Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 08:00 pm GMT

PDB ID	:	4U4R
Title	:	Crystal structure of Lactimidomycin bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-24
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

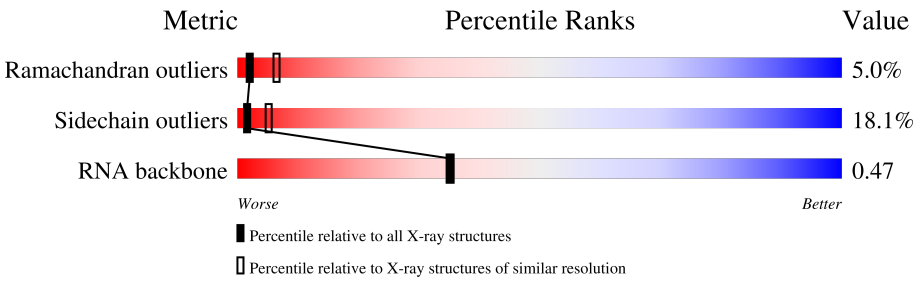
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	67% 25% 6% •
1	6	1800	65% 29% 6%
2	S0	251	61% 20% • 18%
2	s0	251	64% 16% • 18%
3	S1	254	63% 20% • 16%
3	s1	254	70% 14% • 15%
4	S2	253	68% 17% • 14%
4	s2	253	68% 17% • 14%

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Mol	Chain	Length	Quality of chain
5	S3	239	77% 16% • 7%
5	s3	239	75% 17% • 7%
6	S4	260	82% 16% •
6	s4	260	83% 17% •
7	S5	224	70% 20% • 8%
7	s5	224	70% 20% • 8%
8	S6	236	79% 17% •
8	s6	236	74% 18% 8%
9	S7	189	76% 20% • •
9	s7	189	76% 20% • •
10	S8	200	76% 16% • 6%
10	s8	200	80% 14% • 6%
11	S9	196	72% 21% • 6%
11	s9	196	76% 16% • 6%
12	C0	105	68% 23% • 9%
12	c0	105	68% 21% • 9%
13	C1	155	79% 20% •
13	c1	155	75% 19% • 6%
14	C2	142	58% 27% • 13%
14	c2	142	59% 25% • • 13%
15	C3	150	81% 19% •
15	c3	150	81% 18% •
16	C4	136	72% 18% • • 7%
16	c4	136	74% 15% • 6%
17	C5	141	71% 16% • 12%

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Mol	Chain	Length	Quality of chain
17	c5	141	70% 23%
18	C6	142	80% 18%
18	c6	142	81% 18%
19	C7	136	66% 21% 12%
19	c7	136	71% 15% 14%
20	C8	145	78% 19%
20	c8	145	78% 20%
21	C9	143	83% 15%
21	c9	143	83% 16%
22	D0	120	67% 22% 11%
22	d0	120	68% 22% 8%
23	D1	87	77% 23%
23	d1	87	75% 25%
24	D2	129	87% 12%
24	d2	129	88% 12%
25	D3	144	79% 17%
25	d3	144	88% 10%
26	D4	134	82% 16%
26	d4	134	82% 16%
27	D5	107	42% 21% 35%
27	d5	107	52% 12% 36%
28	D6	97	74% 19% 5%
28	d6	97	78% 21%
29	D7	81	80% 16%
29	d7	81	78% 20%

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Mol	Chain	Length	Quality of chain
30	D8	66	74% 20% 5%
30	d8	66	79% 14% 5%
31	D9	55	75% 20%
31	d9	55	73% 24%
32	E0	60	83% 15%
33	E1	76	55% 30% 8% 7%
33	e1	76	57% 37% 5%
34	SR	318	89% 10%
34	sR	318	89% 10%
35	SM	273	46% 10% 42%
35	sM	273	32% 5% 62%
36	1	3396	51% 34% 7% 7%
36	5	3396	51% 35% 7% 7%
37	3	121	70% 27%
37	7	121	63% 31% 6%
38	4	158	58% 35% 7%
38	8	158	63% 30% 7%
39	L2	253	84% 15%
39	l2	253	81% 16%
40	L3	386	81% 18%
40	l3	386	81% 17%
41	L4	361	80% 18%
41	l4	361	81% 18%
42	L5	296	78% 20%
42	l5	296	79% 19%

