



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 08:51 pm GMT

PDB ID : 4U3N
Title : Crystal structure of CCA trinucleotide bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-22
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

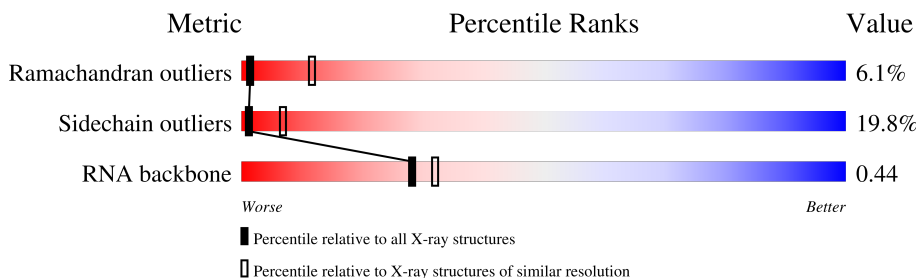
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	64% (green), 29% (yellow), . (orange), . (red), . (grey)
1	6	1800	64% (green), 30% (yellow), 5% (orange)
2	S0	251	64% (green), 15% (yellow), . (orange), 18% (grey)
2	s0	251	61% (green), 20% (yellow), . (orange), 18% (grey)
3	S1	254	57% (green), 24% (yellow), . (orange), 16% (grey)
3	s1	254	65% (green), 19% (yellow), . (orange), 15% (grey)
4	S2	253	63% (green), 22% (yellow), . (orange), 14% (grey)
4	s2	253	64% (green), 20% (yellow), . (orange), 14% (grey)

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Mol	Chain	Length	Quality of chain
5	S3	239	73% 17% 7%
5	s3	239	72% 20% 7%
6	S4	260	78% 21%
6	s4	260	79% 20%
7	S5	224	73% 18% 8%
7	s5	224	67% 23% 8%
8	S6	236	76% 19%
8	s6	236	73% 19% 8%
9	S7	189	72% 23%
9	s7	189	75% 21%
10	S8	200	74% 19% 6%
10	s8	200	74% 18% 6%
11	S9	196	73% 19% 6%
11	s9	196	76% 17% 6%
12	C0	105	71% 18% 9%
13	C1	155	78% 19%
13	c1	155	77% 15% 6%
14	C2	142	60% 24% 13%
14	c2	142	56% 29% 13%
15	C3	150	79% 18%
15	c3	150	78% 20%
16	C4	136	70% 19% 7%
16	c4	136	67% 26% 6%
17	C5	141	67% 18% 12%
17	c5	141	67% 26%

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Mol	Chain	Length	Quality of chain
18	C6	142	74% 22% . . .
18	c6	142	78% 20% .
19	C7	136	70% 15% . 12%
19	c7	136	60% 25% . . 14%
20	C8	145	74% 20% 6%
20	c8	145	76% 21% .
21	C9	143	75% 22% .
21	c9	143	81% 17% .
22	D0	120	72% 18% 11%
22	d0	120	57% 33% . 8%
23	D1	87	75% 23% .
23	d1	87	80% 18% .
24	D2	129	81% 18% .
24	d2	129	86% 13% .
25	D3	144	79% 17% . .
25	d3	144	78% 19% .
26	D4	134	81% 16% .
26	d4	134	78% 21% . .
27	D5	107	43% 18% 5% 35%
27	d5	107	47% 17% . 36%
28	D6	97	74% 20% 6%
28	d6	97	72% 25% .
29	D7	81	77% 20% .
29	d7	81	80% 17% .
30	D8	66	67% 24% 5% 5%

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Mol	Chain	Length	Quality of chain
30	d8	66	67% 27% 5%
31	D9	55	82% 13%
31	d9	55	67% 29%
32	E0	60	85% 13%
33	E1	76	51% 37% 7%
34	SR	318	78% 21%
34	sR	318	89% 10%
35	SM	273	46% 11% 42%
35	sM	273	29% 8% 62%
36	1	3396	55% 32% 6% 7%
36	5	3396	54% 34% 6% 7%
37	3	121	79% 21%
37	7	121	62% 34%
38	4	158	61% 36%
38	8	158	65% 32%
39	L2	253	81% 17%
39	l2	253	80% 19%
40	L3	386	81% 18%
40	l3	386	82% 16%
41	L4	361	80% 18%
41	l4	361	80% 19%
42	L5	296	79% 19%
42	l5	296	80% 18%
43	L6	175	74% 15% 11%
43	l6	175	73% 16% 10%







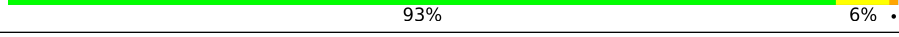

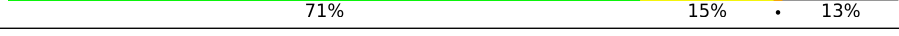

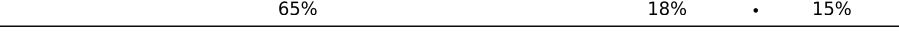
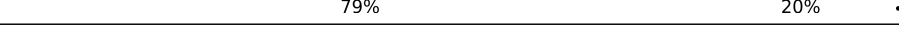

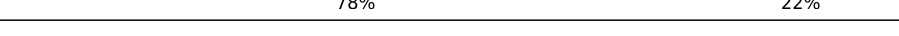


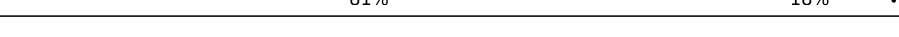

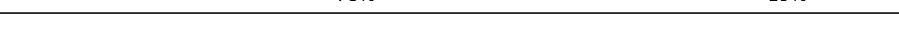






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Mol	Chain	Length	Quality of chain
44	L7	243	79% 11% 9%
44	l7	243	80% 11% 8%
45	L8	255	74% 16% 9%
45	l8	255	72% 18% 9%
46	L9	191	81% 19%
46	l9	191	77% 21%
47	M0	220	74% 21%
47	m0	220	76% 19%
48	M1	173	73% 20% 5%
48	m1	173	73% 22%
49	M3	198	77% 19%
49	m3	198	80% 16%
50	M4	137	80% 19%
50	m4	137	82% 16%
51	M5	203	85% 14%
51	m5	203	83% 16%
52	M6	198	83% 15%
52	m6	198	84% 15%
53	M7	183	81% 18%
53	m7	183	70% 15% 15%
54	M8	185	82% 17%
54	m8	185	83% 17%
55	M9	188	87% 13%
55	m9	188	81% 18%
56	N0	172	80% 17%









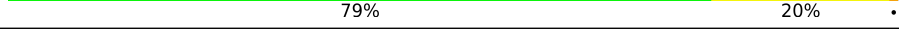

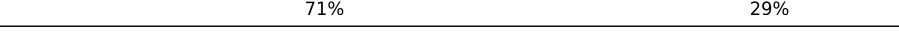
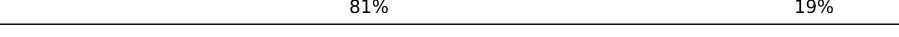

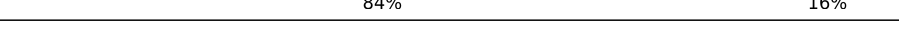


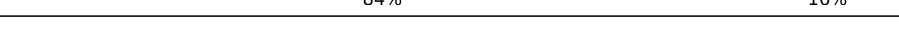

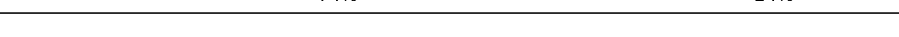






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Mol	Chain	Length	Quality of chain
56	n0	172	 80% 19%
57	N1	159	 77% 21%
57	n1	159	 79% 21%
58	N2	120	 63% 18% 17%
58	n2	120	 65% 16% 18%
59	N3	136	 85% 15%
59	n3	136	 93% 6%
60	N4	155	 54% 8% 37%
60	n4	155	 71% 15% 13%
61	N5	141	 72% 13% 14%
61	n5	141	 65% 18% 15%
62	N6	126	 79% 20%
62	n6	126	 71% 28%
63	N7	135	 78% 22%
63	n7	135	 76% 21%
64	N8	148	 78% 19%
64	n8	148	 81% 18%
65	N9	58	 78% 22%
65	n9	58	 78% 19%
66	O0	104	 72% 20% 7%
66	o0	104	 80% 16%
67	O1	112	 77% 19%
67	o1	112	 69% 29%
68	O2	129	 78% 21%
68	o2	129	 78% 19%

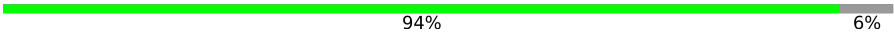



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Mol	Chain	Length	Quality of chain
69	O3	106	 84% 15%
69	o3	106	 83% 15%
70	O4	119	 76% 18% 6%
70	o4	119	 79% 15% 6%
71	O5	119	 75% 23%
71	o5	119	 79% 20%
72	O6	99	 76% 21%
72	o6	99	 74% 23%
73	O7	87	 79% 20%
73	o7	87	 77% 21%
74	O8	77	 71% 29%
74	o8	77	 81% 19%
75	O9	50	 76% 22%
75	o9	50	 84% 16%
76	Q0	52	 75% 23%
76	q0	52	 75% 25%
77	Q1	25	 84% 16%
77	q1	25	 72% 28%
78	Q2	105	 74% 24%
78	q2	105	 75% 23%
79	Q3	91	 85% 14%
79	q3	91	 82% 18%
80	c0	105	 68% 21% 9%
81	e0	62	 69% 29%
82	e1	76	 55% 36% 8%

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Mol	Chain	Length	Quality of chain
83	m2	160	 94% 6%
84	p0	311	 37% 8% 54%
85	p1	47	 100%
86	p2	46	 100%

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 411288 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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
			Total	C	N	O	S			
14	C2	124	892	562	156	172	2	0	0	0

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	l3	386	3075	1950	584	533	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	2748	1729	522	494	3	0	0	0
41	l4	361	2748	1729	522	494	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	2375	1501	414	458	2	0	0	0
42	l5	294	2359	1489	412	456	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	1239	800	222	216	1	0	0	0
43	l6	157	1248	806	224	217	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	1784	1151	324	308	1	0	0	0
44	l7	223	1791	1155	325	310	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	1804	1151	323	327	3	0	0	0
45	l8	231	1763	1130	316	314	3	0	0	0

- 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
51	M5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	m5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
80	c0	96	Total 762	C 491	N 125	O 144	S 2	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 81 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
82	e1	76	Total 608	C 388	N 117	O 99	S 4	0	0	0

- Molecule 83 is a protein called UNKNOWN PROTEIN m2.

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

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 85 is a protein called UNKNOWN PROTEIN p1.

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

- Molecule 86 is a protein called UNKNOWN PROTEIN p2.

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

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	2	124	Total	Mg	0	0
			124	124		
87	S4	2	Total	Mg	0	0
			2	2		
87	S8	1	Total	Mg	0	0
			1	1		
87	D3	1	Total	Mg	0	0
			1	1		
87	SM	1	Total	Mg	0	0
			1	1		
87	1	477	Total	Mg	0	0
			477	477		
87	3	14	Total	Mg	0	0
			14	14		
87	4	19	Total	Mg	0	0
			19	19		
87	L2	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	L3	3	Total 3	Mg 3	0	0
87	L4	1	Total 1	Mg 1	0	0
87	L5	1	Total 1	Mg 1	0	0
87	L7	4	Total 4	Mg 4	0	0
87	L8	1	Total 1	Mg 1	0	0
87	M0	2	Total 2	Mg 2	0	0
87	M1	1	Total 1	Mg 1	0	0
87	M3	2	Total 2	Mg 2	0	0
87	M5	2	Total 2	Mg 2	0	0
87	M6	1	Total 1	Mg 1	0	0
87	M7	4	Total 4	Mg 4	0	0
87	M9	1	Total 1	Mg 1	0	0
87	N0	1	Total 1	Mg 1	0	0
87	N3	3	Total 3	Mg 3	0	0
87	N5	1	Total 1	Mg 1	0	0
87	N8	5	Total 5	Mg 5	0	0
87	O2	1	Total 1	Mg 1	0	0
87	O4	1	Total 1	Mg 1	0	0
87	O5	1	Total 1	Mg 1	0	0
87	O7	1	Total 1	Mg 1	0	0
87	6	144	Total 144	Mg 144	0	0

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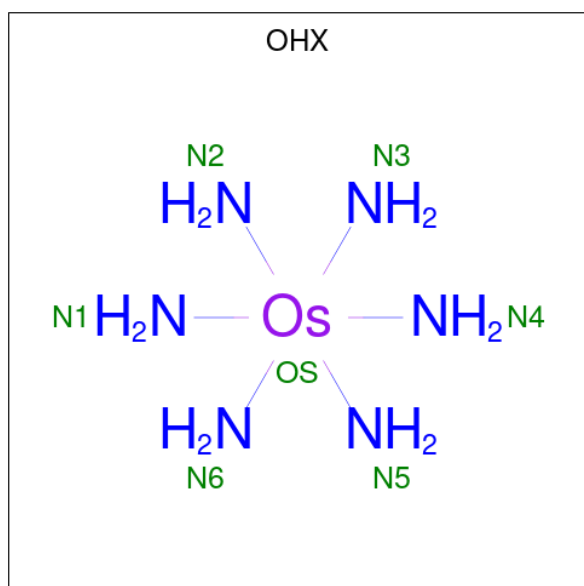
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	s1	1	Total 1	Mg 1	0	0
87	s6	1	Total 1	Mg 1	0	0
87	s8	3	Total 3	Mg 3	0	0
87	c1	1	Total 1	Mg 1	0	0
87	c7	2	Total 2	Mg 2	0	0
87	c8	1	Total 1	Mg 1	0	0
87	c9	1	Total 1	Mg 1	0	0
87	d3	1	Total 1	Mg 1	0	0
87	d4	1	Total 1	Mg 1	0	0
87	d6	1	Total 1	Mg 1	0	0
87	sM	1	Total 1	Mg 1	0	0
87	5	502	Total 502	Mg 502	0	0
87	7	15	Total 15	Mg 15	0	0
87	8	16	Total 16	Mg 16	0	0
87	l2	1	Total 1	Mg 1	0	0
87	l3	3	Total 3	Mg 3	0	0
87	l4	2	Total 2	Mg 2	0	0
87	l5	2	Total 2	Mg 2	0	0
87	l7	1	Total 1	Mg 1	0	0
87	m1	2	Total 2	Mg 2	0	0
87	m5	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	m6	2	Total Mg 2 2	0	0
87	m7	5	Total Mg 5 5	0	0
87	n0	3	Total Mg 3 3	0	0
87	n3	2	Total Mg 2 2	0	0
87	n6	2	Total Mg 2 2	0	0
87	n8	3	Total Mg 3 3	0	0
87	o1	1	Total Mg 1 1	0	0
87	o3	1	Total Mg 1 1	0	0
87	o4	1	Total Mg 1 1	0	0
87	q0	1	Total Mg 1 1	0	0
87	q1	1	Total Mg 1 1	0	0
87	q3	2	Total Mg 2 2	0	0

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
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88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
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88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0
88	2	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
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88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
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88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	2	1	7	6	1	0	0
88	S8	1	7	6	1	0	0
88	C3	1	7	6	1	0	0
88	C5	1	7	6	1	0	0
88	C8	1	7	6	1	0	0
88	D3	1	7	6	1	0	0
88	D9	1	7	6	1	0	0
88	SR	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
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88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
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88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0
88	1	1	Total	N	Os		
			7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
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88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
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88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
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88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
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88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
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88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
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88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	1	1	7	6	1	0	0
88	3	1	7	6	1	0	0
88	3	1	7	6	1	0	0
88	3	1	7	6	1	0	0
88	3	1	7	6	1	0	0
88	3	1	7	6	1	0	0
88	3	1	7	6	1	0	0
88	3	1	7	6	1	0	0
88	3	1	7	6	1	0	0
88	3	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	3	1	7	6	1	0	0
88	3	1	7	6	1	0	0
88	3	1	7	6	1	0	0
88	3	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	4	1	7	6	1	0	0
88	L3	1	7	6	1	0	0
88	L3	1	7	6	1	0	0
88	L3	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	L4	1	7	6	1	0	0
88	M0	1	7	6	1	0	0
88	M5	1	7	6	1	0	0
88	M7	1	7	6	1	0	0
88	M7	1	7	6	1	0	0
88	M8	1	7	6	1	0	0
88	M9	1	7	6	1	0	0
88	N9	1	7	6	1	0	0
88	O3	1	7	6	1	0	0
88	O7	1	7	6	1	0	0
88	O7	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
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88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	6	1	7	6	1	0	0
88	6	1	7	6	1	0	0
88	s1	1	7	6	1	0	0
88	s1	1	7	6	1	0	0
88	s8	1	7	6	1	0	0
88	c1	1	7	6	1	0	0
88	c3	1	7	6	1	0	0
88	c5	1	7	6	1	0	0
88	c8	1	7	6	1	0	0
88	d4	1	7	6	1	0	0
88	d9	1	7	6	1	0	0
88	sR	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0
88	5	1	Total	N	Os		
			7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
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88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	5	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	7	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	8	1	7	6	1	0	0
88	13	1	7	6	1	0	0
88	13	1	7	6	1	0	0
88	13	1	7	6	1	0	0

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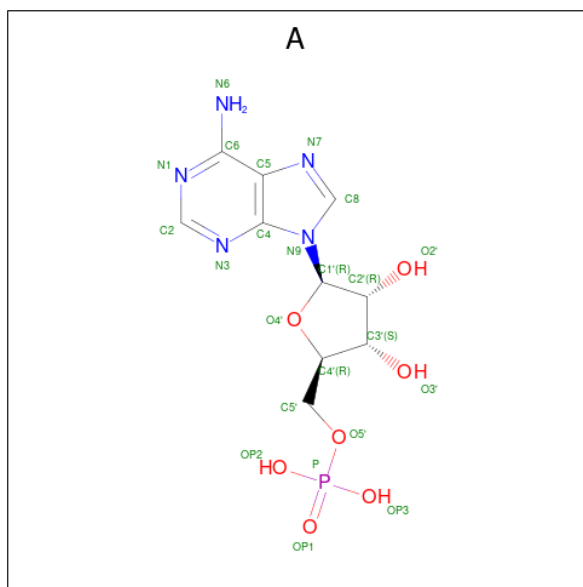
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
88	l4	1	7	6	1	0	0
88	l4	1	7	6	1	0	0
88	l5	1	7	6	1	0	0
88	l5	1	7	6	1	0	0
88	l5	1	7	6	1	0	0
88	l5	1	7	6	1	0	0
88	l9	1	7	6	1	0	0
88	m0	1	7	6	1	0	0
88	m0	1	7	6	1	0	0
88	m1	1	7	6	1	0	0
88	m4	1	7	6	1	0	0
88	m5	1	7	6	1	0	0
88	m6	1	7	6	1	0	0
88	n3	1	7	6	1	0	0
88	n3	1	7	6	1	0	0
88	n9	1	7	6	1	0	0
88	o3	1	7	6	1	0	0
88	o7	1	7	6	1	0	0
88	q2	1	7	6	1	0	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

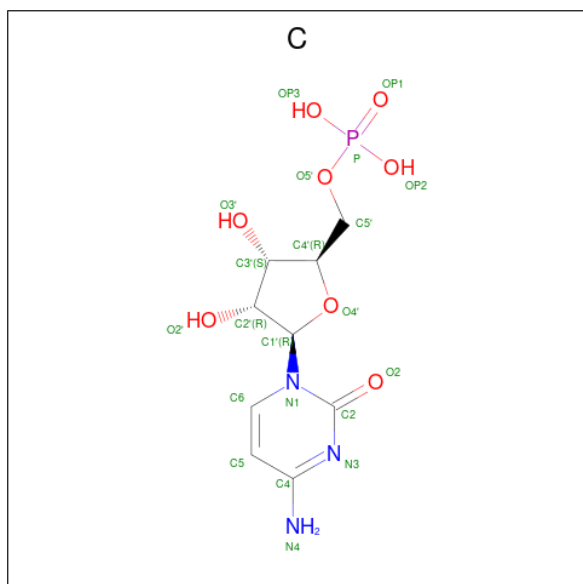
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
89	D6	1	Total Zn 1 1	0	0
89	D7	1	Total Zn 1 1	0	0
89	D9	1	Total Zn 1 1	0	0
89	E1	1	Total Zn 1 1	0	0
89	O7	1	Total Zn 1 1	0	0
89	Q0	1	Total Zn 1 1	0	0
89	Q2	1	Total Zn 1 1	0	0
89	Q3	1	Total Zn 1 1	0	0
89	d6	1	Total Zn 1 1	0	0
89	d7	1	Total Zn 1 1	0	0
89	d9	1	Total Zn 1 1	0	0
89	e1	1	Total Zn 1 1	0	0
89	o7	1	Total Zn 1 1	0	0
89	q0	1	Total Zn 1 1	0	0
89	q2	1	Total Zn 1 1	0	0
89	q3	1	Total Zn 1 1	0	0

- Molecule 90 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
90	1	1	22	10	5	6	1	0	0
90	5	1	22	10	5	6	1	0	0

- Molecule 91 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: $C_9H_{14}N_3O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
91	Q2	1	20	9	3	7	1	0	0

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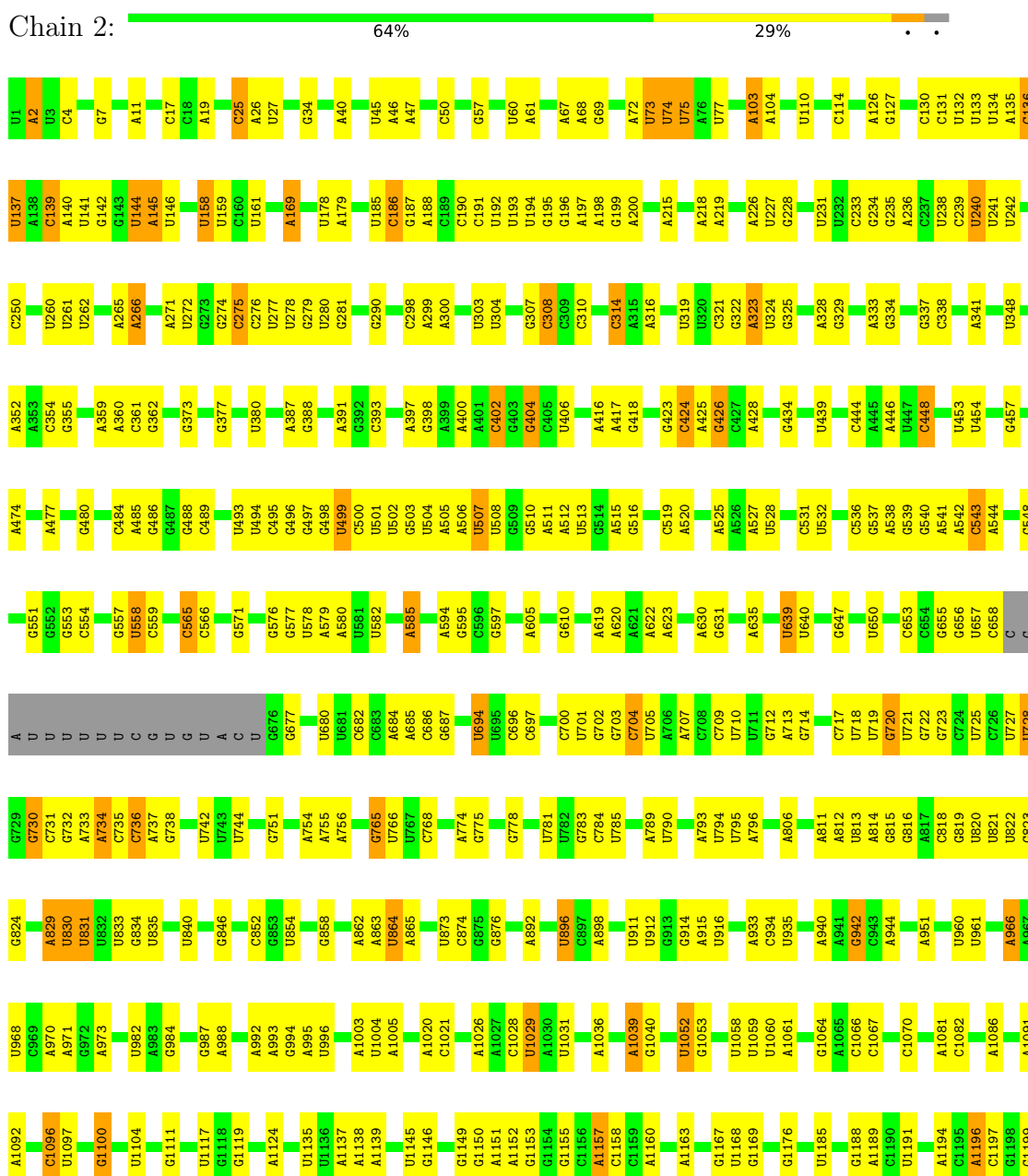
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
91	Q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
91	q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
91	q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

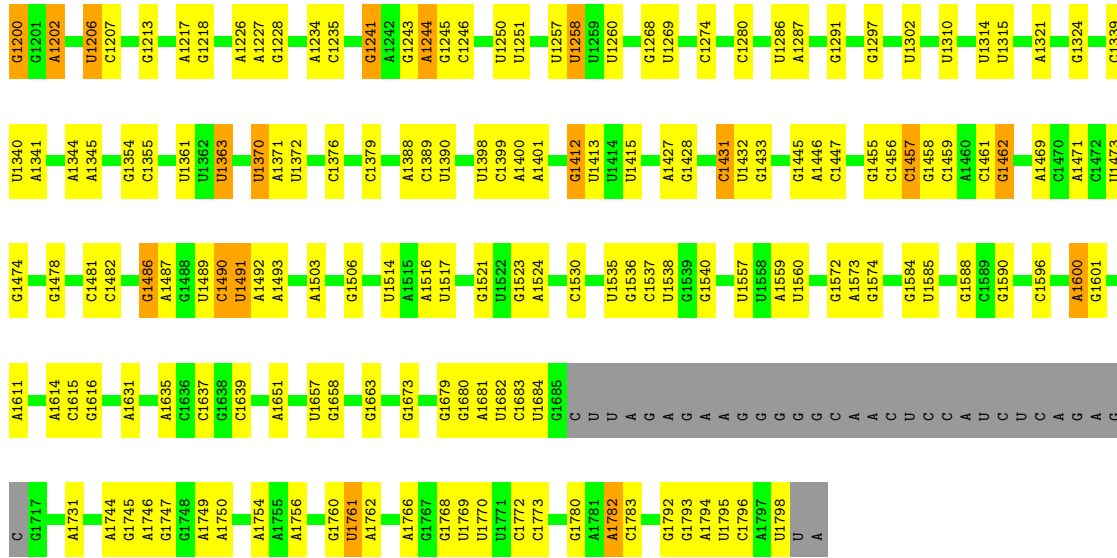
3 Residue-property plots [i](#)

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.

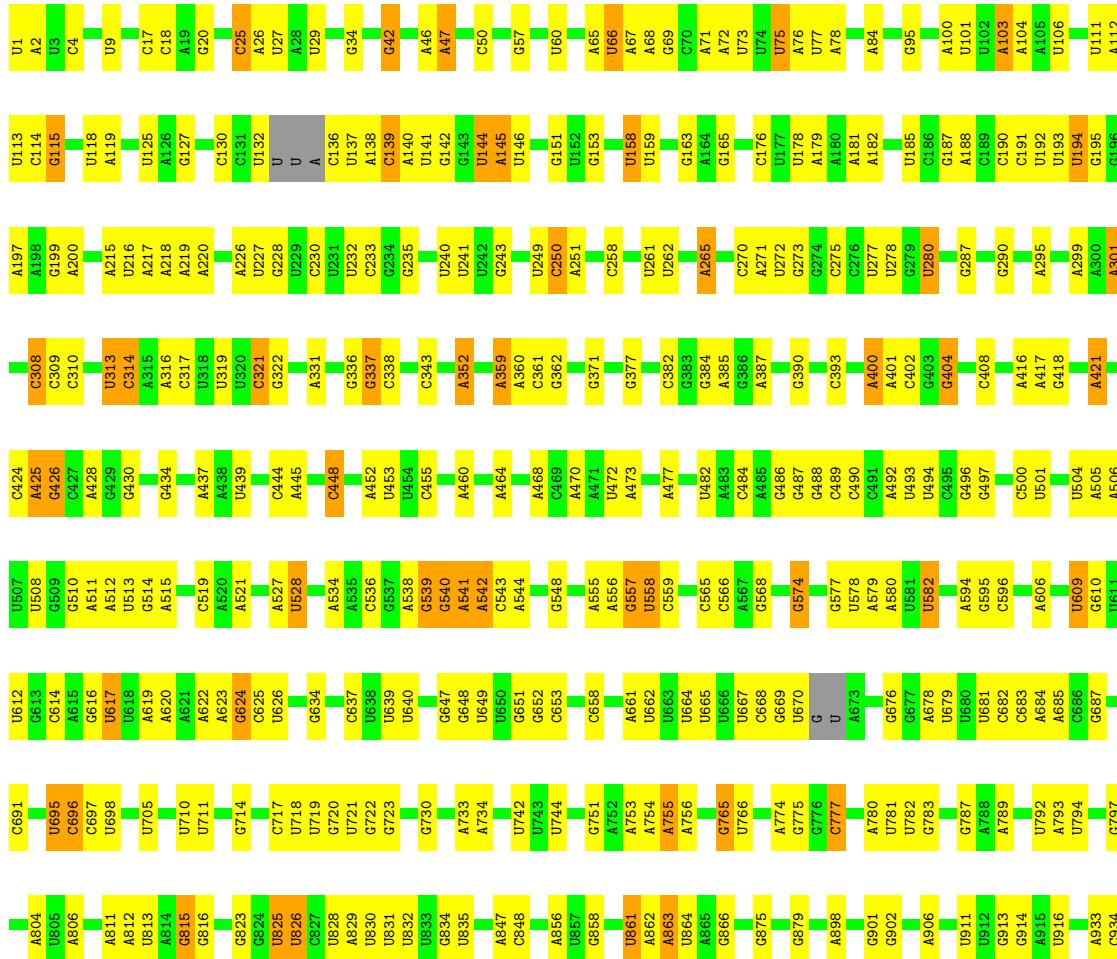
Note EDS failed to run properly.

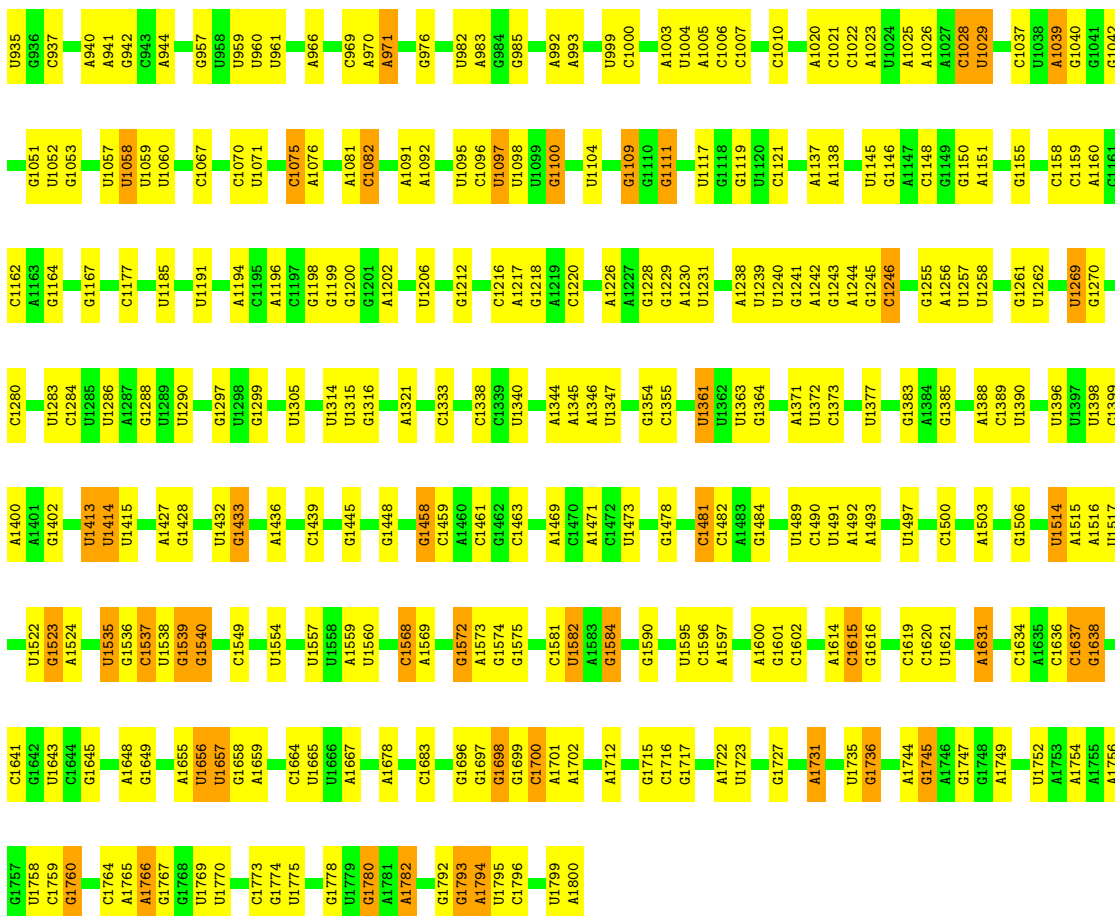
- Molecule 1: 18S ribosomal RNA



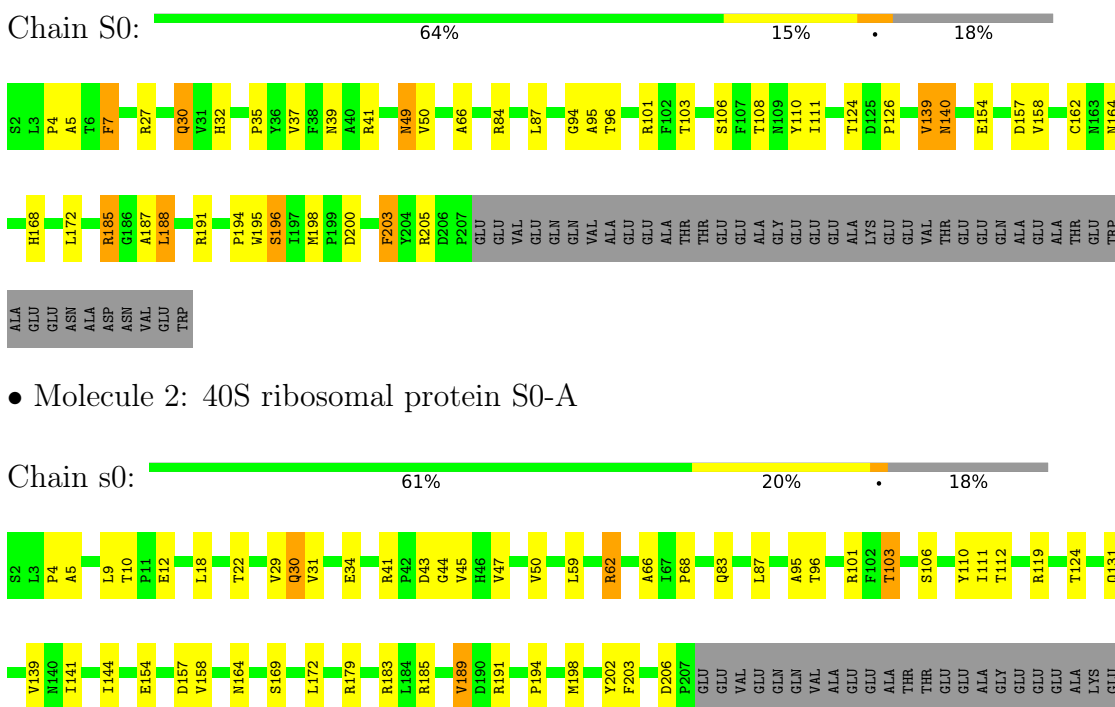


• Molecule 1: 18S ribosomal RNA





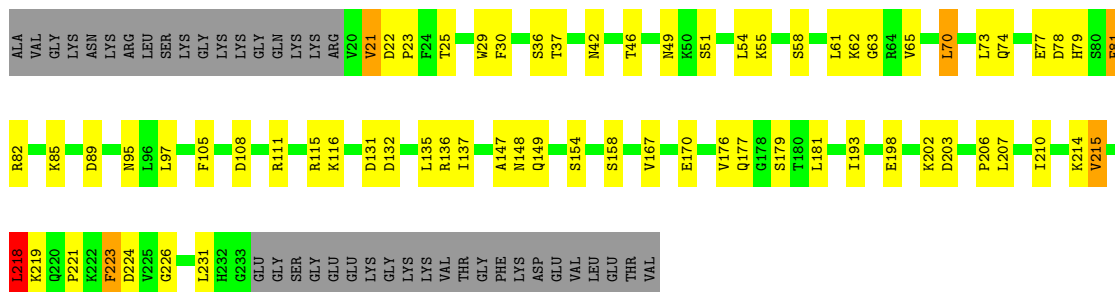
• Molecule 2: 40S ribosomal protein S0-A



GLU VAL THR GLU GLU GLN GLN GLU ALA GLU ALA THR GLU TRP GLU ALA GLU ASN ASP VAL VAL TRP

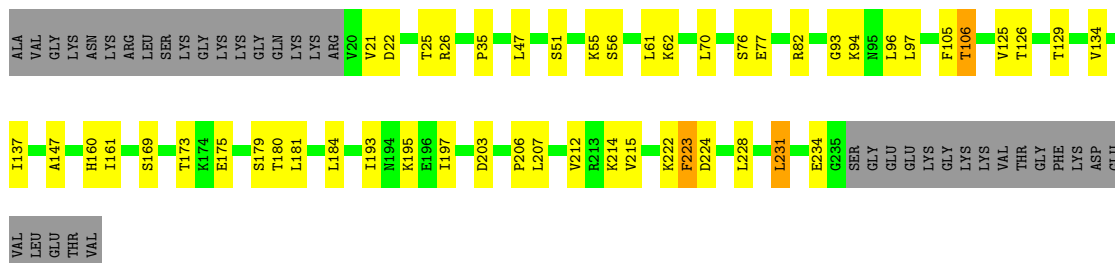
• Molecule 3: 40S ribosomal protein S1-A

Chain S1: 57% 24% 16%



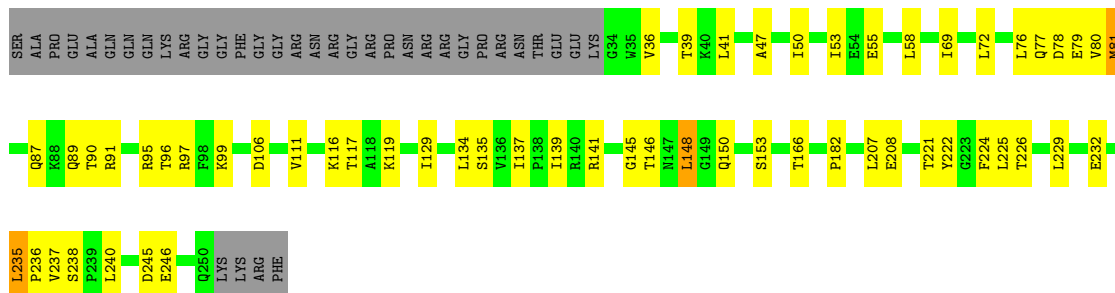
• Molecule 3: 40S ribosomal protein S1-A

Chain s1: 65% 19% 15%



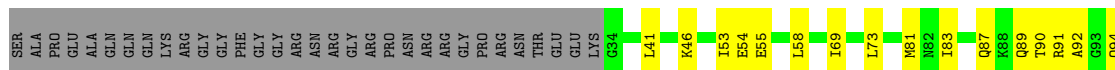
• Molecule 4: 40S ribosomal protein S2

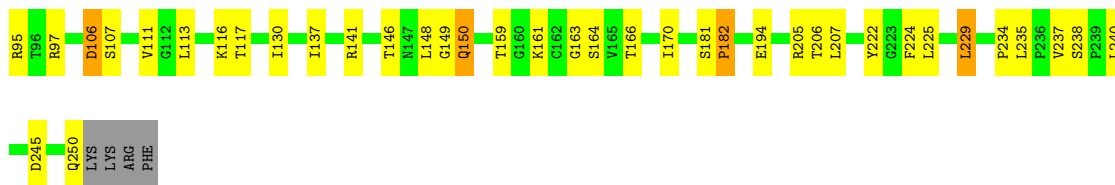
Chain S2: 63% 22% 14%



• Molecule 4: 40S ribosomal protein S2

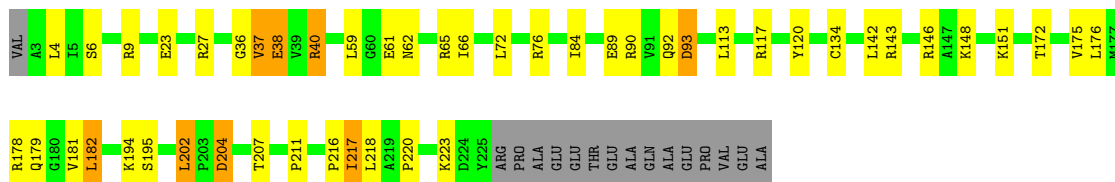
Chain s2: 64% 20% 14%





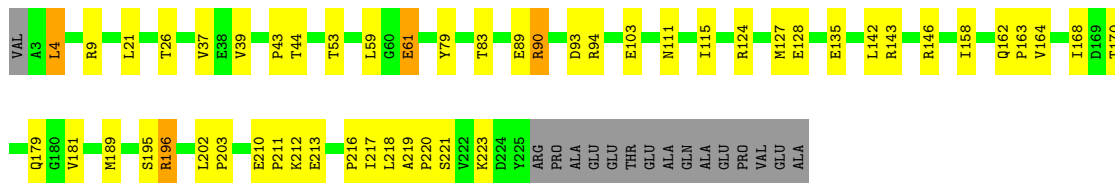
- Molecule 5: 40S ribosomal protein S3

Chain S3: 73% 17% 7%



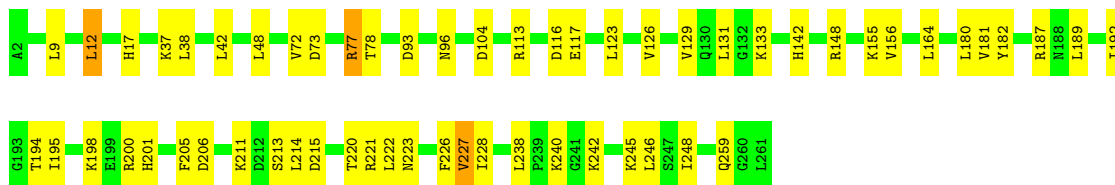
- Molecule 5: 40S ribosomal protein S3

Chain s3: 72% 20% 7%



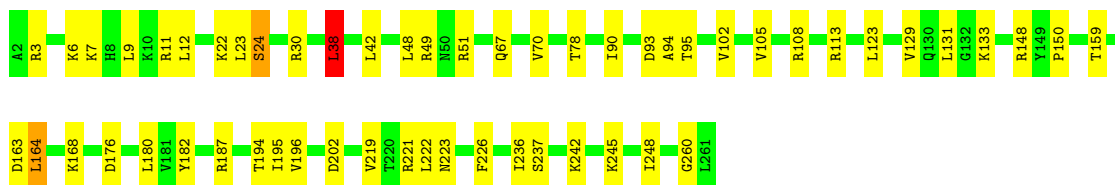
- Molecule 6: 40S ribosomal protein S4-A

Chain S4: 78% 21% 1%



- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 79% 20% 1%



- Molecule 7: 40S ribosomal protein S5

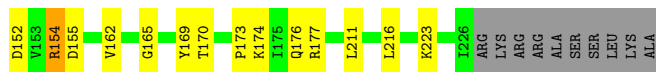
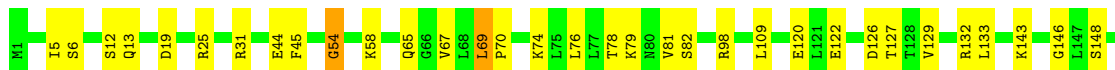
Chain S5: 73% 18% 8%



• Molecule 7: 40S ribosomal protein S5



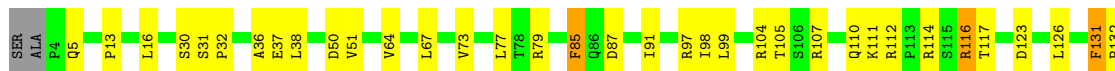
• Molecule 8: 40S ribosomal protein S6-A



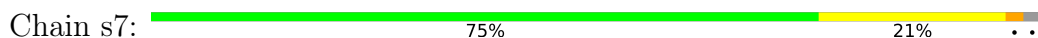
• Molecule 8: 40S ribosomal protein S6-A

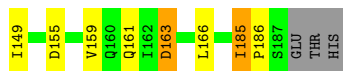


• Molecule 9: 40S ribosomal protein S7-A

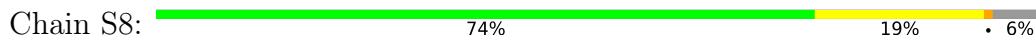


• Molecule 9: 40S ribosomal protein S7-A

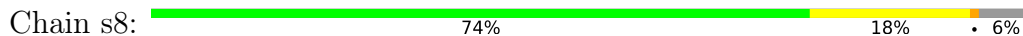




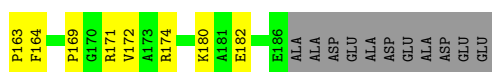
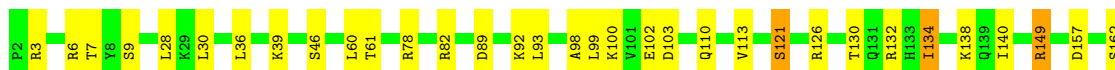
- Molecule 10: 40S ribosomal protein S8-A



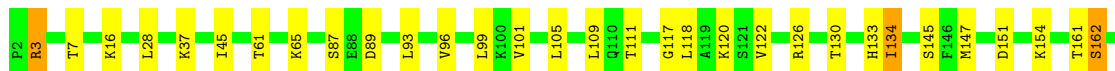
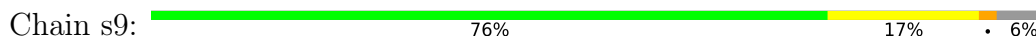
- Molecule 10: 40S ribosomal protein S8-A



- Molecule 11: 40S ribosomal protein S9-A



- Molecule 11: 40S ribosomal protein S9-A

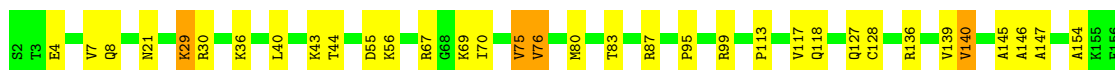
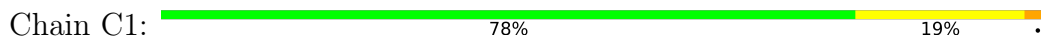


- Molecule 12: 40S ribosomal protein S10-A

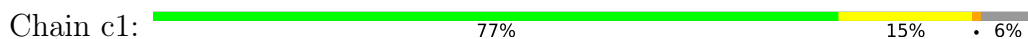




• Molecule 13: 40S ribosomal protein S11-A

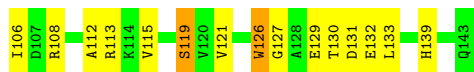


• Molecule 13: 40S ribosomal protein S11-A



PHE

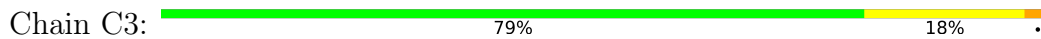
• Molecule 14: 40S ribosomal protein S12



• Molecule 14: 40S ribosomal protein S12

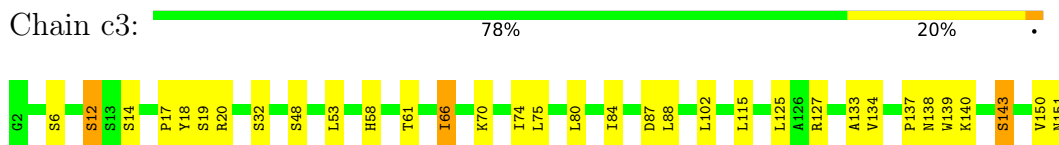


• Molecule 15: 40S ribosomal protein S13

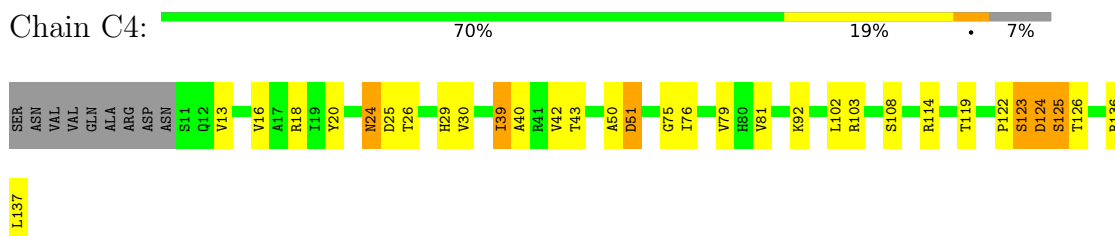


M151

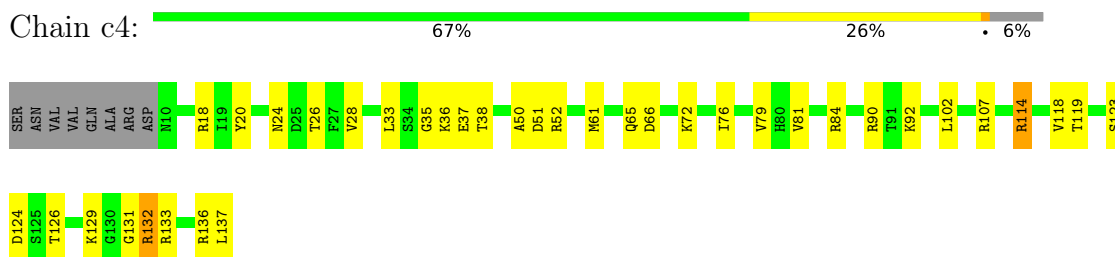
• Molecule 15: 40S ribosomal protein S13



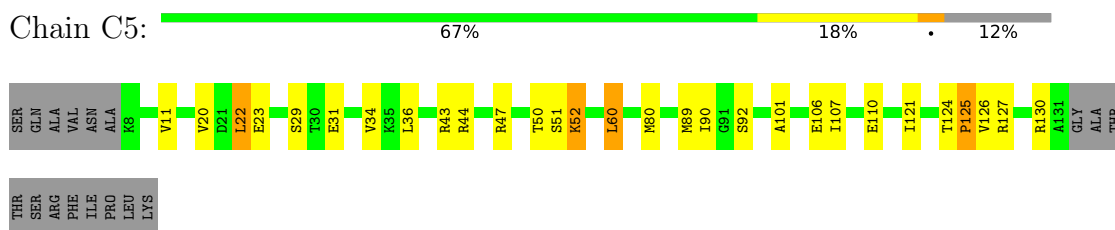
• Molecule 16: 40S ribosomal protein S14-A



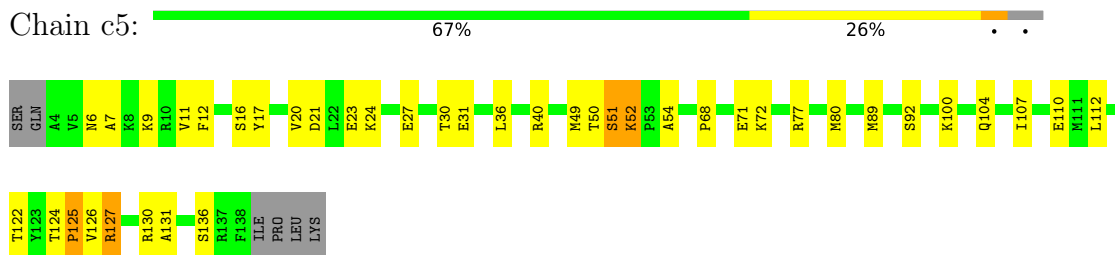
• Molecule 16: 40S ribosomal protein S14-A



• Molecule 17: 40S ribosomal protein S15

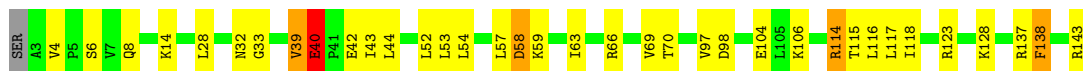


• Molecule 17: 40S ribosomal protein S15

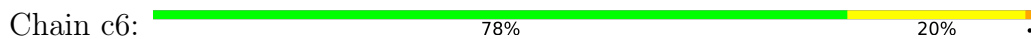


• Molecule 18: 40S ribosomal protein S16-A





- Molecule 18: 40S ribosomal protein S16-A



- Molecule 19: 40S ribosomal protein S17-A



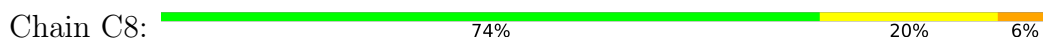
ARG
VAL

- Molecule 19: 40S ribosomal protein S17-A



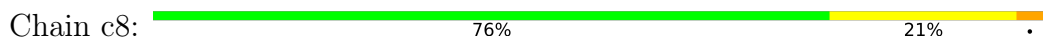
L113
K116
S120
V123
I122
ASN
VAL
SER
ALA
GLN
ARG
ASP
ARG
ARG
TYR
LYS
LYS
ARG
VAL

- Molecule 20: 40S ribosomal protein S18-A

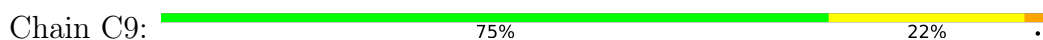


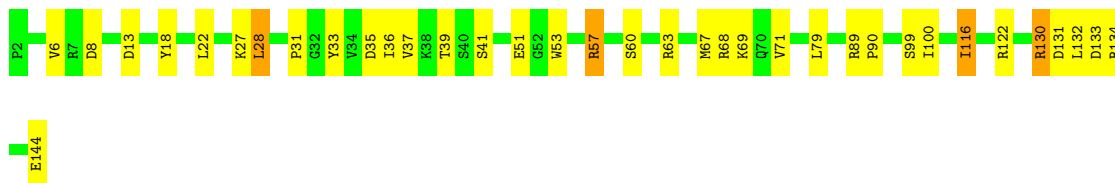
R143
R144
R145
A146

- Molecule 20: 40S ribosomal protein S18-A



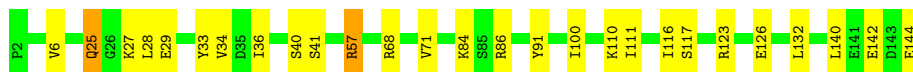
- Molecule 21: 40S ribosomal protein S19-A





- Molecule 21: 40S ribosomal protein S19-A

Chain c9: 81% 17%



- Molecule 22: 40S ribosomal protein S20

Chain D0: 72% 18% 11%



- Molecule 22: 40S ribosomal protein S20

Chain d0: 57% 33% 8%



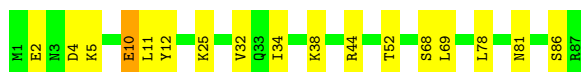
- Molecule 23: 40S ribosomal protein S21-A

Chain D1: 75% 23%



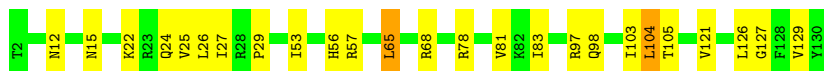
- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 80% 18%

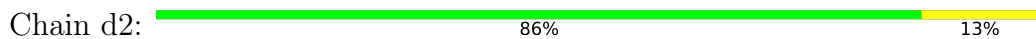


- Molecule 24: 40S ribosomal protein S22-A

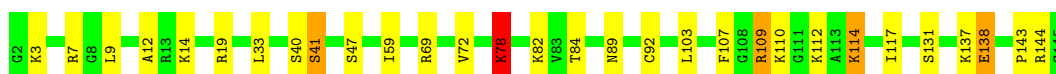
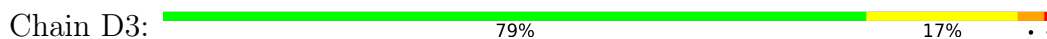
Chain D2: 81% 18%



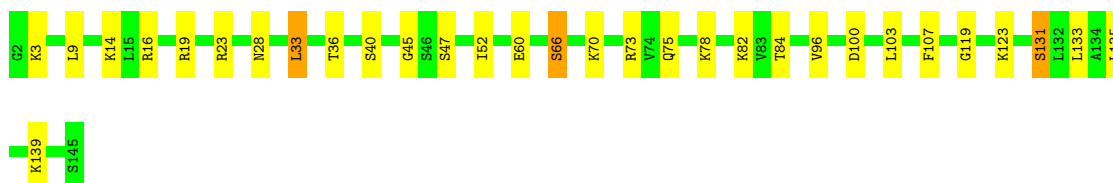
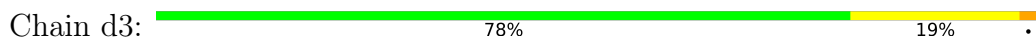
- Molecule 24: 40S ribosomal protein S22-A



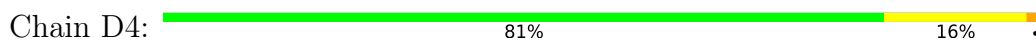
- Molecule 25: 40S ribosomal protein S23-A



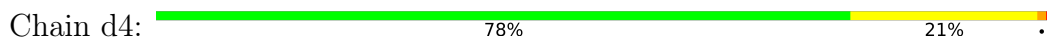
- Molecule 25: 40S ribosomal protein S23-A



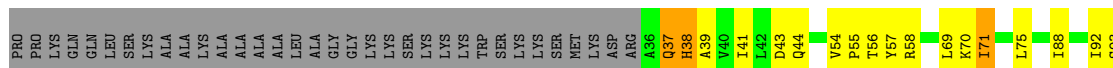
- Molecule 26: 40S ribosomal protein S24-A



- Molecule 26: 40S ribosomal protein S24-A



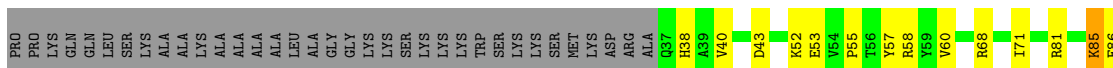
- Molecule 27: 40S ribosomal protein S25-A





- Molecule 27: 40S ribosomal protein S25-A

Chain d5: 47% 17% 36%



- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 74% 20% 6%



- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 72% 25%



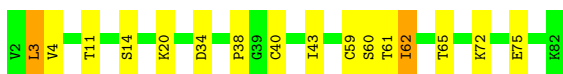
- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 77% 20%



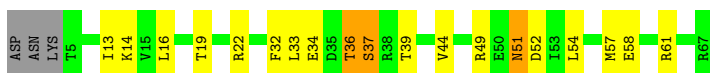
- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 80% 17%



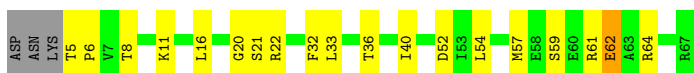
- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 67% 24% 5% 5%




- Molecule 30: 40S ribosomal protein S28-A

Chain d8:  67% 27% 5%



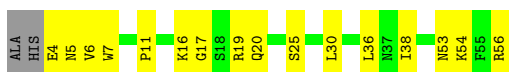
- Molecule 31: 40S ribosomal protein S29-A

Chain D9:  82% 13% 5%



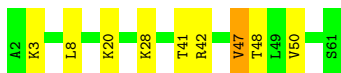
- Molecule 31: 40S ribosomal protein S29-A

Chain d9:  67% 29% 4%



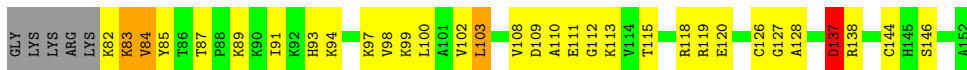
- Molecule 32: 40S ribosomal protein S30-A

Chain E0:  85% 13% 2%




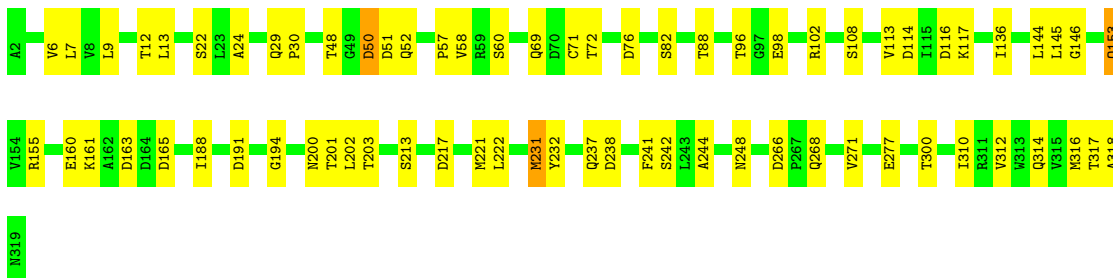
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:  51% 37% 12%




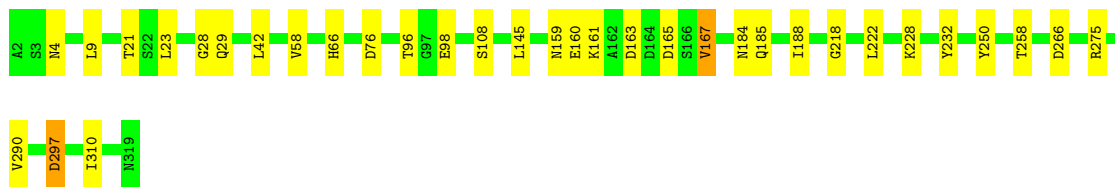
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:  78% 21% 1%

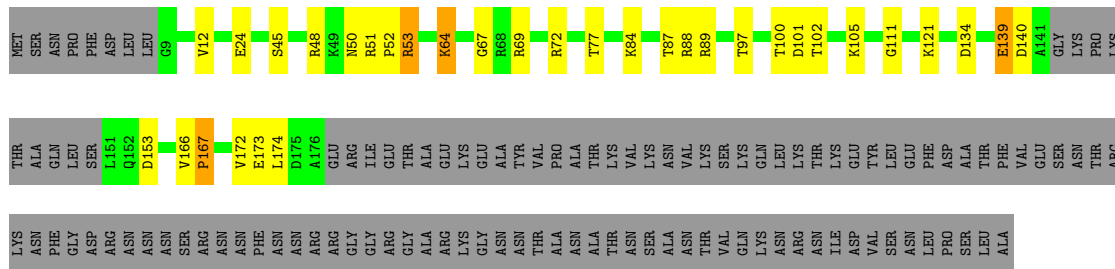


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

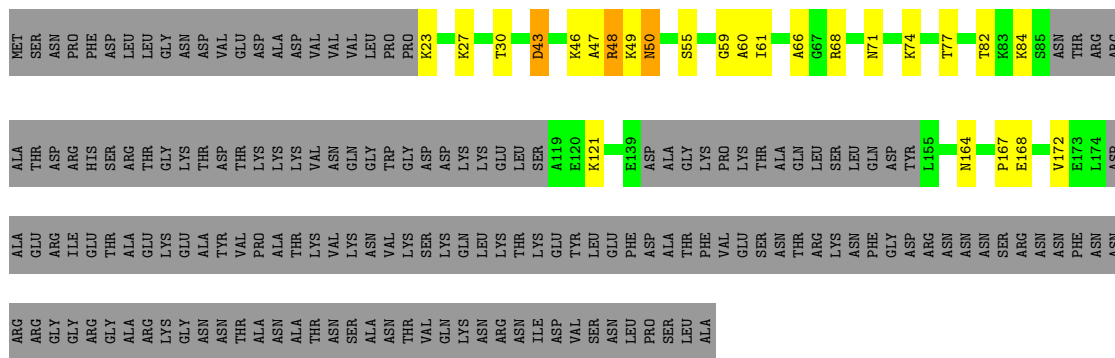
Chain sR:  89% 10% 1%



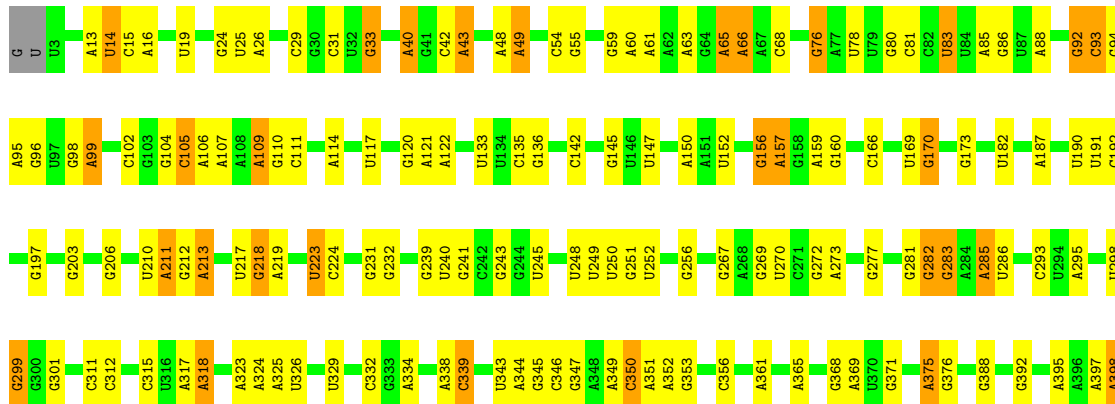
• Molecule 35: Suppressor protein STM1



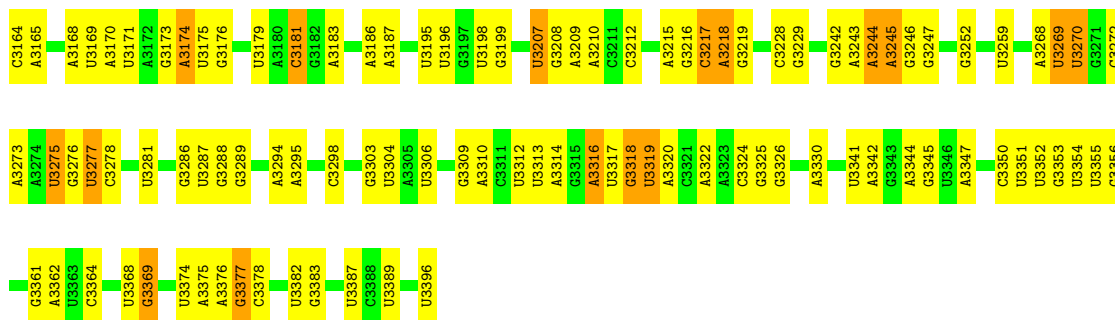
• Molecule 35: Suppressor protein STM1



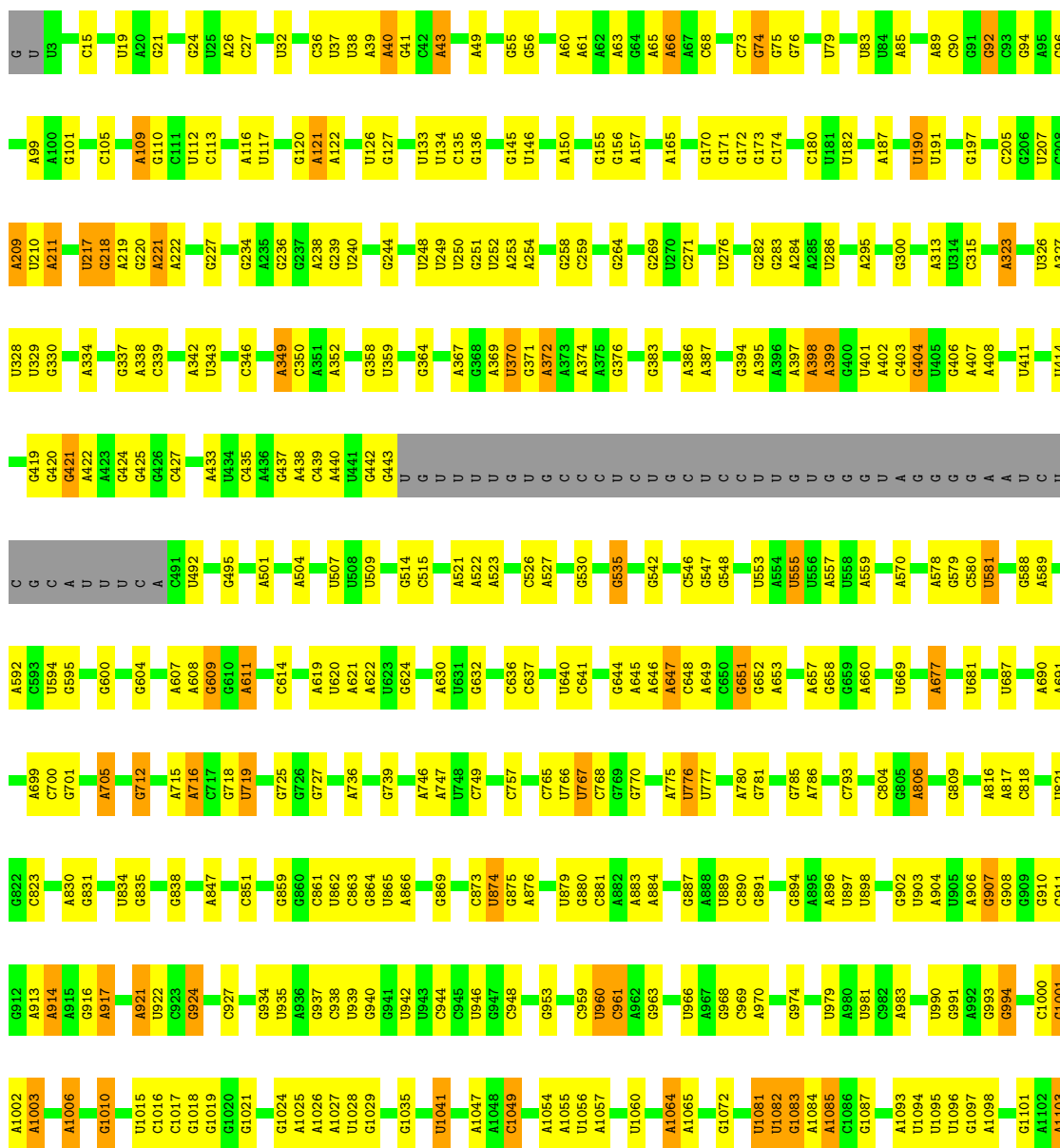
• Molecule 36: 25S ribosomal RNA



A3049	U2944	C2756	C92664	U2588	C	C2422	C9388	A2255	C2156	G	G1838
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U3055	G2946	G2761	C2675	C2594	U	U2428	C2343	C2257	A2158	G	U1840
U3056	A2762	U2762	A2676	A2595	C	U2428	C2350	G2261	G2165	A	A1841
U3057	U2949	U2763	G2677	G2600	C	C2431	U2351	G2272	G2169	C	A1842
G3058	G2950	C2764	A2678	A2601	U	A2432	G2355	G2273	U2170	C	G1845
G3059	U2953	U2766	A2679	A2602	U	U2433	A2357	A2274	U2176	G	C1846
U3066	U2954	C2768	U2681	G2604	U	U2434	A2357	A2275	C	A1849	
G3069	A2958	C2772	G2687	G2605	A	U2436	U2366	A2276	C	A1850	
C3076	A2967	C2773	U2688	G2606	U2501	G2437	C2360	C2277	C	U1855	
A3077	A2872	G2777	A2689	G2607	G2502	C2444	A2361	A2279	U	C1856	
A3078	U2873	G2778	G2690	G2608	G2503	U2445	C2362	A2280	G	C1857	
U3079	G2874	A2780	A2691	A2609	U2514	U	A2363	A2281	C	A1859	
G3080	G2977	U2875	C2692	G2610	U2514	U	C2365	U2282	C	G1860	
C3081	U2978	G2786	A2694	U2611	A2515	G	C2366	G2283	U	U1866	
U3086	U2979	G2787	A2695	U2612	A	U	U2366	C2284	C	C1867	
A3087	U2980	C2791	A2696	G2614	A2520	G	G2369	C2285	A	G1868	
A3088	U2981	G2791	A2697	U2617	U2521	G	G2370	U2286	U	U1871	
C2983	C2982	U2795	G2698	G2618	G2522	G	G2371	U2289	U	A1879	
A3091	C2983	G2796	G2699	G2619	A2523	U	A2372	U2290	C	U1880	
C3092	U2986	C2797	U2700	G2620	U2532	U	C2374	U2291	A	G1882	
A3103	A2987	C2798	A2702	G2621	G2533	A	G2375	G2201	C	U1884	
U3107	C2988	U2799	G2703	G2622	G2534	G	G2376	G2202	G	U1885	
U3111	U2989	G2800	A2704	G2623	U2537	A	C2383	A2208	C	A1886	
G3112	G2990	A2801	A2705	G2624	U2538	U	A2384	U2209	C	A1891	
A3113	U2991	A2802	G2714	C2625	U2539	A	G2385	G2210	C	G1892	
A3114	G2993	A2803	G2714	U2629	A2540	A	U2388	U2211	U	A1893	
U3119	U2996	C2810	U2718	G2630	U2541	G	G2391	G2212	G	A1901	
C3120	G2997	G2816	U2719	U2631	U2542	U	G2392	C2213	C	G1902	
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A3122	A3006	U2818	U2722	U2633	U2547	G	G2393	A2215	C	G1904	
A3123	U3007	A2819	U2725	A2635	C2548	A	G2394	U2216	C	G1905	
A3129	A3008	G2823	C2726	A2636	U2549	G	G2395	A2223	A	G1906	
A3130	G3009	G2827	A2727	A2637	U2550	U	C2397	A2224	U	A1909	
U3131	U3010	U2828	G2728	G2638	U2551	C	U2401	U2225	C	A1910	
C3132	A3011	G2829	U2729	G2639	C2552	U	A2402	U2226	G	A1911	
G3140	A3012	U2829	G2730	A2640	U2553	G	A2403	C2227	C	A1912	
A3141	A3016	G2830	U2731	U2641	A2554	G	A2404	A2228	C	A1913	
A3142	G3022	C2832	G2732	A2642	G2555	G	A2406	A2232	U	U1920	
C3143	C3025	G2834	C2737	C2644	U2561	C	C2407	G2233	C	G1928	
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A3153	A3029	A2836	A2746	U2652	C2568	G	G2409	C2237	A	G1839	
C3154	G3030	A2837	A2748	C2653	U2569	G	U2410	A2242	G	G1940	
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U3156	U3037	G2844	U2750	G2657	C2572	A	G2412	A2244	C	G1929	
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		U2847	G2754	G2662	U2585	U	U2417	G2249	C	G1940	
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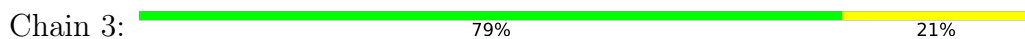
• Molecule 36: 25S ribosomal RNA



G1104	C1192	U1309	U1398	U1494	C1582	U1716	G1833	G1938	U	A2139	G2234	A2317	G2391
U1109	A1193	G1310	A1399	U1495	A1583	U1717	A1841	G1929	A	U2140	C2235	U2318	C2392
U1110	C1196	G1313	G1400	U1496	G1587	U1718	A1842	A1930	G	G2236	G2237	A2320	G2393
U1111	C1199	G1314	U1405	C1497	A1588	U1724	C1843	U1931	G	A2144	C2237	A2321	G2394
G1112	G1199	C1315	U1406	G1500	A1589	C1725	C1845	G1935	C	A2147	A2243	G2323	G2395
G1113	A1200	C1316	U1416	A1503	G1592	G1730	A1847	A1936	U	U2148	A2244	A2324	A2397
U1114	C1201	C1316	G1417	A1504	A1593	U1731	G1848	U1937	C	U2152	C2245	G2325	A2398
G1115	A1202	G1321	A1418	C1505	A1594	A1741	C1849	U1938	G	A2156	G2246	A2326	A2399
G1116	A1203	G1322	A1419	C1506	A1595	U1742	A1850	G1939	G	C2156	G2247	A2326	A2401
G1117	A1204	U1329	C1420	G1507	U1598	U1746	G1851	G1940	C	G2157	G2248	G2327	G2401
U1124	A1205	U1330	G1421	C1508	G1598	U1750	G1852	U1941	U	A2158	G2249	A2332	A2402
U1125	G1207	A1331	G1422	U1511	A1602	A1751	A1858	U1942	A	C2163	G2251	U2334	G2404
U1128	U1208	A1332	A1428	U1512	A1603	G1751	G1863	G1953	G	U2164	A2252	U2335	A2405
A1129	G1209	U1336	G1429	G1513	G1604	U1752	A1864	G	C	A2166	G2253	U2336	C2406
A1130	U1213	G1340	U1431	G1514	A1605	C1755	A1865	U	C	G2165	G2254	G2337	C2407
G1131	G1213	G1340	G1432	A1515	A1609	U1763	G1868	G	C	A2167	A2256	C2338	U2408
C1141	A1217	A1343	A1433	C1516	C1609	C1762	C1869	U	C	A2168	U2260	A2341	U2411
G1142	U1218	G1346	G1434	U1517	U1620	U1764	A1874	G	C	U2169	U2261	U2342	G2412
A1143	G1222	U1347	A1435	U1518	U1621	U1765	G1875	A	A	U2175	C2267	U2344	U2416
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G1147	U1232	G1349	U1438	G1528	U1629	G1769	U1880	C	C	C2179	A2271	U2349	G2418
G1148	C1232	A1350	G1441	U1533	G1635	G1770	A1881	C	C	C2179	G2272	C2350	A2419
U1149	U1236	A1352	G1442	G1536	C1639	G1780	G1882	U	A	G2185	A2273	U2351	C2420
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G1152	C1238	A1355	U1445	A1546	U1642	U1783	U1885	U	A	U2191	A2280	C2354	U2423
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G1170	G1246	G1370	A1461	G1560	G1658	G1796	A1895	U	C	U2200	C2290	C2366	U2434
G1172	U1258	G1371	A1462	G1561	C1562	A1797	A1896	C	C	G2201	C2291	A2367	G2437
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G1178	C1284	U1384	U1480	U1570	G1677	U1815	A1902	C	C	U2210	G	U2377	A2443
A1179	G1285	G1385	A1481	A1571	U1572	A1816	A1903	U	C	U2211	U2300	C2377	C2444
A1180	C1292	A1386	A1482	G1573	C1574	G1817	A1909	C	C	G2212	G2121	U2380	A
U1181	A1302	G1389	U1483	C1574	U1574	U1818	A1917	U	C	G2213	G2122	G2381	A
C1183	A1303	G1391	U1484	G1575	C1575	U1821	C1917	C	C	G2130	A2131	G2382	G
C1187	A1304	C1392	A1489	G1576	U1576	C1822	U1920	U	C	C2132	A2223	C2308	G
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C1189	G1306	U1395	A1491	C1578	U1578	G1829	A1922	U	A	U2134	A2228	A2386	G
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							G1927	G	G	A2138	A2233	G2316	G

A	A	A	A	A	G	U	G	G	G	G	A	G	C	C	U	U	U	U	U	U	A	G2503	U2504	U2505	U2506	C2507	U2508	U2509	U2510	A2511	U2512	U2513	U2514	U2515	U2516	U2517																																																																																																																																								
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A2946	G2947	G2950	G2951	G2952	U2953	U2954	U2955	U2956	U2957	C2960	G2961	U2962	C2963	U2964	U2965	G2968	A2969	C2970	A2971	G2972	U2978	U2979	U2980	U2981	U2982	C2983	C2984	U2985	U2986	G2990	A2991	U2992	U2996	G2997	A3000	C3004	A3005	A3008	U3121	A3122	A3123	G3124	U3207	G3208	A3209	C3212	A3213	A3215																																																																																																																												
C3034	C3039	A3040	G3041	U3042	C3043	U3047	A3048	A3049	U3050	U3054	U3055	U3056	U3057	G3059	C3060	U3068	A3070	U3071	U3078	U3079	C3084	G3085	A3086	C3089	C3092	G3102	A3103	U3104	U3105	A3106	G3107	G3108	U3111	C3115	C3120	U3121	A3122	A3123	G3124	U3207	G3208	A3209	C3212	A3213	A3215																																																																																																																															
A3141	A3142	C3143	G3144	C3145	G3146	G3147	U3148	G3149	A3150	U3151	U3152	U3153	C3154	U3155	U3156	U3157	G3158	C3159	C3164	C3165	C3166	A3167	A3168	U3171	A3172	G3173	A3174	U3175	G3176	G3177	A3178	U3179	A3180	C3181	G3182	A3183	A3187	C3190	U3196	U3197	G3198	G3199	G3200	U3207	G3208	A3209	C3212	A3213	A3215																																																																																																																											
G3216	C3217	A3218	G3219	G3220	C3221	U3222	A3223	G3224	A3227	C3228	G3229	G3230	U3231	G3238	G3239	A3244	A3245	G3246	G3247	G3253	G3256	U3269	U3270	G3271	U3275	G3276	U3277	C3278	U3279	U3280	U3281	U3282	U3283	G3284	C3285	G3286	U3287	G3288	G3289	G3290	A3294	G3303	U3304																																																																																																																																	
A3307	C3308	G3309	A3310	U3313	A3314	G3315	U3316	U3317	G3318	U3319	A3320	C3321	A3322	C3323	G3324	G3325	A3330	U3331	A3335	A3339	G3340	U3341	A3342	G3343	A3344	G3345	U3346	A3347	U3351	U3352	G3353	U3354	U3355	G3356	U3357	U3358	A3362	U3365	U3368	G3369	U3373	U3374	G3377	C3378	U3380	U3381																																																																																																																														
U3387	C3388	U3389	G3390	U3393	U3394	U3396																																																																																																																																																																						

• Molecule 37: 5S ribosomal RNA



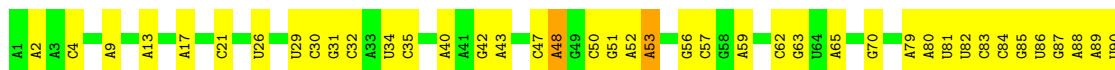
G1	A11	U12	A13	U14	C15	A22	C28	U83	G41	A42	U64	G65	A66	G67	C74	G75	A76	A79	G80	U81	G82	U83	A84	G91	A92	A102	U106	G112	C113	U114	U121
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• Molecule 37: 5S ribosomal RNA





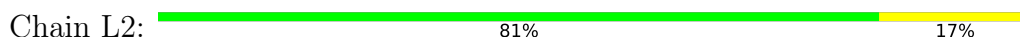
- Molecule 38: 5.8S ribosomal RNA



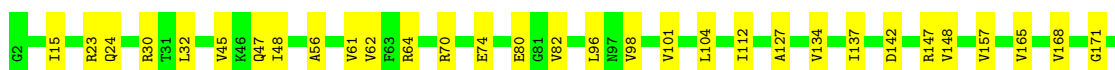
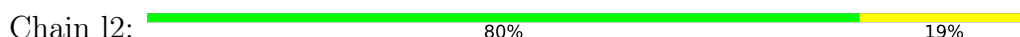
- Molecule 38: 5.8S ribosomal RNA



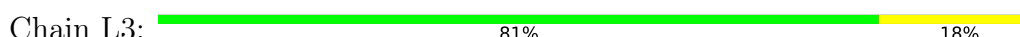
- Molecule 39: 60S ribosomal protein L2-A



- Molecule 39: 60S ribosomal protein L2-A



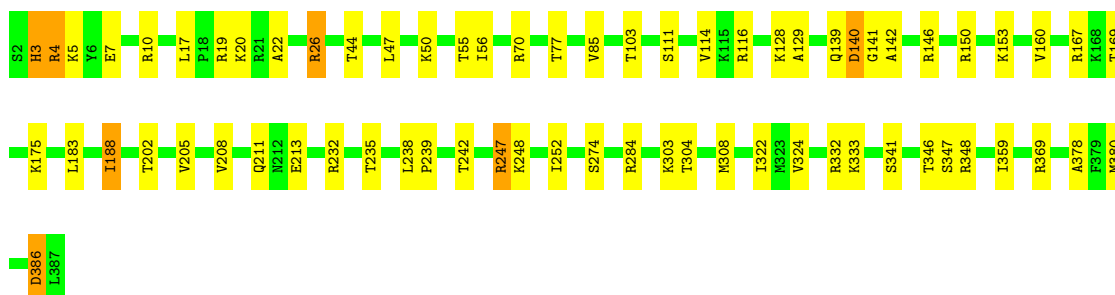
- Molecule 40: 60S ribosomal protein L3





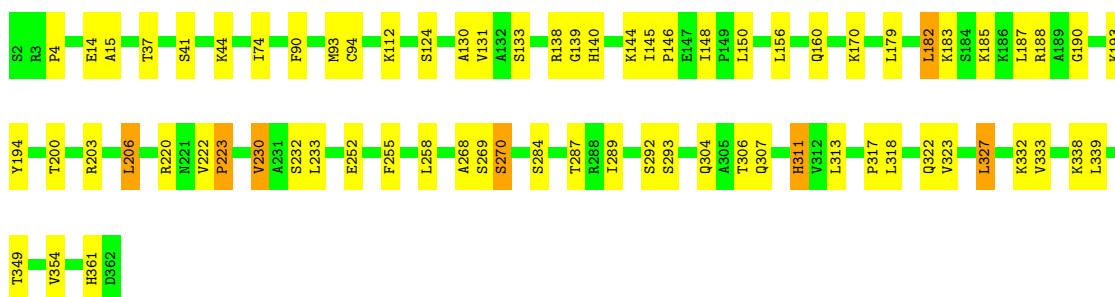
- Molecule 40: 60S ribosomal protein L3

Chain l3: 82% 16%



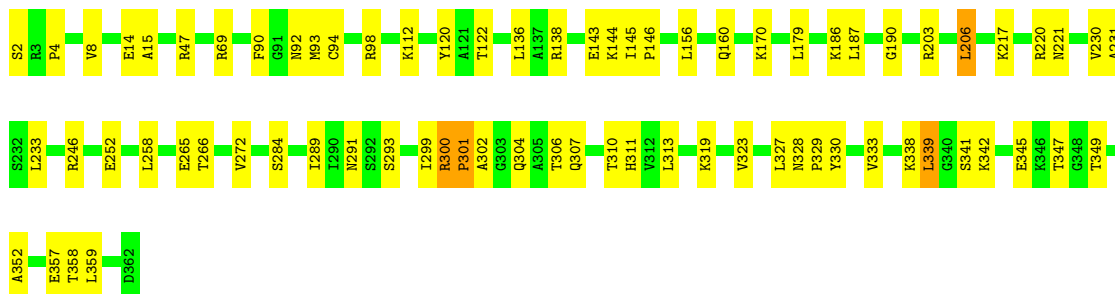
- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 80% 18%

