N7-C8-N9	-5.00	111.30	113.80
36	5	1117	G	C6-C5-N7	-5.00	127.40	130.40
36	5	1158	A	C4-C5-C6	5.00	119.50	117.00
36	5	1835	A	N1-C6-N6	5.00	121.60	118.60
36	5	3189	G	O5'-P-OP1	-5.00	101.20	105.70

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
19	C7	85	VAL	Peptide
25	D3	78	LYS	Peptide
27	D5	94	LYS	Peptide
28	D6	97	PRO	Peptide
33	E1	146	SER	Peptide
39	L2	142	ASP	Peptide

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Mol	Chain	Res	Type	Group
40	L3	141	GLY	Peptide
43	L6	51	ARG	Peptide
45	L8	30	THR	Peptide
46	L9	21	LYS	Peptide
48	M1	8	PRO	Peptide
52	M6	110	PRO	Peptide
56	N0	22	PRO	Peptide
65	N9	19	ASN	Peptide
65	N9	23	LYS	Peptide
67	O1	5	LYS	Peptide
72	O6	2	THR	Peptide
6	S4	167	GLY	Peptide
9	S7	131	PHE	Peptide
9	S7	30	SER	Peptide
18	c6	40	GLU	Peptide
39	l2	143	GLU	Peptide
43	l6	51	ARG	Peptide
44	l7	192	GLY	Peptide
81	m2	29	UNK	Peptide
52	m6	110	PRO	Peptide
54	m8	169	GLY	Peptide
56	n0	133	ALA	Peptide
59	n3	41	GLY	Peptide
64	n8	66	ALA	Peptide
7	s5	99	MET	Peptide
9	s7	130	VAL	Peptide
10	s8	60	ILE	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%)	139 (68%)	40 (20%)	25 (12%)	0	1
2	s0	204/251 (81%)	148 (72%)	37 (18%)	19 (9%)	0	4
3	S1	212/254 (84%)	147 (69%)	38 (18%)	27 (13%)	0	1
3	s1	214/254 (84%)	164 (77%)	34 (16%)	16 (8%)	1	7
4	S2	215/253 (85%)	177 (82%)	26 (12%)	12 (6%)	2	11
4	s2	215/253 (85%)	171 (80%)	27 (13%)	17 (8%)	1	6
5	S3	221/239 (92%)	176 (80%)	32 (14%)	13 (6%)	1	10
5	s3	221/239 (92%)	172 (78%)	30 (14%)	19 (9%)	1	5
6	S4	258/260 (99%)	205 (80%)	39 (15%)	14 (5%)	2	12
6	s4	258/260 (99%)	206 (80%)	34 (13%)	18 (7%)	1	7
7	S5	204/224 (91%)	149 (73%)	38 (19%)	17 (8%)	1	5
7	s5	204/224 (91%)	145 (71%)	44 (22%)	15 (7%)	1	7
8	S6	224/236 (95%)	194 (87%)	20 (9%)	10 (4%)	2	15
8	s6	216/236 (92%)	184 (85%)	20 (9%)	12 (6%)	2	11
9	S7	182/189 (96%)	132 (72%)	33 (18%)	17 (9%)	0	4
9	s7	184/189 (97%)	142 (77%)	23 (12%)	19 (10%)	0	3
10	S8	184/200 (92%)	150 (82%)	23 (12%)	11 (6%)	1	10
10	s8	184/200 (92%)	155 (84%)	21 (11%)	8 (4%)	2	16
11	S9	183/196 (93%)	146 (80%)	24 (13%)	13 (7%)	1	7
11	s9	183/196 (93%)	144 (79%)	25 (14%)	14 (8%)	1	6
12	C0	94/105 (90%)	68 (72%)	17 (18%)	9 (10%)	0	4
12	c0	92/105 (88%)	60 (65%)	16 (17%)	16 (17%)	0	1
13	C1	153/155 (99%)	118 (77%)	22 (14%)	13 (8%)	1	5
13	c1	144/155 (93%)	112 (78%)	25 (17%)	7 (5%)	2	14
14	C2	122/142 (86%)	70 (57%)	28 (23%)	24 (20%)	0	0
14	c2	122/142 (86%)	68 (56%)	36 (30%)	18 (15%)	0	1
15	C3	148/150 (99%)	120 (81%)	16 (11%)	12 (8%)	1	6
15	c3	148/150 (99%)	112 (76%)	23 (16%)	13 (9%)	1	5
16	C4	125/136 (92%)	92 (74%)	22 (18%)	11 (9%)	1	5
16	c4	126/136 (93%)	94 (75%)	22 (18%)	10 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	C5	122/141 (86%)	89 (73%)	24 (20%)	9 (7%)	1	7
17	c5	133/141 (94%)	87 (65%)	28 (21%)	18 (14%)	0	1
18	C6	139/142 (98%)	108 (78%)	18 (13%)	13 (9%)	0	4
18	c6	140/142 (99%)	111 (79%)	19 (14%)	10 (7%)	1	7
19	C7	116/136 (85%)	86 (74%)	19 (16%)	11 (10%)	0	4
19	c7	113/136 (83%)	84 (74%)	21 (19%)	8 (7%)	1	7
20	C8	143/145 (99%)	110 (77%)	22 (15%)	11 (8%)	1	6
20	c8	143/145 (99%)	112 (78%)	21 (15%)	10 (7%)	1	7
21	C9	141/143 (99%)	114 (81%)	20 (14%)	7 (5%)	2	14
21	c9	141/143 (99%)	109 (77%)	27 (19%)	5 (4%)	3	21
22	D0	105/120 (88%)	87 (83%)	13 (12%)	5 (5%)	2	14
22	d0	108/120 (90%)	83 (77%)	13 (12%)	12 (11%)	0	2
23	D1	85/87 (98%)	54 (64%)	21 (25%)	10 (12%)	0	2
23	d1	85/87 (98%)	66 (78%)	12 (14%)	7 (8%)	1	5
24	D2	127/129 (98%)	103 (81%)	20 (16%)	4 (3%)	4	23
24	d2	127/129 (98%)	111 (87%)	14 (11%)	2 (2%)	9	36
25	D3	142/144 (99%)	107 (75%)	22 (16%)	13 (9%)	1	4
25	d3	142/144 (99%)	120 (84%)	16 (11%)	6 (4%)	3	17
26	D4	132/134 (98%)	107 (81%)	20 (15%)	5 (4%)	3	19
26	d4	132/134 (98%)	101 (76%)	22 (17%)	9 (7%)	1	8
27	D5	68/107 (64%)	39 (57%)	18 (26%)	11 (16%)	0	1
27	d5	67/107 (63%)	51 (76%)	13 (19%)	3 (4%)	2	15
28	D6	95/97 (98%)	55 (58%)	21 (22%)	19 (20%)	0	0
28	d6	95/97 (98%)	72 (76%)	14 (15%)	9 (10%)	0	4
29	D7	79/81 (98%)	58 (73%)	16 (20%)	5 (6%)	1	9
29	d7	79/81 (98%)	64 (81%)	10 (13%)	5 (6%)	1	9
30	D8	61/66 (92%)	45 (74%)	11 (18%)	5 (8%)	1	5
30	d8	61/66 (92%)	40 (66%)	15 (25%)	6 (10%)	0	3
31	D9	51/55 (93%)	43 (84%)	6 (12%)	2 (4%)	3	18
31	d9	51/55 (93%)	41 (80%)	4 (8%)	6 (12%)	0	2
32	E0	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	E1	69/76 (91%)	31 (45%)	22 (32%)	16 (23%)	0	0
33	e1	74/76 (97%)	35 (47%)	18 (24%)	21 (28%)	0	0
34	SR	316/318 (99%)	263 (83%)	41 (13%)	12 (4%)	3	19
34	sR	316/318 (99%)	269 (85%)	37 (12%)	10 (3%)	4	22
35	SM	155/273 (57%)	101 (65%)	33 (21%)	21 (14%)	0	1
35	sM	98/273 (36%)	56 (57%)	29 (30%)	13 (13%)	0	1
39	L2	250/253 (99%)	208 (83%)	30 (12%)	12 (5%)	2	14
39	l2	250/253 (99%)	206 (82%)	26 (10%)	18 (7%)	1	7
40	L3	384/386 (100%)	319 (83%)	46 (12%)	19 (5%)	2	14
40	l3	384/386 (100%)	331 (86%)	40 (10%)	13 (3%)	3	22
41	L4	359/361 (99%)	289 (80%)	42 (12%)	28 (8%)	1	6
41	l4	359/361 (99%)	290 (81%)	44 (12%)	25 (7%)	1	7
42	L5	294/296 (99%)	235 (80%)	42 (14%)	17 (6%)	1	11
42	l5	292/296 (99%)	244 (84%)	36 (12%)	12 (4%)	3	17
43	L6	152/175 (87%)	126 (83%)	21 (14%)	5 (3%)	4	22
43	l6	153/175 (87%)	129 (84%)	21 (14%)	3 (2%)	7	32
44	L7	220/243 (90%)	175 (80%)	35 (16%)	10 (4%)	2	15
44	l7	221/243 (91%)	179 (81%)	34 (15%)	8 (4%)	3	20
45	L8	231/255 (91%)	176 (76%)	42 (18%)	13 (6%)	2	11
45	l8	229/255 (90%)	179 (78%)	32 (14%)	18 (8%)	1	6
46	L9	189/191 (99%)	159 (84%)	23 (12%)	7 (4%)	3	20
46	l9	189/191 (99%)	159 (84%)	24 (13%)	6 (3%)	4	22
47	M0	207/220 (94%)	165 (80%)	27 (13%)	15 (7%)	1	7
47	m0	209/220 (95%)	155 (74%)	39 (19%)	15 (7%)	1	7
48	M1	167/173 (96%)	120 (72%)	27 (16%)	20 (12%)	0	2
48	m1	167/173 (96%)	134 (80%)	22 (13%)	11 (7%)	1	8
49	M3	191/198 (96%)	151 (79%)	29 (15%)	11 (6%)	1	11
49	m3	192/198 (97%)	159 (83%)	17 (9%)	16 (8%)	1	5
50	M4	134/137 (98%)	108 (81%)	17 (13%)	9 (7%)	1	8
50	m4	135/137 (98%)	113 (84%)	18 (13%)	4 (3%)	4	24
51	M5	201/203 (99%)	176 (88%)	20 (10%)	5 (2%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	m5	201/203 (99%)	167 (83%)	26 (13%)	8 (4%)	3	18
52	M6	195/198 (98%)	172 (88%)	18 (9%)	5 (3%)	5	27
52	m6	195/198 (98%)	164 (84%)	22 (11%)	9 (5%)	2	15
53	M7	181/183 (99%)	139 (77%)	32 (18%)	10 (6%)	2	11
53	m7	153/183 (84%)	134 (88%)	17 (11%)	2 (1%)	12	40
54	M8	183/185 (99%)	154 (84%)	24 (13%)	5 (3%)	5	26
54	m8	183/185 (99%)	151 (82%)	27 (15%)	5 (3%)	5	26
55	M9	186/188 (99%)	157 (84%)	25 (13%)	4 (2%)	6	30
55	m9	186/188 (99%)	154 (83%)	28 (15%)	4 (2%)	6	30
56	N0	170/172 (99%)	151 (89%)	13 (8%)	6 (4%)	3	21
56	n0	170/172 (99%)	157 (92%)	11 (6%)	2 (1%)	13	42
57	N1	157/159 (99%)	134 (85%)	16 (10%)	7 (4%)	2	15
57	n1	157/159 (99%)	128 (82%)	23 (15%)	6 (4%)	3	19
58	N2	98/120 (82%)	74 (76%)	16 (16%)	8 (8%)	1	5
58	n2	96/120 (80%)	79 (82%)	11 (12%)	6 (6%)	1	9
59	N3	134/136 (98%)	119 (89%)	12 (9%)	3 (2%)	6	30
59	n3	134/136 (98%)	124 (92%)	9 (7%)	1 (1%)	22	54
60	N4	96/155 (62%)	69 (72%)	19 (20%)	8 (8%)	1	5
60	n4	133/155 (86%)	108 (81%)	14 (10%)	11 (8%)	1	5
61	N5	119/141 (84%)	107 (90%)	11 (9%)	1 (1%)	19	51
61	n5	118/141 (84%)	92 (78%)	17 (14%)	9 (8%)	1	6
62	N6	124/126 (98%)	107 (86%)	13 (10%)	4 (3%)	4	22
62	n6	124/126 (98%)	109 (88%)	11 (9%)	4 (3%)	4	22
63	N7	133/135 (98%)	105 (79%)	20 (15%)	8 (6%)	1	10
63	n7	133/135 (98%)	99 (74%)	24 (18%)	10 (8%)	1	7
64	N8	146/148 (99%)	112 (77%)	25 (17%)	9 (6%)	1	10
64	n8	146/148 (99%)	114 (78%)	24 (16%)	8 (6%)	2	11
65	N9	56/58 (97%)	48 (86%)	7 (12%)	1 (2%)	8	35
65	n9	56/58 (97%)	36 (64%)	14 (25%)	6 (11%)	0	3
66	O0	95/104 (91%)	81 (85%)	12 (13%)	2 (2%)	7	31
66	o0	98/104 (94%)	90 (92%)	7 (7%)	1 (1%)	15	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	O1	107/112 (96%)	92 (86%)	8 (8%)	7 (6%)	1	9
67	o1	107/112 (96%)	83 (78%)	12 (11%)	12 (11%)	0	2
68	O2	125/129 (97%)	109 (87%)	12 (10%)	4 (3%)	4	22
68	o2	125/129 (97%)	101 (81%)	17 (14%)	7 (6%)	2	11
69	O3	104/106 (98%)	88 (85%)	14 (14%)	2 (2%)	8	34
69	o3	104/106 (98%)	90 (86%)	10 (10%)	4 (4%)	3	19
70	O4	110/119 (92%)	87 (79%)	19 (17%)	4 (4%)	3	20
70	o4	110/119 (92%)	93 (84%)	13 (12%)	4 (4%)	3	20
71	O5	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	3	22
71	o5	117/119 (98%)	93 (80%)	20 (17%)	4 (3%)	3	22
72	O6	97/99 (98%)	80 (82%)	9 (9%)	8 (8%)	1	5
72	o6	97/99 (98%)	77 (79%)	12 (12%)	8 (8%)	1	5
73	O7	85/87 (98%)	69 (81%)	15 (18%)	1 (1%)	13	42
73	o7	85/87 (98%)	67 (79%)	15 (18%)	3 (4%)	3	21
74	O8	75/77 (97%)	60 (80%)	12 (16%)	3 (4%)	3	18
74	o8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	2	12
75	O9	48/50 (96%)	38 (79%)	8 (17%)	2 (4%)	3	17
75	o9	48/50 (96%)	40 (83%)	8 (17%)	0	100	100
76	Q0	50/52 (96%)	45 (90%)	3 (6%)	2 (4%)	3	18
76	q0	50/52 (96%)	43 (86%)	5 (10%)	2 (4%)	3	18
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	19 (83%)	2 (9%)	2 (9%)	1	5
78	Q2	103/105 (98%)	72 (70%)	23 (22%)	8 (8%)	1	6
78	q2	103/105 (98%)	93 (90%)	8 (8%)	2 (2%)	8	34
79	Q3	89/91 (98%)	76 (85%)	8 (9%)	5 (6%)	2	11
79	q3	89/91 (98%)	75 (84%)	10 (11%)	4 (4%)	2	15
80	e0	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	8
82	p0	139/311 (45%)	119 (86%)	14 (10%)	6 (4%)	2	16
All	All	22333/24141 (92%)	17773 (80%)	3160 (14%)	1400 (6%)	1	9

All (1400) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	66	ALA
2	S0	102	PHE
2	S0	103	THR
2	S0	139	VAL
2	S0	140	ASN
2	S0	158	VAL
2	S0	190	ASP
2	S0	191	ARG
2	S0	202	TYR
3	S1	37	THR
3	S1	49	ASN
3	S1	58	SER
3	S1	63	GLY
3	S1	81	PHE
3	S1	93	GLY
3	S1	132	ASP
3	S1	179	SER
4	S2	135	SER
5	S3	62	ASN
5	S3	65	ARG
5	S3	93	ASP
5	S3	195	SER
5	S3	211	PRO
5	S3	220	PRO
6	S4	104	ASP
6	S4	200	ARG
7	S5	39	GLU
7	S5	63	GLN
7	S5	101	GLY
8	S6	173	PRO
8	S6	174	LYS
9	S7	12	ALA
9	S7	64	VAL
9	S7	131	PHE
9	S7	134	GLU
9	S7	159	VAL
10	S8	149	SER
11	S9	134	ILE
11	S9	164	PHE
11	S9	168	ARG
11	S9	169	PRO

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Mol	Chain	Res	Type
12	C0	54	TYR
12	C0	60	SER
12	C0	87	VAL
12	C0	88	PRO
13	C1	3	THR
13	C1	7	VAL
13	C1	30	ARG
14	C2	42	ALA
14	C2	55	GLY
14	C2	125	ASN
14	C2	126	TRP
14	C2	131	ASP
15	C3	3	ARG
15	C3	22	ALA
15	C3	27	LYS
15	C3	68	GLY
15	C3	138	ASN
16	C4	39	ILE
16	C4	50	ALA
16	C4	51	ASP
16	C4	124	ASP
16	C4	125	SER
17	C5	54	ALA
17	C5	80	MET
17	C5	125	PRO
17	C5	126	VAL
18	C6	41	PRO
18	C6	59	LYS
18	C6	115	THR
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	113	LEU
20	C8	14	ILE
20	C8	60	GLU
20	C8	83	ALA
20	C8	91	ASP
20	C8	92	ILE
21	C9	31	PRO
21	C9	53	TRP
26	D4	6	THR
26	D4	51	GLU

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Mol	Chain	Res	Type
27	D5	39	ALA
27	D5	43	ASP
27	D5	44	GLN
27	D5	54	VAL
27	D5	86	GLU
27	D5	97	LYS
28	D6	19	LYS
28	D6	36	ILE
28	D6	45	VAL
28	D6	46	GLU
28	D6	65	PRO
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
29	D7	38	PRO
29	D7	62	ILE
32	E0	47	VAL
33	E1	84	VAL
33	E1	87	THR
33	E1	98	VAL
33	E1	102	VAL
33	E1	138	ARG
34	SR	117	LYS
34	SR	160	GLU
34	SR	161	LYS
35	SM	32	SER
35	SM	52	PRO
35	SM	87	THR
35	SM	89	ARG
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
39	L2	202	VAL
39	L2	246	LEU
40	L3	136	LYS
40	L3	138	ALA
40	L3	139	GLN
40	L3	188	ILE
40	L3	212	ASN
40	L3	243	HIS
40	L3	300	ARG
40	L3	385	LYS

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Mol	Chain	Res	Type
41	L4	4	PRO
41	L4	132	ALA
41	L4	146	PRO
41	L4	175	HIS
41	L4	268	ALA
41	L4	270	SER
41	L4	293	SER
41	L4	306	THR
41	L4	317	PRO
41	L4	318	LEU
42	L5	57	ASN
42	L5	153	THR
42	L5	233	ALA
42	L5	234	ASP
42	L5	253	PHE
42	L5	258	LYS
43	L6	59	GLU
43	L6	98	VAL
44	L7	26	VAL
45	L8	25	PRO
45	L8	31	PRO
45	L8	115	ALA
45	L8	116	VAL
47	M0	145	LYS
47	M0	194	GLY
48	M1	8	PRO
48	M1	9	MET
48	M1	11	ASP
48	M1	94	ARG
48	M1	95	ASN
48	M1	115	LYS
48	M1	165	GLN
48	M1	167	TYR
49	M3	129	ASN
49	M3	136	GLU
49	M3	166	ALA
49	M3	193	ALA
50	M4	8	LYS
50	M4	9	ALA
50	M4	136	ALA
52	M6	110	PRO
52	M6	111	PRO

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Mol	Chain	Res	Type
53	M7	109	ALA
53	M7	159	LYS
54	M8	41	ASP
54	M8	99	THR
55	M9	47	ASN
56	N0	130	GLU
56	N0	142	GLN
57	N1	159	PHE
58	N2	59	ASP
58	N2	60	GLY
58	N2	107	PHE
60	N4	64	THR
60	N4	81	PRO
60	N4	97	LYS
63	N7	35	SER
63	N7	128	GLN
64	N8	76	ASP
67	O1	5	LYS
67	O1	83	GLU
68	O2	127	ALA
71	O5	118	ILE
72	O6	33	ALA
72	O6	34	SER
72	O6	99	ARG
75	O9	4	GLN
75	O9	50	ASN
76	Q0	78	ILE
78	Q2	8	ARG
78	Q2	15	LYS
78	Q2	30	ALA
78	Q2	33	ALA
78	Q2	100	LYS
2	s0	4	PRO
2	s0	29	VAL
2	s0	95	ALA
2	s0	189	VAL
2	s0	206	ASP
3	s1	206	PRO
3	s1	210	ILE
4	s2	92	ALA
4	s2	106	ASP
4	s2	107	SER

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Mol	Chain	Res	Type
5	s3	115	ILE
5	s3	195	SER
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	95	THR
6	s4	104	ASP
6	s4	195	ILE
6	s4	196	VAL
7	s5	28	PRO
7	s5	36	ALA
7	s5	43	PHE
7	s5	55	ASP
7	s5	184	PHE
7	s5	205	SER
8	s6	70	PRO
8	s6	153	VAL
8	s6	154	ARG
8	s6	156	PHE
8	s6	173	PRO
8	s6	174	LYS
9	s7	10	SER
9	s7	64	VAL
9	s7	66	SER
9	s7	74	GLN
9	s7	131	PHE
9	s7	163	ASP
11	s9	118	LEU
11	s9	183	ALA
12	c0	31	LYS
12	c0	82	LEU
12	c0	83	PRO
12	c0	88	PRO
12	c0	97	PRO
13	c1	82	ARG
13	c1	129	ARG
14	c2	115	VAL
14	c2	131	ASP
15	c3	19	SER
15	c3	87	ASP
15	c3	88	LEU

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Mol	Chain	Res	Type
16	c4	35	GLY
16	c4	98	GLY
17	c5	11	VAL
17	c5	14	THR
17	c5	51	SER
17	c5	52	LYS
17	c5	68	PRO
17	c5	125	PRO
17	c5	126	VAL
18	c6	39	VAL
18	c6	40	GLU
18	c6	42	GLU
18	c6	113	ASP
18	c6	116	LEU
19	c7	82	ASP
19	c7	86	PRO
19	c7	88	VAL
19	c7	99	VAL
19	c7	104	ASN
20	c8	145	ARG
22	d0	15	GLN
22	d0	51	VAL
22	d0	97	VAL
22	d0	118	VAL
23	d1	4	ASP
23	d1	29	HIS
24	d2	68	ARG
25	d3	138	GLU
26	d4	30	PRO
26	d4	32	ARG
26	d4	33	ALA
26	d4	35	VAL
26	d4	52	LYS
26	d4	121	THR
27	d5	85	LYS
28	d6	8	ASN
28	d6	63	ALA
29	d7	38	PRO
29	d7	59	CYS
29	d7	60	SER
30	d8	61	ARG
31	d9	6	VAL

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Mol	Chain	Res	Type
31	d9	16	LYS
80	e0	45	VAL
80	e0	54	ARG
80	e0	60	PRO
33	e1	79	LYS
33	e1	84	VAL
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	102	VAL
33	e1	103	LEU
33	e1	106	TYR
34	sR	160	GLU
34	sR	161	LYS
34	sR	163	ASP
34	sR	165	ASP
34	sR	318	ALA
35	sM	50	ASN
35	sM	55	SER
39	l2	24	GLN
39	l2	96	LEU
39	l2	115	ASN
39	l2	212	GLY
39	l2	229	ALA
39	l2	249	SER
40	l3	139	GLN
40	l3	235	THR
40	l3	347	SER
41	l4	4	PRO
41	l4	90	PHE
41	l4	301	PRO
41	l4	302	ALA
41	l4	329	PRO
41	l4	330	TYR
41	l4	342	LYS
41	l4	361	HIS
42	l5	132	THR
42	l5	258	LYS
42	l5	260	PHE
43	l6	98	VAL
44	l7	191	VAL
44	l7	193	PRO

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Mol	Chain	Res	Type
44	l7	228	SER
45	l8	25	PRO
45	l8	26	LEU
45	l8	34	PHE
45	l8	122	LYS
47	m0	82	ARG
48	m1	8	PRO
48	m1	10	ARG
48	m1	108	GLU
48	m1	111	ASP
49	m3	47	ALA
49	m3	129	ASN
49	m3	134	GLU
49	m3	152	THR
49	m3	193	ALA
51	m5	91	GLU
52	m6	16	VAL
52	m6	110	PRO
54	m8	91	ALA
54	m8	99	THR
54	m8	112	ALA
55	m9	36	ASN
56	n0	2	ALA
57	n1	122	GLN
57	n1	135	PRO
57	n1	146	ASN
58	n2	49	ASN
60	n4	26	SER
60	n4	63	ILE
60	n4	71	ARG
60	n4	76	VAL
61	n5	25	LYS
61	n5	44	PRO
61	n5	45	LYS
61	n5	48	SER
61	n5	58	ASP
62	n6	83	ASP
62	n6	84	LYS
62	n6	126	LEU
63	n7	36	HIS
63	n7	129	TRP
64	n8	15	VAL

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Mol	Chain	Res	Type
64	n8	76	ASP
65	n9	23	LYS
65	n9	39	PHE
66	o0	104	LEU
67	o1	5	LYS
67	o1	45	GLY
67	o1	84	ASP
68	o2	4	LEU
68	o2	5	PRO
68	o2	27	ARG
69	o3	90	PRO
70	o4	67	LYS
70	o4	79	SER
72	o6	33	ALA
72	o6	34	SER
72	o6	64	SER
72	o6	98	ARG
74	o8	3	ARG
74	o8	17	ARG
76	q0	80	PRO
78	q2	60	LYS
82	p0	93	LEU
2	S0	5	ALA
2	S0	26	ALA
2	S0	27	ARG
2	S0	30	GLN
2	S0	49	ASN
2	S0	111	ILE
2	S0	185	ARG
2	S0	187	ALA
3	S1	54	LEU
3	S1	62	LYS
3	S1	82	ARG
3	S1	158	SER
3	S1	177	GLN
3	S1	206	PRO
3	S1	221	PRO
4	S2	107	SER
4	S2	144	TRP
4	S2	148	LEU
5	S3	51	ARG
5	S3	64	ARG

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Mol	Chain	Res	Type
5	S3	112	GLY
5	S3	216	PRO
5	S3	218	LEU
6	S4	26	CYS
6	S4	142	HIS
7	S5	26	ALA
7	S5	51	VAL
7	S5	58	LEU
7	S5	81	ARG
7	S5	153	GLY
9	S7	11	GLN
9	S7	32	PRO
9	S7	73	VAL
9	S7	116	ARG
9	S7	126	LEU
9	S7	155	ASP
10	S8	40	ALA
10	S8	120	THR
11	S9	118	LEU
11	S9	120	LYS
11	S9	163	PRO
12	C0	34	GLU
13	C1	29	LYS
13	C1	55	ASP
13	C1	145	ALA
13	C1	146	ALA
13	C1	154	ALA
14	C2	66	VAL
14	C2	89	ILE
14	C2	91	VAL
14	C2	93	ASP
14	C2	106	ILE
14	C2	127	GLY
15	C3	24	ALA
16	C4	42	VAL
16	C4	108	SER
16	C4	126	THR
18	C6	39	VAL
18	C6	42	GLU
20	C8	100	THR
21	C9	29	GLU
21	C9	50	ALA

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Mol	Chain	Res	Type
21	C9	69	LYS
21	C9	130	ARG
22	D0	118	VAL
23	D1	49	GLU
25	D3	61	SER
25	D3	70	LYS
25	D3	128	SER
27	D5	71	ILE
28	D6	11	ASN
28	D6	47	ALA
29	D7	51	GLN
29	D7	63	LEU
30	D8	36	THR
31	D9	8	PHE
33	E1	103	LEU
33	E1	110	ALA
33	E1	111	GLU
33	E1	128	ALA
34	SR	48	THR
34	SR	51	ASP
35	SM	139	GLU
35	SM	153	ASP
35	SM	165	LYS
39	L2	13	GLY
39	L2	143	GLU
39	L2	144	ASN
39	L2	250	GLN
40	L3	140	ASP
40	L3	386	ASP
41	L4	90	PHE
41	L4	190	GLY
41	L4	232	SER
41	L4	292	SER
41	L4	304	GLN
41	L4	320	ASN
41	L4	338	LYS
42	L5	59	ASP
42	L5	252	ALA
43	L6	150	LYS
44	L7	24	GLU
45	L8	39	ALA
45	L8	93	LEU