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Mol	Chain	Length	Quality of chain
43	L6	175	76% 13% • 11%
43	l6	175	74% 15% • 10%
44	L7	243	80% 9% • 9%
44	l7	243	79% 11% • 8%
45	L8	255	75% 16% 9%
45	l8	255	70% 20% • 9%
46	L9	191	82% 17% •
46	l9	191	80% 20% •
47	M0	220	78% 17% •
47	m0	220	77% 20% •
48	M1	173	75% 20% • •
48	m1	173	79% 17% • •
49	M3	198	79% 17% • •
49	m3	198	80% 17% • •
50	M4	137	80% 18% • •
50	m4	137	87% 11% •
51	M5	203	83% 16% •
51	m5	203	85% 14% •
52	M6	198	84% 12% • • •
52	m6	198	82% 15% • • •
53	M7	183	82% 17% •
53	m7	183	74% 10% • 15%
54	M8	185	83% 16% •
54	m8	185	81% 18% •
55	M9	188	89% 10% •

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Mol	Chain	Length	Quality of chain
55	m9	188	81% 19%
56	N0	172	82% 17%
56	n0	172	84% 15%
57	N1	159	80% 19%
57	n1	159	86% 12%
58	N2	120	72% 11% 17%
58	n2	120	69% 12% 18%
59	N3	136	87% 12%
59	n3	136	90% 8%
60	N4	155	57% 5% 37%
60	n4	155	75% 10% 13%
61	N5	141	67% 18% 14%
61	n5	141	66% 18% 15%
62	N6	126	80% 17%
62	n6	126	76% 23%
63	N7	135	76% 23%
63	n7	135	78% 21%
64	N8	148	81% 16%
64	n8	148	80% 18%
65	N9	58	79% 21%
65	n9	58	69% 28%
66	O0	104	78% 14% 7%
66	o0	104	79% 17%
67	O1	112	76% 20%
67	o1	112	79% 17%

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Mol	Chain	Length	Quality of chain
68	O2	129	85% 12%
68	o2	129	82% 14%
69	O3	106	85% 13%
69	o3	106	87% 12%
70	O4	119	77% 16% 6%
70	o4	119	81% 13% 6%
71	O5	119	78% 20%
71	o5	119	76% 23%
72	O6	99	71% 28%
72	o6	99	69% 27%
73	O7	87	79% 21%
73	o7	87	83% 17%
74	O8	77	79% 21%
74	o8	77	82% 17%
75	O9	50	80% 18%
75	o9	50	78% 22%
76	Q0	52	83% 15%
76	q0	52	85% 13%
77	Q1	25	68% 32%
77	q1	25	64% 32%
78	Q2	105	82% 17%
78	q2	105	79% 21%
79	Q3	91	87% 13%
79	q3	91	85% 15%
80	e0	62	76% 23%

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Mol	Chain	Length	Quality of chain
81	m2	160	94% 6%
82	p0	311	39% 7% 54%
83	p1	47	100%
84	p2	46	100%

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 411226 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	37283	16668	6591	12274	1750	0	0	0
1	6	1795	38238	17095	6758	12590	1795	0	0	0

- 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	1577	1014	278	283	2	0	0	0
2	s0	206	1583	1017	281	283	2	0	0	0

- 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	1709	1084	310	311	4	0	0	0
3	s1	216	1722	1091	312	315	4	0	0	0

- 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	1635	1047	289	297	2	0	0	0
4	s2	217	1635	1047	289	297	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	S9	185	1494	943	289	261	1	0	0	0
			Total	C	N	O	S			
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
			Total	C	N	O	S			
12	c0	96	762	491	125	144	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	C1	155	1214	775	230	206	3	0	0	0
			Total	C	N	O	S			
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	890	560	156	172	2	0	0	0
14	c2	124	890	560	156	172	2	0	0	0

- 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	926	577	177	170	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	L3	386	3075	1950	584	533	8	0	0	0
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	1518	963	274	277	4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	847	534	170	138	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
78	q2	105	847	534	170	138	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	694	429	138	121	6	0	0	0
79	q3	91	694	429	138	121	6	0	0	0

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

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

- Molecule 81 is a protein called Unknown protein m2.

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

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

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

- Molecule 83 is a protein called Unknown protein p1.