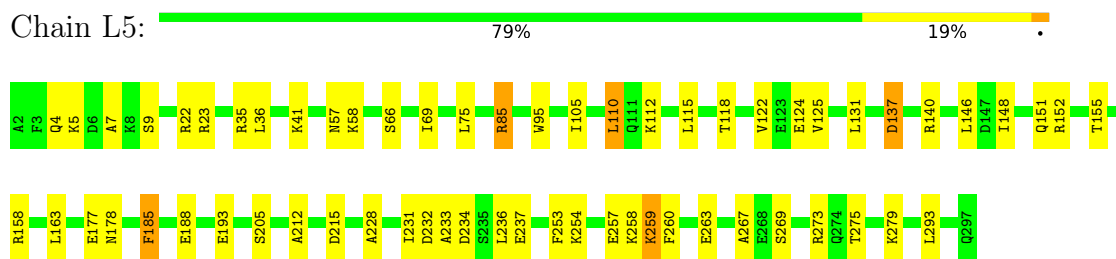


- Molecule 41: 60S ribosomal protein L4-A

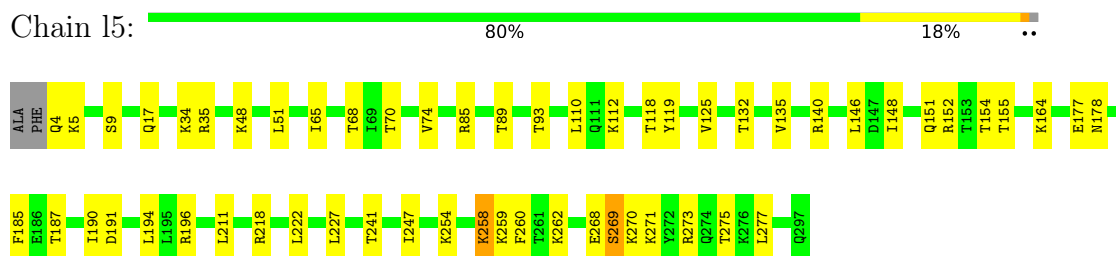
Chain l4: 80% 19%



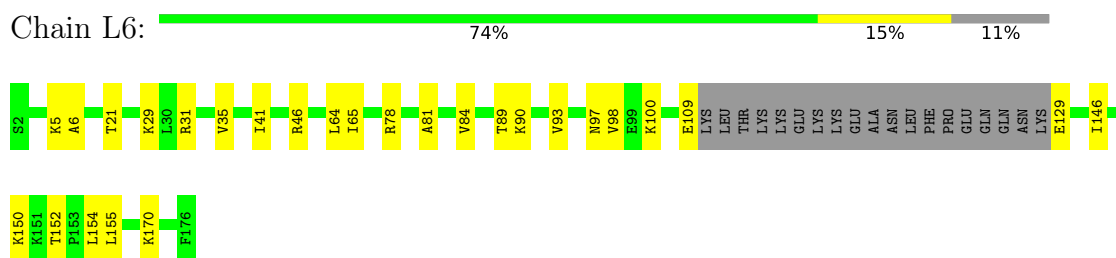
- Molecule 42: 60S ribosomal protein L5



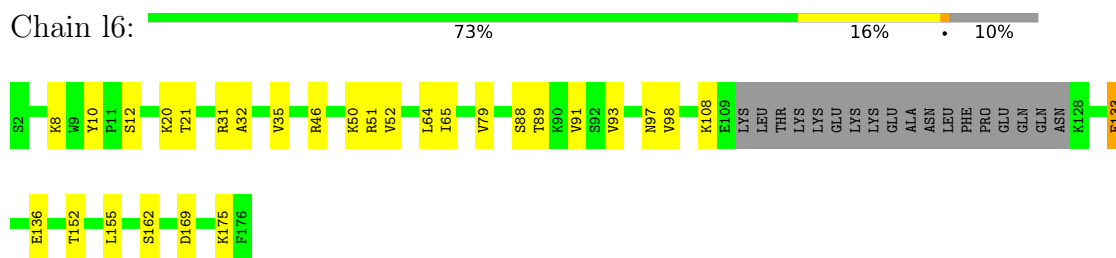
- Molecule 42: 60S ribosomal protein L5



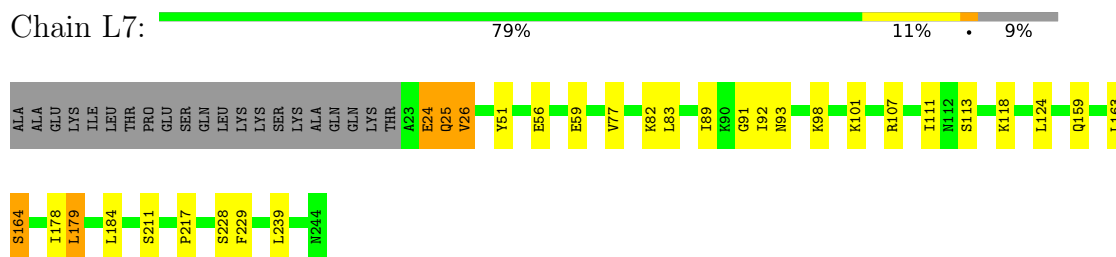
- Molecule 43: 60S ribosomal protein L6-A




- Molecule 43: 60S ribosomal protein L6-A

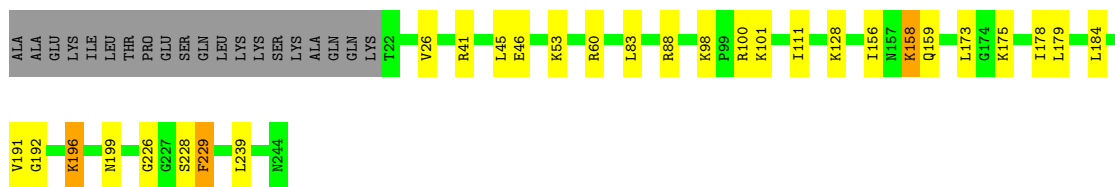


- Molecule 44: 60S ribosomal protein L7-A



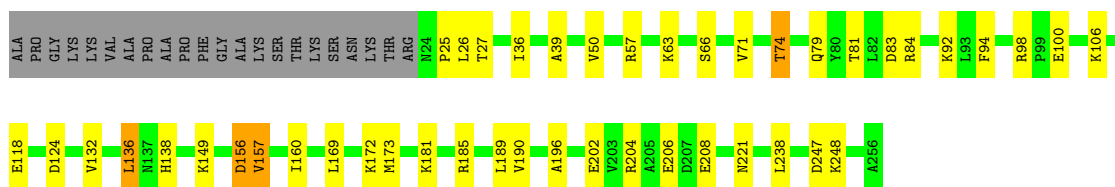
- Molecule 44: 60S ribosomal protein L7-A

Chain 17:  80% 11% 8%



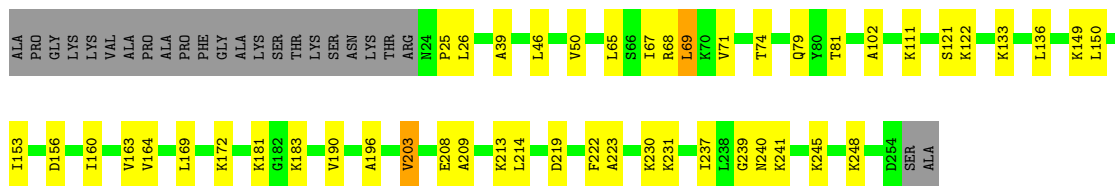
- Molecule 45: 60S ribosomal protein L8-A

Chain 18:  74% 16% 9%




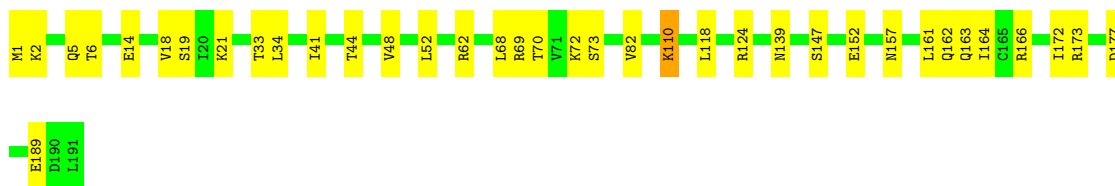
- Molecule 45: 60S ribosomal protein L8-A

Chain 18:  72% 18% 9%




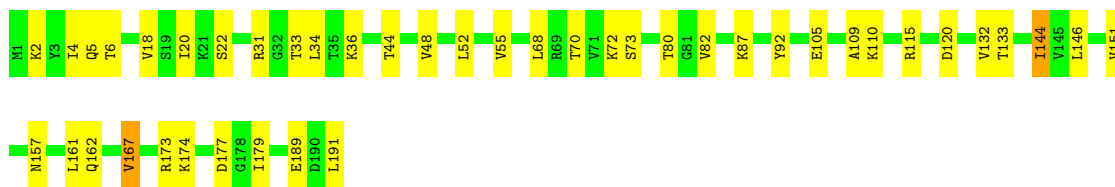
- Molecule 46: 60S ribosomal protein L9-A

Chain 19:  81% 19%

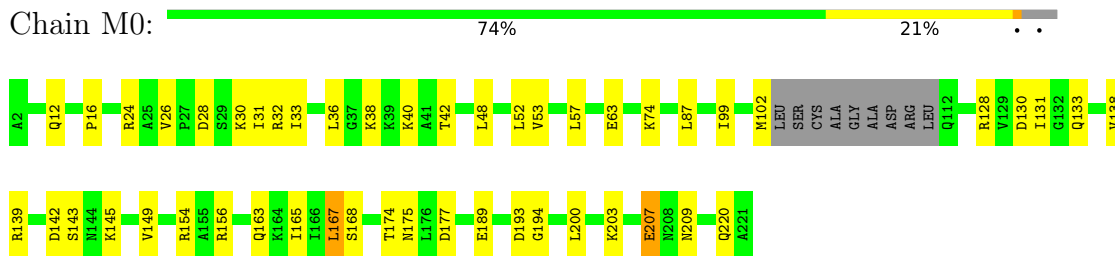


- Molecule 46: 60S ribosomal protein L9-A

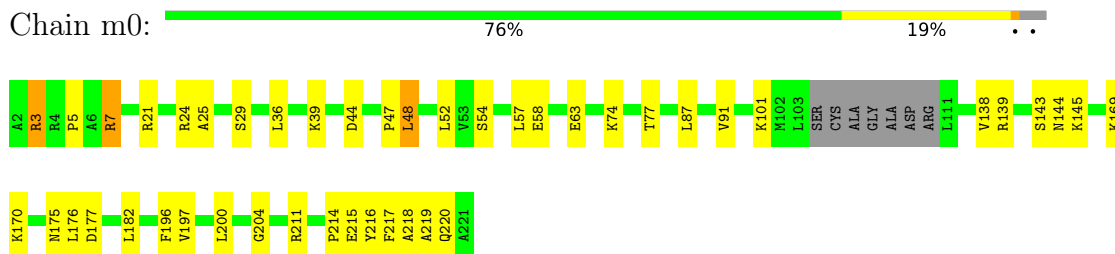
Chain 19:  77% 21%



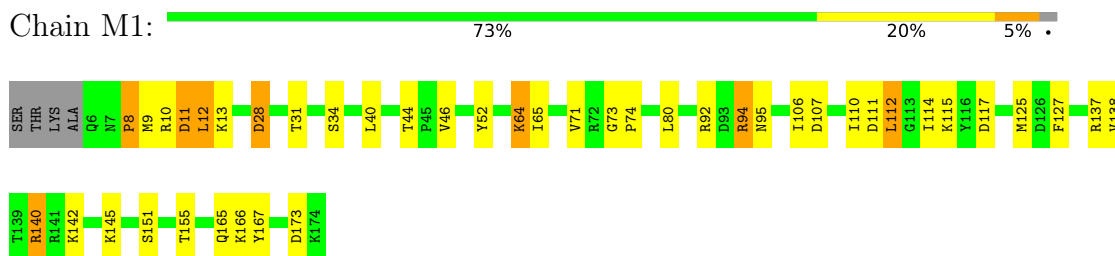
- Molecule 47: 60S ribosomal protein L10



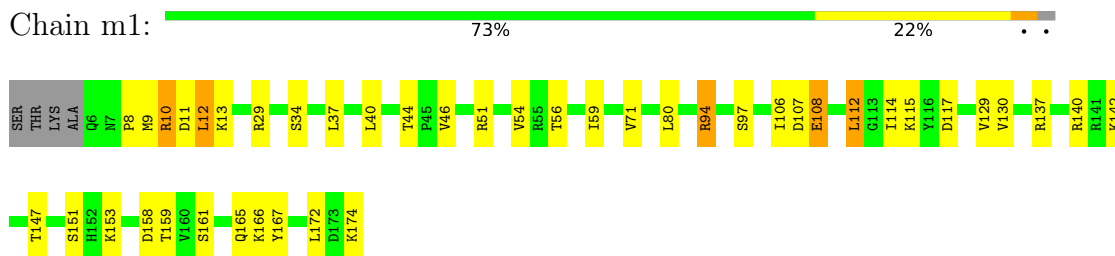
- Molecule 47: 60S ribosomal protein L10



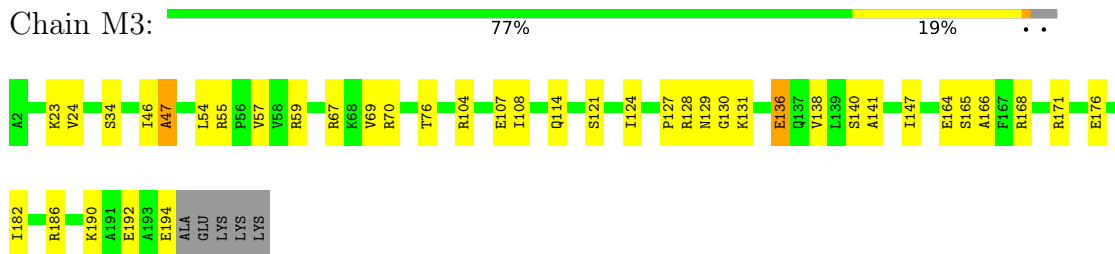
- Molecule 48: 60S ribosomal protein L11-B



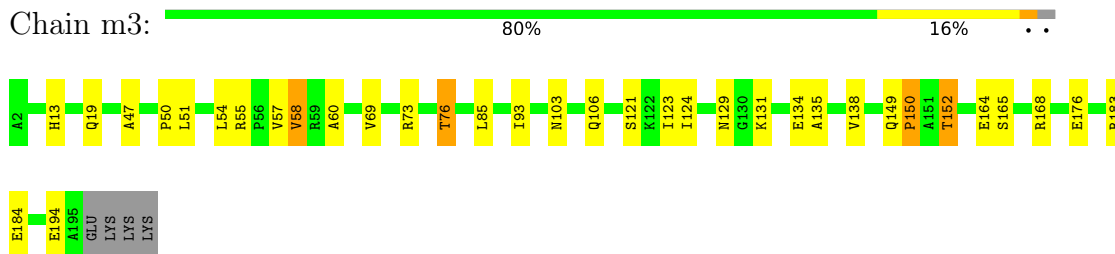
- Molecule 48: 60S ribosomal protein L11-B



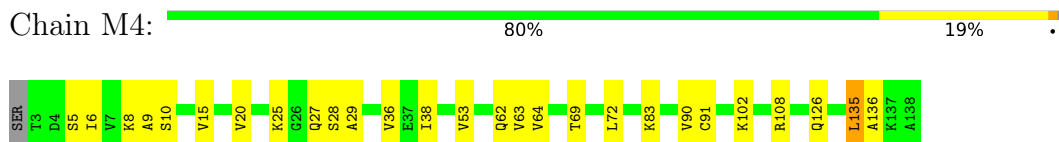
- Molecule 49: 60S ribosomal protein L13-A



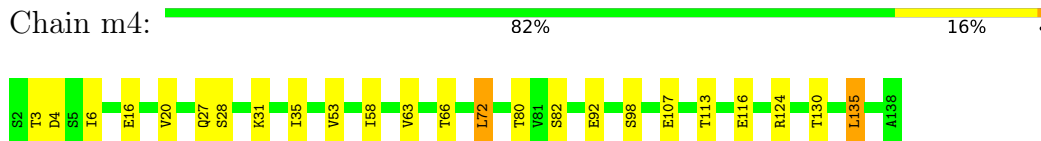
- Molecule 49: 60S ribosomal protein L13-A



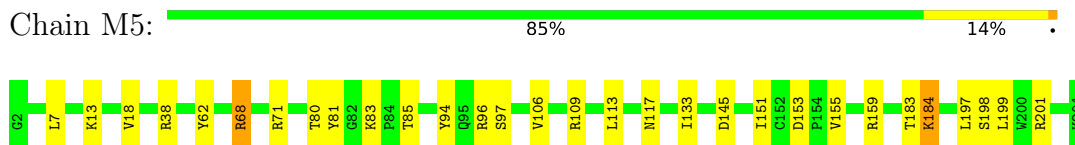
- Molecule 50: 60S ribosomal protein L14-A



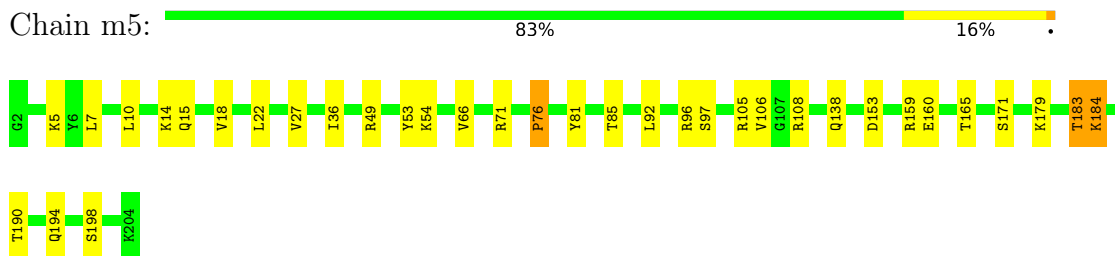
- Molecule 50: 60S ribosomal protein L14-A



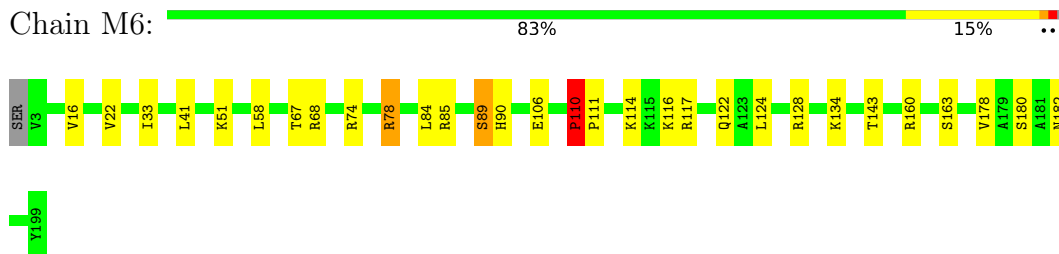
- Molecule 51: 60S ribosomal protein L15-A




- Molecule 51: 60S ribosomal protein L15-A



- Molecule 52: 60S ribosomal protein L16-A




- Molecule 52: 60S ribosomal protein L16-A

Chain m6:  84% 15% ...



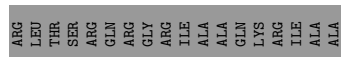
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:  81% 18% .




- Molecule 53: 60S ribosomal protein L17-A

Chain m7:  70% 15% 15%




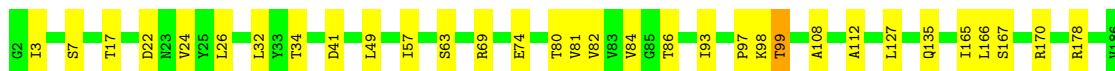
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:  82% 17% .




- Molecule 54: 60S ribosomal protein L18-A

Chain m8:  83% 17% .




- Molecule 55: 60S ribosomal protein L19-A

Chain M9:  87% 13%

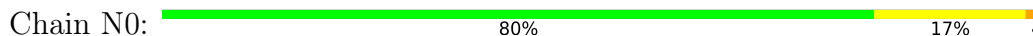


- Molecule 55: 60S ribosomal protein L19-A

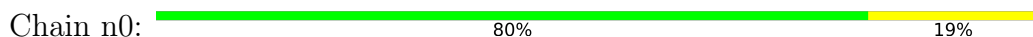
Chain m9:  81% 18% .



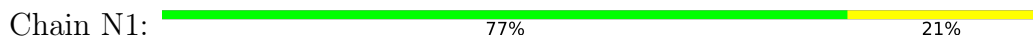
• Molecule 56: 60S ribosomal protein L20-A



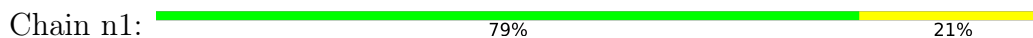
• Molecule 56: 60S ribosomal protein L20-A



• Molecule 57: 60S ribosomal protein L21-A



• Molecule 57: 60S ribosomal protein L21-A



• Molecule 58: 60S ribosomal protein L22-A



GLU
ASP
GLU
GLU

- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 65% 16% 18%



GLU
ASP
GLU
GLU

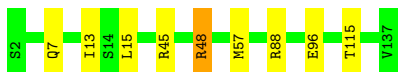
- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 85% 15%



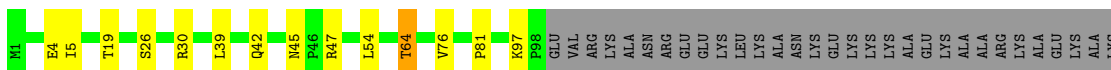
- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 93% 6%



- Molecule 60: 60S ribosomal protein L24-A

Chain N4: 54% 8% 37%



SER ALA GLY THR 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

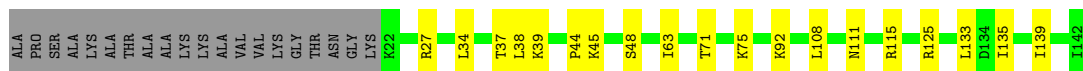
Chain n4: 71% 15% 13%



ALA
ALA
THR
SER
ARG

- Molecule 61: 60S ribosomal protein L25

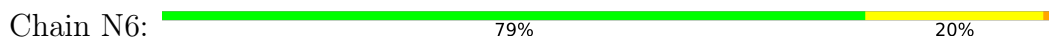
Chain N5: 72% 13% 14%



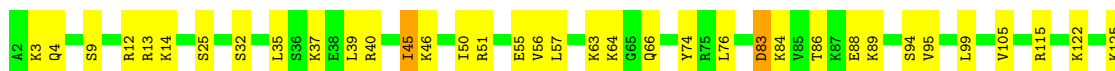
- Molecule 61: 60S ribosomal protein L25



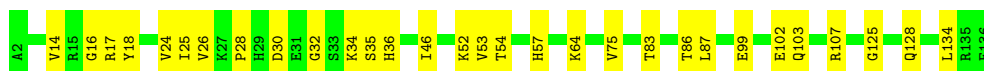
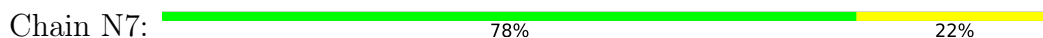
- Molecule 62: 60S ribosomal protein L26-A



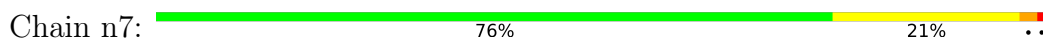
- Molecule 62: 60S ribosomal protein L26-A



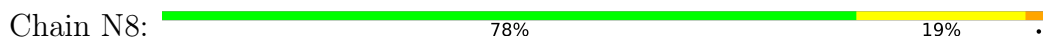
- Molecule 63: 60S ribosomal protein L27-A



- Molecule 63: 60S ribosomal protein L27-A

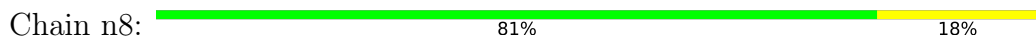


- Molecule 64: 60S ribosomal protein L28

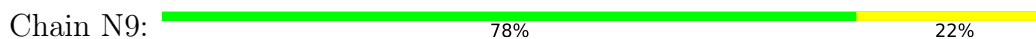




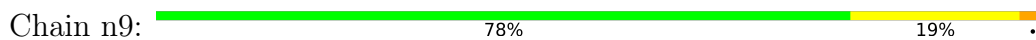
- Molecule 64: 60S ribosomal protein L28



- Molecule 65: 60S ribosomal protein L29



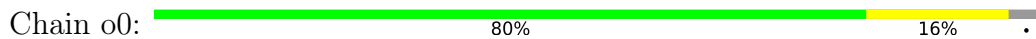
- Molecule 65: 60S ribosomal protein L29



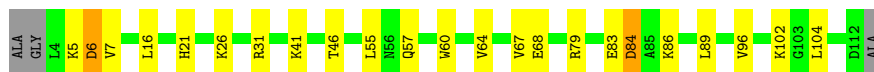
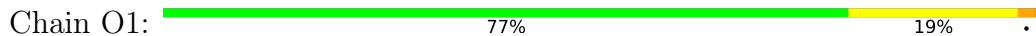
- Molecule 66: 60S ribosomal protein L30



- Molecule 66: 60S ribosomal protein L30



- Molecule 67: 60S ribosomal protein L31-A

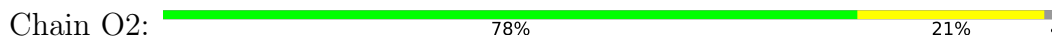


- Molecule 67: 60S ribosomal protein L31-A

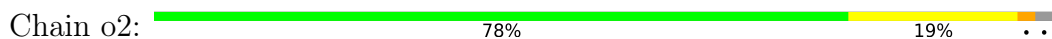




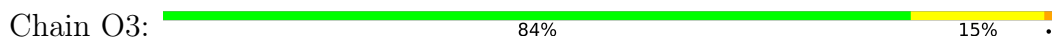
- Molecule 68: 60S ribosomal protein L32



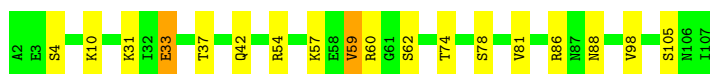
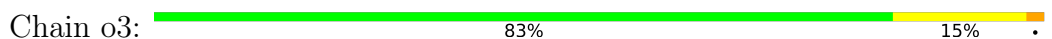
- Molecule 68: 60S ribosomal protein L32



- Molecule 69: 60S ribosomal protein L33-A



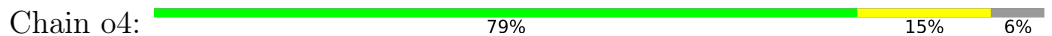
- Molecule 69: 60S ribosomal protein L33-A



- Molecule 70: 60S ribosomal protein L34-A



- Molecule 70: 60S ribosomal protein L34-A



- Molecule 71: 60S ribosomal protein L35-A





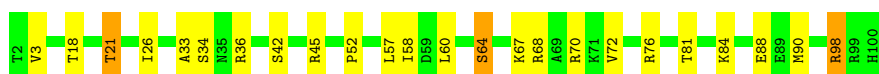
- Molecule 71: 60S ribosomal protein L35-A

Chain o5: 79% 20%



- Molecule 72: 60S ribosomal protein L36-A

Chain O6: 76% 21%



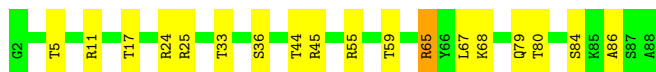
- Molecule 72: 60S ribosomal protein L36-A

Chain o6: 74% 23%



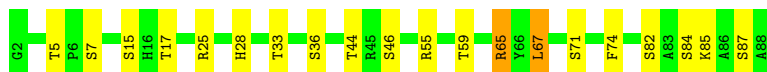
- Molecule 73: 60S ribosomal protein L37-A

Chain O7: 79% 20%



- Molecule 73: 60S ribosomal protein L37-A

Chain o7: 77% 21%



- Molecule 74: 60S ribosomal protein L38

Chain O8: 71% 29%

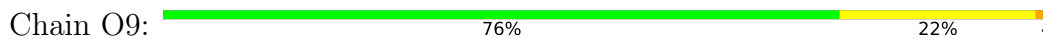


- Molecule 74: 60S ribosomal protein L38

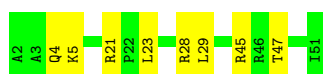
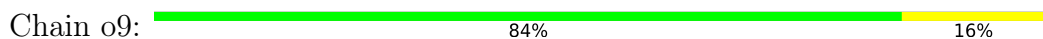
Chain o8: 81% 19%



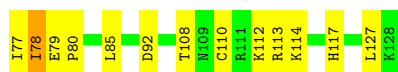
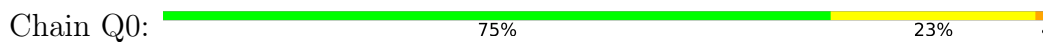
- Molecule 75: 60S ribosomal protein L39



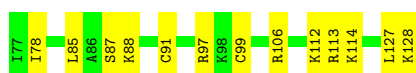
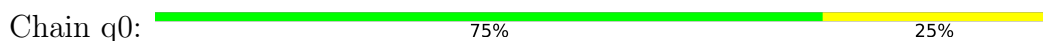
- Molecule 75: 60S ribosomal protein L39



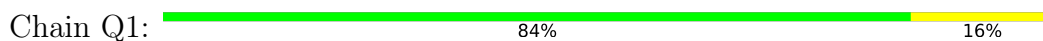
- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



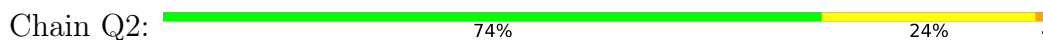
- Molecule 77: 60S ribosomal protein L41-A

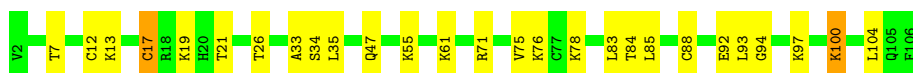


- Molecule 77: 60S ribosomal protein L41-A

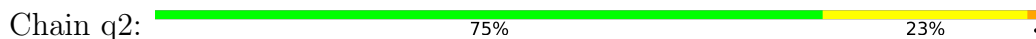


- Molecule 78: 60S ribosomal protein L42-A

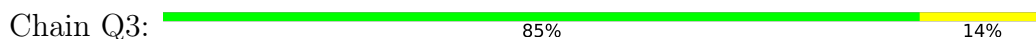




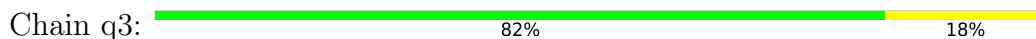
- Molecule 78: 60S ribosomal protein L42-A



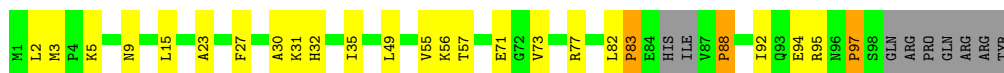
- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 40S ribosomal protein S10-A



- Molecule 81: 40S ribosomal protein S30-A

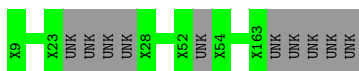


- Molecule 82: Ubiquitin-40S ribosomal protein S31

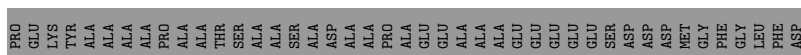
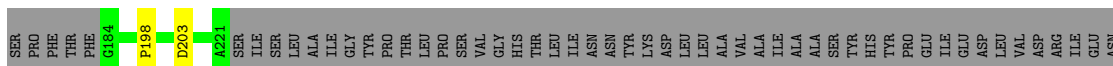
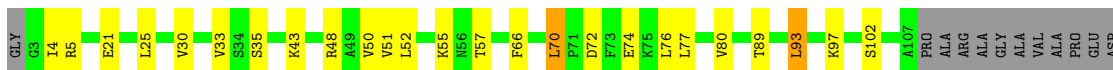
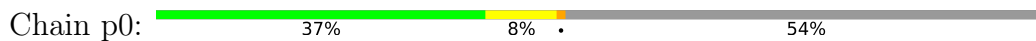


- Molecule 83: UNKNOWN PROTEIN m2





- Molecule 84: 60S acidic ribosomal protein P0



- Molecule 85: UNKNOWN PROTEIN p1



There are no outlier residues recorded for this chain.

- Molecule 86: UNKNOWN PROTEIN p2



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.02Å 287.59Å 304.52Å 90.00° 99.02° 90.00°	Depositor
Resolution (Å)	49.82 – 3.20	Depositor
% Data completeness (in resolution range)	100.0 (49.82-3.20)	Depositor
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.181 , 0.237	Depositor
Wilson B-factor (Å ²)	70.5	Xtrriage
Anisotropy	0.157	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	411288	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: OHX, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.68	1/41698 (0.0%)	1.28	292/64972 (0.4%)
1	6	0.81	13/42765 (0.0%)	1.38	456/66634 (0.7%)
2	S0	0.43	0/1617	0.67	0/2215
2	s0	0.49	0/1623	0.72	0/2222
3	S1	0.37	0/1735	0.69	2/2335 (0.1%)
3	s1	0.51	0/1748	0.70	1/2352 (0.0%)
4	S2	0.45	0/1665	0.65	0/2263
4	s2	0.54	0/1665	0.72	1/2263 (0.0%)
5	S3	0.45	0/1759	0.68	2/2368 (0.1%)
5	s3	0.45	0/1759	0.60	0/2368
6	S4	0.47	0/2109	0.71	0/2839
6	s4	0.52	0/2109	0.75	2/2839 (0.1%)
7	S5	0.38	0/1629	0.60	0/2202
7	s5	0.46	0/1629	0.71	1/2202 (0.0%)
8	S6	0.45	0/1823	0.63	1/2439 (0.0%)
8	s6	0.51	0/1779	0.68	0/2379
9	S7	0.42	0/1506	0.63	0/2028
9	s7	0.44	0/1516	0.70	1/2043 (0.0%)
10	S8	0.51	0/1514	0.76	1/2021 (0.0%)
10	s8	0.59	0/1514	0.77	1/2021 (0.0%)
11	S9	0.43	0/1519	0.65	0/2035
11	s9	0.53	0/1519	0.75	1/2035 (0.0%)
12	C0	0.43	0/790	0.66	1/1069 (0.1%)
13	C1	0.55	0/1240	0.69	0/1675
13	c1	0.60	0/1194	0.80	2/1610 (0.1%)
14	C2	0.35	0/900	0.65	1/1224 (0.1%)
14	c2	0.32	0/900	0.60	1/1224 (0.1%)
15	C3	0.47	0/1215	0.69	3/1638 (0.2%)
15	c3	0.54	0/1215	0.75	1/1638 (0.1%)
16	C4	0.37	0/901	0.64	0/1217
16	c4	0.52	0/960	0.73	0/1290
17	C5	0.44	0/998	0.66	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	c5	0.47	0/1060	0.66	0/1426
18	C6	0.43	0/1125	0.69	2/1510 (0.1%)
18	c6	0.48	0/1131	0.71	1/1518 (0.1%)
19	C7	0.40	0/935	0.66	0/1254
19	c7	0.48	0/914	0.72	0/1224
20	C8	0.43	0/1211	0.66	1/1628 (0.1%)
20	c8	0.50	0/1211	0.70	2/1628 (0.1%)
21	C9	0.44	0/1130	0.67	1/1517 (0.1%)
21	c9	0.49	0/1130	0.72	2/1517 (0.1%)
22	D0	0.45	0/865	0.66	0/1169
22	d0	0.49	0/892	0.70	0/1205
23	D1	0.39	0/693	0.59	0/935
23	d1	0.49	0/693	0.70	0/935
24	D2	0.46	0/1038	0.75	2/1395 (0.1%)
24	d2	0.64	0/1038	0.78	1/1395 (0.1%)
25	D3	0.58	0/1139	0.74	0/1518
25	d3	0.64	0/1139	0.82	2/1518 (0.1%)
26	D4	0.41	0/1087	0.59	0/1449
26	d4	0.51	0/1087	0.69	0/1449
27	D5	0.39	0/571	0.77	2/768 (0.3%)
27	d5	0.42	0/566	0.69	0/761
28	D6	0.40	0/782	0.60	0/1047
28	d6	0.53	0/782	0.69	0/1047
29	D7	0.42	0/620	0.68	0/838
29	d7	0.44	0/620	0.68	0/838
30	D8	0.34	0/499	0.62	0/670
30	d8	0.38	0/499	0.64	0/670
31	D9	0.50	0/452	0.74	1/600 (0.2%)
31	d9	0.56	0/452	0.71	0/600
32	E0	0.40	0/483	0.64	0/643
33	E1	0.41	0/577	0.78	0/770
34	SR	0.39	0/2494	0.63	0/3393
34	sR	0.39	0/2495	0.60	0/3395
35	SM	0.45	0/1113	0.68	2/1502 (0.1%)
35	sM	0.41	0/683	0.63	1/923 (0.1%)
36	1	1.01	59/75394 (0.1%)	1.57	1453/117545 (1.2%)
36	5	1.05	74/75414 (0.1%)	1.58	1442/117575 (1.2%)
37	3	0.87	0/2883	1.32	14/4491 (0.3%)
37	7	1.02	1/2883 (0.0%)	1.60	54/4491 (1.2%)
38	4	0.95	1/3746 (0.0%)	1.51	47/5832 (0.8%)
38	8	0.89	0/3746	1.43	43/5832 (0.7%)
39	L2	0.65	0/1948	0.81	2/2617 (0.1%)
39	l2	0.64	0/1946	0.83	0/2614

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	L3	0.62	0/3146	0.77	0/4228
40	l3	0.76	0/3146	0.84	3/4228 (0.1%)
41	L4	0.70	1/2800 (0.0%)	0.88	3/3790 (0.1%)
41	l4	0.68	1/2800 (0.0%)	0.85	3/3790 (0.1%)
42	L5	0.51	0/2425	0.67	0/3271
42	l5	0.65	0/2408	0.76	0/3248
43	L6	0.65	0/1260	0.79	0/1694
43	l6	0.66	0/1269	0.76	1/1705 (0.1%)
44	L7	0.68	0/1821	0.85	2/2451 (0.1%)
44	l7	0.74	0/1828	0.80	2/2461 (0.1%)
45	L8	0.51	0/1836	0.69	0/2481
45	l8	0.52	0/1795	0.67	0/2429
46	L9	0.60	0/1539	0.71	0/2073
46	l9	0.70	0/1539	0.80	0/2073
47	M0	0.64	0/1741	0.76	2/2335 (0.1%)
47	m0	0.67	0/1758	0.80	3/2358 (0.1%)
48	M1	0.49	0/1374	0.71	1/1842 (0.1%)
48	m1	0.59	0/1374	0.81	2/1842 (0.1%)
49	M3	0.68	0/1568	0.80	1/2106 (0.0%)
49	m3	0.61	0/1573	0.78	0/2113
50	M4	0.61	0/1068	0.74	0/1438
50	m4	0.68	0/1074	0.80	1/1446 (0.1%)
51	M5	0.65	0/1757	0.79	1/2354 (0.0%)
51	m5	0.64	0/1757	0.77	0/2354
52	M6	0.70	0/1585	0.86	3/2128 (0.1%)
52	m6	0.84	0/1585	0.92	3/2128 (0.1%)
53	M7	0.67	0/1443	0.80	1/1944 (0.1%)
53	m7	0.78	0/1250	0.81	0/1683
54	M8	0.67	0/1465	0.85	2/1965 (0.1%)
54	m8	0.66	0/1465	0.86	2/1965 (0.1%)
55	M9	0.51	0/1538	0.66	0/2050
55	m9	0.57	0/1538	0.65	0/2050
56	N0	0.64	0/1481	0.82	3/1990 (0.2%)
56	n0	0.73	0/1481	0.83	2/1990 (0.1%)
57	N1	0.68	0/1300	0.79	0/1743
57	n1	0.74	0/1300	0.79	0/1743
58	N2	0.44	0/812	0.63	0/1099
58	n2	0.46	0/794	0.62	0/1076
59	N3	0.62	0/1018	0.78	1/1369 (0.1%)
59	n3	0.69	0/1018	0.83	1/1369 (0.1%)
60	N4	0.50	0/712	0.64	0/958
60	n4	0.61	0/1052	0.70	0/1398
61	N5	0.53	0/979	0.74	1/1321 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	n5	0.58	0/974	0.74	1/1314 (0.1%)
62	N6	0.63	0/1004	0.82	1/1341 (0.1%)
62	n6	0.57	0/1004	0.78	1/1341 (0.1%)
63	N7	0.49	0/1118	0.66	0/1497
63	n7	0.47	0/1118	0.67	0/1497
64	N8	0.72	0/1204	0.86	1/1612 (0.1%)
64	n8	0.69	0/1204	0.82	0/1612
65	N9	0.60	0/473	0.78	0/629
65	n9	0.63	0/473	0.89	1/629 (0.2%)
66	O0	0.47	0/751	0.64	0/1008
66	o0	0.49	0/775	0.69	0/1040
67	O1	0.60	0/890	0.74	0/1196
67	o1	0.66	0/897	0.81	0/1205
68	O2	0.79	0/1041	0.87	0/1394
68	o2	0.74	0/1041	0.87	2/1394 (0.1%)
69	O3	0.79	0/868	0.85	0/1168
69	o3	0.79	0/868	0.83	0/1168
70	O4	0.59	0/890	0.79	2/1189 (0.2%)
70	o4	0.57	0/890	0.81	0/1189
71	O5	0.62	0/978	0.77	0/1301
71	o5	0.53	0/974	0.67	0/1297
72	O6	0.57	0/778	0.74	0/1034
72	o6	0.55	0/777	0.70	0/1033
73	O7	0.67	0/696	0.94	4/923 (0.4%)
73	o7	0.64	0/696	0.81	1/923 (0.1%)
74	O8	0.48	0/618	0.64	1/826 (0.1%)
74	o8	0.45	0/614	0.64	0/822
75	O9	0.64	0/443	0.83	0/588
75	o9	0.63	0/443	0.76	0/588
76	Q0	0.64	0/423	0.73	0/562
76	q0	0.81	1/423 (0.2%)	0.85	0/562
77	Q1	0.66	0/234	0.84	0/300
77	q1	0.65	0/234	0.98	2/300 (0.7%)
78	Q2	0.74	1/860 (0.1%)	0.83	0/1136
78	q2	0.69	0/860	0.79	1/1136 (0.1%)
79	Q3	0.67	0/701	0.77	0/934
79	q3	0.65	0/701	0.80	0/934
80	c0	0.40	0/777	0.66	3/1049 (0.3%)
81	e0	0.49	0/499	0.72	0/665
82	e1	0.38	0/619	0.74	1/822 (0.1%)
84	p0	0.44	0/1092	0.63	1/1474 (0.1%)
All	All	0.80	153/430074 (0.0%)	1.26	3913/631364 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	s1	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
10	s8	0	1
13	C1	0	1
15	c3	0	1
16	C4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	3
22	d0	0	1
25	D3	0	1
26	d4	0	2
27	D5	0	3
27	d5	0	1
33	E1	0	1
39	L2	0	1
39	l2	0	2
42	l5	0	2
43	l6	0	1
44	l7	0	2
45	L8	0	2
48	M1	0	2
51	m5	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	2
56	n0	0	1
57	N1	0	1
60	n4	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	1
82	e1	0	1
All	All	0	52

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-11.64	1.28	1.38
36	5	3008	A	N9-C4	-8.98	1.32	1.37
36	5	2358	A	N9-C4	-8.04	1.33	1.37
36	1	1114	U	C2-N3	-7.72	1.32	1.37
36	1	2714	G	N9-C4	-7.69	1.31	1.38
36	1	338	A	N7-C5	-7.29	1.34	1.39
36	5	1152	G	N3-C4	-7.21	1.30	1.35
36	5	2280	A	N9-C4	-7.10	1.33	1.37
36	1	884	A	N9-C4	-6.99	1.33	1.37
36	5	3008	A	N3-C4	-6.99	1.30	1.34
36	1	2197	C	C2-O2	6.95	1.30	1.24
36	5	2147	A	C5-C6	-6.88	1.34	1.41
36	1	2983	C	N3-C4	-6.78	1.29	1.33
36	5	1451	C	N1-C6	-6.74	1.33	1.37
1	6	163	G	N9-C4	-6.72	1.32	1.38
1	2	1754	A	N9-C4	-6.71	1.33	1.37
78	Q2	17	CYS	CB-SG	6.67	1.93	1.82
36	5	1178	G	C5-C6	-6.63	1.35	1.42
36	1	1446	A	N3-C4	-6.63	1.30	1.34
36	1	2714	G	N9-C8	6.60	1.42	1.37
36	5	2733	A	N3-C4	-6.55	1.30	1.34
1	6	1744	A	N9-C4	-6.55	1.33	1.37
36	1	2188	A	N9-C4	-6.54	1.33	1.37
36	5	2890	A	N7-C5	-6.53	1.35	1.39
36	5	1143	A	N9-C4	-6.53	1.33	1.37
36	5	2726	C	N3-C4	-6.50	1.29	1.33
36	5	1152	G	N9-C8	6.49	1.42	1.37
36	1	2355	G	N7-C5	-6.46	1.35	1.39
36	5	1443	G	N1-C2	-6.37	1.32	1.37
36	5	2139	A	N3-C4	-6.36	1.31	1.34
36	5	2386	A	N7-C5	-6.29	1.35	1.39
36	1	1158	A	N7-C5	-6.29	1.35	1.39
36	5	3245	A	C5-C6	-6.27	1.35	1.41
36	5	2640	A	N9-C4	-6.08	1.34	1.37
37	7	89	G	N9-C8	-6.08	1.33	1.37
36	1	2384	A	N9-C4	6.06	1.41	1.37
1	6	359	A	N9-C4	-6.02	1.34	1.37
36	1	804	C	N1-C6	-6.01	1.33	1.37
36	1	361	A	N3-C4	-6.01	1.31	1.34
1	6	337	G	C2-N3	5.98	1.37	1.32
36	1	942	U	C4-O4	5.98	1.28	1.23
36	5	2647	A	N9-C4	-5.95	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	21	G	N9-C4	-5.92	1.33	1.38
36	5	1374	G	N1-C2	-5.88	1.33	1.37
41	L4	94	CYS	CB-SG	-5.88	1.72	1.81
76	q0	99	CYS	CB-SG	-5.86	1.72	1.81
36	5	1374	G	C6-N1	-5.85	1.35	1.39
36	5	3039	C	N1-C6	-5.82	1.33	1.37
36	5	3040	A	N7-C5	-5.78	1.35	1.39
1	6	119	A	N9-C4	-5.78	1.34	1.37
36	1	2871	G	N7-C5	5.77	1.42	1.39
36	5	2385	G	N9-C4	-5.76	1.33	1.38
36	1	361	A	N9-C4	-5.72	1.34	1.37
36	5	847	A	N9-C4	-5.72	1.34	1.37
36	1	1154	A	N3-C4	-5.72	1.31	1.34
36	5	2617	U	N1-C2	-5.72	1.33	1.38
41	l4	94	CYS	CB-SG	-5.71	1.72	1.81
36	5	523	A	N9-C4	-5.70	1.34	1.37
36	5	2804	A	N9-C4	-5.70	1.34	1.37
36	5	804	C	N1-C6	-5.65	1.33	1.37
36	5	1188	U	C2-N3	-5.64	1.33	1.37
36	1	653	A	N7-C5	-5.63	1.35	1.39
36	1	2422	C	N3-C4	-5.62	1.30	1.33
1	6	163	G	N3-C4	-5.62	1.31	1.35
36	5	3215	A	N9-C4	-5.58	1.34	1.37
36	1	1154	A	C6-N1	-5.58	1.31	1.35
36	5	2910	A	N9-C4	-5.57	1.34	1.37
36	5	2971	A	N9-C4	5.57	1.41	1.37
36	1	426	G	N1-C2	-5.57	1.33	1.37
38	4	111	A	N7-C5	-5.55	1.35	1.39
36	5	1847	A	N9-C4	-5.55	1.34	1.37
36	5	2639	G	N7-C5	-5.55	1.35	1.39
36	5	2811	A	C6-N1	-5.54	1.31	1.35
36	5	1372	C	N1-C6	-5.54	1.33	1.37
1	6	1655	A	N7-C5	-5.53	1.35	1.39
36	5	2318	U	C2-N3	-5.52	1.33	1.37
36	1	706	A	N9-C4	-5.51	1.34	1.37
36	5	2144	A	N9-C4	5.51	1.41	1.37
36	1	653	A	C5-C6	-5.50	1.36	1.41
36	5	2379	U	N3-C4	-5.50	1.33	1.38
36	5	1922	A	N9-C4	-5.49	1.34	1.37
36	5	3103	A	N3-C4	-5.48	1.31	1.34
36	1	1394	A	N9-C4	-5.44	1.34	1.37
36	5	2696	A	N3-C4	-5.42	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	1150	A	N9-C4	-5.41	1.34	1.37
36	1	1164	G	N3-C4	-5.39	1.31	1.35
36	5	1152	G	N1-C2	5.38	1.42	1.37
36	1	2611	U	C2-N3	-5.38	1.33	1.37
36	5	2243	A	N3-C4	-5.38	1.31	1.34
36	1	3129	A	N9-C4	-5.37	1.34	1.37
36	1	3008	A	N9-C4	-5.36	1.34	1.37
36	5	2762	A	N9-C4	-5.36	1.34	1.37
36	1	949	C	N1-C6	-5.36	1.33	1.37
36	1	1883	A	N9-C4	-5.36	1.34	1.37
36	5	61	A	N3-C4	-5.36	1.31	1.34
36	5	1148	G	N9-C8	-5.36	1.34	1.37
1	6	65	A	N9-C4	-5.35	1.34	1.37
36	5	1443	G	C6-N1	-5.35	1.35	1.39
36	1	3123	A	N9-C4	-5.34	1.34	1.37
36	1	816	A	C8-N7	5.34	1.35	1.31
36	1	2946	A	N7-C5	-5.33	1.36	1.39
36	1	2640	A	C6-N1	-5.32	1.31	1.35
36	5	611	A	N7-C5	-5.32	1.36	1.39
36	5	884	A	N9-C4	-5.31	1.34	1.37
36	5	421	G	N1-C2	-5.31	1.33	1.37
36	1	1369	A	N9-C4	-5.29	1.34	1.37
36	5	3209	A	C5-C4	5.29	1.42	1.38
1	6	1655	A	C5-C4	-5.26	1.35	1.38
1	6	17	C	N3-C4	-5.26	1.30	1.33
36	5	647	A	N3-C4	-5.24	1.31	1.34
36	1	2953	U	C4-O4	5.23	1.27	1.23
36	1	1164	G	N9-C4	-5.23	1.33	1.38
36	5	420	G	N9-C8	-5.23	1.34	1.37
36	1	646	A	N7-C5	-5.22	1.36	1.39
36	1	1305	U	C2-O2	5.20	1.27	1.22
36	1	361	A	C6-N1	-5.20	1.31	1.35
36	1	970	A	N3-C4	-5.19	1.31	1.34
36	1	1369	A	N7-C5	-5.18	1.36	1.39
36	5	2163	C	N1-C6	-5.18	1.34	1.37
36	1	2232	A	N9-C4	-5.18	1.34	1.37
1	6	387	A	N9-C4	5.18	1.41	1.37
36	5	2650	U	C4-O4	-5.18	1.19	1.23
36	5	953	G	C5-C4	-5.17	1.34	1.38
36	1	61	A	N3-C4	-5.17	1.31	1.34
36	5	2910	A	N3-C4	-5.17	1.31	1.34
36	1	1330	A	C5-C6	-5.16	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2398	A	C6-N1	-5.16	1.31	1.35
36	5	3172	A	N9-C4	-5.15	1.34	1.37
36	1	3306	U	C2-N3	-5.14	1.34	1.37
36	5	367	A	N3-C4	-5.14	1.31	1.34
36	5	367	A	N9-C4	-5.13	1.34	1.37
36	5	2280	A	N3-C4	-5.11	1.31	1.34
36	5	970	A	N9-C4	-5.11	1.34	1.37
36	1	3316	A	N9-C4	-5.11	1.34	1.37
36	5	699	A	N9-C4	-5.10	1.34	1.37
36	1	432	G	N3-C4	-5.09	1.31	1.35
36	1	948	C	N3-C4	-5.09	1.30	1.33
36	5	3120	C	N1-C6	-5.09	1.34	1.37
36	1	1335	C	N1-C6	-5.08	1.34	1.37
1	6	542	A	N7-C5	-5.08	1.36	1.39
36	1	1308	A	N3-C4	-5.07	1.31	1.34
36	1	948	C	N1-C6	-5.06	1.34	1.37
36	5	1115	G	N7-C5	-5.05	1.36	1.39
36	5	2273	G	C5-C4	-5.04	1.34	1.38
36	1	345	G	N7-C5	-5.04	1.36	1.39
36	5	2363	A	N7-C5	-5.03	1.36	1.39
36	1	368	G	N7-C5	-5.02	1.36	1.39
36	1	699	A	N3-C4	-5.02	1.31	1.34
36	1	1858	A	N3-C4	-5.01	1.31	1.34
1	6	1775	U	C2-N3	-5.01	1.34	1.37
36	1	2169	G	C5-C6	5.01	1.47	1.42
36	5	2695	A	N3-C4	-5.01	1.31	1.34
36	5	1462	A	N9-C4	-5.00	1.34	1.37