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Mol	Chain	Res	Type
45	L8	135	GLY
45	L8	156	ASP
46	L9	50	ASN
46	L9	96	HIS
46	L9	110	LYS
47	M0	91	VAL
47	M0	117	GLY
47	M0	149	VAL
47	M0	207	GLU
48	M1	24	GLY
49	M3	13	HIS
49	M3	25	HIS
49	M3	47	ALA
50	M4	28	SER
50	M4	135	LEU
51	M5	81	TYR
52	M6	90	HIS
53	M7	163	LYS
53	M7	164	LYS
55	M9	53	LYS
56	N0	139	TYR
57	N1	124	VAL
57	N1	144	GLU
58	N2	11	ILE
58	N2	51	GLY
62	N6	43	TYR
62	N6	84	LYS
63	N7	3	LYS
64	N8	66	ALA
64	N8	93	SER
66	O0	96	GLY
67	O1	6	ASP
67	O1	82	GLU
68	O2	27	ARG
69	O3	40	ASP
70	O4	17	SER
71	O5	97	ALA
72	O6	13	LYS
74	O8	33	LYS
78	Q2	32	LYS
79	Q3	84	ARG
2	s0	30	GLN

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Mol	Chain	Res	Type
2	s0	62	ARG
2	s0	158	VAL
2	s0	186	GLY
2	s0	191	ARG
3	s1	26	ARG
3	s1	93	GLY
3	s1	147	ALA
3	s1	209	ASN
3	s1	223	PHE
4	s2	148	LEU
4	s2	163	GLY
4	s2	164	SER
5	s3	61	GLU
5	s3	76	ARG
5	s3	179	GLN
5	s3	219	ALA
6	s4	90	ILE
6	s4	164	LEU
6	s4	242	LYS
7	s5	98	MET
7	s5	151	GLY
7	s5	204	GLY
8	s6	68	LEU
8	s6	131	LYS
9	s7	67	LEU
11	s9	120	LYS
11	s9	121	SER
12	c0	73	VAL
12	c0	92	ILE
12	c0	94	GLU
13	c1	61	THR
14	c2	22	VAL
14	c2	39	ASP
14	c2	66	VAL
14	c2	101	ALA
14	c2	106	ILE
14	c2	119	SER
15	c3	66	ILE
15	c3	139	TRP
16	c4	67	VAL
16	c4	97	GLY
16	c4	131	GLY

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Mol	Chain	Res	Type
16	c4	132	ARG
17	c5	50	THR
17	c5	71	GLU
17	c5	117	GLY
18	c6	120	ASP
19	c7	113	LEU
20	c8	91	ASP
20	c8	135	GLY
21	c9	28	LEU
21	c9	34	VAL
22	d0	17	GLN
22	d0	45	ALA
22	d0	96	PRO
23	d1	6	GLY
23	d1	64	GLU
24	d2	56	HIS
25	d3	70	LYS
25	d3	101	GLU
26	d4	53	ASP
27	d5	87	GLY
28	d6	47	ALA
28	d6	62	TYR
29	d7	20	LYS
30	d8	20	GLY
30	d8	57	MET
30	d8	65	ARG
31	d9	7	TRP
33	e1	81	LYS
33	e1	85	TYR
33	e1	100	LEU
33	e1	127	GLY
33	e1	145	HIS
33	e1	146	SER
33	e1	148	TYR
34	sR	237	GLN
35	sM	47	ALA
35	sM	48	ARG
35	sM	65	THR
35	sM	67	GLY
35	sM	72	ARG
35	sM	120	GLU
39	l2	54	ARG

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Mol	Chain	Res	Type
39	l2	213	GLY
39	l2	215	ASN
39	l2	238	ILE
40	l3	142	ALA
40	l3	187	SER
40	l3	258	ALA
40	l3	348	ARG
41	l4	26	PHE
41	l4	35	VAL
41	l4	142	VAL
41	l4	190	GLY
41	l4	233	LEU
41	l4	272	VAL
41	l4	328	ASN
41	l4	339	LEU
41	l4	349	THR
44	l7	129	LEU
45	l8	120	LYS
45	l8	239	GLY
46	l9	144	ILE
47	m0	101	LYS
47	m0	117	GLY
47	m0	174	THR
47	m0	207	GLU
47	m0	219	ALA
48	m1	115	LYS
48	m1	116	TYR
48	m1	167	TYR
49	m3	29	ALA
49	m3	76	THR
49	m3	93	ILE
49	m3	135	ALA
49	m3	162	ASN
51	m5	81	TYR
52	m6	13	GLY
52	m6	160	ARG
53	m7	66	SER
54	m8	84	VAL
54	m8	98	LYS
55	m9	183	ALA
56	n0	142	GLN
58	n2	104	ARG

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Mol	Chain	Res	Type
60	n4	25	ASP
60	n4	77	LYS
60	n4	83	THR
61	n5	38	LEU
61	n5	47	ALA
61	n5	55	ASN
62	n6	125	LYS
63	n7	7	ALA
63	n7	16	GLY
63	n7	102	GLU
63	n7	125	GLY
64	n8	47	LYS
64	n8	56	VAL
64	n8	84	GLU
65	n9	24	PRO
67	o1	83	GLU
67	o1	86	LYS
67	o1	91	SER
69	o3	60	ARG
71	o5	40	SER
71	o5	119	LYS
72	o6	63	ASN
72	o6	67	LYS
73	o7	67	LEU
78	q2	17	CYS
82	p0	47	GLY
82	p0	68	SER
82	p0	198	PRO
2	S0	195	TRP
3	S1	26	ARG
3	S1	35	PRO
3	S1	36	SER
4	S2	163	GLY
4	S2	236	PRO
5	S3	81	PRO
5	S3	217	ILE
6	S4	17	HIS
6	S4	96	ASN
7	S5	43	PHE
7	S5	64	VAL
8	S6	25	ARG
8	S6	138	ALA

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Mol	Chain	Res	Type
8	S6	148	SER
8	S6	152	ASP
9	S7	30	SER
9	S7	98	ILE
9	S7	112	ARG
10	S8	22	ARG
10	S8	52	ASN
10	S8	59	ARG
10	S8	152	ILE
10	S8	159	GLN
11	S9	60	LEU
11	S9	98	ALA
11	S9	150	LEU
12	C0	25	LYS
12	C0	93	GLN
14	C2	36	LEU
14	C2	37	VAL
14	C2	69	ALA
14	C2	107	ASP
14	C2	115	VAL
17	C5	51	SER
17	C5	52	LYS
17	C5	101	ALA
17	C5	130	ARG
18	C6	33	GLY
18	C6	40	GLU
18	C6	114	ARG
18	C6	116	LEU
19	C7	83	GLN
19	C7	87	GLU
19	C7	115	LEU
20	C8	25	ASN
21	C9	100	ILE
23	D1	4	ASP
23	D1	7	GLN
23	D1	15	ARG
23	D1	43	GLY
24	D2	30	SER
24	D2	100	GLY
25	D3	11	SER
25	D3	41	SER
25	D3	44	GLY

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Mol	Chain	Res	Type
25	D3	112	LYS
25	D3	114	LYS
25	D3	143	PRO
26	D4	34	ASN
27	D5	56	THR
27	D5	70	LYS
28	D6	5	ARG
28	D6	10	ARG
28	D6	61	GLU
28	D6	62	TYR
28	D6	63	ALA
28	D6	75	VAL
28	D6	97	PRO
33	E1	137	ASP
34	SR	318	ALA
35	SM	95	SER
39	L2	127	ALA
39	L2	133	TYR
39	L2	151	PRO
40	L3	3	HIS
40	L3	83	PRO
40	L3	299	ASP
40	L3	351	LEU
41	L4	15	ALA
41	L4	130	ALA
41	L4	220	ARG
41	L4	361	HIS
42	L5	7	ALA
42	L5	22	ARG
42	L5	137	ASP
42	L5	148	ILE
42	L5	259	LYS
42	L5	276	LYS
44	L7	159	GLN
44	L7	163	LEU
46	L9	2	LYS
47	M0	16	PRO
47	M0	23	ASN
47	M0	113	GLN
47	M0	116	ARG
47	M0	218	ALA
48	M1	28	ASP

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Mol	Chain	Res	Type
48	M1	74	PRO
48	M1	152	HIS
48	M1	166	LYS
50	M4	10	SER
50	M4	29	ALA
50	M4	113	THR
51	M5	144	ARG
53	M7	3	ARG
53	M7	157	VAL
53	M7	160	ALA
53	M7	162	GLU
54	M8	98	LYS
55	M9	26	PRO
55	M9	35	ALA
56	N0	24	LEU
57	N1	123	GLY
57	N1	127	GLN
57	N1	132	PRO
58	N2	22	PRO
59	N3	46	LEU
63	N7	102	GLU
64	N8	47	LYS
68	O2	126	LEU
70	O4	26	PRO
70	O4	86	LYS
74	O8	24	THR
2	s0	10	THR
2	s0	163	ASN
2	s0	164	ASN
2	s0	200	ASP
4	s2	91	ARG
4	s2	93	GLY
4	s2	149	GLY
4	s2	234	PRO
4	s2	238	SER
5	s3	90	ARG
5	s3	144	ALA
5	s3	160	SER
5	s3	196	ARG
6	s4	96	ASN
7	s5	35	GLN
7	s5	57	SER

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Mol	Chain	Res	Type
8	s6	165	GLY
8	s6	175	ILE
9	s7	83	LYS
9	s7	133	THR
9	s7	185	ILE
10	s8	12	SER
10	s8	136	SER
10	s8	137	LYS
11	s9	20	GLU
11	s9	88	GLU
11	s9	150	LEU
11	s9	167	ALA
12	c0	2	LEU
12	c0	23	ALA
12	c0	32	HIS
12	c0	35	ILE
14	c2	58	LEU
14	c2	82	PRO
14	c2	108	ARG
15	c3	43	LYS
15	c3	140	LYS
17	c5	7	ALA
17	c5	48	GLY
18	c6	142	TYR
19	c7	116	LYS
20	c8	61	LEU
21	c9	33	TYR
21	c9	100	ILE
22	d0	49	ASN
25	d3	3	LYS
26	d4	49	LYS
28	d6	13	LYS
28	d6	34	LYS
28	d6	61	GLU
30	d8	36	THR
31	d9	11	PRO
31	d9	17	GLY
33	e1	111	GLU
33	e1	131	PHE
34	sR	279	ALA
35	sM	42	ALA
35	sM	46	LYS

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Mol	Chain	Res	Type
35	sM	171	LYS
39	l2	32	LEU
39	l2	127	ALA
40	l3	386	ASP
41	l4	14	GLU
41	l4	24	ALA
41	l4	43	ASN
41	l4	146	PRO
41	l4	311	HIS
42	l5	178	ASN
42	l5	269	SER
42	l5	270	LYS
42	l5	279	LYS
45	l8	39	ALA
45	l8	69	LEU
45	l8	121	SER
45	l8	133	LYS
45	l8	203	VAL
46	l9	2	LYS
46	l9	108	GLY
46	l9	110	LYS
47	m0	196	PHE
47	m0	204	GLY
48	m1	9	MET
48	m1	114	ILE
49	m3	13	HIS
49	m3	141	ALA
50	m4	10	SER
50	m4	136	ALA
51	m5	104	GLU
51	m5	187	ARG
52	m6	90	HIS
52	m6	163	SER
52	m6	186	ALA
57	n1	80	VAL
57	n1	121	ALA
58	n2	23	THR
60	n4	132	GLY
63	n7	134	LEU
64	n8	129	PHE
65	n9	5	LYS
65	n9	21	ILE

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Mol	Chain	Res	Type
67	o1	25	PHE
68	o2	6	HIS
68	o2	124	GLY
68	o2	127	ALA
69	o3	57	LYS
69	o3	59	VAL
71	o5	82	ALA
71	o5	99	GLN
73	o7	55	ARG
74	o8	18	ALA
77	q1	23	ARG
79	q3	10	ILE
79	q3	51	ALA
2	S0	62	ARG
2	S0	192	THR
2	S0	205	ARG
3	S1	156	ALA
3	S1	207	LEU
3	S1	209	ASN
4	S2	39	THR
4	S2	248	SER
6	S4	39	ARG
6	S4	194	THR
6	S4	245	LYS
7	S5	100	ASN
7	S5	150	GLY
7	S5	154	ALA
8	S6	154	ARG
9	S7	132	PRO
11	S9	162	SER
12	C0	94	GLU
13	C1	4	GLU
13	C1	51	GLY
14	C2	87	PRO
14	C2	101	ALA
14	C2	119	SER
15	C3	19	SER
15	C3	28	LEU
15	C3	137	PRO
15	C3	144	ALA
16	C4	40	ALA
16	C4	75	GLY

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Mol	Chain	Res	Type
17	C5	69	GLU
18	C6	113	ASP
18	C6	124	PRO
19	C7	72	LYS
19	C7	84	TYR
20	C8	61	LEU
20	C8	142	GLY
20	C8	144	ARG
22	D0	17	GLN
25	D3	96	VAL
26	D4	5	VAL
28	D6	64	LEU
29	D7	75	GLU
30	D8	22	ARG
30	D8	35	ASP
33	E1	118	ARG
34	SR	98	GLU
34	SR	237	GLN
35	SM	12	VAL
35	SM	82	THR
35	SM	86	ASN
35	SM	88	ARG
35	SM	101	ASP
35	SM	174	LEU
39	L2	251	LYS
40	L3	155	ALA
40	L3	197	GLU
41	L4	5	GLN
41	L4	140	HIS
41	L4	265	GLU
41	L4	269	SER
41	L4	311	HIS
42	L5	260	PHE
44	L7	217	PRO
44	L7	231	ASN
45	L8	36	ILE
45	L8	94	PHE
45	L8	122	LYS
45	L8	157	VAL
46	L9	177	ASP
47	M0	208	ASN
47	M0	215	GLU

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Mol	Chain	Res	Type
48	M1	108	GLU
48	M1	114	ILE
48	M1	117	ASP
48	M1	151	SER
49	M3	76	THR
50	M4	6	ILE
51	M5	145	ASP
53	M7	23	ARG
53	M7	169	THR
54	M8	162	ALA
54	M8	168	THR
59	N3	47	ASN
60	N4	76	VAL
62	N6	125	LYS
62	N6	126	LEU
63	N7	36	HIS
63	N7	82	PRO
64	N8	24	LYS
64	N8	78	LEU
67	O1	7	VAL
67	O1	84	ASP
70	O4	46	ASP
72	O6	64	SER
78	Q2	96	GLU
79	Q3	7	LYS
2	s0	103	THR
3	s1	60	ALA
3	s1	129	THR
3	s1	207	LEU
4	s2	162	CYS
4	s2	235	LEU
5	s3	142	LEU
6	s4	11	ARG
6	s4	17	HIS
6	s4	23	LEU
6	s4	260	GLY
7	s5	56	ALA
8	s6	143	LYS
9	s7	5	GLN
9	s7	116	ARG
10	s8	62	THR
10	s8	94	ASN

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Mol	Chain	Res	Type
10	s8	107	THR
11	s9	115	LYS
12	c0	3	MET
13	c1	114	ALA
16	c4	96	PRO
16	c4	114	ARG
17	c5	9	LYS
17	c5	12	PHE
17	c5	32	ASP
17	c5	130	ARG
18	c6	97	VAL
18	c6	141	SER
20	c8	55	HIS
20	c8	90	ASN
20	c8	102	ALA
21	c9	29	GLU
22	d0	13	GLU
25	d3	67	ALA
27	d5	103	ARG
28	d6	59	TYR
30	d8	33	LEU
31	d9	12	ARG
33	e1	126	CYS
34	sR	4	ASN
35	sM	43	ASP
35	sM	84	LYS
39	l2	15	ILE
39	l2	56	ALA
39	l2	194	ASN
40	l3	200	GLU
40	l3	239	PRO
41	l4	5	GLN
42	l5	11	ALA
43	l6	10	TYR
43	l6	97	ASN
45	l8	51	LYS
45	l8	82	LEU
47	m0	169	LYS
47	m0	176	LEU
49	m3	60	ALA
50	m4	8	LYS
50	m4	137	LYS

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Mol	Chain	Res	Type
51	m5	68	ARG
51	m5	103	GLU
51	m5	183	THR
52	m6	159	LYS
53	m7	67	ILE
55	m9	143	ILE
58	n2	44	GLU
58	n2	105	LEU
59	n3	16	GLY
61	n5	24	LEU
63	n7	103	GLN
64	n8	12	ARG
67	o1	82	GLU
68	o2	29	ALA
72	o6	4	LYS
72	o6	52	PRO
79	q3	49	ARG
2	S0	33	GLN
3	S1	64	ARG
3	S1	111	ARG
4	S2	67	GLN
4	S2	150	GLN
4	S2	234	PRO
6	S4	38	LEU
6	S4	195	ILE
6	S4	259	GLN
7	S5	127	GLN
8	S6	69	LEU
10	S8	10	LYS
10	S8	86	SER
10	S8	158	SER
13	C1	144	ALA
14	C2	21	GLU
14	C2	108	ARG
14	C2	128	ALA
18	C6	58	ASP
18	C6	112	TYR
20	C8	139	LYS
22	D0	16	GLN
22	D0	21	LYS
22	D0	117	VAL
23	D1	8	LEU

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Mol	Chain	Res	Type
23	D1	10	GLU
23	D1	12	TYR
24	D2	78	ARG
25	D3	5	LYS
25	D3	89	ASN
25	D3	110	LYS
27	D5	55	PRO
30	D8	6	PRO
32	E0	51	ASN
33	E1	83	LYS
33	E1	86	THR
33	E1	100	LEU
34	SR	3	SER
35	SM	22	PRO
39	L2	252	THR
40	L3	317	ILE
41	L4	14	GLU
44	L7	164	SER
44	L7	191	VAL
45	L8	76	ALA
47	M0	24	ARG
48	M1	64	LYS
48	M1	112	LEU
48	M1	173	ASP
49	M3	133	PRO
49	M3	141	ALA
51	M5	94	TYR
56	N0	15	PRO
60	N4	96	LEU
64	N8	117	ARG
65	N9	21	ILE
66	O0	20	SER
67	O1	60	TRP
69	O3	59	VAL
71	O5	75	TYR
72	O6	3	VAL
72	O6	52	PRO
73	O7	87	SER
76	Q0	79	GLU
2	s0	199	PRO
3	s1	22	ASP
3	s1	39	GLU

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Mol	Chain	Res	Type
3	s1	218	LEU
5	s3	43	PRO
6	s4	30	ARG
6	s4	118	GLU
6	s4	168	LYS
9	s7	13	PRO
9	s7	155	ASP
10	s8	78	ILE
11	s9	110	GLN
11	s9	168	ARG
12	c0	24	LYS
13	c1	55	ASP
13	c1	130	PRO
14	c2	40	GLY
14	c2	87	PRO
14	c2	103	LEU
14	c2	118	ALA
15	c3	12	SER
15	c3	22	ALA
15	c3	29	SER
15	c3	108	ASP
16	c4	37	GLU
17	c5	127	ARG
18	c6	32	ASN
19	c7	120	SER
20	c8	14	ILE
22	d0	52	LYS
22	d0	119	ALA
26	d4	84	LYS
28	d6	46	GLU
29	d7	24	LEU
80	e0	47	VAL
33	e1	124	PRO
40	l3	22	ALA
41	l4	144	LYS
41	l4	145	ILE
42	l5	158	ARG
42	l5	220	SER
44	l7	32	ALA
44	l7	159	GLN
44	l7	163	LEU
45	l8	76	ALA

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Mol	Chain	Res	Type
45	l8	112	GLU
45	l8	163	VAL
45	l8	237	ILE
45	l8	249	ARG
46	l9	130	ASP
46	l9	167	VAL
47	m0	220	GLN
48	m1	117	ASP
49	m3	62	THR
49	m3	101	ARG
51	m5	90	ASN
52	m6	47	PHE
60	n4	72	SER
63	n7	28	PRO
65	n9	52	LYS
67	o1	40	ALA
67	o1	90	PHE
67	o1	97	LEU
70	o4	76	TYR
73	o7	85	LYS
77	q1	22	ALA
82	p0	33	VAL
82	p0	102	SER
2	S0	194	PRO
3	S1	60	ALA
4	S2	36	VAL
7	S5	45	LYS
9	S7	125	ILE
11	S9	121	SER
15	C3	117	LEU
19	C7	96	SER
24	D2	83	ILE
27	D5	41	ILE
28	D6	88	SER
30	D8	20	GLY
31	D9	11	PRO
33	E1	85	TYR
34	SR	50	ASP
39	L2	14	SER
40	L3	244	ARG
40	L3	307	PRO
41	L4	23	PRO

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Mol	Chain	Res	Type
43	L6	6	ALA
44	L7	91	GLY
46	L9	59	ASN
46	L9	66	ALA
51	M5	77	LYS
52	M6	16	VAL
52	M6	121	PRO
56	N0	129	ILE
57	N1	18	ASP
58	N2	21	SER
58	N2	27	VAL
60	N4	75	THR
61	N5	50	ALA
63	N7	16	GLY
63	N7	103	GLN
64	N8	96	LYS
71	O5	119	LYS
72	O6	94	ILE
78	Q2	34	SER
79	Q3	51	ALA
2	s0	44	GLY
3	s1	154	SER
4	s2	173	PRO
4	s2	233	GLN
5	s3	45	LYS
5	s3	81	PRO
6	s4	31	PRO
6	s4	214	LEU
6	s4	245	LYS
7	s5	100	ASN
9	s7	53	GLY
9	s7	159	VAL
11	s9	164	PHE
12	c0	95	ARG
12	c0	96	ASN
14	c2	54	ARG
15	c3	137	PRO
16	c4	125	SER
17	c5	100	LYS
20	c8	29	VAL
23	d1	42	GLU
25	d3	27	ASN

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Mol	Chain	Res	Type
33	e1	83	LYS
33	e1	112	GLY
39	l2	41	ILE
39	l2	80	GLU
39	l2	125	ALA
42	l5	12	TYR
42	l5	125	VAL
48	m1	12	LEU
57	n1	124	VAL
60	n4	98	PRO
63	n7	130	PHE
70	o4	78	GLY
3	S1	210	ILE
8	S6	146	GLY
34	SR	206	PRO
35	SM	111	GLY
59	N3	134	GLY
68	O2	70	GLY
2	s0	139	VAL
3	s1	114	VAL
4	s2	150	GLN
5	s3	161	GLY
11	s9	162	SER
23	d1	9	VAL
34	sR	49	GLY
40	l3	305	ILE
44	l7	178	ILE
76	q0	78	ILE
3	S1	21	VAL
6	S4	196	VAL
13	C1	130	PRO
15	C3	11	ILE
19	C7	124	VAL
23	D1	46	ILE
35	SM	20	LEU
44	L7	178	ILE
47	M0	148	VAL
60	N4	16	GLY
64	N8	70	LYS
9	s7	100	PRO
9	s7	172	VAL
10	s8	108	PRO

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Mol	Chain	Res	Type
11	s9	165	GLY
22	d0	19	ILE
23	d1	43	GLY
47	m0	47	PRO
55	m9	48	GLY
64	n8	138	ILE
79	q3	71	VAL
7	S5	89	ILE
12	C0	92	ILE
16	C4	57	PRO
43	L6	36	PRO
49	M3	46	ILE
74	O8	37	PRO
79	Q3	50	GLY
79	Q3	71	VAL
4	s2	182	PRO
7	s5	30	PRO
13	c1	7	VAL
14	c2	91	VAL
34	sR	194	GLY
47	m0	70	ILE
49	m3	50	PRO
74	o8	37	PRO
3	S1	176	VAL
6	S4	233	LYS
7	S5	33	VAL
8	S6	70	PRO
11	S9	160	PRO
13	C1	113	PRO
14	C2	82	PRO
33	E1	127	GLY
34	SR	28	GLY
35	SM	172	VAL
42	L5	19	PRO
42	L5	125	VAL
2	s0	68	PRO
3	s1	221	PRO
8	s6	26	VAL
9	s7	144	VAL
14	c2	89	ILE
15	c3	47	PRO
20	c8	28	ILE

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Mol	Chain	Res	Type
40	l3	33	PRO
47	m0	43	VAL
9	S7	172	VAL
14	C2	22	VAL
23	D1	82	VAL
26	D4	35	VAL
32	E0	50	VAL
60	N4	80	ARG
7	s5	29	ILE
47	m0	179	PRO
58	n2	48	GLY
60	n4	15	PRO
67	o1	59	ILE