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

- Molecule 84 is a protein called Unknown protein p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	2	126	126	126	0	0
85	S8	1	1	1	0	0
85	C3	1	1	1	0	0
85	SM	1	1	1	0	0
85	1	475	475	475	0	0
85	3	14	14	14	0	0
85	4	21	21	21	0	0
85	L2	1	1	1	0	0
85	L3	2	2	2	0	0
85	L4	3	3	3	0	0
85	L5	1	1	1	0	0
85	L6	1	1	1	0	0
85	L7	2	2	2	0	0
85	L8	1	1	1	0	0
85	M0	2	2	2	0	0
85	M1	1	1	1	0	0
85	M3	4	4	4	0	0
85	M5	2	2	2	0	0
85	M6	1	1	1	0	0
85	M7	6	6	6	0	0
85	M9	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	N0	1	1	1	0	0
85	N3	3	3	3	0	0
85	N5	1	1	1	0	0
85	N8	2	2	2	0	0
85	O3	1	1	1	0	0
85	O4	1	1	1	0	0
85	O7	1	1	1	0	0
85	Q2	1	1	1	0	0
85	6	147	147	147	0	0
85	s1	1	1	1	0	0
85	s6	1	1	1	0	0
85	s8	2	2	2	0	0
85	c1	1	1	1	0	0
85	c7	1	1	1	0	0
85	c8	2	2	2	0	0
85	d2	1	1	1	0	0
85	d3	1	1	1	0	0
85	d6	1	1	1	0	0
85	sM	2	2	2	0	0
85	5	504	504	504	0	0
85	7	15	15	15	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	8	13	13	13	0	0
85	l2	2	2	2	0	0
85	l3	1	1	1	0	0
85	l4	1	1	1	0	0
85	l5	3	3	3	0	0
85	l7	1	1	1	0	0
85	m1	2	2	2	0	0
85	m4	1	1	1	0	0
85	m5	1	1	1	0	0
85	m6	1	1	1	0	0
85	m7	5	5	5	0	0
85	n0	2	2	2	0	0
85	n3	2	2	2	0	0
85	n6	2	2	2	0	0
85	n8	4	4	4	0	0
85	n9	2	2	2	0	0
85	o1	1	1	1	0	0
85	o3	2	2	2	0	0
85	o4	2	2	2	0	0
85	q0	1	1	1	0	0
85	q1	1	1	1	0	0

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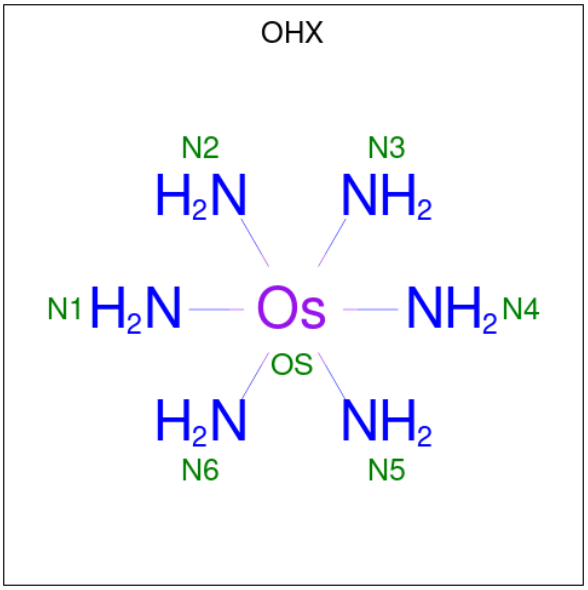
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	q3	1	1	1	0	0

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



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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	S8	1	7	6	1	0	0
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86	C1	1	7	6	1	0	0
			Total	N	Os		
86	C3	1	7	6	1	0	0
			Total	N	Os		
86	C5	1	7	6	1	0	0
			Total	N	Os		
86	C8	1	7	6	1	0	0
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86	D9	1	7	6	1	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	7	6	1	0	0
			Total	N	Os		
86	1	1	7	6	1	0	0
			Total	N	Os		
86	1	1	7	6	1	0	0