All (3913) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-21.84	112.90	126.00
36	5	1152	G	N3-C4-C5	21.63	139.41	128.60
36	5	1152	G	C2-N3-C4	-18.18	102.81	111.90
36	1	2714	G	N3-C4-C5	17.75	137.47	128.60
36	1	1308	A	O5'-P-OP2	-16.96	90.35	110.70
36	1	2714	G	N3-C4-N9	-16.21	116.27	126.00
36	5	1116	G	O5'-P-OP1	-14.88	92.31	105.70
1	6	163	G	N3-C4-N9	-13.88	117.67	126.00
36	5	2199	G	N1-C6-O6	13.59	128.05	119.90
36	5	3245	A	C2-N3-C4	-13.07	104.07	110.60
36	1	1116	G	O5'-P-OP1	-12.94	94.05	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1897	G	N1-C6-O6	12.87	127.62	119.90
36	5	922	U	C5-C6-N1	-12.80	116.30	122.70
36	1	435	C	C6-N1-C2	12.71	125.38	120.30
36	1	1495	U	C5-C6-N1	-12.62	116.39	122.70
36	5	2818	U	O5'-P-OP1	-12.54	94.42	105.70
36	5	1902	G	N1-C6-O6	12.47	127.38	119.90
36	5	2726	C	C5-C4-N4	12.22	128.76	120.20
36	5	3245	A	C5-N7-C8	-12.18	97.81	103.90
1	2	1200	G	N1-C6-O6	12.14	127.18	119.90
36	5	874	U	O5'-P-OP1	-11.95	94.94	105.70
36	1	637	C	C6-N1-C2	11.88	125.05	120.30
36	5	283	G	C4-C5-N7	11.84	115.53	110.80
36	1	2283	G	N1-C6-O6	11.78	126.97	119.90
36	5	2282	U	O5'-P-OP1	-11.75	95.13	105.70
36	5	3245	A	N1-C6-N6	11.69	125.62	118.60
36	1	2870	C	N3-C4-C5	11.52	126.51	121.90
36	5	1902	G	C6-C5-N7	-11.19	123.68	130.40
36	5	1152	G	C8-N9-C1'	11.15	141.49	127.00
36	1	3306	U	C5-C4-O4	11.14	132.58	125.90
36	5	1307	G	P-O3'-C3'	11.13	133.06	119.70
36	5	806	A	O5'-P-OP1	-11.12	95.69	105.70
36	1	343	U	O5'-P-OP2	-11.09	95.72	105.70
36	1	2725	U	C5-C4-O4	11.04	132.52	125.90
36	1	608	A	N1-C6-N6	11.02	125.21	118.60
36	5	2819	A	O5'-P-OP2	-11.00	95.80	105.70
1	6	1029	U	C5-C4-O4	10.89	132.43	125.90
36	1	1149	G	N1-C6-O6	10.84	126.40	119.90
36	5	1897	G	C5-C6-O6	-10.83	122.10	128.60
38	4	94	C	C6-N1-C2	10.81	124.62	120.30
1	6	1773	C	N3-C4-C5	-10.79	117.58	121.90
36	1	639	G	C5-C6-O6	-10.77	122.14	128.60
36	1	2714	G	C2-N3-C4	-10.73	106.54	111.90
36	5	1897	G	C4-C5-N7	10.73	115.09	110.80
36	5	1152	G	C5-N7-C8	-10.71	98.94	104.30
36	1	2797	C	O5'-P-OP1	-10.71	96.06	105.70
36	5	424	G	C5-C6-O6	-10.70	122.18	128.60
36	5	2211	U	C4-C5-C6	10.70	126.12	119.70
36	5	2726	C	N3-C4-N4	-10.66	110.53	118.00
36	5	1909	A	C8-N9-C4	10.66	110.06	105.80
36	1	639	G	N1-C6-O6	10.62	126.28	119.90
1	6	163	G	N3-C4-C5	10.54	133.87	128.60
36	5	1178	G	C5-C6-O6	-10.50	122.30	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1149	G	C5-C6-O6	-10.50	122.30	128.60
36	5	3245	A	C4-C5-N7	10.49	115.95	110.70
1	2	1280	C	N3-C4-C5	-10.48	117.71	121.90
1	2	1039	A	O4'-C1'-N9	10.46	116.57	108.20
36	5	2283	G	C5-C6-O6	-10.44	122.34	128.60
37	7	120	C	C6-N1-C2	10.43	124.47	120.30
36	1	776	U	C4-C5-C6	10.39	125.94	119.70
36	1	2617	U	C5-C4-O4	10.39	132.13	125.90
36	1	1368	U	O5'-P-OP1	-10.38	96.36	105.70
36	5	3245	A	N7-C8-N9	10.34	118.97	113.80
36	5	2147	A	N1-C6-N6	10.27	124.77	118.60
36	5	2272	G	O4'-C1'-N9	10.26	116.41	108.20
36	1	3306	U	N3-C4-O4	-10.26	112.22	119.40
36	5	2283	G	N1-C6-O6	10.26	126.05	119.90
36	5	2830	G	N1-C2-N3	10.19	130.01	123.90
36	5	3245	A	C6-C5-N7	-10.18	125.17	132.30
36	5	1316	C	N1-C2-O2	-10.15	112.81	118.90
1	6	1537	C	C6-N1-C2	-10.14	116.24	120.30
36	1	1381	A	O5'-P-OP2	10.14	122.86	110.70
36	1	2803	A	O5'-P-OP1	-10.11	96.60	105.70
36	5	2524	A	O4'-C1'-N9	10.09	116.27	108.20
1	6	47	A	O5'-P-OP1	-10.07	96.64	105.70
36	5	2620	G	N1-C6-O6	-10.04	113.87	119.90
36	5	1897	G	C6-C5-N7	-10.04	124.38	130.40
36	1	1437	C	C6-N1-C2	-9.99	116.30	120.30
38	4	99	C	C6-N1-C2	9.96	124.28	120.30
1	2	553	G	C5-C6-O6	-9.92	122.65	128.60
36	5	3218	A	N1-C6-N6	9.92	124.55	118.60
36	5	1148	G	C5-C6-O6	-9.89	122.67	128.60
36	1	2373	A	O5'-P-OP1	-9.87	96.82	105.70
36	1	3362	A	N7-C8-N9	9.84	118.72	113.80
36	1	1838	G	N1-C6-O6	9.81	125.79	119.90
36	1	2983	C	C5-C6-N1	-9.80	116.10	121.00
1	2	554	C	N1-C2-O2	9.79	124.78	118.90
36	1	3269	U	O5'-P-OP2	-9.78	96.90	105.70
36	1	3278	C	N1-C2-O2	9.77	124.76	118.90
1	6	542	A	O5'-P-OP1	-9.76	96.91	105.70
36	1	1495	U	C4-C5-C6	9.74	125.55	119.70
36	1	1367	G	N1-C6-O6	9.73	125.74	119.90
36	1	3362	A	C5-N7-C8	-9.70	99.05	103.90
36	5	1321	G	N1-C6-O6	9.68	125.71	119.90
36	1	1495	U	N1-C2-N3	9.68	120.71	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2354	C	N1-C2-O2	-9.67	113.10	118.90
36	5	1897	G	C5-N7-C8	-9.67	99.47	104.30
36	5	3115	C	N1-C2-O2	-9.66	113.11	118.90
36	1	2726	C	N3-C2-O2	-9.57	115.20	121.90
36	5	2234	G	C5-C6-O6	-9.53	122.89	128.60
36	5	1390	A	C8-N9-C4	-9.51	102.00	105.80
36	5	1178	G	C4-C5-N7	9.49	114.60	110.80
36	1	1192	C	N1-C2-O2	9.47	124.58	118.90
36	5	646	A	C2-N3-C4	-9.47	105.87	110.60
36	5	2282	U	O5'-P-OP2	9.45	122.05	110.70
36	1	2679	A	N1-C6-N6	9.45	124.27	118.60
36	5	1208	U	C5-C4-O4	9.45	131.57	125.90
36	1	2846	U	N3-C2-O2	-9.43	115.60	122.20
36	5	1152	G	C4-N9-C1'	-9.43	114.24	126.50
1	2	1200	G	C5-C6-O6	-9.39	122.97	128.60
1	2	1773	C	N3-C4-C5	-9.35	118.16	121.90
3	S1	218	LEU	CA-CB-CG	9.30	136.69	115.30
36	1	1849	C	N1-C2-O2	-9.30	113.32	118.90
1	2	453	U	N3-C2-O2	-9.29	115.69	122.20
36	1	770	G	O4'-C1'-N9	9.29	115.64	108.20
36	5	283	G	C5-C6-O6	-9.29	123.03	128.60
36	1	716	A	N1-C6-N6	9.26	124.15	118.60
37	7	92	A	N1-C6-N6	9.24	124.14	118.60
36	5	917	A	O5'-P-OP2	-9.23	97.39	105.70
36	5	2385	G	O5'-P-OP1	-9.22	97.40	105.70
36	5	2199	G	C5-C6-O6	-9.21	123.07	128.60
36	5	2385	G	N3-C4-C5	9.21	133.20	128.60
36	1	1365	G	N3-C4-C5	-9.18	124.01	128.60
38	4	113	U	C5-C6-N1	-9.18	118.11	122.70
36	1	776	U	C5-C6-N1	-9.16	118.12	122.70
36	5	2913	C	N1-C2-O2	-9.13	113.42	118.90
36	1	3377	G	N3-C4-N9	9.12	131.47	126.00
36	1	2846	U	C5-C4-O4	9.11	131.37	125.90
36	5	2899	C	C6-N1-C2	-9.10	116.66	120.30
36	1	2314	U	N3-C4-O4	9.05	125.73	119.40
36	5	966	U	N3-C2-O2	-9.05	115.87	122.20
36	1	2273	G	C8-N9-C4	9.04	110.02	106.40
36	1	2679	A	C2-N3-C4	-9.04	106.08	110.60
37	7	101	G	N1-C6-O6	9.03	125.32	119.90
36	5	437	G	N9-C4-C5	9.02	109.01	105.40
1	2	553	G	N1-C6-O6	9.01	125.31	119.90
36	1	2827	U	C5-C4-O4	9.00	131.30	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3306	U	N3-C2-O2	-8.99	115.91	122.20
36	5	2917	G	C5-C6-O6	-8.98	123.21	128.60
36	5	2156	C	C6-N1-C2	8.98	123.89	120.30
1	6	65	A	C2-N3-C4	-8.97	106.11	110.60
36	5	1848	G	C5-C6-O6	-8.97	123.22	128.60
36	1	1377	G	C5-C6-O6	-8.95	123.23	128.60
36	1	1113	G	N1-C6-O6	8.95	125.27	119.90
36	1	2726	C	N3-C4-N4	-8.95	111.74	118.00
36	5	406	G	O4'-C1'-N9	8.91	115.33	108.20
36	5	2199	G	C6-C5-N7	-8.90	125.06	130.40
36	5	942	U	N1-C2-O2	-8.90	116.57	122.80
36	1	2314	U	C2-N1-C1'	8.89	128.37	117.70
36	5	1316	C	N3-C4-C5	-8.89	118.34	121.90
36	5	1848	G	N1-C6-O6	8.88	125.23	119.90
1	2	565	C	C6-N1-C2	8.88	123.85	120.30
36	5	2935	U	O5'-P-OP2	-8.88	97.71	105.70
36	1	2355	G	C6-C5-N7	-8.88	125.08	130.40
36	5	1481	A	C8-N9-C4	-8.87	102.25	105.80
36	1	611	A	O5'-P-OP2	-8.86	97.73	105.70
36	1	1902	G	N1-C6-O6	8.85	125.21	119.90
48	m1	112	LEU	CA-CB-CG	8.85	135.65	115.30
36	5	1112	A	C6-N1-C2	-8.84	113.30	118.60
36	1	3057	U	N3-C2-O2	-8.83	116.02	122.20
36	1	2197	C	N1-C2-N3	-8.82	113.02	119.20
36	5	1143	A	C2-N3-C4	-8.82	106.19	110.60
36	1	406	G	O4'-C1'-N9	8.78	115.22	108.20
36	1	2827	U	N3-C4-O4	-8.78	113.25	119.40
36	1	312	C	C6-N1-C2	8.77	123.81	120.30
36	5	504	A	N1-C6-N6	8.75	123.85	118.60
36	5	2372	A	C8-N9-C4	-8.75	102.30	105.80
36	5	2954	U	C2-N1-C1'	8.74	128.18	117.70
36	5	1303	A	C8-N9-C4	8.72	109.29	105.80
36	1	3362	A	C6-C5-N7	-8.72	126.20	132.30
1	2	380	U	N3-C2-O2	-8.72	116.10	122.20
1	2	639	U	N3-C2-O2	-8.71	116.10	122.20
36	5	2354	C	N3-C4-C5	-8.71	118.42	121.90
36	1	2337	C	C6-N1-C2	-8.69	116.82	120.30
38	8	8	C	C6-N1-C2	-8.69	116.82	120.30
36	1	3377	G	C8-N9-C1'	-8.69	115.71	127.00
36	1	699	A	C2-N3-C4	-8.68	106.26	110.60
36	1	2865	U	N3-C4-C5	8.68	119.81	114.60
1	6	163	G	N3-C2-N2	-8.67	113.83	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2308	C	N1-C2-O2	-8.66	113.70	118.90
36	5	1200	A	C4-C5-C6	8.64	121.32	117.00
1	2	1773	C	C6-N1-C2	-8.63	116.85	120.30
36	1	2408	U	O5'-P-OP1	-8.64	97.93	105.70
36	5	1239	C	C5-C6-N1	8.64	125.32	121.00
1	2	1745	G	N3-C4-N9	8.62	131.17	126.00
36	5	1308	A	O5'-P-OP1	-8.62	97.94	105.70
36	5	942	U	N3-C4-O4	8.61	125.43	119.40
1	6	647	G	N3-C4-N9	-8.60	120.84	126.00
36	5	2317	A	O5'-P-OP2	-8.60	97.96	105.70
36	1	1489	A	N1-C6-N6	8.59	123.75	118.60
36	5	2341	A	C8-N9-C4	8.59	109.24	105.80
1	6	1745	G	N3-C4-N9	8.59	131.15	126.00
36	5	1305	U	O5'-P-OP1	-8.58	97.97	105.70
36	1	2572	C	C2-N1-C1'	8.57	128.23	118.80
36	5	437	G	C8-N9-C4	-8.57	102.97	106.40
36	1	1535	A	N1-C6-N6	8.57	123.74	118.60
36	1	2550	U	N3-C2-O2	-8.57	116.20	122.20
36	5	934	G	N3-C4-N9	8.54	131.13	126.00
36	1	3362	A	N1-C6-N6	8.54	123.72	118.60
36	1	2617	U	N1-C2-N3	8.53	120.02	114.90
36	5	3143	C	N1-C2-O2	-8.52	113.79	118.90
36	5	644	G	C4-C5-N7	-8.51	107.39	110.80
36	5	2724	U	C6-N1-C2	-8.50	115.90	121.00
36	1	2283	G	C8-N9-C4	8.49	109.80	106.40
36	5	2680	A	N1-C6-N6	-8.49	113.51	118.60
36	5	1152	G	N3-C2-N2	-8.48	113.96	119.90
36	1	1838	G	C6-C5-N7	-8.48	125.31	130.40
36	5	2288	G	C5-C6-O6	-8.48	123.51	128.60
1	6	1793	G	N1-C6-O6	-8.48	114.81	119.90
37	7	101	G	C5-C6-O6	-8.47	123.52	128.60
36	1	3344	A	C2-N3-C4	-8.47	106.36	110.60
36	1	2996	U	C2-N1-C1'	8.47	127.86	117.70
36	5	424	G	C4-C5-N7	8.45	114.18	110.80
37	7	81	U	N3-C4-O4	-8.44	113.49	119.40
36	1	3362	A	O4'-C1'-N9	8.44	114.95	108.20
36	5	1755	C	C6-N1-C2	8.43	123.67	120.30
1	2	1269	U	C2-N1-C1'	8.42	127.80	117.70
38	8	17	A	N1-C6-N6	8.42	123.65	118.60
36	5	2372	A	P-O3'-C3'	8.41	129.79	119.70
36	1	1409	G	N1-C6-O6	-8.40	114.86	119.90
36	1	1149	G	C5-C6-O6	-8.39	123.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	209	A	N1-C6-N6	8.39	123.64	118.60
1	2	1096	C	C2-N1-C1'	8.39	128.03	118.80
36	5	994	G	O5'-P-OP2	-8.37	98.17	105.70
1	6	408	C	C6-N1-C2	-8.37	116.95	120.30
36	1	3377	G	N9-C4-C5	-8.36	102.06	105.40
36	1	1367	G	C5-C6-O6	-8.35	123.59	128.60
1	6	777	C	C6-N1-C2	-8.33	116.97	120.30
36	1	2714	G	C8-N9-C1'	8.32	137.82	127.00
36	1	3217	C	C2-N1-C1'	8.32	127.95	118.80
1	2	137	U	O5'-P-OP1	-8.32	98.22	105.70
36	1	2868	U	N1-C2-O2	8.31	128.62	122.80
36	1	2836	C	C5-C4-N4	8.31	126.02	120.20
36	5	2290	C	C6-N1-C2	8.31	123.62	120.30
36	1	1192	C	C2-N1-C1'	8.31	127.94	118.80
36	5	36	C	C5-C6-N1	8.31	125.15	121.00
1	2	966	A	N1-C6-N6	8.30	123.58	118.60
36	5	3123	A	C8-N9-C4	8.29	109.12	105.80
36	1	2572	C	N1-C2-O2	8.29	123.87	118.90
36	5	2211	U	N1-C2-N3	8.28	119.87	114.90
36	5	437	G	N3-C4-N9	-8.27	121.04	126.00
36	1	415	G	C2-N3-C4	-8.27	107.77	111.90
36	1	3275	U	C5-C6-N1	8.27	126.83	122.70
73	O7	65	ARG	NE-CZ-NH1	8.27	124.43	120.30
36	1	2357	A	C5-C6-N6	-8.26	117.09	123.70
36	5	2978	U	C5-C6-N1	-8.26	118.57	122.70
44	17	229	PHE	CB-CG-CD1	8.25	126.58	120.80
36	1	636	C	N3-C4-C5	8.24	125.20	121.90
36	5	1148	G	N1-C6-O6	8.24	124.84	119.90
36	1	1148	G	C8-N9-C4	8.23	109.69	106.40
36	1	2355	G	N1-C6-O6	8.23	124.84	119.90
36	1	2434	U	C5-C4-O4	8.23	130.84	125.90
36	5	2572	C	N1-C2-O2	8.23	123.84	118.90
52	M6	78	ARG	NE-CZ-NH1	8.22	124.41	120.30
36	5	3377	G	C5-C6-O6	-8.21	123.67	128.60
36	5	866	A	C8-N9-C4	8.20	109.08	105.80
36	5	2211	U	N3-C2-O2	-8.20	116.46	122.20
36	1	2726	C	C5-C4-N4	8.20	125.94	120.20
36	1	2823	G	C4-C5-N7	-8.18	107.53	110.80
36	5	2278	C	C5-C6-N1	8.17	125.09	121.00
36	1	1279	C	C6-N1-C2	-8.17	117.03	120.30
36	1	2314	U	C5-C6-N1	8.16	126.78	122.70
36	5	2147	A	C5-C6-N6	-8.15	117.18	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	144	U	N3-C2-O2	-8.14	116.50	122.20
36	1	645	A	C6-N1-C2	-8.13	113.72	118.60
36	5	1178	G	C6-C5-N7	-8.13	125.52	130.40
65	n9	23	LYS	C-N-CD	8.12	145.44	128.40
36	5	2964	G	C4-C5-N7	-8.11	107.56	110.80
36	5	938	C	C5-C4-N4	-8.11	114.52	120.20
1	6	265	A	C8-N9-C4	8.11	109.04	105.80
1	6	385	A	N1-C6-N6	-8.09	113.75	118.60
36	1	894	G	N3-C2-N2	-8.07	114.25	119.90
36	1	2201	G	N1-C6-O6	8.07	124.75	119.90
36	1	2603	G	C4-C5-N7	8.07	114.03	110.80
36	5	2639	G	C6-C5-N7	-8.06	125.56	130.40
1	2	1324	G	N3-C4-N9	-8.06	121.16	126.00
36	5	3218	A	C4-C5-N7	8.05	114.73	110.70
36	5	1124	U	N3-C4-C5	8.05	119.43	114.60
36	1	1124	U	N3-C4-C5	8.04	119.43	114.60
36	1	14	U	O5'-P-OP2	-8.04	98.46	105.70
36	5	2273	G	C5-C6-N1	8.04	115.52	111.50
36	5	1443	G	C5-C6-O6	8.03	133.42	128.60
36	1	3362	A	C4-C5-N7	8.01	114.70	110.70
36	5	3309	G	C4-N9-C1'	8.01	136.91	126.50
36	5	2318	U	N1-C2-O2	8.00	128.40	122.80
36	5	1879	A	O5'-P-OP1	8.00	120.30	110.70
1	6	1782	A	C8-N9-C4	-7.99	102.61	105.80
36	5	1148	G	N9-C4-C5	-7.99	102.20	105.40
36	5	2735	U	C6-N1-C2	-7.98	116.21	121.00
36	5	1869	C	C6-N1-C2	7.97	123.49	120.30
36	5	1879	A	N1-C6-N6	7.97	123.38	118.60
36	5	2982	A	C2-N3-C4	7.97	114.58	110.60
1	6	1280	C	N3-C4-C5	-7.95	118.72	121.90
36	5	2917	G	N3-C4-N9	7.95	130.77	126.00
36	1	2169	G	N1-C6-O6	-7.95	115.13	119.90
36	5	1500	G	C8-N9-C4	7.95	109.58	106.40
1	2	453	U	C2-N1-C1'	7.95	127.24	117.70
36	1	988	U	C5-C6-N1	-7.94	118.73	122.70
36	1	1346	G	C2-N3-C4	-7.94	107.93	111.90
36	5	934	G	C2-N3-C4	7.93	115.87	111.90
36	1	716	A	N9-C4-C5	-7.92	102.63	105.80
36	5	437	G	N3-C2-N2	-7.92	114.35	119.90
36	1	2831	G	N1-C6-O6	7.92	124.65	119.90
1	2	647	G	N3-C4-N9	-7.92	121.25	126.00
36	5	1187	C	C6-N1-C2	7.92	123.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2308	C	C2-N3-C4	-7.92	115.94	119.90
1	2	145	A	C8-N9-C4	-7.91	102.63	105.80
36	1	1421	G	O5'-P-OP2	-7.91	98.58	105.70
36	5	1148	G	C8-N9-C4	7.91	109.56	106.40
1	6	777	C	C5-C6-N1	7.89	124.95	121.00
36	1	3362	A	C2-N3-C4	-7.89	106.66	110.60
36	5	1314	C	C2-N1-C1'	7.87	127.46	118.80
36	1	1157	G	C5-C6-O6	7.85	133.31	128.60
36	1	2818	U	O5'-P-OP1	-7.85	98.64	105.70
36	1	1129	A	C8-N9-C4	7.85	108.94	105.80
36	5	1481	A	N7-C8-N9	7.84	117.72	113.80
1	6	1747	G	C8-N9-C4	7.84	109.54	106.40
38	8	99	C	C6-N1-C2	7.84	123.44	120.30
36	5	776	U	C5-C6-N1	-7.84	118.78	122.70
36	5	1178	G	N1-C6-O6	7.83	124.60	119.90
36	5	2358	A	C2-N3-C4	-7.83	106.68	110.60
36	5	2358	A	C8-N9-C4	7.83	108.93	105.80
36	1	878	G	N3-C4-N9	-7.83	121.30	126.00
36	1	2606	G	N3-C4-N9	7.82	130.69	126.00
36	5	3209	A	O4'-C1'-N9	7.82	114.45	108.20
36	1	640	U	N3-C4-O4	7.81	124.87	119.40
1	6	426	G	O5'-P-OP2	-7.81	98.67	105.70
36	5	968	G	C8-N9-C4	7.81	109.53	106.40
36	5	1724	U	N1-C2-O2	-7.81	117.34	122.80
36	5	1306	G	C5-C6-O6	-7.80	123.92	128.60
36	5	3218	A	C6-C5-N7	-7.80	126.84	132.30
36	1	3344	A	O4'-C1'-N9	7.80	114.44	108.20
1	6	858	G	C4-C5-N7	7.79	113.92	110.80
36	5	1110	U	N1-C2-O2	7.79	128.25	122.80
1	6	1537	C	N3-C4-C5	-7.79	118.78	121.90
36	1	2197	C	C6-N1-C2	7.79	123.42	120.30
36	5	804	C	N3-C4-C5	-7.78	118.79	121.90
36	1	793	C	N1-C2-O2	-7.77	114.24	118.90
36	1	2714	G	C4-N9-C1'	-7.77	116.41	126.50
36	5	3214	U	C5-C4-O4	7.76	130.56	125.90
36	1	1495	U	C2-N3-C4	-7.75	122.35	127.00
36	1	800	G	N3-C2-N2	-7.75	114.47	119.90
1	6	542	A	O4'-C1'-N9	7.75	114.40	108.20
36	1	716	A	C4-C5-N7	7.75	114.57	110.70
1	6	194	U	C2-N1-C1'	7.75	127.00	117.70
36	1	660	A	N1-C6-N6	-7.75	113.95	118.60
36	1	1308	A	C8-N9-C4	-7.75	102.70	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	55	U	C6-N1-C2	-7.75	116.35	121.00
36	1	86	G	N9-C4-C5	7.74	108.50	105.40
36	1	409	A	O5'-P-OP2	-7.73	98.74	105.70
38	8	55	U	N1-C2-N3	7.73	119.54	114.90
36	5	2963	C	C6-N1-C2	7.72	123.39	120.30
1	6	1305	U	N1-C2-O2	-7.71	117.40	122.80
36	5	1513	G	C8-N9-C4	-7.71	103.32	106.40
1	2	1324	G	N9-C4-C5	7.71	108.48	105.40
36	5	38	U	O5'-P-OP2	-7.69	98.78	105.70
36	5	3326	G	C8-N9-C4	7.68	109.47	106.40
1	6	1537	C	N1-C2-O2	-7.67	114.30	118.90
36	5	1481	A	P-O3'-C3'	7.67	128.91	119.70
36	1	371	G	C5-C6-O6	-7.67	124.00	128.60
36	5	2622	C	N3-C4-C5	-7.67	118.83	121.90
37	7	92	A	N9-C4-C5	-7.66	102.73	105.80
36	5	2195	C	O5'-P-OP2	-7.66	98.81	105.70
1	2	453	U	N1-C2-O2	7.66	128.16	122.80
36	5	3218	A	C5-N7-C8	-7.66	100.07	103.90
36	1	1305	U	N1-C2-O2	7.65	128.16	122.80
1	2	314	C	O5'-P-OP1	-7.65	98.81	105.70
36	1	2983	C	C4-C5-C6	7.65	121.22	117.40
36	5	1158	A	N1-C6-N6	7.65	123.19	118.60
36	5	1902	G	C5-C6-O6	-7.64	124.01	128.60
10	s8	29	LEU	CA-CB-CG	7.63	132.86	115.30
36	1	1365	G	N3-C4-N9	7.62	130.57	126.00
1	6	1022	C	C6-N1-C2	7.62	123.35	120.30
1	6	163	G	N9-C4-C5	7.61	108.45	105.40
36	5	2726	C	N3-C2-O2	-7.61	116.57	121.90
36	1	1841	A	O5'-P-OP1	-7.61	98.85	105.70
1	6	976	G	C4-C5-N7	7.61	113.84	110.80
36	1	1389	G	N3-C4-N9	7.61	130.56	126.00
36	1	2644	C	C6-N1-C2	-7.60	117.26	120.30
36	5	657	A	N1-C6-N6	-7.60	114.04	118.60
36	1	76	G	C8-N9-C4	-7.60	103.36	106.40
36	5	1437	C	C6-N1-C2	-7.60	117.26	120.30
36	1	1902	G	C6-C5-N7	-7.59	125.84	130.40
36	5	3369	G	C2-N3-C4	7.58	115.69	111.90
36	5	1239	C	C6-N1-C2	-7.58	117.27	120.30
38	8	96	A	C8-N9-C4	7.58	108.83	105.80
1	6	1025	A	N1-C2-N3	7.58	133.09	129.30
36	1	2868	U	N3-C2-O2	-7.57	116.90	122.20
36	1	610	G	C5-C6-N1	7.57	115.29	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	780	A	N1-C6-N6	-7.57	114.06	118.60
36	1	637	C	C5-C6-N1	-7.56	117.22	121.00
36	5	705	A	O5'-P-OP2	-7.56	98.89	105.70
36	5	922	U	C2-N3-C4	-7.56	122.46	127.00
36	5	2147	A	C6-C5-N7	-7.56	127.01	132.30
36	5	404	G	O5'-P-OP2	-7.55	98.91	105.70
12	C0	88	PRO	N-CA-CB	7.55	112.36	103.30
36	5	2639	G	C8-N9-C4	-7.55	103.38	106.40
1	2	1280	C	C6-N1-C2	-7.55	117.28	120.30
36	1	1495	U	N1-C2-O2	-7.54	117.52	122.80
1	6	858	G	O4'-C1'-N9	7.54	114.23	108.20
36	1	1308	A	O5'-P-OP1	7.54	119.75	110.70
1	6	1749	A	C2-N3-C4	-7.54	106.83	110.60
36	5	2808	A	C2-N3-C4	-7.54	106.83	110.60
1	2	7	G	N1-C6-O6	-7.53	115.38	119.90
36	1	392	G	C8-N9-C4	7.53	109.41	106.40
1	6	1773	C	N3-C4-N4	7.53	123.27	118.00
36	5	2965	U	N1-C2-O2	-7.53	117.53	122.80
36	1	2944	U	N1-C2-O2	7.53	128.07	122.80
36	1	2121	G	N1-C6-O6	-7.52	115.39	119.90
36	1	142	C	C6-N1-C2	-7.51	117.29	120.30
36	5	2704	A	O5'-P-OP1	-7.51	98.94	105.70
36	5	3154	C	C2-N1-C1'	7.51	127.06	118.80
36	1	2726	C	N1-C2-N3	7.51	124.45	119.20
1	6	421	A	N1-C6-N6	7.50	123.10	118.60
1	6	1097	U	P-O3'-C3'	7.50	128.70	119.70
38	4	94	C	N3-C4-C5	7.50	124.90	121.90
36	1	49	A	N1-C6-N6	7.50	123.10	118.60
36	1	2636	A	C8-N9-C4	-7.50	102.80	105.80
36	1	1445	U	C2-N1-C1'	-7.49	108.71	117.70
36	5	1321	G	C5-C6-O6	-7.49	124.10	128.60
36	1	3183	A	N1-C6-N6	7.49	123.09	118.60
37	7	101	G	C6-C5-N7	-7.49	125.91	130.40
36	5	2639	G	C5-C6-O6	-7.49	124.11	128.60
36	5	1434	G	N1-C6-O6	7.49	124.39	119.90
36	1	2644	C	N3-C2-O2	-7.48	116.66	121.90
1	2	1490	C	C6-N1-C2	-7.47	117.31	120.30
36	1	2662	G	C2-N3-C4	-7.47	108.16	111.90
36	1	3277	U	N3-C2-O2	-7.47	116.97	122.20
1	6	106	U	C5-C4-O4	7.46	130.38	125.90
1	6	453	U	C2-N1-C1'	7.46	126.65	117.70
36	1	2637	A	O5'-P-OP1	-7.46	98.99	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	558	U	N3-C2-O2	-7.46	116.98	122.20
36	1	730	C	C6-N1-C2	7.46	123.28	120.30
36	1	921	A	C8-N9-C4	-7.46	102.82	105.80
36	1	1902	G	C4-C5-N7	7.46	113.78	110.80
36	1	1303	A	C5-C6-N6	-7.45	117.74	123.70
36	5	2293	C	N3-C4-C5	7.45	124.88	121.90
36	1	645	A	N1-C6-N6	-7.45	114.13	118.60
36	1	961	C	C4-C5-C6	7.44	121.12	117.40
36	5	776	U	C4-C5-C6	7.44	124.16	119.70
1	2	558	U	N1-C2-O2	7.43	128.00	122.80
1	2	1280	C	N3-C4-N4	7.43	123.20	118.00
36	5	2211	U	C5-C6-N1	-7.42	118.99	122.70
36	1	501	A	C8-N9-C4	7.42	108.77	105.80
36	1	776	U	N1-C2-N3	7.42	119.35	114.90
36	1	2719	U	C2-N1-C1'	-7.41	108.80	117.70
36	1	3326	G	C8-N9-C4	7.41	109.36	106.40
1	2	1291	G	N3-C4-N9	-7.41	121.56	126.00
36	1	433	A	N1-C6-N6	7.40	123.04	118.60
36	1	2384	A	C5-C6-N6	-7.40	117.78	123.70
36	5	646	A	N1-C2-N3	7.40	133.00	129.30
36	5	2385	G	N3-C4-N9	-7.40	121.56	126.00
36	1	901	G	C5-C6-O6	-7.40	124.16	128.60
36	1	2314	U	C5-C4-O4	-7.39	121.47	125.90
36	1	1308	A	N7-C8-N9	7.38	117.49	113.80
36	1	2977	G	O5'-P-OP1	-7.38	99.06	105.70
36	1	2283	G	C5-C6-O6	-7.38	124.17	128.60
36	1	3217	C	N1-C2-O2	7.38	123.33	118.90
1	2	380	U	N1-C2-O2	7.38	127.96	122.80
36	5	2353	G	N1-C6-O6	7.38	124.33	119.90
36	1	3057	U	N1-C2-N3	7.37	119.32	114.90
36	5	1314	C	C6-N1-C1'	-7.37	111.95	120.80
36	1	921	A	N9-C4-C5	7.37	108.75	105.80
36	1	1466	G	N9-C4-C5	-7.36	102.45	105.40
36	5	2199	G	N3-C2-N2	-7.36	114.75	119.90
1	2	1456	C	N3-C2-O2	-7.36	116.75	121.90
36	5	1438	U	N3-C2-O2	-7.36	117.05	122.20
36	1	2982	A	O5'-P-OP1	-7.35	99.08	105.70
36	1	2625	C	N1-C2-O2	-7.35	114.49	118.90
36	1	716	A	C5-C6-N6	-7.34	117.83	123.70
36	1	1161	G	N1-C6-O6	-7.33	115.50	119.90
56	NO	155	ARG	NE-CZ-NH1	-7.33	116.63	120.30
36	1	2169	G	C4-C5-N7	-7.33	107.87	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1192	C	N3-C2-O2	-7.33	116.77	121.90
36	5	2964	G	N1-C6-O6	-7.32	115.50	119.90
31	D9	36	LEU	CA-CB-CG	7.32	132.14	115.30
36	5	3362	A	C2-N3-C4	-7.32	106.94	110.60
36	1	2606	G	C6-C5-N7	-7.32	126.01	130.40
36	5	2245	C	C6-N1-C2	-7.32	117.37	120.30
36	5	1848	G	C4-C5-N7	7.32	113.73	110.80
36	1	1433	A	C5-C6-N1	7.31	121.36	117.70
36	5	2675	C	C6-N1-C2	-7.31	117.37	120.30
36	1	672	A	N1-C6-N6	7.31	122.99	118.60
1	6	1091	A	N1-C6-N6	7.31	122.99	118.60
36	5	1010	G	O5'-P-OP2	-7.31	99.12	105.70
1	2	1096	C	C5-C6-N1	7.31	124.66	121.00
37	7	49	G	C4-C5-C6	7.31	123.19	118.80
36	1	417	A	N1-C6-N6	7.30	122.98	118.60
36	1	2884	C	N3-C4-C5	7.30	124.82	121.90
1	2	554	C	C2-N1-C1'	7.30	126.83	118.80
36	1	3081	C	C5-C6-N1	-7.30	117.35	121.00
37	7	85	G	N1-C6-O6	-7.30	115.52	119.90
36	5	2887	A	N1-C6-N6	7.30	122.98	118.60
36	1	3217	C	C6-N1-C1'	-7.29	112.05	120.80
10	S8	29	LEU	CA-CB-CG	7.29	132.07	115.30
36	5	2278	C	C4-C5-C6	-7.29	113.75	117.40
36	5	1200	A	N1-C6-N6	7.29	122.97	118.60
36	5	2234	G	C8-N9-C4	7.29	109.31	106.40
1	6	539	G	N3-C4-N9	-7.28	121.63	126.00
36	5	2572	C	C2-N1-C1'	7.28	126.81	118.80
36	1	347	G	C4-C5-N7	7.28	113.71	110.80
36	5	1445	U	C2-N3-C4	-7.28	122.63	127.00
36	5	2147	A	C4-C5-N7	7.28	114.34	110.70
1	6	1540	G	N1-C6-O6	-7.28	115.53	119.90
37	7	49	G	N1-C6-O6	7.28	124.27	119.90
36	1	972	A	C8-N9-C4	7.27	108.71	105.80
36	1	1658	G	N1-C6-O6	-7.27	115.54	119.90
36	1	608	A	N9-C4-C5	-7.27	102.89	105.80
1	6	265	A	N9-C4-C5	-7.27	102.89	105.80
36	1	3269	U	N3-C2-O2	-7.26	117.12	122.20
36	1	232	G	N3-C4-C5	-7.26	124.97	128.60
38	4	113	U	C5-C4-O4	7.26	130.25	125.90
36	1	49	A	C2-N3-C4	-7.25	106.97	110.60
36	5	1497	C	O5'-P-OP1	-7.25	99.17	105.70
36	5	209	A	C5-C6-N6	-7.25	117.90	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	65	A	P-O3'-C3'	7.25	128.40	119.70
36	1	942	U	C4-C5-C6	7.25	124.05	119.70
36	5	2943	G	C6-C5-N7	-7.25	126.05	130.40
36	1	2942	C	N3-C4-C5	7.25	124.80	121.90
36	1	3212	C	C6-N1-C2	7.25	123.20	120.30
1	2	728	U	C2-N1-C1'	7.25	126.39	117.70
36	1	1360	C	C6-N1-C2	7.24	123.20	120.30
36	1	1182	A	C8-N9-C4	7.23	108.69	105.80
36	5	2735	U	C5-C6-N1	7.23	126.31	122.70
36	5	2916	U	O5'-P-OP1	-7.22	99.20	105.70
1	2	1119	G	N3-C2-N2	7.22	124.95	119.90
36	1	432	G	C5-C6-N1	-7.21	107.89	111.50
1	2	1651	A	C2-N3-C4	-7.21	107.00	110.60
36	5	1730	G	C8-N9-C4	7.21	109.28	106.40
36	1	3362	A	C8-N9-C4	-7.21	102.92	105.80
1	2	300	A	O5'-P-OP1	-7.21	99.22	105.70
36	5	2730	G	C5-C6-O6	-7.21	124.28	128.60
1	2	1119	G	N1-C2-N2	-7.20	109.72	116.20
1	6	387	A	C2-N3-C4	7.20	114.20	110.60
1	6	696	C	O4'-C1'-N1	7.20	113.96	108.20
36	1	1658	G	N9-C4-C5	7.20	108.28	105.40
1	6	65	A	C5-C6-N1	-7.19	114.11	117.70
36	1	576	C	C6-N1-C2	7.19	123.18	120.30
36	1	197	G	C5-C6-O6	-7.18	124.29	128.60
36	1	1909	A	N1-C6-N6	7.18	122.91	118.60
1	2	354	C	C6-N1-C2	-7.18	117.43	120.30
36	1	1210	U	C5-C6-N1	-7.17	119.11	122.70
38	4	113	U	N1-C2-N3	7.17	119.20	114.90
36	1	878	G	N3-C2-N2	-7.16	114.89	119.90
36	1	885	U	C5-C6-N1	-7.16	119.12	122.70
1	6	65	A	N1-C6-N6	7.15	122.89	118.60
36	5	3018	C	O5'-P-OP2	-7.15	99.26	105.70
36	1	1433	A	C2-N3-C4	7.15	114.17	110.60
59	n3	48	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	6	1700	C	C2-N1-C1'	7.15	126.66	118.80
36	5	1449	A	N1-C6-N6	7.15	122.89	118.60
36	1	2417	U	N1-C2-O2	-7.14	117.80	122.80
36	5	644	G	C5-C6-O6	7.14	132.89	128.60
1	6	1731	A	N1-C6-N6	-7.14	114.32	118.60
36	5	658	G	C8-N9-C4	-7.14	103.54	106.40
36	5	2743	A	C8-N9-C4	7.14	108.66	105.80
36	1	2397	A	O5'-P-OP2	-7.14	99.28	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	356	C	O5'-P-OP2	-7.14	99.28	105.70
36	1	969	C	N1-C2-O2	-7.14	114.62	118.90
36	1	1838	G	C4-C5-N7	7.13	113.65	110.80
36	5	1116	G	N9-C4-C5	7.13	108.25	105.40
1	6	813	U	C2-N1-C1'	7.13	126.26	117.70
36	5	2921	U	N3-C4-O4	7.13	124.39	119.40
36	1	650	C	N1-C2-O2	-7.13	114.62	118.90
36	5	394	G	C5-C6-O6	7.13	132.88	128.60
36	1	415	G	N3-C4-C5	7.12	132.16	128.60
36	5	1302	A	N1-C6-N6	-7.12	114.33	118.60
36	5	2858	U	C6-N1-C2	-7.12	116.73	121.00
1	6	609	U	N3-C4-O4	-7.12	114.42	119.40
36	5	580	C	C6-N1-C2	-7.12	117.45	120.30
36	5	2954	U	C6-N1-C1'	-7.12	111.23	121.20
36	1	2725	U	N3-C2-O2	-7.12	117.22	122.20
36	1	2351	U	N3-C2-O2	-7.11	117.22	122.20
36	1	608	A	C6-C5-N7	-7.11	127.32	132.30
36	1	960	U	C6-N1-C2	7.11	125.27	121.00
36	1	1911	A	N1-C6-N6	7.11	122.86	118.60
36	5	1315	U	N1-C2-N3	-7.11	110.64	114.90
1	6	610	G	C8-N9-C1'	-7.11	117.76	127.00
1	6	622	A	O5'-P-OP1	-7.11	99.31	105.70
36	5	1116	G	N3-C4-C5	-7.10	125.05	128.60
1	2	558	U	C2-N1-C1'	7.10	126.22	117.70
36	5	283	G	N9-C4-C5	-7.10	102.56	105.40
36	5	966	U	O5'-P-OP2	-7.10	99.31	105.70
36	5	1869	C	N3-C4-C5	7.10	124.74	121.90
36	5	2616	C	C5-C4-N4	-7.10	115.23	120.20
36	5	3154	C	N1-C2-O2	7.10	123.16	118.90
36	1	332	C	C5-C6-N1	-7.10	117.45	121.00
36	1	2737	C	N1-C2-O2	-7.09	114.64	118.90
36	5	1724	U	N1-C2-N3	7.09	119.16	114.90
36	1	2978	U	O4'-C1'-N1	7.09	113.87	108.20
36	1	2121	G	N3-C2-N2	7.09	124.86	119.90
36	1	1381	A	O5'-P-OP1	-7.09	99.32	105.70
36	5	2318	U	N3-C4-O4	-7.09	114.44	119.40
36	5	927	C	O5'-P-OP1	-7.08	99.32	105.70
36	1	371	G	C4-C5-N7	7.08	113.63	110.80
36	1	1156	C	C5-C6-N1	-7.08	117.46	121.00
1	6	1764	C	C6-N1-C2	7.08	123.13	120.30
36	5	1902	G	C4-C5-C6	7.08	123.05	118.80
36	1	2572	C	C6-N1-C2	-7.08	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2714	G	C4-C5-C6	-7.08	114.55	118.80
36	5	2416	U	C6-N1-C2	-7.08	116.75	121.00
1	6	582	U	N3-C2-O2	-7.08	117.25	122.20
36	1	609	G	O5'-P-OP2	-7.07	99.33	105.70
1	6	337	G	C6-C5-N7	-7.07	126.16	130.40
36	5	1149	G	N1-C6-O6	7.07	124.14	119.90
36	5	2136	C	C5-C6-N1	-7.07	117.46	121.00
36	1	281	G	C5-C6-O6	-7.07	124.36	128.60
36	1	392	G	N9-C4-C5	-7.07	102.57	105.40
1	6	1361	U	C2-N1-C1'	7.07	126.18	117.70
36	1	1192	C	N3-C2-O2	-7.07	116.95	121.90
36	1	2273	G	N7-C8-N9	-7.07	109.57	113.10
36	5	1006	A	O5'-P-OP2	-7.07	99.34	105.70
36	1	2117	A	N1-C6-N6	-7.07	114.36	118.60
38	4	30	C	O5'-P-OP1	-7.07	99.34	105.70
36	5	609	G	N1-C6-O6	7.07	124.14	119.90
36	5	834	U	C6-N1-C2	7.06	125.24	121.00
36	1	901	G	N1-C6-O6	7.06	124.14	119.90
36	1	1795	U	O5'-P-OP1	-7.06	99.34	105.70
1	2	553	G	C6-C5-N7	-7.06	126.16	130.40
36	5	3108	G	N1-C6-O6	7.06	124.13	119.90
36	5	1192	C	N1-C2-O2	7.06	123.13	118.90
36	5	2887	A	C5-C6-N6	-7.05	118.06	123.70
36	5	2434	U	C5-C4-O4	7.05	130.13	125.90
36	1	994	G	C5-C6-N1	7.05	115.03	111.50
36	5	535	G	O5'-P-OP2	-7.05	99.36	105.70
36	5	1130	A	C8-N9-C4	7.05	108.62	105.80
1	2	393	C	C6-N1-C2	7.05	123.12	120.30
1	2	1455	G	C5-C6-N1	-7.05	107.98	111.50
1	6	453	U	N3-C2-O2	-7.05	117.27	122.20
36	5	283	G	C5-N7-C8	-7.05	100.78	104.30
36	1	1144	U	N3-C4-O4	-7.04	114.47	119.40
1	2	1745	G	C5-C6-N1	7.03	115.02	111.50
36	5	934	G	C8-N9-C1'	-7.03	117.87	127.00
36	5	942	U	N3-C2-O2	7.03	127.12	122.20
36	1	2298	U	N3-C4-O4	-7.02	114.48	119.40
1	6	337	G	C4-N9-C1'	7.02	135.63	126.50
36	5	2617	U	N1-C2-O2	-7.02	117.89	122.80
36	1	2982	A	C6-N1-C2	-7.02	114.39	118.60
36	5	2354	C	N3-C2-O2	7.01	126.81	121.90
1	6	112	A	N1-C6-N6	7.01	122.81	118.60
1	6	390	G	O5'-P-OP2	-7.01	99.39	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2327	U	C5-C6-N1	-7.01	119.19	122.70
1	6	1700	C	N1-C2-O2	7.01	123.11	118.90
36	5	1389	G	C6-C5-N7	-7.01	126.20	130.40
36	5	2199	G	C4-C5-C6	7.01	123.00	118.80
36	1	1902	G	C5-C6-O6	-7.00	124.40	128.60
38	4	103	G	N3-C4-C5	-7.00	125.10	128.60
1	6	647	G	N3-C4-C5	7.00	132.10	128.60
36	5	699	A	C2-N3-C4	-7.00	107.10	110.60
36	5	922	U	C4-C5-C6	7.00	123.90	119.70
36	5	2961	G	C8-N9-C4	-7.00	103.60	106.40
36	1	2169	G	C6-C5-N7	7.00	134.60	130.40
36	5	2621	G	N1-C6-O6	7.00	124.10	119.90
36	1	2983	C	N3-C4-N4	-6.99	113.11	118.00
36	1	3049	A	C8-N9-C4	6.99	108.60	105.80
36	1	2823	G	N3-C2-N2	-6.99	115.01	119.90
36	1	2114	C	O5'-P-OP2	-6.99	99.41	105.70
36	5	2838	A	O5'-P-OP1	6.99	119.08	110.70
36	1	2601	A	C8-N9-C4	6.99	108.59	105.80
36	1	2719	U	N1-C2-O2	-6.99	117.91	122.80
36	5	424	G	C5-C6-N1	6.99	114.99	111.50
36	5	1868	G	N9-C4-C5	-6.99	102.61	105.40
36	1	919	U	O5'-P-OP1	6.98	119.08	110.70
36	1	699	A	N1-C2-N3	6.98	132.79	129.30
36	5	1902	G	C8-N9-C1'	-6.98	117.93	127.00
36	1	895	A	C2-N3-C4	-6.97	107.11	110.60
36	1	2993	G	N9-C4-C5	-6.97	102.61	105.40
36	1	197	G	N9-C4-C5	-6.97	102.61	105.40
36	1	2384	A	N1-C6-N6	6.97	122.78	118.60
36	1	25	U	N3-C4-C5	-6.97	110.42	114.60
36	5	2953	U	C5-C4-O4	-6.97	121.72	125.90
36	1	941	G	C5-C6-O6	-6.97	124.42	128.60
36	5	1416	C	N3-C2-O2	-6.97	117.02	121.90
36	5	1433	A	N1-C6-N6	-6.97	114.42	118.60
36	1	939	U	O5'-P-OP1	6.96	119.06	110.70
36	1	1202	A	C2-N3-C4	-6.96	107.12	110.60
36	5	701	G	C4-C5-N7	-6.96	108.01	110.80
36	5	2248	C	N1-C2-O2	-6.96	114.72	118.90
36	5	2358	A	N3-C4-C5	6.96	131.67	126.80
38	8	95	G	N3-C4-C5	6.96	132.08	128.60
1	2	1761	U	P-O3'-C3'	6.96	128.05	119.70
36	1	1431	G	N1-C6-O6	-6.96	115.73	119.90
36	5	1208	U	N3-C4-O4	-6.96	114.53	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2870	C	C6-N1-C1'	6.95	129.15	120.80
36	1	1346	G	O5'-P-OP2	-6.95	99.45	105.70
1	2	73	U	O4'-C1'-N1	6.95	113.76	108.20
36	5	66	A	N1-C6-N6	6.95	122.77	118.60
36	5	3215	A	C2-N3-C4	-6.95	107.13	110.60
36	5	1113	G	C2-N3-C4	-6.94	108.43	111.90
36	5	2634	U	C2-N3-C4	-6.94	122.84	127.00
36	1	1158	A	C6-N1-C2	-6.93	114.44	118.60
36	1	2403	G	O5'-P-OP2	-6.93	99.46	105.70
1	6	251	A	C8-N9-C4	6.93	108.57	105.80
36	5	1307	G	OP2-P-O3'	6.93	120.45	105.20
36	1	197	G	C6-C5-N7	-6.93	126.24	130.40
36	1	2889	C	N3-C2-O2	-6.93	117.05	121.90
36	1	3199	G	C6-C5-N7	6.93	134.56	130.40
36	5	2620	G	C6-C5-N7	6.93	134.56	130.40
36	5	847	A	C8-N9-C4	6.93	108.57	105.80
36	1	197	G	C4-C5-N7	6.93	113.57	110.80
36	5	2308	C	N1-C2-O2	-6.92	114.75	118.90
37	7	29	C	C6-N1-C2	6.92	123.07	120.30
36	1	282	G	C8-N9-C4	-6.92	103.63	106.40
36	1	2846	U	N1-C2-O2	6.92	127.64	122.80
36	1	2643	A	C8-N9-C4	6.92	108.57	105.80
1	6	1028	C	C5-C6-N1	-6.92	117.54	121.00
36	5	3309	G	N3-C4-C5	-6.92	125.14	128.60
36	5	2917	G	N1-C6-O6	6.92	124.05	119.90
36	5	2411	U	N3-C4-C5	6.91	118.75	114.60
1	6	1146	G	N1-C6-O6	6.91	124.05	119.90
1	6	609	U	C5-C4-O4	6.91	130.04	125.90
36	5	2992	U	C5-C4-O4	-6.91	121.76	125.90
1	2	1768	G	C6-C5-N7	6.90	134.54	130.40
36	5	712	G	O5'-P-OP2	-6.90	99.49	105.70
36	5	2618	G	C5-C6-O6	-6.90	124.46	128.60
36	5	3245	A	N1-C2-N3	6.90	132.75	129.30
36	5	1055	A	O5'-P-OP2	-6.90	99.49	105.70
36	1	3028	G	N3-C4-N9	6.90	130.14	126.00
36	1	1344	G	C8-N9-C4	6.89	109.16	106.40
1	2	1269	U	N3-C4-O4	6.89	124.22	119.40
36	1	2983	C	C5-C4-N4	6.89	125.02	120.20
36	1	1292	C	C6-N1-C2	6.89	123.06	120.30
1	6	1793	G	C4-C5-N7	-6.89	108.04	110.80
36	5	994	G	C5-C6-N1	6.89	114.94	111.50
36	1	2664	C	C6-N1-C2	-6.89	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1370	G	N3-C4-C5	-6.89	125.16	128.60
36	1	640	U	C5-C4-O4	-6.88	121.77	125.90
37	7	91	G	N9-C4-C5	-6.88	102.65	105.40
36	1	2394	G	N1-C6-O6	-6.88	115.77	119.90
36	5	1188	U	C5-C6-N1	-6.88	119.26	122.70
36	5	2816	G	C8-N9-C4	6.88	109.15	106.40
36	1	2572	C	N3-C2-O2	-6.88	117.09	121.90
1	6	976	G	C6-C5-N7	-6.88	126.27	130.40
36	1	369	A	C2-N3-C4	6.87	114.04	110.60
36	1	114	A	O5'-P-OP1	-6.87	99.52	105.70
36	5	1939	G	C4-N9-C1'	6.87	135.43	126.50
36	1	696	C	C6-N1-C2	6.87	123.05	120.30
36	1	3377	G	C6-C5-N7	-6.87	126.28	130.40
36	5	1902	G	C4-N9-C1'	6.87	135.43	126.50
36	1	85	A	C2-N3-C4	-6.87	107.17	110.60
36	1	776	U	C5-C4-O4	6.87	130.02	125.90
36	5	3022	G	C8-N9-C4	6.87	109.15	106.40
36	1	2339	C	OP1-P-O3'	6.86	120.30	105.20
36	1	3344	A	N7-C8-N9	6.86	117.23	113.80
36	1	1316	C	N1-C2-O2	-6.86	114.78	118.90
36	5	2639	G	N7-C8-N9	6.86	116.53	113.10
36	5	3164	C	O4'-C1'-N1	6.86	113.69	108.20
1	2	1768	G	N3-C4-N9	-6.86	121.89	126.00
36	5	2830	G	C6-N1-C2	-6.86	120.99	125.10
36	1	699	A	O5'-P-OP2	-6.85	99.53	105.70
1	6	976	G	C5-N7-C8	-6.85	100.87	104.30
36	5	2353	G	C6-C5-N7	-6.85	126.29	130.40
36	1	1901	A	N1-C6-N6	-6.85	114.49	118.60
36	5	2970	C	N3-C4-C5	-6.85	119.16	121.90
1	6	163	G	C8-N9-C1'	6.85	135.90	127.00
36	5	425	G	C2-N3-C4	-6.85	108.48	111.90
36	1	2629	U	O5'-P-OP2	-6.84	99.54	105.70
1	6	1773	C	C6-N1-C2	-6.84	117.56	120.30
36	5	2954	U	O4'-C1'-N1	6.84	113.67	108.20
36	1	2836	C	N3-C4-N4	-6.84	113.21	118.00
36	1	1149	G	N3-C2-N2	-6.84	115.11	119.90
1	6	558	U	C2-N1-C1'	6.84	125.91	117.70
36	1	54	C	O5'-P-OP1	-6.84	99.55	105.70
1	6	1198	G	C6-C5-N7	6.83	134.50	130.40
36	5	2391	G	O5'-P-OP2	6.83	118.90	110.70
1	2	1324	G	N3-C2-N2	-6.83	115.12	119.90
1	6	624	G	C8-N9-C4	6.83	109.13	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1439	C	C5-C6-N1	6.83	124.42	121.00
36	1	1118	C	C6-N1-C2	-6.83	117.57	120.30
1	6	902	G	N1-C6-O6	6.83	124.00	119.90
36	5	21	G	C2-N3-C4	-6.83	108.48	111.90
36	5	2724	U	N1-C2-N3	6.83	119.00	114.90
36	5	2630	C	N1-C2-O2	-6.82	114.81	118.90
36	5	1155	C	O5'-P-OP1	-6.82	99.56	105.70
36	5	386	A	N1-C6-N6	6.82	122.69	118.60
36	5	1124	U	C4-C5-C6	-6.82	115.61	119.70
36	1	109	A	OP1-P-O3'	6.82	120.19	105.20
36	1	416	A	C8-N9-C4	6.82	108.53	105.80
36	1	25	U	N3-C4-O4	6.81	124.17	119.40
1	2	1611	A	N1-C2-N3	6.81	132.71	129.30
36	1	369	A	C8-N9-C4	-6.81	103.08	105.80
1	6	609	U	C5-C6-N1	-6.81	119.29	122.70
36	5	1789	G	C4-N9-C1'	-6.81	117.64	126.50
36	5	313	A	N1-C6-N6	6.80	122.68	118.60
36	1	213	A	N1-C6-N6	6.80	122.68	118.60
36	5	2870	C	C2-N1-C1'	-6.80	111.32	118.80
36	1	1156	C	C4-C5-C6	6.79	120.80	117.40
47	m0	57	LEU	CA-CB-CG	6.79	130.92	115.30
1	6	982	U	O5'-P-OP1	-6.79	99.59	105.70
36	5	966	U	N1-C2-O2	6.79	127.55	122.80
36	1	332	C	C6-N1-C2	6.79	123.01	120.30
36	5	3133	C	N3-C4-C5	-6.79	119.19	121.90
36	1	218	G	O5'-P-OP1	-6.78	99.60	105.70
35	SM	167	PRO	N-CA-CB	6.78	111.43	103.30
36	1	802	C	C4-C5-C6	6.78	120.79	117.40
35	sM	167	PRO	N-CA-CB	6.77	111.43	103.30
36	5	3120	C	N3-C2-O2	-6.77	117.16	121.90
1	2	507	U	C2-N1-C1'	6.77	125.83	117.70
36	5	3214	U	N3-C2-O2	-6.77	117.46	122.20
1	2	831	U	C2-N1-C1'	6.77	125.82	117.70
47	M0	57	LEU	CA-CB-CG	6.77	130.87	115.30
36	5	1897	G	N7-C8-N9	6.77	116.48	113.10
36	5	2197	C	C6-N1-C2	6.77	123.01	120.30
36	5	2964	G	C5-C6-O6	6.77	132.66	128.60
36	5	3335	A	C2-N3-C4	-6.77	107.22	110.60
1	6	1269	U	C6-N1-C2	-6.77	116.94	121.00
36	5	2971	A	C2-N3-C4	6.77	113.98	110.60
36	1	2714	G	C5-N7-C8	-6.76	100.92	104.30
1	2	334	G	C4-N9-C1'	-6.76	117.71	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	881	C	C6-N1-C2	-6.76	117.59	120.30
36	5	3200	G	N1-C6-O6	6.76	123.96	119.90
36	1	1203	A	C8-N9-C4	6.76	108.50	105.80
36	5	437	G	N1-C2-N2	6.76	122.28	116.20
36	1	942	U	N3-C4-O4	6.76	124.13	119.40
36	1	2212	C	C6-N1-C2	6.75	123.00	120.30
36	5	1500	G	N7-C8-N9	-6.75	109.72	113.10
36	5	2572	C	N3-C2-O2	-6.75	117.17	121.90
36	1	1307	G	P-O3'-C3'	6.75	127.80	119.70
36	5	1936	A	N1-C6-N6	6.75	122.65	118.60
36	1	324	A	C4-C5-C6	6.75	120.37	117.00
36	1	919	U	O5'-P-OP2	-6.75	99.63	105.70
36	1	2357	A	N1-C6-N6	6.75	122.65	118.60
36	5	1112	A	C5-C6-N6	-6.74	118.31	123.70
36	1	859	G	N9-C4-C5	-6.74	102.70	105.40
36	5	234	G	N1-C6-O6	6.74	123.94	119.90
36	1	1322	U	O5'-P-OP2	-6.74	99.64	105.70
1	6	425	A	N1-C6-N6	-6.74	114.56	118.60
1	2	1196	A	P-O3'-C3'	6.73	127.78	119.70
36	1	2617	U	C5-C6-N1	-6.73	119.33	122.70
36	1	969	C	N3-C4-C5	6.73	124.59	121.90
36	5	718	G	O4'-C1'-N9	6.73	113.58	108.20
36	5	2253	G	O5'-P-OP2	-6.73	99.65	105.70
36	5	2406	C	N1-C2-O2	-6.73	114.86	118.90
36	5	3092	C	C2-N3-C4	-6.73	116.54	119.90
36	5	776	U	C5-C4-O4	6.72	129.93	125.90
36	5	3309	G	C8-N9-C1'	-6.72	118.26	127.00
1	6	421	A	C8-N9-C4	6.72	108.49	105.80
36	5	1595	U	N1-C2-O2	-6.72	118.10	122.80
36	1	1389	G	N9-C4-C5	-6.72	102.71	105.40
36	5	1661	G	N1-C6-O6	6.72	123.93	119.90
36	1	915	A	N1-C6-N6	-6.71	114.57	118.60
36	1	969	C	C2-N1-C1'	-6.71	111.41	118.80
36	1	2647	A	C6-N1-C2	-6.71	114.57	118.60
36	1	859	G	C6-C5-N7	-6.71	126.38	130.40
36	1	1154	A	O5'-P-OP1	-6.71	99.66	105.70
36	5	2524	A	N7-C8-N9	6.71	117.15	113.80
36	5	2825	C	C6-N1-C2	6.71	122.98	120.30
36	1	361	A	N1-C6-N6	-6.71	114.58	118.60
36	1	232	G	N3-C4-N9	6.71	130.02	126.00
36	5	2699	G	N1-C6-O6	6.71	123.92	119.90
36	1	375	A	O5'-P-OP2	-6.70	99.67	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2996	U	C6-N1-C1'	-6.70	111.82	121.20
36	1	3318	G	C8-N9-C4	-6.70	103.72	106.40
36	5	1940	G	C8-N9-C4	6.70	109.08	106.40
36	1	1884	A	N1-C6-N6	6.70	122.62	118.60
36	5	1310	G	N1-C6-O6	-6.70	115.88	119.90
36	1	2622	C	C6-N1-C2	-6.70	117.62	120.30
36	1	1150	A	N1-C6-N6	-6.70	114.58	118.60
36	1	1820	U	P-O3'-C3'	6.70	127.73	119.70
36	5	1390	A	N9-C4-C5	6.70	108.48	105.80
36	1	2339	C	O5'-P-OP2	-6.69	99.68	105.70
36	5	3068	U	N1-C2-N3	6.69	118.92	114.90
1	6	1137	A	C8-N9-C4	6.69	108.48	105.80
1	2	647	G	N3-C2-N2	-6.69	115.22	119.90
36	1	942	U	N3-C4-C5	-6.69	110.59	114.60
36	1	2885	C	C6-N1-C2	6.69	122.97	120.30
1	6	858	G	C6-C5-N7	-6.69	126.39	130.40
36	1	2418	G	C2-N3-C4	6.69	115.24	111.90
36	5	3212	C	C6-N1-C2	6.68	122.97	120.30
36	1	1158	A	C5-C6-N6	-6.68	118.35	123.70
36	1	1535	A	C4-C5-N7	6.68	114.04	110.70
36	1	2643	A	N1-C6-N6	6.68	122.61	118.60
36	5	1149	G	N3-C4-N9	6.68	130.01	126.00
36	5	2797	C	N3-C4-C5	-6.68	119.23	121.90
1	6	176	C	N1-C2-O2	6.68	122.91	118.90
37	7	103	A	N1-C6-N6	6.68	122.61	118.60
36	1	281	G	N3-C4-N9	6.68	130.01	126.00
36	1	2176	U	N3-C2-O2	-6.68	117.52	122.20
15	C3	114	ARG	NE-CZ-NH1	6.68	123.64	120.30
36	1	2996	U	N1-C2-O2	6.68	127.47	122.80
36	1	637	C	C2-N1-C1'	-6.68	111.45	118.80
36	5	1433	A	N1-C2-N3	6.68	132.64	129.30
36	1	959	C	C6-N1-C2	6.67	122.97	120.30
36	5	2234	G	N9-C4-C5	-6.67	102.73	105.40
36	5	371	G	C5-C6-O6	-6.67	124.60	128.60
1	2	144	U	N3-C2-O2	-6.67	117.53	122.20
1	6	610	G	C4-N9-C1'	6.67	135.17	126.50
36	5	2353	G	C5-C6-O6	-6.67	124.60	128.60
1	6	1667	A	OP1-P-OP2	-6.67	109.59	119.60
36	1	1117	G	N1-C6-O6	6.67	123.90	119.90
36	1	1466	G	C4-C5-N7	6.67	113.47	110.80
36	5	821	U	N3-C4-O4	-6.67	114.73	119.40
36	1	43	A	O5'-P-OP1	-6.66	99.70	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	273	A	N1-C6-N6	-6.66	114.61	118.60
36	5	2550	U	C5-C4-O4	6.66	129.89	125.90
1	2	831	U	C5-C6-N1	6.66	126.03	122.70
36	5	2884	C	C5-C4-N4	-6.66	115.54	120.20
36	1	2606	G	C8-N9-C1'	-6.65	118.35	127.00
15	C3	22	ALA	C-N-CD	-6.65	105.96	120.60
1	6	317	C	C2-N3-C4	-6.65	116.57	119.90
1	6	377	G	N3-C2-N2	6.65	124.56	119.90
36	5	1152	G	C4-C5-N7	6.65	113.46	110.80
36	5	2763	U	C5-C4-O4	-6.65	121.91	125.90
36	1	2718	U	N3-C2-O2	-6.65	117.55	122.20
36	5	1151	U	N1-C2-O2	-6.65	118.15	122.80
36	5	3047	U	N3-C4-C5	-6.65	110.61	114.60
36	1	3278	C	C2-N1-C1'	6.64	126.11	118.80
36	5	222	A	O5'-P-OP2	-6.64	99.72	105.70
36	5	2234	G	N1-C6-O6	6.64	123.89	119.90
1	2	448	C	C6-N1-C2	-6.64	117.64	120.30
1	2	830	U	N3-C2-O2	-6.64	117.55	122.20
36	1	1497	C	N3-C4-C5	-6.64	119.24	121.90
1	6	258	C	C6-N1-C2	6.64	122.95	120.30
1	2	1768	G	C4-C5-N7	-6.64	108.14	110.80
36	5	942	U	C5-C4-O4	-6.64	121.92	125.90
36	5	3190	C	N3-C4-C5	-6.64	119.25	121.90
1	2	831	U	C6-N1-C2	-6.63	117.02	121.00
36	5	609	G	C5-C6-N1	-6.63	108.18	111.50
36	5	2163	C	C4-C5-C6	6.63	120.72	117.40
36	1	3181	C	C6-N1-C2	-6.63	117.65	120.30
36	1	3377	G	C4-N9-C1'	6.63	135.12	126.50
36	1	2384	A	N3-C4-N9	6.63	132.70	127.40
36	5	1116	G	C4-C5-N7	-6.63	108.15	110.80
36	1	646	A	C8-N9-C4	-6.63	103.15	105.80
36	5	1171	G	N1-C2-N2	-6.63	110.24	116.20
36	5	2643	A	C8-N9-C4	6.63	108.45	105.80
36	1	1144	U	C5-C6-N1	-6.62	119.39	122.70
1	6	937	C	C6-N1-C2	-6.62	117.65	120.30
36	5	1483	G	O4'-C1'-N9	6.62	113.50	108.20
36	5	2318	U	N3-C2-O2	-6.62	117.57	122.20
36	1	2764	C	N1-C2-O2	-6.62	114.93	118.90
36	1	1445	U	C5-C6-N1	-6.62	119.39	122.70
36	5	2600	C	C6-N1-C2	-6.62	117.65	120.30
1	6	1117	U	O5'-P-OP1	6.61	118.63	110.70
1	6	1643	U	C2-N3-C4	-6.61	123.03	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2857	C	C6-N1-C2	6.61	122.94	120.30
1	2	1773	C	N3-C4-N4	6.61	122.62	118.00
36	1	2617	U	N3-C4-O4	-6.60	114.78	119.40
36	5	424	G	N9-C4-C5	-6.60	102.76	105.40
36	1	1315	U	C5-C6-N1	-6.60	119.40	122.70
36	1	2343	C	N3-C4-C5	6.60	124.54	121.90
36	1	1148	G	N7-C8-N9	-6.59	109.81	113.10
1	6	75	U	N1-C2-O2	6.59	127.41	122.80
37	7	100	C	C6-N1-C2	6.59	122.94	120.30
36	1	2943	G	C6-C5-N7	-6.59	126.45	130.40
1	6	1537	C	C6-N1-C1'	6.58	128.70	120.80
36	1	2978	U	N3-C2-O2	-6.58	117.59	122.20
1	2	639	U	N1-C2-O2	6.58	127.41	122.80
36	1	66	A	O5'-P-OP1	-6.58	99.78	105.70
36	5	2136	C	C4-C5-C6	6.58	120.69	117.40
36	5	2710	C	N1-C2-O2	-6.58	114.95	118.90
1	2	934	C	C2-N1-C1'	6.57	126.03	118.80
1	2	1456	C	C2-N1-C1'	6.57	126.03	118.80
36	5	1343	A	O5'-P-OP2	-6.57	99.78	105.70
36	1	1481	A	N1-C6-N6	6.57	122.54	118.60
38	4	56	G	O5'-P-OP2	-6.57	99.79	105.70
36	1	1556	C	C2-N1-C1'	6.57	126.03	118.80
36	1	2356	A	N1-C6-N6	6.57	122.54	118.60
36	1	2726	C	C2-N3-C4	-6.57	116.62	119.90
37	7	100	C	C5-C6-N1	-6.57	117.72	121.00
1	6	317	C	C5-C6-N1	-6.56	117.72	121.00
36	1	2601	A	C5-C6-N1	6.56	120.98	117.70
36	5	1416	C	N1-C2-O2	6.56	122.84	118.90
36	5	3339	A	N1-C6-N6	6.56	122.54	118.60
1	6	1793	G	C5-C6-O6	6.56	132.54	128.60
36	5	2144	A	O4'-C1'-N9	6.56	113.45	108.20
36	1	369	A	N3-C4-C5	-6.56	122.21	126.80
36	1	1303	A	N1-C6-N6	6.56	122.53	118.60
36	1	895	A	C4-C5-N7	6.55	113.98	110.70
36	1	2197	C	N1-C2-O2	6.55	122.83	118.90
36	5	1519	G	N1-C6-O6	6.55	123.83	119.90
36	1	2209	U	C5-C6-N1	6.55	125.97	122.70
1	6	384	G	C8-N9-C4	6.55	109.02	106.40
36	5	1085	A	O5'-P-OP1	-6.55	99.81	105.70
36	5	3324	C	C6-N1-C2	6.55	122.92	120.30
36	1	1124	U	C4-C5-C6	-6.55	115.77	119.70
36	1	3217	C	N3-C2-O2	-6.55	117.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	217	U	OP1-P-O3'	6.55	119.60	105.20
36	5	408	A	O5'-P-OP1	-6.55	99.81	105.70
36	1	1308	A	C5-C6-N1	-6.54	114.43	117.70
36	5	2355	G	C4-C5-N7	6.54	113.42	110.80
36	5	2649	A	C4-C5-N7	6.54	113.97	110.70
1	6	1117	U	O5'-P-OP2	-6.54	99.81	105.70
1	6	1600	A	C2-N3-C4	-6.54	107.33	110.60
36	5	1010	G	N3-C4-C5	-6.54	125.33	128.60
36	1	1119	C	C6-N1-C2	6.54	122.92	120.30
1	6	421	A	N9-C4-C5	-6.54	103.18	105.80
36	5	1167	U	N3-C4-O4	6.54	123.98	119.40
1	6	158	U	P-O3'-C3'	6.54	127.55	119.70
36	5	3330	A	C5-C6-N1	6.54	120.97	117.70
1	2	1761	U	C6-N1-C2	-6.54	117.08	121.00
36	1	285	A	N1-C6-N6	6.54	122.52	118.60
36	1	1114	U	N1-C2-O2	6.54	127.37	122.80
1	6	265	A	N1-C6-N6	6.54	122.52	118.60
36	5	217	U	C5-C6-N1	-6.54	119.43	122.70
36	5	349	A	N1-C6-N6	-6.53	114.68	118.60
1	2	1503	A	N1-C6-N6	6.53	122.52	118.60
36	1	439	C	C2-N1-C1'	6.53	125.98	118.80
38	8	3	A	C5-C6-N1	6.53	120.97	117.70
36	5	934	G	C4-N9-C1'	6.53	134.99	126.50
36	1	2618	G	C5-C6-N1	6.53	114.76	111.50
36	5	2411	U	C2-N3-C4	-6.53	123.08	127.00
36	5	2611	U	O5'-P-OP1	6.53	118.53	110.70
36	1	76	G	N3-C4-C5	-6.53	125.34	128.60
36	1	2802	A	OP2-P-O3'	6.52	119.55	105.20
41	14	339	LEU	CA-CB-CG	6.52	130.30	115.30
36	1	647	A	C8-N9-C4	6.52	108.41	105.80
36	5	2724	U	N3-C2-O2	-6.52	117.64	122.20
36	1	2374	C	C4-C5-C6	6.52	120.66	117.40
36	1	2355	G	N9-C4-C5	-6.52	102.79	105.40
1	6	308	C	N3-C4-N4	-6.52	113.44	118.00
36	5	739	G	N1-C6-O6	-6.52	115.99	119.90
36	5	2726	C	C6-N1-C2	-6.51	117.69	120.30
36	1	2156	C	C6-N1-C2	6.51	122.91	120.30
1	6	1029	U	N3-C4-O4	-6.51	114.84	119.40
36	1	939	U	N1-C2-O2	-6.51	118.24	122.80
36	1	2796	G	C2-N3-C4	-6.51	108.64	111.90
36	5	211	A	O5'-P-OP1	-6.51	99.84	105.70
36	1	517	G	N1-C6-O6	-6.51	116.00	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	645	A	C5-C6-N1	6.51	120.95	117.70
1	2	831	U	N3-C2-O2	-6.50	117.65	122.20
36	5	3377	G	C5-C6-N1	6.50	114.75	111.50
37	7	36	C	C6-N1-C2	6.50	122.90	120.30
36	5	2355	G	C5-C6-O6	-6.50	124.70	128.60
36	1	2112	U	P-O3'-C3'	6.50	127.50	119.70
36	5	2272	G	N1-C6-O6	-6.50	116.00	119.90
36	5	2953	U	N3-C2-O2	6.50	126.75	122.20
1	2	1096	C	C6-N1-C1'	-6.49	113.01	120.80
36	5	940	G	C5-C6-O6	-6.49	124.71	128.60
36	5	2354	C	N3-C4-N4	6.49	122.54	118.00
36	1	2541	U	C2-N1-C1'	6.49	125.49	117.70
1	6	101	U	N3-C2-O2	-6.49	117.66	122.20
36	1	1279	C	C5-C6-N1	6.49	124.24	121.00
36	5	1161	G	O5'-P-OP1	-6.49	99.86	105.70
36	1	2892	A	N1-C6-N6	-6.49	114.71	118.60
36	1	2130	G	N1-C6-O6	-6.48	116.01	119.90
36	5	1443	G	N1-C2-N2	-6.48	110.37	116.20
36	1	2725	U	N3-C4-O4	-6.48	114.86	119.40
36	1	3344	A	C5-N7-C8	-6.48	100.66	103.90
36	5	326	U	N3-C4-C5	-6.48	110.71	114.60
36	5	2887	A	C6-C5-N7	-6.48	127.77	132.30
36	5	3039	C	O5'-P-OP2	-6.48	99.87	105.70
36	1	2827	U	C5-C6-N1	-6.48	119.46	122.70
1	6	382	C	C2-N3-C4	-6.48	116.66	119.90
36	5	1843	C	C5-C4-N4	-6.47	115.67	120.20
36	5	1060	U	C5-C6-N1	-6.47	119.46	122.70
1	6	1637	C	C2-N1-C1'	6.47	125.92	118.80
1	2	1745	G	N9-C4-C5	-6.47	102.81	105.40
36	1	783	A	N1-C6-N6	6.47	122.48	118.60
1	2	1761	U	C5-C4-O4	6.46	129.78	125.90
36	1	2719	U	C6-N1-C1'	6.46	130.25	121.20
36	5	907	G	N3-C2-N2	6.46	124.42	119.90
1	6	1596	C	N3-C2-O2	-6.46	117.38	121.90
36	5	1434	G	C5-C6-O6	-6.46	124.72	128.60
36	1	2411	U	N3-C4-O4	-6.46	114.88	119.40
1	6	542	A	N7-C8-N9	6.46	117.03	113.80
36	5	880	G	C5-C6-O6	-6.46	124.73	128.60
36	5	1473	G	C8-N9-C4	6.46	108.98	106.40
36	5	2917	G	C6-C5-N7	-6.45	126.53	130.40
1	6	1657	U	N1-C2-O2	6.45	127.32	122.80
36	5	1302	A	N9-C4-C5	6.45	108.38	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	577	G	N1-C6-O6	6.45	123.77	119.90
36	5	3362	A	N7-C8-N9	6.45	117.02	113.80
36	5	2639	G	N1-C6-O6	6.45	123.77	119.90
36	1	894	G	N3-C4-N9	-6.45	122.13	126.00
36	1	1198	C	O5'-P-OP1	-6.45	99.90	105.70
36	1	1367	G	O5'-P-OP1	-6.45	99.90	105.70
36	1	2950	G	O4'-C1'-N9	6.45	113.36	108.20
36	1	3362	A	N1-C2-N3	6.45	132.52	129.30
36	5	3008	A	O5'-P-OP2	-6.45	99.90	105.70
1	6	1414	U	N3-C2-O2	-6.44	117.69	122.20
36	5	652	G	C6-C5-N7	-6.44	126.53	130.40
1	6	1109	G	C8-N9-C4	-6.44	103.82	106.40
36	5	2351	U	N1-C2-N3	6.44	118.76	114.90
38	8	95	G	C4-N9-C1'	-6.44	118.13	126.50
36	1	3209	A	N1-C6-N6	6.44	122.46	118.60
38	8	44	A	C5-C6-N6	-6.44	118.55	123.70
1	2	1462	G	C8-N9-C4	6.43	108.97	106.40
1	6	1280	C	C6-N1-C2	-6.43	117.73	120.30
36	1	1152	G	O5'-P-OP1	-6.43	99.91	105.70
36	1	1796	G	C8-N9-C4	-6.43	103.83	106.40
1	6	858	G	N7-C8-N9	6.43	116.32	113.10
36	5	2912	G	O5'-P-OP1	-6.43	99.91	105.70
36	1	1891	A	C8-N9-C4	6.43	108.37	105.80
36	5	3018	C	C6-N1-C2	-6.43	117.73	120.30
36	5	1592	G	C5-C6-N1	-6.42	108.29	111.50
36	5	3071	U	C5-C4-O4	6.42	129.75	125.90
1	6	902	G	C5-C6-N1	-6.42	108.29	111.50
36	5	1938	U	C6-N1-C2	6.42	124.85	121.00
36	1	2827	U	C2-N1-C1'	-6.42	109.99	117.70
36	5	1060	U	N3-C4-O4	-6.42	114.91	119.40
36	5	2531	C	N1-C2-O2	6.42	122.75	118.90
1	6	1735	U	N1-C2-O2	6.42	127.29	122.80
1	6	1794	A	O5'-P-OP1	-6.42	99.92	105.70
36	5	903	U	C5-C6-N1	-6.42	119.49	122.70
36	5	1112	A	C5-C6-N1	6.42	120.91	117.70
36	5	1466	G	OP1-P-OP2	-6.42	109.97	119.60
36	5	2287	C	C6-N1-C2	-6.42	117.73	120.30
36	5	3089	C	N3-C4-C5	6.42	124.47	121.90
36	5	3151	U	C6-N1-C2	6.42	124.85	121.00
38	8	45	C	C6-N1-C2	-6.42	117.73	120.30
1	6	163	G	C8-N9-C4	-6.41	103.83	106.40
36	5	637	C	N1-C2-O2	-6.41	115.05	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	3	84	A	N1-C6-N6	6.41	122.45	118.60
36	1	894	G	N9-C4-C5	6.41	107.96	105.40
1	6	453	U	N1-C2-O2	6.41	127.28	122.80
36	1	984	G	C6-N1-C2	-6.40	121.26	125.10
36	1	857	G	N1-C6-O6	6.40	123.74	119.90
1	6	75	U	C2-N1-C1'	6.40	125.38	117.70
1	2	554	C	C6-N1-C1'	-6.40	113.12	120.80
36	1	1481	A	C6-C5-N7	-6.40	127.82	132.30
36	5	2231	C	O4'-C1'-N1	6.40	113.32	108.20
36	1	1133	A	C8-N9-C4	6.40	108.36	105.80
36	5	1370	G	C6-N1-C2	-6.39	121.26	125.10
36	5	1868	G	C8-N9-C4	6.39	108.96	106.40
38	4	125	U	N1-C2-O2	6.39	127.27	122.80
1	6	687	G	N3-C4-N9	-6.39	122.17	126.00
36	1	232	G	C6-C5-N7	-6.39	126.57	130.40
1	6	425	A	C5-C6-N1	6.39	120.89	117.70
7	s5	92	ARG	NE-CZ-NH1	6.39	123.49	120.30
36	1	156	G	C5-C6-N1	6.39	114.69	111.50
36	1	894	G	N1-C2-N2	6.39	121.95	116.20
36	5	2943	G	C2-N3-C4	-6.39	108.71	111.90
1	2	694	U	C2-N1-C1'	6.38	125.36	117.70
38	4	125	U	C2-N1-C1'	6.38	125.36	117.70
36	5	934	G	N3-C4-C5	-6.38	125.41	128.60
37	7	77	G	N1-C6-O6	6.38	123.73	119.90
40	l3	26	ARG	NE-CZ-NH1	-6.38	117.11	120.30
36	1	326	U	N3-C4-O4	6.38	123.87	119.40
36	5	2139	A	N1-C2-N3	6.38	132.49	129.30
36	1	96	G	N1-C6-O6	6.38	123.73	119.90
36	1	968	G	C5-C6-O6	-6.38	124.77	128.60
1	6	858	G	C5-N7-C8	-6.38	101.11	104.30
1	6	1584	G	C5-C6-O6	-6.38	124.77	128.60
21	c9	57	ARG	NE-CZ-NH1	6.38	123.49	120.30
36	1	2355	G	C5-C6-O6	-6.38	124.77	128.60
1	6	901	G	C4-C5-N7	6.38	113.35	110.80
36	5	2350	C	O5'-P-OP2	-6.38	99.96	105.70
36	5	2860	U	C5-C4-O4	6.38	129.73	125.90
36	1	1269	U	C2-N1-C1'	6.38	125.35	117.70
36	5	894	G	C5-C6-O6	-6.38	124.78	128.60
36	5	1112	A	N3-C4-N9	6.37	132.50	127.40
36	5	3218	A	N9-C4-C5	-6.37	103.25	105.80
36	1	1405	U	C6-N1-C2	6.37	124.82	121.00
36	1	961	C	N3-C4-N4	6.37	122.46	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	307	G	N3-C4-N9	6.37	129.82	126.00
36	1	1849	C	N3-C2-O2	6.37	126.36	121.90
36	1	2610	G	N1-C6-O6	6.37	123.72	119.90
36	5	2391	G	OP1-P-OP2	-6.37	110.05	119.60
37	7	101	G	C4-C5-N7	6.36	113.34	110.80
36	1	2124	G	C5-C6-O6	-6.36	124.78	128.60
1	6	336	G	O5'-P-OP2	-6.36	99.98	105.70
1	6	1000	C	C2-N1-C1'	6.36	125.80	118.80
36	5	1833	G	N1-C6-O6	-6.36	116.08	119.90
36	1	1113	G	C5-C6-O6	-6.36	124.78	128.60
1	6	115	G	O5'-P-OP2	-6.36	99.98	105.70
1	6	136	C	C2-N1-C1'	6.36	125.79	118.80
36	5	2620	G	N9-C4-C5	6.35	107.94	105.40
36	1	1151	U	N3-C4-C5	-6.35	110.79	114.60
80	c0	97	PRO	N-CA-CB	6.35	110.92	103.30
36	5	1437	C	C2-N1-C1'	6.35	125.78	118.80
36	5	3208	G	N3-C4-N9	-6.35	122.19	126.00
36	5	2112	U	C6-N1-C2	-6.35	117.19	121.00
36	1	2624	G	N1-C6-O6	6.34	123.71	119.90
36	1	3140	G	N3-C4-N9	6.34	129.81	126.00
36	5	2724	U	C5-C4-O4	6.34	129.71	125.90
24	D2	65	LEU	CA-CB-CG	6.34	129.89	115.30
36	1	1743	G	C8-N9-C4	6.34	108.94	106.40
36	5	2882	U	N1-C2-N3	6.34	118.71	114.90
56	N0	155	ARG	NE-CZ-NH2	6.34	123.47	120.30
36	5	21	G	N3-C4-C5	6.34	131.77	128.60
36	5	398	A	O5'-P-OP2	-6.34	99.99	105.70
36	5	1316	C	N3-C2-O2	6.34	126.34	121.90
36	1	86	G	O5'-P-OP2	-6.34	99.99	105.70
36	5	112	U	O4'-C1'-N1	6.34	113.27	108.20
36	5	146	U	N3-C4-O4	-6.34	114.96	119.40
36	5	2403	G	O5'-P-OP1	6.34	118.31	110.70
1	6	250	C	C5-C6-N1	6.34	124.17	121.00
36	5	1604	G	C4-N9-C1'	6.34	134.74	126.50
36	5	3343	G	N3-C4-N9	6.34	129.80	126.00
36	5	1592	G	C8-N9-C4	-6.33	103.87	106.40
36	1	701	G	N1-C6-O6	6.33	123.70	119.90
36	1	3269	U	N1-C2-N3	6.33	118.70	114.90
1	6	387	A	N1-C6-N6	-6.33	114.80	118.60
1	6	1091	A	C5-C6-N1	-6.33	114.53	117.70
36	1	2249	G	N3-C4-N9	6.33	129.80	126.00
36	5	3387	U	C5-C6-N1	-6.33	119.53	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1377	G	C4-C5-N7	6.33	113.33	110.80
36	1	1402	C	N3-C4-C5	6.33	124.43	121.90
36	5	1340	G	C8-N9-C4	6.33	108.93	106.40
36	1	2121	G	N3-C4-C5	-6.33	125.44	128.60
36	5	1316	C	N3-C4-N4	6.33	122.43	118.00
36	5	2117	A	N1-C6-N6	-6.33	114.81	118.60
36	5	2957	G	O5'-P-OP1	-6.33	100.01	105.70
36	1	717	C	C6-N1-C2	-6.32	117.77	120.30
36	1	1341	U	N3-C2-O2	-6.32	117.77	122.20
1	6	1473	U	N3-C2-O2	-6.32	117.77	122.20
38	8	139	U	N3-C4-O4	-6.32	114.97	119.40
1	6	1514	U	C5-C4-O4	6.32	129.69	125.90
36	1	664	U	N3-C4-O4	6.32	123.83	119.40
36	5	934	G	C5-C6-O6	-6.32	124.81	128.60
36	5	2397	A	N1-C6-N6	-6.32	114.81	118.60
1	6	17	C	O5'-P-OP2	-6.32	100.01	105.70
36	5	27	C	N1-C2-O2	-6.32	115.11	118.90
36	1	919	U	N3-C4-O4	-6.32	114.98	119.40
36	1	3207	U	C5-C4-O4	6.32	129.69	125.90
36	1	281	G	C6-C5-N7	-6.31	126.61	130.40
36	1	1122	U	N3-C4-O4	-6.31	114.98	119.40
36	5	1441	G	C5-C6-N1	6.31	114.66	111.50
36	5	56	G	N1-C6-O6	-6.31	116.11	119.90
36	5	1438	U	C2-N1-C1'	6.31	125.27	117.70
36	1	2693	C	C6-N1-C2	6.31	122.82	120.30
1	6	1568	C	P-O3'-C3'	6.31	127.27	119.70
36	5	1445	U	N1-C2-O2	-6.31	118.39	122.80
36	1	120	G	C8-N9-C4	6.30	108.92	106.40
1	6	1146	G	C6-C5-N7	-6.30	126.62	130.40
3	s1	231	LEU	CA-CB-CG	6.30	129.80	115.30
36	5	2167	A	C8-N9-C4	-6.30	103.28	105.80
1	2	1768	G	C5-C6-O6	6.30	132.38	128.60
36	1	24	G	N3-C2-N2	-6.30	115.49	119.90
36	1	106	A	C8-N9-C4	6.30	108.32	105.80
36	1	3361	G	N3-C2-N2	6.30	124.31	119.90
36	5	2385	G	C4-N9-C1'	-6.30	118.31	126.50
36	5	3217	C	C2-N1-C1'	-6.30	111.87	118.80
38	4	40	A	N1-C6-N6	6.30	122.38	118.60
36	5	776	U	N1-C2-N3	6.30	118.68	114.90
36	5	1878	G	C4-N9-C1'	6.30	134.69	126.50
1	2	186	C	C2-N1-C1'	6.29	125.72	118.80
36	1	1866	C	C6-N1-C2	6.29	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1076	A	C8-N9-C4	6.29	108.32	105.80
36	5	1112	A	N3-C4-C5	-6.29	122.39	126.80
36	1	3010	U	C5-C4-O4	-6.29	122.12	125.90
36	5	2304	C	N1-C2-O2	-6.29	115.13	118.90
1	6	1164	G	C8-N9-C4	6.29	108.92	106.40
36	1	2621	G	N3-C2-N2	-6.29	115.50	119.90
38	4	21	C	C6-N1-C2	6.29	122.81	120.30
36	5	864	G	O5'-P-OP2	-6.29	100.04	105.70
36	1	1396	C	C5-C4-N4	-6.28	115.80	120.20
36	5	2396	G	N9-C4-C5	6.28	107.91	105.40
36	5	2817	A	C5-C6-N6	-6.28	118.67	123.70
1	6	425	A	C4-C5-C6	-6.28	113.86	117.00
1	6	1648	A	C8-N9-C4	6.28	108.31	105.80
36	5	2816	G	N7-C8-N9	-6.28	109.96	113.10
1	2	966	A	C5-C6-N6	-6.28	118.68	123.70
36	1	1463	U	C5-C6-N1	-6.28	119.56	122.70
36	1	783	A	N9-C4-C5	-6.27	103.29	105.80
36	5	3133	C	C4-C5-C6	6.27	120.54	117.40
1	6	1119	G	O5'-P-OP2	-6.27	100.06	105.70
36	1	2237	C	N1-C2-O2	6.27	122.66	118.90
36	1	2866	U	N3-C2-O2	-6.27	117.81	122.20
1	6	1269	U	N3-C2-O2	-6.27	117.81	122.20
36	5	1669	C	C6-N1-C2	6.27	122.81	120.30
36	5	2387	A	N1-C6-N6	6.27	122.36	118.60
36	5	3208	G	N9-C4-C5	6.27	107.91	105.40
1	6	337	G	C8-N9-C1'	-6.27	118.85	127.00
36	5	3308	C	C4-C5-C6	6.27	120.53	117.40
36	5	2622	C	C4-C5-C6	6.26	120.53	117.40
36	1	890	C	N3-C4-C5	6.26	124.40	121.90
1	6	1091	A	C2-N3-C4	-6.26	107.47	110.60
36	1	1111	U	C6-N1-C2	6.25	124.75	121.00
36	5	234	G	C5-C6-O6	-6.25	124.85	128.60
36	1	921	A	N1-C6-N6	-6.25	114.85	118.60
36	1	1481	A	C5-C6-N1	-6.25	114.58	117.70
36	1	3103	A	O5'-P-OP2	-6.25	100.08	105.70
36	5	2236	G	C6-C5-N7	-6.25	126.65	130.40
36	5	2248	C	OP1-P-O3'	6.25	118.94	105.20
36	1	2653	C	C5-C6-N1	-6.25	117.88	121.00
36	5	2341	A	O5'-P-OP2	-6.25	100.08	105.70
36	5	2917	G	C8-N9-C1'	-6.25	118.88	127.00
1	2	1200	G	N3-C2-N2	-6.25	115.53	119.90
36	1	979	U	C6-N1-C2	-6.24	117.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	917	A	O5'-P-OP1	6.24	118.19	110.70
1	6	577	G	N7-C8-N9	6.24	116.22	113.10
36	1	83	U	C5-C4-O4	-6.24	122.16	125.90
36	5	2960	C	N3-C4-C5	6.24	124.40	121.90
36	5	3034	C	C6-N1-C2	6.24	122.80	120.30
36	1	2949	U	C5-C6-N1	-6.24	119.58	122.70
1	2	1456	C	O4'-C1'-N1	6.23	113.19	108.20
38	4	40	A	C5-C6-N6	-6.23	118.71	123.70
1	6	1000	C	N3-C2-O2	-6.23	117.54	121.90
36	5	101	G	C6-C5-N7	-6.23	126.66	130.40
36	5	3141	A	C4-C5-C6	6.23	120.12	117.00
77	q1	23	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	6	119	A	C2-N3-C4	-6.23	107.49	110.60
1	6	815	G	C6-C5-N7	-6.23	126.66	130.40
36	5	146	U	C5-C6-N1	-6.23	119.59	122.70
36	5	804	C	C4-C5-C6	6.23	120.51	117.40
36	1	1129	A	N9-C4-C5	-6.22	103.31	105.80
1	6	1025	A	C2-N3-C4	-6.22	107.49	110.60
36	5	632	G	N3-C4-C5	-6.22	125.49	128.60
36	1	2283	G	N9-C4-C5	-6.22	102.91	105.40
36	1	2356	A	C5-C6-N6	-6.22	118.72	123.70
36	5	1863	G	C5-C6-N1	6.22	114.61	111.50
36	5	1081	U	C2-N1-C1'	6.22	125.16	117.70
36	5	1082	U	C2-N1-C1'	6.22	125.16	117.70
36	5	1156	C	N1-C2-O2	-6.22	115.17	118.90
36	1	1390	A	C8-N9-C4	-6.21	103.31	105.80
36	1	2871	G	C4-C5-C6	-6.21	115.07	118.80
36	1	2371	G	C5-C6-O6	-6.21	124.87	128.60
1	6	1582	U	C5-C6-N1	-6.21	119.59	122.70
36	1	2737	C	N3-C2-O2	6.21	126.25	121.90
36	1	25	U	C4-C5-C6	6.21	123.42	119.70
36	1	1556	C	N1-C2-O2	6.21	122.62	118.90
36	1	2585	G	N3-C4-C5	-6.21	125.50	128.60
1	2	1258	U	N3-C2-O2	-6.21	117.86	122.20
1	6	634	G	O5'-P-OP2	-6.21	100.11	105.70
36	5	2430	A	N1-C6-N6	6.20	122.32	118.60
36	1	608	A	C5-C6-N6	-6.20	118.74	123.70
1	6	1665	U	C6-N1-C2	6.20	124.72	121.00
1	2	1269	U	O4'-C1'-N1	6.20	113.16	108.20
36	1	3361	G	N3-C4-N9	6.20	129.72	126.00
36	1	1495	U	C2-N1-C1'	-6.20	110.26	117.70
36	1	2860	U	C5-C4-O4	-6.20	122.18	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1879	A	C6-C5-N7	-6.20	127.96	132.30
36	5	3362	A	C5-N7-C8	-6.20	100.80	103.90
36	5	2434	U	N3-C4-O4	-6.20	115.06	119.40
1	6	985	G	N3-C2-N2	-6.20	115.56	119.90
36	1	2762	A	O5'-P-OP1	6.19	118.13	110.70
36	1	1920	U	N3-C2-O2	-6.19	117.87	122.20
1	6	20	G	C5-C6-O6	-6.19	124.89	128.60
36	5	906	A	N1-C2-N3	6.19	132.40	129.30
36	5	2996	U	N1-C2-O2	6.19	127.14	122.80
36	5	1886	A	N1-C6-N6	6.19	122.31	118.60
1	2	553	G	C4-C5-N7	6.19	113.28	110.80
36	1	3199	G	C4-N9-C1'	-6.19	118.45	126.50
41	L4	327	LEU	CA-CB-CG	6.19	129.53	115.30
1	6	20	G	N1-C6-O6	6.19	123.61	119.90
38	8	55	U	N3-C4-C5	-6.19	110.89	114.60
36	5	969	C	O5'-P-OP1	-6.18	100.13	105.70
36	5	2350	C	O5'-P-OP1	6.18	118.12	110.70
36	1	949	C	C4-C5-C6	6.18	120.49	117.40
1	2	1096	C	N1-C2-O2	6.18	122.61	118.90
36	1	2404	A	C2-N3-C4	6.18	113.69	110.60
1	2	987	G	N1-C6-O6	-6.18	116.19	119.90
1	6	1722	A	C8-N9-C4	6.18	108.27	105.80
36	1	2603	G	N9-C4-C5	-6.18	102.93	105.40
38	8	95	G	N3-C4-N9	-6.18	122.29	126.00
1	2	158	U	P-O3'-C3'	6.17	127.11	119.70
36	5	3042	U	N1-C2-N3	6.17	118.60	114.90
36	1	2643	A	N9-C4-C5	-6.17	103.33	105.80
1	6	577	G	C5-N7-C8	-6.17	101.21	104.30
36	5	2332	A	C8-N9-C4	6.17	108.27	105.80
36	1	890	C	O5'-P-OP2	-6.17	100.15	105.70
36	1	2617	U	C4-C5-C6	6.17	123.40	119.70
80	c0	83	PRO	N-CA-CB	6.17	110.70	103.30
36	5	2584	G	C4-N9-C1'	6.17	134.52	126.50
1	2	373	G	N3-C4-C5	-6.17	125.52	128.60
36	1	1144	U	N3-C4-C5	6.17	118.30	114.60
1	6	426	G	N3-C4-C5	-6.17	125.52	128.60
36	5	570	A	N1-C6-N6	6.17	122.30	118.60
36	5	1902	G	C4-C5-N7	6.17	113.27	110.80
36	1	988	U	C2-N1-C1'	-6.17	110.30	117.70
1	6	1145	U	C4-C5-C6	6.16	123.40	119.70
1	6	1539	G	N3-C4-C5	6.16	131.68	128.60
36	5	3256	G	N1-C6-O6	6.16	123.60	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	44	A	N1-C6-N6	6.16	122.30	118.60
1	6	163	G	N1-C2-N2	6.16	121.75	116.20
36	5	2890	A	C4-C5-C6	6.16	120.08	117.00
1	6	144	U	O4'-C1'-N1	6.16	113.13	108.20
36	1	1390	A	N9-C4-C5	6.16	108.26	105.80
36	1	2884	C	C6-N1-C2	6.16	122.76	120.30
1	6	310	C	N3-C4-C5	-6.16	119.44	121.90
36	5	1392	G	C8-N9-C4	6.16	108.86	106.40
36	1	2658	G	C8-N9-C4	6.16	108.86	106.40
36	5	2699	G	C5-C6-O6	-6.16	124.91	128.60
36	1	2606	G	C4-N9-C1'	6.15	134.50	126.50
1	6	539	G	N3-C4-C5	6.15	131.68	128.60
36	5	1057	A	O5'-P-OP2	-6.15	100.16	105.70
36	1	1296	C	C6-N1-C2	-6.15	117.84	120.30
36	1	1318	A	C5-N7-C8	-6.15	100.83	103.90
1	6	1778	G	N1-C6-O6	-6.15	116.21	119.90
37	7	91	G	C6-C5-N7	-6.15	126.71	130.40
1	2	1745	G	N3-C2-N2	6.14	124.20	119.90
36	1	3278	C	N3-C2-O2	-6.14	117.60	121.90
36	5	2917	G	C4-N9-C1'	6.14	134.49	126.50
36	5	2341	A	N7-C8-N9	-6.14	110.73	113.80
36	1	939	U	O5'-P-OP2	-6.14	100.17	105.70
36	1	1835	A	C8-N9-C4	6.14	108.26	105.80
36	1	2434	U	N3-C4-O4	-6.14	115.10	119.40
11	s9	3	ARG	NE-CZ-NH2	6.14	123.37	120.30
36	5	2245	C	N3-C4-C5	-6.14	119.44	121.90
36	5	2849	C	N3-C2-O2	6.14	126.20	121.90
37	7	81	U	N3-C4-C5	6.14	118.28	114.60
1	2	1363	U	N1-C2-O2	6.14	127.10	122.80
36	1	2726	C	C6-N1-C2	-6.13	117.85	120.30
36	5	2943	G	O5'-P-OP2	-6.13	100.18	105.70
61	N5	34	LEU	CA-CB-CG	6.13	129.41	115.30
36	1	170	G	O5'-P-OP1	-6.13	100.18	105.70
36	1	1476	G	N1-C6-O6	-6.13	116.22	119.90
36	1	3022	G	O4'-C1'-N9	6.13	113.10	108.20
38	4	31	G	C8-N9-C4	6.13	108.85	106.40
36	5	2139	A	C6-N1-C2	-6.13	114.92	118.60
36	1	2731	U	N1-C2-O2	-6.13	118.51	122.80
1	2	453	U	C5-C4-O4	6.12	129.57	125.90
36	1	984	G	C5-C6-O6	-6.12	124.93	128.60
36	1	1433	A	C5-C6-N6	-6.12	118.81	123.70
36	1	197	G	N1-C6-O6	6.12	123.57	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1157	G	N9-C4-C5	6.12	107.85	105.40
36	1	1397	C	C2-N3-C4	-6.12	116.84	119.90
36	5	1903	U	C5-C4-O4	6.12	129.57	125.90
36	5	2953	U	N3-C4-O4	6.12	123.68	119.40
36	5	41	G	C5-N7-C8	-6.11	101.25	104.30
36	5	645	A	C6-N1-C2	-6.11	114.93	118.60
36	5	1302	A	C5-C6-N6	6.11	128.59	123.70
36	1	3364	C	O5'-P-OP1	-6.11	100.20	105.70
36	5	2354	C	C4-C5-C6	6.11	120.45	117.40
48	m1	12	LEU	CA-CB-CG	6.11	129.35	115.30
36	1	672	A	C2-N3-C4	-6.11	107.55	110.60
36	5	220	G	OP1-P-O3'	6.11	118.63	105.20
1	2	1754	A	N3-C4-C5	6.10	131.07	126.80
36	1	142	C	C5-C6-N1	6.10	124.05	121.00
36	5	63	A	N9-C4-C5	-6.10	103.36	105.80
1	2	1530	C	O5'-P-OP2	-6.10	100.21	105.70
1	6	1774	G	O5'-P-OP2	6.10	118.02	110.70
36	5	2351	U	C6-N1-C2	-6.10	117.34	121.00
36	1	2418	G	N3-C4-C5	-6.09	125.55	128.60
36	5	75	G	C6-C5-N7	-6.09	126.74	130.40
36	5	420	G	C8-N9-C4	6.09	108.84	106.40
36	5	501	A	N1-C6-N6	-6.09	114.94	118.60
36	5	969	C	C4-C5-C6	6.09	120.45	117.40
36	1	96	G	N3-C4-C5	6.09	131.65	128.60
36	1	2124	G	N1-C6-O6	6.09	123.56	119.90
36	1	2889	C	N1-C2-O2	6.09	122.56	118.90
36	5	969	C	C5-C6-N1	-6.09	117.95	121.00
36	5	2430	A	C6-C5-N7	-6.09	128.03	132.30
36	1	3377	G	N3-C2-N2	6.09	124.16	119.90
38	4	113	U	C2-N1-C1'	-6.09	110.39	117.70
36	5	835	G	O4'-C1'-N9	6.09	113.07	108.20
36	5	1371	G	N1-C6-O6	-6.09	116.25	119.90
36	1	2993	G	C8-N9-C4	6.09	108.84	106.40
36	1	49	A	C8-N9-C4	6.09	108.23	105.80
36	5	1116	G	N3-C2-N2	-6.09	115.64	119.90
36	1	1503	A	C8-N9-C4	6.09	108.23	105.80
1	6	625	C	C6-N1-C2	6.09	122.73	120.30
36	5	79	U	C5-C6-N1	6.08	125.74	122.70
36	1	339	C	C5-C4-N4	6.08	124.46	120.20
36	1	878	G	N3-C4-C5	6.08	131.64	128.60
36	5	961	C	OP1-P-OP2	-6.08	110.48	119.60
36	5	2970	C	O5'-P-OP1	-6.08	100.22	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2925	C	O5'-P-OP1	-6.08	100.23	105.70
1	6	65	A	N3-C4-C5	6.08	131.06	126.80
36	5	2971	A	O5'-P-OP2	-6.08	100.23	105.70
36	1	1465	A	C2-N3-C4	-6.08	107.56	110.60
36	1	2435	G	C2-N3-C4	-6.08	108.86	111.90
36	5	3216	G	C6-C5-N7	-6.08	126.75	130.40
1	6	542	A	P-O3'-C3'	6.08	126.99	119.70
36	5	75	G	N3-C4-N9	6.08	129.65	126.00
36	1	1151	U	C6-N1-C2	-6.07	117.36	121.00
9	s7	131	PHE	C-N-CD	6.07	141.15	128.40
36	5	2381	G	N3-C4-C5	-6.07	125.56	128.60
1	6	1	U	O4'-C1'-N1	6.07	113.06	108.20
36	5	3030	G	C5-N7-C8	6.07	107.34	104.30
1	2	829	A	P-O3'-C3'	6.07	126.98	119.70
36	1	1346	G	C5-C6-N1	-6.07	108.46	111.50
38	4	103	G	C5-C6-N1	6.07	114.53	111.50
36	5	2978	U	N3-C2-O2	-6.07	117.95	122.20
36	1	3319	U	P-O3'-C3'	6.07	126.98	119.70
21	c9	57	ARG	NE-CZ-NH2	-6.07	117.27	120.30
36	5	2830	G	N1-C2-N2	-6.07	110.74	116.20
1	2	448	C	N3-C4-C5	-6.07	119.47	121.90
36	1	2242	A	N1-C2-N3	6.07	132.33	129.30
1	6	46	A	C2-N3-C4	-6.07	107.57	110.60
1	6	528	U	N3-C2-O2	-6.07	117.95	122.20
36	1	1850	A	N1-C6-N6	6.07	122.24	118.60
36	5	2897	A	C6-N1-C2	-6.07	114.96	118.60
1	2	1412	G	O4'-C1'-N9	6.06	113.05	108.20
36	5	63	A	N1-C6-N6	6.06	122.24	118.60
36	1	395	A	C8-N9-C4	-6.06	103.38	105.80
36	1	416	A	C5-N7-C8	6.06	106.93	103.90
36	1	2123	G	C8-N9-C4	6.06	108.83	106.40
36	5	2811	A	N1-C2-N3	6.06	132.33	129.30
36	5	3107	U	O5'-P-OP2	-6.06	100.25	105.70
1	6	343	C	N1-C2-O2	-6.06	115.27	118.90
36	1	3344	A	C6-C5-N7	-6.06	128.06	132.30
36	5	342	A	N1-C2-N3	-6.06	126.27	129.30
36	1	324	A	C8-N9-C4	-6.05	103.38	105.80
36	1	942	U	OP1-P-OP2	-6.05	110.52	119.60
36	1	1310	G	C5-C6-O6	6.05	132.23	128.60
36	5	2617	U	N3-C4-C5	-6.05	110.97	114.60
1	2	966	A	N9-C4-C5	-6.05	103.38	105.80
1	2	1189	A	C8-N9-C4	6.05	108.22	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1058	U	O5'-P-OP1	6.05	117.96	110.70
36	1	1548	C	N1-C2-O2	-6.05	115.27	118.90
1	6	787	G	C4-N9-C1'	6.05	134.37	126.50
36	5	770	G	O4'-C1'-N9	6.05	113.04	108.20
1	2	377	G	C8-N9-C4	6.05	108.82	106.40
21	C9	57	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	6	1389	C	C6-N1-C2	-6.05	117.88	120.30
1	6	1657	U	N3-C2-O2	-6.05	117.97	122.20
36	5	3362	A	N1-C2-N3	6.05	132.32	129.30
36	1	1534	A	N1-C6-N6	6.05	122.23	118.60
37	7	103	A	C5-C6-N6	-6.05	118.86	123.70
18	C6	28	LEU	CA-CB-CG	6.05	129.21	115.30
1	6	385	A	C5-C6-N6	6.05	128.54	123.70
1	6	425	A	OP2-P-O3'	6.05	118.50	105.20
36	5	614	C	C6-N1-C2	6.05	122.72	120.30
36	5	911	C	C5-C6-N1	-6.05	117.98	121.00
36	5	2620	G	C5-C6-N1	6.05	114.52	111.50
36	5	2756	C	C6-N1-C2	6.05	122.72	120.30
36	1	1336	U	O5'-P-OP1	6.04	117.95	110.70
36	1	1417	G	C8-N9-C4	6.04	108.82	106.40
1	6	1522	U	N3-C2-O2	-6.04	117.97	122.20
36	1	1296	C	C4-C5-C6	6.04	120.42	117.40
36	5	271	C	N1-C2-O2	6.04	122.53	118.90
36	1	1535	A	C5-C6-N6	-6.04	118.87	123.70
1	2	694	U	N1-C2-O2	6.04	127.03	122.80
36	1	3368	U	C2-N1-C1'	-6.04	110.46	117.70
36	5	3047	U	C4-C5-C6	6.04	123.32	119.70
36	1	1365	G	N1-C2-N2	-6.03	110.77	116.20
36	1	1891	A	C2-N3-C4	-6.03	107.58	110.60
36	1	2283	G	N3-C4-C5	6.03	131.62	128.60
38	4	113	U	C4-C5-C6	6.03	123.32	119.70
36	5	894	G	C4-C5-N7	6.03	113.21	110.80
36	5	2649	A	C5-N7-C8	-6.03	100.88	103.90
36	1	696	C	N3-C4-C5	6.03	124.31	121.90
36	1	3050	U	N1-C2-O2	6.03	127.02	122.80
38	4	65	A	C8-N9-C4	6.03	108.21	105.80
1	6	976	G	C2-N3-C4	-6.03	108.89	111.90
1	6	1007	C	N3-C4-N4	-6.03	113.78	118.00
36	5	1181	U	N3-C2-O2	-6.03	117.98	122.20
36	1	1103	A	P-O3'-C3'	6.03	126.93	119.70
36	1	2886	U	N3-C4-O4	6.03	123.62	119.40
36	5	1896	A	O5'-P-OP1	-6.03	100.28	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2960	C	C2-N3-C4	-6.03	116.89	119.90
36	5	3212	C	C2-N1-C1'	-6.03	112.17	118.80
36	1	1192	C	C6-N1-C1'	-6.03	113.57	120.80
36	5	1495	U	C5-C6-N1	6.03	125.71	122.70
36	5	2147	A	N9-C4-C5	-6.03	103.39	105.80
36	1	63	A	C8-N9-C4	-6.02	103.39	105.80
36	5	1152	G	N1-C2-N3	6.02	127.51	123.90
36	5	2411	U	C6-N1-C2	6.02	124.61	121.00
36	1	857	G	C5-C6-N1	-6.02	108.49	111.50
36	1	2413	A	C8-N9-C4	6.02	108.21	105.80
36	5	3368	U	C2-N1-C1'	-6.02	110.48	117.70
36	1	3181	C	N3-C2-O2	-6.02	117.69	121.90
1	6	542	A	C8-N9-C4	-6.02	103.39	105.80
1	6	1162	C	C6-N1-C2	-6.02	117.89	120.30
36	1	648	C	O5'-P-OP1	-6.02	100.29	105.70
1	6	301	A	O5'-P-OP2	-6.02	100.29	105.70
36	5	1113	G	C5-C6-N1	-6.02	108.49	111.50
36	1	2153	U	C6-N1-C2	-6.01	117.39	121.00
73	O7	45	ARG	NE-CZ-NH1	-6.01	117.29	120.30
36	5	1841	A	O5'-P-OP1	-6.01	100.29	105.70
1	6	309	C	C4-C5-C6	6.01	120.41	117.40
1	6	1164	G	C5-C6-O6	-6.01	124.99	128.60
1	6	999	U	N3-C4-C5	6.01	118.21	114.60
36	5	3216	G	N1-C6-O6	6.01	123.51	119.90
1	2	507	U	N1-C2-O2	6.01	127.00	122.80
36	5	1372	C	N3-C4-C5	-6.01	119.50	121.90
50	m4	72	LEU	CA-CB-CG	6.01	129.12	115.30
36	5	2917	G	N3-C4-C5	-6.01	125.60	128.60
1	2	987	G	C5-C6-O6	6.00	132.20	128.60
1	6	815	G	N7-C8-N9	6.00	116.10	113.10
1	6	1010	C	O5'-P-OP2	-6.00	100.30	105.70
36	5	283	G	C5-C6-N1	6.00	114.50	111.50
36	5	1110	U	N3-C2-O2	-6.00	118.00	122.20
36	1	2621	G	O5'-P-OP1	6.00	117.90	110.70
36	5	1200	A	C6-C5-N7	-6.00	128.10	132.30
36	1	917	A	O5'-P-OP1	6.00	117.90	110.70
36	5	2710	C	N3-C2-O2	6.00	126.10	121.90
36	5	330	G	C8-N9-C4	6.00	108.80	106.40
37	7	49	G	C5-C6-N1	-6.00	108.50	111.50
36	1	273	A	C5-N7-C8	6.00	106.90	103.90
36	1	1838	G	C5-C6-O6	-6.00	125.00	128.60
36	1	3034	C	N3-C2-O2	-6.00	117.70	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	280	U	C2-N1-C1'	6.00	124.90	117.70
36	5	2717	U	N1-C2-N3	6.00	118.50	114.90
36	1	339	C	OP1-P-OP2	-6.00	110.60	119.60
36	1	935	U	N3-C2-O2	-6.00	118.00	122.20
37	7	37	G	N9-C4-C5	-6.00	103.00	105.40
36	1	1062	A	N1-C6-N6	-5.99	115.00	118.60
36	5	1449	A	C6-C5-N7	-5.99	128.10	132.30
36	5	66	A	N9-C4-C5	-5.99	103.40	105.80
36	5	831	G	C5-C6-O6	-5.99	125.00	128.60
36	1	1157	G	N1-C6-O6	-5.99	116.31	119.90
36	1	2613	U	N3-C4-C5	-5.99	111.01	114.60
36	1	2643	A	O5'-P-OP1	-5.99	100.31	105.70
36	5	209	A	C6-C5-N7	-5.99	128.11	132.30
36	1	1269	U	N1-C2-O2	5.99	126.99	122.80
36	5	1056	U	N1-C2-N3	5.99	118.49	114.90
36	1	1157	G	OP2-P-O3'	5.98	118.36	105.20
36	1	3344	A	C8-N9-C4	-5.98	103.41	105.80
1	6	1560	U	N3-C2-O2	-5.98	118.01	122.20
36	5	1495	U	C2-N1-C1'	5.98	124.88	117.70
36	5	2156	C	N3-C4-C5	5.98	124.29	121.90
38	4	53	A	C2-N3-C4	5.98	113.59	110.60
1	2	765	G	O4'-C1'-N9	-5.98	103.42	108.20
1	2	1324	G	C8-N9-C1'	5.98	134.77	127.00
1	6	582	U	C2-N1-C1'	5.98	124.88	117.70
36	5	1533	U	N3-C2-O2	-5.98	118.02	122.20
36	1	1445	U	C2-N3-C4	-5.98	123.41	127.00
36	5	394	G	N1-C6-O6	-5.98	116.31	119.90
36	5	2306	C	O5'-P-OP2	-5.98	100.32	105.70
36	5	2707	C	N3-C4-C5	5.98	124.29	121.90
1	2	1082	C	C6-N1-C2	-5.98	117.91	120.30
36	1	1445	U	N1-C2-O2	-5.98	118.62	122.80
1	6	426	G	C4-N9-C1'	5.97	134.27	126.50
1	6	1145	U	N3-C4-O4	5.97	123.58	119.40
1	6	1745	G	N9-C4-C5	-5.97	103.01	105.40
36	5	283	G	C6-C5-N7	-5.97	126.82	130.40
36	5	2412	G	N3-C4-C5	-5.97	125.61	128.60
36	1	1868	G	C4-C5-N7	5.97	113.19	110.80
36	1	670	C	C4-C5-C6	5.97	120.39	117.40
36	1	2727	A	C2-N3-C4	5.97	113.58	110.60
37	3	84	A	C6-C5-N7	-5.97	128.12	132.30
36	1	1556	C	C6-N1-C2	-5.97	117.91	120.30
36	5	652	G	C4-C5-C6	5.97	122.38	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2255	A	O5'-P-OP1	-5.97	100.33	105.70
36	5	343	U	O5'-P-OP1	-5.97	100.33	105.70
36	1	86	G	C8-N9-C4	-5.97	104.01	106.40
1	6	295	A	C8-N9-C4	5.97	108.19	105.80
1	6	1020	A	C8-N9-C4	-5.97	103.41	105.80
36	5	890	C	C6-N1-C2	5.97	122.69	120.30
36	5	3339	A	C5-C6-N6	-5.97	118.93	123.70
36	1	81	C	C5-C6-N1	-5.96	118.02	121.00
36	1	1313	G	C5-C6-N1	5.96	114.48	111.50
36	5	1000	C	C6-N1-C2	5.96	122.69	120.30
36	1	518	G	O4'-C1'-N9	5.96	112.97	108.20
37	7	37	G	N3-C4-N9	5.96	129.58	126.00
1	6	596	C	C6-N1-C2	5.96	122.68	120.30
36	5	2640	A	C8-N9-C4	5.96	108.18	105.80
36	5	3154	C	C6-N1-C2	-5.96	117.92	120.30
36	1	435	C	C5-C6-N1	-5.96	118.02	121.00
36	1	783	A	C8-N9-C4	5.96	108.18	105.80
36	1	2779	A	O5'-P-OP2	-5.96	100.34	105.70
36	1	2867	C	C5-C6-N1	-5.96	118.02	121.00
36	1	2993	G	OP1-P-OP2	5.96	128.54	119.60
36	1	3049	A	N1-C6-N6	5.96	122.17	118.60
36	1	797	U	OP2-P-O3'	5.96	118.30	105.20
36	1	1162	U	N3-C2-O2	-5.96	118.03	122.20
1	6	858	G	C4-N9-C1'	5.96	134.24	126.50
1	2	543	C	N1-C2-O2	5.95	122.47	118.90
36	1	231	G	O5'-P-OP2	-5.95	100.34	105.70
36	1	906	A	C5-C6-N6	-5.95	118.94	123.70
36	1	943	U	N3-C2-O2	-5.95	118.03	122.20
36	1	1556	C	N3-C2-O2	-5.95	117.73	121.90
36	5	1167	U	C5-C4-O4	-5.95	122.33	125.90
36	5	2392	C	N1-C2-O2	-5.95	115.33	118.90
36	1	2418	G	N3-C4-N9	5.95	129.57	126.00
1	2	1324	G	C4-C5-N7	-5.95	108.42	110.80
36	1	104	G	C5-C6-O6	-5.95	125.03	128.60
36	1	347	G	C5-C6-O6	-5.95	125.03	128.60
38	4	97	A	N1-C6-N6	-5.95	115.03	118.60
36	5	3245	A	C8-N9-C4	-5.95	103.42	105.80
73	o7	65	ARG	NE-CZ-NH1	5.95	123.28	120.30
36	1	3377	G	N1-C2-N2	-5.95	110.85	116.20
36	5	1924	U	C6-N1-C2	5.95	124.57	121.00
1	2	1768	G	C4-N9-C1'	-5.95	118.77	126.50
36	1	232	G	C4-C5-C6	5.95	122.37	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1774	G	N1-C6-O6	-5.94	116.33	119.90
36	1	875	G	N3-C2-N2	-5.94	115.74	119.90
36	5	2421	U	N1-C2-N3	5.94	118.47	114.90
1	2	334	G	N3-C4-C5	5.94	131.57	128.60
36	1	633	C	C4-C5-C6	5.94	120.37	117.40
36	5	2283	G	O5'-P-OP2	-5.94	100.35	105.70
36	1	2218	G	C8-N9-C4	5.94	108.78	106.40
1	6	804	A	N1-C6-N6	5.94	122.16	118.60
36	5	1109	U	N1-C2-O2	5.94	126.96	122.80
36	5	1391	C	N1-C2-O2	-5.94	115.34	118.90
36	5	2953	U	N1-C2-O2	-5.94	118.64	122.80
1	2	19	A	N1-C6-N6	5.94	122.16	118.60
1	2	1462	G	N9-C4-C5	-5.94	103.03	105.40
36	1	639	G	C6-C5-N7	-5.94	126.84	130.40
36	5	2743	A	N7-C8-N9	-5.94	110.83	113.80
36	5	150	A	N1-C6-N6	5.93	122.16	118.60
36	5	1056	U	C6-N1-C2	-5.93	117.44	121.00
36	5	1398	U	C5-C4-O4	5.93	129.46	125.90
36	5	1678	G	N1-C6-O6	-5.93	116.34	119.90
36	1	281	G	N1-C6-O6	5.93	123.46	119.90
36	5	1899	G	N9-C4-C5	5.93	107.77	105.40
36	1	78	U	N1-C2-N3	5.93	118.46	114.90
36	5	37	U	N1-C2-N3	5.93	118.46	114.90
36	5	1303	A	N7-C8-N9	-5.93	110.83	113.80
36	1	908	G	C4-N9-C1'	5.93	134.21	126.50
36	1	677	A	C8-N9-C4	5.93	108.17	105.80
36	1	2641	U	C5-C6-N1	-5.93	119.74	122.70
36	1	2946	A	N1-C6-N6	5.93	122.16	118.60
1	6	1765	A	O5'-P-OP1	-5.93	100.37	105.70
36	1	282	G	O5'-P-OP1	-5.92	100.37	105.70
36	1	1913	A	C8-N9-C4	5.92	108.17	105.80
36	5	2333	C	C6-N1-C2	5.92	122.67	120.30
37	7	91	G	C4-C5-N7	5.92	113.17	110.80
36	1	3322	A	N1-C6-N6	5.92	122.15	118.60
36	5	875	G	N3-C4-C5	-5.92	125.64	128.60
36	5	1931	U	C5-C6-N1	-5.92	119.74	122.70
36	5	3304	U	OP1-P-OP2	5.92	128.48	119.60
36	1	1296	C	N1-C2-N3	5.92	123.34	119.20
36	1	1133	A	N9-C4-C5	-5.92	103.43	105.80
36	1	2550	U	N1-C2-N3	5.92	118.45	114.90
80	c0	88	PRO	N-CA-CB	5.92	110.40	103.30
36	1	677	A	N1-C6-N6	5.92	122.15	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1909	A	C5-C6-N6	-5.92	118.97	123.70
1	6	1389	C	C2-N1-C1'	5.92	125.31	118.80
36	5	609	G	C6-C5-N7	-5.92	126.85	130.40
36	1	652	G	N3-C2-N2	5.91	124.04	119.90
36	1	1142	G	O5'-P-OP2	-5.91	100.38	105.70
36	1	1335	C	C2-N3-C4	-5.91	116.94	119.90
36	5	370	U	N3-C2-O2	-5.91	118.06	122.20
36	5	383	G	C8-N9-C4	5.91	108.77	106.40
36	5	504	A	C4-C5-N7	5.91	113.66	110.70
36	5	2816	G	C5-C6-O6	-5.91	125.05	128.60
36	1	1904	C	C6-N1-C2	-5.91	117.94	120.30
1	6	1597	A	C8-N9-C4	5.91	108.16	105.80
36	5	1178	G	C5-N7-C8	-5.91	101.34	104.30
1	2	1749	A	C8-N9-C4	5.91	108.16	105.80
36	1	739	G	C8-N9-C4	5.91	108.76	106.40
36	5	1909	A	N7-C8-N9	-5.91	110.85	113.80
36	5	3266	G	C5-C6-O6	5.91	132.15	128.60
36	5	884	A	N3-C4-N9	-5.91	122.67	127.40
36	1	2610	G	C5-C6-O6	-5.91	125.06	128.60
37	3	92	A	N1-C2-N3	5.91	132.25	129.30
36	5	1181	U	C4-C5-C6	5.91	123.24	119.70
36	5	1939	G	C6-C5-N7	-5.91	126.86	130.40
36	5	2377	G	C8-N9-C4	5.90	108.76	106.40
1	6	1478	G	N3-C4-N9	5.90	129.54	126.00
36	5	1847	A	O5'-P-OP2	-5.90	100.39	105.70
36	5	1937	U	C5-C6-N1	-5.90	119.75	122.70
36	1	2384	A	C6-C5-N7	-5.90	128.17	132.30
36	5	2383	C	N3-C4-N4	5.90	122.13	118.00
1	2	1202	A	C8-N9-C4	-5.90	103.44	105.80
36	5	220	G	O5'-P-OP2	-5.90	100.39	105.70
36	5	1239	C	C2-N1-C1'	5.90	125.29	118.80
36	1	2695	A	C8-N9-C4	-5.90	103.44	105.80
41	L4	139	GLY	N-CA-C	-5.90	98.36	113.10
1	6	1389	C	N1-C2-O2	5.90	122.44	118.90
36	5	2215	A	C2-N3-C4	-5.90	107.65	110.60
36	5	1592	G	C5-C6-O6	5.90	132.14	128.60
36	1	365	A	N1-C2-N3	5.89	132.25	129.30
36	1	1416	C	N3-C2-O2	-5.89	117.77	121.90
36	1	3275	U	OP1-P-O3'	5.89	118.17	105.20
38	4	103	G	N3-C4-N9	5.89	129.54	126.00
36	5	938	C	C6-N1-C2	5.89	122.66	120.30
37	3	33	U	N3-C2-O2	-5.89	118.08	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	400	A	N1-C6-N6	5.89	122.14	118.60
36	5	3374	U	N3-C4-C5	5.89	118.14	114.60
1	2	1432	U	C5-C6-N1	-5.89	119.76	122.70
36	5	3008	A	O5'-P-OP1	5.89	117.77	110.70
36	5	3105	U	C5-C6-N1	-5.89	119.76	122.70
1	2	736	C	C2-N1-C1'	5.89	125.28	118.80
36	1	1489	A	C5-C6-N6	-5.89	118.99	123.70
36	1	2193	U	N3-C2-O2	-5.89	118.08	122.20
36	1	2601	A	N7-C8-N9	-5.89	110.86	113.80
1	6	1600	A	N1-C6-N6	5.89	122.13	118.60
1	6	1432	U	C5-C6-N1	-5.88	119.76	122.70
36	5	2698	G	C8-N9-C4	5.88	108.75	106.40
36	5	907	G	N1-C2-N2	-5.88	110.91	116.20
36	5	1843	C	C2-N1-C1'	5.88	125.27	118.80
36	5	2169	G	N1-C6-O6	-5.88	116.37	119.90
1	2	314	C	N3-C4-C5	5.88	124.25	121.90
36	5	3123	A	N9-C4-C5	-5.88	103.45	105.80
36	1	2408	U	N3-C4-C5	-5.88	111.07	114.60
36	1	3114	A	C8-N9-C4	5.88	108.15	105.80
38	4	13	A	N1-C6-N6	5.88	122.13	118.60
1	6	1535	U	N3-C2-O2	-5.88	118.08	122.20
36	5	2735	U	C2-N1-C1'	5.88	124.75	117.70
36	5	3054	U	O5'-P-OP2	-5.88	100.41	105.70
36	1	517	G	N3-C4-C5	-5.88	125.66	128.60
36	5	1893	A	C8-N9-C4	5.88	108.15	105.80
36	1	1906	G	O5'-P-OP1	-5.88	100.41	105.70
1	2	186	C	C5-C6-N1	5.87	123.94	121.00
1	6	1029	U	C2-N1-C1'	-5.87	110.65	117.70
36	5	504	A	C5-C6-N6	-5.87	119.00	123.70
36	5	1200	A	N3-C4-C5	-5.87	122.69	126.80
36	1	350	C	C6-N1-C2	-5.87	117.95	120.30
36	1	957	C	N1-C2-O2	-5.87	115.38	118.90
36	5	3245	A	C5-C6-N1	-5.87	114.76	117.70
1	2	720	G	OP1-P-O3'	5.87	118.11	105.20
36	1	1124	U	N1-C2-O2	5.87	126.91	122.80
1	6	163	G	C5-N7-C8	-5.87	101.37	104.30
36	5	2952	G	N1-C6-O6	-5.87	116.38	119.90
52	m6	27	LEU	CA-CB-CG	-5.87	101.81	115.30
1	2	404	G	C5-C6-O6	-5.87	125.08	128.60
36	5	3015	G	C5-C6-N1	-5.87	108.57	111.50
1	2	635	A	N1-C6-N6	5.86	122.12	118.60
36	1	2301	U	O5'-P-OP2	-5.86	100.42	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2942	C	N1-C2-O2	-5.86	115.38	118.90
36	1	3324	C	C6-N1-C2	5.86	122.64	120.30
36	5	3050	U	C5-C4-O4	5.86	129.42	125.90
36	1	2636	A	N7-C8-N9	5.86	116.73	113.80
1	6	1	U	C2-N1-C1'	5.86	124.73	117.70
1	6	1643	U	C5-C6-N1	-5.86	119.77	122.70
36	5	1694	U	N1-C2-N3	5.86	118.42	114.90
36	1	282	G	C2'-C3'-O3'	5.86	123.08	113.70
36	5	41	G	C4-C5-N7	5.86	113.14	110.80
36	5	1010	G	C2-N3-C4	5.86	114.83	111.90
36	1	788	C	C6-N1-C2	5.86	122.64	120.30
1	2	1600	A	C2-N3-C4	-5.86	107.67	110.60
1	6	961	U	C6-N1-C2	-5.86	117.49	121.00
36	1	582	G	N1-C6-O6	-5.85	116.39	119.90
36	1	895	A	C5-N7-C8	-5.85	100.97	103.90
36	1	3326	G	N9-C4-C5	-5.85	103.06	105.40
36	1	346	C	C5-C6-N1	-5.85	118.07	121.00
36	1	700	C	C6-N1-C2	5.85	122.64	120.30
36	5	1158	A	C5-C6-N6	-5.85	119.02	123.70
36	5	2524	A	C5-N7-C8	-5.85	100.97	103.90
36	1	1171	G	N7-C8-N9	-5.85	110.17	113.10
1	6	1029	U	C6-N1-C1'	5.85	129.39	121.20
36	1	1047	A	C5-N7-C8	-5.85	100.98	103.90
36	1	1856	C	C5-C4-N4	-5.85	116.11	120.20
36	1	3057	U	C6-N1-C2	-5.85	117.49	121.00
36	1	1868	G	C6-C5-N7	-5.85	126.89	130.40
36	5	1436	U	N3-C2-O2	-5.85	118.11	122.20
36	5	2295	A	O5'-P-OP2	-5.85	100.44	105.70
36	1	2871	G	C4-N9-C1'	-5.85	118.90	126.50
36	5	2288	G	N9-C4-C5	-5.85	103.06	105.40
47	m0	48	LEU	CA-CB-CG	5.85	128.75	115.30
36	1	808	A	N1-C2-N3	5.84	132.22	129.30
36	1	1905	G	N3-C4-N9	-5.84	122.49	126.00
36	1	3326	G	N3-C2-N2	5.84	123.99	119.90
36	5	427	C	O5'-P-OP1	-5.84	100.44	105.70
36	5	1115	G	C8-N9-C4	-5.84	104.06	106.40
36	5	2800	G	N3-C2-N2	-5.84	115.81	119.90
1	2	298	C	C6-N1-C2	5.84	122.64	120.30
36	5	1879	A	C4-C5-N7	5.84	113.62	110.70
36	5	3362	A	O4'-C1'-N9	5.84	112.87	108.20
36	5	3018	C	O5'-P-OP1	5.84	117.71	110.70
1	2	1600	A	C5-C6-N1	-5.84	114.78	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	339	C	N3-C4-N4	-5.84	113.91	118.00
36	1	24	G	C8-N9-C4	5.84	108.73	106.40
36	5	300	G	O5'-P-OP1	-5.84	100.45	105.70
36	5	1433	A	N9-C4-C5	5.84	108.14	105.80
36	5	3351	U	N3-C2-O2	-5.84	118.11	122.20
37	7	101	G	N9-C4-C5	-5.84	103.07	105.40
1	6	1782	A	N7-C8-N9	5.83	116.72	113.80
36	1	361	A	C8-N9-C4	5.83	108.13	105.80
36	1	1617	G	C8-N9-C4	5.83	108.73	106.40
36	5	939	U	O5'-P-OP2	-5.83	100.45	105.70
36	5	2919	A	C5-C6-N6	5.83	128.37	123.70
1	2	169	A	N1-C6-N6	5.83	122.10	118.60
36	1	2606	G	N9-C4-C5	-5.83	103.07	105.40
36	5	1902	G	C5-C6-N1	-5.83	108.58	111.50
36	5	2233	A	C8-N9-C4	5.83	108.13	105.80
36	5	2403	G	O5'-P-OP2	-5.83	100.45	105.70
1	6	310	C	N3-C4-N4	5.83	122.08	118.00
1	6	331	A	N1-C6-N6	-5.83	115.10	118.60
36	5	1116	G	N1-C2-N3	5.83	127.40	123.90
36	5	3287	U	N1-C2-O2	5.83	126.88	122.80
36	1	1604	G	C2-N3-C4	5.83	114.81	111.90
36	1	2372	A	C4-C5-C6	5.83	119.91	117.00
36	5	1847	A	N3-C4-C5	5.83	130.88	126.80
36	1	2314	U	C6-N1-C1'	-5.82	113.05	121.20
36	5	838	G	N1-C6-O6	-5.82	116.41	119.90
36	5	2271	A	N1-C2-N3	-5.82	126.39	129.30
36	1	2284	C	N3-C2-O2	-5.82	117.83	121.90
38	4	9	A	N1-C6-N6	-5.82	115.11	118.60
36	5	3041	U	N3-C4-C5	5.82	118.09	114.60
36	1	1224	C	C6-N1-C2	-5.82	117.97	120.30
36	1	1798	A	C2-N3-C4	-5.82	107.69	110.60
36	1	2916	U	OP1-P-O3'	5.82	118.00	105.20
36	1	3312	U	C5-C6-N1	-5.82	119.79	122.70
36	1	324	A	N1-C2-N3	5.82	132.21	129.30
36	5	2197	C	N3-C4-C5	5.82	124.23	121.90
36	5	2211	U	C5-C4-O4	5.82	129.39	125.90
36	5	2323	G	N9-C4-C5	5.82	107.73	105.40
1	2	1600	A	P-O3'-C3'	5.82	126.68	119.70
36	1	1537	A	N1-C6-N6	5.82	122.09	118.60
38	4	99	C	N3-C4-C5	5.82	124.23	121.90
37	7	92	A	C8-N9-C4	5.81	108.12	105.80
36	5	2639	G	C4-N9-C1'	5.81	134.06	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	89	G	C8-N9-C4	5.81	108.72	106.40
36	1	1114	U	N3-C2-O2	-5.81	118.13	122.20
36	1	2123	G	N7-C8-N9	-5.81	110.19	113.10
36	1	2791	G	C8-N9-C4	-5.81	104.08	106.40
70	O4	51	LEU	CA-CB-CG	5.81	128.66	115.30
36	5	1792	C	C6-N1-C2	5.81	122.62	120.30
36	5	2267	C	N3-C4-C5	5.81	124.22	121.90
36	1	1928	G	N3-C4-N9	-5.81	122.52	126.00
36	5	3147	G	C2-N3-C4	-5.81	109.00	111.90
37	7	98	C	O5'-P-OP2	-5.81	100.47	105.70
36	1	81	C	C6-N1-C2	5.81	122.62	120.30
36	1	1884	A	C5-C6-N6	-5.81	119.05	123.70
36	1	3318	G	C4-N9-C1'	5.81	134.05	126.50
38	8	17	A	N9-C4-C5	-5.81	103.48	105.80
36	1	919	U	N3-C4-C5	5.81	118.08	114.60
36	1	2617	U	N3-C2-O2	-5.81	118.14	122.20
36	1	3312	U	C6-N1-C2	5.81	124.48	121.00
1	6	359	A	N3-C4-C5	5.81	130.86	126.80
36	5	2383	C	N1-C2-O2	-5.81	115.42	118.90
36	5	2797	C	N1-C2-O2	-5.81	115.42	118.90
36	1	1099	A	OP1-P-OP2	-5.80	110.89	119.60
36	1	2935	U	C5-C6-N1	5.80	125.60	122.70
37	3	82	G	N1-C2-N3	5.80	127.38	123.90
1	6	1581	C	C6-N1-C2	5.80	122.62	120.30
36	5	3285	C	N1-C2-O2	5.80	122.38	118.90
36	1	1110	U	N3-C4-C5	5.80	118.08	114.60
36	1	3123	A	C2-N3-C4	-5.80	107.70	110.60
36	5	1207	G	N7-C8-N9	-5.80	110.20	113.10
1	2	73	U	OP1-P-O3'	5.80	117.96	105.20
36	1	1379	G	N1-C2-N3	5.80	127.38	123.90
36	1	780	A	N9-C4-C5	5.80	108.12	105.80
36	1	1369	A	O5'-P-OP1	-5.80	100.48	105.70
36	1	152	U	N3-C4-C5	-5.80	111.12	114.60
36	5	337	G	N3-C4-C5	-5.80	125.70	128.60
36	1	2394	G	C5-C6-O6	5.79	132.08	128.60
36	1	3270	U	C2-N1-C1'	-5.79	110.75	117.70
36	5	2288	G	C6-N1-C2	-5.79	121.62	125.10
36	5	2772	C	P-O3'-C3'	5.79	126.65	119.70
36	1	645	A	N3-C4-C5	-5.79	122.75	126.80
36	1	1715	A	O4'-C1'-N9	-5.79	103.57	108.20
36	1	3025	C	C6-N1-C2	5.79	122.62	120.30
36	5	776	U	N3-C2-O2	-5.79	118.15	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1084	A	C2-N3-C4	-5.79	107.70	110.60
36	1	2699	G	C5-C6-O6	-5.79	125.13	128.60
36	5	1724	U	C6-N1-C1'	5.79	129.31	121.20
1	6	1637	C	N1-C2-O2	5.79	122.37	118.90
36	5	2881	C	C6-N1-C2	5.79	122.62	120.30
36	5	2965	U	C5-C4-O4	-5.79	122.43	125.90
36	1	1307	G	N1-C6-O6	-5.79	116.43	119.90
36	5	2137	U	O5'-P-OP1	-5.79	100.49	105.70
36	1	2243	A	N1-C6-N6	-5.79	115.13	118.60
1	6	473	A	N1-C6-N6	-5.79	115.13	118.60
36	5	1389	G	C5-C6-O6	-5.79	125.13	128.60
36	5	2634	U	N3-C4-C5	5.78	118.07	114.60
36	1	2356	A	C4-C5-N7	5.78	113.59	110.70
36	5	1183	C	C6-N1-C2	5.78	122.61	120.30
36	1	2870	C	C2-N3-C4	-5.78	117.01	119.90
36	5	690	A	C8-N9-C4	5.78	108.11	105.80
36	5	2865	U	C5-C4-O4	-5.78	122.43	125.90
36	1	1389	G	C8-N9-C1'	-5.78	119.49	127.00
36	1	3143	C	N1-C2-O2	-5.78	115.43	118.90
36	5	1782	U	N1-C2-O2	-5.78	118.75	122.80
1	2	734	A	OP1-P-O3'	5.78	117.91	105.20
36	1	345	G	C4-C5-C6	5.78	122.27	118.80
36	1	650	C	C6-N1-C2	5.78	122.61	120.30
36	1	1405	U	N3-C2-O2	5.78	126.24	122.20
36	5	622	A	N1-C6-N6	5.78	122.07	118.60
1	2	942	G	N1-C6-O6	-5.78	116.44	119.90
1	6	863	A	N1-C6-N6	5.78	122.06	118.60
36	1	1397	C	N3-C4-C5	5.77	124.21	121.90
37	3	33	U	N1-C2-O2	5.77	126.84	122.80
36	5	921	A	C8-N9-C4	-5.77	103.49	105.80
1	2	1029	U	C5-C6-N1	-5.77	119.81	122.70
36	1	29	C	C5-C4-N4	-5.77	116.16	120.20
36	5	1826	C	C6-N1-C2	5.77	122.61	120.30
36	1	835	G	O4'-C1'-N9	5.77	112.82	108.20
36	1	992	A	C5-C6-N1	5.77	120.59	117.70
36	5	1449	A	C2-N3-C4	-5.77	107.71	110.60
36	5	1493	G	O4'-C1'-N9	5.77	112.82	108.20
36	5	1899	G	C5-C6-O6	5.77	132.06	128.60
1	2	940	A	N9-C4-C5	5.77	108.11	105.80
36	1	1151	U	N3-C4-O4	5.77	123.44	119.40
36	1	1433	A	N3-C4-C5	-5.77	122.76	126.80
36	1	2199	G	C5-C6-O6	5.77	132.06	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2861	U	OP2-P-O3'	5.77	117.89	105.20
36	5	640	U	N3-C4-O4	5.77	123.44	119.40
36	1	81	C	C2-N3-C4	-5.77	117.02	119.90
36	1	347	G	N9-C4-C5	-5.77	103.09	105.40
36	1	439	C	N1-C2-O2	5.77	122.36	118.90
36	1	2795	U	N1-C2-N3	5.77	118.36	114.90
1	6	455	C	N3-C4-N4	5.77	122.04	118.00
36	5	2799	A	O5'-P-OP2	-5.77	100.51	105.70
36	1	1116	G	N1-C6-O6	5.77	123.36	119.90
1	2	1119	G	N1-C6-O6	-5.76	116.44	119.90
36	1	1369	A	C2-N3-C4	-5.76	107.72	110.60
1	6	352	A	OP2-P-O3'	5.76	117.88	105.20
36	1	788	C	C2-N1-C1'	-5.76	112.46	118.80
36	5	1547	G	C8-N9-C4	5.76	108.70	106.40
1	2	543	C	N3-C2-O2	-5.76	117.87	121.90
36	1	2261	G	N3-C4-N9	5.76	129.46	126.00
36	5	2843	U	O5'-P-OP1	-5.76	100.51	105.70
37	7	98	C	C6-N1-C2	5.76	122.61	120.30
36	1	2305	G	C6-C5-N7	-5.76	126.94	130.40
38	4	43	A	O5'-P-OP1	-5.76	100.52	105.70
1	6	1664	C	N1-C2-O2	-5.76	115.45	118.90
36	1	2343	C	C5-C4-N4	-5.75	116.17	120.20
1	6	194	U	N1-C2-O2	5.75	126.83	122.80
36	1	25	U	N1-C2-O2	-5.75	118.77	122.80
36	1	3076	C	C6-N1-C2	-5.75	118.00	120.30
36	5	2728	G	O4'-C1'-N9	5.75	112.80	108.20
36	5	2868	U	N1-C2-O2	5.75	126.83	122.80
36	1	3368	U	C6-N1-C1'	5.75	129.25	121.20
1	6	25	C	P-O3'-C3'	5.75	126.60	119.70
1	6	901	G	O4'-C1'-N9	5.75	112.80	108.20
36	1	968	G	C6-C5-N7	-5.75	126.95	130.40
36	5	369	A	C8-N9-C4	-5.75	103.50	105.80
36	5	2887	A	C4-C5-C6	5.75	119.88	117.00
38	4	29	U	N3-C4-O4	5.75	123.42	119.40
36	5	2808	A	N9-C4-C5	-5.75	103.50	105.80
36	1	2165	G	N1-C6-O6	5.75	123.35	119.90
36	1	2836	C	N3-C2-O2	-5.75	117.88	121.90
36	5	1368	U	N3-C2-O2	5.75	126.22	122.20
36	1	917	A	N1-C6-N6	-5.74	115.15	118.60
36	5	911	C	C2-N3-C4	-5.74	117.03	119.90
1	2	329	G	N1-C2-N3	5.74	127.34	123.90
1	2	426	G	C4-N9-C1'	5.74	133.96	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2408	U	C4-C5-C6	5.74	123.14	119.70
36	5	2372	A	N7-C8-N9	5.74	116.67	113.80
1	2	1600	A	N1-C6-N6	5.74	122.04	118.60
36	1	92	G	C5-C6-N1	5.74	114.37	111.50
1	6	1413	U	OP2-P-O3'	5.74	117.82	105.20
1	6	1473	U	C6-N1-C2	-5.74	117.56	121.00
36	5	876	A	C8-N9-C4	5.74	108.10	105.80
36	5	3335	A	N1-C6-N6	5.74	122.04	118.60
54	m8	127	LEU	CA-CB-CG	5.74	128.50	115.30
1	2	507	U	N3-C2-O2	-5.74	118.18	122.20
1	2	1269	U	C6-N1-C1'	-5.74	113.17	121.20
36	1	1310	G	N1-C6-O6	-5.74	116.46	119.90
1	6	151	G	N3-C2-N2	-5.74	115.89	119.90
36	5	2387	A	C5-C6-N6	-5.74	119.11	123.70
36	5	2921	U	C5-C4-O4	-5.74	122.46	125.90
36	5	2931	C	C6-N1-C2	5.74	122.59	120.30
36	1	2376	G	C5-C6-N1	5.73	114.37	111.50
1	6	163	G	C2-N3-C4	-5.73	109.03	111.90
36	5	2600	C	C2-N1-C1'	5.73	125.11	118.80
1	2	585	A	N1-C6-N6	5.73	122.04	118.60
1	2	734	A	P-O3'-C3'	5.73	126.58	119.70
36	1	942	U	N1-C2-N3	5.73	118.34	114.90
36	1	1157	G	C4-C5-N7	-5.73	108.51	110.80
36	5	1846	C	C5-C6-N1	-5.73	118.13	121.00
36	1	1113	G	N3-C2-N2	-5.73	115.89	119.90
36	5	3373	U	C5-C6-N1	-5.73	119.83	122.70
36	1	816	A	C8-N9-C4	-5.73	103.51	105.80
36	1	1520	G	N3-C4-N9	5.73	129.44	126.00
36	5	2355	G	N1-C6-O6	5.73	123.34	119.90
36	1	1151	U	C5-C6-N1	5.73	125.56	122.70
36	1	2308	C	C5-C6-N1	-5.73	118.14	121.00
25	d3	33	LEU	CA-CB-CG	-5.73	102.13	115.30
36	5	83	U	C5-C4-O4	-5.73	122.46	125.90
36	5	2112	U	O5'-P-OP1	-5.73	100.54	105.70
36	1	715	A	N7-C8-N9	5.73	116.66	113.80
36	1	931	C	N3-C2-O2	-5.73	117.89	121.90
1	6	194	U	C5-C6-N1	5.73	125.56	122.70
36	1	324	A	C6-N1-C2	-5.72	115.17	118.60
36	1	1365	G	C6-N1-C2	-5.72	121.67	125.10
36	5	907	G	N9-C4-C5	-5.72	103.11	105.40
36	1	1417	G	N3-C4-C5	5.72	131.46	128.60
36	1	2936	A	O5'-P-OP2	-5.72	100.55	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1595	U	O4'-C1'-N1	5.72	112.78	108.20
6	s4	38	LEU	CA-CB-CG	5.72	128.46	115.30
36	5	1939	G	C8-N9-C1'	-5.72	119.56	127.00
36	1	1658	G	C5-C6-O6	5.72	132.03	128.60
1	6	1042	G	C8-N9-C4	5.72	108.69	106.40
36	1	419	G	N9-C4-C5	-5.72	103.11	105.40
36	1	1497	C	C6-N1-C2	-5.72	118.01	120.30
1	6	1619	C	C6-N1-C2	-5.72	118.01	120.30
36	5	101	G	C4-N9-C1'	5.72	133.94	126.50
36	5	804	C	N3-C4-N4	5.72	122.00	118.00
36	5	1152	G	N9-C4-C5	5.72	107.69	105.40
36	5	1662	G	N1-C6-O6	5.72	123.33	119.90
36	5	1899	G	C4-C5-N7	-5.72	108.51	110.80
36	5	3041	U	N3-C4-O4	-5.72	115.40	119.40
1	2	554	C	C2-N3-C4	5.72	122.76	119.90
36	5	3317	U	O4'-C1'-N1	5.72	112.77	108.20
36	1	1482	A	C5-N7-C8	-5.72	101.04	103.90
36	1	1490	A	C2-N3-C4	-5.72	107.74	110.60
37	3	81	U	C6-N1-C2	5.72	124.43	121.00
1	6	1111	G	C6-C5-N7	-5.72	126.97	130.40
1	6	1745	G	C5-C6-N1	5.72	114.36	111.50
36	5	2825	C	N3-C2-O2	5.72	125.90	121.90
18	C6	53	LEU	CA-CB-CG	-5.71	102.16	115.30
1	6	1389	C	N3-C2-O2	-5.71	117.90	121.90
36	5	61	A	O5'-P-OP1	-5.71	100.56	105.70
36	5	1868	G	N1-C6-O6	5.71	123.33	119.90
36	5	2288	G	N3-C4-N9	5.71	129.43	126.00
36	1	1116	G	N3-C2-N2	-5.71	115.90	119.90
1	6	787	G	N3-C4-C5	-5.71	125.75	128.60
1	6	1523	G	N1-C6-O6	-5.71	116.47	119.90
36	5	767	U	O4'-C1'-N1	5.71	112.77	108.20
36	5	2350	C	OP1-P-OP2	-5.71	111.03	119.60
36	1	969	C	C2-N3-C4	-5.71	117.05	119.90
36	1	1303	A	N9-C4-C5	-5.71	103.52	105.80
36	1	2714	G	N3-C2-N2	-5.71	115.90	119.90
1	6	861	U	N3-C2-O2	-5.71	118.20	122.20
36	5	1939	G	C4-C5-C6	5.71	122.22	118.80
36	5	2775	U	C5-C6-N1	-5.71	119.85	122.70
1	2	499	U	P-O3'-C3'	5.71	126.55	119.70
1	2	571	G	C4-C5-N7	-5.71	108.52	110.80
1	2	1486	G	C8-N9-C4	-5.71	104.12	106.40
1	6	610	G	N3-C4-N9	5.71	129.42	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2841	G	OP1-P-OP2	5.71	128.16	119.60
36	1	2618	G	C6-N1-C2	-5.70	121.68	125.10
1	6	825	U	N3-C2-O2	5.70	126.19	122.20
36	5	504	A	N9-C4-C5	-5.70	103.52	105.80
36	5	1868	G	C4-C5-N7	5.70	113.08	110.80
36	5	1892	G	C5-N7-C8	5.70	107.15	104.30
36	1	1158	A	N1-C6-N6	5.70	122.02	118.60
36	1	582	G	C5-C6-O6	5.70	132.02	128.60
36	1	810	A	N1-C6-N6	-5.70	115.18	118.60
36	1	2309	A	N1-C6-N6	5.70	122.02	118.60
1	6	961	U	N3-C4-C5	-5.70	111.18	114.60
36	5	414	U	N3-C2-O2	5.70	126.19	122.20
36	5	1445	U	N1-C2-N3	5.70	118.32	114.90
36	5	1602	A	OP2-P-O3'	5.70	117.74	105.20
1	2	1747	G	C8-N9-C4	5.70	108.68	106.40
36	1	182	U	C2-N1-C1'	-5.70	110.86	117.70
36	1	2873	U	N3-C2-O2	-5.70	118.21	122.20
36	5	1909	A	N9-C4-C5	-5.70	103.52	105.80
36	1	674	G	C8-N9-C4	-5.70	104.12	106.40
36	1	2873	U	C5-C4-O4	5.70	129.32	125.90
1	6	574	G	C8-N9-C4	5.70	108.68	106.40
36	5	581	U	C5-C4-O4	-5.70	122.48	125.90
36	5	658	G	O5'-P-OP2	-5.70	100.58	105.70
36	5	1903	U	C2-N3-C4	5.70	130.42	127.00
36	5	3218	A	C2-N3-C4	-5.70	107.75	110.60
1	6	1649	G	N3-C2-N2	5.69	123.89	119.90
14	c2	58	LEU	CA-CB-CG	5.69	128.40	115.30
36	5	1370	G	C5-C6-N1	5.69	114.35	111.50
36	5	3147	G	N1-C2-N3	5.69	127.32	123.90
36	1	1327	C	C6-N1-C2	-5.69	118.02	120.30
36	5	1389	G	N1-C6-O6	5.69	123.32	119.90
36	5	2849	C	N1-C2-O2	-5.69	115.48	118.90
36	1	203	G	C8-N9-C4	5.69	108.68	106.40
36	1	1399	A	C8-N9-C4	5.69	108.08	105.80
36	1	1834	U	N1-C2-N3	5.69	118.31	114.90
36	1	3107	U	O5'-P-OP2	-5.69	100.58	105.70
36	1	99	A	O4'-C1'-N9	5.69	112.75	108.20
1	2	940	A	N1-C6-N6	-5.69	115.19	118.60
1	2	1486	G	C5-N7-C8	-5.69	101.46	104.30
36	1	808	A	C6-N1-C2	-5.69	115.19	118.60
59	N3	48	ARG	NE-CZ-NH1	5.69	123.14	120.30
20	C8	3	LEU	CA-CB-CG	5.68	128.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	e1	100	LEU	CA-CB-CG	5.68	128.37	115.30
36	5	2699	G	N9-C4-C5	-5.68	103.13	105.40
36	1	1589	A	O5'-P-OP2	-5.68	100.58	105.70
36	5	3326	G	N9-C4-C5	-5.68	103.13	105.40
36	1	2679	A	C6-C5-N7	-5.68	128.32	132.30
1	6	864	U	N3-C2-O2	-5.68	118.22	122.20
36	5	1595	U	N3-C2-O2	5.68	126.17	122.20
36	5	1650	G	N1-C6-O6	-5.68	116.49	119.90
36	5	1886	A	C4-C5-N7	5.68	113.54	110.70
36	5	2428	U	O5'-P-OP1	5.68	117.52	110.70
36	5	2839	G	C8-N9-C4	5.68	108.67	106.40
36	5	2849	C	OP2-P-O3'	5.68	117.69	105.20
36	1	1476	G	C6-C5-N7	5.68	133.81	130.40
36	1	1951	C	C2-N1-C1'	5.68	125.05	118.80
36	1	2383	C	C5-C4-N4	-5.68	116.23	120.20
36	1	3318	G	C6-C5-N7	-5.68	126.99	130.40
38	4	29	U	C5-C4-O4	-5.68	122.49	125.90
38	8	99	C	N1-C2-O2	5.68	122.31	118.90
1	2	1588	G	N1-C6-O6	-5.67	116.50	119.90
36	1	2818	U	C5-C6-N1	5.67	125.54	122.70
1	6	813	U	C6-N1-C1'	-5.67	113.26	121.20
36	1	650	C	OP2-P-O3'	5.67	117.68	105.20
36	5	1303	A	N9-C4-C5	-5.67	103.53	105.80
36	1	2363	A	C5-C6-N6	-5.67	119.16	123.70
36	1	1433	A	N3-C4-N9	5.67	131.93	127.40
36	1	2289	U	N1-C2-N3	5.67	118.30	114.90
36	1	3181	C	N1-C2-N3	5.67	123.17	119.20
36	5	411	U	C5-C6-N1	-5.67	119.87	122.70
36	5	2680	A	C5-N7-C8	5.67	106.73	103.90
36	5	2956	A	C4-C5-C6	5.67	119.83	117.00
36	5	3078	U	N3-C2-O2	-5.67	118.23	122.20
36	5	3197	G	N3-C4-N9	-5.67	122.60	126.00
1	2	1241	G	C4-C5-N7	5.66	113.06	110.80
36	1	345	G	N3-C4-C5	-5.66	125.77	128.60
36	1	2618	G	N1-C6-O6	-5.66	116.50	119.90
36	1	2816	G	O4'-C1'-N9	5.66	112.73	108.20
36	5	1003	A	C8-N9-C4	5.66	108.07	105.80
36	5	1307	G	C2'-C3'-O3'	5.66	122.76	113.70
36	5	2167	A	N9-C4-C5	5.66	108.06	105.80
36	1	1845	G	N1-C6-O6	-5.66	116.50	119.90
36	5	2197	C	C5-C4-N4	-5.66	116.24	120.20
36	5	3351	U	N1-C2-O2	5.66	126.76	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2961	G	N9-C4-C5	5.66	107.67	105.40
1	2	1370	U	P-O3'-C3'	5.66	126.49	119.70
1	6	95	G	C5-C6-O6	5.66	132.00	128.60
1	6	813	U	N1-C2-O2	5.66	126.76	122.80
36	5	921	A	OP2-P-O3'	5.66	117.65	105.20
36	5	2399	A	C8-N9-C4	5.66	108.06	105.80
1	6	95	G	N1-C6-O6	-5.66	116.51	119.90
36	1	1929	G	N9-C4-C5	-5.65	103.14	105.40
36	1	783	A	C5-C6-N6	-5.65	119.18	123.70
36	1	1348	U	O4'-C1'-N1	5.65	112.72	108.20
36	1	1520	G	N3-C4-C5	-5.65	125.77	128.60
36	1	1881	A	N1-C6-N6	-5.65	115.21	118.60
36	1	2148	U	N1-C2-O2	-5.65	118.84	122.80
38	4	47	C	C5-C6-N1	-5.65	118.17	121.00
1	6	637	C	N3-C4-C5	5.65	124.16	121.90
36	5	1561	G	O4'-C1'-N9	5.65	112.72	108.20
36	5	3148	U	C6-N1-C2	5.65	124.39	121.00
1	6	176	C	N3-C2-O2	-5.65	117.95	121.90
36	5	1443	G	C8-N9-C1'	-5.65	119.66	127.00
36	5	3131	U	N3-C4-C5	5.65	117.99	114.60
37	7	120	C	N3-C4-C5	5.65	124.16	121.90
36	1	1362	G	C8-N9-C4	5.65	108.66	106.40
36	1	2679	A	O4'-C1'-N9	5.65	112.72	108.20
36	1	2700	G	N3-C4-N9	5.65	129.39	126.00
36	1	3275	U	C6-N1-C2	-5.65	117.61	121.00
36	5	2260	U	N3-C2-O2	-5.65	118.25	122.20
36	1	590	G	C8-N9-C4	5.65	108.66	106.40
36	1	3269	U	C5-C4-O4	5.65	129.29	125.90
54	M8	99	THR	N-CA-C	5.65	126.24	111.00
36	5	1389	G	N3-C4-N9	5.65	129.39	126.00
36	5	2343	C	O5'-P-OP2	-5.65	100.62	105.70
36	1	2392	C	C6-N1-C2	5.64	122.56	120.30
36	1	2875	U	C3'-C2'-C1'	-5.64	96.98	101.50
36	5	902	G	C8-N9-C4	5.64	108.66	106.40
36	5	1898	G	N1-C6-O6	5.64	123.29	119.90
36	1	3318	G	N7-C8-N9	5.64	115.92	113.10
36	1	2361	A	N1-C2-N3	5.64	132.12	129.30
36	5	1376	C	OP1-P-OP2	5.64	128.06	119.60
1	2	1560	U	N3-C2-O2	-5.64	118.25	122.20
1	6	1602	C	N3-C2-O2	-5.64	117.95	121.90
36	5	197	G	C6-C5-N7	-5.64	127.02	130.40
36	5	1451	C	C6-N1-C2	5.64	122.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2964	G	C5-N7-C8	5.64	107.12	104.30
36	5	3115	C	O5'-P-OP2	-5.64	100.62	105.70
36	1	1884	A	C4-C5-N7	5.64	113.52	110.70
1	6	430	G	O5'-P-OP1	-5.64	100.63	105.70
1	2	7	G	C4-C5-N7	-5.64	108.55	110.80
36	1	1658	G	C8-N9-C4	-5.64	104.14	106.40
36	1	2855	U	C5-C6-N1	-5.64	119.88	122.70
36	5	3008	A	N1-C2-N3	5.64	132.12	129.30
1	2	1761	U	N3-C4-C5	-5.63	111.22	114.60
36	1	1585	C	C6-N1-C2	5.63	122.55	120.30
36	5	1452	A	C5-N7-C8	-5.63	101.08	103.90
36	5	1917	C	C4-C5-C6	5.63	120.22	117.40
36	1	611	A	O5'-P-OP1	5.63	117.46	110.70
36	1	1489	A	N9-C4-C5	-5.63	103.55	105.80
36	1	3303	G	C8-N9-C4	5.63	108.65	106.40
36	5	3303	G	O4'-C1'-N9	5.63	112.71	108.20
36	1	2926	A	N1-C6-N6	5.63	121.98	118.60
38	4	4	C	O5'-P-OP2	-5.63	100.64	105.70
1	6	308	C	C5-C4-N4	5.63	124.14	120.20
36	5	526	C	N3-C4-C5	5.63	124.15	121.90
36	5	990	U	N1-C2-O2	5.63	126.74	122.80
37	7	32	U	C5-C6-N1	-5.63	119.89	122.70
36	1	1363	A	O5'-P-OP2	-5.63	100.64	105.70
1	6	1283	U	C5-C6-N1	-5.63	119.89	122.70
36	5	313	A	C5-C6-N6	-5.63	119.20	123.70
36	5	399	A	C8-N9-C4	5.63	108.05	105.80
36	5	2848	G	O5'-P-OP1	-5.63	100.64	105.70
38	8	113	U	C2-N1-C1'	5.63	124.45	117.70
1	2	1749	A	C2-N3-C4	-5.62	107.79	110.60
36	1	1796	G	N3-C4-C5	-5.62	125.79	128.60
36	1	2603	G	N3-C2-N2	5.62	123.84	119.90
41	14	300	ARG	NE-CZ-NH1	5.62	123.11	120.30
36	1	2418	G	OP1-P-O3'	5.62	117.57	105.20
36	1	3081	C	C4-C5-C6	5.62	120.21	117.40
36	1	3377	G	C8-N9-C4	5.62	108.65	106.40
1	6	1164	G	N9-C4-C5	-5.62	103.15	105.40
36	1	1413	G	C8-N9-C4	5.62	108.65	106.40
36	1	2787	G	C5-C6-N1	5.62	114.31	111.50
1	6	542	A	C6-C5-N7	-5.62	128.37	132.30
1	6	1760	G	C5-C6-O6	-5.62	125.23	128.60
36	1	3132	C	N3-C2-O2	-5.62	117.97	121.90
36	1	3183	A	N9-C4-C5	-5.62	103.55	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	88	A	C8-N9-C4	5.62	108.05	105.80
36	5	2924	U	N1-C2-O2	-5.62	118.87	122.80
36	1	748	U	C5-C4-O4	-5.62	122.53	125.90
36	5	372	A	O5'-P-OP2	-5.62	100.64	105.70
36	5	938	C	N3-C4-C5	5.62	124.15	121.90
36	5	2695	A	N9-C4-C5	5.62	108.05	105.80
36	5	2941	A	N1-C6-N6	-5.62	115.23	118.60
36	1	2585	G	C2-N3-C4	5.62	114.71	111.90
36	1	2610	G	C4-C5-N7	5.62	113.05	110.80
36	5	3218	A	P-O3'-C3'	5.62	126.44	119.70
36	1	48	A	N1-C2-N3	5.62	132.11	129.30
36	1	1369	A	O5'-P-OP2	5.62	117.44	110.70
36	5	974	G	N3-C4-C5	-5.62	125.79	128.60
36	1	669	U	C6-N1-C2	5.61	124.37	121.00
36	5	1922	A	C8-N9-C4	5.61	108.05	105.80
36	5	2951	G	N1-C6-O6	-5.61	116.53	119.90
37	3	28	C	N3-C4-N4	5.61	121.93	118.00
36	5	1929	G	C4-C5-N7	5.61	113.05	110.80
36	5	890	C	OP2-P-O3'	5.61	117.54	105.20
36	5	1001	G	O5'-P-OP1	-5.61	100.65	105.70
36	5	2191	U	N3-C4-O4	-5.61	115.47	119.40
1	2	996	U	N1-C2-O2	5.61	126.73	122.80
36	5	3154	C	N3-C2-O2	-5.61	117.97	121.90
1	2	2	A	O4'-C1'-N9	-5.61	103.71	108.20
36	5	939	U	N3-C2-O2	5.61	126.13	122.20
36	5	3060	C	N3-C4-N4	5.61	121.93	118.00
36	1	2376	G	OP1-P-OP2	5.61	128.01	119.60
36	5	2334	U	N3-C2-O2	-5.61	118.28	122.20
1	2	11	A	O5'-P-OP1	-5.60	100.66	105.70
36	1	1204	A	N1-C6-N6	5.60	121.96	118.60
36	1	2920	U	C2-N3-C4	-5.60	123.64	127.00
36	1	1159	A	N1-C6-N6	-5.60	115.24	118.60
36	1	2169	G	C5-C6-O6	5.60	131.96	128.60
36	5	145	G	N3-C4-N9	-5.60	122.64	126.00
36	5	1491	A	N1-C2-N3	5.60	132.10	129.30
1	2	1052	U	C2-N1-C1'	5.60	124.42	117.70
36	5	2965	U	N3-C4-O4	5.60	123.32	119.40
1	2	864	U	N3-C2-O2	-5.60	118.28	122.20
36	1	1425	U	C5-C6-N1	-5.60	119.90	122.70
36	1	2719	U	C5-C6-N1	-5.60	119.90	122.70
36	5	630	A	C8-N9-C4	5.60	108.04	105.80
36	5	869	G	C5-C6-N1	5.60	114.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1315	U	C6-N1-C2	5.60	124.36	121.00
36	5	2897	A	N1-C2-N3	5.60	132.10	129.30
36	1	719	U	O5'-P-OP1	-5.60	100.66	105.70
1	6	387	A	N3-C4-C5	-5.60	122.88	126.80
36	5	41	G	C5-C6-O6	-5.60	125.24	128.60
36	5	645	A	N1-C6-N6	-5.60	115.24	118.60
36	5	2941	A	O4'-C1'-N9	-5.60	103.72	108.20
36	1	2197	C	C5-C4-N4	-5.60	116.28	120.20
36	5	624	G	C8-N9-C4	5.60	108.64	106.40
38	8	23	U	N1-C2-N3	5.60	118.26	114.90
1	2	402	C	O5'-P-OP1	-5.59	100.66	105.70
36	1	652	G	N1-C2-N2	-5.59	111.16	116.20
36	5	687	U	N3-C2-O2	5.59	126.12	122.20
36	5	1443	G	N3-C2-N2	5.59	123.82	119.90
36	5	2271	A	C8-N9-C4	5.59	108.04	105.80
1	2	736	C	C5-C6-N1	5.59	123.80	121.00
36	1	914	A	N1-C2-N3	5.59	132.10	129.30
36	1	2110	G	O4'-C1'-N9	5.59	112.67	108.20
36	5	1517	G	N9-C4-C5	5.59	107.64	105.40
36	5	2130	G	C8-N9-C4	5.59	108.64	106.40
1	2	1486	G	N7-C8-N9	5.59	115.89	113.10
36	1	145	G	C5-C6-O6	-5.59	125.25	128.60
36	5	2134	G	N1-C6-O6	-5.59	116.55	119.90
36	1	1203	A	N9-C4-C5	-5.59	103.56	105.80
36	5	40	A	N1-C6-N6	5.59	121.95	118.60
77	q1	23	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	2	1389	C	N1-C2-O2	5.58	122.25	118.90
36	1	182	U	N3-C4-O4	-5.58	115.49	119.40
36	1	2698	G	C5-C6-N1	5.58	114.29	111.50
36	5	1049	C	N3-C4-C5	5.58	124.13	121.90
36	5	1917	C	N1-C2-O2	-5.58	115.55	118.90
36	5	2680	A	C4-C5-N7	-5.58	107.91	110.70
36	5	3005	A	O5'-P-OP2	-5.58	100.67	105.70
56	n0	155	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	2	934	C	C5-C6-N1	5.58	123.79	121.00
36	1	2369	G	C5-C6-O6	-5.58	125.25	128.60
36	1	2608	G	N1-C6-O6	5.58	123.25	119.90
1	6	1758	U	N1-C2-O2	5.58	126.71	122.80
36	5	1372	C	C4-C5-C6	5.58	120.19	117.40
36	5	2706	G	O5'-P-OP2	-5.58	100.68	105.70
36	5	1939	G	N3-C4-C5	-5.58	125.81	128.60
1	2	1754	A	C8-N9-C4	5.58	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2193	U	N1-C2-O2	5.58	126.71	122.80
36	1	2285	C	C6-N1-C2	5.58	122.53	120.30
36	5	641	C	C5-C4-N4	-5.58	116.30	120.20
36	5	2349	U	OP1-P-O3'	5.58	117.47	105.20
36	5	2851	A	N1-C2-N3	5.58	132.09	129.30
36	1	281	G	C8-N9-C1'	-5.58	119.75	127.00
1	6	1023	A	N1-C6-N6	5.58	121.95	118.60
36	5	101	G	O4'-C1'-N9	5.58	112.66	108.20
1	6	1481	C	N3-C2-O2	-5.58	118.00	121.90
36	5	2426	U	C5-C4-O4	5.58	129.25	125.90
36	1	361	A	N7-C8-N9	-5.57	111.01	113.80
36	1	2993	G	N3-C4-N9	5.57	129.34	126.00
36	1	3278	C	C2-N3-C4	5.57	122.69	119.90
36	5	946	U	N3-C4-O4	5.57	123.30	119.40
36	5	2298	U	C5-C6-N1	-5.57	119.91	122.70
62	N6	57	LEU	CA-CB-CG	5.57	128.12	115.30
36	1	1130	A	N1-C2-N3	-5.57	126.52	129.30
1	6	863	A	C5-C6-N6	-5.57	119.24	123.70
36	5	1436	U	N1-C2-O2	5.57	126.70	122.80
36	1	429	U	N3-C2-O2	-5.57	118.30	122.20
36	5	3362	A	C8-N9-C4	-5.57	103.57	105.80
36	5	1346	G	C8-N9-C4	5.57	108.63	106.40
36	5	3144	G	N7-C8-N9	5.57	115.88	113.10
36	1	19	U	N1-C2-N3	5.57	118.24	114.90
36	1	2393	G	C5-C6-N1	5.57	114.28	111.50
36	1	2791	G	N9-C4-C5	5.57	107.63	105.40
36	5	1609	C	N3-C4-N4	5.57	121.90	118.00
36	5	2598	G	N1-C6-O6	5.57	123.24	119.90
1	2	647	G	N9-C4-C5	5.56	107.63	105.40
1	2	973	A	O5'-P-OP2	-5.56	100.69	105.70
36	1	145	G	N1-C6-O6	5.56	123.24	119.90
36	5	3322	A	C2-N3-C4	-5.56	107.82	110.60
36	1	1002	A	C8-N9-C4	5.56	108.03	105.80
1	6	29	U	C5-C6-N1	-5.56	119.92	122.70
1	6	542	A	C4-N9-C1'	5.56	136.31	126.30
36	5	1158	A	N9-C4-C5	-5.56	103.58	105.80
36	5	3347	A	C8-N9-C4	5.56	108.03	105.80
36	1	1437	C	C2-N1-C1'	5.56	124.92	118.80
36	1	2275	A	O5'-P-OP1	-5.56	100.69	105.70
1	6	521	A	N1-C6-N6	-5.56	115.26	118.60
36	1	2830	G	N3-C2-N2	-5.56	116.01	119.90
1	6	577	G	C4-C5-N7	5.56	113.02	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1698	G	P-O3'-C3'	5.56	126.37	119.70
36	5	3177	G	C2-N3-C4	-5.56	109.12	111.90
36	1	1604	G	C4-N9-C1'	5.56	133.72	126.50
64	N8	57	GLY	N-CA-C	5.56	127.00	113.10
36	5	1193	A	C6-C5-N7	-5.56	128.41	132.30
36	5	1213	G	N1-C6-O6	-5.56	116.57	119.90
44	L7	179	LEU	CA-CB-CG	5.56	128.08	115.30
36	5	647	A	C4-C5-C6	5.56	119.78	117.00
1	2	1744	A	O5'-P-OP1	-5.55	100.70	105.70
36	1	109	A	N1-C6-N6	-5.55	115.27	118.60
36	1	2827	U	C6-N1-C1'	5.55	128.98	121.20
36	5	2929	C	C4-C5-C6	5.55	120.18	117.40
36	1	353	G	C4-C5-N7	5.55	113.02	110.80
36	5	881	C	N3-C2-O2	-5.55	118.01	121.90
36	5	1941	C	N1-C2-O2	-5.55	115.57	118.90
36	5	3309	G	C8-N9-C4	-5.55	104.18	106.40
1	2	968	U	N3-C2-O2	-5.55	118.31	122.20
36	1	1553	U	N3-C4-O4	5.55	123.29	119.40
36	1	2786	G	C5-N7-C8	5.55	107.08	104.30
36	1	95	A	N1-C2-N3	5.55	132.07	129.30
36	1	682	U	C5-C4-O4	5.55	129.23	125.90
38	4	40	A	C4-C5-N7	5.55	113.47	110.70
36	5	1329	U	N3-C2-O2	-5.55	118.32	122.20
36	5	2817	A	OP2-P-O3'	5.55	117.41	105.20
36	1	211	A	C2-N3-C4	-5.55	107.83	110.60
36	5	2391	G	N1-C6-O6	-5.55	116.57	119.90
36	5	2811	A	C2-N3-C4	-5.55	107.83	110.60
36	5	3216	G	C5-C6-O6	-5.55	125.27	128.60
36	1	2572	C	C5-C6-N1	5.55	123.77	121.00
1	6	1636	C	C4-C5-C6	5.55	120.17	117.40
36	5	197	G	N7-C8-N9	5.55	115.87	113.10
36	5	387	A	C2-N3-C4	-5.55	107.83	110.60
36	5	1895	A	C6-N1-C2	-5.55	115.27	118.60
1	2	314	C	C6-N1-C2	5.54	122.52	120.30
1	2	865	A	C2-N3-C4	-5.54	107.83	110.60
36	1	1385	C	N1-C2-O2	-5.54	115.57	118.90
38	8	140	G	C8-N9-C4	-5.54	104.18	106.40
36	1	1405	U	N3-C4-C5	5.54	117.92	114.60
36	1	1902	G	C5-N7-C8	-5.54	101.53	104.30
36	1	2391	G	C4-C5-C6	5.54	122.12	118.80
1	6	118	U	N3-C4-O4	-5.54	115.52	119.40
1	6	541	A	C8-N9-C4	-5.54	103.58	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	39	A	N1-C6-N6	5.54	121.92	118.60
1	2	1363	U	N3-C2-O2	-5.54	118.32	122.20
36	1	2284	C	C2-N1-C1'	5.54	124.89	118.80
38	4	107	G	N1-C6-O6	-5.54	116.58	119.90
36	1	3034	C	N1-C2-O2	5.54	122.22	118.90
38	4	56	G	C8-N9-C4	5.54	108.61	106.40
36	5	127	G	N1-C6-O6	5.54	123.22	119.90
36	5	1902	G	N9-C4-C5	-5.54	103.18	105.40
36	5	2572	C	C6-N1-C2	-5.54	118.08	120.30
36	1	988	U	C5-C4-O4	5.54	129.22	125.90
37	7	49	G	C6-C5-N7	-5.54	127.08	130.40
1	2	831	U	N1-C2-O2	5.54	126.67	122.80
1	2	1200	G	C6-C5-N7	-5.54	127.08	130.40
36	1	433	A	C5-C6-N6	-5.54	119.27	123.70
36	5	2389	C	N3-C4-C5	5.54	124.11	121.90
36	5	2550	U	N3-C4-O4	-5.54	115.53	119.40
1	2	577	G	C4-C5-N7	5.53	113.01	110.80
36	1	909	G	N3-C4-C5	5.53	131.37	128.60
1	6	1745	G	N3-C4-C5	-5.53	125.83	128.60
36	5	641	C	N1-C2-O2	-5.53	115.58	118.90
36	5	806	A	O5'-P-OP2	5.53	117.34	110.70
37	7	93	C	O5'-P-OP1	5.53	117.34	110.70
38	8	32	C	C6-N1-C2	5.53	122.51	120.30
1	2	1157	A	P-O3'-C3'	5.53	126.34	119.70
36	1	1949	G	C6-C5-N7	-5.53	127.08	130.40
36	1	2656	A	C8-N9-C4	-5.53	103.59	105.80
18	c6	117	LEU	CA-CB-CG	5.53	128.02	115.30
36	1	521	A	N1-C6-N6	5.53	121.92	118.60
36	1	637	C	N3-C4-C5	5.53	124.11	121.90
36	1	2572	C	C6-N1-C1'	-5.53	114.16	120.80
37	7	37	G	C5-C6-O6	-5.53	125.28	128.60
36	1	1133	A	N1-C6-N6	5.53	121.92	118.60
36	5	2334	U	N1-C2-N3	5.53	118.22	114.90
36	5	2938	G	OP1-P-OP2	5.53	127.89	119.60
36	1	1352	A	P-O3'-C3'	5.53	126.33	119.70
1	6	65	A	C4-C5-N7	5.53	113.46	110.70
36	5	2983	C	N1-C2-O2	-5.52	115.59	118.90
36	1	2356	A	N9-C4-C5	-5.52	103.59	105.80
36	1	2619	G	O5'-P-OP1	-5.52	100.73	105.70
1	6	1649	G	C5-C6-O6	5.52	131.91	128.60
36	5	2715	A	N9-C4-C5	5.52	108.01	105.80
36	5	3115	C	N1-C2-N3	5.52	123.07	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	26	U	N3-C2-O2	-5.52	118.33	122.20
36	5	749	C	C4-C5-C6	5.52	120.16	117.40
1	2	240	U	OP2-P-O3'	5.52	117.34	105.20
36	1	1000	C	C6-N1-C1'	-5.52	114.18	120.80
36	1	2121	G	N1-C2-N2	-5.52	111.23	116.20
36	5	1205	A	C8-N9-C4	-5.52	103.59	105.80
36	5	1673	G	N1-C6-O6	-5.52	116.59	119.90
1	2	1782	A	N9-C4-C5	5.52	108.01	105.80
36	1	1458	U	C5-C6-N1	-5.52	119.94	122.70
36	1	3111	U	N3-C4-O4	-5.52	115.54	119.40
1	6	165	G	C6-C5-N7	-5.52	127.09	130.40
1	6	308	C	C5-C6-N1	-5.52	118.24	121.00
36	5	2351	U	N3-C2-O2	-5.52	118.34	122.20
36	1	312	C	N3-C4-C5	5.52	124.11	121.90
36	1	1345	G	OP2-P-O3'	5.52	117.34	105.20
1	6	866	G	C8-N9-C4	5.52	108.61	106.40
1	6	1473	U	C5-C4-O4	5.52	129.21	125.90
36	1	206	G	N1-C6-O6	-5.51	116.59	119.90
36	1	212	G	N3-C4-N9	5.51	129.31	126.00
36	1	609	G	N1-C2-N2	5.51	121.16	116.20
36	1	1346	G	N3-C4-C5	5.51	131.36	128.60
36	1	2606	G	N1-C2-N2	-5.51	111.24	116.20
36	5	875	G	C4-C5-N7	-5.51	108.59	110.80
36	5	1141	C	N3-C4-C5	5.51	124.11	121.90
36	5	1395	G	OP2-P-O3'	5.51	117.33	105.20
36	5	2514	U	O5'-P-OP1	-5.51	100.74	105.70
1	2	1679	G	N1-C6-O6	-5.51	116.59	119.90
36	1	317	A	C2-N3-C4	-5.51	107.84	110.60
36	1	626	U	N3-C4-C5	5.51	117.91	114.60
36	1	1269	U	N3-C2-O2	-5.51	118.34	122.20
36	1	1929	G	C4-C5-N7	5.51	113.00	110.80
36	1	3174	A	C5-N7-C8	-5.51	101.14	103.90
36	5	2620	G	C2-N3-C4	5.51	114.66	111.90
1	2	310	C	N3-C4-C5	-5.51	119.70	121.90
1	6	1100	G	N3-C4-C5	-5.51	125.84	128.60
1	6	1602	C	N1-C2-O2	5.51	122.20	118.90
36	5	1200	A	N3-C4-N9	5.51	131.81	127.40
36	5	1858	A	O5'-P-OP2	-5.51	100.74	105.70
36	1	2644	C	N1-C2-O2	5.51	122.20	118.90
36	5	1589	A	C5-C6-N1	5.51	120.45	117.70
36	5	2709	C	C5-C4-N4	-5.51	116.34	120.20
1	2	720	G	P-O3'-C3'	5.50	126.31	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1332	A	C6-N1-C2	-5.50	115.30	118.60
36	5	3266	G	N9-C4-C5	5.50	107.60	105.40
36	1	645	A	N1-C2-N3	5.50	132.05	129.30
36	1	914	A	O5'-P-OP1	-5.50	100.75	105.70
36	1	1407	A	N1-C6-N6	-5.50	115.30	118.60
38	4	13	A	C5-C6-N6	-5.50	119.30	123.70
36	5	1113	G	N1-C2-N3	5.50	127.20	123.90
36	5	2176	U	N3-C2-O2	-5.50	118.35	122.20
1	2	1274	C	N3-C2-O2	-5.50	118.05	121.90
36	1	2601	A	C2-N3-C4	5.50	113.35	110.60
1	6	1058	U	OP1-P-O3'	5.50	117.30	105.20
36	5	2715	A	C8-N9-C4	-5.50	103.60	105.80
36	5	3321	C	N1-C2-O2	-5.50	115.60	118.90
1	2	830	U	N1-C2-O2	5.50	126.65	122.80
36	1	1099	A	N1-C6-N6	5.50	121.90	118.60
36	1	1181	U	N3-C2-O2	-5.50	118.35	122.20
1	6	314	C	OP2-P-O3'	5.50	117.29	105.20
36	5	190	U	O4'-C1'-N1	5.50	112.60	108.20
36	5	2398	A	N1-C6-N6	-5.50	115.30	118.60
37	7	80	G	C4-C5-N7	5.50	113.00	110.80
47	m0	7	ARG	NE-CZ-NH1	-5.50	117.55	120.30
36	5	2278	C	OP1-P-OP2	-5.50	111.36	119.60
36	1	343	U	OP2-P-O3'	5.49	117.29	105.20
36	1	1330	A	C4-C5-N7	5.49	113.45	110.70
36	1	2433	U	C5-C6-N1	-5.49	119.95	122.70
36	5	1496	C	O5'-P-OP1	5.49	117.29	110.70
36	5	3004	C	C6-N1-C2	5.49	122.50	120.30
36	5	3120	C	O5'-P-OP1	-5.49	100.76	105.70
36	1	1405	U	C5-C4-O4	-5.49	122.61	125.90
36	1	2550	U	C5-C4-O4	5.49	129.19	125.90
36	1	312	C	C5-C4-N4	-5.49	116.36	120.20
36	1	918	C	O5'-P-OP2	-5.49	100.76	105.70
36	1	2214	A	N1-C6-N6	5.49	121.89	118.60
36	1	2816	G	C6-N1-C2	-5.49	121.81	125.10
1	6	377	G	C5-C6-N1	5.49	114.25	111.50
36	5	2434	U	C5-C6-N1	-5.49	119.95	122.70
1	2	852	C	C5-C6-N1	5.49	123.74	121.00
36	1	156	G	C2-N3-C4	5.49	114.64	111.90
36	1	581	U	OP2-P-O3'	5.49	117.27	105.20
1	6	382	C	N3-C4-C5	5.49	124.09	121.90
1	6	858	G	N1-C6-O6	5.49	123.19	119.90
36	5	2196	C	C5-C6-N1	-5.49	118.26	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2889	C	N3-C2-O2	-5.49	118.06	121.90
36	5	3380	U	C5-C4-O4	5.49	129.19	125.90
36	1	2728	G	N3-C4-C5	-5.49	125.86	128.60
36	5	92	G	N3-C4-N9	5.49	129.29	126.00
36	1	223	U	C6-N1-C2	5.49	124.29	121.00
36	1	2403	G	O5'-P-OP1	5.49	117.28	110.70
36	5	323	A	C8-N9-C4	-5.49	103.61	105.80
36	5	408	A	OP1-P-OP2	5.49	127.83	119.60
36	5	2867	C	N3-C2-O2	5.49	125.74	121.90
1	2	1455	G	C4-C5-N7	-5.48	108.61	110.80
36	1	2865	U	C6-N1-C2	5.48	124.29	121.00
36	1	3374	U	C5-C4-O4	-5.48	122.61	125.90
1	6	359	A	C4-N9-C1'	-5.48	116.43	126.30
37	7	92	A	C5-C6-N6	-5.48	119.31	123.70
1	2	1100	G	N1-C6-O6	5.48	123.19	119.90
1	2	1782	A	C5-C6-N6	5.48	128.09	123.70
36	1	49	A	C5-C6-N1	-5.48	114.96	117.70
36	1	3387	U	C6-N1-C2	5.48	124.29	121.00
36	1	3362	A	C5-C6-N6	-5.48	119.32	123.70
36	5	914	A	C6-N1-C2	-5.48	115.31	118.60
1	2	1457	C	C6-N1-C2	-5.48	118.11	120.30
36	1	2201	G	C5-C6-N1	-5.48	108.76	111.50
36	1	2702	A	C8-N9-C4	-5.48	103.61	105.80
36	1	3269	U	C6-N1-C2	-5.48	117.71	121.00
1	6	1299	G	N3-C4-C5	-5.48	125.86	128.60
56	n0	40	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	2	1297	G	C4-N9-C1'	-5.48	119.38	126.50
36	1	1165	A	C8-N9-C4	5.47	107.99	105.80
36	1	2245	C	C5-C4-N4	5.47	124.03	120.20
36	1	2610	G	C6-C5-N7	-5.47	127.11	130.40
36	1	2657	A	N1-C6-N6	-5.47	115.31	118.60
73	O7	65	ARG	NE-CZ-NH2	-5.47	117.56	120.30
36	5	924	G	C5-C6-N1	-5.47	108.76	111.50
36	5	1443	G	N1-C6-O6	-5.47	116.61	119.90
38	8	17	A	C4-C5-N7	5.47	113.44	110.70
36	1	908	G	O4'-C1'-N9	-5.47	103.82	108.20
36	1	1202	A	C8-N9-C4	5.47	107.99	105.80
1	6	1614	A	N1-C6-N6	5.47	121.88	118.60
36	5	1213	G	C6-C5-N7	5.47	133.68	130.40
36	5	1938	U	N3-C4-C5	5.47	117.88	114.60
36	1	931	C	N1-C2-O2	5.47	122.18	118.90
36	1	972	A	N7-C8-N9	-5.47	111.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2416	U	C5-C6-N1	5.47	125.44	122.70
1	2	1761	U	N1-C2-N3	5.47	118.18	114.90
36	1	2198	A	N9-C4-C5	5.47	107.99	105.80
36	5	1848	G	C6-C5-N7	-5.47	127.12	130.40
36	5	2299	A	C5-C6-N1	-5.47	114.97	117.70
36	5	2383	C	C6-N1-C2	-5.47	118.11	120.30
36	1	1156	C	C2-N3-C4	-5.47	117.17	119.90
36	5	1724	U	C4-C5-C6	5.47	122.98	119.70
36	1	636	C	C5-C4-N4	-5.47	116.37	120.20
36	1	1116	G	C4-C5-C6	5.47	122.08	118.80
36	5	2123	G	C2-N3-C4	5.47	114.63	111.90
36	1	1435	A	N1-C6-N6	5.46	121.88	118.60
36	5	2132	C	C6-N1-C2	-5.46	118.11	120.30
36	5	2719	U	C2-N1-C1'	-5.46	111.14	117.70
36	5	2780	A	O5'-P-OP2	-5.46	100.78	105.70
36	5	197	G	C4-C5-N7	5.46	112.98	110.80
36	5	2531	C	C2-N1-C1'	5.46	124.81	118.80
36	1	273	A	N7-C8-N9	-5.46	111.07	113.80
36	1	1445	U	C6-N1-C1'	5.46	128.85	121.20
36	1	2121	G	N3-C4-N9	5.46	129.28	126.00
36	5	352	A	O4'-C1'-N9	5.46	112.57	108.20
36	5	2921	U	C2-N1-C1'	5.46	124.25	117.70
36	1	964	G	OP2-P-O3'	5.46	117.21	105.20
36	1	976	U	O5'-P-OP2	-5.46	100.79	105.70
1	6	1649	G	N1-C2-N2	-5.46	111.29	116.20
36	5	1161	G	C2-N3-C4	5.46	114.63	111.90
36	5	1171	G	N3-C2-N2	5.46	123.72	119.90
36	5	2699	G	C8-N9-C4	5.46	108.58	106.40
36	5	2900	A	OP2-P-O3'	5.46	117.21	105.20
36	1	2623	G	N9-C4-C5	-5.46	103.22	105.40
1	6	448	C	OP1-P-O3'	5.46	117.20	105.20
36	5	838	G	C5-C6-O6	5.46	131.87	128.60
36	5	2919	A	C4-C5-N7	-5.46	107.97	110.70
36	5	2978	U	O4'-C1'-N1	5.46	112.56	108.20
1	2	728	U	N1-C2-O2	5.46	126.62	122.80
1	6	1473	U	C2-N1-C1'	5.46	124.25	117.70
36	5	2833	A	C6-N1-C2	-5.46	115.33	118.60
36	5	3310	A	N1-C2-N3	5.46	132.03	129.30
36	1	95	A	C2-N3-C4	-5.45	107.87	110.60
36	1	3216	G	N1-C6-O6	-5.45	116.63	119.90
36	5	2273	G	C8-N9-C4	5.45	108.58	106.40
36	5	2338	C	N3-C4-C5	-5.45	119.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	283	G	C8-N9-C1'	-5.45	119.91	127.00
36	1	926	A	N7-C8-N9	-5.45	111.07	113.80
1	6	309	C	O5'-P-OP1	-5.45	100.79	105.70
1	6	1484	G	O5'-P-OP1	-5.45	100.79	105.70
36	5	1128	U	C2-N3-C4	-5.45	123.73	127.00
36	1	345	G	C4-N9-C1'	5.45	133.59	126.50
36	1	1633	C	C5-C6-N1	5.45	123.72	121.00
1	6	1596	C	N3-C4-N4	-5.45	114.19	118.00
36	5	2344	U	C5-C6-N1	-5.45	119.97	122.70
36	5	2808	A	C8-N9-C4	5.45	107.98	105.80
36	1	435	C	N3-C4-C5	5.45	124.08	121.90
36	1	716	A	C5-N7-C8	-5.45	101.18	103.90
41	L4	206	LEU	CA-CB-CG	5.45	127.83	115.30
36	5	326	U	C5-C6-N1	5.45	125.42	122.70
36	5	2123	G	N1-C6-O6	-5.45	116.63	119.90
36	5	3374	U	C6-N1-C2	5.45	124.27	121.00
62	n6	76	LEU	CA-CB-CG	5.45	127.82	115.30
36	5	2673	A	C8-N9-C4	5.44	107.98	105.80
1	2	457	G	N3-C4-N9	5.44	129.26	126.00
36	5	1156	C	C5-C4-N4	-5.44	116.39	120.20
36	5	2396	G	C8-N9-C4	-5.44	104.22	106.40
38	8	112	U	C2-N1-C1'	-5.44	111.17	117.70
36	1	40	A	O5'-P-OP1	-5.44	100.80	105.70
36	1	818	C	C6-N1-C2	-5.44	118.12	120.30
36	1	2314	U	O4'-C1'-N1	5.44	112.55	108.20
52	M6	110	PRO	C-N-CD	-5.44	108.63	120.60
36	5	1159	A	C2-N3-C4	-5.44	107.88	110.60
1	6	875	G	N1-C6-O6	-5.44	116.64	119.90
36	5	1188	U	C2-N3-C4	-5.44	123.74	127.00
1	2	1746	A	N1-C2-N3	-5.44	126.58	129.30
36	1	1476	G	C5-C6-O6	5.44	131.86	128.60
36	1	2210	G	N1-C6-O6	-5.44	116.64	119.90
36	1	2756	C	C6-N1-C2	-5.44	118.12	120.30
36	1	2944	U	N3-C2-O2	-5.44	118.39	122.20
36	5	716	A	N9-C4-C5	-5.44	103.62	105.80
36	5	2341	A	C5-C6-N1	5.44	120.42	117.70
36	5	2855	U	N3-C4-C5	5.44	117.86	114.60
44	17	229	PHE	CB-CG-CD2	-5.44	116.99	120.80
36	1	33	G	N3-C4-N9	-5.44	122.74	126.00
36	1	639	G	N3-C2-N2	-5.43	116.10	119.90
1	6	612	U	O5'-P-OP1	5.43	117.22	110.70
36	5	2714	G	N1-C6-O6	-5.43	116.64	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1466	G	C8-N9-C4	5.43	108.57	106.40
36	1	2747	A	N1-C6-N6	-5.43	115.34	118.60
1	6	1584	G	N1-C6-O6	5.43	123.16	119.90
36	5	197	G	C4-N9-C1'	5.43	133.56	126.50
36	5	1536	G	N3-C2-N2	-5.43	116.10	119.90
36	5	3084	C	C5-C6-N1	-5.43	118.28	121.00
40	l3	4	ARG	NE-CZ-NH1	5.43	123.02	120.30
36	1	2953	U	N1-C2-O2	-5.43	119.00	122.80
36	5	1451	C	C5-C4-N4	-5.43	116.40	120.20
1	2	142	G	N3-C4-C5	5.43	131.31	128.60
36	1	968	G	N3-C4-C5	-5.43	125.89	128.60
36	1	1313	G	C5-C6-O6	-5.43	125.34	128.60
36	5	1142	G	C8-N9-C4	-5.43	104.23	106.40
36	5	1511	U	N1-C2-O2	5.43	126.60	122.80
36	5	3111	U	N3-C4-O4	-5.43	115.60	119.40
14	C2	103	LEU	CA-CB-CG	5.43	127.78	115.30
36	1	29	C	N3-C4-N4	5.43	121.80	118.00
1	6	321	C	N3-C2-O2	-5.43	118.10	121.90
36	5	2388	U	N3-C4-O4	5.43	123.20	119.40
36	5	2800	G	C5-C6-O6	-5.43	125.34	128.60
36	1	416	A	N7-C8-N9	-5.42	111.09	113.80
52	M6	84	LEU	CB-CG-CD1	-5.42	101.78	111.00
37	7	68	C	N1-C2-O2	5.42	122.16	118.90
36	5	960	U	N3-C2-O2	-5.42	118.40	122.20
36	1	61	A	OP2-P-O3'	5.42	117.13	105.20
36	1	926	A	C8-N9-C4	5.42	107.97	105.80
1	6	1109	G	N9-C4-C5	5.42	107.57	105.40
36	5	2619	G	C6-N1-C2	-5.42	121.85	125.10
36	1	1886	A	N1-C6-N6	-5.42	115.35	118.60
36	1	2298	U	C5-C6-N1	-5.42	119.99	122.70
36	1	2756	C	C2-N1-C1'	5.42	124.76	118.80
36	1	2913	C	N3-C2-O2	-5.42	118.11	121.90
36	1	31	C	O5'-P-OP2	-5.42	100.82	105.70
36	1	671	U	O5'-P-OP2	-5.42	100.82	105.70
36	1	1082	U	C2-N1-C1'	5.42	124.20	117.70
1	6	765	G	N1-C2-N3	-5.42	120.65	123.90
36	5	3015	G	C2-N3-C4	-5.42	109.19	111.90
36	1	893	C	C6-N1-C2	-5.42	118.13	120.30
36	1	1409	G	C5-C6-N1	5.42	114.21	111.50
36	1	2303	A	C2-N3-C4	-5.42	107.89	110.60
36	1	2355	G	N3-C4-N9	5.42	129.25	126.00
36	1	2795	U	N3-C2-O2	-5.42	118.41	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3046	A	O5'-P-OP1	-5.42	100.83	105.70
1	6	1572	G	C4-N9-C1'	5.42	133.54	126.50
36	1	784	A	O4'-C1'-N9	5.41	112.53	108.20
36	1	1366	A	C5-C6-N6	-5.41	119.37	123.70
36	5	2981	U	C2-N1-C1'	5.41	124.20	117.70
36	1	2237	C	C6-N1-C2	5.41	122.47	120.30
36	1	2321	A	C4-C5-C6	-5.41	114.29	117.00
36	5	433	A	O5'-P-OP2	-5.41	100.83	105.70
36	5	719	U	N3-C2-O2	-5.41	118.41	122.20
36	5	3260	G	C5-C6-O6	5.41	131.85	128.60
36	1	1061	A	N1-C6-N6	5.41	121.85	118.60
36	5	1181	U	C5-C6-N1	-5.41	120.00	122.70
36	5	2813	A	C4-C5-C6	5.41	119.70	117.00
38	8	34	U	O4'-C1'-N1	5.41	112.53	108.20
36	1	1370	G	C5-C6-O6	-5.41	125.36	128.60
36	1	1379	G	C2-N3-C4	-5.41	109.20	111.90
36	1	2356	A	C5-N7-C8	-5.41	101.20	103.90
36	1	3175	U	N3-C2-O2	-5.41	118.41	122.20
36	5	90	C	N3-C4-N4	5.41	121.78	118.00
36	5	2921	U	C4-C5-C6	5.41	122.94	119.70
36	5	2956	A	N1-C2-N3	5.41	132.00	129.30
36	5	3022	G	N7-C8-N9	-5.41	110.40	113.10
36	1	2101	C	P-O3'-C3'	5.41	126.19	119.70
36	5	1202	A	OP1-P-OP2	5.41	127.71	119.60
36	5	2614	G	OP1-P-OP2	5.41	127.71	119.60
36	5	2733	A	OP1-P-O3'	5.41	117.09	105.20
38	8	23	U	N1-C2-O2	-5.41	119.02	122.80
36	1	3081	C	C2-N3-C4	-5.40	117.20	119.90
54	M8	178	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	6	1121	C	O5'-P-OP2	-5.40	100.84	105.70
36	5	55	G	OP2-P-O3'	5.40	117.08	105.20
36	5	358	G	N9-C1'-C2'	-5.40	106.06	112.00
36	5	1788	C	O5'-P-OP2	-5.40	100.84	105.70
36	1	299	G	C8-N9-C1'	-5.40	119.98	127.00
36	1	351	A	N1-C2-N3	5.40	132.00	129.30
36	1	351	A	N1-C6-N6	-5.40	115.36	118.60
36	1	1364	C	C5-C4-N4	-5.40	116.42	120.20
36	5	1484	U	C6-N1-C2	5.40	124.24	121.00
36	5	2619	G	C5-C6-O6	-5.40	125.36	128.60
36	5	2805	G	C5-C6-O6	-5.40	125.36	128.60
36	1	1411	C	C2-N3-C4	-5.40	117.20	119.90
36	1	2766	U	OP1-P-O3'	5.40	117.08	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2388	U	N3-C2-O2	5.40	125.98	122.20
36	5	2943	G	O5'-P-OP1	5.40	117.18	110.70
36	1	1365	G	C4-N9-C1'	5.40	133.51	126.50
36	5	2411	U	C5-C6-N1	-5.40	120.00	122.70
36	5	3351	U	C2-N1-C1'	5.40	124.18	117.70
52	m6	94	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	6	308	C	C6-N1-C1'	5.39	127.27	120.80
36	5	2199	G	C8-N9-C1'	-5.39	119.99	127.00
36	1	752	C	C6-N1-C2	5.39	122.46	120.30
36	1	1187	C	C6-N1-C2	5.39	122.46	120.30
36	1	2796	G	N1-C2-N3	5.39	127.14	123.90
36	5	271	C	N3-C2-O2	-5.39	118.12	121.90
36	1	301	G	C8-N9-C4	5.39	108.56	106.40
36	1	715	A	O4'-C1'-N9	5.39	112.51	108.20
1	6	84	A	N1-C6-N6	-5.39	115.36	118.60
36	5	3092	C	N3-C2-O2	-5.39	118.13	121.90
5	S3	182	LEU	CA-CB-CG	5.39	127.69	115.30
36	1	283	G	O4'-C1'-N9	-5.39	103.89	108.20
36	1	910	G	C4-C5-C6	5.39	122.03	118.80
36	1	3055	U	C5-C4-O4	-5.39	122.67	125.90
1	6	1340	U	N3-C2-O2	-5.39	118.43	122.20
38	8	84	C	C6-N1-C2	-5.39	118.14	120.30
36	1	2303	A	N1-C6-N6	5.39	121.83	118.60
36	1	3278	C	C5-C6-N1	5.39	123.69	121.00
1	6	957	G	N1-C6-O6	5.39	123.13	119.90
36	5	1112	A	C4-C5-C6	5.39	119.69	117.00
36	1	182	U	C5-C4-O4	5.39	129.13	125.90
36	1	1111	U	C5-C6-N1	-5.39	120.01	122.70
36	1	1305	U	O5'-P-OP1	-5.39	100.85	105.70
1	6	1283	U	C2-N1-C1'	-5.39	111.24	117.70
1	6	1458	G	C8-N9-C1'	-5.39	120.00	127.00
36	5	326	U	N3-C4-O4	5.39	123.17	119.40
36	5	2827	U	O4'-C1'-N1	5.39	112.51	108.20
36	5	2866	U	O5'-P-OP1	-5.39	100.85	105.70
36	1	2719	U	N1-C2-N3	5.38	118.13	114.90
36	1	2866	U	N1-C2-O2	5.38	126.57	122.80
1	6	1058	U	P-O3'-C3'	5.38	126.16	119.70
36	5	1370	G	N1-C6-O6	-5.38	116.67	119.90
36	1	703	G	N1-C6-O6	-5.38	116.67	119.90
38	4	121	U	C5-C4-O4	5.38	129.13	125.90
1	6	139	C	P-O3'-C3'	5.38	126.16	119.70
36	5	2166	A	C2-N3-C4	-5.38	107.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2733	A	N1-C2-N3	5.38	131.99	129.30
36	1	312	C	N3-C2-O2	5.38	125.67	121.90
36	1	804	C	N3-C4-C5	-5.38	119.75	121.90
36	1	2633	U	N3-C2-O2	-5.38	118.43	122.20
36	5	669	U	C2-N3-C4	-5.38	123.77	127.00
36	5	1083	G	N3-C4-C5	-5.38	125.91	128.60
36	1	2293	C	C5-C4-N4	-5.38	116.43	120.20
36	5	2524	A	N9-C1'-C2'	5.38	120.99	114.00
36	5	2892	A	N1-C2-N3	5.38	131.99	129.30
36	5	2941	A	C5-C6-N6	5.38	128.00	123.70
36	5	425	G	C8-N9-C4	5.38	108.55	106.40
36	5	1903	U	O5'-P-OP2	5.38	117.16	110.70
37	7	57	G	N3-C4-C5	5.38	131.29	128.60
37	7	105	C	C6-N1-C2	-5.38	118.15	120.30
36	1	2298	U	C5-C4-O4	5.38	129.13	125.90
36	1	2766	U	N3-C4-O4	-5.38	115.64	119.40
36	5	644	G	N3-C4-C5	-5.38	125.91	128.60
36	5	1803	C	C6-N1-C2	5.38	122.45	120.30
36	5	1892	G	C4-C5-N7	-5.38	108.65	110.80
36	5	3317	U	N3-C4-O4	-5.38	115.64	119.40
36	5	1207	G	OP1-P-OP2	5.38	127.66	119.60
1	6	103	A	P-O3'-C3'	5.37	126.15	119.70
1	6	1700	C	C6-N1-C1'	-5.37	114.35	120.80
36	5	74	G	C8-N9-C4	-5.37	104.25	106.40
36	5	990	U	N3-C4-C5	5.37	117.82	114.60
36	5	2332	A	N9-C4-C5	-5.37	103.65	105.80
36	1	2619	G	OP1-P-OP2	5.37	127.66	119.60
36	1	2930	A	C5-C6-N6	-5.37	119.40	123.70
1	6	1148	C	C5-C6-N1	-5.37	118.31	121.00
1	6	1600	A	C5-N7-C8	-5.37	101.21	103.90
36	5	719	U	N1-C2-O2	5.37	126.56	122.80
36	5	1144	U	N1-C2-N3	5.37	118.12	114.90
36	5	2382	G	N7-C8-N9	-5.37	110.41	113.10
37	7	41	G	N1-C6-O6	5.37	123.12	119.90
1	6	1744	A	C8-N9-C4	5.37	107.95	105.80
36	5	690	A	N7-C8-N9	-5.37	111.12	113.80
36	5	2859	U	N1-C2-N3	5.37	118.12	114.90
36	5	2952	G	N3-C2-N2	5.37	123.66	119.90
37	7	87	G	N3-C2-N2	-5.37	116.14	119.90
1	2	499	U	C3'-C2'-C1'	5.37	105.79	101.50
36	5	1367	G	C5-C6-N1	-5.37	108.82	111.50
1	6	1549	C	C6-N1-C2	-5.37	118.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2634	U	C5-C4-O4	-5.37	122.68	125.90
1	2	355	G	C8-N9-C4	5.36	108.55	106.40
36	1	2355	G	C4-C5-C6	5.36	122.02	118.80
6	s4	222	LEU	CA-CB-CG	5.36	127.64	115.30
36	5	2179	C	C6-N1-C2	5.36	122.44	120.30
36	1	3245	A	OP1-P-O3'	5.36	117.00	105.20
36	1	752	C	C2-N3-C4	-5.36	117.22	119.90
36	1	1336	U	O5'-P-OP2	-5.36	100.88	105.70
36	1	1521	G	C2-N3-C4	-5.36	109.22	111.90
36	1	1830	G	N3-C4-N9	-5.36	122.78	126.00
36	1	2614	G	C5-N7-C8	5.36	106.98	104.30
36	1	2772	C	C2-N1-C1'	5.36	124.70	118.80
1	6	1111	G	C4-C5-N7	5.36	112.94	110.80
36	5	346	C	N1-C2-O2	5.36	122.12	118.90
36	5	2208	A	O4'-C1'-N9	5.36	112.49	108.20
36	1	1661	G	N9-C4-C5	-5.36	103.26	105.40
36	1	2257	C	N3-C2-O2	-5.36	118.15	121.90
1	6	265	A	C5-C6-N6	-5.36	119.41	123.70
36	5	1208	U	N3-C2-O2	-5.36	118.45	122.20
1	6	387	A	C4-C5-N7	-5.36	108.02	110.70
1	6	387	A	N9-C4-C5	5.36	107.94	105.80
1	6	1246	C	C2-N1-C1'	5.36	124.69	118.80
36	5	862	U	N3-C2-O2	5.36	125.95	122.20
36	5	1846	C	C6-N1-C1'	-5.36	114.37	120.80
36	5	2299	A	O5'-P-OP2	-5.36	100.88	105.70
36	1	1082	U	C6-N1-C2	-5.35	117.79	121.00
36	1	1199	C	N3-C2-O2	-5.35	118.15	121.90
36	1	2600	C	N3-C4-N4	-5.35	114.25	118.00
36	1	2653	C	C4-C5-C6	5.35	120.08	117.40
13	c1	120	GLY	N-CA-C	-5.35	99.71	113.10
36	5	3043	C	N3-C4-C5	5.35	124.04	121.90
36	5	1605	A	O4'-C1'-N9	5.35	112.48	108.20
36	5	2882	U	O5'-P-OP2	-5.35	100.88	105.70
36	5	1152	G	C8-N9-C4	-5.35	104.26	106.40
36	5	2231	C	N3-C4-C5	-5.35	119.76	121.90
36	5	2858	U	N1-C2-N3	5.35	118.11	114.90
1	2	1447	C	C6-N1-C2	5.35	122.44	120.30
36	1	1516	C	C6-N1-C2	-5.35	118.16	120.30
36	1	1581	C	N3-C2-O2	-5.35	118.16	121.90
36	1	2187	G	C8-N9-C4	-5.35	104.26	106.40
36	1	2823	G	N9-C4-C5	5.35	107.54	105.40
36	5	327	A	C8-N9-C4	5.35	107.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1546	A	N1-C6-N6	5.35	121.81	118.60
36	1	299	G	C6-C5-N7	-5.34	127.19	130.40
36	1	1838	G	N9-C4-C5	-5.34	103.26	105.40
36	1	2875	U	P-O3'-C3'	-5.34	113.29	119.70
36	5	994	G	OP1-P-O3'	5.34	116.96	105.20
36	1	1660	C	N3-C2-O2	5.34	125.64	121.90
1	6	1333	C	N3-C4-C5	5.34	124.04	121.90
36	1	2550	U	N3-C4-O4	-5.34	115.66	119.40
36	1	2662	G	N1-C2-N3	5.34	127.11	123.90
24	d2	68	ARG	NE-CZ-NH1	-5.34	117.63	120.30
36	5	1169	A	C8-N9-C4	5.34	107.94	105.80
36	5	1886	A	O5'-P-OP1	5.34	117.11	110.70
36	5	2372	A	OP2-P-O3'	5.34	116.95	105.20
36	1	715	A	P-O3'-C3'	5.34	126.11	119.70
36	1	1181	U	O5'-P-OP2	-5.34	100.89	105.70
36	1	3306	U	N1-C2-N3	5.34	118.10	114.90
1	6	614	C	C5-C6-N1	-5.34	118.33	121.00
36	5	326	U	C6-N1-C2	-5.34	117.80	121.00
36	5	1199	C	C4-C5-C6	5.34	120.07	117.40
36	5	2621	G	N3-C2-N2	-5.34	116.16	119.90
36	5	2830	G	N3-C4-C5	-5.34	125.93	128.60
36	1	2402	A	OP1-P-OP2	5.34	127.61	119.60
1	2	139	C	P-O3'-C3'	5.34	126.10	119.70
36	5	1222	G	N9-C4-C5	-5.34	103.27	105.40
36	5	2639	G	C5-N7-C8	-5.34	101.63	104.30
36	5	3105	U	C2-N3-C4	-5.34	123.80	127.00
36	5	3128	G	N9-C4-C5	-5.34	103.27	105.40
36	1	2911	A	N7-C8-N9	-5.33	111.13	113.80
1	6	1754	A	N1-C6-N6	-5.33	115.40	118.60
36	5	1124	U	C5-C6-N1	5.33	125.37	122.70
36	5	1496	C	C2-N1-C1'	5.33	124.67	118.80
40	l3	4	ARG	CG-CD-NE	5.33	123.00	111.80
36	1	2764	C	N3-C4-C5	-5.33	119.77	121.90
36	1	3344	A	N1-C2-N3	5.33	131.97	129.30
37	3	84	A	C4-C5-C6	5.33	119.67	117.00
1	6	609	U	O5'-P-OP2	-5.33	100.90	105.70
36	1	1535	A	C6-C5-N7	-5.33	128.57	132.30
36	1	1716	U	P-O3'-C3'	5.33	126.10	119.70
36	5	1438	U	N1-C2-N3	5.33	118.10	114.90
36	5	2919	A	N1-C6-N6	-5.33	115.40	118.60
1	2	1491	U	N3-C2-O2	-5.33	118.47	122.20
36	1	1398	U	N3-C4-O4	-5.33	115.67	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2958	A	C5-C6-N1	5.33	120.36	117.70
36	5	437	G	C8-N9-C1'	5.33	133.93	127.00
36	5	2968	G	C4-C5-N7	-5.33	108.67	110.80
36	1	76	G	N9-C4-C5	5.33	107.53	105.40
36	1	1133	A	C5-C6-N6	-5.33	119.44	123.70
36	5	328	U	C2-N1-C1'	-5.33	111.31	117.70
1	2	1169	G	C8-N9-C4	-5.33	104.27	106.40
36	1	2197	C	C2-N3-C4	5.33	122.56	119.90
36	1	3028	G	N3-C4-C5	-5.33	125.94	128.60
36	5	589	A	N1-C6-N6	5.33	121.80	118.60
38	8	129	C	N1-C2-O2	-5.33	115.70	118.90
1	2	934	C	N3-C4-N4	5.32	121.73	118.00
36	1	343	U	N3-C4-O4	5.32	123.13	119.40
36	1	968	G	N1-C6-O6	5.32	123.09	119.90
36	1	2541	U	P-O3'-C3'	5.32	126.09	119.70
36	5	1489	A	N1-C6-N6	5.32	121.79	118.60
36	1	1082	U	C5-C6-N1	5.32	125.36	122.70
36	1	3312	U	N3-C4-O4	-5.32	115.67	119.40
38	8	17	A	C6-C5-N7	-5.32	128.57	132.30
1	2	694	U	N3-C2-O2	-5.32	118.47	122.20
36	1	2409	G	C8-N9-C4	-5.32	104.27	106.40
61	n5	34	LEU	CA-CB-CG	5.32	127.53	115.30
36	1	664	U	C5-C4-O4	-5.32	122.71	125.90
36	1	1157	G	C8-N9-C4	-5.32	104.27	106.40
36	1	2846	U	C6-N1-C2	-5.32	117.81	121.00
36	1	954	U	N1-C2-O2	-5.32	119.08	122.80
36	1	1406	A	N1-C6-N6	5.32	121.79	118.60
36	1	2278	C	OP2-P-O3'	5.32	116.90	105.20
36	1	2871	G	C8-N9-C1'	5.32	133.91	127.00
36	5	109	A	C8-N9-C4	-5.32	103.67	105.80
36	5	1516	C	C5-C6-N1	-5.32	118.34	121.00
1	2	398	G	C8-N9-C4	-5.32	104.27	106.40
1	2	1768	G	C8-N9-C1'	5.32	133.91	127.00
36	1	894	G	C8-N9-C1'	5.32	133.91	127.00
1	6	617	U	C2-N1-C1'	5.32	124.08	117.70
36	5	514	G	N1-C6-O6	5.32	123.09	119.90
36	5	2718	U	N3-C2-O2	-5.32	118.48	122.20
36	5	2816	G	C4-N9-C1'	-5.32	119.59	126.50
1	6	308	C	C2-N3-C4	-5.31	117.24	119.90
36	5	1942	U	N1-C2-N3	5.31	118.09	114.90
36	5	2901	G	C5-C6-O6	-5.31	125.41	128.60
36	1	627	U	N3-C2-O2	5.31	125.92	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3268	A	N1-C6-N6	5.31	121.79	118.60
36	5	421	G	N1-C2-N3	5.31	127.09	123.90
36	5	1151	U	N3-C4-O4	5.31	123.12	119.40
36	5	1604	G	C8-N9-C1'	-5.31	120.09	127.00
36	5	2765	C	C6-N1-C2	-5.31	118.17	120.30
36	1	1535	A	C5-N7-C8	-5.31	101.25	103.90
36	5	875	G	N1-C6-O6	-5.31	116.71	119.90
43	l6	169	ASP	CB-CG-OD1	-5.31	113.52	118.30
8	S6	54	GLY	N-CA-C	5.31	126.37	113.10
36	1	1377	G	N1-C6-O6	5.31	123.08	119.90
36	1	2225	U	C5-C6-N1	-5.31	120.05	122.70
36	1	2634	U	C2-N3-C4	-5.31	123.82	127.00
36	1	2750	U	C5-C6-N1	-5.31	120.05	122.70
39	L2	191	LEU	CA-CB-CG	-5.31	103.09	115.30
36	5	1056	U	OP2-P-O3'	5.31	116.88	105.20
36	5	2978	U	C4-C5-C6	5.31	122.88	119.70
36	5	3309	G	O4'-C1'-N9	5.31	112.44	108.20
36	1	1699	A	N1-C6-N6	5.31	121.78	118.60
36	5	2650	U	N3-C4-C5	5.31	117.78	114.60
36	5	2887	A	OP1-P-OP2	5.31	127.56	119.60
36	1	2818	U	O4'-C1'-N1	-5.30	103.96	108.20
36	1	3112	G	OP1-P-O3'	5.30	116.87	105.20
38	4	32	C	O5'-P-OP2	-5.30	100.93	105.70
36	5	1110	U	N3-C4-O4	-5.30	115.69	119.40
36	5	2355	G	C6-C5-N7	-5.30	127.22	130.40
36	5	2360	C	OP2-P-O3'	5.30	116.87	105.20
36	1	2406	C	O5'-P-OP2	-5.30	100.93	105.70
1	6	1602	C	N3-C4-N4	-5.30	114.29	118.00
36	5	2186	U	C5-C6-N1	5.30	125.35	122.70
36	5	2405	C	N3-C2-O2	-5.30	118.19	121.90
36	5	2643	A	N9-C4-C5	-5.30	103.68	105.80
36	1	3174	A	N7-C8-N9	5.30	116.45	113.80
1	6	1361	U	N1-C2-O2	5.30	126.51	122.80
36	5	746	A	N1-C6-N6	5.30	121.78	118.60
36	5	2653	C	N1-C2-O2	-5.30	115.72	118.90
36	1	142	C	C2-N1-C1'	5.30	124.63	118.80
36	1	2371	G	C4-C5-N7	5.30	112.92	110.80
36	5	1886	A	C5-C6-N6	-5.30	119.46	123.70
36	1	950	G	N1-C6-O6	-5.30	116.72	119.90
36	1	2692	A	N1-C6-N6	5.30	121.78	118.60
36	5	622	A	C5-C6-N6	-5.30	119.46	123.70
36	5	2818	U	C5'-C4'-O4'	-5.30	102.74	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	299	G	N9-C4-C5	-5.30	103.28	105.40
36	1	2827	U	N1-C2-N3	5.30	118.08	114.90
36	1	3361	G	N9-C4-C5	-5.29	103.28	105.40
37	3	80	G	C6-C5-N7	-5.29	127.22	130.40
1	6	971	A	OP1-P-OP2	-5.29	111.66	119.60
36	5	991	G	N1-C6-O6	-5.29	116.72	119.90
36	5	2730	G	C4-C5-N7	5.29	112.92	110.80
36	1	501	A	N9-C4-C5	-5.29	103.68	105.80
36	1	997	A	C8-N9-C4	-5.29	103.68	105.80
36	5	793	C	O5'-P-OP2	-5.29	100.94	105.70
36	5	2197	C	N3-C2-O2	5.29	125.61	121.90
36	5	2599	U	C5-C6-N1	-5.29	120.05	122.70
36	5	3374	U	N3-C4-O4	-5.29	115.69	119.40
1	2	324	U	C6-N1-C2	-5.29	117.83	121.00
36	1	979	U	N3-C2-O2	-5.29	118.50	122.20
36	1	991	G	C6-C5-N7	-5.29	127.22	130.40
36	1	1581	C	N1-C2-O2	5.29	122.08	118.90
1	6	1297	G	N7-C8-N9	-5.29	110.45	113.10
36	5	2148	U	N1-C2-O2	-5.29	119.10	122.80
36	1	1120	A	N1-C2-N3	5.29	131.94	129.30
36	1	2223	A	OP2-P-O3'	5.29	116.84	105.20
1	2	994	G	C4-C5-N7	-5.29	108.68	110.80
36	1	81	C	N3-C4-C5	5.29	124.02	121.90
36	1	501	A	N1-C6-N6	5.29	121.77	118.60
36	1	2986	U	N3-C4-C5	-5.29	111.43	114.60
36	5	921	A	C6-N1-C2	-5.29	115.43	118.60
36	5	1054	A	C8-N9-C4	5.29	107.92	105.80
36	5	1694	U	N3-C2-O2	-5.29	118.50	122.20
37	7	93	C	C5-C6-N1	-5.29	118.36	121.00
1	2	1153	G	N1-C6-O6	-5.29	116.73	119.90
36	1	1330	A	N1-C6-N6	5.29	121.77	118.60
36	1	2823	G	C5-N7-C8	5.29	106.94	104.30
1	6	1095	U	N3-C4-O4	-5.29	115.70	119.40
36	5	2584	G	OP2-P-O3'	5.29	116.83	105.20
36	1	908	G	N1-C6-O6	5.29	123.07	119.90
36	1	1390	A	N1-C2-N3	5.29	131.94	129.30
36	1	1620	U	C2-N1-C1'	5.29	124.04	117.70
1	6	617	U	N3-C2-O2	-5.29	118.50	122.20
36	5	2862	U	N1-C2-N3	5.29	118.07	114.90
1	2	266	A	C8-N9-C4	5.28	107.91	105.80
1	6	337	G	N7-C8-N9	5.28	115.74	113.10
36	5	2882	U	C6-N1-C2	-5.28	117.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1745	G	C6-N1-C2	-5.28	121.93	125.10
36	1	1389	G	C6-C5-N7	-5.28	127.23	130.40
36	1	1699	A	C8-N9-C4	5.28	107.91	105.80
36	1	2283	G	C5-C6-N1	-5.28	108.86	111.50
1	6	1793	G	C6-C5-N7	5.28	133.57	130.40
36	5	1208	U	N1-C2-N3	5.28	118.07	114.90
36	5	1725	C	O4'-C1'-N1	5.28	112.42	108.20
36	5	3231	U	C5-C4-O4	5.28	129.07	125.90
1	6	755	A	P-O3'-C3'	5.28	126.03	119.70
1	2	1572	G	C4-C5-N7	5.28	112.91	110.80
36	1	267	G	N1-C6-O6	5.28	123.07	119.90
36	1	1320	C	C2-N1-C1'	5.28	124.60	118.80
1	6	1745	G	C5-C6-O6	-5.28	125.43	128.60
36	5	968	G	N7-C8-N9	-5.28	110.46	113.10
36	5	1064	A	P-O3'-C3'	5.28	126.03	119.70
36	5	2943	G	C4-C5-N7	5.28	112.91	110.80
1	2	75	U	N1-C2-O2	5.28	126.49	122.80
1	2	1206	U	C6-N1-C2	-5.28	117.83	121.00
36	1	420	G	N3-C4-N9	5.28	129.17	126.00
36	1	1119	C	C5-C6-N1	-5.28	118.36	121.00
1	6	1037	C	C6-N1-C2	5.28	122.41	120.30
36	5	1799	A	C8-N9-C4	-5.28	103.69	105.80
36	5	2618	G	C5-C6-N1	5.28	114.14	111.50
1	6	582	U	N1-C2-O2	5.27	126.49	122.80
36	5	2820	A	N1-C6-N6	5.27	121.77	118.60
36	1	3312	U	N3-C4-C5	5.27	117.76	114.60
1	6	377	G	N1-C6-O6	-5.27	116.74	119.90
1	6	1028	C	C4-C5-C6	5.27	120.04	117.40
36	5	1371	G	C4-C5-N7	-5.27	108.69	110.80
36	5	3269	U	P-O3'-C3'	5.27	126.03	119.70
36	1	152	U	C6-N1-C2	-5.27	117.84	121.00
36	1	281	G	C4-N9-C1'	5.27	133.35	126.50
36	1	708	G	C8-N9-C4	5.27	108.51	106.40
36	1	1171	G	C8-N9-C4	5.27	108.51	106.40
36	5	1181	U	N1-C2-N3	5.27	118.06	114.90
36	1	3199	G	C8-N9-C1'	5.27	133.85	127.00
36	1	3218	A	P-O3'-C3'	5.27	126.02	119.70
1	6	337	G	C4-C5-N7	5.27	112.91	110.80
36	5	887	G	C2-N3-C4	-5.27	109.27	111.90
84	p0	70	LEU	CA-CB-CG	5.27	127.42	115.30
36	1	2118	C	N3-C2-O2	5.27	125.59	121.90
36	1	2355	G	C4-C5-N7	5.27	112.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	218	G	OP1-P-OP2	5.27	127.50	119.60
36	5	1452	A	C4-C5-N7	5.27	113.33	110.70
36	5	2430	A	C4-C5-C6	5.27	119.63	117.00
36	5	3227	A	N1-C6-N6	5.27	121.76	118.60
36	1	518	G	C4-C5-N7	5.27	112.91	110.80
1	6	1006	C	N1-C2-O2	-5.27	115.74	118.90
1	6	1638	G	N9-C4-C5	5.27	107.51	105.40
37	7	105	C	N3-C4-C5	-5.27	119.79	121.90
1	2	1324	G	N1-C2-N2	5.26	120.94	116.20
36	1	3277	U	N1-C2-O2	5.26	126.48	122.80
36	5	1116	G	C4-C5-C6	5.26	121.96	118.80
36	5	3015	G	OP2-P-O3'	5.26	116.78	105.20
36	1	3215	A	C8-N9-C4	5.26	107.91	105.80
36	5	2950	G	C8-N9-C4	-5.26	104.30	106.40
36	1	2727	A	OP2-P-O3'	5.26	116.77	105.20
1	6	385	A	N9-C4-C5	5.26	107.91	105.80
36	5	648	C	O5'-P-OP1	-5.26	100.96	105.70
36	5	1307	G	OP1-P-OP2	5.26	127.49	119.60
36	5	2379	U	C5-C6-N1	-5.26	120.07	122.70
36	5	2617	U	N1-C2-N3	5.26	118.06	114.90
36	5	2888	U	C5-C4-O4	-5.26	122.74	125.90
1	2	1363	U	C2-N1-C1'	5.26	124.01	117.70
36	1	2176	U	N1-C2-O2	5.26	126.48	122.80
36	1	2257	C	C6-N1-C2	-5.26	118.20	120.30
38	4	40	A	C6-C5-N7	-5.26	128.62	132.30
1	6	65	A	C5-N7-C8	-5.26	101.27	103.90
36	5	1041	U	O5'-P-OP2	-5.26	100.97	105.70
36	5	3200	G	C6-C5-N7	-5.26	127.25	130.40
36	1	1868	G	C5-N7-C8	-5.26	101.67	104.30
36	1	2879	C	N3-C4-C5	-5.26	119.80	121.90
36	5	2165	G	C6-C5-N7	-5.26	127.25	130.40
36	1	2720	G	C8-N9-C4	5.26	108.50	106.40
1	6	1641	C	N1-C2-O2	-5.26	115.75	118.90
36	5	1381	A	C2-N3-C4	-5.26	107.97	110.60
38	8	24	G	N1-C6-O6	-5.26	116.75	119.90
1	6	400	A	C5-C6-N6	-5.25	119.50	123.70
36	5	2199	G	C5-C6-N1	-5.25	108.87	111.50
38	8	17	A	C5-C6-N6	-5.25	119.50	123.70
36	1	98	G	C2-N3-C4	-5.25	109.27	111.90
36	1	332	C	C2-N1-C1'	-5.25	113.02	118.80
36	1	1417	G	N7-C8-N9	-5.25	110.47	113.10
1	6	1584	G	N9-C4-C5	-5.25	103.30	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	325	G	N3-C4-C5	5.25	131.22	128.60
1	2	1585	U	O5'-P-OP2	-5.25	100.97	105.70
36	1	392	G	C4-C5-N7	5.25	112.90	110.80
36	1	2276	G	C8-N9-C4	-5.25	104.30	106.40
36	5	1789	G	C8-N9-C4	5.25	108.50	106.40
36	5	1885	U	C5-C6-N1	-5.25	120.07	122.70
1	2	1768	G	N9-C4-C5	5.25	107.50	105.40
36	1	2434	U	C5-C6-N1	-5.25	120.08	122.70
36	1	2791	G	N3-C2-N2	-5.25	116.23	119.90
37	3	79	A	N1-C2-N3	5.25	131.92	129.30
38	8	44	A	C4-C5-N7	5.25	113.32	110.70
1	2	1596	C	N3-C2-O2	-5.25	118.23	121.90
1	6	1766	A	OP1-P-O3'	5.25	116.74	105.20
36	5	2763	U	C2-N3-C4	-5.25	123.85	127.00
36	5	3041	U	C4-C5-C6	-5.25	116.55	119.70
36	1	2335	G	N1-C6-O6	-5.25	116.75	119.90
36	1	2967	A	N1-C6-N6	5.25	121.75	118.60
1	6	1037	C	N3-C4-C5	5.25	124.00	121.90
36	5	1874	A	C2-N3-C4	-5.25	107.98	110.60
36	5	2920	U	N1-C2-N3	5.25	118.05	114.90
36	1	3016	A	N1-C6-N6	5.24	121.75	118.60
36	1	3361	G	C4-C5-N7	5.24	112.90	110.80
36	5	2374	C	C2-N1-C1'	5.24	124.57	118.80
36	1	1204	A	N9-C4-C5	-5.24	103.70	105.80
36	1	2104	A	C8-N9-C4	5.24	107.90	105.80
1	6	540	G	N1-C2-N3	-5.24	120.75	123.90
1	6	815	G	C4-C5-N7	5.24	112.90	110.80
36	5	2651	G	OP2-P-O3'	5.24	116.73	105.20
36	5	3086	A	O5'-P-OP2	5.24	116.99	110.70
36	1	900	G	C4-C5-N7	-5.24	108.70	110.80
36	1	1102	A	C2-N3-C4	-5.24	107.98	110.60
36	1	2306	C	N3-C4-N4	-5.24	114.33	118.00
36	5	1848	G	N9-C4-C5	-5.24	103.31	105.40
36	5	2412	G	N1-C6-O6	-5.24	116.76	119.90
37	7	91	G	N3-C4-N9	5.24	129.14	126.00
36	1	1505	C	OP2-P-O3'	5.24	116.72	105.20
36	1	2350	C	C2-N3-C4	-5.24	117.28	119.90
36	5	145	G	N3-C4-C5	5.24	131.22	128.60
36	5	1797	A	OP1-P-OP2	-5.24	111.74	119.60
36	5	2273	G	N7-C8-N9	-5.24	110.48	113.10
1	2	362	G	N1-C2-N3	5.24	127.04	123.90
1	2	1246	C	N3-C2-O2	-5.24	118.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	587	U	C5-C6-N1	-5.24	120.08	122.70
36	1	793	C	O5'-P-OP2	-5.24	100.99	105.70
36	1	1496	C	C2-N1-C1'	5.24	124.56	118.80
36	5	1882	G	C5-C6-O6	-5.24	125.46	128.60
36	5	3377	G	C2-N3-C4	5.24	114.52	111.90
1	6	901	G	C5-N7-C8	-5.23	101.68	104.30
1	6	1458	G	C4-N9-C1'	5.23	133.30	126.50
36	1	2988	C	N1-C2-O2	-5.23	115.76	118.90
1	6	1600	A	C5-C6-N1	-5.23	115.08	117.70
36	5	27	C	C6-N1-C1'	5.23	127.08	120.80
36	5	197	G	C5-N7-C8	-5.23	101.68	104.30
36	5	530	G	N1-C6-O6	-5.23	116.76	119.90
36	5	669	U	C5-C6-N1	-5.23	120.08	122.70
1	2	704	C	O4'-C1'-N1	5.23	112.38	108.20
1	2	730	G	C4-N9-C1'	5.23	133.30	126.50
36	1	1883	A	C8-N9-C4	5.23	107.89	105.80
36	1	2357	A	C4-C5-N7	5.23	113.31	110.70
1	6	1478	G	N3-C4-C5	-5.23	125.98	128.60
36	5	1879	A	N9-C4-C5	-5.23	103.71	105.80
36	5	1884	A	C2-N3-C4	-5.23	107.98	110.60
1	2	704	C	N1-C2-O2	5.23	122.04	118.90
36	1	1445	U	N1-C2-N3	5.23	118.04	114.90
36	5	644	G	C5-N7-C8	5.23	106.91	104.30
36	5	718	G	C4-N9-C1'	5.23	133.30	126.50
38	8	8	C	N1-C2-N3	5.23	122.86	119.20
36	1	1097	G	C2-N3-C4	5.23	114.51	111.90
36	1	2321	A	C8-N9-C4	5.23	107.89	105.80
1	6	404	G	O5'-P-OP1	-5.23	101.00	105.70
36	1	2818	U	O5'-P-OP2	-5.23	101.00	105.70
1	6	136	C	N1-C2-O2	5.23	122.04	118.90
36	5	19	U	N3-C4-O4	5.23	123.06	119.40
36	1	419	G	N3-C2-N2	5.22	123.56	119.90
36	1	663	C	N1-C2-O2	-5.22	115.77	118.90
36	1	1167	U	C5-C6-N1	-5.22	120.09	122.70
36	1	2606	G	N3-C2-N2	5.22	123.56	119.90
36	1	2607	G	O5'-P-OP2	-5.22	101.00	105.70
1	6	145	A	OP1-P-O3'	5.22	116.69	105.20
36	5	859	G	C4-C5-N7	5.22	112.89	110.80
36	5	1843	C	N3-C4-N4	5.22	121.66	118.00
36	5	2615	G	C6-C5-N7	-5.22	127.27	130.40
36	5	2970	C	C4-C5-C6	5.22	120.01	117.40
15	C3	22	ALA	C-N-CA	5.22	143.93	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	SM	134	ASP	CB-CG-OD2	5.22	123.00	118.30
36	1	3123	A	N3-C4-C5	5.22	130.46	126.80
1	6	308	C	C2-N1-C1'	-5.22	113.06	118.80
36	5	2620	G	C8-N9-C1'	5.22	133.79	127.00
36	5	3128	G	C5-C6-O6	-5.22	125.47	128.60
1	2	1798	U	N3-C2-O2	-5.22	118.55	122.20
36	1	283	G	C4-N9-C1'	5.22	133.29	126.50
36	5	2278	C	OP2-P-O3'	5.22	116.69	105.20
36	5	2940	A	N1-C6-N6	5.22	121.73	118.60
36	5	3341	U	C5-C6-N1	5.22	125.31	122.70
38	8	95	G	C8-N9-C1'	5.22	133.79	127.00
1	2	334	G	N3-C4-N9	-5.22	122.87	126.00
1	2	1798	U	C2-N1-C1'	5.22	123.96	117.70
1	6	1150	G	C8-N9-C4	5.22	108.49	106.40
36	5	2279	A	OP1-P-OP2	-5.22	111.77	119.60
36	5	2408	U	O5'-P-OP2	-5.22	101.00	105.70
68	o2	4	LEU	C-N-CD	5.22	139.36	128.40
36	1	613	G	N1-C6-O6	5.22	123.03	119.90
36	1	3303	G	O4'-C1'-N9	5.22	112.38	108.20
20	c8	116	LEU	CA-CB-CG	5.22	127.30	115.30
1	6	1297	G	C8-N9-C4	5.22	108.49	106.40
36	5	716	A	C8-N9-C4	5.22	107.89	105.80
36	5	1114	U	N1-C2-O2	5.22	126.45	122.80
36	5	1336	U	O5'-P-OP2	-5.22	101.00	105.70
36	5	2231	C	C2-N1-C1'	5.22	124.54	118.80
36	5	2957	G	C2-N3-C4	-5.22	109.29	111.90
1	2	73	U	P-O3'-C3'	5.21	125.96	119.70
36	1	96	G	N3-C4-N9	-5.21	122.87	126.00
36	1	1476	G	C4-C5-N7	-5.21	108.71	110.80
36	1	1741	A	C2-N3-C4	-5.21	107.99	110.60
1	6	695	U	N3-C2-O2	-5.21	118.55	122.20
36	5	2619	G	C5-C6-N1	5.21	114.11	111.50
36	1	351	A	C5-C6-N6	5.21	127.87	123.70
36	1	585	A	C2-N3-C4	-5.21	107.99	110.60
36	1	939	U	C5-C4-O4	-5.21	122.77	125.90
36	1	1081	U	C5-C6-N1	5.21	125.31	122.70
36	1	1367	G	C4-C5-N7	5.21	112.89	110.80
36	1	2918	G	C2-N3-C4	5.21	114.51	111.90
36	1	3208	G	N9-C4-C5	5.21	107.48	105.40
38	4	21	C	C2-N1-C1'	-5.21	113.07	118.80
1	6	1722	A	C2-N3-C4	-5.21	107.99	110.60
36	5	1125	U	N3-C4-O4	-5.21	115.75	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1238	C	P-O3'-C3'	5.21	125.95	119.70
36	5	1389	G	C4-C5-N7	5.21	112.89	110.80
36	1	651	G	OP2-P-O3'	5.21	116.66	105.20
36	5	374	A	N9-C4-C5	5.21	107.88	105.80
1	2	1213	G	C5-C6-O6	5.21	131.72	128.60
36	1	49	A	N9-C4-C5	-5.21	103.72	105.80
36	1	780	A	C5-C6-N6	5.21	127.87	123.70
36	1	785	G	C2-N3-C4	5.21	114.50	111.90
36	1	1307	G	C5-C6-N1	5.21	114.10	111.50
36	1	2279	A	O5'-P-OP1	-5.21	101.01	105.70
36	1	2613	U	C4-C5-C6	5.21	122.83	119.70
36	5	2727	A	O5'-P-OP2	-5.21	101.01	105.70
36	1	2286	U	O5'-P-OP2	-5.21	101.02	105.70
36	1	3326	G	N7-C8-N9	-5.21	110.50	113.10
36	5	2817	A	N1-C6-N6	5.21	121.72	118.60
36	5	101	G	C8-N9-C4	-5.21	104.32	106.40
36	5	509	U	N3-C4-C5	5.21	117.72	114.60
36	5	2942	C	N1-C2-O2	-5.21	115.78	118.90
1	2	424	C	C2-N3-C4	5.20	122.50	119.90
36	1	55	G	OP2-P-O3'	5.20	116.65	105.20
36	1	1881	A	C5-C6-N1	5.20	120.30	117.70
36	1	2603	G	C5-C6-O6	-5.20	125.48	128.60
36	5	890	C	P-O3'-C3'	5.20	125.94	119.70
36	5	1060	U	C2-N1-C1'	-5.20	111.45	117.70
36	5	1868	G	C6-C5-N7	-5.20	127.28	130.40
36	5	2164	A	C4-C5-C6	5.20	119.60	117.00
36	5	3183	A	C8-N9-C4	5.20	107.88	105.80
36	5	3000	A	C8-N9-C4	5.20	107.88	105.80
1	2	1213	G	N1-C6-O6	-5.20	116.78	119.90
36	1	1433	A	C6-N1-C2	-5.20	115.48	118.60
36	1	1860	G	C8-N9-C4	5.20	108.48	106.40
36	1	2833	A	C8-N9-C4	5.20	107.88	105.80
1	6	337	G	N3-C4-N9	5.20	129.12	126.00
36	5	32	U	N3-C2-O2	-5.20	118.56	122.20
36	5	207	U	C2-N3-C4	-5.20	123.88	127.00
36	5	859	G	C6-C5-N7	-5.20	127.28	130.40
36	5	1506	A	C8-N9-C4	-5.20	103.72	105.80
36	5	2682	C	C2'-C3'-O3'	5.20	122.02	113.70
36	1	1202	A	C5-C6-N1	-5.20	115.10	117.70
1	6	1022	C	C5-C6-N1	-5.20	118.40	121.00
36	5	234	G	C4-C5-N7	5.20	112.88	110.80
36	5	1149	G	N9-C1'-C2'	-5.20	106.28	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1716	U	P-O3'-C3'	5.20	125.94	119.70
36	5	2164	A	N1-C6-N6	5.20	121.72	118.60
38	8	55	U	N3-C2-O2	-5.20	118.56	122.20
36	1	1199	C	N1-C2-O2	5.20	122.02	118.90
36	1	2369	G	N3-C4-N9	5.20	129.12	126.00
36	1	2760	C	N3-C4-C5	-5.20	119.82	121.90
36	5	700	C	C6-N1-C2	5.20	122.38	120.30
36	5	3177	G	C8-N9-C4	5.20	108.48	106.40
38	8	32	C	C2-N1-C1'	-5.20	113.08	118.80
78	q2	93	LEU	CA-CB-CG	5.20	127.25	115.30
1	2	388	G	C5-C6-O6	-5.20	125.48	128.60
36	1	3148	U	N3-C4-C5	5.20	117.72	114.60
1	6	65	A	C6-N1-C2	5.20	121.72	118.60
1	6	1517	U	C2-N1-C1'	-5.20	111.47	117.70
4	s2	229	LEU	CA-CB-CG	5.20	127.25	115.30
36	5	1662	G	C6-C5-N7	-5.20	127.28	130.40
36	5	2372	A	N3-C4-C5	-5.20	123.16	126.80
36	5	2726	C	N1-C2-N3	5.20	122.84	119.20
1	2	896	U	N1-C2-O2	5.19	126.44	122.80
36	1	2632	G	N1-C6-O6	-5.19	116.78	119.90
36	1	3252	G	N3-C4-C5	5.19	131.20	128.60
36	5	2924	U	N3-C2-O2	5.19	125.84	122.20
36	1	2943	G	C4-C5-N7	5.19	112.88	110.80
1	6	1039	A	O4'-C1'-N9	5.19	112.35	108.20
36	5	1384	U	N3-C2-O2	-5.19	118.56	122.20
36	5	2986	U	N3-C4-O4	5.19	123.03	119.40
36	1	653	A	C2-N3-C4	-5.19	108.00	110.60
36	1	2621	G	O5'-P-OP2	-5.19	101.03	105.70
36	5	880	G	C6-N1-C2	-5.19	121.99	125.10
36	5	2928	C	C6-N1-C2	-5.19	118.22	120.30
36	5	1306	G	N1-C6-O6	5.19	123.01	119.90
36	5	1929	G	C5-C6-O6	-5.19	125.49	128.60
36	5	2250	G	N3-C4-N9	5.19	129.11	126.00
36	1	2409	G	N3-C4-C5	-5.19	126.01	128.60
36	1	2831	G	C6-C5-N7	-5.19	127.29	130.40
36	5	1150	A	O5'-P-OP2	-5.19	101.03	105.70
1	2	1745	G	C6-N1-C2	-5.19	121.99	125.10
36	1	107	A	N1-C6-N6	5.19	121.71	118.60
36	1	1097	G	P-O3'-C3'	5.19	125.92	119.70
36	5	3365	U	C5-C4-O4	-5.19	122.79	125.90
1	2	1745	G	N3-C4-C5	-5.18	126.01	128.60
36	1	80	G	C6-N1-C2	-5.18	121.99	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1791	C	C6-N1-C2	5.18	122.37	120.30
36	1	1807	G	N3-C4-N9	5.18	129.11	126.00
36	1	2603	G	OP1-P-O3'	5.18	116.61	105.20
1	6	577	G	C6-C5-N7	-5.18	127.29	130.40
36	5	2661	G	OP1-P-O3'	5.18	116.61	105.20
1	2	1637	C	N1-C2-O2	5.18	122.01	118.90
36	1	318	A	O5'-P-OP1	-5.18	101.03	105.70
36	1	339	C	N3-C2-O2	-5.18	118.27	121.90
1	6	941	A	N1-C6-N6	-5.18	115.49	118.60
36	5	43	A	O4'-C1'-N9	5.18	112.35	108.20
36	5	863	C	C5-C6-N1	-5.18	118.41	121.00
36	5	898	U	N1-C2-N3	-5.18	111.79	114.90
36	5	1879	A	OP1-P-OP2	-5.18	111.83	119.60
36	5	2912	G	O5'-P-OP2	5.18	116.92	110.70
36	1	1505	C	C2-N3-C4	-5.18	117.31	119.90
36	1	2431	C	C5-C6-N1	-5.18	118.41	121.00
36	5	1549	U	C6-N1-C2	5.18	124.11	121.00
1	2	1036	A	C8-N9-C4	5.18	107.87	105.80
36	1	613	G	C5-C6-O6	-5.18	125.49	128.60
36	1	1885	U	N3-C4-O4	5.18	123.03	119.40
36	1	2603	G	C6-C5-N7	-5.18	127.29	130.40
38	4	113	U	C6-N1-C1'	5.18	128.45	121.20
73	O7	11	ARG	NE-CZ-NH1	-5.18	117.71	120.30
36	5	75	G	N3-C4-C5	-5.18	126.01	128.60
36	5	1598	G	C8-N9-C4	5.18	108.47	106.40
36	5	1847	A	C2-N3-C4	-5.18	108.01	110.60
36	5	2774	C	N3-C4-C5	-5.18	119.83	121.90
36	5	3172	A	C2-N3-C4	-5.18	108.01	110.60
1	2	631	G	C4-C5-N7	-5.18	108.73	110.80
36	1	1116	G	C8-N9-C4	-5.18	104.33	106.40
36	5	1449	A	N1-C2-N3	5.18	131.89	129.30
1	2	1772	C	OP1-P-O3'	5.18	116.59	105.20
36	1	2369	G	N3-C4-C5	-5.18	126.01	128.60
36	1	2624	G	C6-C5-N7	-5.18	127.29	130.40
1	6	1596	C	C5-C4-N4	5.18	123.82	120.20
36	5	121	A	C8-N9-C4	5.18	107.87	105.80
36	5	343	U	N1-C2-N3	5.18	118.01	114.90
36	5	435	C	O5'-P-OP2	-5.18	101.04	105.70
36	5	818	C	N1-C2-O2	-5.18	115.79	118.90
36	5	1147	G	C2-N3-C4	5.18	114.49	111.90
36	1	2606	G	C4-C5-N7	5.17	112.87	110.80
1	6	9	U	C5-C4-O4	-5.17	122.80	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	115	G	C8-N9-C4	5.17	108.47	106.40
1	6	125	U	C6-N1-C2	5.17	124.10	121.00
1	6	1095	U	N3-C4-C5	5.17	117.70	114.60
36	1	1724	U	P-O3'-C3'	5.17	125.91	119.70
36	5	1438	U	C6-N1-C2	-5.17	117.90	121.00
38	8	22	U	C5-C6-N1	-5.17	120.11	122.70
1	2	75	U	N3-C2-O2	-5.17	118.58	122.20
36	1	1751	G	C8-N9-C4	5.17	108.47	106.40
1	6	558	U	C5-C6-N1	5.17	125.28	122.70
36	5	522	A	C2-N3-C4	-5.17	108.01	110.60
36	5	935	U	N3-C4-O4	5.17	123.02	119.40
36	1	159	A	C8-N9-C4	5.17	107.87	105.80
36	1	934	G	C8-N9-C1'	-5.17	120.28	127.00
1	6	787	G	N3-C4-N9	5.17	129.10	126.00
36	1	681	U	C5-C6-N1	-5.17	120.11	122.70
36	1	2831	G	C5-C6-N1	-5.17	108.92	111.50
49	M3	47	ALA	C-N-CD	5.17	139.25	128.40
36	5	757	C	OP2-P-O3'	5.17	116.57	105.20
1	2	874	C	C5-C6-N1	5.17	123.58	121.00
36	1	2283	G	C2-N3-C4	-5.17	109.32	111.90
36	5	718	G	C8-N9-C1'	-5.17	120.28	127.00
36	5	847	A	N7-C8-N9	-5.17	111.22	113.80
36	5	2526	C	C6-N1-C1'	-5.17	114.60	120.80
36	5	2817	A	N3-C4-N9	5.17	131.53	127.40
38	8	90	U	C6-N1-C2	5.17	124.10	121.00
1	2	1268	G	O5'-P-OP2	-5.17	101.05	105.70
36	1	1180	A	N1-C6-N6	-5.17	115.50	118.60
36	1	1741	A	N1-C2-N3	5.17	131.88	129.30
36	1	2571	U	N3-C2-O2	-5.17	118.58	122.20
1	6	616	G	C2-N3-C4	5.17	114.48	111.90
1	2	110	U	N3-C4-C5	5.16	117.70	114.60
36	1	715	A	C8-N9-C4	-5.16	103.73	105.80
1	6	42	G	C5-C6-N1	5.16	114.08	111.50
1	2	934	C	C6-N1-C1'	-5.16	114.61	120.80
36	1	1305	U	C2-N1-C1'	5.16	123.89	117.70
20	c8	15	LEU	CA-CB-CG	5.16	127.17	115.30
36	5	1433	A	C5-C6-N6	5.16	127.83	123.70
36	5	1789	G	C8-N9-C1'	5.16	133.71	127.00
1	2	1754	A	C2-N3-C4	-5.16	108.02	110.60
3	S1	70	LEU	CA-CB-CG	5.16	127.17	115.30
36	1	2928	C	O5'-P-OP1	-5.16	101.06	105.70
1	6	313	U	C5-C6-N1	-5.16	120.12	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2665	U	O5'-P-OP2	-5.16	101.06	105.70
38	8	42	G	O5'-P-OP2	-5.16	101.06	105.70
36	1	25	U	N1-C2-N3	5.16	118.00	114.90
36	1	942	U	O5'-P-OP1	5.16	116.89	110.70
1	6	957	G	N3-C2-N2	-5.16	116.29	119.90
1	2	25	C	P-O3'-C3'	5.16	125.89	119.70
36	1	1040	A	N1-C6-N6	5.16	121.69	118.60
36	5	677	A	C2-N3-C4	-5.16	108.02	110.60
36	5	1179	A	C8-N9-C4	5.16	107.86	105.80
36	5	1431	G	C2-N3-C4	5.16	114.48	111.90
1	2	565	C	N3-C4-C5	5.16	123.96	121.90
36	1	1124	U	C5-C4-O4	-5.16	122.81	125.90
36	1	1425	U	C5-C4-O4	5.16	128.99	125.90
36	1	2537	U	P-O3'-C3'	5.15	125.89	119.70
36	5	3343	G	N3-C2-N2	5.15	123.51	119.90
1	2	1124	A	O5'-P-OP2	5.15	116.88	110.70
1	2	1651	A	C5-C6-N1	-5.15	115.12	117.70
36	1	1335	C	N3-C2-O2	-5.15	118.29	121.90
38	4	96	A	N1-C6-N6	5.15	121.69	118.60
36	5	1420	C	OP2-P-O3'	5.15	116.54	105.20
36	5	1902	G	O5'-P-OP1	-5.15	101.06	105.70
36	5	2695	A	N1-C6-N6	-5.15	115.51	118.60
36	1	1203	A	C2-N3-C4	-5.15	108.03	110.60
36	1	1691	U	O5'-P-OP2	-5.15	101.06	105.70
36	1	1940	G	N1-C2-N2	-5.15	111.56	116.20
36	1	2621	G	N1-C2-N2	5.15	120.84	116.20
36	1	3377	G	C4-C5-N7	5.15	112.86	110.80
36	1	650	C	N3-C2-O2	5.15	125.50	121.90
36	5	1190	A	O4'-C1'-N9	-5.15	104.08	108.20
36	1	1838	G	C5-N7-C8	-5.15	101.73	104.30
36	1	2722	U	C5-C6-N1	-5.15	120.13	122.70
38	4	42	G	OP1-P-O3'	5.15	116.53	105.20
1	6	1340	U	C5-C4-O4	5.15	128.99	125.90
36	5	2375	G	N1-C6-O6	-5.15	116.81	119.90
36	5	2385	G	C8-N9-C1'	5.15	133.69	127.00
36	5	2626	A	N1-C2-N3	5.15	131.87	129.30
1	6	113	U	C2-N1-C1'	-5.15	111.52	117.70
1	6	144	U	C6-N1-C2	-5.15	117.91	121.00
36	5	749	C	C6-N1-C2	-5.15	118.24	120.30
1	2	103	A	P-O3'-C3'	5.14	125.87	119.70
1	2	1244	A	P-O3'-C3'	5.14	125.87	119.70
1	2	1324	G	C6-C5-N7	5.14	133.49	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1410	U	C5-C4-O4	5.14	128.99	125.90
36	1	1939	G	N3-C2-N2	-5.14	116.30	119.90
36	1	2860	U	C4-C5-C6	-5.14	116.61	119.70
1	6	1659	A	N1-C6-N6	5.14	121.69	118.60
36	5	2237	C	OP2-P-O3'	5.14	116.52	105.20
36	5	2387	A	C6-C5-N7	-5.14	128.70	132.30
36	5	3124	G	C8-N9-C4	-5.14	104.34	106.40
36	1	2818	U	P-O3'-C3'	5.14	125.87	119.70
74	O8	14	LEU	CA-CB-CG	5.14	127.12	115.30
36	5	2201	G	N3-C2-N2	5.14	123.50	119.90
36	5	3381	U	C5-C4-O4	5.14	128.98	125.90
1	2	1611	A	O4'-C1'-N9	5.14	112.31	108.20
36	1	281	G	N9-C4-C5	-5.14	103.34	105.40
36	1	2700	G	C6-C5-N7	-5.14	127.32	130.40
36	5	1556	C	C6-N1-C2	-5.14	118.24	120.30
36	1	2234	G	C4-N9-C1'	5.14	133.18	126.50
36	1	2810	C	C6-N1-C2	5.14	122.36	120.30
1	6	862	A	N1-C6-N6	-5.14	115.52	118.60
36	5	2990	G	N3-C4-N9	5.14	129.08	126.00
36	1	608	A	C4-C5-C6	5.13	119.57	117.00
36	1	857	G	C2-N3-C4	-5.13	109.33	111.90
1	6	426	G	N1-C6-O6	-5.13	116.82	119.90
36	5	2649	A	N1-C6-N6	5.13	121.68	118.60
36	5	2725	U	N1-C2-O2	5.13	126.39	122.80
38	4	113	U	N3-C4-O4	-5.13	115.81	119.40
36	1	1342	C	N3-C4-C5	5.13	123.95	121.90
36	5	644	G	N9-C4-C5	5.13	107.45	105.40
36	5	3182	G	OP1-P-OP2	-5.13	111.90	119.60
1	2	328	A	N1-C6-N6	5.13	121.68	118.60
1	2	334	G	C8-N9-C1'	5.13	133.67	127.00
1	6	95	G	N9-C4-C5	5.13	107.45	105.40
36	5	1151	U	N3-C4-C5	-5.13	111.52	114.60
36	5	1480	G	N3-C4-C5	5.13	131.16	128.60
36	5	2325	G	C5-C6-N1	-5.13	108.94	111.50
36	1	623	U	C2-N1-C1'	-5.13	111.55	117.70
36	1	874	U	N3-C4-C5	5.13	117.68	114.60
36	1	1216	C	C5-C6-N1	5.13	123.56	121.00
36	1	2403	G	C4-C5-C6	5.13	121.88	118.80
36	5	555	U	C2-N1-C1'	5.13	123.86	117.70
37	7	36	C	N3-C4-N4	-5.13	114.41	118.00
36	1	658	G	C4-C5-N7	-5.13	108.75	110.80
1	6	1177	C	C6-N1-C2	5.13	122.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	205	C	O5'-P-OP1	-5.13	101.09	105.70
36	5	1810	A	C8-N9-C4	5.13	107.85	105.80
36	1	1928	G	N3-C4-C5	5.12	131.16	128.60
36	1	2305	G	C5-C6-O6	-5.12	125.53	128.60
36	1	2384	A	N3-C4-C5	-5.12	123.21	126.80
1	6	1645	G	C5-C6-N1	5.12	114.06	111.50
1	2	1269	U	C5-C4-O4	-5.12	122.83	125.90
1	2	1455	G	O5'-P-OP2	-5.12	101.09	105.70
36	1	2357	A	C5-C6-N1	5.12	120.26	117.70
36	5	651	G	C6-C5-N7	-5.12	127.33	130.40
36	5	2804	A	N1-C2-N3	5.12	131.86	129.30
1	2	571	G	N7-C8-N9	-5.12	110.54	113.10
1	2	1782	A	C8-N9-C4	-5.12	103.75	105.80
36	1	157	A	C4-C5-C6	5.12	119.56	117.00
36	1	3143	C	C6-N1-C2	5.12	122.35	120.30
36	1	3269	U	P-O3'-C3'	5.12	125.84	119.70
36	1	3369	G	O4'-C1'-N9	5.12	112.30	108.20
53	M7	56	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	6	1503	A	O4'-C1'-N9	5.12	112.30	108.20
36	5	1384	U	N1-C2-O2	5.12	126.39	122.80
1	2	323	A	O5'-P-OP2	-5.12	101.09	105.70
1	2	426	G	C8-N9-C1'	-5.12	120.34	127.00
36	1	888	A	N1-C6-N6	5.12	121.67	118.60
1	6	1023	A	C5-C6-N6	-5.12	119.60	123.70
36	5	2152	A	N1-C6-N6	5.12	121.67	118.60
36	5	2273	G	C4-N9-C1'	-5.12	119.84	126.50
36	1	1122	U	C5-C4-O4	5.12	128.97	125.90
36	1	1633	C	C2-N1-C1'	5.12	124.43	118.80
1	6	101	U	N1-C2-O2	5.12	126.38	122.80
1	6	1514	U	N3-C4-O4	-5.12	115.82	119.40
36	5	2231	C	C6-N1-C2	-5.12	118.25	120.30
36	5	3331	U	C5-C6-N1	-5.12	120.14	122.70
36	5	1367	G	C4-C5-C6	5.12	121.87	118.80
36	1	24	G	N7-C8-N9	-5.12	110.54	113.10
36	1	898	U	N1-C2-O2	5.12	126.38	122.80
36	1	2696	A	OP2-P-O3'	5.12	116.45	105.20
1	6	1	U	N1-C2-O2	5.12	126.38	122.80
1	6	815	G	C5-N7-C8	-5.12	101.74	104.30
36	5	1359	C	N3-C4-N4	5.12	121.58	118.00
36	5	1846	C	C4-C5-C6	5.12	119.96	117.40
1	6	1631	A	N1-C6-N6	-5.11	115.53	118.60
36	5	809	G	C8-N9-C4	5.11	108.44	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1207	G	O5'-P-OP1	-5.11	101.10	105.70
36	5	1213	G	C4-C5-N7	-5.11	108.75	110.80
68	o2	4	LEU	C-N-CA	-5.11	100.53	122.00
27	D5	75	LEU	CB-CG-CD1	-5.11	102.31	111.00
36	1	1659	U	N1-C2-O2	-5.11	119.22	122.80
36	5	1115	G	C4-N9-C1'	5.11	133.15	126.50
36	5	2937	G	C8-N9-C4	5.11	108.44	106.40
1	2	397	A	N1-C6-N6	-5.11	115.53	118.60
44	L7	107	ARG	NE-CZ-NH1	-5.11	117.75	120.30
13	c1	5	LEU	CA-CB-CG	5.11	127.05	115.30
36	5	2199	G	C4-N9-C1'	5.11	133.14	126.50
36	5	2817	A	C6-N1-C2	-5.11	115.53	118.60
36	5	2952	G	C5-C6-N1	5.11	114.06	111.50
36	1	426	G	N3-C4-N9	5.11	129.06	126.00
1	6	1614	A	C4-C5-N7	5.11	113.25	110.70
36	5	349	A	C6-C5-N7	5.11	135.88	132.30
36	5	2968	G	N1-C6-O6	-5.11	116.83	119.90
36	1	1604	G	C8-N9-C4	-5.11	104.36	106.40
15	c3	75	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	2	308	C	C5-C6-N1	-5.11	118.45	121.00
1	2	1560	U	C2-N1-C1'	5.11	123.83	117.70
36	1	388	G	N3-C2-N2	-5.11	116.33	119.90
1	6	1759	C	C6-N1-C2	5.11	122.34	120.30
36	5	1390	A	N1-C6-N6	-5.11	115.54	118.60
36	5	1390	A	N7-C8-N9	5.11	116.35	113.80
36	5	94	G	C2-N3-C4	-5.10	109.35	111.90
36	5	2620	G	C4-N9-C1'	-5.10	119.86	126.50
1	2	728	U	C6-N1-C1'	-5.10	114.06	121.20
36	1	776	U	N1-C2-O2	-5.10	119.23	122.80
36	1	810	A	C5-C6-N1	5.10	120.25	117.70
36	1	890	C	N3-C4-N4	-5.10	114.43	118.00
1	6	826	U	C5-C6-N1	5.10	125.25	122.70
1	6	934	C	C2-N1-C1'	5.10	124.41	118.80
1	6	1436	A	C8-N9-C4	-5.10	103.76	105.80
36	5	2621	G	C5-C6-O6	-5.10	125.54	128.60
36	5	3245	A	C5-C6-N6	-5.10	119.62	123.70
36	1	334	A	C5-C6-N6	-5.10	119.62	123.70
36	1	1791	C	C5-C6-N1	-5.10	118.45	121.00
36	1	2846	U	N3-C4-O4	-5.10	115.83	119.40
36	1	3079	U	C2-N1-C1'	-5.10	111.58	117.70
36	1	3268	A	C6-C5-N7	-5.10	128.73	132.30
37	7	1	G	C6-C5-N7	-5.10	127.34	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	752	C	N3-C4-C5	5.10	123.94	121.90
36	1	1204	A	C8-N9-C4	5.10	107.84	105.80
36	1	2384	A	C4-C5-C6	5.10	119.55	117.00
1	6	1656	U	O5'-P-OP1	5.10	116.82	110.70
36	5	1878	G	C8-N9-C4	-5.10	104.36	106.40
36	5	2333	C	OP2-P-O3'	5.10	116.41	105.20
36	5	1923	C	C6-N1-C2	-5.10	118.26	120.30
36	5	2804	A	C2-N3-C4	-5.10	108.05	110.60
38	8	12	A	C4-C5-N7	5.10	113.25	110.70
36	1	585	A	O5'-P-OP2	-5.09	101.11	105.70
36	1	2925	C	O5'-P-OP2	5.09	116.81	110.70
36	1	2935	U	OP2-P-O3'	5.09	116.41	105.20
36	5	407	A	N9-C4-C5	-5.09	103.76	105.80
36	5	2271	A	C4-C5-C6	-5.09	114.45	117.00
36	5	3122	A	OP2-P-O3'	5.09	116.41	105.20
38	8	125	U	C2-N1-C1'	5.09	123.81	117.70
27	D5	95	HIS	N-CA-C	5.09	124.75	111.00
36	5	1303	A	C5-C6-N6	-5.09	119.63	123.70
36	1	954	U	N3-C2-O2	5.09	125.76	122.20
36	1	1658	G	C4-C5-N7	-5.09	108.76	110.80
1	6	136	C	C6-N1-C1'	-5.09	114.69	120.80
36	5	946	U	N1-C2-N3	5.09	117.95	114.90
36	5	1117	G	O5'-P-OP1	-5.09	101.12	105.70
36	5	1927	G	C5-C6-O6	-5.09	125.55	128.60
36	5	2400	G	C8-N9-C4	5.09	108.44	106.40
36	1	1366	A	N1-C6-N6	5.09	121.65	118.60
36	1	2117	A	N9-C4-C5	5.09	107.84	105.80
36	1	2318	U	N3-C4-C5	5.09	117.65	114.60
36	5	315	C	N3-C4-C5	5.09	123.94	121.90
36	5	1938	U	C5-C6-N1	-5.09	120.16	122.70
36	5	2112	U	P-O3'-C3'	5.09	125.81	119.70
36	5	2283	G	C8-N9-C4	5.09	108.44	106.40
36	5	2869	U	O5'-P-OP1	-5.09	101.12	105.70
1	2	1745	G	C8-N9-C1'	-5.09	120.39	127.00
36	1	2705	A	C2-N3-C4	5.09	113.14	110.60
1	6	66	U	P-O3'-C3'	5.09	125.81	119.70
1	6	371	G	C6-C5-N7	-5.09	127.35	130.40
36	5	2978	U	C5-C4-O4	5.09	128.95	125.90
1	2	136	C	C6-N1-C2	-5.09	118.27	120.30
1	2	610	G	C8-N9-C1'	-5.09	120.39	127.00
36	1	1537	A	C5-C6-N6	-5.09	119.63	123.70
36	1	1929	G	N3-C2-N2	5.09	123.46	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2417	U	N1-C2-N3	5.09	117.95	114.90
36	1	2623	G	N1-C6-O6	5.09	122.95	119.90
36	1	3079	U	C6-N1-C1'	5.09	128.32	121.20
38	4	17	A	N1-C6-N6	5.09	121.65	118.60
38	4	107	G	C6-C5-N7	5.09	133.45	130.40
1	6	452	A	N1-C6-N6	5.09	121.65	118.60
1	2	1773	C	N1-C2-O2	-5.08	115.85	118.90
36	1	1779	C	OP1-P-OP2	5.08	127.23	119.60
36	1	1911	A	C5-C6-N6	-5.08	119.63	123.70
36	1	2859	U	C5-C6-N1	-5.08	120.16	122.70
1	6	626	U	C6-N1-C2	5.08	124.05	121.00
1	2	404	G	C4-C5-N7	5.08	112.83	110.80
36	1	1124	U	C5-C6-N1	5.08	125.24	122.70
1	6	558	U	P-O3'-C3'	5.08	125.80	119.70
1	6	1615	C	N1-C1'-C2'	-5.08	106.41	112.00
1	6	1736	G	O5'-P-OP1	-5.08	101.12	105.70
36	1	900	G	N7-C8-N9	-5.08	110.56	113.10
36	1	2679	A	C5-C6-N1	-5.08	115.16	117.70
1	6	1747	G	O5'-P-OP2	-5.08	101.13	105.70
36	5	2514	U	C6-N1-C2	-5.08	117.95	121.00
36	5	75	G	C5-C6-O6	-5.08	125.55	128.60
36	5	2940	A	C6-C5-N7	-5.08	128.74	132.30
36	1	293	C	N3-C4-N4	5.08	121.56	118.00
36	1	967	A	N1-C2-N3	5.08	131.84	129.30
36	1	2640	A	C6-N1-C2	-5.08	115.55	118.60
1	6	359	A	C4-C5-C6	-5.08	114.46	117.00
36	5	79	U	C5-C4-O4	-5.08	122.85	125.90
41	14	206	LEU	CA-CB-CG	5.08	126.98	115.30
1	2	1376	C	C6-N1-C2	5.08	122.33	120.30
36	1	86	G	N3-C4-N9	-5.08	122.95	126.00
36	1	88	A	N1-C6-N6	5.08	121.64	118.60
36	1	325	A	C6-N1-C2	-5.08	115.56	118.60
36	1	1117	G	C5-C6-O6	-5.08	125.56	128.60
36	1	2631	U	C2-N3-C4	-5.08	123.95	127.00
1	6	18	C	N3-C4-C5	-5.08	119.87	121.90
36	5	1429	G	C4-C5-N7	5.08	112.83	110.80
36	5	1788	C	N3-C4-C5	-5.08	119.87	121.90
36	5	1789	G	N3-C4-C5	5.08	131.14	128.60
36	5	2758	A	N9-C4-C5	5.08	107.83	105.80
52	m6	16	VAL	CG1-CB-CG2	-5.08	102.78	110.90
36	1	417	A	C2-N3-C4	-5.07	108.06	110.60
36	1	965	A	N1-C6-N6	5.07	121.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1611	G	C5-C6-N1	-5.07	108.96	111.50
36	1	2610	G	O5'-P-OP1	5.07	116.79	110.70
38	4	48	A	C2-N3-C4	5.07	113.14	110.60
36	1	282	G	N1-C6-O6	-5.07	116.86	119.90
36	1	946	U	N1-C2-N3	5.07	117.94	114.90
36	1	1589	A	O4'-C1'-N9	-5.07	104.14	108.20
36	1	2394	G	C4-C5-N7	-5.07	108.77	110.80
1	6	1198	G	C4-C5-N7	-5.07	108.77	110.80
25	d3	45	GLY	N-CA-C	-5.07	100.42	113.10
36	1	105	C	C2-N1-C1'	5.07	124.38	118.80
36	1	371	G	N9-C4-C5	-5.07	103.37	105.40
36	1	2391	G	OP1-P-O3'	5.07	116.35	105.20
36	5	904	A	C5-C6-N6	-5.07	119.64	123.70
36	5	2388	U	OP2-P-O3'	5.07	116.36	105.20
36	5	2850	G	C5-C6-N1	5.07	114.04	111.50
37	7	102	A	C8-N9-C4	5.07	107.83	105.80
54	m8	99	THR	N-CA-C	5.07	124.69	111.00
1	2	1168	U	C2-N1-C1'	5.07	123.78	117.70
36	1	652	G	C5-C6-O6	5.07	131.64	128.60
36	1	827	A	C8-N9-C4	5.07	107.83	105.80
1	6	472	U	N3-C2-O2	-5.07	118.65	122.20
1	2	275	C	C5-C6-N1	5.07	123.53	121.00
1	2	406	U	C6-N1-C2	5.07	124.04	121.00
24	D2	104	LEU	CA-CB-CG	5.07	126.96	115.30
38	4	140	G	N9-C4-C5	5.07	107.43	105.40
1	6	1	U	N3-C2-O2	-5.07	118.65	122.20
1	6	176	C	C2-N1-C1'	5.07	124.37	118.80
1	6	1396	U	C2-N1-C1'	5.07	123.78	117.70
36	5	906	A	C6-N1-C2	-5.07	115.56	118.60
36	1	3344	A	C4-C5-N7	5.07	113.23	110.70
70	O4	58	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	6	687	G	N3-C2-N2	-5.07	116.35	119.90
36	5	282	G	C5-C6-O6	5.07	131.64	128.60
36	5	2894	C	C6-N1-C2	5.07	122.33	120.30
36	1	1183	C	C6-N1-C2	5.06	122.33	120.30
36	1	2121	G	C5-C6-N1	5.06	114.03	111.50
36	5	1101	G	N1-C6-O6	-5.06	116.86	119.90
36	5	3143	C	N3-C2-O2	5.06	125.44	121.90
36	1	3368	U	C5-C4-O4	5.06	128.94	125.90
1	6	1075	C	N1-C2-O2	-5.06	115.86	118.90
36	5	1152	G	N7-C8-N9	5.06	115.63	113.10
37	7	98	C	N3-C4-C5	5.06	123.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	12	A	N1-C2-N3	-5.06	126.77	129.30
36	1	922	U	C2-N1-C1'	5.06	123.77	117.70
36	1	1144	U	C2-N3-C4	-5.06	123.96	127.00
1	6	1735	U	C6-N1-C2	5.06	124.04	121.00
36	5	527	A	C5-C6-N1	5.06	120.23	117.70
36	5	3105	U	O5'-P-OP1	-5.06	101.14	105.70
1	2	1169	G	N3-C4-C5	-5.06	126.07	128.60
1	2	1611	A	C2-N3-C4	-5.06	108.07	110.60
36	1	2305	G	N1-C6-O6	5.06	122.94	119.90
36	5	2904	U	C5-C6-N1	-5.06	120.17	122.70
1	2	74	U	O4'-C1'-N1	5.06	112.25	108.20
36	1	961	C	C5-C6-N1	-5.06	118.47	121.00
36	1	2810	C	C5-C6-N1	-5.06	118.47	121.00
36	5	75	G	C4-N9-C1'	5.06	133.08	126.50
36	5	990	U	N3-C2-O2	-5.06	118.66	122.20
36	5	2940	A	N1-C2-N3	5.06	131.83	129.30
1	2	571	G	C5-N7-C8	5.06	106.83	104.30
36	1	2249	G	N9-C4-C5	-5.06	103.38	105.40
1	6	813	U	N3-C2-O2	-5.06	118.66	122.20
36	5	2327	U	C6-N1-C2	5.06	124.03	121.00
1	2	1124	A	O5'-P-OP1	-5.05	101.15	105.70
36	1	662	U	N3-C2-O2	-5.05	118.66	122.20
36	1	1203	A	N3-C4-C5	5.05	130.34	126.80
36	1	2986	U	N1-C2-N3	5.05	117.93	114.90
36	5	2862	U	C5-C6-N1	-5.05	120.17	122.70
1	2	1100	G	C6-C5-N7	-5.05	127.37	130.40
36	1	281	G	C4-C5-N7	5.05	112.82	110.80
36	1	1179	A	C2-N3-C4	-5.05	108.07	110.60
1	6	1600	A	C6-C5-N7	-5.05	128.76	132.30
36	5	3217	C	C6-N1-C1'	5.05	126.86	120.80
36	1	3066	U	C5-C6-N1	-5.05	120.17	122.70
36	5	221	A	C2-N3-C4	-5.05	108.07	110.60
36	5	2774	C	C6-N1-C2	-5.05	118.28	120.30
36	5	2990	G	C5-C6-O6	-5.05	125.57	128.60
36	1	2328	U	C5-C6-N1	-5.05	120.17	122.70
36	1	2688	U	N1-C2-N3	-5.05	111.87	114.90
1	6	377	G	N1-C2-N2	-5.05	111.66	116.20
1	6	437	A	C8-N9-C4	5.05	107.82	105.80
36	5	2395	G	C4-C5-N7	5.05	112.82	110.80
1	2	474	A	C8-N9-C4	5.05	107.82	105.80
1	2	647	G	N3-C4-C5	5.05	131.12	128.60
1	2	1145	U	N1-C2-O2	-5.05	119.27	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	899	U	N3-C2-O2	-5.05	118.67	122.20
36	1	1373	A	C5-C6-N1	5.05	120.22	117.70
36	1	1578	C	C2-N1-C1'	5.05	124.35	118.80
36	1	2273	G	N9-C4-C5	-5.05	103.38	105.40
36	1	2638	C	N1-C2-O2	5.05	121.93	118.90
1	6	65	A	N9-C4-C5	-5.05	103.78	105.80
1	6	558	U	N1-C2-O2	5.05	126.33	122.80
1	6	1752	U	C5-C6-N1	-5.05	120.18	122.70
36	5	530	G	O5'-P-OP2	-5.05	101.16	105.70
36	5	2287	C	N1-C2-O2	-5.05	115.87	118.90
36	5	3175	U	O5'-P-OP2	-5.05	101.16	105.70
36	1	1366	A	C4-C5-N7	5.04	113.22	110.70
51	M5	68	ARG	NE-CZ-NH1	5.04	122.82	120.30
36	1	701	G	C5-C6-O6	-5.04	125.57	128.60
36	1	1294	A	O4'-C1'-N9	5.04	112.23	108.20
36	1	2316	G	N3-C4-N9	5.04	129.03	126.00
36	1	2571	U	C2-N1-C1'	5.04	123.75	117.70
36	5	328	U	N3-C4-O4	-5.04	115.87	119.40
36	5	1236	G	N1-C6-O6	5.04	122.93	119.90
36	5	1347	U	N1-C2-O2	-5.04	119.27	122.80
36	5	1662	G	C5-C6-O6	-5.04	125.57	128.60
36	5	1850	A	C2-N3-C4	-5.04	108.08	110.60
36	5	2320	A	N1-C6-N6	-5.04	115.57	118.60
1	2	1673	G	C6-C5-N7	-5.04	127.38	130.40
36	1	2869	U	O5'-P-OP2	5.04	116.75	110.70
36	1	3049	A	N9-C4-C5	-5.04	103.78	105.80
1	6	103	A	C5-N7-C8	-5.04	101.38	103.90
1	6	557	G	C4-N9-C1'	5.04	133.05	126.50
1	6	911	U	N3-C2-O2	-5.04	118.67	122.20
1	6	1361	U	C6-N1-C1'	-5.04	114.14	121.20
36	5	3217	C	N3-C4-N4	-5.04	114.47	118.00
36	5	1143	A	N1-C2-N3	5.04	131.82	129.30
36	5	2940	A	C4-C5-C6	5.04	119.52	117.00
36	1	749	C	O5'-P-OP2	-5.04	101.17	105.70
36	1	1699	A	N9-C4-C5	-5.04	103.78	105.80
36	1	1902	G	N9-C4-C5	-5.04	103.38	105.40
36	1	2631	U	C5-C6-N1	-5.04	120.18	122.70
1	6	1082	C	C6-N1-C2	-5.04	118.28	120.30
36	5	364	G	O5'-P-OP2	5.04	116.75	110.70
36	5	1191	U	N1-C2-O2	-5.04	119.27	122.80
36	1	1412	G	C5-N7-C8	-5.04	101.78	104.30
36	5	1371	G	N3-C4-C5	-5.04	126.08	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3221	C	C6-N1-C2	-5.04	118.28	120.30
36	1	398	A	C2-N3-C4	5.04	113.12	110.60
36	1	1318	A	N7-C8-N9	5.04	116.32	113.80
36	1	1549	U	C5-C4-O4	-5.04	122.88	125.90
37	3	114	U	N3-C4-O4	-5.04	115.88	119.40
36	5	1922	A	C2-N3-C4	-5.04	108.08	110.60
36	1	1660	C	N1-C2-O2	-5.03	115.88	118.90
47	M0	167	LEU	CA-CB-CG	5.03	126.88	115.30
36	5	2185	G	C5-C6-N1	-5.03	108.98	111.50
36	5	2938	G	C5-C6-N1	5.03	114.02	111.50
36	5	3145	C	C6-N1-C2	5.03	122.31	120.30
36	5	37	U	C5-C4-O4	5.03	128.92	125.90
36	5	960	U	OP2-P-O3'	5.03	116.27	105.20
36	5	1724	U	C2-N1-C1'	-5.03	111.66	117.70
36	5	2943	G	C5-N7-C8	-5.03	101.78	104.30
1	2	1135	U	N1-C2-N3	-5.03	111.88	114.90
36	1	432	G	C4-C5-C6	5.03	121.82	118.80
36	1	1509	A	C8-N9-C4	5.03	107.81	105.80
36	5	105	C	C6-N1-C2	5.03	122.31	120.30
36	5	881	C	N1-C2-O2	5.03	121.92	118.90
36	5	1504	A	C2-N3-C4	-5.03	108.08	110.60
36	5	2353	G	C4-C5-N7	5.03	112.81	110.80
36	5	3309	G	N3-C4-N9	5.03	129.02	126.00
36	1	878	G	C2-N3-C4	-5.03	109.39	111.90
36	1	3325	G	N1-C6-O6	-5.03	116.88	119.90
36	5	1103	A	OP2-P-O3'	5.03	116.26	105.20
36	1	273	A	C4-C5-N7	-5.03	108.19	110.70
36	1	594	U	C5-C4-O4	5.03	128.92	125.90
36	1	1389	G	C4-N9-C1'	5.03	133.03	126.50
36	1	2130	G	N3-C4-C5	-5.03	126.09	128.60
36	5	2984	C	C2-N3-C4	-5.03	117.39	119.90
1	6	1503	A	N7-C8-N9	5.03	116.31	113.80
36	5	1060	U	N3-C4-C5	5.03	117.61	114.60
1	2	1503	A	C5-N7-C8	-5.02	101.39	103.90
1	2	1600	A	N9-C4-C5	-5.02	103.79	105.80
36	1	1371	G	C8-N9-C4	5.02	108.41	106.40
36	5	2175	U	C5-C6-N1	-5.02	120.19	122.70
36	1	282	G	P-O3'-C3'	5.02	125.73	119.70
36	1	1180	A	C4-C5-N7	-5.02	108.19	110.70
36	1	1373	A	O5'-P-OP2	-5.02	101.18	105.70
36	1	2200	U	N3-C4-O4	5.02	122.92	119.40
36	1	2303	A	N1-C2-N3	5.02	131.81	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2604	U	C5-C6-N1	-5.02	120.19	122.70
36	1	3057	U	N3-C4-O4	-5.02	115.88	119.40
37	3	67	G	N3-C4-C5	5.02	131.11	128.60
36	5	647	A	N1-C2-N3	5.02	131.81	129.30
36	5	1200	A	C5-C6-N6	-5.02	119.68	123.70
48	M1	112	LEU	CA-CB-CG	5.02	126.85	115.30
36	5	1628	C	C6-N1-C2	-5.02	118.29	120.30
1	2	1431	C	C6-N1-C2	5.02	122.31	120.30
36	1	2323	G	N3-C2-N2	5.02	123.41	119.90
36	1	2364	G	C4-C5-N7	-5.02	108.79	110.80
36	1	2373	A	C8-N9-C4	-5.02	103.79	105.80
36	1	2745	G	C8-N9-C4	5.02	108.41	106.40
39	L2	122	ASP	CB-CG-OD2	5.02	122.82	118.30
1	6	797	G	N3-C4-C5	5.02	131.11	128.60
1	6	1433	G	C5-C6-O6	5.02	131.61	128.60
1	6	1780	G	N3-C2-N2	5.02	123.41	119.90
36	5	313	A	C6-C5-N7	-5.02	128.79	132.30
36	5	2393	G	C5-C6-N1	5.02	114.01	111.50
37	7	97	A	C6-N1-C2	-5.02	115.59	118.60
38	8	140	G	N7-C8-N9	5.02	115.61	113.10
36	1	718	G	N3-C4-C5	5.02	131.11	128.60
36	1	994	G	N3-C4-N9	5.02	129.01	126.00
36	1	1158	A	C4-C5-C6	5.02	119.51	117.00
36	1	1510	G	C6-C5-N7	-5.02	127.39	130.40
36	1	3298	C	C6-N1-C2	5.02	122.31	120.30
1	6	797	G	C8-N9-C4	5.02	108.41	106.40
36	5	74	G	N7-C8-N9	5.02	115.61	113.10
36	5	1659	U	C5-C6-N1	5.02	125.21	122.70
36	5	2320	A	O5'-P-OP2	-5.02	101.19	105.70
36	5	2531	C	N3-C2-O2	-5.02	118.39	121.90
36	5	2866	U	N3-C2-O2	-5.02	118.69	122.20
36	5	2867	C	C6-N1-C2	5.02	122.31	120.30
36	5	2916	U	C4-C5-C6	5.02	122.71	119.70
36	5	3215	A	N1-C6-N6	5.02	121.61	118.60
37	7	29	C	C5-C6-N1	-5.02	118.49	121.00
5	S3	202	LEU	CA-CB-CG	5.02	126.84	115.30
37	3	15	C	C6-N1-C2	5.02	122.31	120.30
36	5	2811	A	N1-C6-N6	-5.02	115.59	118.60
36	5	3200	G	C5-C6-O6	-5.02	125.59	128.60
36	1	104	G	C4-C5-N7	5.01	112.81	110.80
36	1	957	C	N3-C2-O2	5.01	125.41	121.90
36	1	1346	G	N1-C6-O6	5.01	122.91	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2242	A	OP2-P-O3'	5.01	116.23	105.20
36	1	2732	G	C2-N3-C4	-5.01	109.39	111.90
36	1	3050	U	N3-C2-O2	-5.01	118.69	122.20
36	1	3361	G	N1-C2-N2	-5.01	111.69	116.20
1	6	1146	G	C5-C6-O6	-5.01	125.59	128.60
1	6	1463	C	C6-N1-C2	5.01	122.31	120.30
36	5	276	U	N1-C2-O2	-5.01	119.29	122.80
36	5	1321	G	C6-C5-N7	-5.01	127.39	130.40
36	5	1446	A	C8-N9-C4	5.01	107.81	105.80
37	7	103	A	C4-C5-N7	5.01	113.21	110.70
36	1	590	G	N9-C4-C5	-5.01	103.39	105.40
36	1	2643	A	C2-N3-C4	-5.01	108.09	110.60
36	5	2817	A	N3-C4-C5	-5.01	123.29	126.80
36	1	3244	A	N1-C6-N6	5.01	121.61	118.60
1	6	985	G	C2-N3-C4	-5.01	109.39	111.90
36	5	934	G	N1-C2-N3	-5.01	120.89	123.90
1	2	687	G	C8-N9-C4	-5.01	104.40	106.40
1	2	1241	G	O4'-C1'-N9	5.01	112.21	108.20
36	1	1306	G	N1-C2-N3	5.01	126.91	123.90
56	N0	115	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	6	308	C	N3-C2-O2	-5.01	118.39	121.90
36	5	1546	A	C5-C6-N6	-5.01	119.69	123.70
36	1	2133	U	C2-N1-C1'	-5.01	111.69	117.70
1	2	75	U	C2-N1-C1'	5.01	123.71	117.70
1	2	453	U	C6-N1-C2	-5.01	118.00	121.00
36	1	1393	A	C6-N1-C2	-5.01	115.60	118.60
36	1	2285	C	C5-C6-N1	-5.01	118.50	121.00
36	1	2403	G	C6-C5-N7	-5.01	127.40	130.40
1	6	1700	C	N3-C2-O2	-5.00	118.40	121.90
36	5	2116	G	N3-C4-N9	5.00	129.00	126.00
36	5	2620	G	C5-C6-O6	5.00	131.60	128.60
36	5	3314	A	N1-C6-N6	5.00	121.60	118.60
36	1	93	C	C6-N1-C2	-5.00	118.30	120.30
1	6	1657	U	C2-N1-C1'	5.00	123.70	117.70
36	5	749	C	N3-C4-C5	-5.00	119.90	121.90
36	5	1701	C	N3-C2-O2	-5.00	118.40	121.90
37	7	92	A	C4-C5-N7	5.00	113.20	110.70
37	7	109	G	C5-C6-O6	-5.00	125.60	128.60