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%)	135 (82%)	29 (18%)	2	8
2	s0	165/209 (79%)	131 (79%)	34 (21%)	1	4
3	S1	191/223 (86%)	149 (78%)	42 (22%)	1	3
3	s1	192/223 (86%)	156 (81%)	36 (19%)	1	6
4	S2	176/204 (86%)	134 (76%)	42 (24%)	0	2
4	s2	176/204 (86%)	128 (73%)	48 (27%)	0	1
5	S3	182/194 (94%)	141 (78%)	41 (22%)	1	3
5	s3	182/194 (94%)	144 (79%)	38 (21%)	1	4
6	S4	221/221 (100%)	177 (80%)	44 (20%)	1	5
6	s4	221/221 (100%)	183 (83%)	38 (17%)	2	9
7	S5	173/190 (91%)	143 (83%)	30 (17%)	2	8
7	s5	173/190 (91%)	144 (83%)	29 (17%)	2	9
8	S6	188/201 (94%)	154 (82%)	34 (18%)	1	7
8	s6	187/201 (93%)	153 (82%)	34 (18%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	S7	165/169 (98%)	135 (82%)	30 (18%)	1	7
9	s7	165/169 (98%)	130 (79%)	35 (21%)	1	4
10	S8	150/161 (93%)	117 (78%)	33 (22%)	1	3
10	s8	150/161 (93%)	124 (83%)	26 (17%)	2	8
11	S9	158/165 (96%)	120 (76%)	38 (24%)	0	2
11	s9	158/165 (96%)	120 (76%)	38 (24%)	0	2
12	C0	77/98 (79%)	66 (86%)	11 (14%)	3	15
12	c0	73/98 (74%)	63 (86%)	10 (14%)	3	16
13	C1	129/136 (95%)	109 (84%)	20 (16%)	2	12
13	c1	129/136 (95%)	104 (81%)	25 (19%)	1	5
14	C2	88/118 (75%)	67 (76%)	21 (24%)	0	2
14	c2	88/118 (75%)	71 (81%)	17 (19%)	1	6
15	C3	127/127 (100%)	104 (82%)	23 (18%)	1	7
15	c3	127/127 (100%)	93 (73%)	34 (27%)	0	1
16	C4	81/104 (78%)	61 (75%)	20 (25%)	0	2
16	c4	97/104 (93%)	69 (71%)	28 (29%)	0	1
17	C5	101/117 (86%)	83 (82%)	18 (18%)	2	8
17	c5	103/117 (88%)	90 (87%)	13 (13%)	4	19
18	C6	117/118 (99%)	92 (79%)	25 (21%)	1	4
18	c6	118/118 (100%)	91 (77%)	27 (23%)	1	3
19	C7	94/124 (76%)	70 (74%)	24 (26%)	0	2
19	c7	92/124 (74%)	74 (80%)	18 (20%)	1	5
20	C8	128/128 (100%)	102 (80%)	26 (20%)	1	5
20	c8	128/128 (100%)	99 (77%)	29 (23%)	1	3
21	C9	115/115 (100%)	93 (81%)	22 (19%)	1	6
21	c9	115/115 (100%)	91 (79%)	24 (21%)	1	4
22	D0	100/113 (88%)	81 (81%)	19 (19%)	1	6
22	d0	103/113 (91%)	76 (74%)	27 (26%)	0	2
23	D1	74/74 (100%)	56 (76%)	18 (24%)	0	2
23	d1	74/74 (100%)	53 (72%)	21 (28%)	0	1
24	D2	110/110 (100%)	92 (84%)	18 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	d2	110/110 (100%)	96 (87%)	14 (13%)	4	19
25	D3	119/119 (100%)	100 (84%)	19 (16%)	2	11
25	d3	119/119 (100%)	94 (79%)	25 (21%)	1	4
26	D4	112/112 (100%)	92 (82%)	20 (18%)	2	8
26	d4	112/112 (100%)	91 (81%)	21 (19%)	1	6
27	D5	61/88 (69%)	42 (69%)	19 (31%)	0	1
27	d5	61/88 (69%)	53 (87%)	8 (13%)	4	17
28	D6	83/83 (100%)	60 (72%)	23 (28%)	0	1
28	d6	83/83 (100%)	62 (75%)	21 (25%)	0	2
29	D7	70/70 (100%)	58 (83%)	12 (17%)	2	9
29	d7	70/70 (100%)	62 (89%)	8 (11%)	5	22
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1	4
30	d8	56/59 (95%)	46 (82%)	10 (18%)	2	8
31	D9	47/48 (98%)	41 (87%)	6 (13%)	4	18
31	d9	47/48 (98%)	35 (74%)	12 (26%)	0	2
32	E0	51/51 (100%)	42 (82%)	9 (18%)	2	8
33	E1	62/66 (94%)	41 (66%)	21 (34%)	0	1
33	e1	66/66 (100%)	50 (76%)	16 (24%)	0	2
34	SR	260/261 (100%)	227 (87%)	33 (13%)	4	19
34	sR	260/261 (100%)	221 (85%)	39 (15%)	3	13
35	SM	97/228 (42%)	75 (77%)	22 (23%)	1	3
35	sM	54/228 (24%)	42 (78%)	12 (22%)	1	3
39	L2	193/195 (99%)	155 (80%)	38 (20%)	1	5
39	l2	192/195 (98%)	150 (78%)	42 (22%)	1	3
40	L3	321/322 (100%)	250 (78%)	71 (22%)	1	3
40	l3	320/322 (99%)	250 (78%)	70 (22%)	1	3
41	L4	288/288 (100%)	224 (78%)	64 (22%)	1	3
41	l4	288/288 (100%)	222 (77%)	66 (23%)	1	3
42	L5	244/244 (100%)	199 (82%)	45 (18%)	1	7
42	l5	243/244 (100%)	190 (78%)	53 (22%)	1	4
43	L6	134/152 (88%)	115 (86%)	19 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	l6	135/152 (89%)	114 (84%)	21 (16%)	2	12
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4	18
44	l7	187/204 (92%)	158 (84%)	29 (16%)	2	12
45	L8	187/207 (90%)	145 (78%)	42 (22%)	1	3
45	l8	177/207 (86%)	143 (81%)	34 (19%)	1	6
46	L9	171/171 (100%)	136 (80%)	35 (20%)	1	4
46	l9	171/171 (100%)	127 (74%)	44 (26%)	0	2
47	M0	177/186 (95%)	143 (81%)	34 (19%)	1	6
47	m0	179/186 (96%)	146 (82%)	33 (18%)	1	7
48	M1	147/150 (98%)	116 (79%)	31 (21%)	1	4
48	m1	147/150 (98%)	110 (75%)	37 (25%)	0	2
49	M3	154/158 (98%)	130 (84%)	24 (16%)	2	12
49	m3	154/158 (98%)	123 (80%)	31 (20%)	1	5
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	8
50	m4	108/108 (100%)	89 (82%)	19 (18%)	2	8
51	M5	175/175 (100%)	142 (81%)	33 (19%)	1	6
51	m5	175/175 (100%)	142 (81%)	33 (19%)	1	6
52	M6	160/161 (99%)	133 (83%)	27 (17%)	2	9
52	m6	160/161 (99%)	126 (79%)	34 (21%)	1	4
53	M7	140/145 (97%)	110 (79%)	30 (21%)	1	4
53	m7	125/145 (86%)	100 (80%)	25 (20%)	1	5
54	M8	150/150 (100%)	132 (88%)	18 (12%)	5	20
54	m8	150/150 (100%)	120 (80%)	30 (20%)	1	5
55	M9	153/153 (100%)	125 (82%)	28 (18%)	1	7
55	m9	153/153 (100%)	126 (82%)	27 (18%)	2	8
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1	5
56	n0	156/156 (100%)	120 (77%)	36 (23%)	1	3
57	N1	136/136 (100%)	109 (80%)	27 (20%)	1	5
57	n1	136/136 (100%)	104 (76%)	32 (24%)	1	3
58	N2	87/106 (82%)	77 (88%)	10 (12%)	5	22
58	n2	85/106 (80%)	69 (81%)	16 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	N3	104/104 (100%)	84 (81%)	20 (19%)	1	6
59	n3	104/104 (100%)	90 (86%)	14 (14%)	4	16
60	N4	57/129 (44%)	51 (90%)	6 (10%)	7	25
60	n4	100/129 (78%)	83 (83%)	17 (17%)	2	9
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	3
61	n5	104/117 (89%)	82 (79%)	22 (21%)	1	4
62	N6	109/109 (100%)	83 (76%)	26 (24%)	0	2
62	n6	109/109 (100%)	85 (78%)	24 (22%)	1	3
63	N7	115/115 (100%)	89 (77%)	26 (23%)	1	3
63	n7	115/115 (100%)	90 (78%)	25 (22%)	1	4
64	N8	118/118 (100%)	96 (81%)	22 (19%)	1	7
64	n8	118/118 (100%)	94 (80%)	24 (20%)	1	5
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	5
65	n9	46/46 (100%)	35 (76%)	11 (24%)	0	2
66	O0	81/87 (93%)	61 (75%)	20 (25%)	0	2
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1	5
67	O1	92/96 (96%)	73 (79%)	19 (21%)	1	4
67	o1	94/96 (98%)	70 (74%)	24 (26%)	0	2
68	O2	109/110 (99%)	86 (79%)	23 (21%)	1	4
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	3
69	O3	90/90 (100%)	74 (82%)	16 (18%)	2	8
69	o3	90/90 (100%)	70 (78%)	20 (22%)	1	3
70	O4	95/101 (94%)	74 (78%)	21 (22%)	1	3
70	o4	95/101 (94%)	73 (77%)	22 (23%)	1	3
71	O5	104/104 (100%)	84 (81%)	20 (19%)	1	6
71	o5	103/104 (99%)	80 (78%)	23 (22%)	1	3
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1	4
72	o6	80/81 (99%)	58 (72%)	22 (28%)	0	1
73	O7	70/70 (100%)	55 (79%)	15 (21%)	1	4
73	o7	70/70 (100%)	57 (81%)	13 (19%)	1	7
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	o8	67/68 (98%)	51 (76%)	16 (24%)	0	2
75	O9	45/45 (100%)	38 (84%)	7 (16%)	2	12
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	8
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	3	13
76	q0	47/47 (100%)	33 (70%)	14 (30%)	0	1
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	0	2
78	q2	90/90 (100%)	73 (81%)	17 (19%)	1	6
79	Q3	71/71 (100%)	58 (82%)	13 (18%)	1	7
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1	3
80	e0	53/53 (100%)	38 (72%)	15 (28%)	0	1
82	p0	105/253 (42%)	84 (80%)	21 (20%)	1	5
All	All	18729/20239 (92%)	14954 (80%)	3775 (20%)	1	5

All (3775) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	7	PHE
2	S0	12	GLU
2	S0	17	LEU
2	S0	22	THR
2	S0	32	HIS
2	S0	37	VAL
2	S0	41	ARG
2	S0	50	VAL
2	S0	59	LEU
2	S0	84	ARG
2	S0	86	VAL
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	101	ARG
2	S0	111	ILE
2	S0	131	GLN
2	S0	140	ASN
2	S0	150	ASP

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Mol	Chain	Res	Type
2	S0	156	VAL
2	S0	157	ASP
2	S0	170	ILE
2	S0	172	LEU
2	S0	179	ARG
2	S0	184	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	196	SER
2	S0	197	ILE
3	S1	21	VAL
3	S1	25	THR
3	S1	26	ARG
3	S1	29	TRP
3	S1	30	PHE
3	S1	36	SER
3	S1	39	GLU
3	S1	42	ASN
3	S1	46	THR
3	S1	51	SER
3	S1	61	LEU
3	S1	70	LEU
3	S1	77	GLU
3	S1	78	ASP
3	S1	80	SER
3	S1	81	PHE
3	S1	85	LYS
3	S1	89	ASP
3	S1	96	LEU
3	S1	97	LEU
3	S1	105	PHE
3	S1	111	ARG
3	S1	112	SER
3	S1	117	TRP
3	S1	126	THR
3	S1	129	THR
3	S1	135	LEU
3	S1	144	ARG
3	S1	146	GLN
3	S1	148	ASN
3	S1	153	HIS
3	S1	154	SER

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Mol	Chain	Res	Type
3	S1	169	SER
3	S1	177	GLN
3	S1	179	SER
3	S1	181	LEU
3	S1	191	GLU
3	S1	193	ILE
3	S1	202	LYS
3	S1	215	VAL
3	S1	222	LYS
3	S1	223	PHE
4	S2	41	LEU
4	S2	50	ILE
4	S2	53	ILE
4	S2	56	ILE
4	S2	60	SER
4	S2	69	ILE
4	S2	72	LEU
4	S2	73	LEU
4	S2	77	GLN
4	S2	79	GLU
4	S2	80	VAL
4	S2	87	GLN
4	S2	89	GLN
4	S2	91	ARG
4	S2	94	GLN
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	111	VAL
4	S2	116	LYS
4	S2	117	THR
4	S2	134	LEU
4	S2	140	ARG
4	S2	141	ARG
4	S2	146	THR
4	S2	148	LEU
4	S2	159	THR
4	S2	166	THR
4	S2	187	LEU
4	S2	190	LEU
4	S2	207	LEU
4	S2	208	GLU

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Mol	Chain	Res	Type
4	S2	221	THR
4	S2	224	PHE
4	S2	225	LEU
4	S2	226	THR
4	S2	229	LEU
4	S2	235	LEU
4	S2	237	VAL
4	S2	240	LEU
4	S2	245	ASP
4	S2	246	GLU
5	S3	4	LEU
5	S3	7	LYS
5	S3	9	ARG
5	S3	14	ASP
5	S3	21	LEU
5	S3	23	GLU
5	S3	44	THR
5	S3	65	ARG
5	S3	70	THR
5	S3	76	ARG
5	S3	84	ILE
5	S3	89	GLU
5	S3	92	GLN
5	S3	93	ASP
5	S3	94	ARG
5	S3	99	VAL
5	S3	103	GLU
5	S3	104	SER
5	S3	111	ASN
5	S3	113	LEU
5	S3	115	ILE
5	S3	117	ARG
5	S3	128	GLU
5	S3	134	CYS
5	S3	139	SER
5	S3	143	ARG
5	S3	151	LYS
5	S3	157	LEU
5	S3	158	ILE
5	S3	172	THR
5	S3	176	LEU
5	S3	177	MET

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Mol	Chain	Res	Type
5	S3	178	ARG
5	S3	181	VAL
5	S3	182	LEU
5	S3	190	ARG
5	S3	195	SER
5	S3	202	LEU
5	S3	204	ASP
5	S3	215	GLU
5	S3	222	VAL
6	S4	9	LEU
6	S4	12	LEU
6	S4	21	ASP
6	S4	38	LEU
6	S4	42	LEU
6	S4	45	ILE
6	S4	49	ARG
6	S4	56	LEU
6	S4	67	GLN
6	S4	68	ARG
6	S4	69	HIS
6	S4	70	VAL
6	S4	77	ARG
6	S4	78	THR
6	S4	92	LEU
6	S4	96	ASN
6	S4	102	VAL
6	S4	108	ARG
6	S4	116	ASP
6	S4	126	VAL
6	S4	129	VAL
6	S4	131	LEU
6	S4	133	LYS
6	S4	156	VAL
6	S4	180	LEU
6	S4	182	TYR
6	S4	184	THR
6	S4	187	ARG
6	S4	192	ILE
6	S4	197	HIS
6	S4	211	LYS
6	S4	212	ASP
6	S4	215	ASP

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Mol	Chain	Res	Type
6	S4	219	VAL
6	S4	221	ARG
6	S4	223	ASN
6	S4	226	PHE
6	S4	227	VAL
6	S4	233	LYS
6	S4	238	LEU
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	259	GLN
7	S5	23	VAL
7	S5	25	LEU
7	S5	32	GLU
7	S5	38	THR
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS
7	S5	49	GLU
7	S5	53	VAL
7	S5	65	ARG
7	S5	70	VAL
7	S5	76	ARG
7	S5	79	ASN
7	S5	81	ARG
7	S5	86	GLN
7	S5	89	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	97	LEU
7	S5	99	MET
7	S5	131	GLN
7	S5	147	THR
7	S5	148	ARG
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	162	VAL
7	S5	163	SER
7	S5	186	ASN
7	S5	217	LEU
8	S6	6	SER

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Mol	Chain	Res	Type
8	S6	15	THR
8	S6	21	GLU
8	S6	25	ARG
8	S6	30	LYS
8	S6	58	LYS
8	S6	71	THR
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	98	ARG
8	S6	101	ILE
8	S6	109	LEU
8	S6	115	LYS
8	S6	120	GLU
8	S6	124	LEU
8	S6	125	THR
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	129	VAL
8	S6	132	ARG
8	S6	133	LEU
8	S6	151	ASP
8	S6	155	ASP
8	S6	169	TYR
8	S6	170	THR
8	S6	175	ILE
8	S6	176	GLN
8	S6	182	GLN
8	S6	193	LEU
8	S6	201	GLN
8	S6	212	LEU
8	S6	223	LYS
9	S7	11	GLN
9	S7	28	GLU
9	S7	38	LEU
9	S7	46	ILE
9	S7	50	ASP
9	S7	51	VAL
9	S7	60	ILE
9	S7	66	SER
9	S7	67	LEU

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Mol	Chain	Res	Type
9	S7	70	PHE
9	S7	74	GLN
9	S7	85	PHE
9	S7	97	ARG
9	S7	104	ARG
9	S7	106	SER
9	S7	110	GLN
9	S7	114	ARG
9	S7	116	ARG
9	S7	118	LEU
9	S7	126	LEU
9	S7	129	LEU
9	S7	144	VAL
9	S7	147	ASN
9	S7	149	ILE
9	S7	156	SER
9	S7	163	ASP
9	S7	166	LEU
9	S7	167	GLU
9	S7	168	SER
9	S7	185	ILE
10	S8	4	SER
10	S8	8	ARG
10	S8	9	HIS
10	S8	14	THR
10	S8	20	GLN
10	S8	21	PHE
10	S8	22	ARG
10	S8	25	ARG
10	S8	26	LYS
10	S8	29	LEU
10	S8	31	ARG
10	S8	36	THR
10	S8	46	VAL
10	S8	49	ARG
10	S8	56	ARG
10	S8	58	LEU
10	S8	73	SER
10	S8	75	LYS
10	S8	82	VAL
10	S8	97	THR
10	S8	103	GLN

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Mol	Chain	Res	Type
10	S8	107	THR
10	S8	121	LEU
10	S8	135	LYS
10	S8	138	ASN
10	S8	151	LYS
10	S8	152	ILE
10	S8	160	PHE
10	S8	164	ARG
10	S8	168	CYS
10	S8	184	LEU
10	S8	193	LEU
10	S8	196	LEU
11	S9	3	ARG
11	S9	6	ARG
11	S9	9	SER
11	S9	14	THR
11	S9	16	LYS
11	S9	22	SER
11	S9	28	LEU
11	S9	30	LEU
11	S9	39	LYS
11	S9	40	LYS
11	S9	46	SER
11	S9	59	LEU
11	S9	78	ARG
11	S9	82	ARG
11	S9	83	VAL
11	S9	87	SER
11	S9	89	ASP
11	S9	93	LEU
11	S9	97	LEU
11	S9	99	LEU
11	S9	101	VAL
11	S9	105	LEU
11	S9	109	LEU
11	S9	118	LEU
11	S9	121	SER
11	S9	122	VAL
11	S9	126	ARG
11	S9	134	ILE
11	S9	138	LYS
11	S9	140	ILE

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Mol	Chain	Res	Type
11	S9	149	ARG
11	S9	151	ASP
11	S9	157	ASP
11	S9	161	THR
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	182	GLU
12	C0	8	ARG
12	C0	27	PHE
12	C0	31	LYS
12	C0	46	LEU
12	C0	55	VAL
12	C0	56	LYS
12	C0	71	GLU
12	C0	76	LEU
12	C0	78	GLU
12	C0	81	ASN
12	C0	82	LEU
13	C1	2	SER
13	C1	10	GLU
13	C1	21	ASN
13	C1	29	LYS
13	C1	37	ASN
13	C1	40	LEU
13	C1	44	THR
13	C1	56	LYS
13	C1	63	LEU
13	C1	67	ARG
13	C1	69	LYS
13	C1	83	THR
13	C1	109	VAL
13	C1	119	VAL
13	C1	123	VAL
13	C1	127	GLN
13	C1	131	ILE
13	C1	136	ARG
13	C1	141	LYS
13	C1	143	SER
14	C2	28	LEU
14	C2	36	LEU
14	C2	37	VAL

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Mol	Chain	Res	Type
14	C2	43	ARG
14	C2	45	LEU
14	C2	46	ARG
14	C2	50	LYS
14	C2	52	LEU
14	C2	54	ARG
14	C2	66	VAL
14	C2	71	ILE
14	C2	74	LEU
14	C2	86	VAL
14	C2	89	ILE
14	C2	97	LEU
14	C2	103	LEU
14	C2	121	VAL
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	139	HIS
15	C3	6	SER
15	C3	9	LYS
15	C3	13	SER
15	C3	19	SER
15	C3	27	LYS
15	C3	34	ILE
15	C3	39	LYS
15	C3	64	ARG
15	C3	66	ILE
15	C3	73	ARG
15	C3	76	LYS
15	C3	94	LYS
15	C3	99	ARG
15	C3	102	LEU
15	C3	109	LYS
15	C3	110	ASP
15	C3	114	ARG
15	C3	115	LEU
15	C3	125	LEU
15	C3	134	VAL
15	C3	142	GLU
15	C3	145	THR
15	C3	151	ASN
16	C4	13	VAL

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Mol	Chain	Res	Type
16	C4	16	VAL
16	C4	29	HIS
16	C4	30	VAL
16	C4	39	ILE
16	C4	42	VAL
16	C4	43	THR
16	C4	48	VAL
16	C4	81	VAL
16	C4	84	ARG
16	C4	92	LYS
16	C4	93	THR
16	C4	108	SER
16	C4	118	VAL
16	C4	123	SER
16	C4	129	LYS
16	C4	132	ARG
16	C4	133	ARG
16	C4	136	ARG
16	C4	137	LEU
17	C5	13	LYS
17	C5	22	LEU
17	C5	26	LEU
17	C5	31	GLU
17	C5	34	VAL
17	C5	35	LYS
17	C5	36	LEU
17	C5	44	ARG
17	C5	52	LYS
17	C5	69	GLU
17	C5	84	ILE
17	C5	86	VAL
17	C5	89	MET
17	C5	110	GLU
17	C5	121	ILE
17	C5	124	THR
17	C5	125	PRO
17	C5	128	HIS
18	C6	4	VAL
18	C6	14	LYS
18	C6	19	VAL
18	C6	29	ILE
18	C6	36	ILE

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Mol	Chain	Res	Type
18	C6	43	ILE
18	C6	44	LEU
18	C6	47	LYS
18	C6	53	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	66	ARG
18	C6	68	ARG
18	C6	69	VAL
18	C6	70	THR
18	C6	82	ARG
18	C6	98	ASP
18	C6	106	LYS
18	C6	118	ILE
18	C6	121	SER
18	C6	123	ARG
18	C6	127	LYS
18	C6	137	ARG
18	C6	138	PHE
18	C6	141	SER
19	C7	3	ARG
19	C7	5	ARG
19	C7	6	THR
19	C7	25	THR
19	C7	30	THR
19	C7	32	LYS
19	C7	34	LEU
19	C7	38	ILE
19	C7	42	GLN
19	C7	46	LEU
19	C7	49	LYS
19	C7	54	THR
19	C7	62	GLN
19	C7	69	ILE
19	C7	72	LYS
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	87	GLU
19	C7	104	ASN
19	C7	105	GLN
19	C7	113	LEU

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Mol	Chain	Res	Type
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	8	GLN
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE
20	C8	18	LEU
20	C8	20	THR
20	C8	28	ILE
20	C8	40	ARG
20	C8	60	GLU
20	C8	61	LEU
20	C8	71	GLN
20	C8	77	THR
20	C8	80	LYS
20	C8	86	LEU
20	C8	93	THR
20	C8	94	ASP
20	C8	97	ASP
20	C8	108	LYS
20	C8	110	ARG
20	C8	115	ARG
20	C8	120	ARG
20	C8	132	ARG
20	C8	136	GLN
20	C8	141	THR
21	C9	4	VAL
21	C9	6	VAL
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	48	GLN
21	C9	57	ARG
21	C9	67	MET
21	C9	89	ARG

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Mol	Chain	Res	Type
21	C9	105	LEU
21	C9	116	ILE
21	C9	126	GLU
21	C9	127	ASN
21	C9	130	ARG
21	C9	131	ASP
21	C9	139	THR
21	C9	144	GLU
22	D0	18	GLN
22	D0	22	ILE
22	D0	23	ARG
22	D0	27	THR
22	D0	29	THR
22	D0	31	VAL
22	D0	33	GLN
22	D0	34	LEU
22	D0	47	GLN
22	D0	48	HIS
22	D0	51	VAL
22	D0	57	ARG
22	D0	61	LYS
22	D0	74	GLU
22	D0	76	SER
22	D0	89	ARG
22	D0	99	ILE
22	D0	103	ILE
22	D0	121	ASN
23	D1	3	ASN
23	D1	5	LYS
23	D1	9	VAL
23	D1	10	GLU
23	D1	11	LEU
23	D1	18	SER
23	D1	31	SER
23	D1	32	VAL
23	D1	41	GLU
23	D1	52	THR
23	D1	56	SER
23	D1	59	VAL
23	D1	61	SER
23	D1	65	SER
23	D1	69	LEU

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Mol	Chain	Res	Type
23	D1	74	GLN
23	D1	82	VAL
23	D1	84	SER
24	D2	7	LEU
24	D2	23	ARG
24	D2	24	GLN
24	D2	25	VAL
24	D2	53	ILE
24	D2	56	HIS
24	D2	65	LEU
24	D2	71	LYS
24	D2	81	VAL
24	D2	87	GLU
24	D2	93	LEU
24	D2	97	ARG
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR
24	D2	121	VAL
24	D2	129	VAL
25	D3	7	ARG
25	D3	16	ARG
25	D3	19	ARG
25	D3	31	LYS
25	D3	34	LEU
25	D3	53	VAL
25	D3	59	ILE
25	D3	71	CYS
25	D3	73	ARG
25	D3	75	GLN
25	D3	78	LYS
25	D3	84	THR
25	D3	96	VAL
25	D3	103	LEU
25	D3	107	PHE
25	D3	109	ARG
25	D3	114	LYS
25	D3	138	GLU
25	D3	144	ARG
26	D4	14	SER
26	D4	17	LEU

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Mol	Chain	Res	Type
26	D4	28	LEU
26	D4	29	HIS
26	D4	32	ARG
26	D4	34	ASN
26	D4	52	LYS
26	D4	57	VAL
26	D4	61	ARG
26	D4	74	LEU
26	D4	78	SER
26	D4	79	VAL
26	D4	84	LYS
26	D4	96	LEU
26	D4	98	GLU
26	D4	99	LYS
26	D4	102	LYS
26	D4	112	LYS
26	D4	124	ARG
26	D4	127	LYS
27	D5	37	GLN
27	D5	42	LEU
27	D5	43	ASP
27	D5	48	ASP
27	D5	58	ARG
27	D5	59	TYR
27	D5	60	VAL
27	D5	62	VAL
27	D5	63	SER
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	85	LYS
27	D5	92	ILE
27	D5	95	HIS
27	D5	96	SER
27	D5	100	ILE
27	D5	103	ARG
27	D5	105	THR
28	D6	7	SER
28	D6	15	ARG
28	D6	18	VAL
28	D6	30	ILE
28	D6	36	ILE

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Mol	Chain	Res	Type
28	D6	38	ARG
28	D6	39	MET
28	D6	44	ILE
28	D6	45	VAL
28	D6	52	ASP
28	D6	61	GLU
28	D6	64	LEU
28	D6	66	LYS
28	D6	68	TYR
28	D6	69	ASN
28	D6	70	LYS
28	D6	76	SER
28	D6	79	ILE
28	D6	82	ARG
28	D6	83	ILE
28	D6	85	ARG
28	D6	87	ARG
28	D6	90	GLU
29	D7	3	LEU
29	D7	20	LYS
29	D7	26	GLN
29	D7	30	SER
29	D7	33	LEU
29	D7	43	ILE
29	D7	45	THR
29	D7	55	THR
29	D7	63	LEU
29	D7	67	THR
29	D7	74	SER
29	D7	79	PHE
30	D8	5	THR
30	D8	14	LYS
30	D8	19	THR
30	D8	34	GLU
30	D8	36	THR
30	D8	38	ARG
30	D8	39	THR
30	D8	49	ARG
30	D8	51	ASN
30	D8	54	LEU
30	D8	58	GLU
30	D8	61	ARG

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Mol	Chain	Res	Type
31	D9	6	VAL
31	D9	7	TRP
31	D9	12	ARG
31	D9	40	ARG
31	D9	41	GLN
31	D9	49	ASP
32	E0	16	SER
32	E0	20	LYS
32	E0	26	LYS
32	E0	28	LYS
32	E0	38	LEU
32	E0	42	ARG
32	E0	47	VAL
32	E0	49	LEU
32	E0	50	VAL
33	E1	86	THR
33	E1	89	LYS
33	E1	91	ILE
33	E1	97	LYS
33	E1	98	VAL
33	E1	103	LEU
33	E1	108	VAL
33	E1	113	LYS
33	E1	115	THR
33	E1	117	LEU
33	E1	118	ARG
33	E1	120	GLU
33	E1	126	CYS
33	E1	130	VAL
33	E1	135	HIS
33	E1	137	ASP
33	E1	139	LEU
33	E1	140	TYR
33	E1	145	HIS
33	E1	146	SER
33	E1	151	ASN
34	SR	6	VAL
34	SR	7	LEU
34	SR	10	ARG
34	SR	29	GLN
34	SR	52	GLN
34	SR	60	SER

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Mol	Chain	Res	Type
34	SR	66	HIS
34	SR	76	ASP
34	SR	100	TYR
34	SR	102	ARG
34	SR	117	LYS
34	SR	136	ILE
34	SR	143	THR
34	SR	144	LEU
34	SR	145	LEU
34	SR	149	ASP
34	SR	188	ILE
34	SR	193	ILE
34	SR	195	HIS
34	SR	207	ASP
34	SR	232	TYR
34	SR	238	ASP
34	SR	256	THR
34	SR	258	THR
34	SR	266	ASP
34	SR	270	LEU
34	SR	277	GLU
34	SR	291	SER
34	SR	292	LEU
34	SR	300	THR
34	SR	308	ASN
34	SR	314	GLN
34	SR	317	THR
35	SM	24	GLU
35	SM	34	LYS
35	SM	45	SER
35	SM	51	ARG
35	SM	61	ILE
35	SM	62	ARG
35	SM	68	ARG
35	SM	72	ARG
35	SM	77	THR
35	SM	84	LYS
35	SM	89	ARG
35	SM	91	THR
35	SM	97	THR
35	SM	100	THR
35	SM	102	THR

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Mol	Chain	Res	Type
35	SM	105	LYS
35	SM	106	VAL
35	SM	116	GLU
35	SM	117	LEU
35	SM	121	LYS
35	SM	130	GLU
35	SM	139	GLU
39	L2	14	SER
39	L2	22	LEU
39	L2	23	ARG
39	L2	32	LEU
39	L2	33	ASP
39	L2	36	GLU
39	L2	44	ILE
39	L2	45	VAL
39	L2	48	ILE
39	L2	70	ARG
39	L2	71	LEU
39	L2	73	GLU
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	114	SER
39	L2	148	VAL
39	L2	165	VAL
39	L2	179	LEU
39	L2	180	LEU
39	L2	193	ARG
39	L2	196	TRP
39	L2	200	ARG
39	L2	202	VAL
39	L2	204	MET
39	L2	206	PRO
39	L2	207	VAL
39	L2	223	SER
39	L2	225	ILE
39	L2	227	ARG
39	L2	230	VAL