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	7	6	1	0	0
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86	4	1	7	6	1	0	0
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86	4	1	7	6	1	0	0
			Total	N	Os		
86	L3	1	7	6	1	0	0
			Total	N	Os		
86	L3	1	7	6	1	0	0
			Total	N	Os		
86	L4	1	7	6	1	0	0
			Total	N	Os		
86	L6	1	7	6	1	0	0
			Total	N	Os		
86	M0	1	7	6	1	0	0
			Total	N	Os		
86	M5	1	7	6	1	0	0
			Total	N	Os		
86	M5	1	7	6	1	0	0
			Total	N	Os		
86	M6	1	7	6	1	0	0
			Total	N	Os		
86	M7	1	7	6	1	0	0
			Total	N	Os		
86	M7	1	7	6	1	0	0
			Total	N	Os		
86	M9	1	7	6	1	0	0
			Total	N	Os		
86	N9	1	7	6	1	0	0
			Total	N	Os		
86	O2	1	7	6	1	0	0
			Total	N	Os		
86	O3	1	7	6	1	0	0
			Total	N	Os		
86	O7	1	7	6	1	0	0
			Total	N	Os		
86	O7	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	O9	1	7	6	1	0	0
			Total	N	Os		
86	Q2	1	7	6	1	0	0
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86	6	1	7	6	1	0	0
			Total	N	Os		
86	6	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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86	6	1	7	6	1	0	0

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	6	1	7	6	1	0	0
			Total	N	Os		
86	6	1	7	6	1	0	0
			Total	N	Os		
86	6	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
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86	6	1	7	6	1	0	0
			Total	N	Os		
86	s1	1	7	6	1	0	0
			Total	N	Os		
86	s1	1	7	6	1	0	0
			Total	N	Os		
86	s4	1	7	6	1	0	0
			Total	N	Os		
86	s8	1	7	6	1	0	0
			Total	N	Os		
86	s9	1	7	6	1	0	0
			Total	N	Os		
86	c1	1	7	6	1	0	0
			Total	N	Os		
86	c3	1	7	6	1	0	0
			Total	N	Os		
86	c5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	c8	1	7	6	1	0	0
86	d4	1	7	6	1	0	0
86	d9	1	7	6	1	0	0
86	sR	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
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86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
86	l3	1	7	6	1	0	0
			Total	N	Os		
86	l3	1	7	6	1	0	0
			Total	N	Os		
86	l4	1	7	6	1	0	0
			Total	N	Os		
86	l4	1	7	6	1	0	0
			Total	N	Os		
86	l5	1	7	6	1	0	0
			Total	N	Os		
86	l5	1	7	6	1	0	0
			Total	N	Os		
86	l5	1	7	6	1	0	0
			Total	N	Os		
86	l9	1	7	6	1	0	0
			Total	N	Os		
86	m0	1	7	6	1	0	0
			Total	N	Os		
86	m0	1	7	6	1	0	0
			Total	N	Os		
86	m1	1	7	6	1	0	0
			Total	N	Os		
86	m4	1	7	6	1	0	0
			Total	N	Os		
86	m5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	m6	1	7	6	1	0	0
86	m7	1	7	6	1	0	0
86	m8	1	7	6	1	0	0
86	n3	1	7	6	1	0	0
86	n9	1	7	6	1	0	0
86	o2	1	7	6	1	0	0
86	o3	1	7	6	1	0	0
86	o4	1	7	6	1	0	0
86	o7	1	7	6	1	0	0
86	q2	1	7	6	1	0	0

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

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

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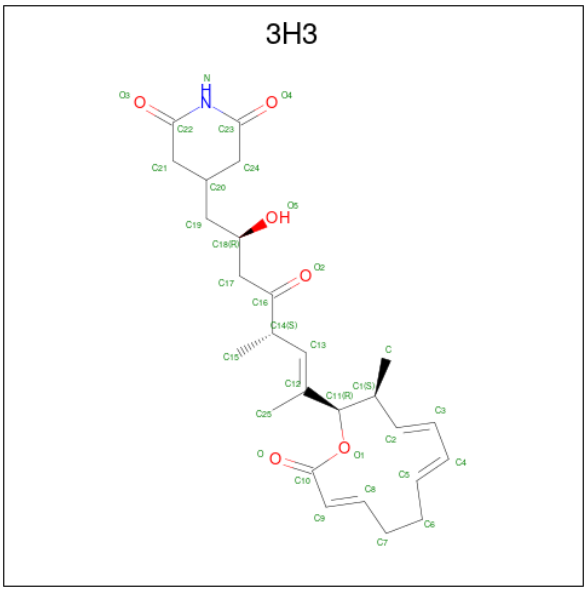
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	d7	1	Total Zn 1 1	0	0
87	d9	1	Total Zn 1 1	0	0
87	e1	1	Total Zn 1 1	0	0
87	o7	1	Total Zn 1 1	0	0
87	q0	1	Total Zn 1 1	0	0
87	q2	1	Total Zn 1 1	0	0
87	q3	1	Total Zn 1 1	0	0