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	C1	127	GLN	Peptide
16	C4	124	ASP	Peptide
18	C6	40	GLU	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
25	D3	78	LYS	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
27	D5	96	SER	Peptide
33	E1	137	ASP	Peptide
39	L2	19	HIS	Peptide
45	L8	124	ASP	Peptide
45	L8	74	THR	Peptide
48	M1	64	LYS	Peptide
48	M1	8	PRO	Peptide
52	M6	110	PRO	Peptide
56	N0	12	ARG	Peptide
56	N0	22	PRO	Peptide
57	N1	16	GLN	Peptide
65	N9	20	GLY	Peptide
9	S7	131	PHE	Peptide
15	c3	17	PRO	Peptide
17	c5	52	LYS	Peptide
18	c6	40	GLU	Peptide
19	c7	87	GLU	Peptide
19	c7	88	VAL	Peptide
19	c7	96	SER	Peptide
22	d0	70	THR	Peptide
26	d4	29	HIS	Peptide
26	d4	49	LYS	Peptide
27	d5	85	LYS	Peptide
82	e1	146	SER	Peptide
39	l2	171	GLY	Peptide
39	l2	237	LEU	Peptide
42	l5	270	LYS	Peptide
42	l5	271	LYS	Peptide
43	l6	51	ARG	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
51	m5	66	VAL	Peptide
52	m6	110	PRO	Peptide
56	n0	133	ALA	Peptide
60	n4	78	ALA	Peptide