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Mol	Chain	Res	Type
39	L2	231	SER
39	L2	247	ARG
39	L2	252	THR
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	47	LEU
40	L3	55	THR
40	L3	66	LYS
40	L3	69	LYS
40	L3	72	VAL
40	L3	73	VAL
40	L3	79	VAL
40	L3	85	VAL
40	L3	100	ARG
40	L3	103	THR
40	L3	104	THR
40	L3	114	VAL
40	L3	116	ARG
40	L3	120	LYS
40	L3	126	LYS
40	L3	139	GLN
40	L3	146	ARG
40	L3	148	LEU
40	L3	150	ARG
40	L3	151	ILE
40	L3	164	THR
40	L3	169	THR
40	L3	173	GLN
40	L3	178	LEU
40	L3	187	SER
40	L3	188	ILE
40	L3	196	ARG
40	L3	200	GLU
40	L3	202	THR
40	L3	205	VAL
40	L3	212	ASN

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Mol	Chain	Res	Type
40	L3	226	PHE
40	L3	229	VAL
40	L3	236	LYS
40	L3	238	LEU
40	L3	241	LYS
40	L3	244	ARG
40	L3	252	ILE
40	L3	264	VAL
40	L3	284	ARG
40	L3	296	THR
40	L3	304	THR
40	L3	305	ILE
40	L3	308	MET
40	L3	320	ASP
40	L3	324	VAL
40	L3	328	ILE
40	L3	332	ARG
40	L3	335	ILE
40	L3	337	THR
40	L3	338	LEU
40	L3	347	SER
40	L3	349	LYS
40	L3	351	LEU
40	L3	353	GLU
40	L3	354	VAL
40	L3	355	SER
40	L3	364	LYS
40	L3	379	PHE
40	L3	380	MET
40	L3	382	THR
40	L3	383	LEU
40	L3	385	LYS
41	L4	4	PRO
41	L4	6	VAL
41	L4	7	THR
41	L4	14	GLU
41	L4	25	VAL
41	L4	37	THR
41	L4	41	SER
41	L4	47	ARG
41	L4	54	GLU
41	L4	60	THR

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Mol	Chain	Res	Type
41	L4	63	GLU
41	L4	74	ILE
41	L4	93	MET
41	L4	99	MET
41	L4	112	LYS
41	L4	124	SER
41	L4	133	SER
41	L4	138	ARG
41	L4	145	ILE
41	L4	147	GLU
41	L4	150	LEU
41	L4	152	VAL
41	L4	153	SER
41	L4	156	LEU
41	L4	179	LEU
41	L4	180	LYS
41	L4	182	LEU
41	L4	187	LEU
41	L4	193	LYS
41	L4	198	ARG
41	L4	203	ARG
41	L4	206	LEU
41	L4	215	ILE
41	L4	217	LYS
41	L4	220	ARG
41	L4	222	VAL
41	L4	225	VAL
41	L4	230	VAL
41	L4	246	ARG
41	L4	256	THR
41	L4	258	LEU
41	L4	259	ASP
41	L4	264	SER
41	L4	265	GLU
41	L4	267	VAL
41	L4	269	SER
41	L4	275	THR
41	L4	283	THR
41	L4	284	SER
41	L4	287	THR
41	L4	292	SER
41	L4	297	SER

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Mol	Chain	Res	Type
41	L4	306	THR
41	L4	313	LEU
41	L4	316	ASN
41	L4	323	VAL
41	L4	327	LEU
41	L4	332	LYS
41	L4	333	VAL
41	L4	338	LYS
41	L4	339	LEU
41	L4	346	LYS
41	L4	347	THR
41	L4	361	HIS
42	L5	3	PHE
42	L5	5	LYS
42	L5	8	LYS
42	L5	9	SER
42	L5	22	ARG
42	L5	23	ARG
42	L5	34	LYS
42	L5	35	ARG
42	L5	41	LYS
42	L5	66	SER
42	L5	75	LEU
42	L5	81	HIS
42	L5	89	THR
42	L5	105	ILE
42	L5	109	THR
42	L5	110	LEU
42	L5	111	GLN
42	L5	112	LYS
42	L5	115	LEU
42	L5	117	GLU
42	L5	118	THR
42	L5	124	GLU
42	L5	131	LEU
42	L5	132	THR
42	L5	137	ASP
42	L5	140	ARG
42	L5	144	VAL
42	L5	146	LEU
42	L5	148	ILE
42	L5	155	THR

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Mol	Chain	Res	Type
42	L5	159	VAL
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE
42	L5	187	THR
42	L5	196	ARG
42	L5	216	GLU
42	L5	222	LEU
42	L5	227	LEU
42	L5	232	ASP
42	L5	236	LEU
42	L5	257	GLU
42	L5	259	LYS
42	L5	263	GLU
42	L5	273	ARG
43	L6	5	LYS
43	L6	15	VAL
43	L6	18	LEU
43	L6	21	THR
43	L6	46	ARG
43	L6	50	LYS
43	L6	52	VAL
43	L6	64	LEU
43	L6	65	ILE
43	L6	78	ARG
43	L6	84	VAL
43	L6	89	THR
43	L6	90	LYS
43	L6	99	GLU
43	L6	129	GLU
43	L6	134	ARG
43	L6	151	LYS
43	L6	155	LEU
43	L6	173	MET
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	39	GLU
44	L7	40	LYS
44	L7	43	ILE
44	L7	83	LEU
44	L7	88	ARG

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Mol	Chain	Res	Type
44	L7	98	LYS
44	L7	110	ARG
44	L7	111	ILE
44	L7	115	THR
44	L7	120	THR
44	L7	124	LEU
44	L7	128	LYS
44	L7	129	LEU
44	L7	157	ASN
44	L7	178	ILE
44	L7	179	LEU
44	L7	182	ASP
44	L7	184	LEU
44	L7	228	SER
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	27	THR
45	L8	41	GLN
45	L8	43	LYS
45	L8	47	SER
45	L8	50	VAL
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	84	ARG
45	L8	86	THR
45	L8	108	ARG
45	L8	126	SER
45	L8	132	VAL
45	L8	136	LEU
45	L8	144	GLU
45	L8	146	LYS
45	L8	147	LYS
45	L8	150	LEU
45	L8	155	ASN
45	L8	156	ASP
45	L8	163	VAL
45	L8	164	VAL
45	L8	169	LEU
45	L8	173	MET
45	L8	180	VAL

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Mol	Chain	Res	Type
45	L8	181	LYS
45	L8	185	ARG
45	L8	188	THR
45	L8	194	THR
45	L8	197	VAL
45	L8	203	VAL
45	L8	214	LEU
45	L8	217	THR
45	L8	224	ASP
45	L8	227	ASP
45	L8	238	LEU
45	L8	240	ASN
45	L8	241	LYS
45	L8	246	MET
45	L8	248	LYS
45	L8	251	LYS
46	L9	5	GLN
46	L9	9	GLN
46	L9	14	GLU
46	L9	16	VAL
46	L9	18	VAL
46	L9	20	ILE
46	L9	28	VAL
46	L9	41	ILE
46	L9	42	ASP
46	L9	44	THR
46	L9	48	VAL
46	L9	52	LEU
46	L9	53	ILE
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	115	ARG
46	L9	118	LEU
46	L9	129	ARG
46	L9	130	ASP
46	L9	133	THR
46	L9	138	THR
46	L9	141	LYS
46	L9	146	LEU
46	L9	151	VAL
46	L9	157	ASN

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Mol	Chain	Res	Type
46	L9	161	LEU
46	L9	162	GLN
46	L9	164	ILE
46	L9	172	ILE
46	L9	173	ARG
46	L9	174	LYS
46	L9	177	ASP
46	L9	182	SER
46	L9	189	GLU
47	M0	3	ARG
47	M0	15	LYS
47	M0	24	ARG
47	M0	28	ASP
47	M0	30	LYS
47	M0	31	ILE
47	M0	32	ARG
47	M0	33	ILE
47	M0	34	TYR
47	M0	39	LYS
47	M0	40	LYS
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	54	SER
47	M0	57	LEU
47	M0	63	GLU
47	M0	73	ASN
47	M0	74	LYS
47	M0	87	LEU
47	M0	91	VAL
47	M0	102	MET
47	M0	139	ARG
47	M0	143	SER
47	M0	145	LYS
47	M0	156	ARG
47	M0	163	GLN
47	M0	165	ILE
47	M0	169	LYS
47	M0	175	ASN
47	M0	176	LEU
47	M0	189	GLU
47	M0	203	LYS

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Mol	Chain	Res	Type
47	M0	205	SER
48	M1	9	MET
48	M1	10	ARG
48	M1	12	LEU
48	M1	13	LYS
48	M1	16	LYS
48	M1	19	LEU
48	M1	28	ASP
48	M1	34	SER
48	M1	37	LEU
48	M1	39	GLN
48	M1	46	VAL
48	M1	52	TYR
48	M1	53	THR
48	M1	70	THR
48	M1	80	LEU
48	M1	82	ARG
48	M1	92	ARG
48	M1	94	ARG
48	M1	101	ASN
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	115	LYS
48	M1	140	ARG
48	M1	142	LYS
48	M1	147	THR
48	M1	155	THR
48	M1	158	ASP
48	M1	166	LYS
48	M1	168	ASP
48	M1	171	VAL
49	M3	24	VAL
49	M3	33	VAL
49	M3	54	LEU
49	M3	55	ARG
49	M3	59	ARG
49	M3	62	THR
49	M3	67	ARG
49	M3	70	ARG
49	M3	81	LYS
49	M3	107	GLU

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Mol	Chain	Res	Type
49	M3	114	GLN
49	M3	117	LYS
49	M3	124	ILE
49	M3	131	LYS
49	M3	136	GLU
49	M3	138	VAL
49	M3	147	ILE
49	M3	155	GLU
49	M3	157	ARG
49	M3	164	GLU
49	M3	169	THR
49	M3	171	ARG
49	M3	190	LYS
49	M3	194	GLU
50	M4	8	LYS
50	M4	20	VAL
50	M4	24	LYS
50	M4	43	LYS
50	M4	50	LYS
50	M4	53	VAL
50	M4	64	VAL
50	M4	66	THR
50	M4	72	LEU
50	M4	74	ARG
50	M4	90	VAL
50	M4	91	CYS
50	M4	98	SER
50	M4	102	LYS
50	M4	125	LYS
50	M4	126	GLN
50	M4	130	THR
50	M4	133	LYS
50	M4	137	LYS
51	M5	7	LEU
51	M5	10	LEU
51	M5	18	VAL
51	M5	19	LEU
51	M5	22	LEU
51	M5	24	ARG
51	M5	43	THR
51	M5	49	ARG
51	M5	50	ARG

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Mol	Chain	Res	Type
51	M5	56	LYS
51	M5	65	ARG
51	M5	68	ARG
51	M5	71	ARG
51	M5	80	THR
51	M5	85	THR
51	M5	92	LEU
51	M5	93	LYS
51	M5	97	SER
51	M5	98	LEU
51	M5	109	ARG
51	M5	133	ILE
51	M5	138	GLN
51	M5	142	ILE
51	M5	151	ILE
51	M5	155	VAL
51	M5	159	ARG
51	M5	167	THR
51	M5	171	SER
51	M5	184	LYS
51	M5	187	ARG
51	M5	188	ARG
51	M5	190	THR
51	M5	198	SER
52	M6	22	VAL
52	M6	25	LYS
52	M6	34	VAL
52	M6	41	LEU
52	M6	42	ASN
52	M6	44	SER
52	M6	67	THR
52	M6	78	ARG
52	M6	82	LYS
52	M6	84	LEU
52	M6	85	ARG
52	M6	89	SER
52	M6	94	ARG
52	M6	106	GLU
52	M6	108	ILE
52	M6	110	PRO
52	M6	117	ARG
52	M6	122	GLN

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Mol	Chain	Res	Type
52	M6	126	VAL
52	M6	128	ARG
52	M6	140	LYS
52	M6	143	THR
52	M6	144	SER
52	M6	151	ASP
52	M6	180	SER
52	M6	184	THR
52	M6	187	GLU
53	M7	7	THR
53	M7	24	VAL
53	M7	29	THR
53	M7	32	THR
53	M7	36	ILE
53	M7	40	GLU
53	M7	41	LEU
53	M7	49	GLU
53	M7	52	LEU
53	M7	53	ASP
53	M7	56	ARG
53	M7	69	ARG
53	M7	78	VAL
53	M7	79	THR
53	M7	94	LEU
53	M7	112	LEU
53	M7	119	VAL
53	M7	120	ASN
53	M7	126	ARG
53	M7	127	ARG
53	M7	141	SER
53	M7	142	SER
53	M7	144	SER
53	M7	146	ILE
53	M7	148	LEU
53	M7	153	LYS
53	M7	154	GLU
53	M7	171	ARG
53	M7	180	LYS
53	M7	181	ARG
54	M8	3	ILE
54	M8	7	SER
54	M8	26	LEU

Continued on next page...

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Mol	Chain	Res	Type
54	M8	32	LEU
54	M8	34	THR
54	M8	49	LEU
54	M8	57	ILE
54	M8	67	ILE
54	M8	73	GLN
54	M8	95	GLU
54	M8	100	THR
54	M8	105	ARG
54	M8	113	LYS
54	M8	129	VAL
54	M8	135	GLN
54	M8	161	LYS
54	M8	174	ARG
54	M8	178	ARG
55	M9	5	ARG
55	M9	8	LYS
55	M9	17	VAL
55	M9	22	VAL
55	M9	25	ASP
55	M9	27	ASN
55	M9	28	GLU
55	M9	29	THR
55	M9	31	GLU
55	M9	44	LEU
55	M9	55	VAL
55	M9	70	LYS
55	M9	72	GLU
55	M9	75	HIS
55	M9	81	ARG
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	116	ASP
55	M9	117	LYS
55	M9	127	SER
55	M9	134	HIS
55	M9	155	LEU
55	M9	156	ASN
55	M9	164	LEU
55	M9	175	GLN
55	M9	180	LYS

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Mol	Chain	Res	Type
55	M9	182	ASP
56	N0	1	MET
56	N0	3	HIS
56	N0	23	LYS
56	N0	34	GLU
56	N0	45	LEU
56	N0	51	VAL
56	N0	79	VAL
56	N0	80	ARG
56	N0	81	TYR
56	N0	87	THR
56	N0	88	HIS
56	N0	98	SER
56	N0	100	VAL
56	N0	105	THR
56	N0	106	LEU
56	N0	113	ARG
56	N0	115	ARG
56	N0	117	ARG
56	N0	123	ILE
56	N0	131	LYS
56	N0	136	LYS
56	N0	137	ARG
56	N0	138	GLN
56	N0	142	GLN
56	N0	145	THR
56	N0	155	ARG
56	N0	156	VAL
56	N0	162	THR
56	N0	167	ARG
56	N0	171	PHE
56	N0	172	TYR
57	N1	12	ARG
57	N1	16	GLN
57	N1	21	LYS
57	N1	26	HIS
57	N1	27	LEU
57	N1	32	LYS
57	N1	36	VAL
57	N1	52	MET
57	N1	75	ILE
57	N1	78	LYS

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Mol	Chain	Res	Type
57	N1	79	MET
57	N1	83	ARG
57	N1	87	LYS
57	N1	88	ARG
57	N1	89	LEU
57	N1	103	GLN
57	N1	104	GLU
57	N1	124	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	134	GLN
57	N1	139	ARG
57	N1	144	GLU
57	N1	149	GLN
57	N1	151	LEU
57	N1	154	VAL
57	N1	158	THR
58	N2	10	LYS
58	N2	29	ASP
58	N2	39	ASP
58	N2	43	VAL
58	N2	52	ASN
58	N2	54	VAL
58	N2	66	VAL
58	N2	70	LYS
58	N2	88	GLN
58	N2	93	ILE
59	N3	13	ILE
59	N3	14	SER
59	N3	32	ARG
59	N3	44	SER
59	N3	54	LEU
59	N3	58	VAL
59	N3	64	LYS
59	N3	69	LEU
59	N3	72	LYS
59	N3	83	LYS
59	N3	84	SER
59	N3	88	ARG
59	N3	102	ILE
59	N3	104	ASN
59	N3	106	LYS

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Mol	Chain	Res	Type
59	N3	115	THR
59	N3	120	LYS
59	N3	125	LEU
59	N3	135	VAL
59	N3	137	VAL
60	N4	5	ILE
60	N4	7	SER
60	N4	19	THR
60	N4	39	LEU
60	N4	42	GLN
60	N4	64	THR
61	N5	27	ARG
61	N5	38	LEU
61	N5	39	LYS
61	N5	40	LEU
61	N5	59	SER
61	N5	63	ILE
61	N5	75	LYS
61	N5	92	LYS
61	N5	96	LYS
61	N5	108	LEU
61	N5	109	LYS
61	N5	113	LEU
61	N5	115	ARG
61	N5	116	PRO
61	N5	119	THR
61	N5	125	ARG
61	N5	126	LEU
61	N5	133	LEU
61	N5	134	ASP
61	N5	135	ILE
61	N5	138	ARG
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	5	SER
62	N6	6	LEU
62	N6	13	ARG
62	N6	30	LEU
62	N6	35	LEU
62	N6	36	SER
62	N6	37	LYS

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Mol	Chain	Res	Type
62	N6	40	ARG
62	N6	42	GLN
62	N6	45	ILE
62	N6	56	VAL
62	N6	57	LEU
62	N6	58	VAL
62	N6	80	VAL
62	N6	81	GLN
62	N6	88	GLU
62	N6	94	SER
62	N6	97	ILE
62	N6	105	VAL
62	N6	110	HIS
62	N6	115	ARG
62	N6	122	LYS
62	N6	125	LYS
62	N6	126	LEU
62	N6	127	GLU
63	N7	14	VAL
63	N7	17	ARG
63	N7	24	VAL
63	N7	26	VAL
63	N7	27	LYS
63	N7	34	LYS
63	N7	42	LEU
63	N7	46	ILE
63	N7	52	LYS
63	N7	54	THR
63	N7	55	LYS
63	N7	57	HIS
63	N7	60	LYS
63	N7	64	LYS
63	N7	72	ILE
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	87	LEU
63	N7	95	VAL
63	N7	106	GLN
63	N7	107	ARG
63	N7	109	GLU
63	N7	127	ASN

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Mol	Chain	Res	Type
63	N7	135	ARG
63	N7	136	PHE
64	N8	6	THR
64	N8	7	LYS
64	N8	8	THR
64	N8	10	LYS
64	N8	14	HIS
64	N8	19	LYS
64	N8	27	LYS
64	N8	29	PRO
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	88	ASP
64	N8	93	SER
64	N8	96	LYS
64	N8	115	LYS
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
64	N8	139	ARG
65	N9	8	THR
65	N9	13	THR
65	N9	14	ARG
65	N9	18	ARG
65	N9	21	ILE
65	N9	25	LYS
65	N9	33	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	11	ASN
66	O0	12	GLN
66	O0	14	LEU
66	O0	16	LEU
66	O0	20	SER
66	O0	24	THR
66	O0	30	THR
66	O0	32	LYS
66	O0	34	LEU

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Mol	Chain	Res	Type
66	O0	36	GLN
66	O0	41	LEU
66	O0	52	ARG
66	O0	54	SER
66	O0	61	MET
66	O0	66	LYS
66	O0	83	LYS
66	O0	87	VAL
66	O0	99	ASP
66	O0	101	LEU
66	O0	102	THR
67	O1	6	ASP
67	O1	13	THR
67	O1	16	LEU
67	O1	26	LYS
67	O1	31	ARG
67	O1	47	ASP
67	O1	64	VAL
67	O1	68	GLU
67	O1	73	LEU
67	O1	76	SER
67	O1	79	ARG
67	O1	82	GLU
67	O1	84	ASP
67	O1	86	LYS
67	O1	89	LEU
67	O1	94	GLU
67	O1	104	LEU
67	O1	106	THR
67	O1	107	VAL
68	O2	4	LEU
68	O2	19	ARG
68	O2	33	ARG
68	O2	41	VAL
68	O2	44	ARG
68	O2	51	SER
68	O2	54	LYS
68	O2	61	LYS
68	O2	67	SER
68	O2	72	LYS
68	O2	73	THR
68	O2	75	LEU

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Mol	Chain	Res	Type
68	O2	76	VAL
68	O2	81	ASP
68	O2	82	LEU
68	O2	84	THR
68	O2	87	MET
68	O2	89	THR
68	O2	101	SER
68	O2	103	LYS
68	O2	111	ARG
68	O2	123	LYS
68	O2	125	ARG
69	O3	14	LEU
69	O3	15	SER
69	O3	21	ARG
69	O3	22	VAL
69	O3	37	THR
69	O3	40	ASP
69	O3	42	GLN
69	O3	59	VAL
69	O3	60	ARG
69	O3	70	LYS
69	O3	72	THR
69	O3	80	VAL
69	O3	81	VAL
69	O3	86	ARG
69	O3	93	THR
69	O3	106	ASN
70	O4	7	PHE
70	O4	8	ARG
70	O4	20	ILE
70	O4	23	VAL
70	O4	24	LYS
70	O4	29	ILE
70	O4	33	GLN
70	O4	36	LYS
70	O4	44	CYS
70	O4	51	LEU
70	O4	52	GLN
70	O4	56	THR
70	O4	71	THR
70	O4	79	SER
70	O4	81	CYS

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Mol	Chain	Res	Type
70	O4	86	LYS
70	O4	87	GLU
70	O4	97	GLU
70	O4	100	ILE
70	O4	102	LYS
70	O4	103	LYS
71	O5	11	THR
71	O5	20	GLN
71	O5	21	LEU
71	O5	27	GLU
71	O5	31	LEU
71	O5	48	ARG
71	O5	49	LYS
71	O5	62	GLN
71	O5	83	LYS
71	O5	85	THR
71	O5	89	ARG
71	O5	90	ARG
71	O5	100	VAL
71	O5	101	THR
71	O5	102	GLU
71	O5	105	ARG
71	O5	107	LYS
71	O5	114	ARG
71	O5	118	ILE
71	O5	119	LYS
72	O6	2	THR
72	O6	7	ILE
72	O6	9	ILE
72	O6	20	MET
72	O6	21	THR
72	O6	26	ILE
72	O6	29	LYS
72	O6	45	ARG
72	O6	52	PRO
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	76	ARG
72	O6	79	SER
72	O6	81	THR
72	O6	98	ARG

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Mol	Chain	Res	Type
72	O6	99	ARG
73	O7	13	ASN
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	26	SER
73	O7	33	THR
73	O7	35	SER
73	O7	44	THR
73	O7	45	ARG
73	O7	55	ARG
73	O7	58	THR
73	O7	59	THR
73	O7	65	ARG
73	O7	67	LEU
73	O7	84	SER
74	O8	3	ARG
74	O8	5	ILE
74	O8	8	ILE
74	O8	12	LEU
74	O8	25	VAL
74	O8	29	LYS
74	O8	31	LEU
74	O8	32	ASN
74	O8	39	ARG
74	O8	45	VAL
74	O8	50	SER
74	O8	53	THR
74	O8	58	ASP
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	72	THR
74	O8	77	ARG
75	O9	5	LYS
75	O9	21	ARG
75	O9	25	GLN
75	O9	27	ILE
75	O9	29	LEU
75	O9	32	ASN
75	O9	36	ARG
76	Q0	78	ILE

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Mol	Chain	Res	Type
76	Q0	97	ARG
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	126	LYS
76	Q0	127	LEU
76	Q0	128	LYS
77	Q1	2	ARG
77	Q1	4	LYS
77	Q1	6	ARG
77	Q1	9	ARG
77	Q1	11	ARG
77	Q1	17	ARG
77	Q1	19	LYS
78	Q2	2	VAL
78	Q2	3	ASN
78	Q2	8	ARG
78	Q2	12	CYS
78	Q2	21	THR
78	Q2	23	HIS
78	Q2	26	THR
78	Q2	35	LEU
78	Q2	38	GLN
78	Q2	47	GLN
78	Q2	60	LYS
78	Q2	78	LYS
78	Q2	80	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	90	HIS
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	21	SER
79	Q3	25	GLN
79	Q3	45	LYS
79	Q3	46	THR
79	Q3	49	ARG
79	Q3	58	SER

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Mol	Chain	Res	Type
79	Q3	59	CYS
79	Q3	60	CYS
79	Q3	70	THR
79	Q3	73	THR
79	Q3	90	VAL
79	Q3	91	GLU
2	s0	6	THR
2	s0	12	GLU
2	s0	17	LEU
2	s0	18	LEU
2	s0	30	GLN
2	s0	31	VAL
2	s0	34	GLU
2	s0	41	ARG
2	s0	45	VAL
2	s0	50	VAL
2	s0	55	GLU
2	s0	62	ARG
2	s0	71	GLU
2	s0	78	SER
2	s0	87	LEU
2	s0	88	LYS
2	s0	106	SER
2	s0	110	TYR
2	s0	124	THR
2	s0	131	GLN
2	s0	144	ILE
2	s0	151	SER
2	s0	156	VAL
2	s0	157	ASP
2	s0	164	ASN
2	s0	165	ARG
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	200	ASP
3	s1	21	VAL
3	s1	25	THR

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Mol	Chain	Res	Type
3	s1	37	THR
3	s1	47	LEU
3	s1	48	VAL
3	s1	51	SER
3	s1	56	SER
3	s1	70	LEU
3	s1	74	GLN
3	s1	80	SER
3	s1	82	ARG
3	s1	83	LYS
3	s1	89	ASP
3	s1	96	LEU
3	s1	105	PHE
3	s1	110	LEU
3	s1	114	VAL
3	s1	115	ARG
3	s1	119	THR
3	s1	120	LEU
3	s1	125	VAL
3	s1	126	THR
3	s1	129	THR
3	s1	135	LEU
3	s1	137	ILE
3	s1	152	ARG
3	s1	159	SER
3	s1	175	GLU
3	s1	180	THR
3	s1	181	LEU
3	s1	195	LYS
3	s1	202	LYS
3	s1	203	ASP
3	s1	210	ILE
3	s1	212	VAL
3	s1	231	LEU
4	s2	39	THR
4	s2	41	LEU
4	s2	52	THR
4	s2	53	ILE
4	s2	54	GLU
4	s2	58	LEU
4	s2	60	SER
4	s2	69	ILE

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Mol	Chain	Res	Type
4	s2	70	ASP
4	s2	72	LEU
4	s2	79	GLU
4	s2	80	VAL
4	s2	81	MET
4	s2	83	ILE
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	95	ARG
4	s2	97	ARG
4	s2	106	ASP
4	s2	108	ASN
4	s2	111	VAL
4	s2	117	THR
4	s2	130	ILE
4	s2	139	ILE
4	s2	141	ARG
4	s2	146	THR
4	s2	152	HIS
4	s2	158	THR
4	s2	159	THR
4	s2	165	VAL
4	s2	166	THR
4	s2	170	ILE
4	s2	182	PRO
4	s2	185	LYS
4	s2	194	GLU
4	s2	195	ASP
4	s2	207	LEU
4	s2	222	TYR
4	s2	225	LEU
4	s2	226	THR
4	s2	229	LEU
4	s2	233	GLN
4	s2	237	VAL
4	s2	240	LEU
4	s2	244	SER
4	s2	248	SER
5	s3	4	LEU
5	s3	7	LYS

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Mol	Chain	Res	Type
5	s3	9	ARG
5	s3	32	GLU
5	s3	34	TYR
5	s3	35	SER
5	s3	37	VAL
5	s3	41	VAL
5	s3	44	THR
5	s3	50	ILE
5	s3	59	LEU
5	s3	61	GLU
5	s3	67	ASN
5	s3	70	THR
5	s3	83	THR
5	s3	84	ILE
5	s3	89	GLU
5	s3	90	ARG
5	s3	97	SER
5	s3	103	GLU
5	s3	109	LEU
5	s3	111	ASN
5	s3	115	ILE
5	s3	125	TYR
5	s3	128	GLU
5	s3	132	LYS
5	s3	142	LEU
5	s3	146	ARG
5	s3	154	ASP
5	s3	158	ILE
5	s3	169	ASP
5	s3	172	THR
5	s3	185	LYS
5	s3	207	THR
5	s3	212	LYS
5	s3	213	GLU
5	s3	223	LYS
5	s3	224	ASP
6	s4	9	LEU
6	s4	12	LEU
6	s4	23	LEU
6	s4	26	CYS
6	s4	32	SER
6	s4	39	ARG