- Molecule 88 is 4-{(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxooxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl}piperidine-2,6-dione (three-letter code: 3H3) (formula: $C_{26}H_{35}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	1	1	Total C N O 33 26 1 6	0	0
88	5	1	Total C N O 33 26 1 6	0	0

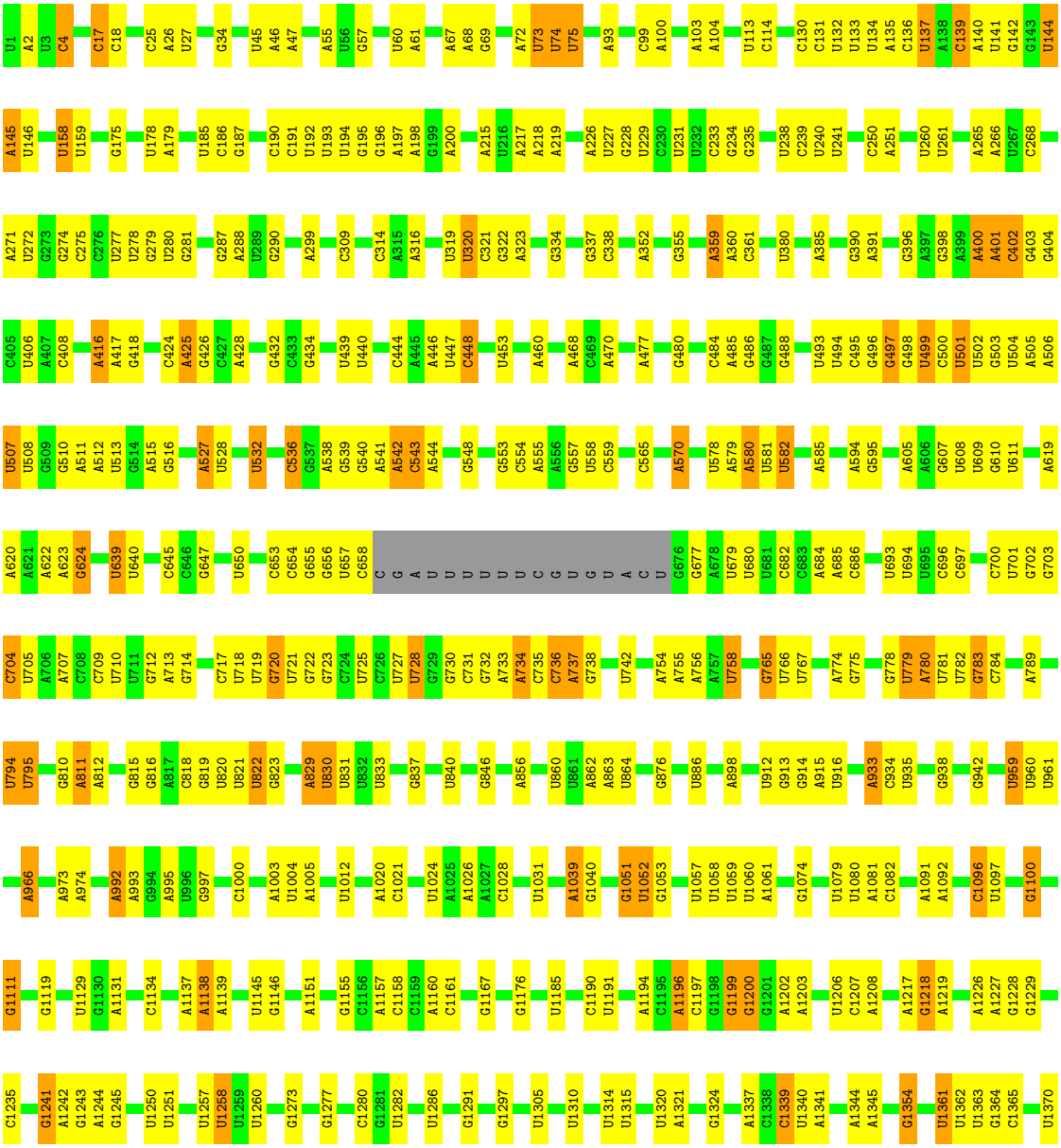
3 Residue-property plots (i)