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Mol	Chain	Res	Type	Group
63	n7	5	LEU	Peptide
64	n8	18	GLY	Peptide
64	n8	66	ALA	Peptide
65	n9	22	LYS	Peptide
3	s1	134	VAL	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide
9	s7	29	ASN	Peptide
10	s8	60	ILE	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%)	143 (70%)	34 (17%)	27 (13%)	0	1
2	s0	204/251 (81%)	152 (74%)	33 (16%)	19 (9%)	0	3
3	S1	212/254 (84%)	141 (66%)	38 (18%)	33 (16%)	0	1
3	s1	214/254 (84%)	171 (80%)	30 (14%)	13 (6%)	1	12
4	S2	215/253 (85%)	173 (80%)	27 (13%)	15 (7%)	1	8
4	s2	215/253 (85%)	184 (86%)	21 (10%)	10 (5%)	2	17
5	S3	221/239 (92%)	182 (82%)	24 (11%)	15 (7%)	1	9
5	s3	221/239 (92%)	174 (79%)	31 (14%)	16 (7%)	1	7
6	S4	258/260 (99%)	206 (80%)	34 (13%)	18 (7%)	1	8
6	s4	258/260 (99%)	210 (81%)	28 (11%)	20 (8%)	1	6
7	S5	204/224 (91%)	154 (76%)	34 (17%)	16 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	s5	204/224 (91%)	154 (76%)	35 (17%)	15 (7%)	1	7
8	S6	224/236 (95%)	197 (88%)	15 (7%)	12 (5%)	2	14
8	s6	216/236 (92%)	184 (85%)	22 (10%)	10 (5%)	2	18
9	S7	182/189 (96%)	136 (75%)	25 (14%)	21 (12%)	0	2
9	s7	184/189 (97%)	141 (77%)	28 (15%)	15 (8%)	1	5
10	S8	184/200 (92%)	148 (80%)	23 (12%)	13 (7%)	1	8
10	s8	184/200 (92%)	155 (84%)	16 (9%)	13 (7%)	1	8
11	S9	183/196 (93%)	147 (80%)	26 (14%)	10 (6%)	2	14
11	s9	183/196 (93%)	148 (81%)	28 (15%)	7 (4%)	3	22
12	C0	94/105 (90%)	68 (72%)	17 (18%)	9 (10%)	0	3
13	C1	153/155 (99%)	114 (74%)	24 (16%)	15 (10%)	0	3
13	c1	144/155 (93%)	122 (85%)	16 (11%)	6 (4%)	3	20
14	C2	122/142 (86%)	67 (55%)	34 (28%)	21 (17%)	0	0
14	c2	122/142 (86%)	67 (55%)	32 (26%)	23 (19%)	0	0
15	C3	148/150 (99%)	122 (82%)	20 (14%)	6 (4%)	3	21
15	c3	148/150 (99%)	120 (81%)	18 (12%)	10 (7%)	1	9
16	C4	125/136 (92%)	90 (72%)	19 (15%)	16 (13%)	0	1
16	c4	126/136 (93%)	96 (76%)	19 (15%)	11 (9%)	1	4
17	C5	122/141 (86%)	88 (72%)	22 (18%)	12 (10%)	0	3
17	c5	133/141 (94%)	94 (71%)	20 (15%)	19 (14%)	0	1
18	C6	139/142 (98%)	117 (84%)	11 (8%)	11 (8%)	1	6
18	c6	140/142 (99%)	120 (86%)	12 (9%)	8 (6%)	1	14
19	C7	116/136 (85%)	87 (75%)	21 (18%)	8 (7%)	1	8
19	c7	113/136 (83%)	84 (74%)	19 (17%)	10 (9%)	1	4
20	C8	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	5
20	c8	143/145 (99%)	115 (80%)	18 (13%)	10 (7%)	1	8
21	C9	141/143 (99%)	120 (85%)	14 (10%)	7 (5%)	2	16
21	c9	141/143 (99%)	114 (81%)	21 (15%)	6 (4%)	2	20
22	D0	105/120 (88%)	82 (78%)	19 (18%)	4 (4%)	3	22
22	d0	108/120 (90%)	87 (81%)	10 (9%)	11 (10%)	0	3
23	D1	85/87 (98%)	64 (75%)	12 (14%)	9 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	d1	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	3	24
24	D2	127/129 (98%)	112 (88%)	12 (9%)	3 (2%)	6	34
24	d2	127/129 (98%)	112 (88%)	14 (11%)	1 (1%)	19	58
25	D3	142/144 (99%)	109 (77%)	19 (13%)	14 (10%)	0	3
25	d3	142/144 (99%)	119 (84%)	18 (13%)	5 (4%)	3	24
26	D4	132/134 (98%)	106 (80%)	18 (14%)	8 (6%)	1	12
26	d4	132/134 (98%)	106 (80%)	16 (12%)	10 (8%)	1	7
27	D5	68/107 (64%)	44 (65%)	11 (16%)	13 (19%)	0	0
27	d5	67/107 (63%)	49 (73%)	11 (16%)	7 (10%)	0	3
28	D6	95/97 (98%)	62 (65%)	19 (20%)	14 (15%)	0	1
28	d6	95/97 (98%)	67 (70%)	18 (19%)	10 (10%)	0	3
29	D7	79/81 (98%)	63 (80%)	9 (11%)	7 (9%)	1	4
29	d7	79/81 (98%)	60 (76%)	12 (15%)	7 (9%)	1	4
30	D8	61/66 (92%)	49 (80%)	6 (10%)	6 (10%)	0	3
30	d8	61/66 (92%)	43 (70%)	13 (21%)	5 (8%)	1	5
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3	22
31	d9	51/55 (93%)	36 (71%)	9 (18%)	6 (12%)	0	2
32	E0	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	9	42
33	E1	69/76 (91%)	38 (55%)	12 (17%)	19 (28%)	0	0
34	SR	316/318 (99%)	244 (77%)	45 (14%)	27 (8%)	1	4
34	sR	316/318 (99%)	261 (83%)	42 (13%)	13 (4%)	3	21
35	SM	155/273 (57%)	111 (72%)	27 (17%)	17 (11%)	0	2
35	sM	98/273 (36%)	57 (58%)	28 (29%)	13 (13%)	0	1
39	L2	250/253 (99%)	224 (90%)	17 (7%)	9 (4%)	3	23
39	l2	250/253 (99%)	214 (86%)	23 (9%)	13 (5%)	2	15
40	L3	384/386 (100%)	322 (84%)	45 (12%)	17 (4%)	2	19
40	l3	384/386 (100%)	339 (88%)	32 (8%)	13 (3%)	3	24
41	L4	359/361 (99%)	297 (83%)	34 (10%)	28 (8%)	1	6
41	l4	359/361 (99%)	299 (83%)	38 (11%)	22 (6%)	1	12
42	L5	294/296 (99%)	237 (81%)	35 (12%)	22 (8%)	1	7
42	l5	292/296 (99%)	253 (87%)	32 (11%)	7 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	L6	152/175 (87%)	134 (88%)	12 (8%)	6 (4%)	3	22
43	l6	153/175 (87%)	130 (85%)	17 (11%)	6 (4%)	3	22
44	L7	220/243 (90%)	184 (84%)	26 (12%)	10 (4%)	2	18
44	l7	221/243 (91%)	189 (86%)	27 (12%)	5 (2%)	6	34
45	L8	231/255 (91%)	189 (82%)	31 (13%)	11 (5%)	2	17
45	l8	229/255 (90%)	188 (82%)	23 (10%)	18 (8%)	1	6
46	L9	189/191 (99%)	166 (88%)	21 (11%)	2 (1%)	14	51
46	l9	189/191 (99%)	166 (88%)	17 (9%)	6 (3%)	4	26
47	M0	207/220 (94%)	171 (83%)	28 (14%)	8 (4%)	3	22
47	m0	209/220 (95%)	172 (82%)	23 (11%)	14 (7%)	1	9
48	M1	167/173 (96%)	122 (73%)	29 (17%)	16 (10%)	0	3
48	m1	167/173 (96%)	141 (84%)	15 (9%)	11 (7%)	1	9
49	M3	191/198 (96%)	154 (81%)	26 (14%)	11 (6%)	1	13
49	m3	192/198 (97%)	150 (78%)	28 (15%)	14 (7%)	1	7
50	M4	134/137 (98%)	113 (84%)	12 (9%)	9 (7%)	1	9
50	m4	135/137 (98%)	118 (87%)	16 (12%)	1 (1%)	22	61
51	M5	201/203 (99%)	183 (91%)	14 (7%)	4 (2%)	7	38
51	m5	201/203 (99%)	181 (90%)	16 (8%)	4 (2%)	7	38
52	M6	195/198 (98%)	176 (90%)	12 (6%)	7 (4%)	3	23
52	m6	195/198 (98%)	179 (92%)	10 (5%)	6 (3%)	4	26
53	M7	181/183 (99%)	144 (80%)	27 (15%)	10 (6%)	2	14
53	m7	153/183 (84%)	132 (86%)	18 (12%)	3 (2%)	7	38
54	M8	183/185 (99%)	154 (84%)	24 (13%)	5 (3%)	5	30
54	m8	183/185 (99%)	151 (82%)	26 (14%)	6 (3%)	4	25
55	M9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	67
55	m9	186/188 (99%)	167 (90%)	14 (8%)	5 (3%)	5	30
56	N0	170/172 (99%)	154 (91%)	13 (8%)	3 (2%)	8	41
56	n0	170/172 (99%)	160 (94%)	7 (4%)	3 (2%)	8	41
57	N1	157/159 (99%)	139 (88%)	11 (7%)	7 (4%)	2	18
57	n1	157/159 (99%)	140 (89%)	12 (8%)	5 (3%)	4	26
58	N2	98/120 (82%)	72 (74%)	15 (15%)	11 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	n2	96/120 (80%)	78 (81%)	15 (16%)	3 (3%)	4	26
59	N3	134/136 (98%)	120 (90%)	12 (9%)	2 (2%)	10	44
59	n3	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
60	N4	96/155 (62%)	78 (81%)	13 (14%)	5 (5%)	2	15
60	n4	133/155 (86%)	109 (82%)	15 (11%)	9 (7%)	1	9
61	N5	119/141 (84%)	106 (89%)	11 (9%)	2 (2%)	9	42
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	1	7
62	N6	124/126 (98%)	104 (84%)	14 (11%)	6 (5%)	2	17
62	n6	124/126 (98%)	112 (90%)	8 (6%)	4 (3%)	4	26
63	N7	133/135 (98%)	111 (84%)	11 (8%)	11 (8%)	1	5
63	n7	133/135 (98%)	101 (76%)	21 (16%)	11 (8%)	1	5
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	2	17
64	n8	146/148 (99%)	119 (82%)	22 (15%)	5 (3%)	3	24
65	N9	56/58 (97%)	47 (84%)	6 (11%)	3 (5%)	2	14
65	n9	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	1	4
66	O0	95/104 (91%)	76 (80%)	15 (16%)	4 (4%)	3	20
66	o0	98/104 (94%)	85 (87%)	13 (13%)	0	100	100
67	O1	107/112 (96%)	91 (85%)	8 (8%)	8 (8%)	1	7
67	o1	107/112 (96%)	85 (79%)	13 (12%)	9 (8%)	1	5
68	O2	125/129 (97%)	108 (86%)	17 (14%)	0	100	100
68	o2	125/129 (97%)	109 (87%)	9 (7%)	7 (6%)	2	14
69	O3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	4	28
69	o3	104/106 (98%)	96 (92%)	4 (4%)	4 (4%)	3	22
70	O4	110/119 (92%)	94 (86%)	14 (13%)	2 (2%)	8	41
70	o4	110/119 (92%)	100 (91%)	9 (8%)	1 (1%)	17	56
71	O5	117/119 (98%)	99 (85%)	10 (8%)	8 (7%)	1	9
71	o5	117/119 (98%)	95 (81%)	17 (14%)	5 (4%)	2	20
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	1	11
72	o6	97/99 (98%)	76 (78%)	15 (16%)	6 (6%)	1	11
73	O7	85/87 (98%)	74 (87%)	8 (9%)	3 (4%)	3	24
73	o7	85/87 (98%)	70 (82%)	11 (13%)	4 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	O8	75/77 (97%)	65 (87%)	7 (9%)	3 (4%)	3	21
74	o8	75/77 (97%)	60 (80%)	12 (16%)	3 (4%)	3	21
75	O9	48/50 (96%)	40 (83%)	6 (12%)	2 (4%)	3	20
75	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
76	Q0	50/52 (96%)	39 (78%)	9 (18%)	2 (4%)	3	21
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	7	38
77	Q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	20
78	Q2	103/105 (98%)	84 (82%)	13 (13%)	6 (6%)	1	13
78	q2	103/105 (98%)	92 (89%)	9 (9%)	2 (2%)	8	39
79	Q3	89/91 (98%)	76 (85%)	10 (11%)	3 (3%)	3	24
79	q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	14	51
80	c0	92/105 (88%)	59 (64%)	16 (17%)	17 (18%)	0	0
81	e0	60/62 (97%)	43 (72%)	10 (17%)	7 (12%)	0	2
82	e1	74/76 (97%)	34 (46%)	21 (28%)	19 (26%)	0	0
84	p0	139/311 (45%)	116 (84%)	16 (12%)	7 (5%)	2	16
All	All	22333/24141 (92%)	18253 (82%)	2722 (12%)	1358 (6%)	1	12