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Mol	Chain	Res	Type
6	s4	42	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	62	LYS
6	s4	89	VAL
6	s4	93	ASP
6	s4	98	ASN
6	s4	104	ASP
6	s4	113	ARG
6	s4	125	LYS
6	s4	126	VAL
6	s4	130	GLN
6	s4	146	THR
6	s4	148	ARG
6	s4	170	THR
6	s4	176	ASP
6	s4	181	VAL
6	s4	182	TYR
6	s4	187	ARG
6	s4	194	THR
6	s4	196	VAL
6	s4	209	HIS
6	s4	214	LEU
6	s4	226	PHE
6	s4	227	VAL
6	s4	236	ILE
6	s4	244	ILE
6	s4	245	LYS
6	s4	246	LEU
6	s4	247	SER
6	s4	248	ILE
6	s4	254	ARG
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU
7	s5	38	THR
7	s5	40	ILE
7	s5	45	LYS
7	s5	58	LEU
7	s5	63	GLN
7	s5	64	VAL
7	s5	68	ILE

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Mol	Chain	Res	Type
7	s5	83	ARG
7	s5	89	ILE
7	s5	93	LEU
7	s5	99	MET
7	s5	102	ARG
7	s5	103	ASN
7	s5	119	ASP
7	s5	125	THR
7	s5	128	ASN
7	s5	130	ILE
7	s5	148	ARG
7	s5	157	ARG
7	s5	163	SER
7	s5	190	ILE
7	s5	192	GLU
7	s5	194	LEU
7	s5	203	LYS
7	s5	216	GLU
7	s5	219	ARG
8	s6	1	MET
8	s6	6	SER
8	s6	10	ASN
8	s6	12	SER
8	s6	15	THR
8	s6	22	HIS
8	s6	43	ASP
8	s6	57	ASP
8	s6	67	VAL
8	s6	71	THR
8	s6	73	ILE
8	s6	74	LYS
8	s6	76	LEU
8	s6	78	THR
8	s6	93	LYS
8	s6	108	VAL
8	s6	109	LEU
8	s6	115	LYS
8	s6	120	GLU
8	s6	121	LEU
8	s6	126	ASP
8	s6	127	THR
8	s6	143	LYS

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Mol	Chain	Res	Type
8	s6	151	ASP
8	s6	153	VAL
8	s6	155	ASP
8	s6	156	PHE
8	s6	162	VAL
8	s6	168	THR
8	s6	182	GLN
8	s6	184	LEU
8	s6	193	LEU
8	s6	211	LEU
8	s6	215	ARG
9	s7	8	ILE
9	s7	11	GLN
9	s7	14	THR
9	s7	28	GLU
9	s7	33	GLU
9	s7	49	ILE
9	s7	50	ASP
9	s7	55	LYS
9	s7	60	ILE
9	s7	67	LEU
9	s7	75	THR
9	s7	77	LEU
9	s7	78	THR
9	s7	97	ARG
9	s7	108	GLN
9	s7	110	GLN
9	s7	112	ARG
9	s7	114	ARG
9	s7	115	SER
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	119	THR
9	s7	123	ASP
9	s7	126	LEU
9	s7	129	LEU
9	s7	135	ILE
9	s7	143	LEU
9	s7	144	VAL
9	s7	160	GLN
9	s7	163	ASP

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Mol	Chain	Res	Type
9	s7	166	LEU
9	s7	176	LEU
9	s7	185	ILE
9	s7	187	SER
10	s8	6	ASP
10	s8	7	SER
10	s8	12	SER
10	s8	18	ARG
10	s8	20	GLN
10	s8	22	ARG
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	46	VAL
10	s8	48	THR
10	s8	58	LEU
10	s8	59	ARG
10	s8	64	ASN
10	s8	66	SER
10	s8	74	LYS
10	s8	76	THR
10	s8	121	LEU
10	s8	152	ILE
10	s8	155	SER
10	s8	161	SER
10	s8	172	ARG
10	s8	175	GLN
10	s8	176	SER
10	s8	183	ILE
10	s8	184	LEU
11	s9	3	ARG
11	s9	9	SER
11	s9	13	SER
11	s9	24	LEU
11	s9	28	LEU
11	s9	33	GLU
11	s9	37	LYS
11	s9	39	LYS
11	s9	46	SER
11	s9	49	LEU
11	s9	52	ILE
11	s9	54	ARG

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Mol	Chain	Res	Type
11	s9	63	ASP
11	s9	78	ARG
11	s9	81	VAL
11	s9	82	ARG
11	s9	90	LYS
11	s9	92	LYS
11	s9	101	VAL
11	s9	105	LEU
11	s9	109	LEU
11	s9	110	GLN
11	s9	126	ARG
11	s9	127	VAL
11	s9	133	HIS
11	s9	134	ILE
11	s9	142	ASN
11	s9	147	MET
11	s9	148	VAL
11	s9	149	ARG
11	s9	157	ASP
11	s9	161	THR
11	s9	162	SER
11	s9	168	ARG
11	s9	172	VAL
11	s9	179	ARG
11	s9	180	LYS
11	s9	182	GLU
12	c0	2	LEU
12	c0	15	LEU
12	c0	20	VAL
12	c0	27	PHE
12	c0	28	ASN
12	c0	40	LEU
12	c0	47	GLN
12	c0	49	LEU
12	c0	55	VAL
12	c0	56	LYS
13	c1	5	LEU
13	c1	10	GLU
13	c1	18	HIS
13	c1	21	ASN
13	c1	26	LYS
13	c1	30	ARG

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Mol	Chain	Res	Type
13	c1	32	LYS
13	c1	33	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	56	LYS
13	c1	60	PHE
13	c1	67	ARG
13	c1	69	LYS
13	c1	72	THR
13	c1	74	THR
13	c1	80	MET
13	c1	82	ARG
13	c1	90	TYR
13	c1	99	ARG
13	c1	117	VAL
13	c1	122	ILE
13	c1	128	CYS
13	c1	129	ARG
13	c1	136	ARG
14	c2	28	LEU
14	c2	30	VAL
14	c2	53	THR
14	c2	59	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	89	ILE
14	c2	97	LEU
14	c2	103	LEU
14	c2	121	VAL
14	c2	132	GLU
14	c2	136	ILE
14	c2	140	PHE
15	c3	6	SER
15	c3	12	SER
15	c3	14	SER
15	c3	16	ILE
15	c3	18	TYR
15	c3	21	ASN

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Mol	Chain	Res	Type
15	c3	23	PRO
15	c3	27	LYS
15	c3	28	LEU
15	c3	32	SER
15	c3	35	GLU
15	c3	39	LYS
15	c3	42	ARG
15	c3	46	THR
15	c3	60	VAL
15	c3	66	ILE
15	c3	70	LYS
15	c3	72	MET
15	c3	76	LYS
15	c3	80	LEU
15	c3	84	ILE
15	c3	99	ARG
15	c3	102	LEU
15	c3	104	ARG
15	c3	106	ARG
15	c3	115	LEU
15	c3	116	ILE
15	c3	121	ARG
15	c3	122	ILE
15	c3	125	LEU
15	c3	127	ARG
15	c3	128	TYR
15	c3	134	VAL
15	c3	149	LEU
16	c4	13	VAL
16	c4	16	VAL
16	c4	19	ILE
16	c4	24	ASN
16	c4	31	THR
16	c4	32	ASP
16	c4	39	ILE
16	c4	43	THR
16	c4	49	LYS
16	c4	52	ARG
16	c4	58	TYR
16	c4	61	MET
16	c4	70	LYS
16	c4	71	CYS

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Mol	Chain	Res	Type
16	c4	76	ILE
16	c4	81	VAL
16	c4	83	ILE
16	c4	93	THR
16	c4	102	LEU
16	c4	107	ARG
16	c4	114	ARG
16	c4	118	VAL
16	c4	119	THR
16	c4	123	SER
16	c4	124	ASP
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
17	c5	12	PHE
17	c5	29	SER
17	c5	36	LEU
17	c5	49	MET
17	c5	52	LYS
17	c5	77	ARG
17	c5	92	SER
17	c5	97	TYR
17	c5	107	ILE
17	c5	110	GLU
17	c5	111	MET
17	c5	124	THR
17	c5	127	ARG
18	c6	17	THR
18	c6	23	LYS
18	c6	26	LYS
18	c6	28	LEU
18	c6	36	ILE
18	c6	37	THR
18	c6	43	ILE
18	c6	44	LEU
18	c6	48	VAL
18	c6	53	LEU
18	c6	54	LEU
18	c6	55	VAL
18	c6	57	LEU
18	c6	63	ILE
18	c6	65	ILE

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Mol	Chain	Res	Type
18	c6	68	ARG
18	c6	69	VAL
18	c6	81	ILE
18	c6	83	GLN
18	c6	110	THR
18	c6	114	ARG
18	c6	117	LEU
18	c6	118	ILE
18	c6	127	LYS
18	c6	128	LYS
18	c6	137	ARG
18	c6	143	ARG
19	c7	3	ARG
19	c7	4	VAL
19	c7	6	THR
19	c7	9	VAL
19	c7	17	ILE
19	c7	34	LEU
19	c7	45	ARG
19	c7	46	LEU
19	c7	47	ARG
19	c7	60	ARG
19	c7	61	ILE
19	c7	69	ILE
19	c7	72	LYS
19	c7	83	GLN
19	c7	85	VAL
19	c7	88	VAL
19	c7	112	SER
19	c7	113	LEU
20	c8	3	LEU
20	c8	4	VAL
20	c8	13	HIS
20	c8	15	LEU
20	c8	25	ASN
20	c8	28	ILE
20	c8	29	VAL
20	c8	33	THR
20	c8	36	LYS
20	c8	38	VAL
20	c8	40	ARG
20	c8	41	ARG

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Mol	Chain	Res	Type
20	c8	57	ARG
20	c8	63	GLN
20	c8	69	ILE
20	c8	77	THR
20	c8	85	PHE
20	c8	94	ASP
20	c8	97	ASP
20	c8	100	THR
20	c8	106	GLU
20	c8	115	ARG
20	c8	116	LEU
20	c8	133	VAL
20	c8	136	GLN
20	c8	138	THR
20	c8	141	THR
20	c8	143	ARG
20	c8	145	ARG
21	c9	6	VAL
21	c9	13	ASP
21	c9	20	SER
21	c9	25	GLN
21	c9	27	LYS
21	c9	28	LEU
21	c9	30	VAL
21	c9	34	VAL
21	c9	57	ARG
21	c9	68	ARG
21	c9	71	VAL
21	c9	75	LYS
21	c9	85	SER
21	c9	86	ARG
21	c9	89	ARG
21	c9	123	ARG
21	c9	125	SER
21	c9	126	GLU
21	c9	133	ASP
21	c9	135	ILE
21	c9	139	THR
21	c9	140	LEU
21	c9	141	GLU
21	c9	142	GLU
22	d0	20	ILE

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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	30	LYS
22	d0	31	VAL
22	d0	34	LEU
22	d0	37	VAL
22	d0	44	ASN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	61	LYS
22	d0	63	LEU
22	d0	70	THR
22	d0	72	ASN
22	d0	74	GLU
22	d0	76	SER
22	d0	77	LYS
22	d0	81	THR
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	105	GLN
22	d0	108	ILE
22	d0	115	GLU
23	d1	2	GLU
23	d1	3	ASN
23	d1	4	ASP
23	d1	5	LYS
23	d1	8	LEU
23	d1	10	GLU
23	d1	12	TYR
23	d1	18	SER
23	d1	25	LYS
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

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Mol	Chain	Res	Type
23	d1	56	SER
23	d1	69	LEU
23	d1	70	ASN
23	d1	78	LEU
23	d1	87	ARG
24	d2	7	LEU
24	d2	20	THR
24	d2	23	ARG
24	d2	25	VAL
24	d2	31	SER
24	d2	47	ILE
24	d2	56	HIS
24	d2	65	LEU
24	d2	93	LEU
24	d2	98	GLN
24	d2	105	THR
24	d2	114	GLU
24	d2	117	ARG
24	d2	129	VAL
25	d3	5	LYS
25	d3	7	ARG
25	d3	9	LEU
25	d3	14	LYS
25	d3	15	LEU
25	d3	19	ARG
25	d3	36	THR
25	d3	40	SER
25	d3	41	SER
25	d3	68	ILE
25	d3	73	ARG
25	d3	83	VAL
25	d3	84	THR
25	d3	96	VAL
25	d3	97	ASP
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	109	ARG
25	d3	112	LYS
25	d3	114	LYS
25	d3	121	ARG
25	d3	125	VAL

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Mol	Chain	Res	Type
25	d3	133	LEU
25	d3	144	ARG
26	d4	10	ARG
26	d4	22	GLN
26	d4	26	ASP
26	d4	36	SER
26	d4	38	ASP
26	d4	42	GLU
26	d4	43	LYS
26	d4	44	LEU
26	d4	46	GLU
26	d4	49	LYS
26	d4	51	GLU
26	d4	62	THR
26	d4	78	SER
26	d4	83	LYS
26	d4	88	THR
26	d4	92	VAL
26	d4	98	GLU
26	d4	102	LYS
26	d4	116	LYS
26	d4	128	LYS
26	d4	131	ARG
27	d5	41	ILE
27	d5	43	ASP
27	d5	51	LEU
27	d5	53	GLU
27	d5	57	TYR
27	d5	81	ARG
27	d5	88	ILE
27	d5	90	LYS
28	d6	5	ARG
28	d6	8	ASN
28	d6	10	ARG
28	d6	12	LYS
28	d6	15	ARG
28	d6	28	LYS
28	d6	33	ASP
28	d6	39	MET
28	d6	44	ILE
28	d6	46	GLU
28	d6	51	ARG

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Mol	Chain	Res	Type
28	d6	53	LEU
28	d6	54	SER
28	d6	55	GLU
28	d6	67	THR
28	d6	76	SER
28	d6	82	ARG
28	d6	85	ARG
28	d6	86	VAL
28	d6	89	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	11	THR
29	d7	26	GLN
29	d7	43	ILE
29	d7	45	THR
29	d7	55	THR
29	d7	59	CYS
29	d7	77	THR
30	d8	11	LYS
30	d8	14	LYS
30	d8	22	ARG
30	d8	28	VAL
30	d8	32	PHE
30	d8	33	LEU
30	d8	52	ASP
30	d8	54	LEU
30	d8	58	GLU
30	d8	66	LEU
31	d9	6	VAL
31	d9	10	HIS
31	d9	12	ARG
31	d9	22	ARG
31	d9	24	CYS
31	d9	25	SER
31	d9	28	THR
31	d9	31	ILE
31	d9	39	CYS
31	d9	42	CYS
31	d9	49	ASP
31	d9	54	LYS
80	e0	4	VAL
80	e0	13	LYS

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Mol	Chain	Res	Type
80	e0	21	VAL
80	e0	22	GLU
80	e0	29	LYS
80	e0	31	LYS
80	e0	36	LYS
80	e0	38	LEU
80	e0	39	LEU
80	e0	42	ARG
80	e0	45	VAL
80	e0	46	ASN
80	e0	49	LEU
80	e0	55	ARG
80	e0	61	SER
33	e1	78	LYS
33	e1	80	ARG
33	e1	87	THR
33	e1	89	LYS
33	e1	90	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	107	LYS
33	e1	113	LYS
33	e1	115	THR
33	e1	116	LYS
33	e1	121	CYS
33	e1	135	HIS
33	e1	147	VAL
33	e1	151	ASN
34	sR	8	VAL
34	sR	10	ARG
34	sR	16	HIS
34	sR	23	LEU
34	sR	25	THR
34	sR	32	LEU
34	sR	58	VAL
34	sR	64	HIS
34	sR	65	SER
34	sR	66	HIS
34	sR	72	THR
34	sR	76	ASP
34	sR	82	SER

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Mol	Chain	Res	Type
34	sR	94	VAL
34	sR	96	THR
34	sR	98	GLU
34	sR	100	TYR
34	sR	123	ILE
34	sR	145	LEU
34	sR	152	SER
34	sR	161	LYS
34	sR	164	ASP
34	sR	168	THR
34	sR	176	LYS
34	sR	178	VAL
34	sR	188	ILE
34	sR	199	ILE
34	sR	210	LEU
34	sR	228	LYS
34	sR	232	TYR
34	sR	250	TYR
34	sR	266	ASP
34	sR	275	ARG
34	sR	282	SER
34	sR	286	GLU
34	sR	297	ASP
34	sR	309	VAL
34	sR	310	ILE
34	sR	319	ASN
35	sM	23	LYS
35	sM	28	SER
35	sM	30	THR
35	sM	41	SER
35	sM	43	ASP
35	sM	61	ILE
35	sM	68	ARG
35	sM	71	ASN
35	sM	74	LYS
35	sM	75	ASP
35	sM	77	THR
35	sM	78	ASP
39	l2	8	GLN
39	l2	15	ILE
39	l2	19	HIS
39	l2	23	ARG

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Mol	Chain	Res	Type
39	l2	28	LYS
39	l2	30	ARG
39	l2	31	THR
39	l2	32	LEU
39	l2	44	ILE
39	l2	45	VAL
39	l2	48	ILE
39	l2	49	VAL
39	l2	62	VAL
39	l2	70	ARG
39	l2	74	GLU
39	l2	80	GLU
39	l2	82	VAL
39	l2	84	THR
39	l2	101	VAL
39	l2	104	LEU
39	l2	114	SER
39	l2	118	GLU
39	l2	119	LYS
39	l2	137	ILE
39	l2	142	ASP
39	l2	146	THR
39	l2	147	ARG
39	l2	148	VAL
39	l2	149	ARG
39	l2	168	VAL
39	l2	179	LEU
39	l2	180	LEU
39	l2	190	ARG
39	l2	193	ARG
39	l2	200	ARG
39	l2	205	ASN
39	l2	207	VAL
39	l2	218	HIS
39	l2	224	THR
39	l2	227	ARG
39	l2	243	THR
39	l2	246	LEU
40	l3	3	HIS
40	l3	4	ARG
40	l3	5	LYS
40	l3	7	GLU

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Mol	Chain	Res	Type
40	l3	10	ARG
40	l3	17	LEU
40	l3	19	ARG
40	l3	24	SER
40	l3	38	SER
40	l3	43	LEU
40	l3	47	LEU
40	l3	50	LYS
40	l3	55	THR
40	l3	56	ILE
40	l3	60	LEU
40	l3	70	ARG
40	l3	73	VAL
40	l3	77	THR
40	l3	85	VAL
40	l3	103	THR
40	l3	104	THR
40	l3	112	ASP
40	l3	113	GLU
40	l3	114	VAL
40	l3	120	LYS
40	l3	123	TYR
40	l3	146	ARG
40	l3	148	LEU
40	l3	150	ARG
40	l3	157	VAL
40	l3	160	VAL
40	l3	165	GLN
40	l3	167	ARG
40	l3	169	THR
40	l3	183	LEU
40	l3	184	ASN
40	l3	188	ILE
40	l3	192	VAL
40	l3	201	LYS
40	l3	202	THR
40	l3	205	VAL
40	l3	208	VAL
40	l3	211	GLN
40	l3	214	MET
40	l3	221	THR
40	l3	229	VAL

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Mol	Chain	Res	Type
40	13	232	ARG
40	13	235	THR
40	13	242	THR
40	13	249	VAL
40	13	252	ILE
40	13	264	VAL
40	13	274	SER
40	13	301	THR
40	13	304	THR
40	13	312	VAL
40	13	316	GLU
40	13	320	ASP
40	13	324	VAL
40	13	328	ILE
40	13	332	ARG
40	13	340	LYS
40	13	344	THR
40	13	348	ARG
40	13	354	VAL
40	13	359	ILE
40	13	361	THR
40	13	369	ARG
40	13	376	LYS
40	13	380	MET
41	14	2	SER
41	14	16	THR
41	14	22	LEU
41	14	25	VAL
41	14	27	SER
41	14	47	ARG
41	14	53	SER
41	14	55	LYS
41	14	63	GLU
41	14	73	ARG
41	14	82	THR
41	14	90	PHE
41	14	92	ASN
41	14	93	MET
41	14	99	MET
41	14	112	LYS
41	14	118	LYS
41	14	120	TYR

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Mol	Chain	Res	Type
41	14	122	THR
41	14	126	ILE
41	14	129	THR
41	14	131	VAL
41	14	136	LEU
41	14	144	LYS
41	14	145	ILE
41	14	148	ILE
41	14	150	LEU
41	14	156	LEU
41	14	159	ILE
41	14	177	ASP
41	14	179	LEU
41	14	181	VAL
41	14	183	LYS
41	14	186	LYS
41	14	187	LEU
41	14	191	LYS
41	14	198	ARG
41	14	201	GLN
41	14	203	ARG
41	14	206	LEU
41	14	222	VAL
41	14	230	VAL
41	14	246	ARG
41	14	258	LEU
41	14	261	VAL
41	14	265	GLU
41	14	266	THR
41	14	267	VAL
41	14	275	THR
41	14	278	SER
41	14	287	THR
41	14	300	ARG
41	14	301	PRO
41	14	304	GLN
41	14	307	GLN
41	14	308	LYS
41	14	312	VAL
41	14	313	LEU
41	14	316	ASN
41	14	322	GLN

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Mol	Chain	Res	Type
41	14	333	VAL
41	14	339	LEU
41	14	345	GLU
41	14	347	THR
41	14	356	THR
41	14	359	LEU
42	15	25	GLU
42	15	34	LYS
42	15	35	ARG
42	15	38	THR
42	15	41	LYS
42	15	51	LEU
42	15	56	THR
42	15	65	ILE
42	15	66	SER
42	15	67	SER
42	15	68	THR
42	15	70	THR
42	15	75	LEU
42	15	110	LEU
42	15	112	LYS
42	15	113	LEU
42	15	118	THR
42	15	120	LYS
42	15	131	LEU
42	15	132	THR
42	15	133	GLU
42	15	135	VAL
42	15	140	ARG
42	15	146	LEU
42	15	148	ILE
42	15	152	ARG
42	15	154	THR
42	15	155	THR
42	15	158	ARG
42	15	164	LYS
42	15	183	TRP
42	15	185	PHE
42	15	186	GLU
42	15	187	THR
42	15	189	GLU
42	15	190	ILE

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Mol	Chain	Res	Type
42	15	194	LEU
42	15	211	LEU
42	15	222	LEU
42	15	224	LYS
42	15	227	LEU
42	15	241	THR
42	15	242	SER
42	15	258	LYS
42	15	259	LYS
42	15	268	GLU
42	15	270	LYS
42	15	271	LYS
42	15	273	ARG
42	15	275	THR
42	15	280	GLU
42	15	281	GLU
42	15	293	LEU
43	16	8	LYS
43	16	15	VAL
43	16	21	THR
43	16	31	ARG
43	16	46	ARG
43	16	50	LYS
43	16	52	VAL
43	16	64	LEU
43	16	82	ARG
43	16	89	THR
43	16	98	VAL
43	16	104	GLU
43	16	109	GLU
43	16	131	LYS
43	16	143	LYS
43	16	146	ILE
43	16	152	THR
43	16	155	LEU
43	16	160	SER
43	16	162	SER
43	16	170	LYS
44	17	26	VAL
44	17	41	ARG
44	17	45	LEU
44	17	46	GLU

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Mol	Chain	Res	Type
44	17	48	ASN
44	17	60	ARG
44	17	62	ILE
44	17	82	LYS
44	17	83	LEU
44	17	88	ARG
44	17	93	ASN
44	17	98	LYS
44	17	124	LEU
44	17	128	LYS
44	17	129	LEU
44	17	130	ILE
44	17	156	ILE
44	17	157	ASN
44	17	158	LYS
44	17	173	LEU
44	17	175	LYS
44	17	179	LEU
44	17	184	LEU
44	17	193	PRO
44	17	196	LYS
44	17	199	ASN
44	17	228	SER
44	17	229	PHE
44	17	239	LEU
45	18	26	LEU
45	18	36	ILE
45	18	40	VAL
45	18	49	TYR
45	18	67	ILE
45	18	68	ARG
45	18	71	VAL
45	18	79	GLN
45	18	81	THR
45	18	95	ASN
45	18	98	ARG
45	18	101	THR
45	18	109	LEU
45	18	136	LEU
45	18	146	LYS
45	18	149	LYS
45	18	155	ASN

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Mol	Chain	Res	Type
45	18	160	ILE
45	18	163	VAL
45	18	164	VAL
45	18	173	MET
45	18	185	ARG
45	18	191	ASN
45	18	192	GLN
45	18	200	LEU
45	18	211	LEU
45	18	214	LEU
45	18	216	SER
45	18	219	ASP
45	18	222	PHE
45	18	230	LYS
45	18	240	ASN
45	18	245	LYS
45	18	248	LYS
46	19	1	MET
46	19	5	GLN
46	19	6	THR
46	19	18	VAL
46	19	31	ARG
46	19	39	LYS
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	73	SER
46	19	77	ASN
46	19	79	ILE
46	19	82	VAL
46	19	84	LYS
46	19	92	TYR
46	19	105	GLU
46	19	106	LYS
46	19	115	ARG
46	19	118	LEU
46	19	120	ASP

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Mol	Chain	Res	Type
46	19	122	LYS
46	19	123	ILE
46	19	124	ARG
46	19	133	THR
46	19	137	SER
46	19	138	THR
46	19	143	GLU
46	19	144	ILE
46	19	149	ASN
46	19	151	VAL
46	19	152	GLU
46	19	157	ASN
46	19	161	LEU
46	19	162	GLN
46	19	163	GLN
46	19	166	ARG
46	19	179	ILE
46	19	181	VAL
46	19	191	LEU
47	m0	24	ARG
47	m0	26	VAL
47	m0	36	LEU
47	m0	42	THR
47	m0	50	VAL
47	m0	52	LEU
47	m0	58	GLU
47	m0	63	GLU
47	m0	71	CYS
47	m0	74	LYS
47	m0	76	MET
47	m0	77	THR
47	m0	78	THR
47	m0	83	ASP
47	m0	87	LEU
47	m0	135	ILE
47	m0	139	ARG
47	m0	140	THR
47	m0	154	ARG
47	m0	156	ARG
47	m0	162	GLN
47	m0	169	LYS
47	m0	176	LEU

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Mol	Chain	Res	Type
47	m0	177	ASP
47	m0	189	GLU
47	m0	197	VAL
47	m0	200	LEU
47	m0	206	LEU
47	m0	208	ASN
47	m0	209	ASN
47	m0	211	ARG
47	m0	212	GLU
47	m0	217	PHE
48	m1	6	GLN
48	m1	10	ARG
48	m1	13	LYS
48	m1	16	LYS
48	m1	18	VAL
48	m1	19	LEU
48	m1	23	VAL
48	m1	30	LEU
48	m1	34	SER
48	m1	37	LEU
48	m1	40	LEU
48	m1	43	GLN
48	m1	44	THR
48	m1	46	VAL
48	m1	56	THR
48	m1	64	LYS
48	m1	71	VAL
48	m1	80	LEU
48	m1	92	ARG
48	m1	93	ASP
48	m1	101	ASN
48	m1	106	ILE
48	m1	107	ASP
48	m1	112	LEU
48	m1	115	LYS
48	m1	129	VAL
48	m1	130	VAL
48	m1	132	ASN
48	m1	137	ARG
48	m1	140	ARG
48	m1	145	LYS
48	m1	153	LYS

Continued on next page...

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Mol	Chain	Res	Type
48	m1	154	THR
48	m1	155	THR
48	m1	159	THR
48	m1	171	VAL
48	m1	174	LYS
49	m3	5	LYS
49	m3	13	HIS
49	m3	46	ILE
49	m3	52	ASP
49	m3	53	LEU
49	m3	54	LEU
49	m3	55	ARG
49	m3	58	VAL
49	m3	63	VAL
49	m3	67	ARG
49	m3	68	LYS
49	m3	69	VAL
49	m3	73	ARG
49	m3	76	THR
49	m3	104	ARG
49	m3	107	GLU
49	m3	108	ILE
49	m3	113	VAL
49	m3	121	SER
49	m3	123	ILE
49	m3	128	ARG
49	m3	131	LYS
49	m3	149	GLN
49	m3	152	THR
49	m3	153	ASP
49	m3	164	GLU
49	m3	168	ARG
49	m3	171	ARG
49	m3	176	GLU
49	m3	180	ARG
49	m3	184	GLU
50	m4	2	SER
50	m4	3	THR
50	m4	12	TRP
50	m4	27	GLN
50	m4	41	GLN
50	m4	43	LYS

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Mol	Chain	Res	Type
50	m4	45	LEU
50	m4	53	VAL
50	m4	55	ARG
50	m4	60	LEU
50	m4	62	GLN
50	m4	63	VAL
50	m4	64	VAL
50	m4	66	THR
50	m4	91	CYS
50	m4	113	THR
50	m4	128	ARG
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	8	GLU
51	m5	15	GLN
51	m5	24	ARG
51	m5	50	ARG
51	m5	54	LYS
51	m5	60	VAL
51	m5	66	VAL
51	m5	72	LYS
51	m5	80	THR
51	m5	85	THR
51	m5	92	LEU
51	m5	96	ARG
51	m5	106	VAL
51	m5	109	ARG
51	m5	125	SER
51	m5	138	GLN
51	m5	144	ARG
51	m5	153	ASP
51	m5	155	VAL
51	m5	159	ARG
51	m5	165	THR
51	m5	170	LYS
51	m5	175	ASN
51	m5	176	LYS
51	m5	180	PHE
51	m5	184	LYS
51	m5	188	ARG
51	m5	190	THR

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Mol	Chain	Res	Type
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	16	VAL
52	m6	21	SER
52	m6	36	VAL
52	m6	49	ARG
52	m6	58	LEU
52	m6	66	LYS
52	m6	67	THR
52	m6	74	ARG
52	m6	78	ARG
52	m6	79	ILE
52	m6	82	LYS
52	m6	84	LEU
52	m6	85	ARG
52	m6	94	ARG
52	m6	100	GLU
52	m6	106	GLU
52	m6	110	PRO
52	m6	117	ARG
52	m6	119	VAL
52	m6	128	ARG
52	m6	140	LYS
52	m6	143	THR
52	m6	152	VAL
52	m6	160	ARG
52	m6	166	GLU
52	m6	171	LYS
52	m6	177	LYS
52	m6	180	SER
52	m6	182	ASN
52	m6	190	VAL
52	m6	197	LEU
53	m7	9	THR
53	m7	16	SER
53	m7	28	ASN
53	m7	32	THR

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Mol	Chain	Res	Type
53	m7	51	VAL
53	m7	52	LEU
53	m7	53	ASP
53	m7	55	GLN
53	m7	69	ARG
53	m7	79	THR
53	m7	80	LYS
53	m7	107	LEU
53	m7	112	LEU
53	m7	118	GLN
53	m7	119	VAL
53	m7	126	ARG
53	m7	127	ARG
53	m7	136	ILE
53	m7	137	ASN
53	m7	138	LYS
53	m7	141	SER
53	m7	142	SER
53	m7	150	VAL
53	m7	153	LYS
53	m7	155	GLU
54	m8	7	SER
54	m8	24	VAL
54	m8	26	LEU
54	m8	31	LYS
54	m8	32	LEU
54	m8	34	THR
54	m8	49	LEU
54	m8	58	ASN
54	m8	63	SER
54	m8	64	VAL
54	m8	66	ARG
54	m8	69	ARG
54	m8	79	LYS
54	m8	81	VAL
54	m8	82	VAL
54	m8	88	THR
54	m8	93	ILE
54	m8	127	LEU
54	m8	129	VAL
54	m8	135	GLN
54	m8	136	ASN

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Mol	Chain	Res	Type
54	m8	137	THR
54	m8	138	LEU
54	m8	141	ARG
54	m8	165	ILE
54	m8	170	ARG
54	m8	174	ARG
54	m8	176	ARG
54	m8	178	ARG
54	m8	185	LYS
55	m9	7	GLN
55	m9	8	LYS
55	m9	10	LEU
55	m9	17	VAL
55	m9	20	ARG
55	m9	29	THR
55	m9	39	ASN
55	m9	43	LYS
55	m9	49	THR
55	m9	56	THR
55	m9	63	THR
55	m9	70	LYS
55	m9	88	ARG
55	m9	99	LEU
55	m9	104	ARG
55	m9	105	LEU
55	m9	119	LEU
55	m9	126	GLU
55	m9	128	LYS
55	m9	138	LEU
55	m9	148	ASP
55	m9	152	GLU
55	m9	153	LYS
55	m9	164	LEU
55	m9	166	ASN
55	m9	173	ARG
55	m9	177	VAL
56	n0	1	MET
56	n0	5	LYS
56	n0	13	ARG
56	n0	16	THR
56	n0	17	GLU
56	n0	19	VAL

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Mol	Chain	Res	Type
56	n0	32	SER
56	n0	40	ARG
56	n0	45	LEU
56	n0	50	LYS
56	n0	60	SER
56	n0	70	THR
56	n0	82	ASP
56	n0	85	SER
56	n0	87	THR
56	n0	88	HIS
56	n0	89	ASN
56	n0	97	VAL
56	n0	100	VAL
56	n0	105	THR
56	n0	113	ARG
56	n0	117	ARG
56	n0	120	SER
56	n0	124	LEU
56	n0	125	LYS
56	n0	130	GLU
56	n0	136	LYS
56	n0	137	ARG
56	n0	142	GLN
56	n0	145	THR
56	n0	148	LEU
56	n0	155	ARG
56	n0	157	GLN
56	n0	160	THR
56	n0	162	THR
56	n0	172	TYR
57	n1	3	LYS
57	n1	10	ARG
57	n1	12	ARG
57	n1	16	GLN
57	n1	17	ARG
57	n1	22	HIS
57	n1	25	VAL
57	n1	27	LEU
57	n1	31	LEU
57	n1	35	LYS
57	n1	36	VAL
57	n1	39	ILE

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Mol	Chain	Res	Type
57	n1	55	LYS
57	n1	78	LYS
57	n1	80	VAL
57	n1	82	ASN
57	n1	83	ARG
57	n1	93	VAL
57	n1	96	ILE
57	n1	97	LYS
57	n1	100	LYS
57	n1	102	ARG
57	n1	104	GLU
57	n1	124	VAL
57	n1	126	VAL
57	n1	128	LEU
57	n1	131	GLN
57	n1	135	PRO
57	n1	139	ARG
57	n1	150	THR
57	n1	154	VAL
57	n1	160	ILE
58	n2	13	LYS
58	n2	14	THR
58	n2	16	THR
58	n2	27	VAL
58	n2	33	TYR
58	n2	38	ILE
58	n2	39	ASP
58	n2	50	LEU
58	n2	58	GLU
58	n2	68	THR
58	n2	74	LYS
58	n2	75	TYR
58	n2	90	ARG
58	n2	94	ARG
58	n2	96	VAL
58	n2	100	THR
59	n3	13	ILE
59	n3	14	SER
59	n3	32	ARG
59	n3	45	ARG
59	n3	48	ARG
59	n3	49	LEU

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Mol	Chain	Res	Type
59	n3	67	PRO
59	n3	69	LEU
59	n3	72	LYS
59	n3	74	MET
59	n3	88	ARG
59	n3	91	VAL
59	n3	120	LYS
59	n3	128	ARG
60	n4	1	MET
60	n4	2	LYS
60	n4	36	SER
60	n4	39	LEU
60	n4	41	LYS
60	n4	54	LEU
60	n4	57	LYS
60	n4	63	ILE
60	n4	89	LEU
60	n4	96	LEU
60	n4	97	LYS
60	n4	98	PRO
60	n4	107	GLU
60	n4	126	GLU
60	n4	127	LYS
60	n4	130	SER
60	n4	135	SER
61	n5	27	ARG
61	n5	33	ARG
61	n5	37	THR
61	n5	39	LYS
61	n5	52	PRO
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	71	THR
61	n5	74	LYS
61	n5	78	ASP
61	n5	86	VAL
61	n5	87	SER
61	n5	105	VAL
61	n5	108	LEU
61	n5	114	VAL
61	n5	115	ARG

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Mol	Chain	Res	Type
61	n5	117	ASN
61	n5	125	ARG
61	n5	135	ILE
61	n5	137	ASN
61	n5	142	ILE
62	n6	4	GLN
62	n6	12	ARG
62	n6	13	ARG
62	n6	32	SER
62	n6	37	LYS
62	n6	45	ILE
62	n6	50	ILE
62	n6	51	ARG
62	n6	56	VAL
62	n6	57	LEU
62	n6	62	SER
62	n6	67	GLU
62	n6	74	TYR
62	n6	84	LYS
62	n6	90	VAL
62	n6	95	VAL
62	n6	99	LEU
62	n6	105	VAL
62	n6	108	LYS
62	n6	111	LEU
62	n6	112	ASP
62	n6	115	ARG
62	n6	120	GLN
62	n6	122	LYS
63	n7	3	LYS
63	n7	5	LEU
63	n7	12	VAL
63	n7	17	ARG
63	n7	21	LYS
63	n7	24	VAL
63	n7	25	ILE
63	n7	28	PRO
63	n7	33	SER
63	n7	34	LYS
63	n7	36	HIS
63	n7	46	ILE
63	n7	52	LYS

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Mol	Chain	Res	Type
63	n7	65	ARG
63	n7	72	ILE
63	n7	77	TYR
63	n7	81	LEU
63	n7	86	THR
63	n7	90	GLU
63	n7	93	LYS
63	n7	95	VAL
63	n7	99	GLU
63	n7	105	SER
63	n7	121	ARG
63	n7	127	ASN
64	n8	3	SER
64	n8	4	ARG
64	n8	8	THR
64	n8	10	LYS
64	n8	14	HIS
64	n8	15	VAL
64	n8	22	ILE
64	n8	26	ARG
64	n8	27	LYS
64	n8	42	ARG
64	n8	47	LYS
64	n8	60	TYR
64	n8	64	GLN
64	n8	65	GLN
64	n8	73	LEU
64	n8	78	LEU
64	n8	82	ILE
64	n8	88	ASP
64	n8	91	LEU
64	n8	92	LYS
64	n8	97	GLU
64	n8	120	ASN
64	n8	123	VAL
64	n8	133	LEU
65	n9	22	LYS
65	n9	23	LYS
65	n9	26	THR
65	n9	31	SER
65	n9	33	LYS
65	n9	38	LYS

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Mol	Chain	Res	Type
65	n9	40	ARG
65	n9	42	ASN
65	n9	50	THR
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	9	SER
66	o0	10	ILE
66	o0	18	ILE
66	o0	19	LYS
66	o0	34	LEU
66	o0	40	LYS
66	o0	41	LEU
66	o0	48	THR
66	o0	55	GLU
66	o0	61	MET
66	o0	64	LYS
66	o0	66	LYS
66	o0	68	TYR
66	o0	69	TYR
66	o0	74	ASN
66	o0	86	ARG
67	o1	6	ASP
67	o1	13	THR
67	o1	16	LEU
67	o1	24	SER
67	o1	26	LYS
67	o1	28	ARG
67	o1	31	ARG
67	o1	34	LYS
67	o1	44	MET
67	o1	46	THR
67	o1	64	VAL
67	o1	70	ARG
67	o1	76	SER
67	o1	83	GLU
67	o1	84	ASP
67	o1	89	LEU
67	o1	91	SER
67	o1	96	VAL
67	o1	98	VAL
67	o1	102	LYS

Continued on next page...

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Mol	Chain	Res	Type
67	o1	104	LEU
67	o1	106	THR
67	o1	110	GLU
67	o1	112	ASP
68	o2	3	SER
68	o2	4	LEU
68	o2	8	LYS
68	o2	9	ILE
68	o2	10	VAL
68	o2	15	LYS
68	o2	24	ARG
68	o2	27	ARG
68	o2	33	ARG
68	o2	34	LYS
68	o2	44	ARG
68	o2	45	ARG
68	o2	52	GLN
68	o2	54	LYS
68	o2	61	LYS
68	o2	62	LYS
68	o2	66	LEU
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	86	THR
68	o2	89	THR
68	o2	101	SER
68	o2	125	ARG
69	o3	4	SER
69	o3	6	ARG
69	o3	15	SER
69	o3	31	LYS
69	o3	42	GLN
69	o3	45	LEU
69	o3	57	LYS
69	o3	58	GLU
69	o3	59	VAL
69	o3	64	ILE
69	o3	70	LYS
69	o3	73	ARG
69	o3	74	THR
69	o3	81	VAL

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Mol	Chain	Res	Type
69	o3	84	THR
69	o3	86	ARG
69	o3	90	PRO
69	o3	93	THR
69	o3	105	SER
69	o3	107	ILE
70	o4	5	VAL
70	o4	15	THR
70	o4	20	ILE
70	o4	22	VAL
70	o4	24	LYS
70	o4	25	THR
70	o4	29	ILE
70	o4	30	LEU
70	o4	35	VAL
70	o4	49	SER
70	o4	57	LEU
70	o4	58	ARG
70	o4	71	THR
70	o4	72	VAL
70	o4	81	CYS
70	o4	83	ASN
70	o4	85	VAL
70	o4	86	LYS
70	o4	88	ARG
70	o4	98	GLN
70	o4	104	VAL
70	o4	107	GLU
71	o5	4	VAL
71	o5	11	THR
71	o5	13	SER
71	o5	20	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	28	LEU
71	o5	36	LEU
71	o5	38	ARG
71	o5	44	ILE
71	o5	45	LYS
71	o5	46	THR
71	o5	47	VAL
71	o5	48	ARG

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Mol	Chain	Res	Type
71	o5	59	ASN
71	o5	66	VAL
71	o5	69	LEU
71	o5	79	ASP
71	o5	81	ARG
71	o5	86	ARG
71	o5	89	ARG
71	o5	107	LYS
71	o5	119	LYS
72	o6	3	VAL
72	o6	7	ILE
72	o6	9	ILE
72	o6	21	THR
72	o6	26	ILE
72	o6	35	ASN
72	o6	36	ARG
72	o6	41	ARG
72	o6	42	SER
72	o6	43	LEU
72	o6	45	ARG
72	o6	56	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	59	ASP
72	o6	68	ARG
72	o6	75	LYS
72	o6	76	ARG
72	o6	79	SER
72	o6	88	GLU
72	o6	94	ILE
72	o6	97	SER
73	o7	17	THR
73	o7	19	CYS
73	o7	25	ARG
73	o7	31	LYS
73	o7	33	THR
73	o7	36	SER
73	o7	44	THR
73	o7	58	THR
73	o7	59	THR
73	o7	65	ARG
73	o7	67	LEU

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Mol	Chain	Res	Type
73	o7	80	THR
73	o7	85	LYS
74	o8	5	ILE
74	o8	12	LEU
74	o8	14	LEU
74	o8	16	ARG
74	o8	17	ARG
74	o8	24	THR
74	o8	41	THR
74	o8	46	ARG
74	o8	50	SER
74	o8	53	THR
74	o8	61	LYS
74	o8	63	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	72	THR
74	o8	73	LEU
75	o9	4	GLN
75	o9	5	LYS
75	o9	6	SER
75	o9	9	ILE
75	o9	15	LYS
75	o9	21	ARG
75	o9	29	LEU
75	o9	47	THR
76	q0	79	GLU
76	q0	83	LYS
76	q0	85	LEU
76	q0	87	SER
76	q0	88	LYS
76	q0	93	LYS
76	q0	99	CYS
76	q0	106	ARG
76	q0	108	THR
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	122	ARG
76	q0	127	LEU
77	q1	6	ARG
77	q1	9	ARG

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Mol	Chain	Res	Type
77	q1	11	ARG
77	q1	13	LEU
77	q1	16	LYS
77	q1	19	LYS
77	q1	21	ARG
77	q1	23	ARG
78	q2	7	THR
78	q2	8	ARG
78	q2	20	HIS
78	q2	35	LEU
78	q2	45	ARG
78	q2	48	SER
78	q2	61	LYS
78	q2	63	LYS
78	q2	78	LYS
78	q2	79	THR
78	q2	80	ARG
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	99	GLN
78	q2	100	LYS
78	q2	104	LEU
79	q3	3	LYS
79	q3	8	VAL
79	q3	16	VAL
79	q3	20	SER
79	q3	24	ARG
79	q3	40	SER
79	q3	46	THR
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	58	SER
79	q3	62	LYS
79	q3	70	THR
79	q3	72	SER
79	q3	73	THR
79	q3	80	ARG
82	p0	4	ILE
82	p0	5	ARG
82	p0	6	GLU

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Mol	Chain	Res	Type
82	p0	15	LEU
82	p0	25	LEU
82	p0	30	VAL
82	p0	41	VAL
82	p0	42	ARG
82	p0	48	ARG
82	p0	51	VAL
82	p0	55	LYS
82	p0	70	LEU
82	p0	72	ASP
82	p0	74	GLU
82	p0	76	LEU
82	p0	89	THR
82	p0	93	LEU
82	p0	97	LYS
82	p0	104	ARG
82	p0	185	LEU
82	p0	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
3	S1	149	GLN
3	S1	211	HIS
4	S2	87	GLN
5	S3	162	GLN
5	S3	165	ASN
7	S5	131	GLN
9	S7	74	GLN
11	S9	139	GLN
13	C1	104	HIS
14	C2	70	ASN
16	C4	12	GLN
17	C5	103	ASN
19	C7	105	GLN
20	C8	19	ASN
20	C8	99	HIS
21	C9	70	GLN
22	D0	33	GLN
23	D1	74	GLN
26	D4	63	GLN
33	E1	135	HIS

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Mol	Chain	Res	Type
34	SR	17	ASN
39	L2	38	HIS
39	L2	79	ASN
40	L3	293	ASN
41	L4	307	GLN
42	L5	40	HIS
44	L7	244	ASN
46	L9	49	ASN
48	M1	39	GLN
51	M5	194	GLN
54	M8	126	GLN
56	N0	65	ASN
56	N0	142	GLN
57	N1	98	HIS
59	N3	98	ASN
61	N5	111	ASN
65	N9	48	HIS
69	O3	106	ASN
74	O8	32	ASN
76	Q0	117	HIS
79	Q3	33	GLN
6	s4	98	ASN
9	s7	71	HIS
11	s9	110	GLN
11	s9	124	HIS
12	c0	32	HIS
12	c0	58	GLN
19	c7	42	GLN
20	c8	25	ASN
20	c8	90	ASN
22	d0	98	GLN
23	d1	3	ASN
24	d2	113	HIS
25	d3	79	ASN
27	d5	37	GLN
30	d8	27	GLN
80	e0	17	GLN
33	e1	95	HIS
34	sR	187	GLN
39	l2	38	HIS
39	l2	218	HIS
40	l3	165	GLN

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Mol	Chain	Res	Type
41	l4	328	ASN
42	l5	94	ASN
42	l5	151	GLN
42	l5	264	GLN
43	l6	61	ASN
44	l7	48	ASN
48	m1	132	ASN
51	m5	194	GLN
54	m8	145	ASN
55	m9	7	GLN
57	n1	98	HIS
57	n1	122	GLN
59	n3	33	ASN
62	n6	120	GLN
63	n7	57	HIS
68	o2	88	HIS
73	o7	13	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	511 (29%)	56 (3%)
1	6	1793/1800 (99%)	498 (27%)	50 (2%)
36	1	3145/3396 (92%)	747 (23%)	83 (2%)
36	5	3145/3396 (92%)	744 (23%)	85 (2%)
37	3	120/121 (99%)	19 (15%)	3 (2%)
37	7	120/121 (99%)	23 (19%)	3 (2%)
38	4	157/158 (99%)	45 (28%)	4 (2%)
38	8	157/158 (99%)	41 (26%)	2 (1%)
All	All	10384/10950 (94%)	2628 (25%)	286 (2%)

All (2628) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	20	G
1	2	21	U
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	39	A
1	2	46	A
1	2	47	A
1	2	57	G
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	76	A
1	2	77	U
1	2	104	A
1	2	114	C
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	167	U
1	2	169	A
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	188	A

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Mol	Chain	Res	Type
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	197	A
1	2	198	A
1	2	200	A
1	2	207	U
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	220	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	242	U
1	2	249	U
1	2	250	C
1	2	260	U
1	2	261	U
1	2	262	U
1	2	265	A
1	2	267	U
1	2	270	C
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	276	C

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Mol	Chain	Res	Type
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	299	A
1	2	302	U
1	2	304	U
1	2	308	C
1	2	309	C
1	2	314	C
1	2	316	A
1	2	319	U
1	2	321	C
1	2	322	G
1	2	332	U
1	2	333	A
1	2	337	G
1	2	338	C
1	2	341	A
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	365	G
1	2	393	C
1	2	399	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	418	G
1	2	419	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	431	C
1	2	433	C
1	2	434	G

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Mol	Chain	Res	Type
1	2	437	A
1	2	439	U
1	2	444	C
1	2	445	A
1	2	446	A
1	2	448	C
1	2	452	A
1	2	468	A
1	2	469	C
1	2	484	C
1	2	485	A
1	2	486	G
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	510	G
1	2	511	A
1	2	513	U
1	2	514	G
1	2	515	A
1	2	518	A
1	2	519	C
1	2	520	A
1	2	524	U
1	2	525	A
1	2	527	A
1	2	532	U
1	2	534	A
1	2	536	C
1	2	538	A

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Mol	Chain	Res	Type
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	546	U
1	2	548	G
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	579	A
1	2	580	A
1	2	584	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	622	A
1	2	623	A
1	2	624	G
1	2	630	A
1	2	639	U
1	2	640	U
1	2	643	G
1	2	650	U
1	2	653	C
1	2	655	G
1	2	656	G
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C

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Mol	Chain	Res	Type
1	2	692	C
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	711	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	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	752	A
1	2	754	A
1	2	755	A

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Mol	Chain	Res	Type
1	2	756	A
1	2	765	G
1	2	766	U
1	2	768	C
1	2	774	A
1	2	775	G
1	2	777	C
1	2	778	G
1	2	779	U
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	789	A
1	2	793	A
1	2	794	U
1	2	795	U
1	2	803	A
1	2	812	A
1	2	813	U
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	824	G
1	2	830	U
1	2	831	U
1	2	833	U
1	2	837	G
1	2	838	G
1	2	840	U
1	2	846	G
1	2	850	A
1	2	854	U
1	2	856	A
1	2	863	A
1	2	864	U
1	2	876	G
1	2	886	U

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Mol	Chain	Res	Type
1	2	887	A
1	2	892	A
1	2	896	U
1	2	898	A
1	2	912	U
1	2	914	G
1	2	916	U
1	2	921	U
1	2	933	A
1	2	935	U
1	2	942	G
1	2	951	A
1	2	960	U
1	2	966	A
1	2	984	G
1	2	988	A
1	2	991	G
1	2	992	A
1	2	993	A
1	2	994	G
1	2	996	U
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1026	A
1	2	1028	C
1	2	1029	U
1	2	1031	U
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1062	A
1	2	1064	G
1	2	1066	C
1	2	1067	C
1	2	1074	G

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Mol	Chain	Res	Type
1	2	1076	A
1	2	1080	U
1	2	1081	A
1	2	1082	C
1	2	1083	G
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1101	G
1	2	1109	G
1	2	1137	A
1	2	1138	A
1	2	1139	A
1	2	1143	A
1	2	1146	G
1	2	1149	G
1	2	1150	G
1	2	1151	A
1	2	1157	A
1	2	1158	C
1	2	1159	C
1	2	1160	A
1	2	1163	A
1	2	1167	G
1	2	1168	U
1	2	1180	C
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	1226	A

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Mol	Chain	Res	Type
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1241	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1258	U
1	2	1260	U
1	2	1267	G
1	2	1268	G
1	2	1276	U
1	2	1285	U
1	2	1286	U
1	2	1287	A
1	2	1314	U
1	2	1315	U
1	2	1316	G
1	2	1319	A
1	2	1321	A
1	2	1325	A
1	2	1337	A
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1350	U
1	2	1355	C
1	2	1361	U
1	2	1363	U
1	2	1364	G
1	2	1370	U
1	2	1371	A
1	2	1390	U
1	2	1395	G
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1410	A

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Mol	Chain	Res	Type
1	2	1412	G
1	2	1413	U
1	2	1414	U
1	2	1415	U
1	2	1418	G
1	2	1420	C
1	2	1421	A
1	2	1424	A
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1433	G
1	2	1446	A
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1461	C
1	2	1465	C
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1475	A
1	2	1482	C
1	2	1483	A
1	2	1485	C
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1503	A
1	2	1506	G
1	2	1514	U
1	2	1516	A
1	2	1517	U
1	2	1523	G
1	2	1524	A
1	2	1526	A
1	2	1530	C
1	2	1535	U
1	2	1536	G

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Mol	Chain	Res	Type
1	2	1537	C
1	2	1538	U
1	2	1542	G
1	2	1557	U
1	2	1559	A
1	2	1572	G
1	2	1574	G
1	2	1584	G
1	2	1600	A
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1625	C
1	2	1631	A
1	2	1636	C
1	2	1637	C
1	2	1652	C
1	2	1657	U
1	2	1658	G
1	2	1683	C
1	2	1684	U
1	2	1719	A
1	2	1731	A
1	2	1738	U
1	2	1754	A
1	2	1755	A
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1768	G
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1791	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

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Mol	Chain	Res	Type
36	1	13	A
36	1	14	U
36	1	15	C
36	1	16	A
36	1	26	A
36	1	37	U
36	1	40	A
36	1	43	A
36	1	49	A
36	1	54	C
36	1	57	A
36	1	59	G
36	1	60	A
36	1	61	A
36	1	65	A
36	1	66	A
36	1	68	C
36	1	74	G
36	1	76	G
36	1	83	U
36	1	93	C
36	1	94	G
36	1	99	A
36	1	109	A
36	1	110	G
36	1	111	C
36	1	113	C
36	1	115	A
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	156	G
36	1	157	A
36	1	160	G
36	1	166	C
36	1	169	U
36	1	187	A
36	1	190	U
36	1	191	U
36	1	195	U

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Mol	Chain	Res	Type
36	1	197	G
36	1	210	U
36	1	211	A
36	1	218	G
36	1	219	A
36	1	232	G
36	1	235	A
36	1	240	U
36	1	241	G
36	1	243	G
36	1	247	C
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	263	C
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	305	U
36	1	306	A
36	1	315	C
36	1	318	A
36	1	323	A
36	1	329	U
36	1	334	A
36	1	339	C
36	1	349	A
36	1	350	C
36	1	359	U
36	1	376	G
36	1	395	A
36	1	398	A
36	1	399	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	404	G
36	1	420	G

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Mol	Chain	Res	Type
36	1	421	G
36	1	422	A
36	1	438	A
36	1	439	C
36	1	440	A
36	1	495	G
36	1	498	A
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	552	G
36	1	553	U
36	1	555	U
36	1	556	U
36	1	557	A
36	1	559	A
36	1	560	G
36	1	569	A
36	1	578	A
36	1	579	G
36	1	588	G
36	1	592	A
36	1	604	G
36	1	609	G
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A
36	1	636	C
36	1	638	C
36	1	648	C
36	1	649	A
36	1	658	G
36	1	660	A
36	1	661	G
36	1	675	C
36	1	677	A

Continued on next page...

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Mol	Chain	Res	Type
36	1	681	U
36	1	691	A
36	1	692	A
36	1	697	A
36	1	705	A
36	1	711	A
36	1	712	G
36	1	715	A
36	1	716	A
36	1	719	U
36	1	725	G
36	1	759	U
36	1	764	U
36	1	766	U
36	1	767	U
36	1	768	C
36	1	776	U
36	1	777	U
36	1	780	A
36	1	781	G
36	1	785	G
36	1	787	G
36	1	802	C
36	1	803	C
36	1	806	A
36	1	817	A
36	1	826	G
36	1	830	A
36	1	831	G
36	1	849	C
36	1	861	C
36	1	874	U
36	1	876	A
36	1	878	G
36	1	879	U
36	1	890	C
36	1	891	G
36	1	896	A
36	1	901	G
36	1	907	G
36	1	908	G
36	1	909	G

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Mol	Chain	Res	Type
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	933	A
36	1	937	G
36	1	938	C
36	1	944	C
36	1	953	G
36	1	958	C
36	1	959	C
36	1	960	U
36	1	962	A
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	994	G
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1012	G
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1021	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1037	C
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1063	G
36	1	1064	A
36	1	1068	C
36	1	1072	G
36	1	1081	U

Continued on next page...