All (1358) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	30	GLN
2	S0	39	ASN
2	S0	66	ALA
2	S0	111	ILE
2	S0	140	ASN
2	S0	158	VAL
2	S0	185	ARG
2	S0	187	ALA
2	S0	191	ARG
3	S1	36	SER
3	S1	37	THR
3	S1	49	ASN
3	S1	63	GLY
3	S1	79	HIS

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Mol	Chain	Res	Type
3	S1	132	ASP
3	S1	147	ALA
3	S1	148	ASN
3	S1	206	PRO
3	S1	223	PHE
3	S1	224	ASP
4	S2	78	ASP
4	S2	80	VAL
4	S2	135	SER
4	S2	148	LEU
5	S3	62	ASN
5	S3	93	ASP
5	S3	211	PRO
5	S3	220	PRO
6	S4	104	ASP
6	S4	142	HIS
6	S4	223	ASN
6	S4	227	VAL
6	S4	228	ILE
7	S5	26	ALA
7	S5	39	GLU
7	S5	43	PHE
7	S5	63	GLN
7	S5	84	LYS
7	S5	153	GLY
8	S6	54	GLY
8	S6	122	GLU
8	S6	173	PRO
8	S6	174	LYS
9	S7	31	SER
9	S7	32	PRO
9	S7	64	VAL
9	S7	85	PHE
9	S7	111	LYS
9	S7	116	ARG
9	S7	131	PHE
9	S7	134	GLU
11	S9	121	SER
11	S9	134	ILE
11	S9	169	PRO
12	C0	60	SER
12	C0	81	ASN

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Mol	Chain	Res	Type
12	C0	87	VAL
12	C0	88	PRO
13	C1	7	VAL
13	C1	75	VAL
13	C1	76	VAL
13	C1	140	VAL
14	C2	108	ARG
14	C2	126	TRP
14	C2	127	GLY
15	C3	27	LYS
16	C4	42	VAL
16	C4	50	ALA
16	C4	126	THR
17	C5	60	LEU
17	C5	125	PRO
17	C5	126	VAL
18	C6	39	VAL
18	C6	42	GLU
18	C6	58	ASP
18	C6	59	LYS
18	C6	97	VAL
18	C6	114	ARG
18	C6	115	THR
18	C6	138	PHE
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
20	C8	14	ILE
20	C8	60	GLU
20	C8	91	ASP
20	C8	92	ILE
21	C9	31	PRO
21	C9	53	TRP
21	C9	116	ILE
24	D2	83	ILE
25	D3	3	LYS
25	D3	12	ALA
25	D3	92	CYS
25	D3	114	LYS
25	D3	137	LYS
27	D5	37	GLN
27	D5	39	ALA

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Mol	Chain	Res	Type
27	D5	43	ASP
27	D5	44	GLN
27	D5	55	PRO
27	D5	56	THR
27	D5	57	TYR
27	D5	97	LYS
28	D6	36	ILE
28	D6	45	VAL
28	D6	46	GLU
28	D6	65	PRO
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
29	D7	38	PRO
29	D7	62	ILE
30	D8	36	THR
30	D8	37	SER
30	D8	61	ARG
32	E0	47	VAL
33	E1	85	TYR
33	E1	103	LEU
33	E1	138	ARG
34	SR	24	ALA
34	SR	57	PRO
34	SR	58	VAL
34	SR	155	ARG
34	SR	160	GLU
34	SR	161	LYS
34	SR	201	THR
34	SR	203	THR
34	SR	318	ALA
35	SM	102	THR
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
40	L3	4	ARG
40	L3	5	LYS
40	L3	83	PRO
40	L3	140	ASP
40	L3	347	SER
40	L3	378	ALA
41	L4	131	VAL

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Mol	Chain	Res	Type
41	L4	182	LEU
41	L4	268	ALA
41	L4	292	SER
41	L4	293	SER
41	L4	311	HIS
41	L4	317	PRO
41	L4	318	LEU
41	L4	338	LYS
41	L4	361	HIS
42	L5	233	ALA
42	L5	234	ASP
42	L5	258	LYS
44	L7	24	GLU
44	L7	26	VAL
45	L8	25	PRO
45	L8	36	ILE
47	M0	189	GLU
47	M0	207	GLU
48	M1	8	PRO
48	M1	9	MET
48	M1	11	ASP
48	M1	12	LEU
48	M1	28	ASP
48	M1	74	PRO
48	M1	165	GLN
49	M3	47	ALA
49	M3	129	ASN
49	M3	141	ALA
50	M4	9	ALA
50	M4	135	LEU
50	M4	136	ALA
52	M6	111	PRO
53	M7	157	VAL
54	M8	98	LYS
54	M8	99	THR
56	N0	13	ARG
57	N1	36	VAL
57	N1	124	VAL
58	N2	44	GLU
58	N2	51	GLY
58	N2	60	GLY
60	N4	26	SER

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Mol	Chain	Res	Type
60	N4	64	THR
60	N4	81	PRO
61	N5	44	PRO
63	N7	18	TYR
63	N7	125	GLY
64	N8	57	GLY
64	N8	76	ASP
67	O1	83	GLU
71	O5	96	GLU
71	O5	97	ALA
71	O5	98	SER
71	O5	119	LYS
72	O6	33	ALA
72	O6	98	ARG
73	O7	84	SER
76	Q0	78	ILE
76	Q0	79	GLU
78	Q2	100	LYS
2	s0	4	PRO
2	s0	30	GLN
2	s0	62	ARG
2	s0	95	ALA
2	s0	158	VAL
2	s0	164	ASN
2	s0	189	VAL
2	s0	203	PHE
2	s0	206	ASP
3	s1	106	THR
3	s1	147	ALA
3	s1	206	PRO
3	s1	223	PHE
4	s2	106	ASP
4	s2	238	SER
5	s3	179	GLN
5	s3	195	SER
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	24	SER
6	s4	95	THR
6	s4	163	ASP

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Mol	Chain	Res	Type
6	s4	196	VAL
6	s4	242	LYS
7	s5	28	PRO
7	s5	43	PHE
7	s5	151	GLY
7	s5	184	PHE
7	s5	209	TYR
8	s6	25	ARG
8	s6	138	ALA
8	s6	173	PRO
8	s6	174	LYS
9	s7	30	SER
9	s7	64	VAL
9	s7	66	SER
9	s7	106	SER
9	s7	131	PHE
9	s7	163	ASP
9	s7	185	ILE
10	s8	101	ILE
10	s8	115	ALA
10	s8	116	HIS
10	s8	136	SER
11	s9	117	GLY
11	s9	147	MET
80	c0	2	LEU
80	c0	32	HIS
80	c0	82	LEU
80	c0	83	PRO
80	c0	88	PRO
80	c0	94	GLU
80	c0	97	PRO
13	c1	61	THR
13	c1	114	ALA
14	c2	22	VAL
15	c3	19	SER
15	c3	66	ILE
15	c3	87	ASP
15	c3	137	PRO
15	c3	143	SER
16	c4	126	THR
16	c4	132	ARG
17	c5	11	VAL

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Mol	Chain	Res	Type
17	c5	17	TYR
17	c5	50	THR
17	c5	51	SER
17	c5	68	PRO
17	c5	125	PRO
17	c5	126	VAL
17	c5	127	ARG
17	c5	131	ALA
18	c6	39	VAL
18	c6	42	GLU
19	c7	88	VAL
20	c8	91	ASP
20	c8	92	ILE
21	c9	25	GLN
21	c9	29	GLU
21	c9	34	VAL
22	d0	15	GLN
22	d0	118	VAL
23	d1	4	ASP
26	d4	30	PRO
26	d4	33	ALA
26	d4	35	VAL
26	d4	52	LYS
26	d4	121	THR
27	d5	38	HIS
27	d5	85	LYS
27	d5	104	ALA
28	d6	13	LYS
28	d6	28	LYS
28	d6	47	ALA
29	d7	38	PRO
29	d7	59	CYS
29	d7	60	SER
31	d9	6	VAL
82	e1	87	THR
82	e1	92	LYS
82	e1	97	LYS
82	e1	98	VAL
82	e1	102	VAL
82	e1	103	LEU
82	e1	106	TYR
82	e1	127	GLY

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Mol	Chain	Res	Type
34	sR	4	ASN
34	sR	96	THR
34	sR	163	ASP
34	sR	165	ASP
34	sR	250	TYR
35	sM	47	ALA
35	sM	48	ARG
35	sM	50	ASN
35	sM	60	ALA
35	sM	172	VAL
39	l2	24	GLN
40	l3	129	ALA
40	l3	140	ASP
40	l3	142	ALA
40	l3	188	ILE
40	l3	347	SER
41	l4	14	GLU
41	l4	145	ILE
41	l4	301	PRO
41	l4	302	ALA
41	l4	329	PRO
41	l4	330	TYR
41	l4	339	LEU
41	l4	342	LYS
42	l5	5	LYS
42	l5	258	LYS
42	l5	260	PHE
42	l5	269	SER
44	l7	158	LYS
45	l8	25	PRO
45	l8	39	ALA
45	l8	122	LYS
45	l8	190	VAL
45	l8	203	VAL
45	l8	223	ALA
47	m0	7	ARG
47	m0	204	GLY
47	m0	219	ALA
47	m0	220	GLN
48	m1	8	PRO
48	m1	9	MET
48	m1	10	ARG

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Mol	Chain	Res	Type
48	m1	108	GLU
48	m1	165	GLN
49	m3	47	ALA
49	m3	50	PRO
49	m3	51	LEU
49	m3	58	VAL
49	m3	150	PRO
49	m3	152	THR
51	m5	183	THR
52	m6	16	VAL
52	m6	110	PRO
53	m7	67	ILE
54	m8	99	THR
55	m9	156	ASN
55	m9	183	ALA
56	n0	2	ALA
57	n1	122	GLN
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	55	ASN
62	n6	83	ASP
63	n7	5	LEU
63	n7	56	LYS
63	n7	125	GLY
63	n7	129	TRP
65	n9	21	ILE
65	n9	23	LYS
65	n9	39	PHE
67	o1	7	VAL
67	o1	45	GLY
67	o1	86	LYS
68	o2	4	LEU
68	o2	5	PRO
68	o2	6	HIS
70	o4	79	SER
72	o6	33	ALA
72	o6	98	ARG
73	o7	84	SER

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Mol	Chain	Res	Type
74	o8	17	ARG
74	o8	18	ALA
74	o8	19	ASP
76	q0	78	ILE
84	p0	93	LEU
84	p0	198	PRO
2	S0	5	ALA
2	S0	49	ASN
2	S0	94	GLY
2	S0	205	ARG
3	S1	51	SER
3	S1	58	SER
3	S1	78	ASP
3	S1	81	PHE
3	S1	177	GLN
3	S1	221	PRO
4	S2	81	MET
4	S2	182	PRO
5	S3	38	GLU
5	S3	40	ARG
5	S3	90	ARG
5	S3	216	PRO
6	S4	12	LEU
6	S4	17	HIS
6	S4	96	ASN
6	S4	195	ILE
6	S4	222	LEU
6	S4	245	LYS
7	S5	51	VAL
7	S5	64	VAL
7	S5	101	GLY
7	S5	127	GLN
7	S5	150	GLY
8	S6	70	PRO
8	S6	154	ARG
9	S7	73	VAL
9	S7	98	ILE
9	S7	155	ASP
9	S7	159	VAL
10	S8	52	ASN
10	S8	81	VAL
10	S8	149	SER

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Mol	Chain	Res	Type
10	S8	186	GLY
11	S9	98	ALA
11	S9	100	LYS
12	C0	35	ILE
12	C0	64	TYR
12	C0	92	ILE
13	C1	29	LYS
13	C1	55	ASP
13	C1	145	ALA
13	C1	154	ALA
14	C2	22	VAL
14	C2	55	GLY
14	C2	66	VAL
14	C2	91	VAL
14	C2	101	ALA
14	C2	119	SER
15	C3	22	ALA
15	C3	68	GLY
16	C4	39	ILE
16	C4	51	ASP
16	C4	124	ASP
17	C5	80	MET
17	C5	101	ALA
18	C6	116	LEU
19	C7	113	LEU
19	C7	115	LEU
19	C7	124	VAL
20	C8	10	SER
20	C8	61	LEU
20	C8	104	ASN
20	C8	144	ARG
21	C9	90	PRO
23	D1	4	ASP
23	D1	7	GLN
23	D1	43	GLY
24	D2	127	GLY
25	D3	40	SER
25	D3	41	SER
25	D3	112	LYS
25	D3	138	GLU
26	D4	5	VAL
26	D4	34	ASN

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Mol	Chain	Res	Type
26	D4	35	VAL
27	D5	41	ILE
28	D6	47	ALA
28	D6	86	VAL
29	D7	63	LEU
30	D8	51	ASN
31	D9	6	VAL
33	E1	83	LYS
33	E1	84	VAL
33	E1	98	VAL
33	E1	127	GLY
35	SM	64	LYS
35	SM	139	GLU
35	SM	173	GLU
39	L2	13	GLY
39	L2	47	GLN
39	L2	246	LEU
40	L3	3	HIS
40	L3	139	GLN
40	L3	262	TRP
40	L3	351	LEU
40	L3	379	PHE
40	L3	385	LYS
40	L3	386	ASP
41	L4	4	PRO
41	L4	130	ALA
41	L4	146	PRO
41	L4	190	GLY
41	L4	232	SER
41	L4	313	LEU
41	L4	339	LEU
42	L5	7	ALA
42	L5	57	ASN
42	L5	85	ARG
42	L5	228	ALA
43	L6	81	ALA
44	L7	25	GLN
44	L7	51	TYR
44	L7	91	GLY
45	L8	94	PHE
45	L8	100	GLU
45	L8	196	ALA

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Mol	Chain	Res	Type
47	M0	16	PRO
47	M0	194	GLY
48	M1	94	ARG
48	M1	117	ASP
48	M1	151	SER
48	M1	167	TYR
49	M3	76	THR
50	M4	8	LYS
50	M4	10	SER
50	M4	28	SER
50	M4	36	VAL
51	M5	184	LYS
52	M6	16	VAL
52	M6	110	PRO
52	M6	182	ASN
53	M7	110	THR
53	M7	161	ALA
55	M9	53	LYS
57	N1	121	ALA
57	N1	159	PHE
58	N2	50	LEU
58	N2	59	ASP
58	N2	91	ASP
59	N3	82	ALA
60	N4	97	LYS
61	N5	45	LYS
62	N6	52	ARG
62	N6	53	ASP
62	N6	84	LYS
63	N7	16	GLY
63	N7	17	ARG
63	N7	35	SER
63	N7	128	GLN
64	N8	66	ALA
66	O0	71	GLN
66	O0	96	GLY
67	O1	6	ASP
67	O1	84	ASP
69	O3	59	VAL
72	O6	3	VAL
75	O9	44	TRP
79	Q3	58	SER

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Mol	Chain	Res	Type
2	s0	44	GLY
2	s0	66	ALA
2	s0	111	ILE
2	s0	139	VAL
2	s0	191	ARG
3	s1	93	GLY
3	s1	161	ILE
3	s1	179	SER
4	s2	92	ALA
4	s2	163	GLY
5	s3	61	GLU
5	s3	90	ARG
5	s3	203	PRO
6	s4	12	LEU
6	s4	93	ASP
6	s4	164	LEU
6	s4	195	ILE
6	s4	202	ASP
7	s5	36	ALA
7	s5	204	GLY
8	s6	68	LEU
9	s7	67	LEU
10	s8	199	LYS
11	s9	118	LEU
80	c0	23	ALA
13	c1	144	ALA
14	c2	26	ASP
14	c2	89	ILE
14	c2	90	LYS
14	c2	101	ALA
14	c2	103	LEU
14	c2	131	ASP
15	c3	12	SER
15	c3	139	TRP
15	c3	140	LYS
16	c4	35	GLY
16	c4	50	ALA
16	c4	90	ARG
16	c4	131	GLY
18	c6	40	GLU
18	c6	97	VAL
18	c6	113	ASP

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Mol	Chain	Res	Type
19	c7	50	ILE
19	c7	51	ALA
19	c7	98	GLY
19	c7	99	VAL
19	c7	113	LEU
20	c8	61	LEU
21	c9	33	TYR
22	d0	17	GLN
22	d0	49	ASN
22	d0	51	VAL
22	d0	52	LYS
22	d0	96	PRO
23	d1	44	ARG
24	d2	68	ARG
25	d3	66	SER
26	d4	49	LYS
27	d5	103	ARG
28	d6	8	ASN
28	d6	63	ALA
29	d7	62	ILE
30	d8	61	ARG
31	d9	5	ASN
31	d9	7	TRP
81	e0	45	VAL
81	e0	51	ASN
82	e1	83	LYS
82	e1	84	VAL
82	e1	100	LEU
34	sR	28	GLY
34	sR	160	GLU
34	sR	218	GLY
39	l2	30	ARG
39	l2	142	ASP
39	l2	212	GLY
39	l2	215	ASN
40	l3	247	ARG
41	l4	4	PRO
41	l4	15	ALA
41	l4	90	PHE
41	l4	143	GLU
41	l4	146	PRO
41	l4	272	VAL

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Mol	Chain	Res	Type
41	l4	311	HIS
42	l5	178	ASN
43	l6	32	ALA
44	l7	191	VAL
45	l8	26	LEU
45	l8	209	ALA
45	l8	239	GLY
46	l9	144	ILE
46	l9	189	GLU
47	m0	25	ALA
47	m0	176	LEU
47	m0	216	TYR
47	m0	218	ALA
48	m1	114	ILE
49	m3	76	THR
49	m3	121	SER
49	m3	134	GLU
49	m3	135	ALA
50	m4	135	LEU
51	m5	184	LYS
52	m6	13	GLY
52	m6	111	PRO
52	m6	186	ALA
53	m7	54	HIS
53	m7	66	SER
54	m8	41	ASP
55	m9	155	LEU
55	m9	182	ASP
58	n2	48	GLY
58	n2	50	LEU
60	n4	64	THR
62	n6	45	ILE
62	n6	84	LYS
62	n6	125	LYS
63	n7	17	ARG
63	n7	36	HIS
65	n9	24	PRO
67	o1	84	ASP
67	o1	91	SER
68	o2	27	ARG
68	o2	124	GLY
69	o3	33	GLU

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Mol	Chain	Res	Type
69	o3	60	ARG
69	o3	88	ASN
71	o5	82	ALA
71	o5	119	LYS
73	o7	85	LYS
78	q2	17	CYS
84	p0	33	VAL
84	p0	102	SER
2	S0	27	ARG
2	S0	95	ALA
2	S0	195	TRP
2	S0	196	SER
3	S1	62	LYS
3	S1	82	ARG
3	S1	131	ASP
3	S1	158	SER
3	S1	179	SER
3	S1	218	LEU
4	S2	39	THR
5	S3	72	LEU
5	S3	217	ILE
5	S3	218	LEU
6	S4	77	ARG
6	S4	201	HIS
6	S4	205	PHE
7	S5	35	GLN
7	S5	58	LEU
8	S6	146	GLY
8	S6	152	ASP
9	S7	5	GLN
9	S7	30	SER
9	S7	36	ALA
9	S7	112	ARG
9	S7	156	SER
9	S7	186	PRO
10	S8	40	ALA
10	S8	120	THR
11	S9	9	SER
11	S9	163	PRO
11	S9	164	PHE
12	C0	94	GLU
13	C1	4	GLU

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Mol	Chain	Res	Type
13	C1	30	ARG
13	C1	113	PRO
13	C1	139	VAL
13	C1	146	ALA
13	C1	147	ALA
14	C2	21	GLU
14	C2	87	PRO
14	C2	105	LYS
14	C2	112	ALA
16	C4	18	ARG
16	C4	40	ALA
16	C4	75	GLY
16	C4	125	SER
17	C5	22	LEU
17	C5	52	LYS
17	C5	130	ARG
20	C8	7	GLU
20	C8	100	THR
21	C9	69	LYS
23	D1	64	GLU
24	D2	57	ARG
25	D3	131	SER
26	D4	6	THR
26	D4	36	SER
26	D4	97	ALA
26	D4	104	SER
27	D5	38	HIS
27	D5	70	LYS
28	D6	11	ASN
30	D8	14	LYS
30	D8	16	LEU
33	E1	87	THR
33	E1	102	VAL
33	E1	118	ARG
34	SR	13	LEU
34	SR	22	SER
34	SR	50	ASP
34	SR	153	GLN
34	SR	194	GLY
34	SR	242	SER
35	SM	52	PRO
35	SM	87	THR

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Mol	Chain	Res	Type
35	SM	174	LEU
39	L2	127	ALA
39	L2	180	LEU
39	L2	251	LYS
40	L3	155	ALA
41	L4	230	VAL
41	L4	304	GLN
42	L5	58	LYS
42	L5	110	LEU
42	L5	124	GLU
42	L5	125	VAL
42	L5	188	GLU
42	L5	259	LYS
42	L5	269	SER
43	L6	97	ASN
43	L6	150	LYS
44	L7	163	LEU
45	L8	39	ALA
47	M0	220	GLN
48	M1	73	GLY
48	M1	95	ASN
48	M1	114	ILE
48	M1	140	ARG
49	M3	130	GLY
49	M3	136	GLU
49	M3	165	SER
51	M5	81	TYR
52	M6	90	HIS
53	M7	3	ARG
53	M7	109	ALA
53	M7	164	LYS
56	N0	2	ALA
56	N0	130	GLU
58	N2	11	ILE
58	N2	20	SER
58	N2	31	ALA
58	N2	52	ASN
62	N6	83	ASP
63	N7	28	PRO
63	N7	102	GLU
64	N8	47	LYS
64	N8	78	LEU

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Mol	Chain	Res	Type
65	N9	44	LYS
67	O1	60	TRP
69	O3	40	ASP
69	O3	88	ASN
70	O4	46	ASP
71	O5	14	LYS
71	O5	27	GLU
71	O5	75	TYR
71	O5	95	PHE
72	O6	64	SER
73	O7	68	LYS
74	O8	33	LYS
75	O9	32	ASN
78	Q2	33	ALA
78	Q2	34	SER
78	Q2	78	LYS
78	Q2	94	GLY
2	s0	103	THR
3	s1	82	ARG
4	s2	107	SER
5	s3	221	SER
6	s4	3	ARG
6	s4	94	ALA
6	s4	245	LYS
7	s5	29	ILE
7	s5	39	GLU
7	s5	55	ASP
9	s7	159	VAL
10	s8	108	PRO
11	s9	65	LYS
80	c0	3	MET
80	c0	30	ALA
80	c0	31	LYS
80	c0	92	ILE
13	c1	133	LYS
14	c2	106	ILE
14	c2	108	ARG
14	c2	119	SER
15	c3	48	SER
15	c3	133	ALA
17	c5	7	ALA
17	c5	9	LYS

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Mol	Chain	Res	Type
17	c5	71	GLU
17	c5	80	MET
18	c6	116	LEU
19	c7	67	ARG
19	c7	120	SER
20	c8	94	ASP
21	c9	40	SER
22	d0	19	ILE
22	d0	55	PRO
22	d0	97	VAL
25	d3	60	GLU
25	d3	70	LYS
26	d4	58	PHE
26	d4	132	ARG
27	d5	93	SER
28	d6	59	TYR
28	d6	82	ARG
29	d7	3	LEU
29	d7	20	LYS
30	d8	57	MET
81	e0	47	VAL
81	e0	54	ARG
82	e1	90	LYS
82	e1	112	GLY
82	e1	131	PHE
34	sR	161	LYS
34	sR	297	ASP
35	sM	66	ALA
35	sM	168	GLU
39	l2	80	GLU
39	l2	127	ALA
39	l2	194	ASN
39	l2	229	ALA
39	l2	249	SER
40	l3	378	ALA
41	l4	233	LEU
41	l4	338	LYS
41	l4	341	SER
43	l6	97	ASN
43	l6	98	VAL
43	l6	133	GLU
44	l7	228	SER

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Mol	Chain	Res	Type
45	l8	69	LEU
45	l8	121	SER
45	l8	133	LYS
45	l8	237	ILE
46	l9	109	ALA
46	l9	110	LYS
47	m0	3	ARG
47	m0	196	PHE
48	m1	94	ARG
49	m3	129	ASN
51	m5	81	TYR
52	m6	4	GLU
55	m9	36	ASN
57	n1	16	GLN
57	n1	121	ALA
60	n4	83	THR
60	n4	93	ARG
60	n4	132	GLY
61	n5	40	LEU
61	n5	47	ALA
61	n5	48	SER
63	n7	134	LEU
67	o1	40	ALA
67	o1	83	GLU
69	o3	59	VAL
71	o5	61	GLN
71	o5	83	LYS
72	o6	4	LYS
73	o7	87	SER
77	q1	4	LYS
79	q3	51	ALA
2	S0	103	THR
2	S0	126	PRO
2	S0	164	ASN
2	S0	188	LEU
2	S0	194	PRO
3	S1	21	VAL
3	S1	54	LEU
3	S1	55	LYS
3	S1	116	LYS
4	S2	150	GLN
5	S3	195	SER

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Mol	Chain	Res	Type
5	S3	204	ASP
6	S4	73	ASP
6	S4	194	THR
6	S4	200	ARG
7	S5	21	THR
7	S5	54	LYS
10	S8	10	LYS
10	S8	19	ALA
10	S8	152	ILE
10	S8	153	GLU
11	S9	162	SER
14	C2	69	ALA
14	C2	106	ILE
14	C2	115	VAL
14	C2	130	THR
15	C3	19	SER
16	C4	25	ASP
16	C4	79	VAL
16	C4	114	ARG
16	C4	123	SER
17	C5	11	VAL
17	C5	51	SER
18	C6	33	GLY
20	C8	8	GLN
21	C9	28	LEU
21	C9	130	ARG
22	D0	16	GLN
22	D0	49	ASN
23	D1	10	GLU
23	D1	12	TYR
23	D1	42	GLU
25	D3	109	ARG
26	D4	51	GLU
28	D6	8	ASN
28	D6	63	ALA
28	D6	64	LEU
29	D7	23	THR
29	D7	51	GLN
33	E1	94	LYS
33	E1	100	LEU
33	E1	111	GLU
34	SR	51	ASP

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Mol	Chain	Res	Type
34	SR	114	ASP
34	SR	217	ASP
34	SR	231	MET
34	SR	237	GLN
34	SR	244	ALA
35	SM	53	ARG
39	L2	70	ARG
39	L2	130	SER
40	L3	141	GLY
41	L4	90	PHE
41	L4	140	HIS
41	L4	270	SER
42	L5	178	ASN
42	L5	185	PHE
42	L5	215	ASP
42	L5	253	PHE
45	L8	136	LEU
45	L8	138	HIS
45	L8	157	VAL
46	L9	2	LYS
48	M1	111	ASP
49	M3	140	SER
49	M3	166	ALA
50	M4	6	ILE
51	M5	145	ASP
52	M6	178	VAL
53	M7	160	ALA
54	M8	21	SER
54	M8	162	ALA
57	N1	114	ALA
59	N3	46	LEU
60	N4	76	VAL
62	N6	25	SER
63	N7	32	GLY
63	N7	103	GLN
66	O0	46	ALA
67	O1	5	LYS
67	O1	7	VAL
67	O1	21	HIS
79	Q3	84	ARG
2	s0	5	ALA
2	s0	68	PRO

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Mol	Chain	Res	Type
3	s1	22	ASP
4	s2	150	GLN
4	s2	235	LEU
5	s3	4	LEU
5	s3	79	TYR
5	s3	196	ARG
5	s3	219	ALA
6	s4	90	ILE
6	s4	168	LYS
6	s4	260	GLY
8	s6	58	LYS
8	s6	70	PRO
9	s7	13	PRO
9	s7	155	ASP
9	s7	186	PRO
10	s8	62	THR
10	s8	100	ALA
10	s8	137	LYS
10	s8	149	SER
80	c0	9	ASN
13	c1	121	ASP
14	c2	21	GLU
14	c2	87	PRO
14	c2	91	VAL
14	c2	130	THR
16	c4	37	GLU
16	c4	114	ARG
17	c5	6	ASN
17	c5	54	ALA
17	c5	100	LYS
17	c5	136	SER
18	c6	142	TYR
19	c7	15	ALA
19	c7	116	LYS
20	c8	7	GLU
20	c8	60	GLU
22	d0	16	GLN
23	d1	10	GLU
25	d3	131	SER
27	d5	71	ILE
28	d6	93	LYS
31	d9	16	LYS

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Mol	Chain	Res	Type
82	e1	79	LYS
82	e1	85	TYR
34	sR	290	VAL
35	sM	43	ASP
35	sM	46	LYS
35	sM	84	LYS
35	sM	121	LYS
35	sM	164	ASN
39	l2	56	ALA
40	l3	3	HIS
40	l3	22	ALA
40	l3	348	ARG
41	l4	190	GLY
41	l4	231	ALA
41	l4	352	ALA
42	l5	119	TYR
43	l6	10	TYR
45	l8	79	GLN
45	l8	222	PHE
45	l8	240	ASN
46	l9	2	LYS
47	m0	101	LYS
48	m1	167	TYR
49	m3	60	ALA
51	m5	76	PRO
54	m8	112	ALA
56	n0	154	HIS
58	n2	60	GLY
60	n4	77	LYS
61	n5	24	LEU
63	n7	6	LYS
64	n8	24	LYS
64	n8	56	VAL
65	n9	26	THR
71	o5	40	SER
72	o6	34	SER
78	q2	33	ALA
84	p0	21	GLU
84	p0	203	ASP
2	S0	203	PHE
3	S1	207	LEU
3	S1	215	VAL

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Mol	Chain	Res	Type
4	S2	47	ALA
4	S2	79	GLU
4	S2	106	ASP
7	S5	65	ARG
8	S6	148	SER
9	S7	13	PRO
9	S7	110	GLN
10	S8	59	ARG
10	S8	105	ASP
12	C0	54	TYR
14	C2	113	ARG
14	C2	131	ASP
15	C3	12	SER
16	C4	24	ASN
17	C5	29	SER
18	C6	40	GLU
19	C7	23	LYS
19	C7	24	LEU
22	D0	17	GLN
22	D0	21	LYS
23	D1	21	ASN
27	D5	88	ILE
29	D7	57	GLU
29	D7	75	GLU
33	E1	99	LYS
33	E1	110	ALA
33	E1	137	ASP
34	SR	98	GLU
34	SR	163	ASP
35	SM	88	ARG
35	SM	153	ASP
39	L2	143	GLU
41	L4	14	GLU
41	L4	15	ALA
41	L4	223	PRO
41	L4	233	LEU
41	L4	269	SER
42	L5	260	PHE
42	L5	267	ALA
43	L6	6	ALA
43	L6	100	LYS
44	L7	159	GLN

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Mol	Chain	Res	Type
44	L7	164	SER
44	L7	217	PRO
45	L8	156	ASP
46	L9	110	LYS
47	M0	38	LYS
50	M4	29	ALA
51	M5	94	TYR
52	M6	89	SER
54	M8	176	ARG
57	N1	127	GLN
58	N2	107	PHE
66	O0	20	SER
72	O6	21	THR
72	O6	34	SER
74	O8	70	PRO
78	Q2	17	CYS
2	s0	10	THR
2	s0	194	PRO
3	s1	160	HIS
3	s1	224	ASP
4	s2	182	PRO
4	s2	234	PRO
5	s3	43	PRO
6	s4	22	LYS
6	s4	30	ARG
6	s4	38	LEU
7	s5	100	ASN
7	s5	171	ALA
9	s7	100	PRO
9	s7	133	THR
10	s8	78	ILE
10	s8	107	THR
10	s8	159	GLN
11	s9	162	SER
80	c0	35	ILE
80	c0	49	LEU
80	c0	95	ARG
13	c1	129	ARG
14	c2	25	GLU
14	c2	39	ASP
14	c2	64	SER
14	c2	82	PRO

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Mol	Chain	Res	Type
16	c4	124	ASP
17	c5	52	LYS
17	c5	130	ARG
20	c8	14	ILE
26	d4	51	GLU
26	d4	78	SER
28	d6	5	ARG
29	d7	75	GLU
81	e0	60	PRO
81	e0	61	SER
82	e1	128	ALA
34	sR	185	GLN
39	l2	247	ARG
39	l2	251	LYS
40	l3	386	ASP
41	l4	328	ASN
44	l7	196	LYS
45	l8	102	ALA
45	l8	196	ALA
46	l9	167	VAL
48	m1	115	LYS
49	m3	13	HIS
49	m3	93	ILE
63	n7	18	TYR
64	n8	76	ASP
64	n8	129	PHE
67	o1	47	ASP
68	o2	17	PHE
2	S0	7	PHE
2	S0	35	PRO
3	S1	23	PRO
3	S1	210	ILE
3	S1	226	GLY
4	S2	235	LEU
4	S2	236	PRO
5	S3	36	GLY
6	S4	164	LEU
11	S9	149	ARG
13	C1	95	PRO
15	C3	3	ARG
17	C5	127	ARG
25	D3	78	LYS

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Mol	Chain	Res	Type
25	D3	89	ASN
31	D9	8	PHE
33	E1	128	ALA
33	E1	144	CYS
34	SR	30	PRO
35	SM	12	VAL
35	SM	67	GLY
35	SM	111	GLY
35	SM	172	VAL
40	L3	188	ILE
41	L4	183	LYS
42	L5	137	ASP
42	L5	212	ALA
44	L7	178	ILE
47	M0	145	LYS
49	M3	127	PRO
49	M3	192	GLU
64	N8	56	VAL
64	N8	97	GLU
65	N9	45	HIS
70	O4	74	ARG
73	O7	86	ALA
74	O8	37	PRO
79	Q3	7	LYS
3	s1	207	LEU
7	s5	152	GLY
11	s9	134	ILE
14	c2	40	GLY
14	c2	45	LEU
30	d8	62	GLU
31	d9	11	PRO
81	e0	38	LEU
82	e1	148	TYR
35	sM	59	GLY
40	l3	239	PRO
42	l5	125	VAL
43	l6	93	VAL
47	m0	47	PRO
48	m1	153	LYS
54	m8	108	ALA
57	n1	136	ARG
60	n4	72	SER

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Mol	Chain	Res	Type
64	n8	68	PHE
67	o1	41	LYS
72	o6	22	PRO
73	o7	67	LEU
4	S2	36	VAL
8	S6	69	LEU
8	S6	162	VAL
8	S6	165	GLY
27	D5	71	ILE
34	SR	113	VAL
34	SR	146	GLY
34	SR	271	VAL
47	M0	149	VAL
53	M7	51	VAL
53	M7	143	PRO
65	N9	21	ILE
6	s4	150	PRO
80	c0	73	VAL
14	c2	63	VAL
14	c2	66	VAL
44	l7	178	ILE
48	m1	117	ASP
61	n5	62	VAL
63	n7	70	PRO
3	S1	176	VAL
5	S3	37	VAL
43	L6	98	VAL
8	s6	165	GLY
11	s9	168	ARG
16	c4	79	VAL
20	c8	29	VAL
31	d9	17	GLY
40	l3	141	GLY
63	n7	103	GLN
2	S0	139	VAL
10	S8	107	THR
14	C2	37	VAL
23	D1	46	ILE
33	E1	112	GLY
40	L3	317	ILE
53	M7	182	ILE
57	N1	123	GLY

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Mol	Chain	Res	Type
63	N7	36	HIS
8	s6	69	LEU
8	s6	157	VAL
18	c6	4	VAL
20	c8	135	GLY
21	c9	100	ILE
25	d3	119	GLY
28	d6	58	VAL
30	d8	20	GLY
54	m8	84	VAL
68	o2	122	PRO
72	o6	9	ILE
4	S2	145	GLY
9	S7	132	PRO
25	D3	143	PRO
28	D6	75	VAL
45	L8	190	VAL
62	N6	92	GLY
67	O1	67	VAL
5	s3	163	PRO
7	s5	101	GLY
9	s7	12	ALA
14	c2	115	VAL
27	d5	55	PRO
47	m0	5	PRO
47	m0	214	PRO
54	m8	97	PRO
56	n0	129	ILE
84	p0	77	LEU
14	C2	102	GLY
16	C4	122	PRO
20	C8	82	PRO
3	s1	35	PRO
4	s2	149	GLY
7	s5	153	GLY
16	c4	76	ILE
20	c8	28	ILE
30	d8	6	PRO
82	e1	124	PRO
34	sR	167	VAL
57	n1	148	PRO

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%)	136 (83%)	28 (17%)	2	10
2	s0	165/209 (79%)	127 (77%)	38 (23%)	1	3
3	S1	191/223 (86%)	151 (79%)	40 (21%)	1	6
3	s1	192/223 (86%)	153 (80%)	39 (20%)	1	6
4	S2	176/204 (86%)	130 (74%)	46 (26%)	0	2
4	s2	176/204 (86%)	129 (73%)	47 (27%)	0	2
5	S3	182/194 (94%)	143 (79%)	39 (21%)	1	5
5	s3	182/194 (94%)	143 (79%)	39 (21%)	1	5
6	S4	221/221 (100%)	178 (80%)	43 (20%)	1	7
6	s4	221/221 (100%)	184 (83%)	37 (17%)	2	10
7	S5	173/190 (91%)	145 (84%)	28 (16%)	2	11
7	s5	173/190 (91%)	133 (77%)	40 (23%)	1	3
8	S6	188/201 (94%)	151 (80%)	37 (20%)	1	7
8	s6	187/201 (93%)	150 (80%)	37 (20%)	1	7
9	S7	165/169 (98%)	136 (82%)	29 (18%)	2	9
9	s7	165/169 (98%)	134 (81%)	31 (19%)	1	8
10	S8	150/161 (93%)	122 (81%)	28 (19%)	1	8
10	s8	150/161 (93%)	124 (83%)	26 (17%)	2	10
11	S9	158/165 (96%)	124 (78%)	34 (22%)	1	5
11	s9	158/165 (96%)	126 (80%)	32 (20%)	1	6
12	C0	77/98 (79%)	64 (83%)	13 (17%)	2	10
13	C1	129/136 (95%)	107 (83%)	22 (17%)	2	10
13	c1	129/136 (95%)	109 (84%)	20 (16%)	2	12
14	C2	88/118 (75%)	66 (75%)	22 (25%)	0	2
14	c2	88/118 (75%)	63 (72%)	25 (28%)	0	1
15	C3	127/127 (100%)	100 (79%)	27 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	c3	127/127 (100%)	103 (81%)	24 (19%)	1	8
16	C4	81/104 (78%)	60 (74%)	21 (26%)	0	2
16	c4	97/104 (93%)	69 (71%)	28 (29%)	0	1
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1	6
17	c5	103/117 (88%)	78 (76%)	25 (24%)	0	2
18	C6	117/118 (99%)	89 (76%)	28 (24%)	0	3
18	c6	118/118 (100%)	95 (80%)	23 (20%)	1	7
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	6
19	c7	92/124 (74%)	66 (72%)	26 (28%)	0	1
20	C8	128/128 (100%)	96 (75%)	32 (25%)	0	2
20	c8	128/128 (100%)	101 (79%)	27 (21%)	1	6
21	C9	115/115 (100%)	83 (72%)	32 (28%)	0	1
21	c9	115/115 (100%)	93 (81%)	22 (19%)	1	8
22	D0	100/113 (88%)	83 (83%)	17 (17%)	2	10
22	d0	103/113 (91%)	71 (69%)	32 (31%)	0	0
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1	6
23	d1	74/74 (100%)	59 (80%)	15 (20%)	1	6
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	6
24	d2	110/110 (100%)	93 (84%)	17 (16%)	2	12
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2	9
25	d3	119/119 (100%)	92 (77%)	27 (23%)	1	4
26	D4	112/112 (100%)	92 (82%)	20 (18%)	2	9
26	d4	112/112 (100%)	91 (81%)	21 (19%)	1	8
27	D5	61/88 (69%)	50 (82%)	11 (18%)	1	9
27	d5	61/88 (69%)	49 (80%)	12 (20%)	1	7
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1	6
28	d6	83/83 (100%)	63 (76%)	20 (24%)	0	3
29	D7	70/70 (100%)	55 (79%)	15 (21%)	1	5
29	d7	70/70 (100%)	59 (84%)	11 (16%)	2	12
30	D8	56/59 (95%)	40 (71%)	16 (29%)	0	1
30	d8	56/59 (95%)	41 (73%)	15 (27%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	D9	47/48 (98%)	41 (87%)	6 (13%)	4	20
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	5
32	E0	51/51 (100%)	42 (82%)	9 (18%)	2	9
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	1
34	SR	260/261 (100%)	214 (82%)	46 (18%)	2	9
34	sR	260/261 (100%)	237 (91%)	23 (9%)	10	36
35	SM	97/228 (42%)	79 (81%)	18 (19%)	1	8
35	sM	54/228 (24%)	40 (74%)	14 (26%)	0	2
39	L2	193/195 (99%)	153 (79%)	40 (21%)	1	6
39	l2	192/195 (98%)	156 (81%)	36 (19%)	1	8
40	L3	320/322 (99%)	260 (81%)	60 (19%)	1	8
40	l3	319/322 (99%)	259 (81%)	60 (19%)	1	8
41	L4	288/288 (100%)	241 (84%)	47 (16%)	2	11
41	l4	288/288 (100%)	236 (82%)	52 (18%)	1	8
42	L5	244/244 (100%)	199 (82%)	45 (18%)	1	8
42	l5	243/244 (100%)	194 (80%)	49 (20%)	1	6
43	L6	134/152 (88%)	113 (84%)	21 (16%)	2	12
43	l6	135/152 (89%)	113 (84%)	22 (16%)	2	11
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4	19
44	l7	187/204 (92%)	163 (87%)	24 (13%)	4	20
45	L8	187/207 (90%)	151 (81%)	36 (19%)	1	8
45	l8	177/207 (86%)	145 (82%)	32 (18%)	1	8
46	L9	171/171 (100%)	135 (79%)	36 (21%)	1	6
46	l9	171/171 (100%)	132 (77%)	39 (23%)	1	4
47	M0	177/186 (95%)	136 (77%)	41 (23%)	1	3
47	m0	179/186 (96%)	148 (83%)	31 (17%)	2	10
48	M1	147/150 (98%)	115 (78%)	32 (22%)	1	5
48	m1	147/150 (98%)	112 (76%)	35 (24%)	0	3
49	M3	154/158 (98%)	124 (80%)	30 (20%)	1	7
49	m3	154/158 (98%)	129 (84%)	25 (16%)	2	11
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	m4	108/108 (100%)	84 (78%)	24 (22%)	1	4
51	M5	175/175 (100%)	148 (85%)	27 (15%)	2	13
51	m5	175/175 (100%)	142 (81%)	33 (19%)	1	8
52	M6	160/161 (99%)	134 (84%)	26 (16%)	2	11
52	m6	160/161 (99%)	136 (85%)	24 (15%)	3	14
53	M7	140/145 (97%)	114 (81%)	26 (19%)	1	8
53	m7	125/145 (86%)	101 (81%)	24 (19%)	1	8
54	M8	150/150 (100%)	123 (82%)	27 (18%)	1	9
54	m8	150/150 (100%)	125 (83%)	25 (17%)	2	10
55	M9	153/153 (100%)	130 (85%)	23 (15%)	3	14
55	m9	153/153 (100%)	121 (79%)	32 (21%)	1	6
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1	6
56	n0	156/156 (100%)	127 (81%)	29 (19%)	1	8
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1	3
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	5
58	N2	87/106 (82%)	72 (83%)	15 (17%)	2	10
58	n2	85/106 (80%)	67 (79%)	18 (21%)	1	5
59	N3	104/104 (100%)	85 (82%)	19 (18%)	1	8
59	n3	104/104 (100%)	95 (91%)	9 (9%)	10	37
60	N4	57/129 (44%)	47 (82%)	10 (18%)	2	9
60	n4	100/129 (78%)	84 (84%)	16 (16%)	2	11
61	N5	104/117 (89%)	88 (85%)	16 (15%)	2	13
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	6
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1	6
62	n6	109/109 (100%)	75 (69%)	34 (31%)	0	0
63	N7	115/115 (100%)	96 (84%)	19 (16%)	2	10
63	n7	115/115 (100%)	89 (77%)	26 (23%)	1	4
64	N8	118/118 (100%)	90 (76%)	28 (24%)	1	3
64	n8	118/118 (100%)	96 (81%)	22 (19%)	1	8
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	7
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	O0	81/87 (93%)	62 (76%)	19 (24%)	1	3
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1	6
67	O1	92/96 (96%)	75 (82%)	17 (18%)	1	8
67	o1	94/96 (98%)	71 (76%)	23 (24%)	0	2
68	O2	109/110 (99%)	82 (75%)	27 (25%)	0	2
68	o2	109/110 (99%)	89 (82%)	20 (18%)	1	8
69	O3	90/90 (100%)	75 (83%)	15 (17%)	2	10
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2	9
70	O4	95/101 (94%)	76 (80%)	19 (20%)	1	6
70	o4	95/101 (94%)	78 (82%)	17 (18%)	2	9
71	O5	104/104 (100%)	79 (76%)	25 (24%)	0	3
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1	6
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0	2
72	o6	80/81 (99%)	57 (71%)	23 (29%)	0	1
73	O7	70/70 (100%)	57 (81%)	13 (19%)	1	8
73	o7	70/70 (100%)	53 (76%)	17 (24%)	0	2
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0	2
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	9
75	O9	45/45 (100%)	34 (76%)	11 (24%)	0	2
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	9
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	0	2
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1	3
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	10
77	q1	23/23 (100%)	18 (78%)	5 (22%)	1	5
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	0	2
78	q2	90/90 (100%)	65 (72%)	25 (28%)	0	1
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	10
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	6
80	c0	73/98 (74%)	65 (89%)	8 (11%)	6	26
81	e0	53/53 (100%)	40 (76%)	13 (24%)	0	2
82	e1	66/66 (100%)	45 (68%)	21 (32%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	p0	105/253 (42%)	84 (80%)	21 (20%)	1	6
All	All	18727/20239 (92%)	15017 (80%)	3710 (20%)	1	7

All (3710) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	7	PHE
2	S0	30	GLN
2	S0	32	HIS
2	S0	37	VAL
2	S0	41	ARG
2	S0	49	ASN
2	S0	50	VAL
2	S0	84	ARG
2	S0	87	LEU
2	S0	96	THR
2	S0	101	ARG
2	S0	106	SER
2	S0	108	THR
2	S0	110	TYR
2	S0	124	THR
2	S0	139	VAL
2	S0	140	ASN
2	S0	154	GLU
2	S0	157	ASP
2	S0	162	CYS
2	S0	168	HIS
2	S0	172	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	196	SER
2	S0	198	MET
2	S0	200	ASP
2	S0	203	PHE
3	S1	21	VAL
3	S1	22	ASP
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	42	ASN
3	S1	46	THR
3	S1	61	LEU

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Mol	Chain	Res	Type
3	S1	65	VAL
3	S1	70	LEU
3	S1	73	LEU
3	S1	74	GLN
3	S1	77	GLU
3	S1	81	PHE
3	S1	85	LYS
3	S1	89	ASP
3	S1	95	ASN
3	S1	97	LEU
3	S1	105	PHE
3	S1	108	ASP
3	S1	111	ARG
3	S1	115	ARG
3	S1	135	LEU
3	S1	136	ARG
3	S1	137	ILE
3	S1	149	GLN
3	S1	154	SER
3	S1	167	VAL
3	S1	170	GLU
3	S1	181	LEU
3	S1	193	ILE
3	S1	198	GLU
3	S1	202	LYS
3	S1	203	ASP
3	S1	214	LYS
3	S1	215	VAL
3	S1	218	LEU
3	S1	219	LYS
3	S1	223	PHE
3	S1	231	LEU
4	S2	41	LEU
4	S2	50	ILE
4	S2	53	ILE
4	S2	55	GLU
4	S2	58	LEU
4	S2	69	ILE
4	S2	72	LEU
4	S2	76	LEU
4	S2	77	GLN
4	S2	81	MET

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Mol	Chain	Res	Type
4	S2	87	GLN
4	S2	89	GLN
4	S2	90	THR
4	S2	91	ARG
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	99	LYS
4	S2	111	VAL
4	S2	116	LYS
4	S2	117	THR
4	S2	119	LYS
4	S2	129	ILE
4	S2	134	LEU
4	S2	137	ILE
4	S2	139	ILE
4	S2	141	ARG
4	S2	146	THR
4	S2	148	LEU
4	S2	153	SER
4	S2	166	THR
4	S2	207	LEU
4	S2	208	GLU
4	S2	221	THR
4	S2	222	TYR
4	S2	224	PHE
4	S2	225	LEU
4	S2	226	THR
4	S2	229	LEU
4	S2	232	GLU
4	S2	235	LEU
4	S2	237	VAL
4	S2	238	SER
4	S2	240	LEU
4	S2	245	ASP
4	S2	246	GLU
5	S3	4	LEU
5	S3	6	SER
5	S3	9	ARG
5	S3	23	GLU
5	S3	27	ARG
5	S3	37	VAL

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Mol	Chain	Res	Type
5	S3	38	GLU
5	S3	40	ARG
5	S3	59	LEU
5	S3	61	GLU
5	S3	65	ARG
5	S3	66	ILE
5	S3	76	ARG
5	S3	84	ILE
5	S3	89	GLU
5	S3	92	GLN
5	S3	93	ASP
5	S3	113	LEU
5	S3	117	ARG
5	S3	120	TYR
5	S3	134	CYS
5	S3	142	LEU
5	S3	143	ARG
5	S3	146	ARG
5	S3	148	LYS
5	S3	151	LYS
5	S3	172	THR
5	S3	175	VAL
5	S3	176	LEU
5	S3	178	ARG
5	S3	179	GLN
5	S3	181	VAL
5	S3	182	LEU
5	S3	194	LYS
5	S3	202	LEU
5	S3	204	ASP
5	S3	207	THR
5	S3	217	ILE
5	S3	223	LYS
6	S4	9	LEU
6	S4	12	LEU
6	S4	37	LYS
6	S4	38	LEU
6	S4	42	LEU
6	S4	48	LEU
6	S4	72	VAL
6	S4	77	ARG
6	S4	78	THR

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Mol	Chain	Res	Type
6	S4	93	ASP
6	S4	113	ARG
6	S4	116	ASP
6	S4	117	GLU
6	S4	123	LEU
6	S4	126	VAL
6	S4	129	VAL
6	S4	131	LEU
6	S4	133	LYS
6	S4	148	ARG
6	S4	155	LYS
6	S4	156	VAL
6	S4	180	LEU
6	S4	181	VAL
6	S4	182	TYR
6	S4	187	ARG
6	S4	189	LEU
6	S4	192	ILE
6	S4	198	LYS
6	S4	206	ASP
6	S4	211	LYS
6	S4	213	SER
6	S4	214	LEU
6	S4	215	ASP
6	S4	220	THR
6	S4	221	ARG
6	S4	226	PHE
6	S4	227	VAL
6	S4	238	LEU
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	248	ILE
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	53	VAL

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Mol	Chain	Res	Type
7	S5	59	VAL
7	S5	65	ARG
7	S5	76	ARG
7	S5	79	ASN
7	S5	80	LYS
7	S5	83	ARG
7	S5	93	LEU
7	S5	94	THR
7	S5	122	ASN
7	S5	131	GLN
7	S5	146	THR
7	S5	147	THR
7	S5	156	ARG
7	S5	157	ARG
7	S5	161	ASP
7	S5	162	VAL
7	S5	166	ARG
7	S5	190	ILE
7	S5	194	LEU
7	S5	196	GLU
8	S6	5	ILE
8	S6	6	SER
8	S6	12	SER
8	S6	13	GLN
8	S6	19	ASP
8	S6	25	ARG
8	S6	31	ARG
8	S6	44	GLU
8	S6	45	PHE
8	S6	58	LYS
8	S6	65	GLN
8	S6	67	VAL
8	S6	69	LEU
8	S6	74	LYS
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	81	VAL
8	S6	82	SER
8	S6	98	ARG
8	S6	109	LEU
8	S6	120	GLU

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Mol	Chain	Res	Type
8	S6	126	ASP
8	S6	127	THR
8	S6	129	VAL
8	S6	132	ARG
8	S6	133	LEU
8	S6	143	LYS
8	S6	154	ARG
8	S6	155	ASP
8	S6	169	TYR
8	S6	170	THR
8	S6	176	GLN
8	S6	177	ARG
8	S6	211	LEU
8	S6	216	LEU
8	S6	223	LYS
9	S7	16	LEU
9	S7	37	GLU
9	S7	38	LEU
9	S7	50	ASP
9	S7	51	VAL
9	S7	67	LEU
9	S7	77	LEU
9	S7	79	ARG
9	S7	85	PHE
9	S7	87	ASP
9	S7	91	ILE
9	S7	97	ARG
9	S7	99	LEU
9	S7	104	ARG
9	S7	105	THR
9	S7	107	ARG
9	S7	114	ARG
9	S7	116	ARG
9	S7	117	THR
9	S7	123	ASP
9	S7	126	LEU
9	S7	147	ASN
9	S7	156	SER
9	S7	161	GLN
9	S7	166	LEU
9	S7	174	ASN
9	S7	176	LEU

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Mol	Chain	Res	Type
9	S7	185	ILE
9	S7	187	SER
10	S8	4	SER
10	S8	5	ARG
10	S8	8	ARG
10	S8	20	GLN
10	S8	21	PHE
10	S8	22	ARG
10	S8	26	LYS
10	S8	29	LEU
10	S8	32	GLN
10	S8	36	THR
10	S8	37	LYS
10	S8	46	VAL
10	S8	58	LEU
10	S8	66	SER
10	S8	73	SER
10	S8	74	LYS
10	S8	75	LYS
10	S8	77	ARG
10	S8	88	ASN
10	S8	97	THR
10	S8	140	GLU
10	S8	151	LYS
10	S8	152	ILE
10	S8	164	ARG
10	S8	184	LEU
10	S8	189	LEU
10	S8	193	LEU
10	S8	196	LEU
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR
11	S9	28	LEU
11	S9	30	LEU
11	S9	36	LEU
11	S9	39	LYS
11	S9	46	SER
11	S9	60	LEU
11	S9	61	THR
11	S9	78	ARG
11	S9	82	ARG

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Mol	Chain	Res	Type
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	99	LEU
11	S9	102	GLU
11	S9	103	ASP
11	S9	110	GLN
11	S9	113	VAL
11	S9	121	SER
11	S9	126	ARG
11	S9	130	THR
11	S9	132	ARG
11	S9	134	ILE
11	S9	138	LYS
11	S9	140	ILE
11	S9	149	ARG
11	S9	157	ASP
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	180	LYS
11	S9	182	GLU
12	C0	5	LYS
12	C0	8	ARG
12	C0	17	GLN
12	C0	20	VAL
12	C0	27	PHE
12	C0	32	HIS
12	C0	55	VAL
12	C0	56	LYS
12	C0	71	GLU
12	C0	76	LEU
12	C0	79	TYR
12	C0	81	ASN
12	C0	82	LEU
13	C1	8	GLN
13	C1	21	ASN
13	C1	29	LYS
13	C1	36	LYS
13	C1	40	LEU
13	C1	43	LYS
13	C1	44	THR

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Mol	Chain	Res	Type
13	C1	56	LYS
13	C1	67	ARG
13	C1	69	LYS
13	C1	70	ILE
13	C1	75	VAL
13	C1	76	VAL
13	C1	80	MET
13	C1	83	THR
13	C1	87	ARG
13	C1	99	ARG
13	C1	117	VAL
13	C1	118	GLN
13	C1	128	CYS
13	C1	136	ARG
13	C1	140	VAL
14	C2	28	LEU
14	C2	36	LEU
14	C2	37	VAL
14	C2	41	LEU
14	C2	43	ARG
14	C2	46	ARG
14	C2	50	LYS
14	C2	54	ARG
14	C2	61	VAL
14	C2	66	VAL
14	C2	71	ILE
14	C2	74	LEU
14	C2	86	VAL
14	C2	89	ILE
14	C2	103	LEU
14	C2	119	SER
14	C2	121	VAL
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	133	LEU
14	C2	139	HIS
15	C3	3	ARG
15	C3	9	LYS
15	C3	16	ILE
15	C3	27	LYS
15	C3	30	SER

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Mol	Chain	Res	Type
15	C3	34	ILE
15	C3	37	ILE
15	C3	39	LYS
15	C3	42	ARG
15	C3	45	LEU
15	C3	46	THR
15	C3	56	ASP
15	C3	64	ARG
15	C3	66	ILE
15	C3	76	LYS
15	C3	83	GLU
15	C3	86	GLU
15	C3	88	LEU
15	C3	102	LEU
15	C3	114	ARG
15	C3	115	LEU
15	C3	125	LEU
15	C3	127	ARG
15	C3	134	VAL
15	C3	140	LYS
15	C3	142	GLU
15	C3	143	SER
16	C4	13	VAL
16	C4	16	VAL
16	C4	20	TYR
16	C4	24	ASN
16	C4	26	THR
16	C4	29	HIS
16	C4	30	VAL
16	C4	39	ILE
16	C4	43	THR
16	C4	51	ASP
16	C4	76	ILE
16	C4	81	VAL
16	C4	92	LYS
16	C4	102	LEU
16	C4	103	ARG
16	C4	108	SER
16	C4	119	THR
16	C4	123	SER
16	C4	125	SER
16	C4	136	ARG

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Mol	Chain	Res	Type
16	C4	137	LEU
17	C5	20	VAL
17	C5	22	LEU
17	C5	23	GLU
17	C5	31	GLU
17	C5	34	VAL
17	C5	36	LEU
17	C5	43	ARG
17	C5	44	ARG
17	C5	47	ARG
17	C5	50	THR
17	C5	52	LYS
17	C5	60	LEU
17	C5	89	MET
17	C5	90	ILE
17	C5	92	SER
17	C5	106	GLU
17	C5	107	ILE
17	C5	110	GLU
17	C5	121	ILE
17	C5	124	THR
17	C5	125	PRO
18	C6	4	VAL
18	C6	6	SER
18	C6	8	GLN
18	C6	14	LYS
18	C6	32	ASN
18	C6	39	VAL
18	C6	40	GLU
18	C6	43	ILE
18	C6	44	LEU
18	C6	52	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	58	ASP
18	C6	63	ILE
18	C6	66	ARG
18	C6	69	VAL
18	C6	70	THR
18	C6	98	ASP
18	C6	104	GLU
18	C6	106	LYS

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Mol	Chain	Res	Type
18	C6	114	ARG
18	C6	117	LEU
18	C6	118	ILE
18	C6	123	ARG
18	C6	128	LYS
18	C6	137	ARG
18	C6	138	PHE
18	C6	143	ARG
19	C7	3	ARG
19	C7	5	ARG
19	C7	25	THR
19	C7	30	THR
19	C7	38	ILE
19	C7	46	LEU
19	C7	48	ASN
19	C7	49	LYS
19	C7	62	GLN
19	C7	69	ILE
19	C7	72	LYS
19	C7	84	TYR
19	C7	87	GLU
19	C7	88	VAL
19	C7	105	GLN
19	C7	107	SER
19	C7	113	LEU
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	7	GLU
20	C8	8	GLN
20	C8	11	PHE
20	C8	12	GLN
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	17	LEU
20	C8	20	THR
20	C8	25	ASN
20	C8	28	ILE
20	C8	40	ARG
20	C8	46	VAL

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Mol	Chain	Res	Type
20	C8	57	ARG
20	C8	60	GLU
20	C8	61	LEU
20	C8	77	THR
20	C8	80	LYS
20	C8	85	PHE
20	C8	86	LEU
20	C8	88	ARG
20	C8	92	ILE
20	C8	93	THR
20	C8	97	ASP
20	C8	104	ASN
20	C8	108	LYS
20	C8	132	ARG
20	C8	136	GLN
20	C8	140	THR
20	C8	143	ARG
21	C9	6	VAL
21	C9	8	ASP
21	C9	13	ASP
21	C9	18	TYR
21	C9	22	LEU
21	C9	27	LYS
21	C9	28	LEU
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	39	THR
21	C9	41	SER
21	C9	51	GLU
21	C9	57	ARG
21	C9	60	SER
21	C9	63	ARG
21	C9	67	MET
21	C9	68	ARG
21	C9	71	VAL
21	C9	79	LEU
21	C9	89	ARG
21	C9	99	SER
21	C9	100	ILE
21	C9	116	ILE

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Mol	Chain	Res	Type
21	C9	122	ARG
21	C9	130	ARG
21	C9	131	ASP
21	C9	132	LEU
21	C9	133	ASP
21	C9	134	ARG
21	C9	144	GLU
22	D0	15	GLN
22	D0	18	GLN
22	D0	23	ARG
22	D0	27	THR
22	D0	31	VAL
22	D0	47	GLN
22	D0	51	VAL
22	D0	57	ARG
22	D0	58	LEU
22	D0	61	LYS
22	D0	62	VAL
22	D0	67	THR
22	D0	74	GLU
22	D0	89	ARG
22	D0	103	ILE
22	D0	105	GLN
22	D0	108	ILE
23	D1	7	GLN
23	D1	9	VAL
23	D1	11	LEU
23	D1	12	TYR
23	D1	18	SER
23	D1	33	GLN
23	D1	36	VAL
23	D1	41	GLU
23	D1	52	THR
23	D1	56	SER
23	D1	68	SER
23	D1	69	LEU
23	D1	78	LEU
23	D1	80	LYS
23	D1	82	VAL
24	D2	12	ASN
24	D2	15	ASN
24	D2	22	LYS

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Mol	Chain	Res	Type
24	D2	24	GLN
24	D2	25	VAL
24	D2	26	LEU
24	D2	27	ILE
24	D2	29	PRO
24	D2	53	ILE
24	D2	56	HIS
24	D2	65	LEU
24	D2	68	ARG
24	D2	78	ARG
24	D2	81	VAL
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	126	LEU
24	D2	129	VAL
25	D3	7	ARG
25	D3	9	LEU
25	D3	14	LYS
25	D3	19	ARG
25	D3	33	LEU
25	D3	41	SER
25	D3	47	SER
25	D3	59	ILE
25	D3	69	ARG
25	D3	72	VAL
25	D3	78	LYS
25	D3	82	LYS
25	D3	84	THR
25	D3	103	LEU
25	D3	107	PHE
25	D3	109	ARG
25	D3	110	LYS
25	D3	114	LYS
25	D3	117	ILE
25	D3	138	GLU
25	D3	144	ARG
26	D4	20	ARG
26	D4	21	LYS

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Mol	Chain	Res	Type
26	D4	27	VAL
26	D4	28	LEU
26	D4	29	HIS
26	D4	32	ARG
26	D4	34	ASN
26	D4	36	SER
26	D4	40	LEU
26	D4	41	ARG
26	D4	51	GLU
26	D4	57	VAL
26	D4	62	THR
26	D4	74	LEU
26	D4	84	LYS
26	D4	96	LEU
26	D4	99	LYS
26	D4	102	LYS
26	D4	124	ARG
26	D4	127	LYS
27	D5	37	GLN
27	D5	38	HIS
27	D5	58	ARG
27	D5	69	LEU
27	D5	71	ILE
27	D5	92	ILE
27	D5	93	SER
27	D5	95	HIS
27	D5	96	SER
27	D5	100	ILE
27	D5	105	THR
28	D6	4	LYS
28	D6	36	ILE
28	D6	41	ILE
28	D6	44	ILE
28	D6	58	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	66	LYS
28	D6	70	LYS
28	D6	71	LEU
28	D6	82	ARG
28	D6	83	ILE
28	D6	84	VAL

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Mol	Chain	Res	Type
28	D6	85	ARG
28	D6	86	VAL
28	D6	88	SER
28	D6	90	GLU
29	D7	3	LEU
29	D7	4	VAL
29	D7	20	LYS
29	D7	29	ARG
29	D7	33	LEU
29	D7	36	LYS
29	D7	42	ASN
29	D7	55	THR
29	D7	56	CYS
29	D7	61	THR
29	D7	62	ILE
29	D7	63	LEU
29	D7	67	THR
29	D7	74	SER
29	D7	75	GLU
30	D8	13	ILE
30	D8	19	THR
30	D8	22	ARG
30	D8	32	PHE
30	D8	33	LEU
30	D8	34	GLU
30	D8	36	THR
30	D8	37	SER
30	D8	39	THR
30	D8	44	VAL
30	D8	49	ARG
30	D8	51	ASN
30	D8	52	ASP
30	D8	54	LEU
30	D8	57	MET
30	D8	58	GLU
31	D9	7	TRP
31	D9	19	ARG
31	D9	22	ARG
31	D9	30	LEU
31	D9	32	ARG
31	D9	36	LEU
32	E0	3	LYS

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Mol	Chain	Res	Type
32	E0	8	LEU
32	E0	20	LYS
32	E0	28	LYS
32	E0	41	THR
32	E0	42	ARG
32	E0	47	VAL
32	E0	48	THR
32	E0	50	VAL
33	E1	82	LYS
33	E1	83	LYS
33	E1	84	VAL
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
33	E1	103	LEU
33	E1	108	VAL
33	E1	109	ASP
33	E1	113	LYS
33	E1	115	THR
33	E1	119	ARG
33	E1	120	GLU
33	E1	126	CYS
33	E1	137	ASP
33	E1	146	SER
34	SR	6	VAL
34	SR	7	LEU
34	SR	9	LEU
34	SR	12	THR
34	SR	29	GLN
34	SR	48	THR
34	SR	50	ASP
34	SR	52	GLN
34	SR	60	SER
34	SR	69	GLN
34	SR	71	CYS
34	SR	72	THR
34	SR	76	ASP
34	SR	82	SER
34	SR	88	THR
34	SR	96	THR
34	SR	102	ARG

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Mol	Chain	Res	Type
34	SR	108	SER
34	SR	116	ASP
34	SR	117	LYS
34	SR	136	ILE
34	SR	144	LEU
34	SR	145	LEU
34	SR	153	GLN
34	SR	165	ASP
34	SR	188	ILE
34	SR	191	ASP
34	SR	200	ASN
34	SR	202	LEU
34	SR	213	SER
34	SR	221	MET
34	SR	222	LEU
34	SR	231	MET
34	SR	232	TYR
34	SR	238	ASP
34	SR	241	PHE
34	SR	248	ASN
34	SR	266	ASP
34	SR	268	GLN
34	SR	277	GLU
34	SR	300	THR
34	SR	310	ILE
34	SR	312	VAL
34	SR	314	GLN
34	SR	316	MET
34	SR	317	THR
35	SM	24	GLU
35	SM	45	SER
35	SM	48	ARG
35	SM	50	ASN
35	SM	51	ARG
35	SM	53	ARG
35	SM	64	LYS
35	SM	69	ARG
35	SM	72	ARG
35	SM	77	THR
35	SM	84	LYS
35	SM	89	ARG
35	SM	97	THR

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Mol	Chain	Res	Type
35	SM	100	THR
35	SM	101	ASP
35	SM	105	LYS
35	SM	121	LYS
35	SM	139	GLU
39	L2	14	SER
39	L2	20	THR
39	L2	31	THR
39	L2	32	LEU
39	L2	41	ILE
39	L2	44	ILE
39	L2	45	VAL
39	L2	46	LYS
39	L2	70	ARG
39	L2	74	GLU
39	L2	82	VAL
39	L2	84	THR
39	L2	96	LEU
39	L2	97	ASN
39	L2	101	VAL
39	L2	104	LEU
39	L2	107	VAL
39	L2	109	GLU
39	L2	116	VAL
39	L2	122	ASP
39	L2	137	ILE
39	L2	139	HIS
39	L2	142	ASP
39	L2	143	GLU
39	L2	148	VAL
39	L2	152	SER
39	L2	157	VAL
39	L2	160	SER
39	L2	165	VAL
39	L2	179	LEU
39	L2	180	LEU
39	L2	181	LYS
39	L2	198	LYS
39	L2	202	VAL
39	L2	204	MET
39	L2	207	VAL
39	L2	227	ARG

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Mol	Chain	Res	Type
39	L2	230	VAL
39	L2	241	ARG
39	L2	245	LEU
40	L3	2	SER
40	L3	7	GLU
40	L3	17	LEU
40	L3	19	ARG
40	L3	21	ARG
40	L3	24	SER
40	L3	25	ILE
40	L3	30	LYS
40	L3	37	ARG
40	L3	47	LEU
40	L3	67	PHE
40	L3	79	VAL
40	L3	81	THR
40	L3	84	VAL
40	L3	85	VAL
40	L3	100	ARG
40	L3	103	THR
40	L3	112	ASP
40	L3	114	VAL
40	L3	116	ARG
40	L3	134	SER
40	L3	139	GLN
40	L3	144	ILE
40	L3	146	ARG
40	L3	148	LEU
40	L3	150	ARG
40	L3	156	SER
40	L3	160	VAL
40	L3	164	THR
40	L3	169	THR
40	L3	187	SER
40	L3	188	ILE
40	L3	192	VAL
40	L3	196	ARG
40	L3	200	GLU
40	L3	205	VAL
40	L3	216	ASP
40	L3	229	VAL
40	L3	232	ARG

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Mol	Chain	Res	Type
40	L3	235	THR
40	L3	236	LYS
40	L3	237	LYS
40	L3	238	LEU
40	L3	252	ILE
40	L3	274	SER
40	L3	284	ARG
40	L3	296	THR
40	L3	300	ARG
40	L3	305	ILE
40	L3	312	VAL
40	L3	328	ILE
40	L3	332	ARG
40	L3	333	LYS
40	L3	338	LEU
40	L3	347	SER
40	L3	354	VAL
40	L3	355	SER
40	L3	367	LYS
40	L3	371	GLN
40	L3	382	THR
41	L4	37	THR
41	L4	41	SER
41	L4	44	LYS
41	L4	74	ILE
41	L4	93	MET
41	L4	112	LYS
41	L4	124	SER
41	L4	133	SER
41	L4	138	ARG
41	L4	144	LYS
41	L4	145	ILE
41	L4	148	ILE
41	L4	150	LEU
41	L4	156	LEU
41	L4	160	GLN
41	L4	170	LYS
41	L4	179	LEU
41	L4	182	LEU
41	L4	185	LYS
41	L4	187	LEU
41	L4	188	ARG

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Mol	Chain	Res	Type
41	L4	193	LYS
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	206	LEU
41	L4	220	ARG
41	L4	222	VAL
41	L4	223	PRO
41	L4	230	VAL
41	L4	252	GLU
41	L4	255	PHE
41	L4	258	LEU
41	L4	270	SER
41	L4	284	SER
41	L4	287	THR
41	L4	289	ILE
41	L4	306	THR
41	L4	307	GLN
41	L4	311	HIS
41	L4	322	GLN
41	L4	323	VAL
41	L4	327	LEU
41	L4	332	LYS
41	L4	333	VAL
41	L4	349	THR
41	L4	354	VAL
42	L5	4	GLN
42	L5	5	LYS
42	L5	9	SER
42	L5	22	ARG
42	L5	23	ARG
42	L5	35	ARG
42	L5	36	LEU
42	L5	41	LYS
42	L5	66	SER
42	L5	69	ILE
42	L5	75	LEU
42	L5	85	ARG
42	L5	95	TRP
42	L5	105	ILE
42	L5	110	LEU
42	L5	112	LYS

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Mol	Chain	Res	Type
42	L5	115	LEU
42	L5	118	THR
42	L5	122	VAL
42	L5	131	LEU
42	L5	137	ASP
42	L5	140	ARG
42	L5	146	LEU
42	L5	148	ILE
42	L5	151	GLN
42	L5	152	ARG
42	L5	155	THR
42	L5	158	ARG
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE
42	L5	193	GLU
42	L5	205	SER
42	L5	231	ILE
42	L5	232	ASP
42	L5	236	LEU
42	L5	237	GLU
42	L5	254	LYS
42	L5	257	GLU
42	L5	259	LYS
42	L5	263	GLU
42	L5	273	ARG
42	L5	275	THR
42	L5	279	LYS
42	L5	293	LEU
43	L6	5	LYS
43	L6	21	THR
43	L6	29	LYS
43	L6	31	ARG
43	L6	35	VAL
43	L6	41	ILE
43	L6	46	ARG
43	L6	64	LEU
43	L6	65	ILE
43	L6	78	ARG
43	L6	84	VAL
43	L6	89	THR
43	L6	90	LYS

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Mol	Chain	Res	Type
43	L6	93	VAL
43	L6	109	GLU
43	L6	129	GLU
43	L6	146	ILE
43	L6	152	THR
43	L6	154	LEU
43	L6	155	LEU
43	L6	170	LYS
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	56	GLU
44	L7	59	GLU
44	L7	77	VAL
44	L7	82	LYS
44	L7	83	LEU
44	L7	89	ILE
44	L7	92	ILE
44	L7	93	ASN
44	L7	98	LYS
44	L7	101	LYS
44	L7	111	ILE
44	L7	113	SER
44	L7	118	LYS
44	L7	124	LEU
44	L7	164	SER
44	L7	179	LEU
44	L7	184	LEU
44	L7	211	SER
44	L7	228	SER
44	L7	229	PHE
44	L7	239	LEU
45	L8	26	LEU
45	L8	27	THR
45	L8	50	VAL
45	L8	57	ARG
45	L8	63	LYS
45	L8	66	SER
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	81	THR

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Mol	Chain	Res	Type
45	L8	83	ASP
45	L8	84	ARG
45	L8	92	LYS
45	L8	98	ARG
45	L8	106	LYS
45	L8	118	GLU
45	L8	132	VAL
45	L8	136	LEU
45	L8	149	LYS
45	L8	156	ASP
45	L8	157	VAL
45	L8	160	ILE
45	L8	169	LEU
45	L8	172	LYS
45	L8	173	MET
45	L8	181	LYS
45	L8	185	ARG
45	L8	189	LEU
45	L8	202	GLU
45	L8	204	ARG
45	L8	206	GLU
45	L8	208	GLU
45	L8	221	ASN
45	L8	238	LEU
45	L8	247	ASP
45	L8	248	LYS
46	L9	1	MET
46	L9	5	GLN
46	L9	6	THR
46	L9	14	GLU
46	L9	18	VAL
46	L9	19	SER
46	L9	21	LYS
46	L9	33	THR
46	L9	34	LEU
46	L9	41	ILE
46	L9	44	THR
46	L9	48	VAL
46	L9	52	LEU
46	L9	62	ARG
46	L9	68	LEU
46	L9	69	ARG

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Mol	Chain	Res	Type
46	L9	70	THR
46	L9	72	LYS
46	L9	73	SER
46	L9	82	VAL
46	L9	110	LYS
46	L9	118	LEU
46	L9	124	ARG
46	L9	139	ASN
46	L9	147	SER
46	L9	152	GLU
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	163	GLN
46	L9	164	ILE
46	L9	166	ARG
46	L9	172	ILE
46	L9	173	ARG
46	L9	177	ASP
46	L9	189	GLU
47	M0	12	GLN
47	M0	24	ARG
47	M0	26	VAL
47	M0	28	ASP
47	M0	30	LYS
47	M0	31	ILE
47	M0	32	ARG
47	M0	33	ILE
47	M0	36	LEU
47	M0	40	LYS
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	53	VAL
47	M0	63	GLU
47	M0	74	LYS
47	M0	87	LEU
47	M0	99	ILE
47	M0	102	MET
47	M0	128	ARG
47	M0	130	ASP
47	M0	131	ILE

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Mol	Chain	Res	Type
47	M0	133	GLN
47	M0	138	VAL
47	M0	139	ARG
47	M0	142	ASP
47	M0	143	SER
47	M0	154	ARG
47	M0	156	ARG
47	M0	163	GLN
47	M0	165	ILE
47	M0	167	LEU
47	M0	168	SER
47	M0	174	THR
47	M0	175	ASN
47	M0	177	ASP
47	M0	193	ASP
47	M0	200	LEU
47	M0	203	LYS
47	M0	207	GLU
47	M0	209	ASN
48	M1	10	ARG
48	M1	11	ASP
48	M1	12	LEU
48	M1	13	LYS
48	M1	28	ASP
48	M1	31	THR
48	M1	34	SER
48	M1	40	LEU
48	M1	44	THR
48	M1	46	VAL
48	M1	52	TYR
48	M1	64	LYS
48	M1	65	ILE
48	M1	71	VAL
48	M1	80	LEU
48	M1	92	ARG
48	M1	94	ARG
48	M1	106	ILE
48	M1	107	ASP
48	M1	110	ILE
48	M1	112	LEU
48	M1	115	LYS
48	M1	125	MET

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Mol	Chain	Res	Type
48	M1	127	PHE
48	M1	137	ARG
48	M1	138	VAL
48	M1	140	ARG
48	M1	142	LYS
48	M1	145	LYS
48	M1	155	THR
48	M1	166	LYS
48	M1	173	ASP
49	M3	23	LYS
49	M3	24	VAL
49	M3	34	SER
49	M3	46	ILE
49	M3	54	LEU
49	M3	55	ARG
49	M3	57	VAL
49	M3	59	ARG
49	M3	67	ARG
49	M3	69	VAL
49	M3	70	ARG
49	M3	104	ARG
49	M3	107	GLU
49	M3	108	ILE
49	M3	114	GLN
49	M3	121	SER
49	M3	124	ILE
49	M3	128	ARG
49	M3	131	LYS
49	M3	136	GLU
49	M3	138	VAL
49	M3	147	ILE
49	M3	164	GLU
49	M3	168	ARG
49	M3	171	ARG
49	M3	176	GLU
49	M3	182	ILE
49	M3	186	ARG
49	M3	190	LYS
49	M3	194	GLU
50	M4	5	SER
50	M4	15	VAL
50	M4	20	VAL

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Mol	Chain	Res	Type
50	M4	25	LYS
50	M4	27	GLN
50	M4	38	ILE
50	M4	53	VAL
50	M4	62	GLN
50	M4	63	VAL
50	M4	64	VAL
50	M4	69	THR
50	M4	72	LEU
50	M4	83	LYS
50	M4	90	VAL
50	M4	91	CYS
50	M4	102	LYS
50	M4	108	ARG
50	M4	126	GLN
50	M4	135	LEU
51	M5	7	LEU
51	M5	13	LYS
51	M5	18	VAL
51	M5	38	ARG
51	M5	62	TYR
51	M5	68	ARG
51	M5	71	ARG
51	M5	80	THR
51	M5	83	LYS
51	M5	85	THR
51	M5	96	ARG
51	M5	97	SER
51	M5	106	VAL
51	M5	109	ARG
51	M5	113	LEU
51	M5	117	ASN
51	M5	133	ILE
51	M5	151	ILE
51	M5	153	ASP
51	M5	155	VAL
51	M5	159	ARG
51	M5	183	THR
51	M5	184	LYS
51	M5	197	LEU
51	M5	198	SER
51	M5	199	LEU

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Mol	Chain	Res	Type
51	M5	201	ARG
52	M6	22	VAL
52	M6	33	ILE
52	M6	41	LEU
52	M6	51	LYS
52	M6	58	LEU
52	M6	67	THR
52	M6	68	ARG
52	M6	74	ARG
52	M6	78	ARG
52	M6	85	ARG
52	M6	89	SER
52	M6	106	GLU
52	M6	110	PRO
52	M6	114	LYS
52	M6	116	LYS
52	M6	117	ARG
52	M6	122	GLN
52	M6	124	LEU
52	M6	128	ARG
52	M6	134	LYS
52	M6	143	THR
52	M6	160	ARG
52	M6	163	SER
52	M6	180	SER
52	M6	189	ASP
52	M6	190	VAL
53	M7	3	ARG
53	M7	7	THR
53	M7	9	THR
53	M7	24	VAL
53	M7	32	THR
53	M7	36	ILE
53	M7	49	GLU
53	M7	52	LEU
53	M7	53	ASP
53	M7	54	HIS
53	M7	56	ARG
53	M7	67	ILE
53	M7	78	VAL
53	M7	119	VAL
53	M7	126	ARG

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Mol	Chain	Res	Type
53	M7	127	ARG
53	M7	128	ARG
53	M7	129	THR
53	M7	142	SER
53	M7	144	SER
53	M7	146	ILE
53	M7	168	LEU
53	M7	171	ARG
53	M7	173	ARG
53	M7	180	LYS
53	M7	181	ARG
54	M8	3	ILE
54	M8	11	LYS
54	M8	17	THR
54	M8	22	ASP
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	41	ASP
54	M8	49	LEU
54	M8	50	LYS
54	M8	63	SER
54	M8	64	VAL
54	M8	67	ILE
54	M8	73	GLN
54	M8	81	VAL
54	M8	86	THR
54	M8	100	THR
54	M8	105	ARG
54	M8	127	LEU
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	146	SER
54	M8	147	ARG
54	M8	159	LYS
54	M8	179	ARG
54	M8	180	ARG
55	M9	10	LEU
55	M9	13	SER
55	M9	31	GLU
55	M9	41	ILE

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Mol	Chain	Res	Type
55	M9	49	THR
55	M9	55	VAL
55	M9	72	GLU
55	M9	74	ARG
55	M9	86	GLU
55	M9	91	SER
55	M9	98	ARG
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	110	ARG
55	M9	115	ILE
55	M9	134	HIS
55	M9	138	LEU
55	M9	155	LEU
55	M9	175	GLN
55	M9	177	VAL
55	M9	180	LYS
55	M9	182	ASP
56	N0	8	GLN
56	N0	12	ARG
56	N0	13	ARG
56	N0	40	ARG
56	N0	45	LEU
56	N0	47	LYS
56	N0	51	VAL
56	N0	58	ILE
56	N0	80	ARG
56	N0	81	TYR
56	N0	87	THR
56	N0	88	HIS
56	N0	92	LYS
56	N0	97	VAL
56	N0	104	GLU
56	N0	106	LEU
56	N0	115	ARG
56	N0	117	ARG
56	N0	123	ILE
56	N0	129	ILE
56	N0	131	LYS
56	N0	137	ARG
56	N0	138	GLN

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Mol	Chain	Res	Type
56	N0	145	THR
56	N0	149	LYS
56	N0	155	ARG
56	N0	156	VAL
56	N0	162	THR
56	N0	169	SER
56	N0	171	PHE
56	N0	172	TYR
57	N1	12	ARG
57	N1	25	VAL
57	N1	26	HIS
57	N1	27	LEU
57	N1	36	VAL
57	N1	43	LYS
57	N1	68	THR
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	80	VAL
57	N1	83	ARG
57	N1	87	LYS
57	N1	88	ARG
57	N1	89	LEU
57	N1	96	ILE
57	N1	103	GLN
57	N1	104	GLU
57	N1	118	GLU
57	N1	120	LYS
57	N1	124	VAL
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	131	GLN
57	N1	136	ARG
57	N1	139	ARG
57	N1	143	THR
57	N1	146	ASN
57	N1	149	GLN
57	N1	158	THR
57	N1	160	ILE
58	N2	10	LYS
58	N2	14	THR

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Mol	Chain	Res	Type
58	N2	16	THR
58	N2	39	ASP
58	N2	43	VAL
58	N2	50	LEU
58	N2	52	ASN
58	N2	56	VAL
58	N2	66	VAL
58	N2	74	LYS
58	N2	82	LYS
58	N2	88	GLN
58	N2	93	ILE
58	N2	98	THR
58	N2	105	LEU
59	N3	12	ARG
59	N3	13	ILE
59	N3	32	ARG
59	N3	33	ASN
59	N3	40	LYS
59	N3	45	ARG
59	N3	48	ARG
59	N3	54	LEU
59	N3	64	LYS
59	N3	69	LEU
59	N3	72	LYS
59	N3	73	VAL
59	N3	74	MET
59	N3	83	LYS
59	N3	102	ILE
59	N3	120	LYS
59	N3	128	ARG
59	N3	135	VAL
59	N3	137	VAL
60	N4	4	GLU
60	N4	5	ILE
60	N4	19	THR
60	N4	30	ARG
60	N4	39	LEU
60	N4	42	GLN
60	N4	45	ASN
60	N4	47	ARG
60	N4	54	LEU
60	N4	64	THR

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Mol	Chain	Res	Type
61	N5	27	ARG
61	N5	37	THR
61	N5	38	LEU
61	N5	39	LYS
61	N5	48	SER
61	N5	63	ILE
61	N5	71	THR
61	N5	75	LYS
61	N5	92	LYS
61	N5	108	LEU
61	N5	111	ASN
61	N5	115	ARG
61	N5	125	ARG
61	N5	133	LEU
61	N5	135	ILE
61	N5	139	ILE
62	N6	3	LYS
62	N6	13	ARG
62	N6	37	LYS
62	N6	38	GLU
62	N6	45	ILE
62	N6	50	ILE
62	N6	51	ARG
62	N6	56	VAL
62	N6	57	LEU
62	N6	64	LYS
62	N6	66	GLN
62	N6	74	TYR
62	N6	76	LEU
62	N6	83	ASP
62	N6	88	GLU
62	N6	94	SER
62	N6	105	VAL
62	N6	111	LEU
62	N6	115	ARG
62	N6	122	LYS
62	N6	125	LYS
62	N6	126	LEU
63	N7	14	VAL
63	N7	24	VAL
63	N7	25	ILE
63	N7	26	VAL

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Mol	Chain	Res	Type
63	N7	30	ASP
63	N7	34	LYS
63	N7	46	ILE
63	N7	52	LYS
63	N7	53	VAL
63	N7	54	THR
63	N7	57	HIS
63	N7	64	LYS
63	N7	75	VAL
63	N7	83	THR
63	N7	86	THR
63	N7	87	LEU
63	N7	99	GLU
63	N7	107	ARG
63	N7	134	LEU
64	N8	3	SER
64	N8	4	ARG
64	N8	8	THR
64	N8	10	LYS
64	N8	16	SER
64	N8	19	LYS
64	N8	34	MET
64	N8	42	ARG
64	N8	43	ILE
64	N8	46	ASP
64	N8	47	LYS
64	N8	60	TYR
64	N8	65	GLN
64	N8	73	LEU
64	N8	76	ASP
64	N8	78	LEU
64	N8	85	ASP
64	N8	88	ASP
64	N8	91	LEU
64	N8	98	THR
64	N8	115	LYS
64	N8	117	ARG
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
64	N8	135	GLU
64	N8	139	ARG

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Mol	Chain	Res	Type
64	N8	146	GLU
65	N9	13	THR
65	N9	14	ARG
65	N9	18	ARG
65	N9	22	LYS
65	N9	23	LYS
65	N9	25	LYS
65	N9	38	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	10	ILE
66	O0	12	GLN
66	O0	16	LEU
66	O0	18	ILE
66	O0	22	LYS
66	O0	36	GLN
66	O0	42	ILE
66	O0	50	VAL
66	O0	54	SER
66	O0	61	MET
66	O0	66	LYS
66	O0	71	GLN
66	O0	76	GLU
66	O0	83	LYS
66	O0	84	LEU
66	O0	93	LEU
66	O0	100	ILE
66	O0	101	LEU
66	O0	102	THR
67	O1	6	ASP
67	O1	16	LEU
67	O1	26	LYS
67	O1	31	ARG
67	O1	41	LYS
67	O1	46	THR
67	O1	55	LEU
67	O1	57	GLN
67	O1	64	VAL
67	O1	68	GLU
67	O1	79	ARG
67	O1	84	ASP
67	O1	86	LYS

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Mol	Chain	Res	Type
67	O1	89	LEU
67	O1	96	VAL
67	O1	102	LYS
67	O1	104	LEU
68	O2	3	SER
68	O2	12	LYS
68	O2	19	ARG
68	O2	27	ARG
68	O2	31	ASN
68	O2	33	ARG
68	O2	34	LYS
68	O2	35	GLN
68	O2	41	VAL
68	O2	44	ARG
68	O2	51	SER
68	O2	52	GLN
68	O2	54	LYS
68	O2	61	LYS
68	O2	66	LEU
68	O2	67	SER
68	O2	73	THR
68	O2	75	LEU
68	O2	82	LEU
68	O2	84	THR
68	O2	91	THR
68	O2	109	LEU
68	O2	111	ARG
68	O2	118	LYS
68	O2	125	ARG
68	O2	126	LEU
68	O2	128	LEU
69	O3	15	SER
69	O3	21	ARG
69	O3	28	SER
69	O3	31	LYS
69	O3	33	GLU
69	O3	37	THR
69	O3	49	ILE
69	O3	54	ARG
69	O3	59	VAL
69	O3	70	LYS
69	O3	80	VAL