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Mol	Chain	Res	Type
36	1	1082	U
36	1	1083	G
36	1	1087	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1131	G
36	1	1144	U
36	1	1153	A
36	1	1159	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1186	G
36	1	1191	U
36	1	1192	C
36	1	1196	C
36	1	1201	C
36	1	1209	G
36	1	1211	U
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	1238	C
36	1	1241	U
36	1	1243	G
36	1	1245	A
36	1	1246	G

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Mol	Chain	Res	Type
36	1	1248	C
36	1	1249	G
36	1	1258	U
36	1	1259	A
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1267	U
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1274	A
36	1	1278	A
36	1	1279	C
36	1	1280	C
36	1	1285	G
36	1	1286	A
36	1	1287	A
36	1	1297	C
36	1	1305	U
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1314	C
36	1	1318	A
36	1	1330	A
36	1	1331	U
36	1	1332	A
36	1	1339	C
36	1	1345	G
36	1	1348	U
36	1	1349	G
36	1	1350	A
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G

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Mol	Chain	Res	Type
36	1	1385	C
36	1	1386	A
36	1	1387	G
36	1	1397	C
36	1	1398	U
36	1	1399	A
36	1	1400	G
36	1	1408	G
36	1	1417	G
36	1	1418	A
36	1	1419	A
36	1	1421	G
36	1	1431	G
36	1	1434	G
36	1	1437	C
36	1	1438	U
36	1	1446	A
36	1	1450	G
36	1	1455	U
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1488	G
36	1	1490	A
36	1	1503	A
36	1	1508	C
36	1	1511	U
36	1	1518	U
36	1	1519	G
36	1	1526	U
36	1	1529	A
36	1	1533	U
36	1	1535	A
36	1	1536	G
36	1	1538	G
36	1	1549	U
36	1	1554	U
36	1	1555	U
36	1	1556	C
36	1	1560	G
36	1	1561	G
36	1	1562	C

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Mol	Chain	Res	Type
36	1	1563	C
36	1	1564	U
36	1	1565	G
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	1575	A
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	1586	G
36	1	1587	A
36	1	1589	A
36	1	1593	A
36	1	1605	A
36	1	1607	U
36	1	1608	C
36	1	1609	C
36	1	1620	U
36	1	1621	A
36	1	1629	U
36	1	1633	C
36	1	1639	C
36	1	1642	A
36	1	1643	A
36	1	1645	U
36	1	1655	G
36	1	1658	G
36	1	1664	G
36	1	1683	A
36	1	1692	U
36	1	1705	U
36	1	1716	U
36	1	1717	U

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Mol	Chain	Res	Type
36	1	1724	U
36	1	1734	G
36	1	1736	G
36	1	1741	A
36	1	1742	U
36	1	1750	A
36	1	1751	G
36	1	1760	A
36	1	1761	C
36	1	1762	C
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1768	U
36	1	1770	G
36	1	1775	G
36	1	1779	C
36	1	1780	G
36	1	1797	A
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	1822	C
36	1	1829	G
36	1	1835	A
36	1	1839	A
36	1	1840	U
36	1	1841	A
36	1	1842	A
36	1	1845	G
36	1	1846	C
36	1	1847	A
36	1	1849	C
36	1	1863	G

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Mol	Chain	Res	Type
36	1	1864	A
36	1	1866	C
36	1	1879	A
36	1	1880	U
36	1	1897	G
36	1	1901	A
36	1	1906	G
36	1	1920	U
36	1	1927	G
36	1	1935	G
36	1	1937	U
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	1954	G
36	1	2094	C
36	1	2097	U
36	1	2101	C
36	1	2102	U
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2121	G
36	1	2122	G
36	1	2126	A
36	1	2130	G
36	1	2131	A
36	1	2134	G
36	1	2140	U
36	1	2158	A
36	1	2169	G
36	1	2187	G
36	1	2188	A
36	1	2194	G
36	1	2198	A
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	2228	A

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Mol	Chain	Res	Type
36	1	2231	C
36	1	2239	G
36	1	2245	C
36	1	2246	G
36	1	2249	G
36	1	2250	G
36	1	2252	A
36	1	2255	A
36	1	2256	A
36	1	2260	U
36	1	2268	U
36	1	2272	G
36	1	2273	G
36	1	2281	A
36	1	2282	U
36	1	2283	G
36	1	2284	C
36	1	2288	G
36	1	2301	U
36	1	2303	A
36	1	2306	C
36	1	2307	G
36	1	2308	C
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	2334	U
36	1	2335	G
36	1	2336	U
36	1	2360	C
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

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Mol	Chain	Res	Type
36	1	2403	G
36	1	2404	A
36	1	2405	C
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2437	G
36	1	2443	A
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2504	U
36	1	2514	U
36	1	2515	A
36	1	2520	A
36	1	2522	G
36	1	2523	A
36	1	2525	G
36	1	2526	C
36	1	2532	U
36	1	2533	G
36	1	2534	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2544	U
36	1	2547	A
36	1	2548	C
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2561	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U

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Mol	Chain	Res	Type
36	1	2572	C
36	1	2573	G
36	1	2581	U
36	1	2585	G
36	1	2591	A
36	1	2593	A
36	1	2594	C
36	1	2602	G
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2618	G
36	1	2626	A
36	1	2628	A
36	1	2629	U
36	1	2637	A
36	1	2638	C
36	1	2648	G
36	1	2652	U
36	1	2656	A
36	1	2672	G
36	1	2674	A
36	1	2677	G
36	1	2689	A
36	1	2690	G
36	1	2691	A
36	1	2694	A
36	1	2695	A
36	1	2696	A
36	1	2705	A
36	1	2706	G
36	1	2714	G
36	1	2728	G
36	1	2729	U
36	1	2737	C
36	1	2744	U
36	1	2752	U
36	1	2753	G
36	1	2755	C
36	1	2762	A
36	1	2764	C
36	1	2771	U

Continued on next page...

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Mol	Chain	Res	Type
36	1	2772	C
36	1	2773	C
36	1	2777	G
36	1	2778	G
36	1	2779	A
36	1	2783	U
36	1	2794	G
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2803	A
36	1	2810	C
36	1	2815	G
36	1	2817	A
36	1	2818	U
36	1	2829	U
36	1	2830	G
36	1	2839	G
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2847	A
36	1	2853	A
36	1	2856	G
36	1	2858	U
36	1	2860	U
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2876	C
36	1	2880	U
36	1	2886	U
36	1	2887	A
36	1	2888	U
36	1	2898	G
36	1	2899	C
36	1	2917	G
36	1	2923	U
36	1	2935	U
36	1	2936	A

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Mol	Chain	Res	Type
36	1	2942	C
36	1	2947	G
36	1	2951	G
36	1	2954	U
36	1	2955	U
36	1	2971	A
36	1	2977	G
36	1	2979	U
36	1	2983	C
36	1	2990	G
36	1	2992	U
36	1	2997	G
36	1	3012	A
36	1	3028	G
36	1	3055	U
36	1	3056	U
36	1	3057	U
36	1	3059	G
36	1	3074	G
36	1	3078	U
36	1	3079	U
36	1	3080	G
36	1	3086	A
36	1	3087	A
36	1	3088	G
36	1	3092	C
36	1	3094	A
36	1	3101	G
36	1	3104	U
36	1	3113	A
36	1	3122	A
36	1	3130	A
36	1	3131	U
36	1	3142	A
36	1	3143	C
36	1	3145	C
36	1	3147	G
36	1	3151	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U

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Mol	Chain	Res	Type
36	1	3157	U
36	1	3164	C
36	1	3165	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	3187	A
36	1	3196	U
36	1	3206	C
36	1	3207	U
36	1	3210	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3220	G
36	1	3223	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	3268	A
36	1	3269	U
36	1	3270	U
36	1	3273	A
36	1	3276	G
36	1	3280	U
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3289	G
36	1	3293	U
36	1	3294	A

Continued on next page...

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Mol	Chain	Res	Type
36	1	3295	A
36	1	3303	G
36	1	3304	U
36	1	3307	A
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	3322	A
36	1	3330	A
36	1	3335	A
36	1	3336	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3350	C
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	3358	U
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	11	A
37	3	13	A
37	3	14	U
37	3	17	A
37	3	21	G
37	3	22	A
37	3	41	G
37	3	42	A

Continued on next page...

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Mol	Chain	Res	Type
37	3	53	U
37	3	54	U
37	3	65	G
37	3	74	C
37	3	76	A
37	3	91	G
37	3	102	A
37	3	109	G
37	3	112	G
37	3	121	U
38	4	20	U
38	4	21	C
38	4	26	U
38	4	34	U
38	4	35	C
38	4	43	A
38	4	48	A
38	4	49	G
38	4	52	A
38	4	53	A
38	4	55	U
38	4	58	G
38	4	59	A
38	4	62	C
38	4	63	G
38	4	70	G
38	4	79	A
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	93	U
38	4	95	G
38	4	96	A
38	4	97	A
38	4	102	U
38	4	104	A

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Mol	Chain	Res	Type
38	4	105	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	125	U
38	4	126	A
38	4	128	U
38	4	138	A
38	4	148	G
38	4	152	G
38	4	155	A
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	6	G
1	6	24	U
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	47	A
1	6	50	C
1	6	57	G
1	6	61	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	114	C
1	6	115	G
1	6	126	A
1	6	127	G
1	6	129	U
1	6	130	C
1	6	132	U
1	6	137	U
1	6	138	A

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Mol	Chain	Res	Type
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	149	C
1	6	153	G
1	6	158	U
1	6	159	U
1	6	166	C
1	6	174	U
1	6	177	U
1	6	178	U
1	6	181	A
1	6	185	U
1	6	187	G
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	195	G
1	6	196	G
1	6	197	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
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	234	G
1	6	235	G
1	6	240	U

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Mol	Chain	Res	Type
1	6	241	U
1	6	250	C
1	6	261	U
1	6	265	A
1	6	269	G
1	6	270	C
1	6	271	A
1	6	272	U
1	6	273	G
1	6	275	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	287	G
1	6	299	A
1	6	301	A
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	330	G
1	6	333	A
1	6	337	G
1	6	338	C
1	6	341	A
1	6	346	G
1	6	350	U
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	393	C
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	418	G
1	6	419	G
1	6	421	A

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Mol	Chain	Res	Type
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	437	A
1	6	439	U
1	6	444	C
1	6	454	U
1	6	464	A
1	6	468	A
1	6	475	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	502	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	507	U
1	6	508	U
1	6	510	G
1	6	511	A
1	6	515	A
1	6	519	C
1	6	520	A
1	6	527	A
1	6	536	C
1	6	539	G
1	6	540	G
1	6	541	A

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Mol	Chain	Res	Type
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	565	C
1	6	566	C
1	6	570	A
1	6	574	G
1	6	579	A
1	6	580	A
1	6	582	U
1	6	594	A
1	6	595	G
1	6	606	A
1	6	609	U
1	6	610	G
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	637	C
1	6	639	U
1	6	640	U
1	6	645	C
1	6	648	G
1	6	650	U
1	6	652	G
1	6	653	C
1	6	654	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

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Mol	Chain	Res	Type
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C
1	6	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	730	G
1	6	742	U
1	6	743	U
1	6	744	U
1	6	751	G
1	6	753	A
1	6	754	A
1	6	755	A
1	6	756	A
1	6	757	A
1	6	765	G
1	6	766	U
1	6	767	U
1	6	768	C
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G
1	6	789	A

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Mol	Chain	Res	Type
1	6	792	U
1	6	793	A
1	6	794	U
1	6	806	A
1	6	808	U
1	6	811	A
1	6	812	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	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	842	C
1	6	847	A
1	6	863	A
1	6	873	U
1	6	886	U
1	6	898	A
1	6	904	G
1	6	905	A
1	6	906	A
1	6	910	C
1	6	912	U
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	945	U
1	6	958	U
1	6	959	U
1	6	960	U
1	6	969	C

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Mol	Chain	Res	Type
1	6	970	A
1	6	971	A
1	6	983	A
1	6	985	G
1	6	988	A
1	6	992	A
1	6	993	A
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1010	C
1	6	1018	U
1	6	1026	A
1	6	1028	C
1	6	1029	U
1	6	1039	A
1	6	1040	G
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1063	U
1	6	1065	A
1	6	1067	C
1	6	1070	C
1	6	1072	C
1	6	1073	G
1	6	1075	C
1	6	1081	A
1	6	1082	C
1	6	1092	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1099	U
1	6	1100	G
1	6	1101	G
1	6	1104	U
1	6	1109	G
1	6	1113	A

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Mol	Chain	Res	Type
1	6	1137	A
1	6	1138	A
1	6	1146	G
1	6	1150	G
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1162	C
1	6	1163	A
1	6	1167	G
1	6	1183	A
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	1208	A
1	6	1213	G
1	6	1214	U
1	6	1217	A
1	6	1218	G
1	6	1219	A
1	6	1220	C
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1236	A
1	6	1238	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	1248	C

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Mol	Chain	Res	Type
1	6	1252	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1259	U
1	6	1261	G
1	6	1262	U
1	6	1275	A
1	6	1284	C
1	6	1286	U
1	6	1288	G
1	6	1291	G
1	6	1300	A
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	1341	A
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	1355	C
1	6	1360	A
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1371	A
1	6	1372	U
1	6	1373	C
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1413	U

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Mol	Chain	Res	Type
1	6	1415	U
1	6	1418	G
1	6	1424	A
1	6	1425	A
1	6	1427	A
1	6	1428	G
1	6	1429	G
1	6	1430	U
1	6	1431	C
1	6	1433	G
1	6	1437	U
1	6	1438	G
1	6	1445	G
1	6	1446	A
1	6	1448	G
1	6	1451	C
1	6	1459	C
1	6	1461	C
1	6	1471	A
1	6	1481	C
1	6	1482	C
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1506	G
1	6	1514	U
1	6	1516	A
1	6	1523	G
1	6	1524	A
1	6	1531	G
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1573	A

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Mol	Chain	Res	Type
1	6	1574	G
1	6	1575	G
1	6	1577	A
1	6	1584	G
1	6	1590	G
1	6	1597	A
1	6	1601	G
1	6	1616	G
1	6	1620	C
1	6	1621	U
1	6	1622	G
1	6	1631	A
1	6	1635	A
1	6	1637	C
1	6	1638	G
1	6	1656	U
1	6	1657	U
1	6	1658	G
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1712	A
1	6	1716	C
1	6	1717	G
1	6	1731	A
1	6	1736	G
1	6	1745	G
1	6	1755	A
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1772	C
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	1790	A

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Mol	Chain	Res	Type
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	14	U
36	5	15	C
36	5	26	A
36	5	40	A
36	5	43	A
36	5	44	U
36	5	49	A
36	5	60	A
36	5	62	A
36	5	65	A
36	5	66	A
36	5	73	C
36	5	74	G
36	5	76	G
36	5	83	U
36	5	85	A
36	5	92	G
36	5	93	C
36	5	96	G
36	5	97	U
36	5	99	A
36	5	101	G
36	5	109	A
36	5	110	G
36	5	111	C
36	5	113	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	124	U
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G

Continued on next page...

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Mol	Chain	Res	Type
36	5	152	U
36	5	156	G
36	5	157	A
36	5	161	G
36	5	165	A
36	5	166	C
36	5	170	G
36	5	171	G
36	5	172	G
36	5	174	C
36	5	180	C
36	5	181	U
36	5	182	U
36	5	186	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	192	C
36	5	200	C
36	5	206	G
36	5	210	U
36	5	211	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	231	G
36	5	234	G
36	5	237	G
36	5	239	G
36	5	240	U
36	5	242	C
36	5	244	G
36	5	245	U
36	5	246	U
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	257	U

Continued on next page...

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Mol	Chain	Res	Type
36	5	269	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	323	A
36	5	329	U
36	5	334	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	351	A
36	5	352	A
36	5	356	C
36	5	370	U
36	5	372	A
36	5	375	A
36	5	376	G
36	5	395	A
36	5	397	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	404	G
36	5	421	G
36	5	422	A
36	5	436	A
36	5	438	A
36	5	439	C
36	5	441	U
36	5	492	U
36	5	495	G
36	5	507	U
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	555	U

Continued on next page...

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Mol	Chain	Res	Type
36	5	557	A
36	5	559	A
36	5	578	A
36	5	579	G
36	5	592	A
36	5	604	G
36	5	607	A
36	5	609	G
36	5	610	G
36	5	611	A
36	5	619	A
36	5	620	U
36	5	621	A
36	5	636	C
36	5	644	G
36	5	649	A
36	5	653	A
36	5	656	A
36	5	660	A
36	5	675	C
36	5	677	A
36	5	681	U
36	5	683	U
36	5	691	A
36	5	705	A
36	5	708	G
36	5	712	G
36	5	715	A
36	5	716	A
36	5	717	C
36	5	725	G
36	5	727	G
36	5	748	U
36	5	763	G
36	5	766	U
36	5	767	U
36	5	776	U
36	5	777	U
36	5	781	G
36	5	785	G
36	5	786	A
36	5	801	A

Continued on next page...

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Mol	Chain	Res	Type
36	5	806	A
36	5	813	G
36	5	817	A
36	5	830	A
36	5	860	G
36	5	861	C
36	5	869	G
36	5	871	U
36	5	874	U
36	5	877	C
36	5	879	U
36	5	891	G
36	5	896	A
36	5	897	U
36	5	898	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	923	C
36	5	924	G
36	5	926	A
36	5	937	G
36	5	944	C
36	5	959	C
36	5	960	U
36	5	964	G
36	5	979	U
36	5	993	G
36	5	994	G
36	5	1000	C
36	5	1001	G
36	5	1002	A
36	5	1006	A
36	5	1010	G
36	5	1015	U
36	5	1017	C
36	5	1019	G

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Mol	Chain	Res	Type
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	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	1051	U
36	5	1064	A
36	5	1065	A
36	5	1072	G
36	5	1075	A
36	5	1081	U
36	5	1082	U
36	5	1083	G
36	5	1087	G
36	5	1088	U
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1117	G
36	5	1118	C
36	5	1131	G
36	5	1138	U
36	5	1144	U
36	5	1152	G
36	5	1153	A
36	5	1159	A
36	5	1160	C
36	5	1162	U
36	5	1165	A
36	5	1172	G
36	5	1173	U

Continued on next page...

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Mol	Chain	Res	Type
36	5	1178	G
36	5	1179	A
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1186	G
36	5	1190	A
36	5	1191	U
36	5	1192	C
36	5	1200	A
36	5	1201	C
36	5	1209	G
36	5	1222	G
36	5	1232	C
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1243	G
36	5	1245	A
36	5	1246	G
36	5	1248	C
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	1274	A
36	5	1285	G
36	5	1301	A
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1311	G
36	5	1313	G
36	5	1324	U
36	5	1330	A
36	5	1348	U
36	5	1349	G

Continued on next page...

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Mol	Chain	Res	Type
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1356	U
36	5	1357	G
36	5	1369	A
36	5	1370	G
36	5	1379	G
36	5	1385	C
36	5	1386	A
36	5	1398	U
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1421	G
36	5	1428	A
36	5	1431	G
36	5	1433	A
36	5	1434	G
36	5	1437	C
36	5	1438	U
36	5	1443	G
36	5	1446	A
36	5	1450	G
36	5	1465	A
36	5	1472	U
36	5	1481	A
36	5	1482	A
36	5	1490	A
36	5	1503	A
36	5	1508	C
36	5	1519	G
36	5	1528	G
36	5	1533	U
36	5	1536	G
36	5	1539	A
36	5	1541	G
36	5	1549	U
36	5	1554	U
36	5	1555	U
36	5	1556	C

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Mol	Chain	Res	Type
36	5	1557	A
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1564	U
36	5	1566	A
36	5	1567	U
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1589	A
36	5	1594	A
36	5	1600	U
36	5	1605	A
36	5	1607	U
36	5	1614	C
36	5	1618	G
36	5	1619	A
36	5	1620	U
36	5	1629	U
36	5	1639	C
36	5	1641	U
36	5	1642	A
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1656	A
36	5	1658	G
36	5	1677	G
36	5	1683	A
36	5	1685	C
36	5	1687	U

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Mol	Chain	Res	Type
36	5	1699	A
36	5	1708	C
36	5	1715	A
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1736	G
36	5	1741	A
36	5	1750	A
36	5	1751	G
36	5	1758	G
36	5	1759	C
36	5	1761	C
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1767	C
36	5	1770	G
36	5	1772	U
36	5	1775	G
36	5	1780	G
36	5	1781	C
36	5	1787	A
36	5	1788	C
36	5	1793	C
36	5	1795	U
36	5	1797	A
36	5	1808	G
36	5	1810	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1820	U
36	5	1821	U
36	5	1839	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1849	C

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Mol	Chain	Res	Type
36	5	1850	A
36	5	1859	A
36	5	1863	G
36	5	1864	A
36	5	1866	C
36	5	1871	U
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1884	A
36	5	1886	A
36	5	1891	A
36	5	1893	A
36	5	1895	A
36	5	1901	A
36	5	1906	G
36	5	1918	C
36	5	1920	U
36	5	1935	G
36	5	1948	G
36	5	1952	G
36	5	1953	G
36	5	2101	C
36	5	2102	U
36	5	2112	U
36	5	2113	A
36	5	2114	C
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	2145	A
36	5	2146	C
36	5	2158	A
36	5	2169	G
36	5	2177	G
36	5	2184	U
36	5	2185	G
36	5	2187	G
36	5	2192	C

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Mol	Chain	Res	Type
36	5	2198	A
36	5	2205	U
36	5	2208	A
36	5	2209	U
36	5	2210	G
36	5	2213	A
36	5	2215	A
36	5	2221	G
36	5	2223	A
36	5	2225	U
36	5	2229	A
36	5	2231	C
36	5	2244	A
36	5	2246	G
36	5	2249	G
36	5	2250	G
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2258	U
36	5	2266	U
36	5	2269	U
36	5	2270	A
36	5	2273	G
36	5	2278	C
36	5	2279	A
36	5	2281	A
36	5	2286	U
36	5	2288	G
36	5	2297	U
36	5	2298	U
36	5	2303	A
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2321	A
36	5	2336	U
36	5	2339	C
36	5	2352	A
36	5	2366	C

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Mol	Chain	Res	Type
36	5	2367	A
36	5	2368	A
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2383	C
36	5	2385	G
36	5	2388	U
36	5	2392	C
36	5	2393	G
36	5	2394	G
36	5	2397	A
36	5	2400	G
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2435	G
36	5	2437	G
36	5	2439	A
36	5	2440	G
36	5	2441	A
36	5	2443	A
36	5	2444	C
36	5	2504	U
36	5	2505	U
36	5	2506	U
36	5	2507	C
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2514	U
36	5	2515	A
36	5	2518	C
36	5	2523	A
36	5	2524	A
36	5	2526	C
36	5	2530	G

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Mol	Chain	Res	Type
36	5	2531	C
36	5	2532	U
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2541	U
36	5	2543	U
36	5	2549	G
36	5	2552	C
36	5	2555	G
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2586	G
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2614	G
36	5	2615	G
36	5	2618	G
36	5	2636	A
36	5	2637	A
36	5	2642	A
36	5	2652	U
36	5	2656	A
36	5	2657	A
36	5	2674	A
36	5	2677	G
36	5	2683	U
36	5	2689	A
36	5	2690	G
36	5	2691	A
36	5	2694	A

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Mol	Chain	Res	Type
36	5	2696	A
36	5	2705	A
36	5	2714	G
36	5	2717	U
36	5	2727	A
36	5	2728	G
36	5	2729	U
36	5	2740	A
36	5	2748	A
36	5	2750	U
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	2783	U
36	5	2796	G
36	5	2797	C
36	5	2800	G
36	5	2801	A
36	5	2802	A
36	5	2810	C
36	5	2814	G
36	5	2817	A
36	5	2818	U
36	5	2821	C
36	5	2822	U
36	5	2828	G
36	5	2837	A
36	5	2838	A
36	5	2839	G
36	5	2843	U
36	5	2845	A
36	5	2849	C
36	5	2853	A
36	5	2858	U
36	5	2867	C
36	5	2871	G

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Mol	Chain	Res	Type
36	5	2872	A
36	5	2876	C
36	5	2880	U
36	5	2887	A
36	5	2889	C
36	5	2899	C
36	5	2923	U
36	5	2928	C
36	5	2935	U
36	5	2936	A
36	5	2939	G
36	5	2941	A
36	5	2942	C
36	5	2947	G
36	5	2957	G
36	5	2966	G
36	5	2972	G
36	5	2973	G
36	5	2983	C
36	5	2990	G
36	5	2993	G
36	5	2995	A
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3013	U
36	5	3028	G
36	5	3039	C
36	5	3056	U
36	5	3059	G
36	5	3069	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3087	A
36	5	3092	C
36	5	3104	U
36	5	3119	U
36	5	3122	A
36	5	3130	A
36	5	3131	U
36	5	3142	A

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Mol	Chain	Res	Type
36	5	3143	C
36	5	3148	U
36	5	3153	U
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3164	C
36	5	3165	A
36	5	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	3180	A
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3198	U
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3224	G
36	5	3227	A
36	5	3228	C
36	5	3229	G
36	5	3239	G
36	5	3243	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3260	G
36	5	3265	C
36	5	3270	U
36	5	3273	A

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Mol	Chain	Res	Type
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3279	A
36	5	3280	U
36	5	3282	U
36	5	3284	G
36	5	3285	C
36	5	3286	G
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3310	A
36	5	3313	U
36	5	3316	A
36	5	3317	U
36	5	3318	G
36	5	3319	U
36	5	3333	G
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3350	C
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3356	G
36	5	3358	U
36	5	3369	G
36	5	3377	G
36	5	3378	C
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	23	A
37	7	27	A
37	7	33	U

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Mol	Chain	Res	Type
37	7	38	U
37	7	41	G
37	7	49	G
37	7	51	A
37	7	52	G
37	7	54	U
37	7	60	G
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	77	G
37	7	99	G
37	7	101	G
37	7	102	A
37	7	103	A
37	7	110	G
37	7	112	G
38	8	21	C
38	8	23	U
38	8	34	U
38	8	35	C
38	8	42	G
38	8	48	A
38	8	49	G
38	8	51	G
38	8	52	A
38	8	59	A
38	8	60	U
38	8	62	C
38	8	63	G
38	8	79	A
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	85	G
38	8	86	U
38	8	87	G
38	8	90	U
38	8	95	G

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Mol	Chain	Res	Type
38	8	96	A
38	8	97	A
38	8	102	U
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	136	G
38	8	137	C
38	8	152	G
38	8	156	U
38	8	157	U
38	8	158	U

All (286) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	68	A
1	2	73	U
1	2	113	U
1	2	130	C
1	2	131	C
1	2	139	C
1	2	158	U
1	2	217	A
1	2	218	A
1	2	232	U
1	2	240	U
1	2	278	U
1	2	280	U
1	2	321	C
1	2	417	A
1	2	468	A
1	2	484	C
1	2	497	G
1	2	499	U
1	2	501	U

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Mol	Chain	Res	Type
1	2	503	G
1	2	512	A
1	2	545	A
1	2	555	A
1	2	558	U
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	734	A
1	2	755	A
1	2	782	U
1	2	794	U
1	2	829	A
1	2	913	G
1	2	1058	U
1	2	1081	A
1	2	1108	G
1	2	1157	A
1	2	1196	A
1	2	1207	C
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1339	C
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1489	U
1	2	1490	C
1	2	1573	A
1	2	1600	A
1	2	1615	C
1	2	1657	U
1	2	1761	U
36	1	43	A
36	1	65	A
36	1	210	U
36	1	239	G
36	1	282	G
36	1	369	A
36	1	547	G

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Mol	Chain	Res	Type
36	1	594	U
36	1	619	A
36	1	637	C
36	1	715	A
36	1	763	G
36	1	873	C
36	1	896	A
36	1	916	G
36	1	932	U
36	1	979	U
36	1	981	U
36	1	993	G
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1196	C
36	1	1273	A
36	1	1307	G
36	1	1317	A
36	1	1329	U
36	1	1331	U
36	1	1352	A
36	1	1355	A
36	1	1419	A
36	1	1481	A
36	1	1484	U
36	1	1554	U
36	1	1562	C
36	1	1716	U
36	1	1751	G
36	1	1778	G
36	1	1815	U
36	1	1816	A
36	1	1820	U
36	1	1841	A
36	1	1846	C
36	1	1849	C
36	1	1858	A
36	1	1879	A
36	1	2101	C
36	1	2112	U
36	1	2209	U

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Mol	Chain	Res	Type
36	1	2249	G
36	1	2281	A
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	2571	U
36	1	2593	A
36	1	2704	A
36	1	2728	G
36	1	2772	C
36	1	2801	A
36	1	2818	U
36	1	2842	U
36	1	2950	G
36	1	3048	A
36	1	3078	U
36	1	3121	U
36	1	3195	U
36	1	3218	A
36	1	3228	C
36	1	3275	U
36	1	3276	G
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
36	1	3382	U
37	3	13	A
37	3	49	G
37	3	52	G
38	4	82	U
38	4	85	G
38	4	111	A
38	4	125	U
1	6	25	C

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Mol	Chain	Res	Type
1	6	76	A
1	6	114	C
1	6	136	C
1	6	145	A
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	272	U
1	6	345	U
1	6	400	A
1	6	417	A
1	6	542	A
1	6	543	C
1	6	555	A
1	6	557	G
1	6	558	U
1	6	651	G
1	6	697	C
1	6	717	C
1	6	755	A
1	6	829	A
1	6	834	G
1	6	1051	G
1	6	1058	U
1	6	1097	U
1	6	1137	A
1	6	1207	C
1	6	1218	G
1	6	1227	A
1	6	1238	A
1	6	1241	G
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1398	U
1	6	1481	C
1	6	1489	U
1	6	1535	U
1	6	1568	C
1	6	1572	G

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Mol	Chain	Res	Type
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	122	A
36	5	151	A
36	5	210	U
36	5	221	A
36	5	238	A
36	5	369	A
36	5	438	A
36	5	594	U
36	5	715	A
36	5	765	C
36	5	816	A
36	5	873	C
36	5	896	A
36	5	916	G
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1178	G
36	5	1181	U
36	5	1196	C
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	1370	G
36	5	1434	G
36	5	1481	A

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Mol	Chain	Res	Type
36	5	1554	U
36	5	1560	G
36	5	1574	C
36	5	1580	A
36	5	1605	A
36	5	1716	U
36	5	1816	A
36	5	1819	U
36	5	1841	A
36	5	1846	C
36	5	1878	G
36	5	2101	C
36	5	2112	U
36	5	2121	G
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2257	C
36	5	2372	A
36	5	2374	C
36	5	2404	A
36	5	2418	G
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2531	C
36	5	2682	C
36	5	2689	A
36	5	2772	C
36	5	2801	A
36	5	2818	U
36	5	2821	C
36	5	2887	A
36	5	2971	A
36	5	3065	G
36	5	3078	U
36	5	3121	U
36	5	3154	C
36	5	3167	A
36	5	3195	U
36	5	3218	A

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Mol	Chain	Res	Type
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	54	U
37	7	76	A
37	7	111	U
38	8	111	A
38	8	126	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2554 ligands modelled in this entry, 1422 are monoatomic - leaving 1132 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	3907	-	0,6,6	-	-	-	-	-
86	OHX	1	3926	-	0,6,6	-	-	-	-	-
86	OHX	1	3887	-	0,6,6	-	-	-	-	-
86	OHX	5	4207	-	0,6,6	-	-	-	-	-
86	OHX	1	3874	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4178	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	3	225	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	M7	205	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	Q2	502	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2151	-	0,6,6	-	-	-	-	-
86	OHX	D9	102	-	0,6,6	-	-	-	-	-
86	OHX	1	4179	-	0,6,6	-	-	-	-	-
86	OHX	6	2100	-	0,6,6	-	-	-	-	-
86	OHX	1	3913	-	0,6,6	-	-	-	-	-
86	OHX	o7	503	-	0,6,6	-	-	-	-	-
86	OHX	5	4149	-	0,6,6	-	-	-	-	-
86	OHX	6	2177	-	0,6,6	-	-	-	-	-
86	OHX	5	3964	-	0,6,6	-	-	-	-	-
86	OHX	1	3903	-	0,6,6	-	-	-	-	-
86	OHX	1	3908	-	0,6,6	-	-	-	-	-
86	OHX	1	4166	-	0,6,6	-	-	-	-	-
86	OHX	O6	201	-	0,6,6	-	-	-	-	-
86	OHX	1	3904	-	0,6,6	-	-	-	-	-
86	OHX	6	2129	-	0,6,6	-	-	-	-	-
86	OHX	6	2163	-	0,6,6	-	-	-	-	-
86	OHX	6	2196	-	0,6,6	-	-	-	-	-
86	OHX	1	3946	-	0,6,6	-	-	-	-	-
86	OHX	5	4062	-	0,6,6	-	-	-	-	-
86	OHX	1	4147	-	0,6,6	-	-	-	-	-
86	OHX	5	4081	-	0,6,6	-	-	-	-	-
86	OHX	5	4241	-	0,6,6	-	-	-	-	-
86	OHX	8	225	-	0,6,6	-	-	-	-	-
86	OHX	1	3867	-	0,6,6	-	-	-	-	-
86	OHX	2	2114	-	0,6,6	-	-	-	-	-
86	OHX	1	3915	-	0,6,6	-	-	-	-	-
86	OHX	1	4142	-	0,6,6	-	-	-	-	-
86	OHX	2	2158	-	0,6,6	-	-	-	-	-
86	OHX	6	2166	-	0,6,6	-	-	-	-	-
86	OHX	5	4217	-	0,6,6	-	-	-	-	-
86	OHX	5	3894	-	0,6,6	-	-	-	-	-
86	OHX	4	227	-	0,6,6	-	-	-	-	-
86	OHX	5	4238	-	0,6,6	-	-	-	-	-
86	OHX	1	4208	-	0,6,6	-	-	-	-	-
86	OHX	5	4159	-	0,6,6	-	-	-	-	-
86	OHX	2	2082	-	0,6,6	-	-	-	-	-
86	OHX	1	3933	-	0,6,6	-	-	-	-	-
86	OHX	6	2103	-	0,6,6	-	-	-	-	-
86	OHX	1	4150	-	0,6,6	-	-	-	-	-
86	OHX	5	3906	-	0,6,6	-	-	-	-	-
86	OHX	1	4031	-	0,6,6	-	-	-	-	-
86	OHX	5	4114	-	0,6,6	-	-	-	-	-
86	OHX	5	4230	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	7	227	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	O4	201	-	0,6,6	-	-	-		
86	OHX	5	4179	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	O7	103	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	C3	202	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	L4	403	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	5	4181	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		
86	OHX	5	3898	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	5	3899	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	1	4210	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	o2	201	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
88	3J6	5	4246	85	21,24,24	1.17	1 (4%)	25,42,42	1.19	2 (8%)
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	5	3896	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	13	405	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	6	2189	1	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
88	3J6	1	4213	85	21,24,24	2.31	3 (14%)	25,42,42	1.98	6 (24%)
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	14	402	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	n3	203	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	1	4188	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3895	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2046	-	0,6,6	-	-	-	-	-
86	OHX	2	2155	-	0,6,6	-	-	-	-	-
86	OHX	1	4201	-	0,6,6	-	-	-	-	-
86	OHX	6	2061	-	0,6,6	-	-	-	-	-
86	OHX	SR	401	-	0,6,6	-	-	-	-	-
86	OHX	1	4086	-	0,6,6	-	-	-	-	-
86	OHX	2	2028	-	0,6,6	-	-	-	-	-
86	OHX	2	2080	-	0,6,6	-	-	-	-	-
86	OHX	5	4022	-	0,6,6	-	-	-	-	-
86	OHX	1	4041	-	0,6,6	-	-	-	-	-
86	OHX	4	231	-	0,6,6	-	-	-	-	-
86	OHX	6	2116	-	0,6,6	-	-	-	-	-
86	OHX	1	3982	-	0,6,6	-	-	-	-	-
86	OHX	5	4010	-	0,6,6	-	-	-	-	-
86	OHX	1	4205	-	0,6,6	-	-	-	-	-
86	OHX	5	4014	-	0,6,6	-	-	-	-	-
86	OHX	1	4040	-	0,6,6	-	-	-	-	-
86	OHX	1	3985	-	0,6,6	-	-	-	-	-
86	OHX	1	3997	-	0,6,6	-	-	-	-	-
86	OHX	1	4136	-	0,6,6	-	-	-	-	-
86	OHX	1	3873	-	0,6,6	-	-	-	-	-
86	OHX	2	2159	-	0,6,6	-	-	-	-	-
86	OHX	1	4045	-	0,6,6	-	-	-	-	-
86	OHX	5	4167	-	0,6,6	-	-	-	-	-
86	OHX	2	2096	-	0,6,6	-	-	-	-	-
86	OHX	1	4101	-	0,6,6	-	-	-	-	-
86	OHX	7	225	-	0,6,6	-	-	-	-	-
86	OHX	6	2140	-	0,6,6	-	-	-	-	-
86	OHX	1	3943	-	0,6,6	-	-	-	-	-
86	OHX	6	2170	-	0,6,6	-	-	-	-	-
86	OHX	1	4027	-	0,6,6	-	-	-	-	-
86	OHX	1	3931	-	0,6,6	-	-	-	-	-
86	OHX	1	3914	-	0,6,6	-	-	-	-	-
86	OHX	6	2147	-	0,6,6	-	-	-	-	-
86	OHX	1	4074	-	0,6,6	-	-	-	-	-
86	OHX	6	2190	-	0,6,6	-	-	-	-	-
86	OHX	5	4047	-	0,6,6	-	-	-	-	-
86	OHX	1	3939	-	0,6,6	-	-	-	-	-
86	OHX	1	4161	-	0,6,6	-	-	-	-	-
86	OHX	5	4232	-	0,6,6	-	-	-	-	-
86	OHX	5	4223	-	0,6,6	-	-	-	-	-
86	OHX	1	4029	-	0,6,6	-	-	-	-	-
86	OHX	1	4036	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	15	307	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	8	231	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	m1	202	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	n6	203	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	3	224	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	5	3943	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	l3	404	-	0,6,6	-	-	-		
86	OHX	2	2178	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	m5	303	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	M0	304	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	5	3897	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	2	2179	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		
86	OHX	1	4209	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	o3	203	-	0,6,6	-	-	-		
86	OHX	L3	405	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	5	4233	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	3	226	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	15	306	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	6	2203	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	19	202	-	0,6,6	-	-	-		
86	OHX	S6	301	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	m0	303	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	5	4226	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	O3	202	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	n9	102	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	6	2045	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	1	4176	-	0,6,6	-	-	-		
86	OHX	S8	302	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	4	221	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	l5	304	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	1	4168	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	5	4228	-	0,6,6	-	-	-		
86	OHX	6	2201	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	O1	201	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	n3	204	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2168	-	0,6,6	-	-	-	-	-
86	OHX	2	2173	-	0,6,6	-	-	-	-	-
86	OHX	1	3889	-	0,6,6	-	-	-	-	-
86	OHX	1	4126	-	0,6,6	-	-	-	-	-
86	OHX	1	4170	-	0,6,6	-	-	-	-	-
86	OHX	5	4147	-	0,6,6	-	-	-	-	-
86	OHX	5	3929	-	0,6,6	-	-	-	-	-
86	OHX	2	2084	-	0,6,6	-	-	-	-	-
86	OHX	14	403	-	0,6,6	-	-	-	-	-
86	OHX	5	4099	-	0,6,6	-	-	-	-	-
86	OHX	1	3888	-	0,6,6	-	-	-	-	-
86	OHX	5	4034	-	0,6,6	-	-	-	-	-
86	OHX	M7	206	-	0,6,6	-	-	-	-	-
86	OHX	5	4003	-	0,6,6	-	-	-	-	-
86	OHX	1	4007	-	0,6,6	-	-	-	-	-
86	OHX	1	3967	-	0,6,6	-	-	-	-	-
86	OHX	6	2187	-	0,6,6	-	-	-	-	-
86	OHX	5	4025	-	0,6,6	-	-	-	-	-
86	OHX	M9	203	-	0,6,6	-	-	-	-	-
86	OHX	5	4072	-	0,6,6	-	-	-	-	-
86	OHX	5	4092	-	0,6,6	-	-	-	-	-
86	OHX	1	4194	-	0,6,6	-	-	-	-	-
86	OHX	1	3924	-	0,6,6	-	-	-	-	-
86	OHX	1	4155	-	0,6,6	-	-	-	-	-
86	OHX	5	3933	-	0,6,6	-	-	-	-	-
86	OHX	1	3927	-	0,6,6	-	-	-	-	-
86	OHX	1	3990	-	0,6,6	-	-	-	-	-
86	OHX	1	4130	-	0,6,6	-	-	-	-	-
86	OHX	2	2153	-	0,6,6	-	-	-	-	-
86	OHX	6	2094	-	0,6,6	-	-	-	-	-
86	OHX	6	2114	-	0,6,6	-	-	-	-	-
86	OHX	6	2204	-	0,6,6	-	-	-	-	-
86	OHX	8	219	-	0,6,6	-	-	-	-	-
86	OHX	5	4194	-	0,6,6	-	-	-	-	-
86	OHX	2	2131	-	0,6,6	-	-	-	-	-
86	OHX	5	3962	-	0,6,6	-	-	-	-	-
86	OHX	1	4189	-	0,6,6	-	-	-	-	-
86	OHX	5	4052	-	0,6,6	-	-	-	-	-
86	OHX	5	4090	-	0,6,6	-	-	-	-	-
86	OHX	5	4136	-	0,6,6	-	-	-	-	-
86	OHX	1	4162	-	0,6,6	-	-	-	-	-
86	OHX	1	4200	-	0,6,6	-	-	-	-	-
86	OHX	6	2128	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4035	-	0,6,6	-	-	-	-	-
86	OHX	1	3993	-	0,6,6	-	-	-	-	-
86	OHX	2	2083	-	0,6,6	-	-	-	-	-
86	OHX	1	3909	-	0,6,6	-	-	-	-	-
86	OHX	2	2037	-	0,6,6	-	-	-	-	-
86	OHX	1	3911	-	0,6,6	-	-	-	-	-
86	OHX	1	4054	-	0,6,6	-	-	-	-	-
86	OHX	5	4085	-	0,6,6	-	-	-	-	-
86	OHX	1	3897	-	0,6,6	-	-	-	-	-
86	OHX	5	3926	-	0,6,6	-	-	-	-	-
86	OHX	1	4204	-	0,6,6	-	-	-	-	-
86	OHX	4	222	-	0,6,6	-	-	-	-	-
86	OHX	5	4093	-	0,6,6	-	-	-	-	-
86	OHX	5	4121	-	0,6,6	-	-	-	-	-
86	OHX	1	4211	-	0,6,6	-	-	-	-	-
86	OHX	2	2109	-	0,6,6	-	-	-	-	-
86	OHX	1	4212	-	0,6,6	-	-	-	-	-
86	OHX	1	4146	-	0,6,6	-	-	-	-	-
86	OHX	5	4056	-	0,6,6	-	-	-	-	-
86	OHX	5	4169	-	0,6,6	-	-	-	-	-
86	OHX	5	4170	-	0,6,6	-	-	-	-	-
86	OHX	2	2138	-	0,6,6	-	-	-	-	-
86	OHX	2	2172	-	0,6,6	-	-	-	-	-
86	OHX	5	4039	-	0,6,6	-	-	-	-	-
86	OHX	5	4019	-	0,6,6	-	-	-	-	-
86	OHX	5	4030	-	0,6,6	-	-	-	-	-
86	OHX	1	4184	-	0,6,6	-	-	-	-	-
86	OHX	1	3870	-	0,6,6	-	-	-	-	-
86	OHX	1	3882	-	0,6,6	-	-	-	-	-
86	OHX	1	4106	-	0,6,6	-	-	-	-	-
86	OHX	1	4137	-	0,6,6	-	-	-	-	-
86	OHX	4	224	-	0,6,6	-	-	-	-	-
86	OHX	6	2048	-	0,6,6	-	-	-	-	-
86	OHX	5	4107	-	0,6,6	-	-	-	-	-
86	OHX	5	3913	-	0,6,6	-	-	-	-	-
86	OHX	5	4216	-	0,6,6	-	-	-	-	-
86	OHX	6	2168	-	0,6,6	-	-	-	-	-
86	OHX	1	4102	-	0,6,6	-	-	-	-	-
86	OHX	m6	203	-	0,6,6	-	-	-	-	-
86	OHX	2	2027	-	0,6,6	-	-	-	-	-
86	OHX	2	2144	-	0,6,6	-	-	-	-	-
86	OHX	6	2079	-	0,6,6	-	-	-	-	-
86	OHX	5	3927	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4008	-	0,6,6	-	-	-	-	-
86	OHX	5	3988	-	0,6,6	-	-	-	-	-
86	OHX	5	4187	-	0,6,6	-	-	-	-	-
86	OHX	m7	206	-	0,6,6	-	-	-	-	-
86	OHX	5	3938	-	0,6,6	-	-	-	-	-
86	OHX	6	2194	-	0,6,6	-	-	-	-	-
86	OHX	1	3948	-	0,6,6	-	-	-	-	-
86	OHX	6	2148	-	0,6,6	-	-	-	-	-
86	OHX	6	2161	-	0,6,6	-	-	-	-	-
86	OHX	6	2052	-	0,6,6	-	-	-	-	-
86	OHX	2	2049	-	0,6,6	-	-	-	-	-
86	OHX	2	2069	-	0,6,6	-	-	-	-	-
86	OHX	5	4053	-	0,6,6	-	-	-	-	-
86	OHX	2	2034	-	0,6,6	-	-	-	-	-
86	OHX	2	2071	-	0,6,6	-	-	-	-	-
86	OHX	3	219	-	0,6,6	-	-	-	-	-
86	OHX	1	3940	-	0,6,6	-	-	-	-	-
86	OHX	6	2088	-	0,6,6	-	-	-	-	-
86	OHX	5	4073	-	0,6,6	-	-	-	-	-
86	OHX	5	4195	-	0,6,6	-	-	-	-	-
86	OHX	5	4202	-	0,6,6	-	-	-	-	-
86	OHX	5	4236	-	0,6,6	-	-	-	-	-
86	OHX	7	222	-	0,6,6	-	-	-	-	-
86	OHX	15	305	-	0,6,6	-	-	-	-	-
86	OHX	5	4011	-	0,6,6	-	-	-	-	-
86	OHX	6	2183	-	0,6,6	-	-	-	-	-
86	OHX	6	2086	-	0,6,6	-	-	-	-	-
86	OHX	5	4027	-	0,6,6	-	-	-	-	-
86	OHX	2	2142	-	0,6,6	-	-	-	-	-
86	OHX	7	218	-	0,6,6	-	-	-	-	-
86	OHX	1	3920	-	0,6,6	-	-	-	-	-
86	OHX	1	4117	-	0,6,6	-	-	-	-	-
86	OHX	2	2097	-	0,6,6	-	-	-	-	-
86	OHX	6	2070	-	0,6,6	-	-	-	-	-
86	OHX	5	4007	-	0,6,6	-	-	-	-	-
86	OHX	1	3959	-	0,6,6	-	-	-	-	-
86	OHX	c3	201	-	0,6,6	-	-	-	-	-
86	OHX	D3	202	-	0,6,6	-	-	-	-	-
86	OHX	5	4029	-	0,6,6	-	-	-	-	-
86	OHX	5	4175	-	0,6,6	-	-	-	-	-
86	OHX	5	4130	-	0,6,6	-	-	-	-	-
86	OHX	5	4218	-	0,6,6	-	-	-	-	-
86	OHX	6	2054	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3893	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		
86	OHX	O9	101	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	1	4197	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	1	4116	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	6	2202	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	1	4119	-	0,6,6	-	-	-		
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2099	-	0,6,6	-	-	-	-	-
86	OHX	5	4082	-	0,6,6	-	-	-	-	-
86	OHX	5	3968	-	0,6,6	-	-	-	-	-
86	OHX	5	4157	-	0,6,6	-	-	-	-	-
86	OHX	5	4137	-	0,6,6	-	-	-	-	-
86	OHX	1	4087	-	0,6,6	-	-	-	-	-
86	OHX	5	4110	-	0,6,6	-	-	-	-	-
86	OHX	5	4197	-	0,6,6	-	-	-	-	-
86	OHX	2	2036	-	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	3J6	5	4246	85	-	3/3/68/68	0/5/4/4
88	3J6	1	4213	85	-	0/3/68/68	0/5/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4213	3J6	C4-C3	7.70	1.66	1.54
88	1	4213	3J6	O2-C11	6.28	1.55	1.44
88	1	4213	3J6	C11-C7	-2.53	1.49	1.56
88	5	4246	3J6	C4-C3	2.33	1.58	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4213	3J6	O2-C12-C11	5.21	64.68	59.35
88	1	4213	3J6	C11-C7-C4	-4.60	103.63	106.74
88	1	4213	3J6	O2-C11-C7	-3.21	113.91	117.98
88	1	4213	3J6	O3-C3-C4	3.06	116.13	112.50
88	1	4213	3J6	C12-O2-C11	-2.81	57.23	60.91
88	5	4246	3J6	C7-C11-C10	-2.78	99.32	104.68
88	1	4213	3J6	O2-C11-C10	2.52	120.38	115.59
88	5	4246	3J6	O3-C3-C2	2.28	109.28	105.54

There are no chirality outliers.

All (3) torsion outliers are listed below:

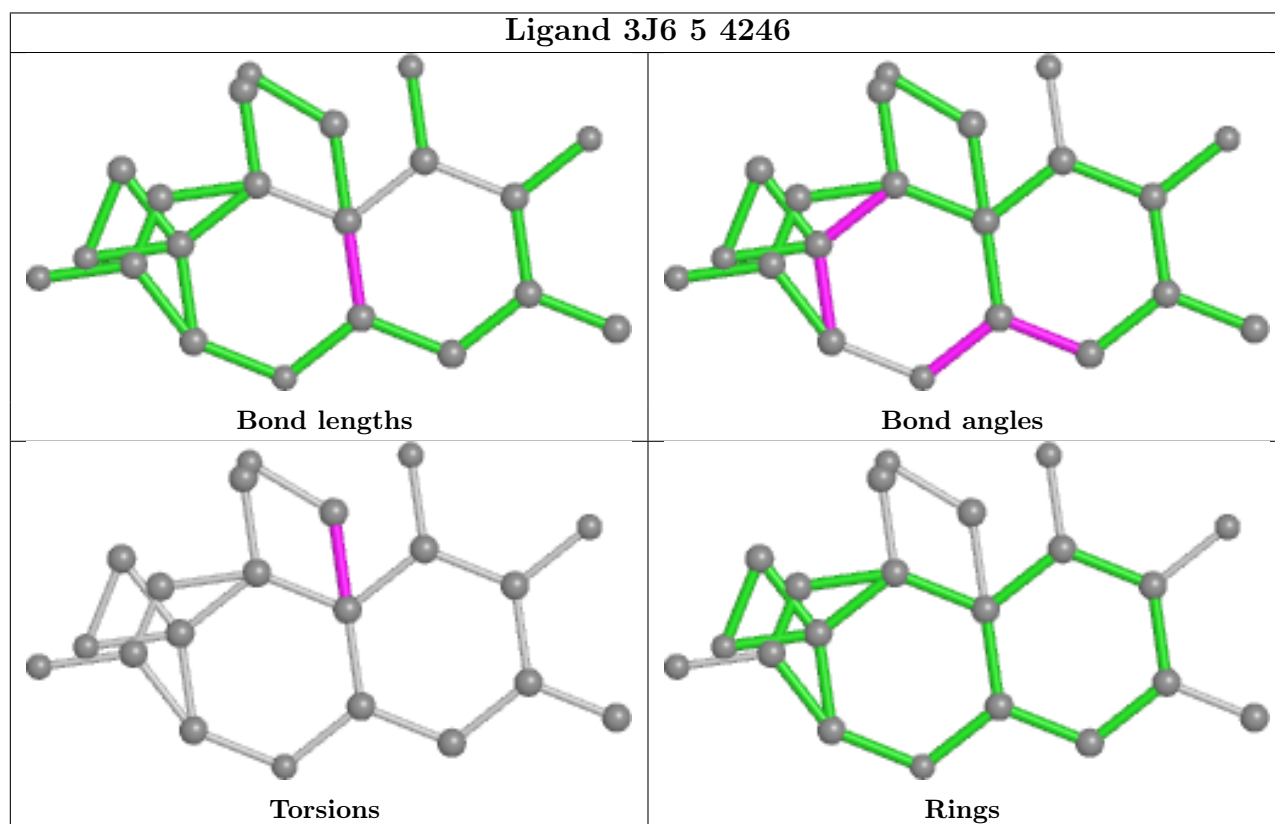
Mol	Chain	Res	Type	Atoms
88	5	4246	3J6	O5-C14-C4-C5
88	5	4246	3J6	O5-C14-C4-C7
88	5	4246	3J6	O5-C14-C4-C3

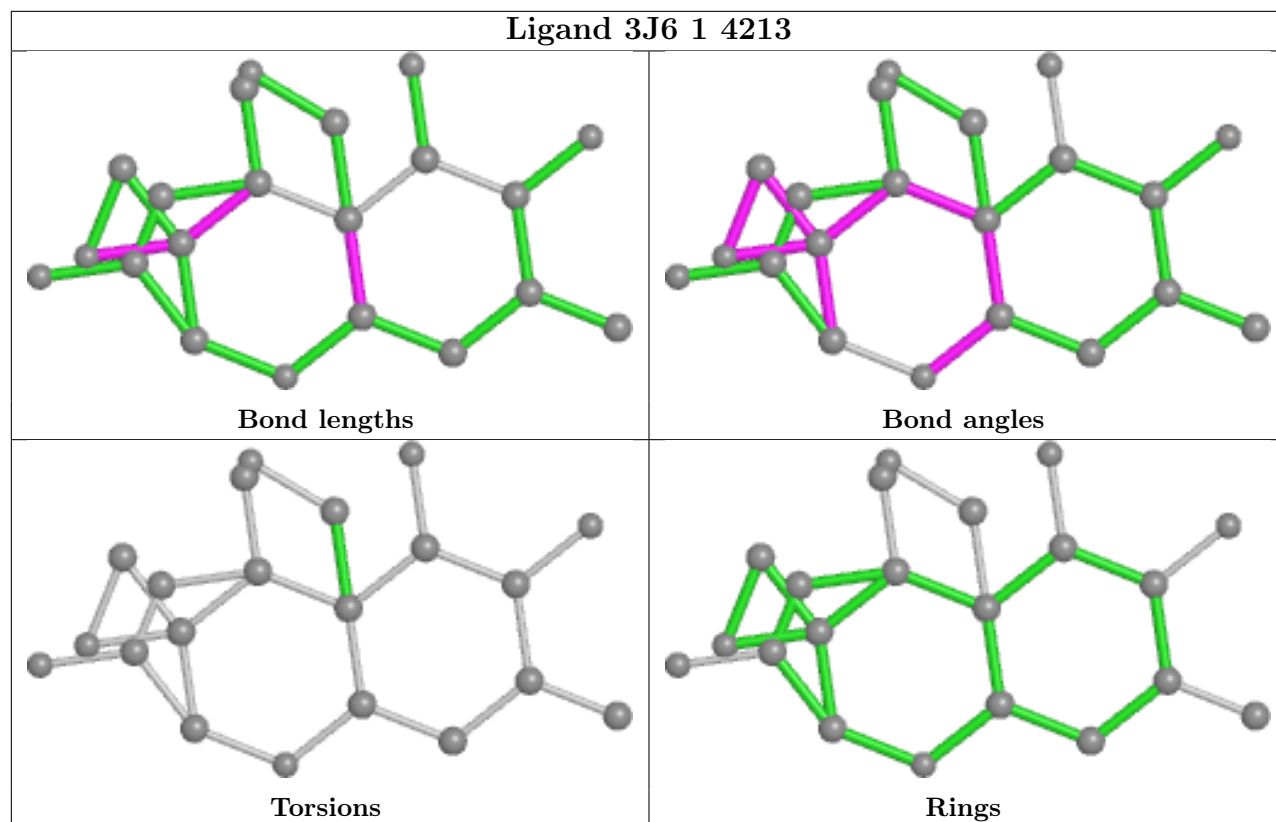
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	S6	301	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.