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Mol	Chain	Res	Type
69	O3	81	VAL
69	O3	98	VAL
69	O3	105	SER
69	O3	106	ASN
70	O4	8	ARG
70	O4	16	ARG
70	O4	20	ILE
70	O4	21	LYS
70	O4	24	LYS
70	O4	29	ILE
70	O4	31	ARG
70	O4	49	SER
70	O4	58	ARG
70	O4	65	VAL
70	O4	71	THR
70	O4	72	VAL
70	O4	79	SER
70	O4	80	ARG
70	O4	81	CYS
70	O4	86	LYS
70	O4	101	VAL
70	O4	102	LYS
70	O4	104	VAL
71	O5	15	GLU
71	O5	21	LEU
71	O5	22	VAL
71	O5	27	GLU
71	O5	38	ARG
71	O5	47	VAL
71	O5	48	ARG
71	O5	49	LYS
71	O5	50	SER
71	O5	62	GLN
71	O5	64	GLU
71	O5	71	LYS
71	O5	73	LYS
71	O5	74	LYS
71	O5	76	GLN
71	O5	81	ARG
71	O5	89	ARG
71	O5	90	ARG
71	O5	93	THR

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Mol	Chain	Res	Type
71	O5	96	GLU
71	O5	102	GLU
71	O5	104	GLN
71	O5	105	ARG
71	O5	107	LYS
71	O5	119	LYS
72	O6	18	THR
72	O6	21	THR
72	O6	26	ILE
72	O6	36	ARG
72	O6	42	SER
72	O6	45	ARG
72	O6	52	PRO
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	64	SER
72	O6	67	LYS
72	O6	68	ARG
72	O6	70	ARG
72	O6	72	VAL
72	O6	76	ARG
72	O6	81	THR
72	O6	84	LYS
72	O6	88	GLU
72	O6	90	MET
72	O6	98	ARG
73	O7	5	THR
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	36	SER
73	O7	44	THR
73	O7	55	ARG
73	O7	59	THR
73	O7	65	ARG
73	O7	67	LEU
73	O7	79	GLN
73	O7	80	THR
74	O8	4	GLU
74	O8	5	ILE

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Mol	Chain	Res	Type
74	O8	6	THR
74	O8	8	ILE
74	O8	12	LEU
74	O8	13	GLU
74	O8	20	VAL
74	O8	22	THR
74	O8	31	LEU
74	O8	32	ASN
74	O8	45	VAL
74	O8	46	ARG
74	O8	53	THR
74	O8	64	LYS
74	O8	65	LEU
74	O8	68	SER
74	O8	77	ARG
74	O8	78	LEU
75	O9	4	GLN
75	O9	5	LYS
75	O9	21	ARG
75	O9	23	LEU
75	O9	28	ARG
75	O9	29	LEU
75	O9	30	ARG
75	O9	32	ASN
75	O9	42	ARG
75	O9	45	ARG
75	O9	51	ILE
76	Q0	77	ILE
76	Q0	78	ILE
76	Q0	80	PRO
76	Q0	85	LEU
76	Q0	92	ASP
76	Q0	108	THR
76	Q0	110	CYS
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	117	HIS
76	Q0	127	LEU
77	Q1	2	ARG
77	Q1	10	THR
77	Q1	14	LYS

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Mol	Chain	Res	Type
77	Q1	15	ARG
78	Q2	7	THR
78	Q2	12	CYS
78	Q2	13	LYS
78	Q2	19	LYS
78	Q2	21	THR
78	Q2	26	THR
78	Q2	35	LEU
78	Q2	47	GLN
78	Q2	55	LYS
78	Q2	61	LYS
78	Q2	71	ARG
78	Q2	75	VAL
78	Q2	76	LYS
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	88	CYS
78	Q2	92	GLU
78	Q2	93	LEU
78	Q2	97	LYS
78	Q2	100	LYS
78	Q2	104	LEU
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	25	GLN
79	Q3	32	GLN
79	Q3	40	SER
79	Q3	45	LYS
79	Q3	49	ARG
79	Q3	56	THR
79	Q3	60	CYS
79	Q3	70	THR
79	Q3	84	ARG
79	Q3	91	GLU
2	s0	9	LEU
2	s0	12	GLU
2	s0	18	LEU
2	s0	22	THR
2	s0	29	VAL
2	s0	30	GLN
2	s0	31	VAL

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Mol	Chain	Res	Type
2	s0	34	GLU
2	s0	41	ARG
2	s0	43	ASP
2	s0	45	VAL
2	s0	47	VAL
2	s0	50	VAL
2	s0	59	LEU
2	s0	62	ARG
2	s0	83	GLN
2	s0	87	LEU
2	s0	96	THR
2	s0	101	ARG
2	s0	103	THR
2	s0	106	SER
2	s0	110	TYR
2	s0	112	THR
2	s0	119	ARG
2	s0	124	THR
2	s0	131	GLN
2	s0	141	ILE
2	s0	144	ILE
2	s0	154	GLU
2	s0	157	ASP
2	s0	169	SER
2	s0	172	LEU
2	s0	179	ARG
2	s0	183	ARG
2	s0	185	ARG
2	s0	189	VAL
2	s0	198	MET
2	s0	202	TYR
3	s1	21	VAL
3	s1	25	THR
3	s1	26	ARG
3	s1	47	LEU
3	s1	51	SER
3	s1	55	LYS
3	s1	56	SER
3	s1	61	LEU
3	s1	62	LYS
3	s1	70	LEU
3	s1	76	SER

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Mol	Chain	Res	Type
3	s1	77	GLU
3	s1	94	LYS
3	s1	96	LEU
3	s1	97	LEU
3	s1	105	PHE
3	s1	106	THR
3	s1	125	VAL
3	s1	126	THR
3	s1	129	THR
3	s1	137	ILE
3	s1	169	SER
3	s1	173	THR
3	s1	175	GLU
3	s1	180	THR
3	s1	181	LEU
3	s1	184	LEU
3	s1	193	ILE
3	s1	195	LYS
3	s1	197	ILE
3	s1	203	ASP
3	s1	212	VAL
3	s1	214	LYS
3	s1	215	VAL
3	s1	222	LYS
3	s1	223	PHE
3	s1	228	LEU
3	s1	231	LEU
3	s1	234	GLU
4	s2	41	LEU
4	s2	46	LYS
4	s2	53	ILE
4	s2	54	GLU
4	s2	55	GLU
4	s2	58	LEU
4	s2	69	ILE
4	s2	73	LEU
4	s2	81	MET
4	s2	83	ILE
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG

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Mol	Chain	Res	Type
4	s2	94	GLN
4	s2	95	ARG
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	113	LEU
4	s2	116	LYS
4	s2	117	THR
4	s2	130	ILE
4	s2	137	ILE
4	s2	141	ARG
4	s2	146	THR
4	s2	148	LEU
4	s2	150	GLN
4	s2	159	THR
4	s2	161	LYS
4	s2	164	SER
4	s2	166	THR
4	s2	170	ILE
4	s2	181	SER
4	s2	182	PRO
4	s2	194	GLU
4	s2	205	ARG
4	s2	206	THR
4	s2	207	LEU
4	s2	222	TYR
4	s2	224	PHE
4	s2	225	LEU
4	s2	229	LEU
4	s2	237	VAL
4	s2	240	LEU
4	s2	245	ASP
4	s2	250	GLN
5	s3	4	LEU
5	s3	9	ARG
5	s3	21	LEU
5	s3	26	THR
5	s3	37	VAL
5	s3	39	VAL
5	s3	44	THR
5	s3	53	THR
5	s3	59	LEU

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Mol	Chain	Res	Type
5	s3	61	GLU
5	s3	83	THR
5	s3	89	GLU
5	s3	90	ARG
5	s3	93	ASP
5	s3	94	ARG
5	s3	103	GLU
5	s3	111	ASN
5	s3	115	ILE
5	s3	124	ARG
5	s3	127	MET
5	s3	128	GLU
5	s3	135	GLU
5	s3	142	LEU
5	s3	143	ARG
5	s3	146	ARG
5	s3	158	ILE
5	s3	162	GLN
5	s3	164	VAL
5	s3	168	ILE
5	s3	170	THR
5	s3	181	VAL
5	s3	189	MET
5	s3	196	ARG
5	s3	202	LEU
5	s3	210	GLU
5	s3	212	LYS
5	s3	213	GLU
5	s3	218	LEU
5	s3	223	LYS
6	s4	6	LYS
6	s4	7	LYS
6	s4	9	LEU
6	s4	11	ARG
6	s4	23	LEU
6	s4	24	SER
6	s4	38	LEU
6	s4	42	LEU
6	s4	48	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	67	GLN

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Mol	Chain	Res	Type
6	s4	70	VAL
6	s4	78	THR
6	s4	102	VAL
6	s4	105	VAL
6	s4	108	ARG
6	s4	113	ARG
6	s4	123	LEU
6	s4	129	VAL
6	s4	131	LEU
6	s4	133	LYS
6	s4	148	ARG
6	s4	159	THR
6	s4	164	LEU
6	s4	176	ASP
6	s4	180	LEU
6	s4	182	TYR
6	s4	187	ARG
6	s4	194	THR
6	s4	219	VAL
6	s4	221	ARG
6	s4	223	ASN
6	s4	226	PHE
6	s4	236	ILE
6	s4	237	SER
6	s4	248	ILE
7	s5	23	VAL
7	s5	25	LEU
7	s5	34	GLN
7	s5	38	THR
7	s5	39	GLU
7	s5	41	LYS
7	s5	43	PHE
7	s5	47	SER
7	s5	63	GLN
7	s5	64	VAL
7	s5	65	ARG
7	s5	68	ILE
7	s5	76	ARG
7	s5	79	ASN
7	s5	83	ARG
7	s5	89	ILE
7	s5	92	ARG

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Mol	Chain	Res	Type
7	s5	93	LEU
7	s5	94	THR
7	s5	107	LYS
7	s5	112	ARG
7	s5	115	LYS
7	s5	119	ASP
7	s5	124	LEU
7	s5	125	THR
7	s5	128	ASN
7	s5	143	ARG
7	s5	146	THR
7	s5	156	ARG
7	s5	157	ARG
7	s5	167	ARG
7	s5	190	ILE
7	s5	194	LEU
7	s5	203	LYS
7	s5	206	SER
7	s5	212	LYS
7	s5	213	LYS
7	s5	216	GLU
7	s5	219	ARG
7	s5	224	ASN
8	s6	6	SER
8	s6	12	SER
8	s6	15	THR
8	s6	21	GLU
8	s6	25	ARG
8	s6	30	LYS
8	s6	31	ARG
8	s6	41	VAL
8	s6	59	GLN
8	s6	67	VAL
8	s6	71	THR
8	s6	76	LEU
8	s6	89	ASP
8	s6	93	LYS
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU
8	s6	111	LEU
8	s6	112	VAL

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Mol	Chain	Res	Type
8	s6	121	LEU
8	s6	122	GLU
8	s6	126	ASP
8	s6	128	THR
8	s6	129	VAL
8	s6	133	LEU
8	s6	143	LYS
8	s6	151	ASP
8	s6	155	ASP
8	s6	162	VAL
8	s6	166	GLU
8	s6	170	THR
8	s6	177	ARG
8	s6	180	THR
8	s6	191	ARG
8	s6	193	LEU
8	s6	212	LEU
8	s6	215	ARG
9	s7	10	SER
9	s7	11	GLN
9	s7	14	THR
9	s7	16	LEU
9	s7	25	VAL
9	s7	33	GLU
9	s7	42	GLN
9	s7	49	ILE
9	s7	50	ASP
9	s7	67	LEU
9	s7	77	LEU
9	s7	84	LYS
9	s7	86	GLN
9	s7	96	ARG
9	s7	97	ARG
9	s7	99	LEU
9	s7	107	ARG
9	s7	110	GLN
9	s7	114	ARG
9	s7	115	SER
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	126	LEU

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Mol	Chain	Res	Type
9	s7	129	LEU
9	s7	144	VAL
9	s7	149	ILE
9	s7	161	GLN
9	s7	163	ASP
9	s7	166	LEU
9	s7	185	ILE
10	s8	7	SER
10	s8	18	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	45	SER
10	s8	46	VAL
10	s8	47	ARG
10	s8	58	LEU
10	s8	61	GLU
10	s8	62	THR
10	s8	74	LYS
10	s8	76	THR
10	s8	77	ARG
10	s8	82	VAL
10	s8	89	GLU
10	s8	93	THR
10	s8	119	GLN
10	s8	120	THR
10	s8	121	LEU
10	s8	138	ASN
10	s8	151	LYS
10	s8	152	ILE
10	s8	155	SER
10	s8	183	ILE
10	s8	184	LEU
10	s8	185	GLU
11	s9	3	ARG
11	s9	7	THR
11	s9	16	LYS
11	s9	28	LEU
11	s9	37	LYS
11	s9	45	ILE
11	s9	61	THR
11	s9	87	SER
11	s9	89	ASP

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Mol	Chain	Res	Type
11	s9	93	LEU
11	s9	96	VAL
11	s9	99	LEU
11	s9	101	VAL
11	s9	105	LEU
11	s9	109	LEU
11	s9	111	THR
11	s9	120	LYS
11	s9	122	VAL
11	s9	126	ARG
11	s9	130	THR
11	s9	133	HIS
11	s9	134	ILE
11	s9	145	SER
11	s9	151	ASP
11	s9	154	LYS
11	s9	161	THR
11	s9	162	SER
11	s9	172	VAL
11	s9	174	ARG
11	s9	180	LYS
11	s9	182	GLU
11	s9	186	GLU
80	c0	5	LYS
80	c0	15	LEU
80	c0	27	PHE
80	c0	55	VAL
80	c0	56	LYS
80	c0	57	THR
80	c0	71	GLU
80	c0	77	ARG
13	c1	5	LEU
13	c1	10	GLU
13	c1	21	ASN
13	c1	26	LYS
13	c1	32	LYS
13	c1	40	LEU
13	c1	44	THR
13	c1	56	LYS
13	c1	60	PHE
13	c1	67	ARG
13	c1	72	THR

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Mol	Chain	Res	Type
13	c1	74	THR
13	c1	77	SER
13	c1	79	LYS
13	c1	80	MET
13	c1	83	THR
13	c1	95	PRO
13	c1	116	ARG
13	c1	129	ARG
13	c1	131	ILE
14	c2	28	LEU
14	c2	30	VAL
14	c2	36	LEU
14	c2	38	HIS
14	c2	43	ARG
14	c2	52	LEU
14	c2	58	LEU
14	c2	59	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	66	VAL
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	86	VAL
14	c2	89	ILE
14	c2	97	LEU
14	c2	103	LEU
14	c2	120	VAL
14	c2	121	VAL
14	c2	126	TRP
14	c2	132	GLU
14	c2	140	PHE
14	c2	141	SER
15	c3	6	SER
15	c3	12	SER
15	c3	14	SER
15	c3	18	TYR
15	c3	20	ARG
15	c3	32	SER
15	c3	53	LEU
15	c3	58	HIS

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Mol	Chain	Res	Type
15	c3	61	THR
15	c3	66	ILE
15	c3	70	LYS
15	c3	74	ILE
15	c3	80	LEU
15	c3	84	ILE
15	c3	88	LEU
15	c3	102	LEU
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	134	VAL
15	c3	138	ASN
15	c3	143	SER
15	c3	150	VAL
15	c3	151	ASN
16	c4	18	ARG
16	c4	20	TYR
16	c4	24	ASN
16	c4	26	THR
16	c4	28	VAL
16	c4	33	LEU
16	c4	36	LYS
16	c4	38	THR
16	c4	51	ASP
16	c4	52	ARG
16	c4	61	MET
16	c4	65	GLN
16	c4	66	ASP
16	c4	72	LYS
16	c4	81	VAL
16	c4	84	ARG
16	c4	92	LYS
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	129	LYS
16	c4	132	ARG
16	c4	133	ARG

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Mol	Chain	Res	Type
16	c4	136	ARG
16	c4	137	LEU
17	c5	12	PHE
17	c5	16	SER
17	c5	20	VAL
17	c5	21	ASP
17	c5	23	GLU
17	c5	24	LYS
17	c5	27	GLU
17	c5	30	THR
17	c5	31	GLU
17	c5	36	LEU
17	c5	40	ARG
17	c5	49	MET
17	c5	51	SER
17	c5	72	LYS
17	c5	77	ARG
17	c5	89	MET
17	c5	92	SER
17	c5	104	GLN
17	c5	107	ILE
17	c5	110	GLU
17	c5	112	LEU
17	c5	122	THR
17	c5	124	THR
17	c5	125	PRO
17	c5	127	ARG
18	c6	19	VAL
18	c6	23	LYS
18	c6	28	LEU
18	c6	37	THR
18	c6	43	ILE
18	c6	48	VAL
18	c6	53	LEU
18	c6	54	LEU
18	c6	55	VAL
18	c6	57	LEU
18	c6	66	ARG
18	c6	68	ARG
18	c6	69	VAL
18	c6	70	THR
18	c6	81	ILE

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Mol	Chain	Res	Type
18	c6	83	GLN
18	c6	100	GLN
18	c6	105	LEU
18	c6	110	THR
18	c6	115	THR
18	c6	117	LEU
18	c6	128	LYS
18	c6	137	ARG
19	c7	3	ARG
19	c7	5	ARG
19	c7	6	THR
19	c7	7	LYS
19	c7	8	THR
19	c7	11	ARG
19	c7	25	THR
19	c7	26	LEU
19	c7	27	ASP
19	c7	34	LEU
19	c7	45	ARG
19	c7	46	LEU
19	c7	47	ARG
19	c7	54	THR
19	c7	61	ILE
19	c7	63	LYS
19	c7	72	LYS
19	c7	73	LEU
19	c7	78	ARG
19	c7	79	GLU
19	c7	82	ASP
19	c7	85	VAL
19	c7	88	VAL
19	c7	104	ASN
19	c7	105	GLN
19	c7	113	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	8	GLN
20	c8	12	GLN
20	c8	13	HIS
20	c8	15	LEU
20	c8	25	ASN

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Mol	Chain	Res	Type
20	c8	26	ILE
20	c8	27	LYS
20	c8	28	ILE
20	c8	36	LYS
20	c8	57	ARG
20	c8	63	GLN
20	c8	69	ILE
20	c8	77	THR
20	c8	86	LEU
20	c8	94	ASP
20	c8	105	VAL
20	c8	110	ARG
20	c8	114	GLU
20	c8	116	LEU
20	c8	133	VAL
20	c8	136	GLN
20	c8	138	THR
20	c8	144	ARG
20	c8	145	ARG
21	c9	6	VAL
21	c9	25	GLN
21	c9	27	LYS
21	c9	28	LEU
21	c9	36	ILE
21	c9	41	SER
21	c9	57	ARG
21	c9	68	ARG
21	c9	71	VAL
21	c9	84	LYS
21	c9	86	ARG
21	c9	91	TYR
21	c9	110	LYS
21	c9	111	ILE
21	c9	116	ILE
21	c9	117	SER
21	c9	123	ARG
21	c9	126	GLU
21	c9	132	LEU
21	c9	140	LEU
21	c9	142	GLU
21	c9	144	GLU
22	d0	13	GLU

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Mol	Chain	Res	Type
22	d0	21	LYS
22	d0	23	ARG
22	d0	27	THR
22	d0	30	LYS
22	d0	31	VAL
22	d0	34	LEU
22	d0	36	ASN
22	d0	38	SER
22	d0	39	SER
22	d0	47	GLN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	62	VAL
22	d0	63	LEU
22	d0	67	THR
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	88	LYS
22	d0	89	ARG
22	d0	99	ILE
22	d0	103	ILE
22	d0	105	GLN
22	d0	107	THR
22	d0	108	ILE
22	d0	109	GLU
22	d0	113	ASP
23	d1	2	GLU
23	d1	5	LYS
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	25	LYS
23	d1	32	VAL
23	d1	34	ILE
23	d1	38	LYS
23	d1	52	THR
23	d1	68	SER

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Mol	Chain	Res	Type
23	d1	69	LEU
23	d1	78	LEU
23	d1	81	ASN
23	d1	86	SER
24	d2	6	VAL
24	d2	20	THR
24	d2	23	ARG
24	d2	24	GLN
24	d2	25	VAL
24	d2	26	LEU
24	d2	43	LYS
24	d2	56	HIS
24	d2	74	VAL
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	105	THR
24	d2	117	ARG
24	d2	121	VAL
24	d2	124	LYS
24	d2	129	VAL
25	d3	3	LYS
25	d3	9	LEU
25	d3	14	LYS
25	d3	16	ARG
25	d3	19	ARG
25	d3	23	ARG
25	d3	28	ASN
25	d3	33	LEU
25	d3	36	THR
25	d3	40	SER
25	d3	47	SER
25	d3	52	ILE
25	d3	66	SER
25	d3	73	ARG
25	d3	75	GLN
25	d3	78	LYS
25	d3	82	LYS
25	d3	84	THR
25	d3	96	VAL
25	d3	100	ASP
25	d3	103	LEU

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Mol	Chain	Res	Type
25	d3	107	PHE
25	d3	123	LYS
25	d3	131	SER
25	d3	133	LEU
25	d3	135	LEU
25	d3	139	LYS
26	d4	2	SER
26	d4	10	ARG
26	d4	13	ILE
26	d4	21	LYS
26	d4	26	ASP
26	d4	29	HIS
26	d4	43	LYS
26	d4	44	LEU
26	d4	46	GLU
26	d4	49	LYS
26	d4	55	VAL
26	d4	62	THR
26	d4	77	ASN
26	d4	88	THR
26	d4	91	LEU
26	d4	92	VAL
26	d4	98	GLU
26	d4	100	VAL
26	d4	114	ARG
26	d4	128	LYS
26	d4	133	ASN
27	d5	40	VAL
27	d5	43	ASP
27	d5	52	LYS
27	d5	53	GLU
27	d5	57	TYR
27	d5	58	ARG
27	d5	60	VAL
27	d5	68	ARG
27	d5	81	ARG
27	d5	86	GLU
27	d5	90	LYS
27	d5	92	ILE
28	d6	4	LYS
28	d6	8	ASN
28	d6	10	ARG

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Mol	Chain	Res	Type
28	d6	24	VAL
28	d6	26	CYS
28	d6	27	SER
28	d6	28	LYS
28	d6	30	ILE
28	d6	34	LYS
28	d6	39	MET
28	d6	41	ILE
28	d6	43	ASN
28	d6	53	LEU
28	d6	54	SER
28	d6	67	THR
28	d6	79	ILE
28	d6	82	ARG
28	d6	85	ARG
28	d6	89	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	4	VAL
29	d7	11	THR
29	d7	14	SER
29	d7	34	ASP
29	d7	40	CYS
29	d7	43	ILE
29	d7	61	THR
29	d7	62	ILE
29	d7	65	THR
29	d7	72	LYS
30	d8	5	THR
30	d8	8	THR
30	d8	11	LYS
30	d8	16	LEU
30	d8	21	SER
30	d8	22	ARG
30	d8	32	PHE
30	d8	33	LEU
30	d8	36	THR
30	d8	40	ILE
30	d8	52	ASP
30	d8	54	LEU
30	d8	59	SER
30	d8	62	GLU

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Mol	Chain	Res	Type
30	d8	64	ARG
31	d9	4	GLU
31	d9	19	ARG
31	d9	20	GLN
31	d9	25	SER
31	d9	30	LEU
31	d9	36	LEU
31	d9	38	ILE
31	d9	53	ASN
31	d9	54	LYS
31	d9	56	ARG
81	e0	4	VAL
81	e0	14	VAL
81	e0	23	LYS
81	e0	24	THR
81	e0	26	LYS
81	e0	29	LYS
81	e0	36	LYS
81	e0	38	LEU
81	e0	41	THR
81	e0	42	ARG
81	e0	44	PHE
81	e0	49	LEU
81	e0	55	ARG
82	e1	80	ARG
82	e1	86	THR
82	e1	90	LYS
82	e1	97	LYS
82	e1	98	VAL
82	e1	100	LEU
82	e1	102	VAL
82	e1	106	TYR
82	e1	107	LYS
82	e1	109	ASP
82	e1	113	LYS
82	e1	115	THR
82	e1	116	LYS
82	e1	118	ARG
82	e1	119	ARG
82	e1	121	CYS
82	e1	135	HIS
82	e1	140	TYR

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Mol	Chain	Res	Type
82	e1	146	SER
82	e1	147	VAL
82	e1	150	VAL
34	sR	9	LEU
34	sR	21	THR
34	sR	23	LEU
34	sR	29	GLN
34	sR	42	LEU
34	sR	58	VAL
34	sR	66	HIS
34	sR	76	ASP
34	sR	98	GLU
34	sR	108	SER
34	sR	145	LEU
34	sR	159	ASN
34	sR	167	VAL
34	sR	184	ASN
34	sR	188	ILE
34	sR	222	LEU
34	sR	228	LYS
34	sR	232	TYR
34	sR	258	THR
34	sR	266	ASP
34	sR	275	ARG
34	sR	297	ASP
34	sR	310	ILE
35	sM	23	LYS
35	sM	27	LYS
35	sM	30	THR
35	sM	43	ASP
35	sM	48	ARG
35	sM	49	LYS
35	sM	50	ASN
35	sM	55	SER
35	sM	61	ILE
35	sM	68	ARG
35	sM	71	ASN
35	sM	74	LYS
35	sM	77	THR
35	sM	82	THR
39	l2	15	ILE
39	l2	23	ARG

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Mol	Chain	Res	Type
39	12	32	LEU
39	12	45	VAL
39	12	47	GLN
39	12	48	ILE
39	12	61	VAL
39	12	62	VAL
39	12	64	ARG
39	12	70	ARG
39	12	74	GLU
39	12	82	VAL
39	12	96	LEU
39	12	98	VAL
39	12	101	VAL
39	12	104	LEU
39	12	112	ILE
39	12	134	VAL
39	12	137	ILE
39	12	147	ARG
39	12	148	VAL
39	12	157	VAL
39	12	165	VAL
39	12	168	VAL
39	12	188	LYS
39	12	191	LEU
39	12	193	ARG
39	12	202	VAL
39	12	204	MET
39	12	227	ARG
39	12	233	GLN
39	12	238	ILE
39	12	241	ARG
39	12	243	THR
39	12	246	LEU
39	12	249	SER
40	13	3	HIS
40	13	4	ARG
40	13	5	LYS
40	13	7	GLU
40	13	10	ARG
40	13	17	LEU
40	13	19	ARG
40	13	20	LYS

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Mol	Chain	Res	Type
40	l3	26	ARG
40	l3	44	THR
40	l3	47	LEU
40	l3	50	LYS
40	l3	55	THR
40	l3	56	ILE
40	l3	70	ARG
40	l3	77	THR
40	l3	85	VAL
40	l3	103	THR
40	l3	111	SER
40	l3	114	VAL
40	l3	116	ARG
40	l3	128	LYS
40	l3	139	GLN
40	l3	140	ASP
40	l3	146	ARG
40	l3	150	ARG
40	l3	153	LYS
40	l3	160	VAL
40	l3	167	ARG
40	l3	169	THR
40	l3	175	LYS
40	l3	183	LEU
40	l3	188	ILE
40	l3	202	THR
40	l3	205	VAL
40	l3	208	VAL
40	l3	211	GLN
40	l3	213	GLU
40	l3	232	ARG
40	l3	235	THR
40	l3	238	LEU
40	l3	242	THR
40	l3	247	ARG
40	l3	248	LYS
40	l3	252	ILE
40	l3	274	SER
40	l3	284	ARG
40	l3	303	LYS
40	l3	304	THR
40	l3	308	MET

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Mol	Chain	Res	Type
40	13	322	ILE
40	13	324	VAL
40	13	332	ARG
40	13	333	LYS
40	13	341	SER
40	13	346	THR
40	13	359	ILE
40	13	369	ARG
40	13	380	MET
40	13	386	ASP
41	14	2	SER
41	14	8	VAL
41	14	47	ARG
41	14	69	ARG
41	14	92	ASN
41	14	93	MET
41	14	98	ARG
41	14	112	LYS
41	14	120	TYR
41	14	122	THR
41	14	136	LEU
41	14	138	ARG
41	14	144	LYS
41	14	156	LEU
41	14	160	GLN
41	14	170	LYS
41	14	179	LEU
41	14	186	LYS
41	14	187	LEU
41	14	203	ARG
41	14	206	LEU
41	14	217	LYS
41	14	220	ARG
41	14	221	ASN
41	14	230	VAL
41	14	246	ARG
41	14	252	GLU
41	14	258	LEU
41	14	265	GLU
41	14	266	THR
41	14	284	SER
41	14	289	ILE

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Mol	Chain	Res	Type
41	14	291	ASN
41	14	293	SER
41	14	299	ILE
41	14	300	ARG
41	14	301	PRO
41	14	304	GLN
41	14	306	THR
41	14	307	GLN
41	14	310	THR
41	14	313	LEU
41	14	319	LYS
41	14	323	VAL
41	14	327	LEU
41	14	333	VAL
41	14	345	GLU
41	14	347	THR
41	14	349	THR
41	14	357	GLU
41	14	358	THR
41	14	359	LEU
42	15	4	GLN
42	15	9	SER
42	15	17	GLN
42	15	34	LYS
42	15	35	ARG
42	15	48	LYS
42	15	51	LEU
42	15	65	ILE
42	15	68	THR
42	15	70	THR
42	15	74	VAL
42	15	85	ARG
42	15	89	THR
42	15	93	THR
42	15	110	LEU
42	15	112	LYS
42	15	118	THR
42	15	132	THR
42	15	135	VAL
42	15	140	ARG
42	15	146	LEU
42	15	148	ILE

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Mol	Chain	Res	Type
42	15	151	GLN
42	15	152	ARG
42	15	154	THR
42	15	155	THR
42	15	164	LYS
42	15	177	GLU
42	15	185	PHE
42	15	187	THR
42	15	190	ILE
42	15	191	ASP
42	15	194	LEU
42	15	196	ARG
42	15	211	LEU
42	15	218	ARG
42	15	222	LEU
42	15	227	LEU
42	15	241	THR
42	15	247	ILE
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS
42	15	262	LYS
42	15	268	GLU
42	15	269	SER
42	15	273	ARG
42	15	275	THR
42	15	277	LEU
43	16	8	LYS
43	16	12	SER
43	16	20	LYS
43	16	21	THR
43	16	31	ARG
43	16	35	VAL
43	16	46	ARG
43	16	50	LYS
43	16	52	VAL
43	16	64	LEU
43	16	65	ILE
43	16	79	VAL
43	16	88	SER
43	16	89	THR
43	16	91	VAL

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Mol	Chain	Res	Type
43	16	108	LYS
43	16	133	GLU
43	16	136	GLU
43	16	152	THR
43	16	155	LEU
43	16	162	SER
43	16	175	LYS
44	17	26	VAL
44	17	41	ARG
44	17	45	LEU
44	17	46	GLU
44	17	53	LYS
44	17	60	ARG
44	17	83	LEU
44	17	88	ARG
44	17	98	LYS
44	17	100	ARG
44	17	101	LYS
44	17	111	ILE
44	17	128	LYS
44	17	156	ILE
44	17	158	LYS
44	17	159	GLN
44	17	173	LEU
44	17	175	LYS
44	17	179	LEU
44	17	184	LEU
44	17	196	LYS
44	17	199	ASN
44	17	229	PHE
44	17	239	LEU
45	18	46	LEU
45	18	50	VAL
45	18	65	LEU
45	18	67	ILE
45	18	68	ARG
45	18	69	LEU
45	18	71	VAL
45	18	74	THR
45	18	81	THR
45	18	111	LYS
45	18	136	LEU

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Mol	Chain	Res	Type
45	18	149	LYS
45	18	150	LEU
45	18	153	ILE
45	18	156	ASP
45	18	160	ILE
45	18	163	VAL
45	18	164	VAL
45	18	169	LEU
45	18	172	LYS
45	18	181	LYS
45	18	183	LYS
45	18	203	VAL
45	18	208	GLU
45	18	213	LYS
45	18	214	LEU
45	18	219	ASP
45	18	230	LYS
45	18	231	LYS
45	18	241	LYS
45	18	245	LYS
45	18	248	LYS
46	19	4	ILE
46	19	5	GLN
46	19	6	THR
46	19	18	VAL
46	19	20	ILE
46	19	22	SER
46	19	31	ARG
46	19	33	THR
46	19	34	LEU
46	19	36	LYS
46	19	44	THR
46	19	48	VAL
46	19	52	LEU
46	19	55	VAL
46	19	68	LEU
46	19	70	THR
46	19	72	LYS
46	19	73	SER
46	19	80	THR
46	19	82	VAL
46	19	87	LYS

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Mol	Chain	Res	Type
46	19	92	TYR
46	19	105	GLU
46	19	115	ARG
46	19	120	ASP
46	19	132	VAL
46	19	133	THR
46	19	144	ILE
46	19	146	LEU
46	19	151	VAL
46	19	157	ASN
46	19	161	LEU
46	19	162	GLN
46	19	167	VAL
46	19	173	ARG
46	19	174	LYS
46	19	177	ASP
46	19	179	ILE
46	19	191	LEU
47	m0	3	ARG
47	m0	21	ARG
47	m0	24	ARG
47	m0	29	SER
47	m0	36	LEU
47	m0	39	LYS
47	m0	44	ASP
47	m0	48	LEU
47	m0	52	LEU
47	m0	54	SER
47	m0	58	GLU
47	m0	63	GLU
47	m0	74	LYS
47	m0	77	THR
47	m0	87	LEU
47	m0	91	VAL
47	m0	138	VAL
47	m0	139	ARG
47	m0	143	SER
47	m0	144	ASN
47	m0	145	LYS
47	m0	169	LYS
47	m0	170	LYS
47	m0	175	ASN

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Mol	Chain	Res	Type
47	m0	177	ASP
47	m0	182	LEU
47	m0	197	VAL
47	m0	200	LEU
47	m0	211	ARG
47	m0	215	GLU
47	m0	217	PHE
48	m1	10	ARG
48	m1	11	ASP
48	m1	12	LEU
48	m1	13	LYS
48	m1	29	ARG
48	m1	34	SER
48	m1	37	LEU
48	m1	40	LEU
48	m1	44	THR
48	m1	46	VAL
48	m1	51	ARG
48	m1	54	VAL
48	m1	56	THR
48	m1	59	ILE
48	m1	71	VAL
48	m1	80	LEU
48	m1	94	ARG
48	m1	97	SER
48	m1	106	ILE
48	m1	107	ASP
48	m1	108	GLU
48	m1	112	LEU
48	m1	129	VAL
48	m1	130	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	142	LYS
48	m1	147	THR
48	m1	151	SER
48	m1	158	ASP
48	m1	159	THR
48	m1	161	SER
48	m1	166	LYS
48	m1	172	LEU
48	m1	174	LYS

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Mol	Chain	Res	Type
49	m3	19	GLN
49	m3	54	LEU
49	m3	55	ARG
49	m3	57	VAL
49	m3	58	VAL
49	m3	69	VAL
49	m3	73	ARG
49	m3	76	THR
49	m3	85	LEU
49	m3	103	ASN
49	m3	106	GLN
49	m3	123	ILE
49	m3	124	ILE
49	m3	131	LYS
49	m3	138	VAL
49	m3	149	GLN
49	m3	150	PRO
49	m3	152	THR
49	m3	164	GLU
49	m3	165	SER
49	m3	168	ARG
49	m3	176	GLU
49	m3	183	ARG
49	m3	184	GLU
49	m3	194	GLU
50	m4	3	THR
50	m4	4	ASP
50	m4	6	ILE
50	m4	16	GLU
50	m4	20	VAL
50	m4	27	GLN
50	m4	28	SER
50	m4	31	LYS
50	m4	35	ILE
50	m4	53	VAL
50	m4	58	ILE
50	m4	63	VAL
50	m4	66	THR
50	m4	72	LEU
50	m4	80	THR
50	m4	82	SER
50	m4	92	GLU

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Mol	Chain	Res	Type
50	m4	98	SER
50	m4	107	GLU
50	m4	113	THR
50	m4	116	GLU
50	m4	124	ARG
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	7	LEU
51	m5	10	LEU
51	m5	14	LYS
51	m5	15	GLN
51	m5	18	VAL
51	m5	22	LEU
51	m5	27	VAL
51	m5	36	ILE
51	m5	49	ARG
51	m5	53	TYR
51	m5	54	LYS
51	m5	71	ARG
51	m5	76	PRO
51	m5	85	THR
51	m5	92	LEU
51	m5	96	ARG
51	m5	97	SER
51	m5	105	ARG
51	m5	106	VAL
51	m5	108	ARG
51	m5	138	GLN
51	m5	153	ASP
51	m5	159	ARG
51	m5	160	GLU
51	m5	165	THR
51	m5	171	SER
51	m5	179	LYS
51	m5	183	THR
51	m5	184	LYS
51	m5	190	THR
51	m5	194	GLN
51	m5	198	SER
52	m6	12	LYS
52	m6	46	GLU

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Mol	Chain	Res	Type
52	m6	60	LYS
52	m6	66	LYS
52	m6	67	THR
52	m6	74	ARG
52	m6	78	ARG
52	m6	79	ILE
52	m6	85	ARG
52	m6	100	GLU
52	m6	106	GLU
52	m6	108	ILE
52	m6	110	PRO
52	m6	117	ARG
52	m6	122	GLN
52	m6	124	LEU
52	m6	128	ARG
52	m6	141	LEU
52	m6	151	ASP
52	m6	152	VAL
52	m6	171	LYS
52	m6	182	ASN
52	m6	184	THR
52	m6	197	LEU
53	m7	7	THR
53	m7	8	SER
53	m7	9	THR
53	m7	18	ARG
53	m7	23	ARG
53	m7	24	VAL
53	m7	31	GLU
53	m7	32	THR
53	m7	41	LEU
53	m7	46	LYS
53	m7	52	LEU
53	m7	56	ARG
53	m7	69	ARG
53	m7	78	VAL
53	m7	79	THR
53	m7	89	LYS
53	m7	94	LEU
53	m7	112	LEU
53	m7	114	VAL
53	m7	119	VAL

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Mol	Chain	Res	Type
53	m7	120	ASN
53	m7	126	ARG
53	m7	144	SER
53	m7	148	LEU
54	m8	3	ILE
54	m8	7	SER
54	m8	17	THR
54	m8	22	ASP
54	m8	24	VAL
54	m8	26	LEU
54	m8	32	LEU
54	m8	34	THR
54	m8	49	LEU
54	m8	57	ILE
54	m8	63	SER
54	m8	69	ARG
54	m8	74	GLU
54	m8	80	THR
54	m8	81	VAL
54	m8	82	VAL
54	m8	86	THR
54	m8	93	ILE
54	m8	98	LYS
54	m8	135	GLN
54	m8	165	ILE
54	m8	166	LEU
54	m8	167	SER
54	m8	170	ARG
54	m8	178	ARG
55	m9	7	GLN
55	m9	10	LEU
55	m9	17	VAL
55	m9	27	ASN
55	m9	36	ASN
55	m9	37	SER
55	m9	43	LYS
55	m9	47	ASN
55	m9	49	THR
55	m9	56	THR
55	m9	63	THR
55	m9	74	ARG
55	m9	78	TYR

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Mol	Chain	Res	Type
55	m9	92	GLN
55	m9	98	ARG
55	m9	99	LEU
55	m9	104	ARG
55	m9	116	ASP
55	m9	117	LYS
55	m9	121	HIS
55	m9	126	GLU
55	m9	146	LYS
55	m9	148	ASP
55	m9	152	GLU
55	m9	153	LYS
55	m9	156	ASN
55	m9	158	GLU
55	m9	162	ARG
55	m9	164	LEU
55	m9	165	LYS
55	m9	167	ARG
55	m9	173	ARG
56	n0	5	LYS
56	n0	13	ARG
56	n0	17	GLU
56	n0	21	GLU
56	n0	23	LYS
56	n0	32	SER
56	n0	45	LEU
56	n0	70	THR
56	n0	71	LYS
56	n0	73	LYS
56	n0	87	THR
56	n0	97	VAL
56	n0	100	VAL
56	n0	104	GLU
56	n0	105	THR
56	n0	117	ARG
56	n0	119	ARG
56	n0	120	SER
56	n0	130	GLU
56	n0	136	LYS
56	n0	137	ARG
56	n0	145	THR
56	n0	148	LEU

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Mol	Chain	Res	Type
56	n0	149	LYS
56	n0	155	ARG
56	n0	157	GLN
56	n0	162	THR
56	n0	169	SER
56	n0	172	TYR
57	n1	9	SER
57	n1	12	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	35	LYS
57	n1	43	LYS
57	n1	55	LYS
57	n1	71	SER
57	n1	80	VAL
57	n1	83	ARG
57	n1	96	ILE
57	n1	97	LYS
57	n1	102	ARG
57	n1	104	GLU
57	n1	118	GLU
57	n1	124	VAL
57	n1	126	VAL
57	n1	127	GLN
57	n1	130	ARG
57	n1	131	GLN
57	n1	139	ARG
57	n1	141	VAL
57	n1	143	THR
57	n1	144	GLU
57	n1	149	GLN
57	n1	150	THR
57	n1	154	VAL
57	n1	158	THR
58	n2	14	THR
58	n2	16	THR
58	n2	21	SER
58	n2	27	VAL
58	n2	28	PHE
58	n2	37	LEU
58	n2	43	VAL

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Mol	Chain	Res	Type
58	n2	50	LEU
58	n2	55	THR
58	n2	57	THR
58	n2	62	VAL
58	n2	68	THR
58	n2	75	TYR
58	n2	90	ARG
58	n2	96	VAL
58	n2	98	THR
58	n2	100	THR
58	n2	104	ARG
59	n3	7	GLN
59	n3	13	ILE
59	n3	15	LEU
59	n3	45	ARG
59	n3	48	ARG
59	n3	57	MET
59	n3	88	ARG
59	n3	96	GLU
59	n3	115	THR
60	n4	1	MET
60	n4	19	THR
60	n4	34	SER
60	n4	39	LEU
60	n4	43	ARG
60	n4	54	LEU
60	n4	57	LYS
60	n4	58	HIS
60	n4	63	ILE
60	n4	82	ILE
60	n4	87	LEU
60	n4	89	LEU
60	n4	97	LYS
60	n4	112	ASN
60	n4	119	GLU
60	n4	127	LYS
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	45	LYS
61	n5	56	ARG

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Mol	Chain	Res	Type
61	n5	57	LEU
61	n5	63	ILE
61	n5	71	THR
61	n5	73	MET
61	n5	86	VAL
61	n5	87	SER
61	n5	105	VAL
61	n5	108	LEU
61	n5	109	LYS
61	n5	115	ARG
61	n5	117	ASN
61	n5	125	ARG
61	n5	131	ASP
61	n5	135	ILE
61	n5	142	ILE
62	n6	3	LYS
62	n6	4	GLN
62	n6	9	SER
62	n6	12	ARG
62	n6	13	ARG
62	n6	14	LYS
62	n6	25	SER
62	n6	32	SER
62	n6	35	LEU
62	n6	37	LYS
62	n6	39	LEU
62	n6	40	ARG
62	n6	45	ILE
62	n6	46	LYS
62	n6	50	ILE
62	n6	51	ARG
62	n6	55	GLU
62	n6	56	VAL
62	n6	57	LEU
62	n6	63	LYS
62	n6	64	LYS
62	n6	66	GLN
62	n6	74	TYR
62	n6	83	ASP
62	n6	86	THR
62	n6	88	GLU
62	n6	89	LYS

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Mol	Chain	Res	Type
62	n6	94	SER
62	n6	95	VAL
62	n6	99	LEU
62	n6	105	VAL
62	n6	115	ARG
62	n6	122	LYS
62	n6	127	GLU
63	n7	3	LYS
63	n7	5	LEU
63	n7	14	VAL
63	n7	21	LYS
63	n7	24	VAL
63	n7	25	ILE
63	n7	34	LYS
63	n7	36	HIS
63	n7	46	ILE
63	n7	52	LYS
63	n7	65	ARG
63	n7	72	ILE
63	n7	81	LEU
63	n7	93	LYS
63	n7	95	VAL
63	n7	98	THR
63	n7	99	GLU
63	n7	102	GLU
63	n7	103	GLN
63	n7	105	SER
63	n7	106	GLN
63	n7	126	LYS
63	n7	127	ASN
63	n7	128	GLN
63	n7	134	LEU
63	n7	135	ARG
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	10	LYS
64	n8	14	HIS
64	n8	15	VAL
64	n8	19	LYS
64	n8	42	ARG
64	n8	47	LYS

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Mol	Chain	Res	Type
64	n8	60	TYR
64	n8	73	LEU
64	n8	76	ASP
64	n8	78	LEU
64	n8	80	THR
64	n8	82	ILE
64	n8	85	ASP
64	n8	91	LEU
64	n8	97	GLU
64	n8	98	THR
64	n8	123	VAL
64	n8	128	ARG
64	n8	133	LEU
65	n9	12	GLN
65	n9	19	ASN
65	n9	21	ILE
65	n9	42	ASN
65	n9	47	LEU
65	n9	50	THR
65	n9	58	LYS
65	n9	59	LYS
66	o0	9	SER
66	o0	10	ILE
66	o0	28	LYS
66	o0	30	THR
66	o0	32	LYS
66	o0	33	SER
66	o0	34	LEU
66	o0	41	LEU
66	o0	61	MET
66	o0	71	GLN
66	o0	81	VAL
66	o0	83	LYS
66	o0	84	LEU
66	o0	86	ARG
66	o0	87	VAL
66	o0	97	ASP
66	o0	101	LEU
67	o1	6	ASP
67	o1	8	VAL
67	o1	16	LEU
67	o1	23	VAL

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Mol	Chain	Res	Type
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	48	ASP
67	o1	53	PRO
67	o1	68	GLU
67	o1	76	SER
67	o1	90	PHE
67	o1	93	VAL
67	o1	94	GLU
67	o1	97	LEU
67	o1	102	LYS
67	o1	104	LEU
67	o1	105	GLN
67	o1	106	THR
67	o1	110	GLU
68	o2	14	THR
68	o2	17	PHE
68	o2	19	ARG
68	o2	21	HIS
68	o2	24	ARG
68	o2	31	ASN
68	o2	33	ARG
68	o2	40	SER
68	o2	49	ASN
68	o2	51	SER
68	o2	61	LYS
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	84	THR
68	o2	87	MET
68	o2	89	THR
68	o2	115	LEU
68	o2	123	LYS
68	o2	125	ARG
69	o3	4	SER
69	o3	10	LYS
69	o3	31	LYS

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Mol	Chain	Res	Type
69	o3	33	GLU
69	o3	37	THR
69	o3	42	GLN
69	o3	54	ARG
69	o3	57	LYS
69	o3	59	VAL
69	o3	62	SER
69	o3	74	THR
69	o3	78	SER
69	o3	81	VAL
69	o3	86	ARG
69	o3	98	VAL
69	o3	105	SER
70	o4	5	VAL
70	o4	10	ARG
70	o4	16	ARG
70	o4	20	ILE
70	o4	24	LYS
70	o4	29	ILE
70	o4	33	GLN
70	o4	40	THR
70	o4	46	ASP
70	o4	47	CYS
70	o4	58	ARG
70	o4	61	GLN
70	o4	85	VAL
70	o4	88	ARG
70	o4	98	GLN
70	o4	101	VAL
70	o4	104	VAL
71	o5	11	THR
71	o5	20	GLN
71	o5	21	LEU
71	o5	31	LEU
71	o5	38	ARG
71	o5	40	SER
71	o5	45	LYS
71	o5	47	VAL
71	o5	48	ARG
71	o5	53	CYS
71	o5	62	GLN
71	o5	68	GLN

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Mol	Chain	Res	Type
71	o5	69	LEU
71	o5	81	ARG
71	o5	85	THR
71	o5	89	ARG
71	o5	100	VAL
71	o5	101	THR
71	o5	107	LYS
71	o5	108	GLN
71	o5	113	GLN
72	o6	3	VAL
72	o6	7	ILE
72	o6	9	ILE
72	o6	12	ASN
72	o6	18	THR
72	o6	26	ILE
72	o6	29	LYS
72	o6	34	SER
72	o6	36	ARG
72	o6	37	THR
72	o6	42	SER
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	60	LEU
72	o6	68	ARG
72	o6	72	VAL
72	o6	74	LYS
72	o6	76	ARG
72	o6	81	THR
72	o6	94	ILE
72	o6	98	ARG
73	o7	5	THR
73	o7	7	SER
73	o7	15	SER
73	o7	17	THR
73	o7	25	ARG
73	o7	28	HIS
73	o7	33	THR
73	o7	36	SER
73	o7	44	THR
73	o7	46	SER

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Mol	Chain	Res	Type
73	o7	55	ARG
73	o7	59	THR
73	o7	65	ARG
73	o7	67	LEU
73	o7	71	SER
73	o7	74	PHE
73	o7	82	SER
74	o8	5	ILE
74	o8	13	GLU
74	o8	20	VAL
74	o8	22	THR
74	o8	24	THR
74	o8	41	THR
74	o8	46	ARG
74	o8	53	THR
74	o8	61	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	72	THR
75	o9	4	GLN
75	o9	5	LYS
75	o9	21	ARG
75	o9	23	LEU
75	o9	28	ARG
75	o9	29	LEU
75	o9	45	ARG
75	o9	47	THR
76	q0	85	LEU
76	q0	87	SER
76	q0	88	LYS
76	q0	91	CYS
76	q0	97	ARG
76	q0	106	ARG
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	127	LEU
76	q0	128	LYS
77	q1	2	ARG
77	q1	6	ARG
77	q1	9	ARG
77	q1	13	LEU

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Mol	Chain	Res	Type
77	q1	21	ARG
78	q2	6	LYS
78	q2	7	THR
78	q2	8	ARG
78	q2	15	LYS
78	q2	16	THR
78	q2	17	CYS
78	q2	22	GLN
78	q2	38	GLN
78	q2	45	ARG
78	q2	47	GLN
78	q2	48	SER
78	q2	61	LYS
78	q2	66	LYS
78	q2	71	ARG
78	q2	73	GLU
78	q2	75	VAL
78	q2	78	LYS
78	q2	79	THR
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	89	LYS
78	q2	91	PHE
78	q2	93	LEU
78	q2	100	LYS
79	q3	10	ILE
79	q3	20	SER
79	q3	24	ARG
79	q3	40	SER
79	q3	42	CYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	57	CYS
79	q3	59	CYS
79	q3	60	CYS
79	q3	70	THR
79	q3	73	THR
79	q3	79	VAL
79	q3	84	ARG
84	p0	4	ILE

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Mol	Chain	Res	Type
84	p0	5	ARG
84	p0	25	LEU
84	p0	30	VAL
84	p0	35	SER
84	p0	43	LYS
84	p0	48	ARG
84	p0	50	VAL
84	p0	51	VAL
84	p0	52	LEU
84	p0	55	LYS
84	p0	57	THR
84	p0	66	PHE
84	p0	70	LEU
84	p0	72	ASP
84	p0	74	GLU
84	p0	76	LEU
84	p0	80	VAL
84	p0	89	THR
84	p0	93	LEU
84	p0	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	S0	163	ASN
5	S3	179	GLN
7	S5	103	ASN
10	S8	138	ASN
12	C0	12	HIS
18	C6	83	GLN
20	C8	99	HIS
23	D1	75	ASN
24	D2	56	HIS
27	D5	95	HIS
35	SM	86	ASN
39	L2	83	HIS
39	L2	209	HIS
42	L5	40	HIS
44	L7	25	GLN
44	L7	81	HIS
44	L7	225	GLN
44	L7	244	ASN

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Mol	Chain	Res	Type
46	L9	156	GLN
47	M0	55	ASN
47	M0	162	GLN
54	M8	152	HIS
57	N1	26	HIS
59	N3	33	ASN
59	N3	98	ASN
3	s1	149	GLN
4	s2	147	ASN
11	s9	124	HIS
80	c0	29	GLN
80	c0	32	HIS
18	c6	83	GLN
20	c8	25	ASN
20	c8	90	ASN
24	d2	24	GLN
27	d5	37	GLN
29	d7	19	HIS
82	e1	93	HIS
34	sR	184	ASN
44	l7	112	ASN
47	m0	59	GLN
47	m0	144	ASN
49	m3	25	HIS
53	m7	34	GLN
63	n7	57	HIS
64	n8	49	HIS
70	o4	18	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	488 (27%)	56 (3%)
1	6	1792/1800 (99%)	474 (26%)	57 (3%)
36	1	3145/3396 (92%)	688 (21%)	83 (2%)
36	5	3145/3396 (92%)	687 (21%)	76 (2%)
37	3	120/121 (99%)	14 (11%)	0
37	7	120/121 (99%)	24 (20%)	1 (0%)
38	4	157/158 (99%)	38 (24%)	2 (1%)
38	8	157/158 (99%)	37 (23%)	2 (1%)
All	All	10383/10950 (94%)	2450 (23%)	277 (2%)

All (2450) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	40	A
1	2	45	U
1	2	46	A
1	2	47	A
1	2	50	C
1	2	57	G
1	2	60	U
1	2	61	A
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	103	A
1	2	104	A
1	2	114	C
1	2	127	G
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	158	U
1	2	159	U
1	2	161	U

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Mol	Chain	Res	Type
1	2	169	A
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	199	G
1	2	200	A
1	2	215	A
1	2	218	A
1	2	219	A
1	2	226	A
1	2	227	U
1	2	228	G
1	2	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	250	C
1	2	260	U
1	2	261	U
1	2	262	U
1	2	265	A
1	2	266	A
1	2	271	A
1	2	272	U

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Mol	Chain	Res	Type
1	2	274	G
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	290	G
1	2	299	A
1	2	303	U
1	2	304	U
1	2	308	C
1	2	314	C
1	2	316	A
1	2	319	U
1	2	321	C
1	2	323	A
1	2	333	A
1	2	337	G
1	2	338	C
1	2	341	A
1	2	348	U
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	387	A
1	2	391	A
1	2	400	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	418	G
1	2	423	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	434	G
1	2	439	U
1	2	444	C

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Mol	Chain	Res	Type
1	2	446	A
1	2	448	C
1	2	454	U
1	2	477	A
1	2	480	G
1	2	484	C
1	2	485	A
1	2	486	G
1	2	488	G
1	2	489	C
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	511	A
1	2	512	A
1	2	513	U
1	2	515	A
1	2	516	G
1	2	519	C
1	2	520	A
1	2	525	A
1	2	527	A
1	2	528	U
1	2	531	C
1	2	532	U
1	2	536	C
1	2	537	G
1	2	538	A
1	2	539	G
1	2	540	G

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Mol	Chain	Res	Type
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	548	G
1	2	551	G
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	566	C
1	2	576	G
1	2	578	U
1	2	579	A
1	2	580	A
1	2	582	U
1	2	585	A
1	2	594	A
1	2	595	G
1	2	597	G
1	2	605	A
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	630	A
1	2	639	U
1	2	640	U
1	2	650	U
1	2	653	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	677	G
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	694	U
1	2	696	C

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Mol	Chain	Res	Type
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	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	744	U
1	2	751	G
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	768	C
1	2	774	A

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Mol	Chain	Res	Type
1	2	775	G
1	2	778	G
1	2	781	U
1	2	783	G
1	2	784	C
1	2	785	U
1	2	789	A
1	2	790	U
1	2	793	A
1	2	794	U
1	2	795	U
1	2	796	A
1	2	806	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G
1	2	824	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	833	U
1	2	834	G
1	2	835	U
1	2	840	U
1	2	846	G
1	2	854	U
1	2	858	G
1	2	862	A
1	2	863	A
1	2	864	U
1	2	873	U
1	2	876	G
1	2	892	A
1	2	896	U

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Mol	Chain	Res	Type
1	2	898	A
1	2	911	U
1	2	912	U
1	2	914	G
1	2	915	A
1	2	916	U
1	2	933	A
1	2	935	U
1	2	942	G
1	2	944	A
1	2	951	A
1	2	960	U
1	2	961	U
1	2	966	A
1	2	970	A
1	2	971	A
1	2	982	U
1	2	984	G
1	2	988	A
1	2	992	A
1	2	993	A
1	2	995	A
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1021	C
1	2	1026	A
1	2	1028	C
1	2	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	1064	G
1	2	1066	C
1	2	1067	C

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Mol	Chain	Res	Type
1	2	1070	C
1	2	1081	A
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	1104	U
1	2	1111	G
1	2	1117	U
1	2	1138	A
1	2	1139	A
1	2	1146	G
1	2	1149	G
1	2	1150	G
1	2	1151	A
1	2	1152	A
1	2	1155	G
1	2	1158	C
1	2	1160	A
1	2	1163	A
1	2	1167	G
1	2	1176	G
1	2	1185	U
1	2	1188	G
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1206	U
1	2	1207	C
1	2	1217	A
1	2	1218	G
1	2	1226	A
1	2	1227	A
1	2	1228	G
1	2	1235	C
1	2	1241	G

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Mol	Chain	Res	Type
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1257	U
1	2	1258	U
1	2	1260	U
1	2	1286	U
1	2	1287	A
1	2	1302	U
1	2	1310	U
1	2	1314	U
1	2	1315	U
1	2	1321	A
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1354	G
1	2	1355	C
1	2	1361	U
1	2	1363	U
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1379	C
1	2	1388	A
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1401	A
1	2	1412	G
1	2	1413	U
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1433	G
1	2	1445	G

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Mol	Chain	Res	Type
1	2	1446	A
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1461	C
1	2	1462	G
1	2	1469	A
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1478	G
1	2	1482	C
1	2	1486	G
1	2	1487	A
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1506	G
1	2	1514	U
1	2	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1540	G
1	2	1557	U
1	2	1559	A
1	2	1574	G
1	2	1584	G
1	2	1590	G
1	2	1600	A
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1631	A
1	2	1635	A

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Mol	Chain	Res	Type
1	2	1639	C
1	2	1657	U
1	2	1658	G
1	2	1663	G
1	2	1680	G
1	2	1681	A
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1731	A
1	2	1750	A
1	2	1756	A
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	13	A
36	1	14	U
36	1	15	C
36	1	16	A
36	1	26	A
36	1	33	G
36	1	40	A
36	1	42	C
36	1	43	A
36	1	49	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	68	C
36	1	76	G

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Mol	Chain	Res	Type
36	1	83	U
36	1	92	G
36	1	93	C
36	1	94	G
36	1	99	A
36	1	102	C
36	1	105	C
36	1	109	A
36	1	110	G
36	1	111	C
36	1	117	U
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	147	U
36	1	150	A
36	1	156	G
36	1	157	A
36	1	160	G
36	1	166	C
36	1	170	G
36	1	173	G
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	210	U
36	1	211	A
36	1	213	A
36	1	218	G
36	1	219	A
36	1	224	C
36	1	240	U
36	1	241	G
36	1	243	G
36	1	245	U
36	1	248	U
36	1	249	U
36	1	250	U
36	1	251	G

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Mol	Chain	Res	Type
36	1	252	U
36	1	256	G
36	1	269	G
36	1	270	U
36	1	272	G
36	1	277	G
36	1	282	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	299	G
36	1	311	C
36	1	315	C
36	1	318	A
36	1	323	A
36	1	329	U
36	1	339	C
36	1	344	A
36	1	349	A
36	1	350	C
36	1	352	A
36	1	375	A
36	1	376	G
36	1	397	A
36	1	398	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	412	G
36	1	420	G
36	1	421	G
36	1	422	A
36	1	438	A
36	1	440	A
36	1	498	A
36	1	520	U
36	1	521	A
36	1	531	G
36	1	535	G
36	1	541	U
36	1	543	C

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Mol	Chain	Res	Type
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G
36	1	551	A
36	1	552	G
36	1	555	U
36	1	557	A
36	1	559	A
36	1	568	G
36	1	578	A
36	1	579	G
36	1	592	A
36	1	594	U
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	624	G
36	1	636	C
36	1	642	U
36	1	643	U
36	1	649	A
36	1	660	A
36	1	661	G
36	1	667	C
36	1	677	A
36	1	681	U
36	1	683	U
36	1	691	A
36	1	699	A
36	1	705	A
36	1	712	G
36	1	715	A
36	1	716	A
36	1	725	G
36	1	764	U
36	1	766	U
36	1	767	U
36	1	776	U

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Mol	Chain	Res	Type
36	1	777	U
36	1	780	A
36	1	781	G
36	1	784	A
36	1	785	G
36	1	791	A
36	1	792	G
36	1	806	A
36	1	816	A
36	1	817	A
36	1	830	A
36	1	849	C
36	1	861	C
36	1	874	U
36	1	879	U
36	1	880	G
36	1	887	G
36	1	890	C
36	1	896	A
36	1	907	G
36	1	908	G
36	1	910	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	919	U
36	1	921	A
36	1	923	C
36	1	924	G
36	1	937	G
36	1	944	C
36	1	953	G
36	1	959	C
36	1	960	U
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	994	G
36	1	1001	G
36	1	1002	A
36	1	1006	A

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Mol	Chain	Res	Type
36	1	1010	G
36	1	1013	G
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1037	C
36	1	1042	U
36	1	1045	C
36	1	1047	A
36	1	1049	C
36	1	1064	A
36	1	1065	A
36	1	1068	C
36	1	1071	U
36	1	1072	G
36	1	1079	A
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1087	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1129	A
36	1	1131	G
36	1	1153	A
36	1	1159	A
36	1	1161	G
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A

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Mol	Chain	Res	Type
36	1	1191	U
36	1	1192	C
36	1	1201	C
36	1	1202	A
36	1	1203	A
36	1	1209	G
36	1	1213	G
36	1	1216	C
36	1	1218	U
36	1	1222	G
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1251	A
36	1	1258	U
36	1	1259	A
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	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	1292	C
36	1	1293	U
36	1	1307	G
36	1	1308	A

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Mol	Chain	Res	Type
36	1	1309	U
36	1	1313	G
36	1	1319	G
36	1	1320	C
36	1	1330	A
36	1	1331	U
36	1	1348	U
36	1	1349	G
36	1	1350	A
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1379	G
36	1	1386	A
36	1	1399	A
36	1	1400	G
36	1	1419	A
36	1	1431	G
36	1	1433	A
36	1	1434	G
36	1	1437	C
36	1	1445	U
36	1	1446	A
36	1	1450	G
36	1	1455	U
36	1	1481	A
36	1	1482	A
36	1	1503	A
36	1	1506	A
36	1	1507	G
36	1	1508	C
36	1	1526	U
36	1	1527	C
36	1	1528	G
36	1	1534	A
36	1	1553	U
36	1	1556	C
36	1	1560	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	1576	G
36	1	1579	C
36	1	1580	A
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1593	A
36	1	1598	G
36	1	1599	G
36	1	1605	A
36	1	1607	U
36	1	1619	A
36	1	1620	U
36	1	1621	A
36	1	1629	U
36	1	1633	C
36	1	1639	C
36	1	1643	A
36	1	1644	C
36	1	1645	U
36	1	1646	G
36	1	1657	C
36	1	1664	G
36	1	1677	G
36	1	1679	A
36	1	1683	A
36	1	1688	U
36	1	1714	A
36	1	1716	U
36	1	1717	U
36	1	1724	U

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Mol	Chain	Res	Type
36	1	1725	C
36	1	1736	G
36	1	1741	A
36	1	1742	U
36	1	1749	A
36	1	1750	A
36	1	1751	G
36	1	1757	A
36	1	1761	C
36	1	1762	C
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1769	G
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	1814	A
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1839	A
36	1	1840	U
36	1	1841	A
36	1	1842	A
36	1	1846	C
36	1	1849	C
36	1	1850	A
36	1	1855	U
36	1	1871	U
36	1	1879	A
36	1	1880	U
36	1	1883	A
36	1	1884	A
36	1	1886	A
36	1	1893	A

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Mol	Chain	Res	Type
36	1	1906	G
36	1	1948	G
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	1954	G
36	1	2094	C
36	1	2101	C
36	1	2102	U
36	1	2110	G
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2114	C
36	1	2121	G
36	1	2122	G
36	1	2131	A
36	1	2134	G
36	1	2140	U
36	1	2144	A
36	1	2158	A
36	1	2169	G
36	1	2170	U
36	1	2179	C
36	1	2187	G
36	1	2188	A
36	1	2195	C
36	1	2205	U
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2223	A
36	1	2225	U
36	1	2228	A
36	1	2244	A
36	1	2245	C
36	1	2249	G
36	1	2254	U
36	1	2255	A
36	1	2256	A
36	1	2272	G
36	1	2273	G

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Mol	Chain	Res	Type
36	1	2281	A
36	1	2282	U
36	1	2284	C
36	1	2301	U
36	1	2303	A
36	1	2304	C
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2317	A
36	1	2319	U
36	1	2324	A
36	1	2330	C
36	1	2334	U
36	1	2335	G
36	1	2336	U
36	1	2361	A
36	1	2366	C
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2388	U
36	1	2393	G
36	1	2395	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2405	C
36	1	2406	C
36	1	2411	U
36	1	2417	U
36	1	2418	G
36	1	2419	A
36	1	2423	U
36	1	2428	U
36	1	2437	G
36	1	2444	C
36	1	2445	A

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Mol	Chain	Res	Type
36	1	2502	A
36	1	2503	G
36	1	2504	U
36	1	2513	U
36	1	2514	U
36	1	2515	A
36	1	2520	A
36	1	2522	G
36	1	2523	A
36	1	2532	U
36	1	2533	G
36	1	2534	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2547	A
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2560	C
36	1	2561	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2585	G
36	1	2586	G
36	1	2588	U
36	1	2593	A
36	1	2594	C
36	1	2595	A
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2622	C

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Mol	Chain	Res	Type
36	1	2623	G
36	1	2637	A
36	1	2638	C
36	1	2652	U
36	1	2656	A
36	1	2674	A
36	1	2675	C
36	1	2677	G
36	1	2681	U
36	1	2687	G
36	1	2689	A
36	1	2691	A
36	1	2694	A
36	1	2696	A
36	1	2705	A
36	1	2714	G
36	1	2728	G
36	1	2729	U
36	1	2749	G
36	1	2753	G
36	1	2755	C
36	1	2762	A
36	1	2772	C
36	1	2773	C
36	1	2777	G
36	1	2778	G
36	1	2780	A
36	1	2796	G
36	1	2797	C
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2803	A
36	1	2810	C
36	1	2817	A
36	1	2818	U
36	1	2819	A
36	1	2829	U
36	1	2830	G
36	1	2833	A
36	1	2834	G
36	1	2837	A

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Mol	Chain	Res	Type
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2847	A
36	1	2860	U
36	1	2871	G
36	1	2872	A
36	1	2887	A
36	1	2889	C
36	1	2898	G
36	1	2899	C
36	1	2914	G
36	1	2923	U
36	1	2927	C
36	1	2935	U
36	1	2936	A
36	1	2939	G
36	1	2942	C
36	1	2945	G
36	1	2947	G
36	1	2954	U
36	1	2971	A
36	1	2980	U
36	1	2983	C
36	1	2990	G
36	1	2992	U
36	1	2997	G
36	1	3006	A
36	1	3012	A
36	1	3030	G
36	1	3034	C
36	1	3037	U
36	1	3056	U
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3069	G
36	1	3078	U
36	1	3079	U
36	1	3086	A
36	1	3087	A
36	1	3091	A

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Mol	Chain	Res	Type
36	1	3092	C
36	1	3113	A
36	1	3119	U
36	1	3122	A
36	1	3130	A
36	1	3131	U
36	1	3142	A
36	1	3143	C
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3164	C
36	1	3165	A
36	1	3168	A
36	1	3169	U
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3186	A
36	1	3187	A
36	1	3195	U
36	1	3196	U
36	1	3198	U
36	1	3207	U
36	1	3210	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3229	G
36	1	3243	A
36	1	3244	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3259	U
36	1	3269	U

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Mol	Chain	Res	Type
36	1	3270	U
36	1	3272	C
36	1	3273	A
36	1	3276	G
36	1	3277	U
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3288	G
36	1	3289	G
36	1	3294	A
36	1	3295	A
36	1	3304	U
36	1	3309	G
36	1	3310	A
36	1	3313	U
36	1	3314	A
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3330	A
36	1	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	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
36	1	3396	U

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Mol	Chain	Res	Type
37	3	11	A
37	3	13	A
37	3	22	A
37	3	41	G
37	3	42	A
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	106	U
37	3	112	G
37	3	121	U
38	4	2	A
38	4	26	U
38	4	34	U
38	4	35	C
38	4	48	A
38	4	50	C
38	4	51	G
38	4	52	A
38	4	53	A
38	4	57	C
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	89	A
38	4	90	U
38	4	95	G
38	4	105	A
38	4	106	C

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Mol	Chain	Res	Type
38	4	111	A
38	4	113	U
38	4	125	U
38	4	126	A
38	4	128	U
38	4	133	G
38	4	138	A
38	4	148	G
38	4	152	G
38	4	158	U
1	6	2	A
1	6	4	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	42	G
1	6	47	A
1	6	50	C
1	6	57	G
1	6	60	U
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	71	A
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	100	A
1	6	103	A
1	6	104	A
1	6	111	U
1	6	114	C
1	6	115	G
1	6	127	G
1	6	130	C
1	6	132	U
1	6	137	U

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Mol	Chain	Res	Type
1	6	138	A
1	6	140	A
1	6	141	U
1	6	142	G
1	6	144	U
1	6	145	A
1	6	146	U
1	6	153	G
1	6	159	U
1	6	178	U
1	6	179	A
1	6	181	A
1	6	182	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	194	U
1	6	195	G
1	6	197	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	235	G
1	6	240	U
1	6	241	U
1	6	243	G
1	6	249	U

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Mol	Chain	Res	Type
1	6	250	C
1	6	261	U
1	6	262	U
1	6	265	A
1	6	270	C
1	6	271	A
1	6	272	U
1	6	273	G
1	6	275	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	287	G
1	6	290	G
1	6	299	A
1	6	301	A
1	6	308	C
1	6	313	U
1	6	314	C
1	6	316	A
1	6	319	U
1	6	321	C
1	6	322	G
1	6	337	G
1	6	338	C
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	362	G
1	6	393	C
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	417	A
1	6	418	G
1	6	421	A
1	6	424	C
1	6	425	A
1	6	426	G

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Mol	Chain	Res	Type
1	6	428	A
1	6	434	G
1	6	439	U
1	6	444	C
1	6	445	A
1	6	448	C
1	6	460	A
1	6	464	A
1	6	468	A
1	6	470	A
1	6	477	A
1	6	482	U
1	6	484	C
1	6	486	G
1	6	487	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	514	G
1	6	515	A
1	6	519	C
1	6	527	A
1	6	528	U
1	6	534	A
1	6	536	C
1	6	538	A
1	6	539	G

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Mol	Chain	Res	Type
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	565	C
1	6	566	C
1	6	568	G
1	6	574	G
1	6	578	U
1	6	579	A
1	6	580	A
1	6	582	U
1	6	594	A
1	6	595	G
1	6	606	A
1	6	609	U
1	6	617	U
1	6	619	A
1	6	620	A
1	6	623	A
1	6	624	G
1	6	639	U
1	6	640	U
1	6	648	G
1	6	649	U
1	6	652	G
1	6	653	C
1	6	658	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	669	G
1	6	670	U

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Mol	Chain	Res	Type
1	6	676	G
1	6	678	A
1	6	679	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C
1	6	695	U
1	6	696	C
1	6	697	C
1	6	698	U
1	6	705	U
1	6	710	U
1	6	711	U
1	6	714	G
1	6	717	C
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	723	G
1	6	730	G
1	6	733	A
1	6	734	A
1	6	742	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	765	G
1	6	766	U
1	6	774	A
1	6	775	G
1	6	777	C
1	6	780	A
1	6	781	U
1	6	782	U

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Mol	Chain	Res	Type
1	6	783	G
1	6	789	A
1	6	792	U
1	6	793	A
1	6	794	U
1	6	806	A
1	6	811	A
1	6	812	A
1	6	815	G
1	6	816	G
1	6	823	G
1	6	825	U
1	6	826	U
1	6	828	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	847	A
1	6	848	C
1	6	856	A
1	6	861	U
1	6	863	A
1	6	879	G
1	6	898	A
1	6	906	A
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	940	A
1	6	942	G
1	6	959	U
1	6	960	U
1	6	966	A
1	6	969	C
1	6	970	A
1	6	971	A
1	6	983	A

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Mol	Chain	Res	Type
1	6	992	A
1	6	993	A
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1021	C
1	6	1026	A
1	6	1028	C
1	6	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	1067	C
1	6	1070	C
1	6	1071	U
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	1100	G
1	6	1104	U
1	6	1109	G
1	6	1111	G
1	6	1138	A
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1167	G
1	6	1185	U
1	6	1191	U
1	6	1194	A
1	6	1196	A

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Mol	Chain	Res	Type
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1206	U
1	6	1212	G
1	6	1216	C
1	6	1217	A
1	6	1218	G
1	6	1220	C
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1231	U
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	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1261	G
1	6	1262	U
1	6	1270	G
1	6	1284	C
1	6	1286	U
1	6	1288	G
1	6	1290	U
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1338	C
1	6	1344	A
1	6	1345	A
1	6	1346	A

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Mol	Chain	Res	Type
1	6	1347	U
1	6	1354	G
1	6	1355	C
1	6	1361	U
1	6	1363	U
1	6	1364	G
1	6	1371	A
1	6	1372	U
1	6	1373	C
1	6	1377	U
1	6	1383	G
1	6	1385	G
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1413	U
1	6	1414	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1433	G
1	6	1445	G
1	6	1448	G
1	6	1458	G
1	6	1459	C
1	6	1461	C
1	6	1469	A
1	6	1471	A
1	6	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	1497	U
1	6	1500	C
1	6	1506	G
1	6	1514	U

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Mol	Chain	Res	Type
1	6	1515	A
1	6	1516	A
1	6	1523	G
1	6	1524	A
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1539	G
1	6	1540	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1568	C
1	6	1569	A
1	6	1572	G
1	6	1573	A
1	6	1574	G
1	6	1575	G
1	6	1582	U
1	6	1584	G
1	6	1590	G
1	6	1601	G
1	6	1616	G
1	6	1621	U
1	6	1631	A
1	6	1634	C
1	6	1637	C
1	6	1638	G
1	6	1656	U
1	6	1657	U
1	6	1658	G
1	6	1678	A
1	6	1683	C
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1712	A
1	6	1715	G

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Mol	Chain	Res	Type
1	6	1716	C
1	6	1717	G
1	6	1723	U
1	6	1727	G
1	6	1731	A
1	6	1736	G
1	6	1745	G
1	6	1756	A
1	6	1760	G
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	24	G
36	5	26	A
36	5	40	A
36	5	43	A
36	5	49	A
36	5	60	A
36	5	65	A
36	5	66	A
36	5	68	C
36	5	73	C
36	5	74	G
36	5	76	G
36	5	85	A
36	5	89	A
36	5	92	G
36	5	96	G
36	5	99	A
36	5	109	A
36	5	110	G

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Mol	Chain	Res	Type
36	5	113	C
36	5	116	A
36	5	117	U
36	5	120	G
36	5	121	A
36	5	122	A
36	5	126	U
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	155	G
36	5	156	G
36	5	157	A
36	5	165	A
36	5	170	G
36	5	171	G
36	5	172	G
36	5	173	G
36	5	174	C
36	5	180	C
36	5	182	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	209	A
36	5	210	U
36	5	211	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	227	G
36	5	236	G
36	5	238	A
36	5	239	G
36	5	240	U
36	5	244	G
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U

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Mol	Chain	Res	Type
36	5	253	A
36	5	254	A
36	5	258	G
36	5	259	C
36	5	264	G
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	338	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	359	U
36	5	370	U
36	5	372	A
36	5	376	G
36	5	395	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	404	G
36	5	419	G
36	5	421	G
36	5	422	A
36	5	438	A
36	5	439	C
36	5	440	A
36	5	442	G
36	5	443	G
36	5	492	U
36	5	495	G
36	5	507	U
36	5	515	C
36	5	521	A
36	5	535	G
36	5	542	G

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Mol	Chain	Res	Type
36	5	546	C
36	5	547	G
36	5	548	G
36	5	553	U
36	5	555	U
36	5	557	A
36	5	559	A
36	5	578	A
36	5	579	G
36	5	581	U
36	5	592	A
36	5	594	U
36	5	595	G
36	5	600	G
36	5	604	G
36	5	607	A
36	5	608	A
36	5	609	G
36	5	611	A
36	5	619	A
36	5	620	U
36	5	621	A
36	5	636	C
36	5	649	A
36	5	651	G
36	5	653	A
36	5	660	A
36	5	677	A
36	5	681	U
36	5	691	A
36	5	705	A
36	5	712	G
36	5	715	A
36	5	716	A
36	5	719	U
36	5	725	G
36	5	727	G
36	5	736	A
36	5	747	A
36	5	766	U
36	5	767	U
36	5	768	C

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Mol	Chain	Res	Type
36	5	775	A
36	5	776	U
36	5	777	U
36	5	780	A
36	5	781	G
36	5	785	G
36	5	786	A
36	5	806	A
36	5	817	A
36	5	823	C
36	5	830	A
36	5	851	C
36	5	861	C
36	5	865	U
36	5	874	U
36	5	879	U
36	5	883	A
36	5	889	U
36	5	891	G
36	5	896	A
36	5	897	U
36	5	907	G
36	5	908	G
36	5	910	G
36	5	913	A
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	924	G
36	5	937	G
36	5	944	C
36	5	948	C
36	5	959	C
36	5	960	U
36	5	961	C
36	5	963	G
36	5	979	U
36	5	981	U
36	5	983	A
36	5	993	G
36	5	994	G

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Mol	Chain	Res	Type
36	5	1001	G
36	5	1002	A
36	5	1003	A
36	5	1006	A
36	5	1010	G
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1019	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1027	A
36	5	1028	U
36	5	1029	G
36	5	1035	G
36	5	1041	U
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1072	G
36	5	1081	U
36	5	1082	U
36	5	1083	G
36	5	1085	A
36	5	1087	G
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1117	G
36	5	1131	G
36	5	1152	G
36	5	1153	A
36	5	1159	A

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Mol	Chain	Res	Type
36	5	1160	C
36	5	1172	G
36	5	1179	A
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1191	U
36	5	1192	C
36	5	1196	C
36	5	1201	C
36	5	1203	A
36	5	1209	G
36	5	1217	A
36	5	1218	U
36	5	1222	G
36	5	1225	A
36	5	1232	C
36	5	1236	G
36	5	1237	G
36	5	1238	C
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	1258	U
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1284	C
36	5	1285	G
36	5	1292	C
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1313	G
36	5	1330	A
36	5	1331	U
36	5	1348	U

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Mol	Chain	Res	Type
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1354	G
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1386	A
36	5	1399	A
36	5	1400	G
36	5	1405	U
36	5	1418	A
36	5	1419	A
36	5	1422	G
36	5	1428	A
36	5	1431	G
36	5	1433	A
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1460	A
36	5	1465	A
36	5	1468	A
36	5	1480	G
36	5	1481	A
36	5	1482	A
36	5	1490	A
36	5	1503	A
36	5	1508	C
36	5	1528	G
36	5	1533	U
36	5	1536	G
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1563	C
36	5	1564	U

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Mol	Chain	Res	Type
36	5	1565	G
36	5	1566	A
36	5	1567	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1593	A
36	5	1620	U
36	5	1629	U
36	5	1635	G
36	5	1639	C
36	5	1641	U
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1655	G
36	5	1658	G
36	5	1677	G
36	5	1682	U
36	5	1713	G
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1725	C
36	5	1741	A
36	5	1746	U
36	5	1750	A
36	5	1751	G
36	5	1756	C
36	5	1762	C
36	5	1764	U

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Mol	Chain	Res	Type
36	5	1765	U
36	5	1766	G
36	5	1769	G
36	5	1770	G
36	5	1780	G
36	5	1795	U
36	5	1797	A
36	5	1810	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1821	U
36	5	1822	C
36	5	1829	G
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1847	A
36	5	1849	C
36	5	1850	A
36	5	1851	G
36	5	1864	A
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1891	A
36	5	1893	A
36	5	1895	A
36	5	1901	A
36	5	1906	G
36	5	1920	U
36	5	1935	G
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2111	G
36	5	2112	U
36	5	2113	A
36	5	2117	A
36	5	2121	G

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Mol	Chain	Res	Type
36	5	2122	G
36	5	2131	A
36	5	2140	U
36	5	2144	A
36	5	2158	A
36	5	2169	G
36	5	2192	C
36	5	2198	A
36	5	2205	U
36	5	2206	G
36	5	2207	A
36	5	2210	G
36	5	2215	A
36	5	2222	A
36	5	2223	A
36	5	2228	A
36	5	2234	G
36	5	2237	C
36	5	2244	A
36	5	2246	G
36	5	2249	G
36	5	2250	G
36	5	2252	A
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2267	C
36	5	2273	G
36	5	2278	C
36	5	2279	A
36	5	2280	A
36	5	2287	C
36	5	2288	G
36	5	2303	A
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2318	U
36	5	2327	U
36	5	2334	U
36	5	2336	U

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Mol	Chain	Res	Type
36	5	2366	C
36	5	2367	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2393	G
36	5	2397	A
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2411	U
36	5	2418	G
36	5	2420	C
36	5	2422	C
36	5	2423	U
36	5	2437	G
36	5	2439	A
36	5	2441	A
36	5	2443	A
36	5	2504	U
36	5	2505	U
36	5	2506	U
36	5	2507	C
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2514	U
36	5	2515	A
36	5	2517	U
36	5	2518	C
36	5	2523	A
36	5	2524	A
36	5	2526	C
36	5	2530	G
36	5	2531	C
36	5	2532	U
36	5	2534	G
36	5	2536	A
36	5	2537	U

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Mol	Chain	Res	Type
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2541	U
36	5	2543	U
36	5	2552	C
36	5	2555	G
36	5	2562	A
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2587	U
36	5	2588	U
36	5	2589	G
36	5	2593	A
36	5	2606	G
36	5	2607	G
36	5	2614	G
36	5	2615	G
36	5	2626	A
36	5	2637	A
36	5	2639	G
36	5	2652	U
36	5	2656	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
36	5	2696	A
36	5	2705	A
36	5	2714	G

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Mol	Chain	Res	Type
36	5	2720	G
36	5	2727	A
36	5	2728	G
36	5	2729	U
36	5	2737	C
36	5	2742	C
36	5	2752	U
36	5	2753	G
36	5	2755	C
36	5	2762	A
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2779	A
36	5	2780	A
36	5	2783	U
36	5	2796	G
36	5	2797	C
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2802	A
36	5	2810	C
36	5	2814	G
36	5	2817	A
36	5	2818	U
36	5	2819	A
36	5	2829	U
36	5	2842	U
36	5	2843	U
36	5	2844	C
36	5	2845	A
36	5	2847	A
36	5	2853	A
36	5	2871	G
36	5	2872	A
36	5	2880	U
36	5	2882	U
36	5	2886	U
36	5	2887	A
36	5	2889	C

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Mol	Chain	Res	Type
36	5	2896	A
36	5	2897	A
36	5	2899	C
36	5	2900	A
36	5	2901	G
36	5	2912	G
36	5	2921	U
36	5	2922	G
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2937	G
36	5	2942	C
36	5	2945	G
36	5	2947	G
36	5	2957	G
36	5	2971	A
36	5	2972	G
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3018	C
36	5	3029	A
36	5	3030	G
36	5	3049	A
36	5	3056	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3092	C
36	5	3102	G
36	5	3104	U
36	5	3122	A
36	5	3123	A
36	5	3127	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	3150	A
36	5	3153	U
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3159	C
36	5	3164	C
36	5	3165	A
36	5	3168	A
36	5	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	3196	U
36	5	3198	U
36	5	3207	U
36	5	3208	G
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3223	A
36	5	3224	G
36	5	3227	A
36	5	3228	C
36	5	3229	G
36	5	3238	G
36	5	3239	G
36	5	3244	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3263	G

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Mol	Chain	Res	Type
36	5	3270	U
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3279	A
36	5	3281	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	3307	A
36	5	3310	A
36	5	3313	U
36	5	3316	A
36	5	3317	U
36	5	3319	U
36	5	3320	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3355	U
36	5	3358	U
36	5	3369	G
36	5	3378	C
36	5	3389	U
36	5	3390	G
36	5	3393	U
36	5	3394	U
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	23	A
37	7	25	G
37	7	27	A

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Mol	Chain	Res	Type
37	7	38	U
37	7	41	G
37	7	45	A
37	7	49	G
37	7	52	G
37	7	53	U
37	7	54	U
37	7	55	A
37	7	60	G
37	7	65	G
37	7	73	C
37	7	74	C
37	7	75	G
37	7	76	A
37	7	91	G
37	7	101	G
37	7	102	A
37	7	112	G
37	7	121	U
38	8	21	C
38	8	34	U
38	8	35	C
38	8	43	A
38	8	48	A
38	8	53	A
38	8	59	A
38	8	62	C
38	8	63	G
38	8	76	C
38	8	79	A
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	86	U
38	8	87	G
38	8	90	U
38	8	95	G
38	8	97	A
38	8	102	U
38	8	104	A

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Mol	Chain	Res	Type
38	8	105	A
38	8	106	C
38	8	108	C
38	8	111	A
38	8	113	U
38	8	115	C
38	8	122	U
38	8	124	G
38	8	125	U
38	8	126	A
38	8	152	G
38	8	156	U
38	8	157	U
38	8	158	U

All (277) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	73	U
1	2	74	U
1	2	103	A
1	2	114	C
1	2	126	A
1	2	130	C
1	2	131	C
1	2	136	C
1	2	139	C
1	2	144	U
1	2	158	U
1	2	187	G
1	2	192	U
1	2	218	A
1	2	240	U
1	2	278	U
1	2	280	U
1	2	322	G
1	2	417	A
1	2	497	G
1	2	499	U

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Mol	Chain	Res	Type
1	2	501	U
1	2	503	G
1	2	512	A
1	2	558	U
1	2	582	U
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	734	A
1	2	755	A
1	2	794	U
1	2	811	A
1	2	823	G
1	2	829	A
1	2	1058	U
1	2	1137	A
1	2	1157	A
1	2	1196	A
1	2	1226	A
1	2	1234	A
1	2	1244	A
1	2	1250	U
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1489	U
1	2	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	169	U
36	1	210	U
36	1	217	U
36	1	223	U
36	1	239	G
36	1	282	G
36	1	285	A
36	1	397	A

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Mol	Chain	Res	Type
36	1	547	G
36	1	588	G
36	1	594	U
36	1	715	A
36	1	719	U
36	1	763	G
36	1	816	A
36	1	896	A
36	1	916	G
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1181	U
36	1	1273	A
36	1	1291	A
36	1	1307	G
36	1	1317	A
36	1	1329	U
36	1	1352	A
36	1	1355	A
36	1	1467	A
36	1	1562	C
36	1	1568	U
36	1	1716	U
36	1	1724	U
36	1	1751	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	2101	C
36	1	2109	U
36	1	2112	U
36	1	2209	U
36	1	2227	C
36	1	2281	A
36	1	2360	C

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Mol	Chain	Res	Type
36	1	2372	A
36	1	2374	C
36	1	2403	G
36	1	2418	G
36	1	2513	U
36	1	2537	U
36	1	2541	U
36	1	2585	G
36	1	2704	A
36	1	2728	G
36	1	2772	C
36	1	2818	U
36	1	2842	U
36	1	2996	U
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3169	U
36	1	3195	U
36	1	3218	A
36	1	3228	C
36	1	3242	G
36	1	3269	U
36	1	3275	U
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
36	1	3377	G
36	1	3382	U
38	4	85	G
38	4	125	U
1	6	25	C
1	6	66	U
1	6	76	A
1	6	103	A
1	6	114	C
1	6	139	C
1	6	145	A
1	6	158	U
1	6	187	G

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Mol	Chain	Res	Type
1	6	192	U
1	6	217	A
1	6	218	A
1	6	240	U
1	6	400	A
1	6	417	A
1	6	468	A
1	6	488	G
1	6	512	A
1	6	542	A
1	6	543	C
1	6	557	G
1	6	558	U
1	6	606	A
1	6	651	G
1	6	664	U
1	6	695	U
1	6	697	C
1	6	717	C
1	6	755	A
1	6	828	U
1	6	829	A
1	6	834	G
1	6	944	A
1	6	1004	U
1	6	1051	G
1	6	1058	U
1	6	1097	U
1	6	1238	A
1	6	1244	A
1	6	1255	G
1	6	1269	U
1	6	1314	U
1	6	1344	A
1	6	1346	A
1	6	1481	C
1	6	1489	U
1	6	1491	U
1	6	1535	U
1	6	1568	C
1	6	1572	G
1	6	1573	A

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Mol	Chain	Res	Type
1	6	1615	C
1	6	1620	C
1	6	1657	U
1	6	1696	G
1	6	1698	G
1	6	1700	C
36	5	43	A
36	5	210	U
36	5	217	U
36	5	238	A
36	5	397	A
36	5	588	G
36	5	647	A
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	960	U
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1236	G
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1481	A
36	5	1514	G
36	5	1554	U
36	5	1560	G
36	5	1580	A
36	5	1716	U
36	5	1815	U
36	5	1816	A

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Mol	Chain	Res	Type
36	5	1841	A
36	5	1846	C
36	5	1878	G
36	5	2101	C
36	5	2112	U
36	5	2204	C
36	5	2209	U
36	5	2255	A
36	5	2372	A
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2531	C
36	5	2539	C
36	5	2586	G
36	5	2682	C
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2817	A
36	5	2818	U
36	5	2887	A
36	5	2896	A
36	5	2971	A
36	5	2979	U
36	5	3055	U
36	5	3078	U
36	5	3121	U
36	5	3167	A
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3269	U
36	5	3271	G
36	5	3275	U
36	5	3289	G
36	5	3340	G
36	5	3341	U
36	5	3354	U
36	5	3357	U
37	7	49	G
38	8	86	U

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Mol	Chain	Res	Type
38	8	156	U

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 2563 ligands modelled in this entry, 1424 are monoatomic - leaving 1139 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	$\# Z > 2$
88	OHX	1	3897	-	0,6,6	-	-	-		
88	OHX	5	4017	-	0,6,6	-	-	-		
88	OHX	5	4215	-	0,6,6	-	-	-		
88	OHX	5	4168	-	0,6,6	-	-	-		
88	OHX	5	4082	-	0,6,6	-	-	-		
88	OHX	5	3980	-	0,6,6	-	-	-		
88	OHX	5	3989	-	0,6,6	-	-	-		
88	OHX	2	2044	-	0,6,6	-	-	-		
88	OHX	5	4074	-	0,6,6	-	-	-		
88	OHX	5	4076	-	0,6,6	-	-	-		
88	OHX	5	3924	-	0,6,6	-	-	-		
88	OHX	5	4165	-	0,6,6	-	-	-		
88	OHX	5	3948	-	0,6,6	-	-	-		
88	OHX	5	3995	-	0,6,6	-	-	-		
88	OHX	m1	203	-	0,6,6	-	-	-		
88	OHX	5	4084	-	0,6,6	-	-	-		
88	OHX	6	2192	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	2	2112	-	0,6,6	-	-	-		
88	OHX	2	2122	-	0,6,6	-	-	-		
88	OHX	1	3952	-	0,6,6	-	-	-		
88	OHX	1	4162	-	0,6,6	-	-	-		
88	OHX	1	4003	-	0,6,6	-	-	-		
88	OHX	2	2169	-	0,6,6	-	-	-		
88	OHX	N9	101	-	0,6,6	-	-	-		
88	OHX	5	4070	-	0,6,6	-	-	-		
88	OHX	1	4048	-	0,6,6	-	-	-		
88	OHX	5	4073	-	0,6,6	-	-	-		
88	OHX	3	223	-	0,6,6	-	-	-		
88	OHX	L3	405	-	0,6,6	-	-	-		
88	OHX	1	4062	-	0,6,6	-	-	-		
88	OHX	1	3958	-	0,6,6	-	-	-		
88	OHX	1	4054	-	0,6,6	-	-	-		
88	OHX	5	4182	-	0,6,6	-	-	-		
91	C	q2	502	-	18,21,22	0.37	0	26,30,33	0.63	0
88	OHX	1	4142	-	0,6,6	-	-	-		
88	OHX	1	3982	-	0,6,6	-	-	-		
88	OHX	5	4208	-	0,6,6	-	-	-		
88	OHX	5	4237	-	0,6,6	-	-	-		
88	OHX	8	219	-	0,6,6	-	-	-		
88	OHX	1	4134	-	0,6,6	-	-	-		
88	OHX	2	2173	-	0,6,6	-	-	-		
88	OHX	4	225	-	0,6,6	-	-	-		
88	OHX	6	2199	-	0,6,6	-	-	-		
88	OHX	SR	401	-	0,6,6	-	-	-		
88	OHX	5	3984	-	0,6,6	-	-	-		
88	OHX	5	4079	-	0,6,6	-	-	-		
88	OHX	5	4218	-	0,6,6	-	-	-		
88	OHX	2	2127	-	0,6,6	-	-	-		
88	OHX	2	2137	-	0,6,6	-	-	-		
88	OHX	5	4201	-	0,6,6	-	-	-		
88	OHX	4	222	-	0,6,6	-	-	-		
88	OHX	2	2149	-	0,6,6	-	-	-		
88	OHX	2	2111	-	0,6,6	-	-	-		
88	OHX	5	4127	-	0,6,6	-	-	-		
88	OHX	1	4035	-	0,6,6	-	-	-		
88	OHX	5	4106	-	0,6,6	-	-	-		
88	OHX	5	3946	-	0,6,6	-	-	-		
88	OHX	1	3927	-	0,6,6	-	-	-		
88	OHX	8	223	-	0,6,6	-	-	-		
88	OHX	o7	502	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	3957	-	0,6,6	-	-	-		
88	OHX	2	2148	-	0,6,6	-	-	-		
88	OHX	5	4022	-	0,6,6	-	-	-		
88	OHX	5	4001	-	0,6,6	-	-	-		
88	OHX	5	3910	-	0,6,6	-	-	-		
88	OHX	2	2142	-	0,6,6	-	-	-		
88	OHX	1	4127	-	0,6,6	-	-	-		
88	OHX	1	4187	-	0,6,6	-	-	-		
88	OHX	6	2169	-	0,6,6	-	-	-		
88	OHX	1	4102	-	0,6,6	-	-	-		
88	OHX	5	4089	-	0,6,6	-	-	-		
88	OHX	8	230	-	0,6,6	-	-	-		
88	OHX	2	2095	-	0,6,6	-	-	-		
88	OHX	5	4232	-	0,6,6	-	-	-		
88	OHX	6	2054	-	0,6,6	-	-	-		
88	OHX	6	2141	-	0,6,6	-	-	-		
88	OHX	1	4166	-	0,6,6	-	-	-		
88	OHX	6	2135	-	0,6,6	-	-	-		
88	OHX	1	4176	-	0,6,6	-	-	-		
88	OHX	1	3898	-	0,6,6	-	-	-		
88	OHX	5	4019	-	0,6,6	-	-	-		
88	OHX	5	4147	-	0,6,6	-	-	-		
88	OHX	2	2153	-	0,6,6	-	-	-		
88	OHX	M7	205	-	0,6,6	-	-	-		
88	OHX	5	4023	-	0,6,6	-	-	-		
88	OHX	1	4178	-	0,6,6	-	-	-		
88	OHX	1	4024	-	0,6,6	-	-	-		
88	OHX	1	4186	-	0,6,6	-	-	-		
88	OHX	7	220	-	0,6,6	-	-	-		
88	OHX	L3	406	-	0,6,6	-	-	-		
88	OHX	5	4009	-	0,6,6	-	-	-		
88	OHX	1	4219	-	0,6,6	-	-	-		
88	OHX	2	2125	-	0,6,6	-	-	-		
88	OHX	1	4068	-	0,6,6	-	-	-		
88	OHX	1	4073	-	0,6,6	-	-	-		
88	OHX	5	3983	-	0,6,6	-	-	-		
88	OHX	2	2093	-	0,6,6	-	-	-		
88	OHX	5	4154	-	0,6,6	-	-	-		
88	OHX	1	4199	-	0,6,6	-	-	-		
88	OHX	6	2106	-	0,6,6	-	-	-		
88	OHX	7	226	-	0,6,6	-	-	-		
88	OHX	5	4095	-	0,6,6	-	-	-		
88	OHX	6	2084	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	6	2179	-	0,6,6	-	-	-		
88	OHX	5	3962	-	0,6,6	-	-	-		
88	OHX	1	4159	-	0,6,6	-	-	-		
88	OHX	2	2029	-	0,6,6	-	-	-		
88	OHX	1	3938	-	0,6,6	-	-	-		
88	OHX	1	4222	-	0,6,6	-	-	-		
88	OHX	2	2176	-	0,6,6	-	-	-		
88	OHX	5	3952	-	0,6,6	-	-	-		
88	OHX	6	2160	-	0,6,6	-	-	-		
88	OHX	2	2079	-	0,6,6	-	-	-		
88	OHX	2	2158	-	0,6,6	-	-	-		
88	OHX	5	4146	-	0,6,6	-	-	-		
88	OHX	6	2062	-	0,6,6	-	-	-		
88	OHX	6	2059	-	0,6,6	-	-	-		
88	OHX	5	3958	-	0,6,6	-	-	-		
88	OHX	5	4129	-	0,6,6	-	-	-		
88	OHX	2	2102	-	0,6,6	-	-	-		
88	OHX	1	3884	-	0,6,6	-	-	-		
88	OHX	5	4034	-	0,6,6	-	-	-		
88	OHX	1	4198	-	0,6,6	-	-	-		
88	OHX	5	3968	-	0,6,6	-	-	-		
88	OHX	6	2060	-	0,6,6	-	-	-		
88	OHX	15	304	-	0,6,6	-	-	-		
88	OHX	O7	104	-	0,6,6	-	-	-		
88	OHX	5	4238	-	0,6,6	-	-	-		
88	OHX	1	4175	-	0,6,6	-	-	-		
88	OHX	1	4098	-	0,6,6	-	-	-		
88	OHX	6	2070	-	0,6,6	-	-	-		
88	OHX	5	3922	-	0,6,6	-	-	-		
88	OHX	2	2161	-	0,6,6	-	-	-		
88	OHX	1	4116	-	0,6,6	-	-	-		
88	OHX	5	3923	-	0,6,6	-	-	-		
88	OHX	2	2045	-	0,6,6	-	-	-		
88	OHX	3	217	-	0,6,6	-	-	-		
88	OHX	1	4104	-	0,6,6	-	-	-		
88	OHX	2	2026	-	0,6,6	-	-	-		
88	OHX	1	4220	-	0,6,6	-	-	-		
88	OHX	6	2154	-	0,6,6	-	-	-		
90	A	5	3401	-	18,24,25	0.68	0	18,35,38	0.99	1 (5%)
88	OHX	2	2052	-	0,6,6	-	-	-		
88	OHX	7	218	-	0,6,6	-	-	-		
88	OHX	2	2134	-	0,6,6	-	-	-		
88	OHX	1	3988	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4096	-	0,6,6	-	-	-		
88	OHX	2	2027	-	0,6,6	-	-	-		
88	OHX	1	3943	-	0,6,6	-	-	-		
88	OHX	2	2155	-	0,6,6	-	-	-		
88	OHX	5	4189	-	0,6,6	-	-	-		
88	OHX	2	2141	-	0,6,6	-	-	-		
88	OHX	6	2187	-	0,6,6	-	-	-		
88	OHX	5	4054	-	0,6,6	-	-	-		
88	OHX	1	4029	-	0,6,6	-	-	-		
88	OHX	6	2050	-	0,6,6	-	-	-		
88	OHX	1	4128	-	0,6,6	-	-	-		
88	OHX	6	2202	-	0,6,6	-	-	-		
88	OHX	1	4157	-	0,6,6	-	-	-		
88	OHX	2	2060	-	0,6,6	-	-	-		
88	OHX	1	3873	-	0,6,6	-	-	-		
88	OHX	5	4149	-	0,6,6	-	-	-		
88	OHX	5	4166	-	0,6,6	-	-	-		
88	OHX	5	4162	-	0,6,6	-	-	-		
88	OHX	1	4124	-	0,6,6	-	-	-		
88	OHX	5	4003	-	0,6,6	-	-	-		
88	OHX	5	4179	-	0,6,6	-	-	-		
88	OHX	1	4096	-	0,6,6	-	-	-		
88	OHX	5	4239	-	0,6,6	-	-	-		
88	OHX	6	2053	-	0,6,6	-	-	-		
88	OHX	6	2173	-	0,6,6	-	-	-		
88	OHX	5	4145	-	0,6,6	-	-	-		
88	OHX	5	4062	-	0,6,6	-	-	-		
88	OHX	6	2104	-	0,6,6	-	-	-		
88	OHX	5	4242	-	0,6,6	-	-	-		
88	OHX	1	4025	-	0,6,6	-	-	-		
88	OHX	5	4068	-	0,6,6	-	-	-		
88	OHX	2	2051	-	0,6,6	-	-	-		
88	OHX	5	3901	-	0,6,6	-	-	-		
88	OHX	5	3966	-	0,6,6	-	-	-		
88	OHX	13	404	-	0,6,6	-	-	-		
88	OHX	6	2047	-	0,6,6	-	-	-		
88	OHX	2	2154	-	0,6,6	-	-	-		
88	OHX	5	3982	-	0,6,6	-	-	-		
88	OHX	2	2157	-	0,6,6	-	-	-		
88	OHX	1	4121	-	0,6,6	-	-	-		
88	OHX	5	3976	-	0,6,6	-	-	-		
88	OHX	5	4027	-	0,6,6	-	-	-		
88	OHX	5	4078	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4245	-	0,6,6	-	-	-		
88	OHX	1	3968	-	0,6,6	-	-	-		
91	C	Q2	502	-	18,21,22	0.40	0	26,30,33	0.75	0
88	OHX	5	4227	-	0,6,6	-	-	-		
88	OHX	5	4063	-	0,6,6	-	-	-		
88	OHX	5	3955	-	0,6,6	-	-	-		
88	OHX	d4	202	-	0,6,6	-	-	-		
88	OHX	5	4139	-	0,6,6	-	-	-		
88	OHX	5	4029	-	0,6,6	-	-	-		
88	OHX	2	2046	-	0,6,6	-	-	-		
88	OHX	1	3974	-	0,6,6	-	-	-		
88	OHX	5	3999	-	0,6,6	-	-	-		
88	OHX	5	4060	-	0,6,6	-	-	-		
88	OHX	5	4125	-	0,6,6	-	-	-		
88	OHX	1	3977	-	0,6,6	-	-	-		
88	OHX	6	2097	-	0,6,6	-	-	-		
88	OHX	2	2171	-	0,6,6	-	-	-		
88	OHX	6	2180	-	0,6,6	-	-	-		
88	OHX	1	3964	-	0,6,6	-	-	-		
88	OHX	1	4110	-	0,6,6	-	-	-		
88	OHX	5	3964	-	0,6,6	-	-	-		
88	OHX	2	2037	-	0,6,6	-	-	-		
88	OHX	2	2028	-	0,6,6	-	-	-		
88	OHX	1	3885	-	0,6,6	-	-	-		
88	OHX	5	4102	-	0,6,6	-	-	-		
88	OHX	8	224	-	0,6,6	-	-	-		
88	OHX	1	3981	-	0,6,6	-	-	-		
88	OHX	5	3990	-	0,6,6	-	-	-		
88	OHX	5	4206	-	0,6,6	-	-	-		
88	OHX	C8	201	-	0,6,6	-	-	-		
88	OHX	5	4105	-	0,6,6	-	-	-		
88	OHX	5	4180	-	0,6,6	-	-	-		
88	OHX	1	4181	-	0,6,6	-	-	-		
88	OHX	6	2130	-	0,6,6	-	-	-		
88	OHX	5	3942	-	0,6,6	-	-	-		
88	OHX	6	2177	-	0,6,6	-	-	-		
88	OHX	6	2123	-	0,6,6	-	-	-		
88	OHX	5	4205	-	0,6,6	-	-	-		
88	OHX	6	2115	-	0,6,6	-	-	-		
88	OHX	5	4225	-	0,6,6	-	-	-		
88	OHX	c1	202	-	0,6,6	-	-	-		
88	OHX	1	4223	-	0,6,6	-	-	-		
88	OHX	6	2152	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	3903	-	0,6,6	-	-	-	-	-
88	OHX	2	2166	-	0,6,6	-	-	-	-	-
88	OHX	5	3935	-	0,6,6	-	-	-	-	-
88	OHX	1	4021	-	0,6,6	-	-	-	-	-
88	OHX	6	2120	-	0,6,6	-	-	-	-	-
88	OHX	2	2144	-	0,6,6	-	-	-	-	-
88	OHX	1	3931	-	0,6,6	-	-	-	-	-
88	OHX	1	4145	-	0,6,6	-	-	-	-	-
88	OHX	14	404	-	0,6,6	-	-	-	-	-
88	OHX	2	2065	-	0,6,6	-	-	-	-	-
88	OHX	1	4131	-	0,6,6	-	-	-	-	-
88	OHX	1	4101	-	0,6,6	-	-	-	-	-
88	OHX	2	2180	-	0,6,6	-	-	-	-	-
88	OHX	1	4183	-	0,6,6	-	-	-	-	-
88	OHX	6	2190	-	0,6,6	-	-	-	-	-
88	OHX	2	2050	-	0,6,6	-	-	-	-	-
88	OHX	14	403	-	0,6,6	-	-	-	-	-
88	OHX	8	217	-	0,6,6	-	-	-	-	-
88	OHX	2	2090	-	0,6,6	-	-	-	-	-
88	OHX	5	4041	-	0,6,6	-	-	-	-	-
88	OHX	5	4142	-	0,6,6	-	-	-	-	-
88	OHX	5	4196	-	0,6,6	-	-	-	-	-
88	OHX	1	3951	-	0,6,6	-	-	-	-	-
88	OHX	6	2185	-	0,6,6	-	-	-	-	-
88	OHX	1	3908	-	0,6,6	-	-	-	-	-
88	OHX	5	4100	-	0,6,6	-	-	-	-	-
88	OHX	2	2105	-	0,6,6	-	-	-	-	-
88	OHX	1	3915	-	0,6,6	-	-	-	-	-
88	OHX	1	4055	-	0,6,6	-	-	-	-	-
88	OHX	3	218	-	0,6,6	-	-	-	-	-
88	OHX	6	2196	-	0,6,6	-	-	-	-	-
88	OHX	5	4000	-	0,6,6	-	-	-	-	-
88	OHX	1	4185	-	0,6,6	-	-	-	-	-
88	OHX	5	4049	-	0,6,6	-	-	-	-	-
88	OHX	5	4080	-	0,6,6	-	-	-	-	-
88	OHX	6	2175	-	0,6,6	-	-	-	-	-
88	OHX	5	4246	-	0,6,6	-	-	-	-	-
88	OHX	5	4153	-	0,6,6	-	-	-	-	-
88	OHX	5	4175	-	0,6,6	-	-	-	-	-
88	OHX	5	4004	-	0,6,6	-	-	-	-	-
88	OHX	5	4249	-	0,6,6	-	-	-	-	-
88	OHX	6	2195	-	0,6,6	-	-	-	-	-
88	OHX	6	2153	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	4032	-	0,6,6	-	-	-		
88	OHX	6	2058	-	0,6,6	-	-	-		
88	OHX	5	4006	-	0,6,6	-	-	-		
88	OHX	1	3879	-	0,6,6	-	-	-		
88	OHX	1	3950	-	0,6,6	-	-	-		
88	OHX	6	2068	-	0,6,6	-	-	-		
88	OHX	6	2144	-	0,6,6	-	-	-		
88	OHX	5	3950	-	0,6,6	-	-	-		
88	OHX	1	4064	-	0,6,6	-	-	-		
88	OHX	5	3963	-	0,6,6	-	-	-		
88	OHX	2	2064	-	0,6,6	-	-	-		
88	OHX	1	3906	-	0,6,6	-	-	-		
88	OHX	1	3949	-	0,6,6	-	-	-		
88	OHX	1	3924	-	0,6,6	-	-	-		
88	OHX	1	3886	-	0,6,6	-	-	-		
88	OHX	1	3970	-	0,6,6	-	-	-		
88	OHX	2	2123	-	0,6,6	-	-	-		
88	OHX	1	3940	-	0,6,6	-	-	-		
88	OHX	1	4052	-	0,6,6	-	-	-		
88	OHX	4	230	-	0,6,6	-	-	-		
88	OHX	6	2150	-	0,6,6	-	-	-		
88	OHX	1	4105	-	0,6,6	-	-	-		
88	OHX	5	3970	-	0,6,6	-	-	-		
88	OHX	2	2108	-	0,6,6	-	-	-		
88	OHX	3	215	-	0,6,6	-	-	-		
88	OHX	19	600	-	0,6,6	-	-	-		
88	OHX	5	3943	-	0,6,6	-	-	-		
88	OHX	6	2117	-	0,6,6	-	-	-		
88	OHX	8	225	-	0,6,6	-	-	-		
88	OHX	5	4016	-	0,6,6	-	-	-		
88	OHX	5	4090	-	0,6,6	-	-	-		
88	OHX	1	4043	-	0,6,6	-	-	-		
88	OHX	1	4172	-	0,6,6	-	-	-		
88	OHX	1	3944	-	0,6,6	-	-	-		
88	OHX	2	2097	-	0,6,6	-	-	-		
88	OHX	2	2177	-	0,6,6	-	-	-		
88	OHX	2	2071	-	0,6,6	-	-	-		
88	OHX	1	3907	-	0,6,6	-	-	-		
88	OHX	1	4117	-	0,6,6	-	-	-		
88	OHX	6	2110	-	0,6,6	-	-	-		
88	OHX	5	3951	-	0,6,6	-	-	-		
88	OHX	5	4059	-	0,6,6	-	-	-		
88	OHX	5	4224	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	2	2055	-	0,6,6	-	-	-		
88	OHX	1	4152	-	0,6,6	-	-	-		
88	OHX	1	3926	-	0,6,6	-	-	-		
88	OHX	2	2175	-	0,6,6	-	-	-		
88	OHX	1	4067	-	0,6,6	-	-	-		
88	OHX	2	2023	-	0,6,6	-	-	-		
88	OHX	1	3928	-	0,6,6	-	-	-		
88	OHX	1	3894	-	0,6,6	-	-	-		
88	OHX	1	3962	-	0,6,6	-	-	-		
88	OHX	1	4031	-	0,6,6	-	-	-		
88	OHX	1	4057	-	0,6,6	-	-	-		
88	OHX	6	2109	-	0,6,6	-	-	-		
88	OHX	6	2189	-	0,6,6	-	-	-		
88	OHX	5	4158	-	0,6,6	-	-	-		
88	OHX	5	4231	-	0,6,6	-	-	-		
88	OHX	1	4195	-	0,6,6	-	-	-		
88	OHX	5	4067	-	0,6,6	-	-	-		
88	OHX	1	4026	-	0,6,6	-	-	-		
88	OHX	6	2102	-	0,6,6	-	-	-		
88	OHX	1	4038	-	0,6,6	-	-	-		
88	OHX	5	4190	-	0,6,6	-	-	-		
88	OHX	2	2115	-	0,6,6	-	-	-		
88	OHX	D9	102	-	0,6,6	-	-	-		
88	OHX	5	3971	-	0,6,6	-	-	-		
88	OHX	5	3991	-	0,6,6	-	-	-		
88	OHX	1	3921	-	0,6,6	-	-	-		
88	OHX	2	2109	-	0,6,6	-	-	-		
88	OHX	1	4009	-	0,6,6	-	-	-		
88	OHX	1	4165	-	0,6,6	-	-	-		
88	OHX	6	2114	-	0,6,6	-	-	-		
88	OHX	1	3995	-	0,6,6	-	-	-		
88	OHX	1	3960	-	0,6,6	-	-	-		
88	OHX	5	3953	-	0,6,6	-	-	-		
88	OHX	5	4240	-	0,6,6	-	-	-		
88	OHX	1	3946	-	0,6,6	-	-	-		
88	OHX	2	2038	-	0,6,6	-	-	-		
88	OHX	1	4085	-	0,6,6	-	-	-		
88	OHX	5	3913	-	0,6,6	-	-	-		
88	OHX	5	3920	-	0,6,6	-	-	-		
88	OHX	1	3985	-	0,6,6	-	-	-		
88	OHX	2	2135	-	0,6,6	-	-	-		
88	OHX	6	2118	-	0,6,6	-	-	-		
88	OHX	5	3956	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	3981	-	0,6,6	-	-	-		
88	OHX	5	4092	-	0,6,6	-	-	-		
88	OHX	n3	204	-	0,6,6	-	-	-		
88	OHX	1	3998	-	0,6,6	-	-	-		
88	OHX	6	2083	-	0,6,6	-	-	-		
88	OHX	6	2165	-	0,6,6	-	-	-		
88	OHX	5	4021	-	0,6,6	-	-	-		
88	OHX	1	4042	-	0,6,6	-	-	-		
88	OHX	5	4111	-	0,6,6	-	-	-		
88	OHX	5	4185	-	0,6,6	-	-	-		
88	OHX	1	4194	-	0,6,6	-	-	-		
88	OHX	5	3938	-	0,6,6	-	-	-		
88	OHX	2	2106	-	0,6,6	-	-	-		
88	OHX	1	3973	-	0,6,6	-	-	-		
88	OHX	1	4034	-	0,6,6	-	-	-		
88	OHX	5	4183	-	0,6,6	-	-	-		
88	OHX	5	4221	-	0,6,6	-	-	-		
88	OHX	5	4110	-	0,6,6	-	-	-		
88	OHX	2	2165	-	0,6,6	-	-	-		
88	OHX	5	4187	-	0,6,6	-	-	-		
88	OHX	5	4200	-	0,6,6	-	-	-		
88	OHX	2	2151	-	0,6,6	-	-	-		
88	OHX	2	2179	-	0,6,6	-	-	-		
88	OHX	6	2174	-	0,6,6	-	-	-		
88	OHX	1	4167	-	0,6,6	-	-	-		
88	OHX	1	3978	-	0,6,6	-	-	-		
88	OHX	5	4210	-	0,6,6	-	-	-		
88	OHX	5	4188	-	0,6,6	-	-	-		
88	OHX	1	4144	-	0,6,6	-	-	-		
88	OHX	5	4123	-	0,6,6	-	-	-		
88	OHX	1	3997	-	0,6,6	-	-	-		
88	OHX	5	4244	-	0,6,6	-	-	-		
88	OHX	3	222	-	0,6,6	-	-	-		
88	OHX	5	4035	-	0,6,6	-	-	-		
88	OHX	1	3992	-	0,6,6	-	-	-		
88	OHX	6	2063	-	0,6,6	-	-	-		
88	OHX	1	4069	-	0,6,6	-	-	-		
88	OHX	2	2114	-	0,6,6	-	-	-		
88	OHX	1	4149	-	0,6,6	-	-	-		
88	OHX	6	2065	-	0,6,6	-	-	-		
88	OHX	5	3937	-	0,6,6	-	-	-		
88	OHX	5	3903	-	0,6,6	-	-	-		
88	OHX	13	406	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	4106	-	0,6,6	-	-	-	-	-
88	OHX	5	4173	-	0,6,6	-	-	-	-	-
88	OHX	1	4083	-	0,6,6	-	-	-	-	-
88	OHX	5	4203	-	0,6,6	-	-	-	-	-
88	OHX	5	4083	-	0,6,6	-	-	-	-	-
88	OHX	1	4224	-	0,6,6	-	-	-	-	-
88	OHX	5	4197	-	0,6,6	-	-	-	-	-
88	OHX	2	2138	-	0,6,6	-	-	-	-	-
88	OHX	5	4252	-	0,6,6	-	-	-	-	-
88	OHX	5	3931	-	0,6,6	-	-	-	-	-
88	OHX	5	4039	-	0,6,6	-	-	-	-	-
88	OHX	1	4050	-	0,6,6	-	-	-	-	-
88	OHX	1	3878	-	0,6,6	-	-	-	-	-
88	OHX	1	4109	-	0,6,6	-	-	-	-	-
88	OHX	O7	103	-	0,6,6	-	-	-	-	-
88	OHX	6	2057	-	0,6,6	-	-	-	-	-
88	OHX	6	2079	-	0,6,6	-	-	-	-	-
88	OHX	1	4204	-	0,6,6	-	-	-	-	-
88	OHX	6	2162	-	0,6,6	-	-	-	-	-
88	OHX	5	4152	-	0,6,6	-	-	-	-	-
88	OHX	3	216	-	0,6,6	-	-	-	-	-
88	OHX	6	2131	-	0,6,6	-	-	-	-	-
88	OHX	1	3991	-	0,6,6	-	-	-	-	-
88	OHX	6	2101	-	0,6,6	-	-	-	-	-
88	OHX	5	3985	-	0,6,6	-	-	-	-	-
88	OHX	5	3994	-	0,6,6	-	-	-	-	-
88	OHX	1	4019	-	0,6,6	-	-	-	-	-
88	OHX	1	4129	-	0,6,6	-	-	-	-	-
88	OHX	2	2174	-	0,6,6	-	-	-	-	-
88	OHX	1	3913	-	0,6,6	-	-	-	-	-
88	OHX	2	2053	-	0,6,6	-	-	-	-	-
88	OHX	1	3892	-	0,6,6	-	-	-	-	-
88	OHX	6	2181	-	0,6,6	-	-	-	-	-
88	OHX	4	227	-	0,6,6	-	-	-	-	-
88	OHX	1	3983	-	0,6,6	-	-	-	-	-
88	OHX	1	4061	-	0,6,6	-	-	-	-	-
88	OHX	1	4033	-	0,6,6	-	-	-	-	-
88	OHX	6	2143	-	0,6,6	-	-	-	-	-
88	OHX	2	2039	-	0,6,6	-	-	-	-	-
88	OHX	1	4022	-	0,6,6	-	-	-	-	-
88	OHX	1	3901	-	0,6,6	-	-	-	-	-
88	OHX	1	3936	-	0,6,6	-	-	-	-	-
88	OHX	4	228	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	4	229	-	0,6,6	-	-	-	-	-
88	OHX	2	2132	-	0,6,6	-	-	-	-	-
88	OHX	1	4015	-	0,6,6	-	-	-	-	-
88	OHX	5	4056	-	0,6,6	-	-	-	-	-
88	OHX	6	2052	-	0,6,6	-	-	-	-	-
88	OHX	6	2061	-	0,6,6	-	-	-	-	-
88	OHX	5	4140	-	0,6,6	-	-	-	-	-
88	OHX	c5	201	-	0,6,6	-	-	-	-	-
88	OHX	5	4052	-	0,6,6	-	-	-	-	-
88	OHX	5	4002	-	0,6,6	-	-	-	-	-
88	OHX	1	3876	-	0,6,6	-	-	-	-	-
88	OHX	1	4156	-	0,6,6	-	-	-	-	-
88	OHX	5	3961	-	0,6,6	-	-	-	-	-
88	OHX	5	4103	-	0,6,6	-	-	-	-	-
88	OHX	m6	203	-	0,6,6	-	-	-	-	-
88	OHX	1	4213	-	0,6,6	-	-	-	-	-
88	OHX	2	2047	-	0,6,6	-	-	-	-	-
88	OHX	8	218	-	0,6,6	-	-	-	-	-
88	OHX	5	3978	-	0,6,6	-	-	-	-	-
88	OHX	1	4217	-	0,6,6	-	-	-	-	-
88	OHX	5	4202	-	0,6,6	-	-	-	-	-
88	OHX	1	4184	-	0,6,6	-	-	-	-	-
88	OHX	2	2035	-	0,6,6	-	-	-	-	-
88	OHX	1	4191	-	0,6,6	-	-	-	-	-
88	OHX	1	3895	-	0,6,6	-	-	-	-	-
88	OHX	6	2119	-	0,6,6	-	-	-	-	-
88	OHX	8	229	-	0,6,6	-	-	-	-	-
88	OHX	5	4058	-	0,6,6	-	-	-	-	-
88	OHX	5	4114	-	0,6,6	-	-	-	-	-
88	OHX	2	2034	-	0,6,6	-	-	-	-	-
88	OHX	S8	302	-	0,6,6	-	-	-	-	-
88	OHX	1	4114	-	0,6,6	-	-	-	-	-
88	OHX	5	4038	-	0,6,6	-	-	-	-	-
88	OHX	5	4042	-	0,6,6	-	-	-	-	-
88	OHX	2	2041	-	0,6,6	-	-	-	-	-
88	OHX	1	4107	-	0,6,6	-	-	-	-	-
88	OHX	1	4158	-	0,6,6	-	-	-	-	-
88	OHX	5	3921	-	0,6,6	-	-	-	-	-
88	OHX	7	217	-	0,6,6	-	-	-	-	-
88	OHX	2	2098	-	0,6,6	-	-	-	-	-
88	OHX	2	2146	-	0,6,6	-	-	-	-	-
88	OHX	m0	302	-	0,6,6	-	-	-	-	-
88	OHX	2	2100	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	3965	-	0,6,6	-	-	-	-	-
88	OHX	1	4177	-	0,6,6	-	-	-	-	-
88	OHX	5	4107	-	0,6,6	-	-	-	-	-
88	OHX	5	4174	-	0,6,6	-	-	-	-	-
88	OHX	1	3976	-	0,6,6	-	-	-	-	-
88	OHX	5	4209	-	0,6,6	-	-	-	-	-
88	OHX	5	4251	-	0,6,6	-	-	-	-	-
88	OHX	5	3912	-	0,6,6	-	-	-	-	-
88	OHX	7	219	-	0,6,6	-	-	-	-	-
88	OHX	6	2157	-	0,6,6	-	-	-	-	-
88	OHX	6	2168	-	0,6,6	-	-	-	-	-
88	OHX	1	3909	-	0,6,6	-	-	-	-	-
88	OHX	1	4214	-	0,6,6	-	-	-	-	-
88	OHX	5	3998	-	0,6,6	-	-	-	-	-
88	OHX	1	3955	-	0,6,6	-	-	-	-	-
88	OHX	2	2076	-	0,6,6	-	-	-	-	-
88	OHX	1	3880	-	0,6,6	-	-	-	-	-
88	OHX	1	4036	-	0,6,6	-	-	-	-	-
88	OHX	6	2136	-	0,6,6	-	-	-	-	-
88	OHX	15	305	-	0,6,6	-	-	-	-	-
88	OHX	6	2139	-	0,6,6	-	-	-	-	-
88	OHX	2	2120	-	0,6,6	-	-	-	-	-
88	OHX	1	4041	-	0,6,6	-	-	-	-	-
88	OHX	5	4061	-	0,6,6	-	-	-	-	-
88	OHX	5	4235	-	0,6,6	-	-	-	-	-
88	OHX	1	4208	-	0,6,6	-	-	-	-	-
88	OHX	M9	202	-	0,6,6	-	-	-	-	-
88	OHX	1	4099	-	0,6,6	-	-	-	-	-
88	OHX	1	4002	-	0,6,6	-	-	-	-	-
88	OHX	1	4008	-	0,6,6	-	-	-	-	-
88	OHX	1	4037	-	0,6,6	-	-	-	-	-
88	OHX	1	4028	-	0,6,6	-	-	-	-	-
88	OHX	5	3927	-	0,6,6	-	-	-	-	-
88	OHX	1	4189	-	0,6,6	-	-	-	-	-
88	OHX	2	2139	-	0,6,6	-	-	-	-	-
88	OHX	sR	401	-	0,6,6	-	-	-	-	-
88	OHX	1	4010	-	0,6,6	-	-	-	-	-
88	OHX	1	3925	-	0,6,6	-	-	-	-	-
88	OHX	5	4144	-	0,6,6	-	-	-	-	-
88	OHX	1	3888	-	0,6,6	-	-	-	-	-
88	OHX	6	2194	-	0,6,6	-	-	-	-	-
88	OHX	1	4164	-	0,6,6	-	-	-	-	-
88	OHX	1	3941	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	3999	-	0,6,6	-	-	-		
88	OHX	1	3933	-	0,6,6	-	-	-		
88	OHX	L3	404	-	0,6,6	-	-	-		
88	OHX	M0	303	-	0,6,6	-	-	-		
88	OHX	6	2077	-	0,6,6	-	-	-		
88	OHX	6	2074	-	0,6,6	-	-	-		
88	OHX	2	2145	-	0,6,6	-	-	-		
88	OHX	5	3944	-	0,6,6	-	-	-		
88	OHX	1	4084	-	0,6,6	-	-	-		
88	OHX	1	3937	-	0,6,6	-	-	-		
88	OHX	5	4204	-	0,6,6	-	-	-		
88	OHX	1	4180	-	0,6,6	-	-	-		
88	OHX	5	4199	-	0,6,6	-	-	-		
88	OHX	5	3969	-	0,6,6	-	-	-		
88	OHX	6	2159	-	0,6,6	-	-	-		
88	OHX	1	3942	-	0,6,6	-	-	-		
88	OHX	1	4132	-	0,6,6	-	-	-		
88	OHX	5	4159	-	0,6,6	-	-	-		
88	OHX	1	4012	-	0,6,6	-	-	-		
88	OHX	2	2162	-	0,6,6	-	-	-		
88	OHX	6	2089	-	0,6,6	-	-	-		
88	OHX	5	4230	-	0,6,6	-	-	-		
88	OHX	7	222	-	0,6,6	-	-	-		
88	OHX	1	4136	-	0,6,6	-	-	-		
88	OHX	8	222	-	0,6,6	-	-	-		
88	OHX	1	4013	-	0,6,6	-	-	-		
88	OHX	2	2081	-	0,6,6	-	-	-		
88	OHX	2	2054	-	0,6,6	-	-	-		
88	OHX	8	221	-	0,6,6	-	-	-		
88	OHX	6	2127	-	0,6,6	-	-	-		
88	OHX	5	4012	-	0,6,6	-	-	-		
88	OHX	5	4033	-	0,6,6	-	-	-		
88	OHX	5	4101	-	0,6,6	-	-	-		
88	OHX	1	4046	-	0,6,6	-	-	-		
88	OHX	6	2049	-	0,6,6	-	-	-		
88	OHX	2	2066	-	0,6,6	-	-	-		
88	OHX	1	3971	-	0,6,6	-	-	-		
88	OHX	2	2118	-	0,6,6	-	-	-		
88	OHX	1	3917	-	0,6,6	-	-	-		
88	OHX	6	2133	-	0,6,6	-	-	-		
88	OHX	5	4192	-	0,6,6	-	-	-		
88	OHX	3	224	-	0,6,6	-	-	-		
88	OHX	1	4143	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	2	2033	-	0,6,6	-	-	-		
88	OHX	L4	402	-	0,6,6	-	-	-		
88	OHX	5	3947	-	0,6,6	-	-	-		
88	OHX	5	4024	-	0,6,6	-	-	-		
88	OHX	5	4191	-	0,6,6	-	-	-		
88	OHX	5	4194	-	0,6,6	-	-	-		
88	OHX	5	4253	-	0,6,6	-	-	-		
88	OHX	2	2049	-	0,6,6	-	-	-		
88	OHX	7	215	-	0,6,6	-	-	-		
88	OHX	2	2133	-	0,6,6	-	-	-		
88	OHX	5	4156	-	0,6,6	-	-	-		
88	OHX	4	226	-	0,6,6	-	-	-		
88	OHX	2	2160	-	0,6,6	-	-	-		
88	OHX	2	2061	-	0,6,6	-	-	-		
88	OHX	6	2140	-	0,6,6	-	-	-		
88	OHX	6	2095	-	0,6,6	-	-	-		
88	OHX	q2	504	-	0,6,6	-	-	-		
88	OHX	8	227	-	0,6,6	-	-	-		
88	OHX	1	4192	-	0,6,6	-	-	-		
88	OHX	c8	202	-	0,6,6	-	-	-		
88	OHX	2	2099	-	0,6,6	-	-	-		
88	OHX	1	4090	-	0,6,6	-	-	-		
88	OHX	5	4037	-	0,6,6	-	-	-		
88	OHX	6	2138	-	0,6,6	-	-	-		
88	OHX	2	2124	-	0,6,6	-	-	-		
88	OHX	15	303	-	0,6,6	-	-	-		
88	OHX	5	3933	-	0,6,6	-	-	-		
88	OHX	5	3949	-	0,6,6	-	-	-		
88	OHX	8	228	-	0,6,6	-	-	-		
88	OHX	6	2155	-	0,6,6	-	-	-		
88	OHX	5	4116	-	0,6,6	-	-	-		
88	OHX	5	3965	-	0,6,6	-	-	-		
88	OHX	5	3979	-	0,6,6	-	-	-		
88	OHX	5	3941	-	0,6,6	-	-	-		
88	OHX	1	4205	-	0,6,6	-	-	-		
88	OHX	5	4157	-	0,6,6	-	-	-		
88	OHX	1	4170	-	0,6,6	-	-	-		
88	OHX	2	2163	-	0,6,6	-	-	-		
88	OHX	1	4216	-	0,6,6	-	-	-		
88	OHX	2	2063	-	0,6,6	-	-	-		
88	OHX	6	2096	-	0,6,6	-	-	-		
88	OHX	2	2121	-	0,6,6	-	-	-		
88	OHX	5	4172	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	3916	-	0,6,6	-	-	-		
88	OHX	5	4026	-	0,6,6	-	-	-		
88	OHX	6	2188	-	0,6,6	-	-	-		
88	OHX	5	3939	-	0,6,6	-	-	-		
88	OHX	6	2076	-	0,6,6	-	-	-		
88	OHX	1	3905	-	0,6,6	-	-	-		
88	OHX	1	4203	-	0,6,6	-	-	-		
88	OHX	1	4018	-	0,6,6	-	-	-		
88	OHX	5	4148	-	0,6,6	-	-	-		
88	OHX	5	4241	-	0,6,6	-	-	-		
88	OHX	1	4133	-	0,6,6	-	-	-		
88	OHX	2	2172	-	0,6,6	-	-	-		
88	OHX	1	4100	-	0,6,6	-	-	-		
88	OHX	5	3934	-	0,6,6	-	-	-		
88	OHX	5	4133	-	0,6,6	-	-	-		
88	OHX	2	2042	-	0,6,6	-	-	-		
88	OHX	2	2096	-	0,6,6	-	-	-		
88	OHX	1	4095	-	0,6,6	-	-	-		
88	OHX	5	4176	-	0,6,6	-	-	-		
88	OHX	2	2074	-	0,6,6	-	-	-		
88	OHX	5	4031	-	0,6,6	-	-	-		
88	OHX	5	4020	-	0,6,6	-	-	-		
88	OHX	5	4046	-	0,6,6	-	-	-		
88	OHX	5	4122	-	0,6,6	-	-	-		
88	OHX	6	2056	-	0,6,6	-	-	-		
88	OHX	5	3945	-	0,6,6	-	-	-		
88	OHX	5	3909	-	0,6,6	-	-	-		
88	OHX	5	4243	-	0,6,6	-	-	-		
88	OHX	s1	303	-	0,6,6	-	-	-		
88	OHX	2	2129	-	0,6,6	-	-	-		
88	OHX	5	3925	-	0,6,6	-	-	-		
88	OHX	2	2067	-	0,6,6	-	-	-		
88	OHX	6	2201	-	0,6,6	-	-	-		
88	OHX	1	4040	-	0,6,6	-	-	-		
88	OHX	1	3993	-	0,6,6	-	-	-		
88	OHX	2	2056	-	0,6,6	-	-	-		
88	OHX	1	4074	-	0,6,6	-	-	-		
88	OHX	1	4078	-	0,6,6	-	-	-		
88	OHX	2	2159	-	0,6,6	-	-	-		
88	OHX	5	4099	-	0,6,6	-	-	-		
88	OHX	2	2057	-	0,6,6	-	-	-		
88	OHX	6	2087	-	0,6,6	-	-	-		
88	OHX	1	4155	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	3930	-	0,6,6	-	-	-		
88	OHX	5	4121	-	0,6,6	-	-	-		
88	OHX	5	4131	-	0,6,6	-	-	-		
88	OHX	5	4047	-	0,6,6	-	-	-		
88	OHX	1	3923	-	0,6,6	-	-	-		
88	OHX	1	4200	-	0,6,6	-	-	-		
88	OHX	2	2128	-	0,6,6	-	-	-		
88	OHX	2	2025	-	0,6,6	-	-	-		
88	OHX	5	4141	-	0,6,6	-	-	-		
88	OHX	1	4014	-	0,6,6	-	-	-		
88	OHX	6	2113	-	0,6,6	-	-	-		
88	OHX	5	3960	-	0,6,6	-	-	-		
88	OHX	1	3900	-	0,6,6	-	-	-		
88	OHX	5	4130	-	0,6,6	-	-	-		
88	OHX	6	2100	-	0,6,6	-	-	-		
88	OHX	2	2117	-	0,6,6	-	-	-		
88	OHX	1	3948	-	0,6,6	-	-	-		
88	OHX	1	3967	-	0,6,6	-	-	-		
88	OHX	5	4223	-	0,6,6	-	-	-		
88	OHX	6	2091	-	0,6,6	-	-	-		
88	OHX	5	4013	-	0,6,6	-	-	-		
88	OHX	6	2080	-	0,6,6	-	-	-		
88	OHX	1	4079	-	0,6,6	-	-	-		
88	OHX	6	2081	-	0,6,6	-	-	-		
88	OHX	5	4088	-	0,6,6	-	-	-		
88	OHX	2	2085	-	0,6,6	-	-	-		
88	OHX	5	4195	-	0,6,6	-	-	-		
88	OHX	5	3993	-	0,6,6	-	-	-		
88	OHX	1	3996	-	0,6,6	-	-	-		
88	OHX	2	2073	-	0,6,6	-	-	-		
88	OHX	1	4123	-	0,6,6	-	-	-		
88	OHX	1	4160	-	0,6,6	-	-	-		
88	OHX	1	4163	-	0,6,6	-	-	-		
88	OHX	1	4225	-	0,6,6	-	-	-		
88	OHX	6	2055	-	0,6,6	-	-	-		
88	OHX	6	2164	-	0,6,6	-	-	-		
88	OHX	5	4050	-	0,6,6	-	-	-		
88	OHX	3	221	-	0,6,6	-	-	-		
88	OHX	6	2044	-	0,6,6	-	-	-		
88	OHX	5	3915	-	0,6,6	-	-	-		
88	OHX	6	2066	-	0,6,6	-	-	-		
88	OHX	1	4092	-	0,6,6	-	-	-		
88	OHX	1	4179	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	6	2147	-	0,6,6	-	-	-		
88	OHX	5	3905	-	0,6,6	-	-	-		
88	OHX	1	4137	-	0,6,6	-	-	-		
88	OHX	5	3908	-	0,6,6	-	-	-		
88	OHX	1	4112	-	0,6,6	-	-	-		
88	OHX	2	2147	-	0,6,6	-	-	-		
88	OHX	2	2152	-	0,6,6	-	-	-		
88	OHX	6	2092	-	0,6,6	-	-	-		
91	C	Q2	503	-	18,21,22	0.72	0	26,30,33	1.15	4 (15%)
88	OHX	5	3917	-	0,6,6	-	-	-		
88	OHX	4	231	-	0,6,6	-	-	-		
88	OHX	6	2161	-	0,6,6	-	-	-		
88	OHX	1	3957	-	0,6,6	-	-	-		
88	OHX	1	3918	-	0,6,6	-	-	-		
88	OHX	5	3932	-	0,6,6	-	-	-		
88	OHX	5	4143	-	0,6,6	-	-	-		
88	OHX	C3	201	-	0,6,6	-	-	-		
88	OHX	1	4060	-	0,6,6	-	-	-		
88	OHX	1	4097	-	0,6,6	-	-	-		
88	OHX	6	2111	-	0,6,6	-	-	-		
88	OHX	1	4138	-	0,6,6	-	-	-		
88	OHX	2	2087	-	0,6,6	-	-	-		
88	OHX	5	4236	-	0,6,6	-	-	-		
88	OHX	1	3911	-	0,6,6	-	-	-		
88	OHX	1	4049	-	0,6,6	-	-	-		
88	OHX	1	4120	-	0,6,6	-	-	-		
88	OHX	5	4177	-	0,6,6	-	-	-		
88	OHX	2	2084	-	0,6,6	-	-	-		
88	OHX	5	3936	-	0,6,6	-	-	-		
88	OHX	6	2193	-	0,6,6	-	-	-		
88	OHX	6	2075	-	0,6,6	-	-	-		
88	OHX	1	4089	-	0,6,6	-	-	-		
88	OHX	5	3992	-	0,6,6	-	-	-		
88	OHX	1	3975	-	0,6,6	-	-	-		
88	OHX	5	4126	-	0,6,6	-	-	-		
88	OHX	5	4254	-	0,6,6	-	-	-		
88	OHX	6	2178	-	0,6,6	-	-	-		
88	OHX	5	4211	-	0,6,6	-	-	-		
88	OHX	5	4226	-	0,6,6	-	-	-		
88	OHX	1	3882	-	0,6,6	-	-	-		
88	OHX	1	4161	-	0,6,6	-	-	-		
88	OHX	6	2107	-	0,6,6	-	-	-		
88	OHX	M8	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4216	-	0,6,6	-	-	-		
88	OHX	2	2036	-	0,6,6	-	-	-		
88	OHX	1	3881	-	0,6,6	-	-	-		
88	OHX	1	4088	-	0,6,6	-	-	-		
88	OHX	1	4150	-	0,6,6	-	-	-		
88	OHX	M7	206	-	0,6,6	-	-	-		
88	OHX	5	4181	-	0,6,6	-	-	-		
88	OHX	1	4016	-	0,6,6	-	-	-		
88	OHX	5	3928	-	0,6,6	-	-	-		
88	OHX	1	3887	-	0,6,6	-	-	-		
88	OHX	1	3935	-	0,6,6	-	-	-		
88	OHX	1	4071	-	0,6,6	-	-	-		
88	OHX	5	4220	-	0,6,6	-	-	-		
88	OHX	8	226	-	0,6,6	-	-	-		
88	OHX	2	2150	-	0,6,6	-	-	-		
91	C	q2	503	-	18,21,22	0.61	0	26,30,33	0.76	1 (3%)
88	OHX	2	2077	-	0,6,6	-	-	-		
88	OHX	2	2088	-	0,6,6	-	-	-		
88	OHX	5	4118	-	0,6,6	-	-	-		
88	OHX	1	3910	-	0,6,6	-	-	-		
88	OHX	1	4146	-	0,6,6	-	-	-		
88	OHX	d9	102	-	0,6,6	-	-	-		
88	OHX	6	2132	-	0,6,6	-	-	-		
88	OHX	5	4044	-	0,6,6	-	-	-		
88	OHX	5	4212	-	0,6,6	-	-	-		
88	OHX	5	4163	-	0,6,6	-	-	-		
88	OHX	1	3939	-	0,6,6	-	-	-		
88	OHX	6	2078	-	0,6,6	-	-	-		
88	OHX	1	4209	-	0,6,6	-	-	-		
88	OHX	1	4065	-	0,6,6	-	-	-		
88	OHX	6	2176	-	0,6,6	-	-	-		
88	OHX	6	2094	-	0,6,6	-	-	-		
88	OHX	2	2075	-	0,6,6	-	-	-		
88	OHX	2	2110	-	0,6,6	-	-	-		
88	OHX	5	4057	-	0,6,6	-	-	-		
88	OHX	1	4058	-	0,6,6	-	-	-		
88	OHX	5	4085	-	0,6,6	-	-	-		
88	OHX	C5	201	-	0,6,6	-	-	-		
88	OHX	6	2182	-	0,6,6	-	-	-		
88	OHX	1	4140	-	0,6,6	-	-	-		
88	OHX	5	4198	-	0,6,6	-	-	-		
88	OHX	2	2089	-	0,6,6	-	-	-		
88	OHX	5	3926	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	3932	-	0,6,6	-	-	-		
88	OHX	1	4080	-	0,6,6	-	-	-		
88	OHX	5	4112	-	0,6,6	-	-	-		
88	OHX	5	4155	-	0,6,6	-	-	-		
88	OHX	1	3986	-	0,6,6	-	-	-		
88	OHX	1	4006	-	0,6,6	-	-	-		
88	OHX	1	4139	-	0,6,6	-	-	-		
88	OHX	1	4023	-	0,6,6	-	-	-		
88	OHX	1	3912	-	0,6,6	-	-	-		
88	OHX	1	4171	-	0,6,6	-	-	-		
88	OHX	2	2069	-	0,6,6	-	-	-		
88	OHX	5	4028	-	0,6,6	-	-	-		
88	OHX	5	4167	-	0,6,6	-	-	-		
88	OHX	6	2172	-	0,6,6	-	-	-		
88	OHX	2	2030	-	0,6,6	-	-	-		
88	OHX	5	3911	-	0,6,6	-	-	-		
88	OHX	1	4111	-	0,6,6	-	-	-		
88	OHX	5	4120	-	0,6,6	-	-	-		
88	OHX	1	3919	-	0,6,6	-	-	-		
88	OHX	1	3899	-	0,6,6	-	-	-		
88	OHX	1	4226	-	0,6,6	-	-	-		
88	OHX	5	4258	-	0,6,6	-	-	-		
88	OHX	1	4153	-	0,6,6	-	-	-		
88	OHX	5	4064	-	0,6,6	-	-	-		
88	OHX	1	4001	-	0,6,6	-	-	-		
88	OHX	5	3967	-	0,6,6	-	-	-		
88	OHX	2	2178	-	0,6,6	-	-	-		
88	OHX	m5	306	-	0,6,6	-	-	-		
88	OHX	5	4077	-	0,6,6	-	-	-		
88	OHX	m4	201	-	0,6,6	-	-	-		
88	OHX	D3	202	-	0,6,6	-	-	-		
88	OHX	5	3906	-	0,6,6	-	-	-		
88	OHX	n9	101	-	0,6,6	-	-	-		
88	OHX	5	4161	-	0,6,6	-	-	-		
88	OHX	5	4135	-	0,6,6	-	-	-		
88	OHX	2	2080	-	0,6,6	-	-	-		
88	OHX	1	4174	-	0,6,6	-	-	-		
88	OHX	1	4075	-	0,6,6	-	-	-		
88	OHX	1	4082	-	0,6,6	-	-	-		
88	OHX	1	4118	-	0,6,6	-	-	-		
88	OHX	1	4197	-	0,6,6	-	-	-		
90	A	1	3401	-	18,24,25	0.72	0	18,35,38	0.96	2 (11%)
88	OHX	1	4044	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	6	2045	-	0,6,6	-	-	-		
88	OHX	6	2156	-	0,6,6	-	-	-		
88	OHX	1	4030	-	0,6,6	-	-	-		
88	OHX	2	2130	-	0,6,6	-	-	-		
88	OHX	1	4072	-	0,6,6	-	-	-		
88	OHX	6	2051	-	0,6,6	-	-	-		
88	OHX	1	4190	-	0,6,6	-	-	-		
88	OHX	5	4193	-	0,6,6	-	-	-		
88	OHX	2	2164	-	0,6,6	-	-	-		
88	OHX	M5	303	-	0,6,6	-	-	-		
88	OHX	1	3893	-	0,6,6	-	-	-		
88	OHX	5	4214	-	0,6,6	-	-	-		
88	OHX	8	220	-	0,6,6	-	-	-		
88	OHX	5	4137	-	0,6,6	-	-	-		
88	OHX	5	4025	-	0,6,6	-	-	-		
88	OHX	2	2113	-	0,6,6	-	-	-		
88	OHX	2	2156	-	0,6,6	-	-	-		
88	OHX	5	3919	-	0,6,6	-	-	-		
88	OHX	5	4018	-	0,6,6	-	-	-		
88	OHX	5	3914	-	0,6,6	-	-	-		
88	OHX	5	4248	-	0,6,6	-	-	-		
88	OHX	2	2119	-	0,6,6	-	-	-		
88	OHX	1	4115	-	0,6,6	-	-	-		
88	OHX	4	224	-	0,6,6	-	-	-		
88	OHX	1	3891	-	0,6,6	-	-	-		
88	OHX	5	3918	-	0,6,6	-	-	-		
88	OHX	2	2092	-	0,6,6	-	-	-		
88	OHX	6	2126	-	0,6,6	-	-	-		
88	OHX	6	2128	-	0,6,6	-	-	-		
88	OHX	5	4124	-	0,6,6	-	-	-		
88	OHX	5	4138	-	0,6,6	-	-	-		
88	OHX	1	3896	-	0,6,6	-	-	-		
88	OHX	5	4171	-	0,6,6	-	-	-		
88	OHX	2	2062	-	0,6,6	-	-	-		
88	OHX	2	2059	-	0,6,6	-	-	-		
88	OHX	1	3902	-	0,6,6	-	-	-		
88	OHX	1	4004	-	0,6,6	-	-	-		
88	OHX	s1	302	-	0,6,6	-	-	-		
88	OHX	6	2149	-	0,6,6	-	-	-		
88	OHX	7	216	-	0,6,6	-	-	-		
88	OHX	1	4093	-	0,6,6	-	-	-		
88	OHX	5	4247	-	0,6,6	-	-	-		
88	OHX	5	4069	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4257	-	0,6,6	-	-	-		
88	OHX	5	4233	-	0,6,6	-	-	-		
88	OHX	5	4072	-	0,6,6	-	-	-		
88	OHX	5	3975	-	0,6,6	-	-	-		
88	OHX	5	4055	-	0,6,6	-	-	-		
88	OHX	1	4151	-	0,6,6	-	-	-		
88	OHX	c3	201	-	0,6,6	-	-	-		
88	OHX	7	225	-	0,6,6	-	-	-		
88	OHX	1	4188	-	0,6,6	-	-	-		
88	OHX	2	2168	-	0,6,6	-	-	-		
88	OHX	1	4077	-	0,6,6	-	-	-		
88	OHX	5	4048	-	0,6,6	-	-	-		
88	OHX	1	4126	-	0,6,6	-	-	-		
88	OHX	6	2073	-	0,6,6	-	-	-		
88	OHX	5	4053	-	0,6,6	-	-	-		
88	OHX	5	4234	-	0,6,6	-	-	-		
88	OHX	5	3973	-	0,6,6	-	-	-		
88	OHX	5	4108	-	0,6,6	-	-	-		
88	OHX	5	3904	-	0,6,6	-	-	-		
88	OHX	s8	304	-	0,6,6	-	-	-		
88	OHX	2	2086	-	0,6,6	-	-	-		
88	OHX	3	225	-	0,6,6	-	-	-		
88	OHX	1	4211	-	0,6,6	-	-	-		
88	OHX	5	4065	-	0,6,6	-	-	-		
88	OHX	4	221	-	0,6,6	-	-	-		
88	OHX	7	223	-	0,6,6	-	-	-		
88	OHX	6	2103	-	0,6,6	-	-	-		
88	OHX	2	2072	-	0,6,6	-	-	-		
88	OHX	5	4104	-	0,6,6	-	-	-		
88	OHX	1	4005	-	0,6,6	-	-	-		
88	OHX	5	3940	-	0,6,6	-	-	-		
88	OHX	1	4119	-	0,6,6	-	-	-		
88	OHX	2	2091	-	0,6,6	-	-	-		
88	OHX	1	3990	-	0,6,6	-	-	-		
88	OHX	1	4108	-	0,6,6	-	-	-		
88	OHX	1	4193	-	0,6,6	-	-	-		
88	OHX	6	2116	-	0,6,6	-	-	-		
88	OHX	2	2170	-	0,6,6	-	-	-		
88	OHX	6	2137	-	0,6,6	-	-	-		
88	OHX	1	3979	-	0,6,6	-	-	-		
88	OHX	6	2090	-	0,6,6	-	-	-		
88	OHX	1	3980	-	0,6,6	-	-	-		
88	OHX	5	3986	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	2	2107	-	0,6,6	-	-	-	-	-
88	OHX	6	2093	-	0,6,6	-	-	-	-	-
88	OHX	1	3966	-	0,6,6	-	-	-	-	-
88	OHX	1	3989	-	0,6,6	-	-	-	-	-
88	OHX	6	2105	1	0,6,6	-	-	-	-	-
88	OHX	5	4219	-	0,6,6	-	-	-	-	-
88	OHX	5	4015	-	0,6,6	-	-	-	-	-
88	OHX	1	3890	-	0,6,6	-	-	-	-	-
88	OHX	2	2043	-	0,6,6	-	-	-	-	-
88	OHX	1	4148	-	0,6,6	-	-	-	-	-
88	OHX	5	4093	-	0,6,6	-	-	-	-	-
88	OHX	O3	201	-	0,6,6	-	-	-	-	-
88	OHX	5	4045	-	0,6,6	-	-	-	-	-
88	OHX	1	3877	-	0,6,6	-	-	-	-	-
88	OHX	1	3874	-	0,6,6	-	-	-	-	-
88	OHX	6	2183	-	0,6,6	-	-	-	-	-
88	OHX	m0	301	-	0,6,6	-	-	-	-	-
88	OHX	5	4134	-	0,6,6	-	-	-	-	-
88	OHX	5	4008	-	0,6,6	-	-	-	-	-
88	OHX	5	4094	-	0,6,6	-	-	-	-	-
88	OHX	1	4091	-	0,6,6	-	-	-	-	-
88	OHX	6	2064	-	0,6,6	-	-	-	-	-
88	OHX	5	4151	-	0,6,6	-	-	-	-	-
88	OHX	o3	202	-	0,6,6	-	-	-	-	-
88	OHX	1	3945	-	0,6,6	-	-	-	-	-
88	OHX	1	3959	-	0,6,6	-	-	-	-	-
88	OHX	1	4066	-	0,6,6	-	-	-	-	-
88	OHX	5	4222	-	0,6,6	-	-	-	-	-
88	OHX	5	3988	-	0,6,6	-	-	-	-	-
88	OHX	1	4196	-	0,6,6	-	-	-	-	-
88	OHX	6	2121	-	0,6,6	-	-	-	-	-
88	OHX	1	4007	-	0,6,6	-	-	-	-	-
88	OHX	1	4070	-	0,6,6	-	-	-	-	-
88	OHX	6	2108	-	0,6,6	-	-	-	-	-
88	OHX	4	220	-	0,6,6	-	-	-	-	-
88	OHX	5	3902	-	0,6,6	-	-	-	-	-
88	OHX	6	2170	-	0,6,6	-	-	-	-	-
88	OHX	6	2184	-	0,6,6	-	-	-	-	-
88	OHX	1	3961	-	0,6,6	-	-	-	-	-
88	OHX	5	4010	-	0,6,6	-	-	-	-	-
88	OHX	l3	405	-	0,6,6	-	-	-	-	-
88	OHX	2	2126	-	0,6,6	-	-	-	-	-
88	OHX	2	2040	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	2	2082	-	0,6,6	-	-	-		
88	OHX	1	4053	-	0,6,6	-	-	-		
88	OHX	6	2198	-	0,6,6	-	-	-		
88	OHX	5	4030	-	0,6,6	-	-	-		
88	OHX	5	4051	-	0,6,6	-	-	-		
88	OHX	1	3987	-	0,6,6	-	-	-		
88	OHX	1	4027	-	0,6,6	-	-	-		
88	OHX	6	2071	-	0,6,6	-	-	-		
88	OHX	2	2136	-	0,6,6	-	-	-		
88	OHX	5	4228	-	0,6,6	-	-	-		
88	OHX	2	2031	-	0,6,6	-	-	-		
88	OHX	1	3930	-	0,6,6	-	-	-		
88	OHX	1	3956	-	0,6,6	-	-	-		
88	OHX	1	4130	-	0,6,6	-	-	-		
88	OHX	6	2099	-	0,6,6	-	-	-		
88	OHX	6	2125	-	0,6,6	-	-	-		
88	OHX	2	2094	-	0,6,6	-	-	-		
88	OHX	5	3977	-	0,6,6	-	-	-		
88	OHX	6	2124	-	0,6,6	-	-	-		
88	OHX	6	2166	-	0,6,6	-	-	-		
88	OHX	5	4014	-	0,6,6	-	-	-		
88	OHX	5	4043	-	0,6,6	-	-	-		
88	OHX	5	4086	-	0,6,6	-	-	-		
88	OHX	5	4098	-	0,6,6	-	-	-		
88	OHX	5	4255	-	0,6,6	-	-	-		
88	OHX	5	4250	-	0,6,6	-	-	-		
88	OHX	5	4075	-	0,6,6	-	-	-		
88	OHX	6	2067	-	0,6,6	-	-	-		
88	OHX	1	3954	-	0,6,6	-	-	-		
88	OHX	1	4141	-	0,6,6	-	-	-		
88	OHX	6	2142	-	0,6,6	-	-	-		
88	OHX	5	4115	-	0,6,6	-	-	-		
88	OHX	1	4206	-	0,6,6	-	-	-		
88	OHX	1	3972	-	0,6,6	-	-	-		
88	OHX	1	4173	-	0,6,6	-	-	-		
88	OHX	5	3907	-	0,6,6	-	-	-		
88	OHX	1	4154	-	0,6,6	-	-	-		
88	OHX	5	4032	-	0,6,6	-	-	-		
88	OHX	5	4164	-	0,6,6	-	-	-		
88	OHX	2	2140	-	0,6,6	-	-	-		
88	OHX	6	2163	-	0,6,6	-	-	-		
88	OHX	1	4221	-	0,6,6	-	-	-		
88	OHX	5	4005	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	2	2116	-	0,6,6	-	-	-		
88	OHX	5	4184	-	0,6,6	-	-	-		
88	OHX	5	4036	-	0,6,6	-	-	-		
88	OHX	5	4136	-	0,6,6	-	-	-		
88	OHX	1	4207	-	0,6,6	-	-	-		
88	OHX	2	2083	-	0,6,6	-	-	-		
88	OHX	1	4202	-	0,6,6	-	-	-		
88	OHX	n3	203	-	0,6,6	-	-	-		
88	OHX	1	4168	-	0,6,6	-	-	-		
88	OHX	1	4059	-	0,6,6	-	-	-		
88	OHX	2	2024	-	0,6,6	-	-	-		
88	OHX	1	3889	-	0,6,6	-	-	-		
88	OHX	3	219	-	0,6,6	-	-	-		
88	OHX	5	3929	-	0,6,6	-	-	-		
88	OHX	5	4256	-	0,6,6	-	-	-		
88	OHX	1	3914	-	0,6,6	-	-	-		
88	OHX	1	3953	-	0,6,6	-	-	-		
88	OHX	2	2078	-	0,6,6	-	-	-		
88	OHX	2	2167	-	0,6,6	-	-	-		
88	OHX	6	2046	-	0,6,6	-	-	-		
88	OHX	5	4109	-	0,6,6	-	-	-		
88	OHX	1	4087	-	0,6,6	-	-	-		
88	OHX	1	3947	-	0,6,6	-	-	-		
88	OHX	1	4212	-	0,6,6	-	-	-		
88	OHX	6	2171	-	0,6,6	-	-	-		
88	OHX	1	4045	-	0,6,6	-	-	-		
88	OHX	1	4113	-	0,6,6	-	-	-		
88	OHX	1	3922	-	0,6,6	-	-	-		
88	OHX	2	2032	-	0,6,6	-	-	-		
88	OHX	6	2086	-	0,6,6	-	-	-		
88	OHX	6	2134	-	0,6,6	-	-	-		
88	OHX	6	2151	-	0,6,6	-	-	-		
88	OHX	2	2131	-	0,6,6	-	-	-		
88	OHX	6	2146	-	0,6,6	-	-	-		
88	OHX	1	4081	-	0,6,6	-	-	-		
88	OHX	4	223	-	0,6,6	-	-	-		
88	OHX	1	4210	-	0,6,6	-	-	-		
88	OHX	4	233	-	0,6,6	-	-	-		
88	OHX	7	221	-	0,6,6	-	-	-		
88	OHX	6	2200	-	0,6,6	-	-	-		
88	OHX	5	4091	-	0,6,6	-	-	-		
88	OHX	6	2048	-	0,6,6	-	-	-		
88	OHX	5	4097	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	6	2072	-	0,6,6	-	-	-		
88	OHX	1	4051	-	0,6,6	-	-	-		
88	OHX	2	2058	-	0,6,6	-	-	-		
88	OHX	2	2068	-	0,6,6	-	-	-		
88	OHX	1	3875	-	0,6,6	-	-	-		
88	OHX	1	4020	-	0,6,6	-	-	-		
88	OHX	1	4086	-	0,6,6	-	-	-		
88	OHX	6	2112	-	0,6,6	-	-	-		
88	OHX	1	4063	-	0,6,6	-	-	-		
88	OHX	1	3904	-	0,6,6	-	-	-		
88	OHX	5	3997	-	0,6,6	-	-	-		
88	OHX	2	2101	-	0,6,6	-	-	-		
88	OHX	6	2148	-	0,6,6	-	-	-		
88	OHX	1	4125	-	0,6,6	-	-	-		
88	OHX	1	4011	-	0,6,6	-	-	-		
88	OHX	6	2145	-	0,6,6	-	-	-		
88	OHX	7	224	-	0,6,6	-	-	-		
88	OHX	5	4011	-	0,6,6	-	-	-		
88	OHX	15	306	-	0,6,6	-	-	-		
88	OHX	6	2122	-	0,6,6	-	-	-		
88	OHX	5	4071	-	0,6,6	-	-	-		
88	OHX	1	4017	-	0,6,6	-	-	-		
88	OHX	5	4213	-	0,6,6	-	-	-		
88	OHX	5	4128	-	0,6,6	-	-	-		
88	OHX	6	2069	-	0,6,6	-	-	-		
88	OHX	1	4122	-	0,6,6	-	-	-		
88	OHX	6	2088	-	0,6,6	-	-	-		
88	OHX	1	3969	-	0,6,6	-	-	-		
88	OHX	6	2085	-	0,6,6	-	-	-		
88	OHX	5	3954	-	0,6,6	-	-	-		
88	OHX	1	4201	-	0,6,6	-	-	-		
88	OHX	6	2098	-	0,6,6	-	-	-		
88	OHX	5	3972	-	0,6,6	-	-	-		
88	OHX	5	4117	-	0,6,6	-	-	-		
88	OHX	2	2143	-	0,6,6	-	-	-		
88	OHX	1	4076	-	0,6,6	-	-	-		
88	OHX	5	4150	-	0,6,6	-	-	-		
88	OHX	5	4217	-	0,6,6	-	-	-		
88	OHX	1	3994	-	0,6,6	-	-	-		
88	OHX	1	3929	-	0,6,6	-	-	-		
88	OHX	5	4178	-	0,6,6	-	-	-		
88	OHX	5	4186	-	0,6,6	-	-	-		
88	OHX	6	2191	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4207	-	0,6,6	-	-	-		
88	OHX	1	4147	-	0,6,6	-	-	-		
88	OHX	1	4215	-	0,6,6	-	-	-		
88	OHX	5	4132	-	0,6,6	-	-	-		
88	OHX	1	4039	-	0,6,6	-	-	-		
88	OHX	6	2082	-	0,6,6	-	-	-		
88	OHX	5	3987	-	0,6,6	-	-	-		
88	OHX	5	4081	-	0,6,6	-	-	-		
88	OHX	1	4182	-	0,6,6	-	-	-		
88	OHX	5	4160	-	0,6,6	-	-	-		
88	OHX	5	4087	-	0,6,6	-	-	-		
88	OHX	5	3959	-	0,6,6	-	-	-		
88	OHX	5	4066	-	0,6,6	-	-	-		
88	OHX	6	2158	-	0,6,6	-	-	-		
88	OHX	1	3883	-	0,6,6	-	-	-		
88	OHX	1	4094	-	0,6,6	-	-	-		
88	OHX	5	3974	-	0,6,6	-	-	-		
88	OHX	6	2197	-	0,6,6	-	-	-		
88	OHX	5	4007	-	0,6,6	-	-	-		
88	OHX	1	3984	-	0,6,6	-	-	-		
88	OHX	1	4218	-	0,6,6	-	-	-		
88	OHX	6	2186	-	0,6,6	-	-	-		
88	OHX	5	4113	-	0,6,6	-	-	-		
88	OHX	1	3963	-	0,6,6	-	-	-		
88	OHX	4	232	-	0,6,6	-	-	-		
88	OHX	3	220	-	0,6,6	-	-	-		
88	OHX	5	4170	-	0,6,6	-	-	-		
88	OHX	1	4103	-	0,6,6	-	-	-		
88	OHX	1	4169	-	0,6,6	-	-	-		
88	OHX	1	3920	-	0,6,6	-	-	-		
88	OHX	1	4000	-	0,6,6	-	-	-		
88	OHX	1	4047	-	0,6,6	-	-	-		
88	OHX	1	4135	-	0,6,6	-	-	-		
88	OHX	6	2129	-	0,6,6	-	-	-		
88	OHX	1	4056	-	0,6,6	-	-	-		
88	OHX	2	2104	-	0,6,6	-	-	-		
88	OHX	5	4169	-	0,6,6	-	-	-		
88	OHX	5	4229	-	0,6,6	-	-	-		
88	OHX	2	2048	-	0,6,6	-	-	-		
88	OHX	5	4040	-	0,6,6	-	-	-		
88	OHX	5	3996	-	0,6,6	-	-	-		
88	OHX	1	3916	-	0,6,6	-	-	-		
88	OHX	6	2167	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4119	-	0,6,6	-	-	-		
88	OHX	2	2103	-	0,6,6	-	-	-		
88	OHX	1	3934	-	0,6,6	-	-	-		
88	OHX	2	2070	-	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
91	C	q2	502	-	-	0/7/25/26	0/2/2/2
91	C	Q2	502	-	-	5/7/25/26	0/2/2/2
91	C	q2	503	-	-	2/7/25/26	0/2/2/2
90	A	5	3401	-	-	2/3/25/26	0/3/3/3
91	C	Q2	503	-	-	2/7/25/26	0/2/2/2
90	A	1	3401	-	-	2/3/25/26	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	Q2	503	C	O2-C2-N1	-2.93	112.84	118.89
91	Q2	503	C	C1'-N1-C6	2.63	126.58	120.84
90	5	3401	A	C5-C6-N6	2.29	123.84	120.35
91	Q2	503	C	N1-C2-N3	2.29	122.97	118.81
91	q2	503	C	C5-C4-N4	-2.22	117.08	120.57
90	1	3401	A	C1'-N9-C4	2.19	130.49	126.64
90	1	3401	A	C4-C5-N7	2.14	111.63	109.40
91	Q2	503	C	C6-N1-C2	-2.04	116.95	120.49

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	Q2	502	C	C2'-C1'-N1-C2
91	Q2	502	C	C2'-C1'-N1-C6
91	Q2	503	C	O4'-C4'-C5'-O5'
91	q2	503	C	O4'-C4'-C5'-O5'
91	q2	503	C	C3'-C4'-C5'-O5'

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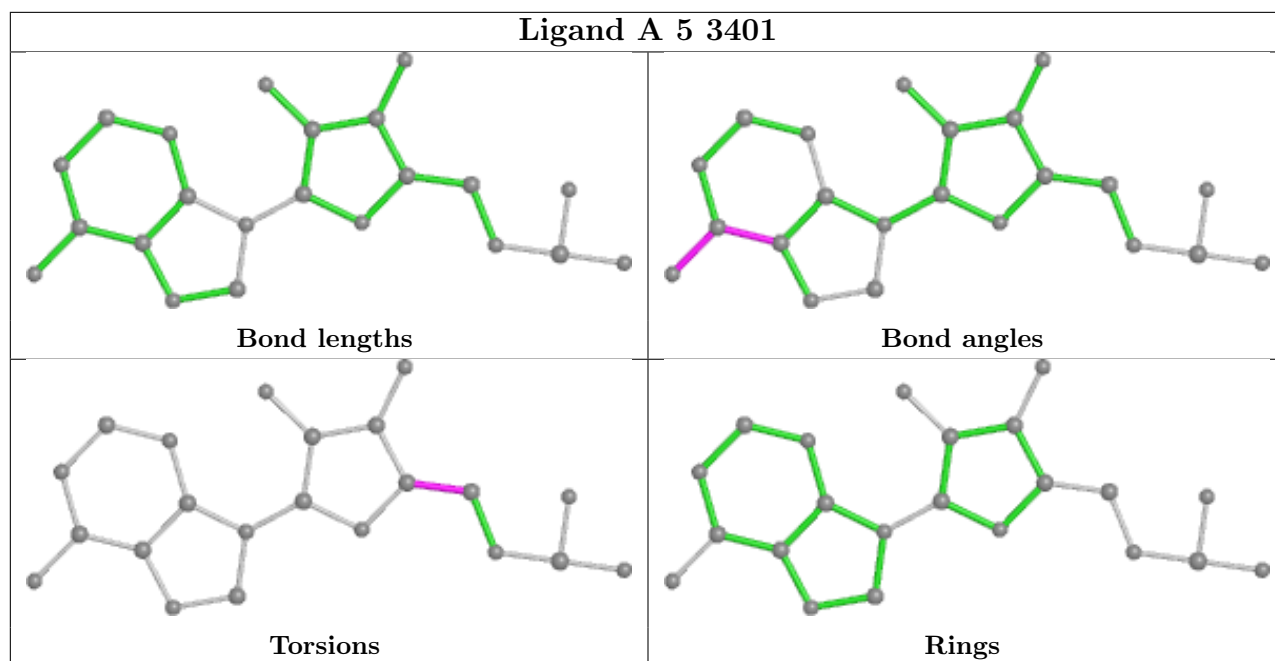
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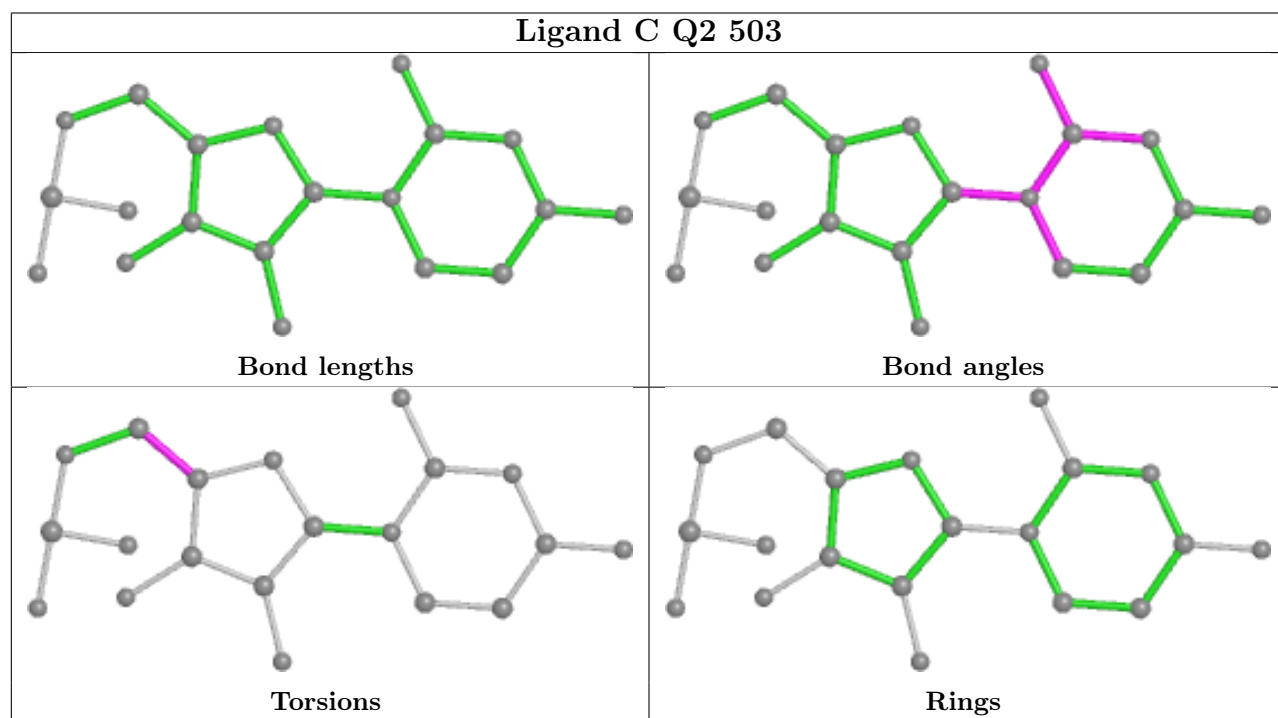
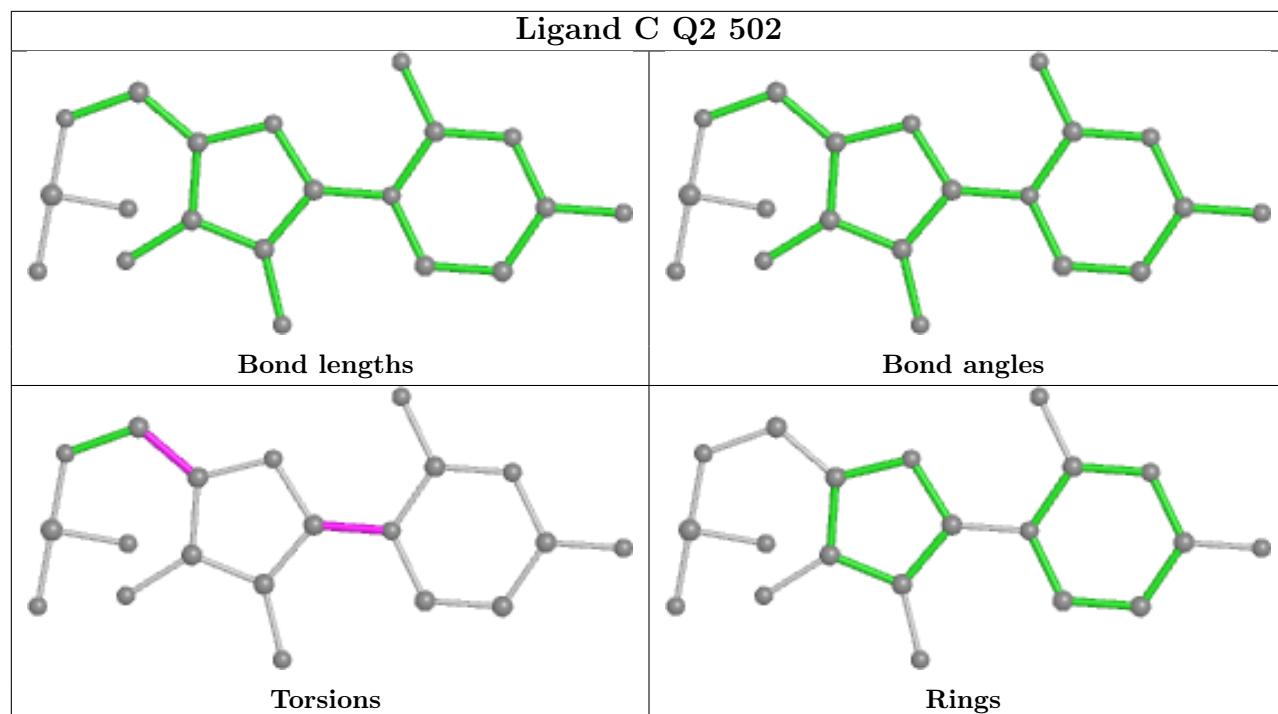
Mol	Chain	Res	Type	Atoms
90	1	3401	A	C3'-C4'-C5'-O5'
91	Q2	503	C	C3'-C4'-C5'-O5'
90	1	3401	A	O4'-C4'-C5'-O5'
90	5	3401	A	C3'-C4'-C5'-O5'
91	Q2	502	C	O4'-C4'-C5'-O5'
91	Q2	502	C	O4'-C1'-N1-C6
91	Q2	502	C	O4'-C1'-N1-C2
90	5	3401	A	O4'-C4'-C5'-O5'

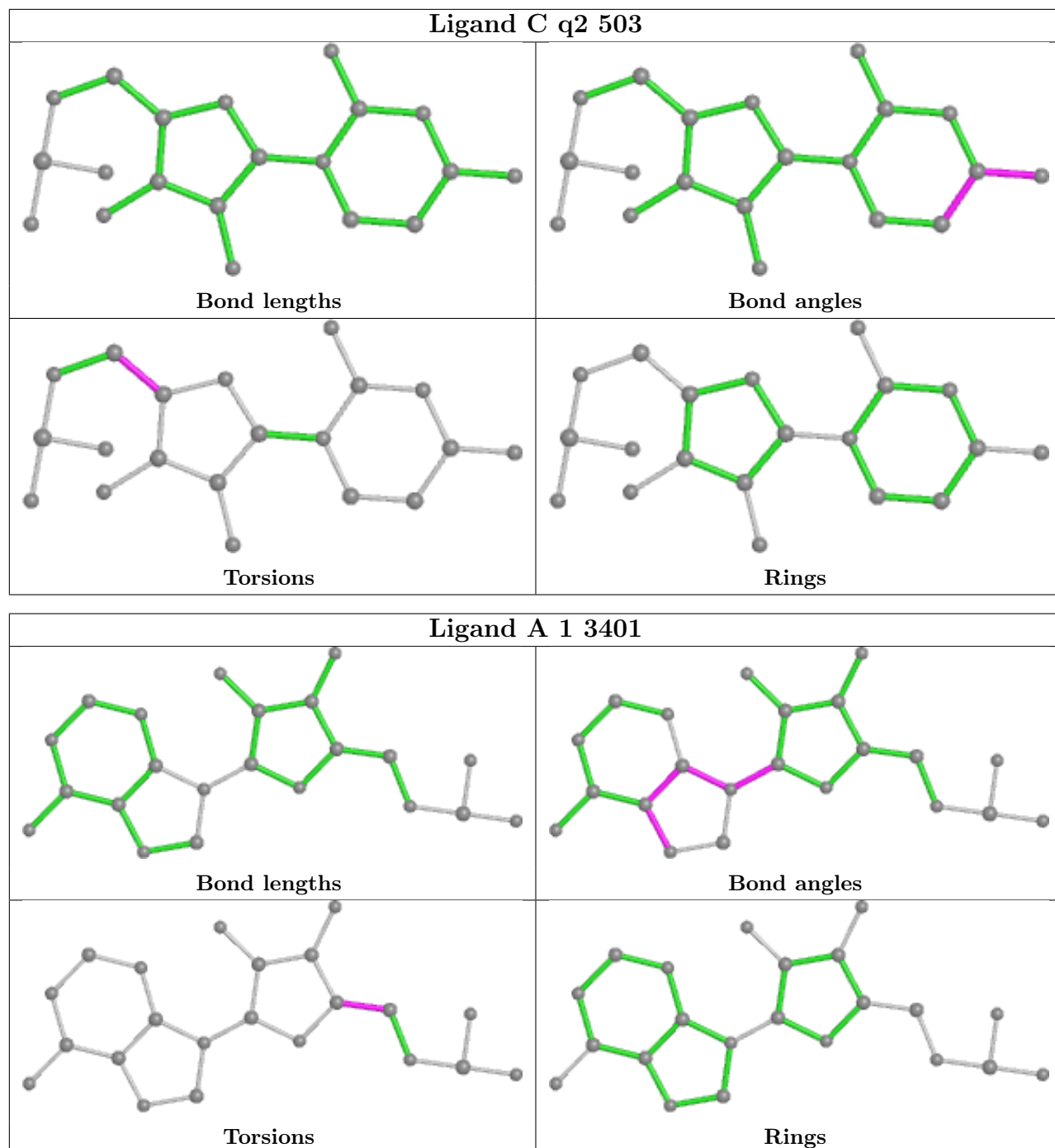
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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