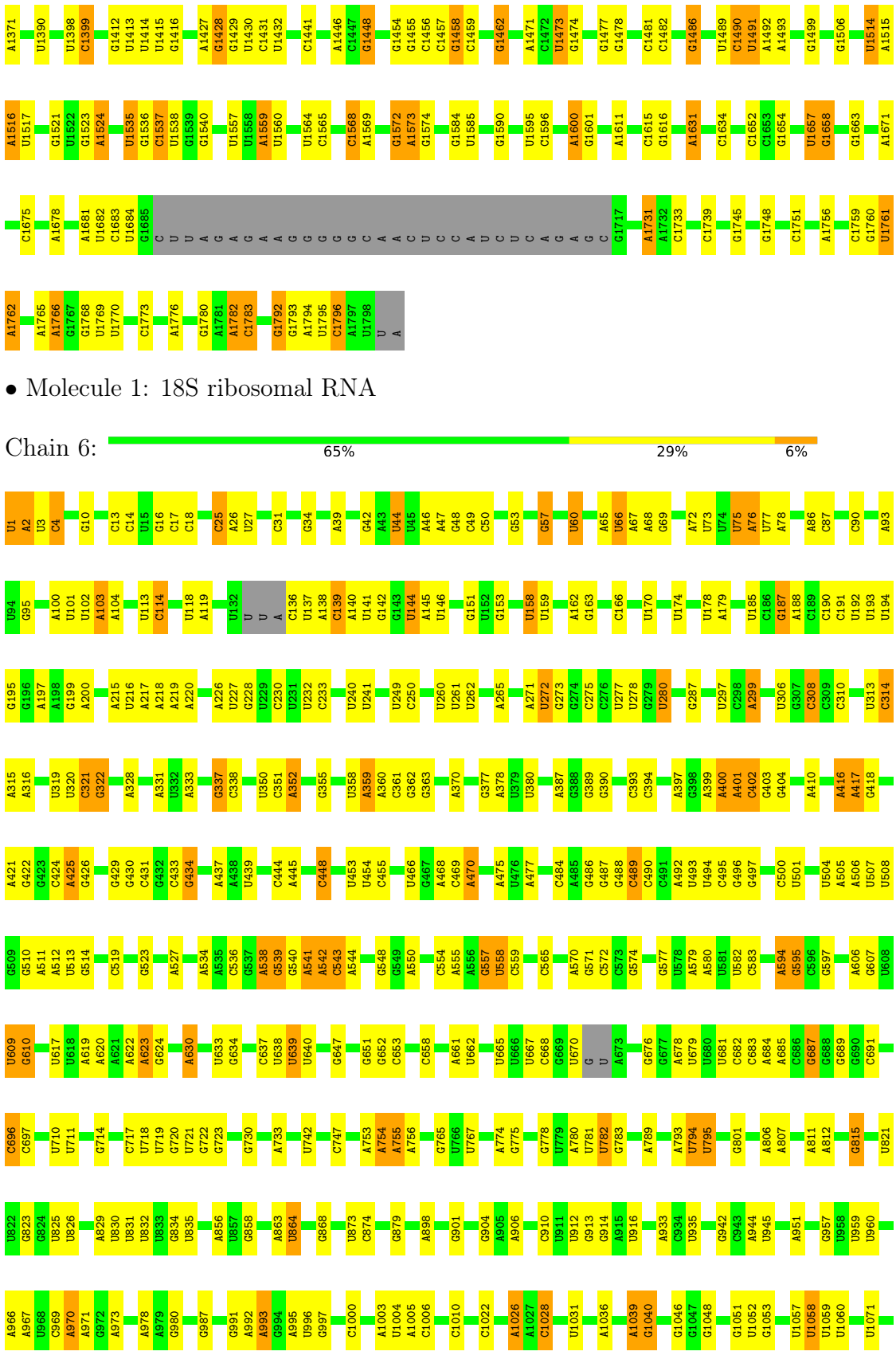
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

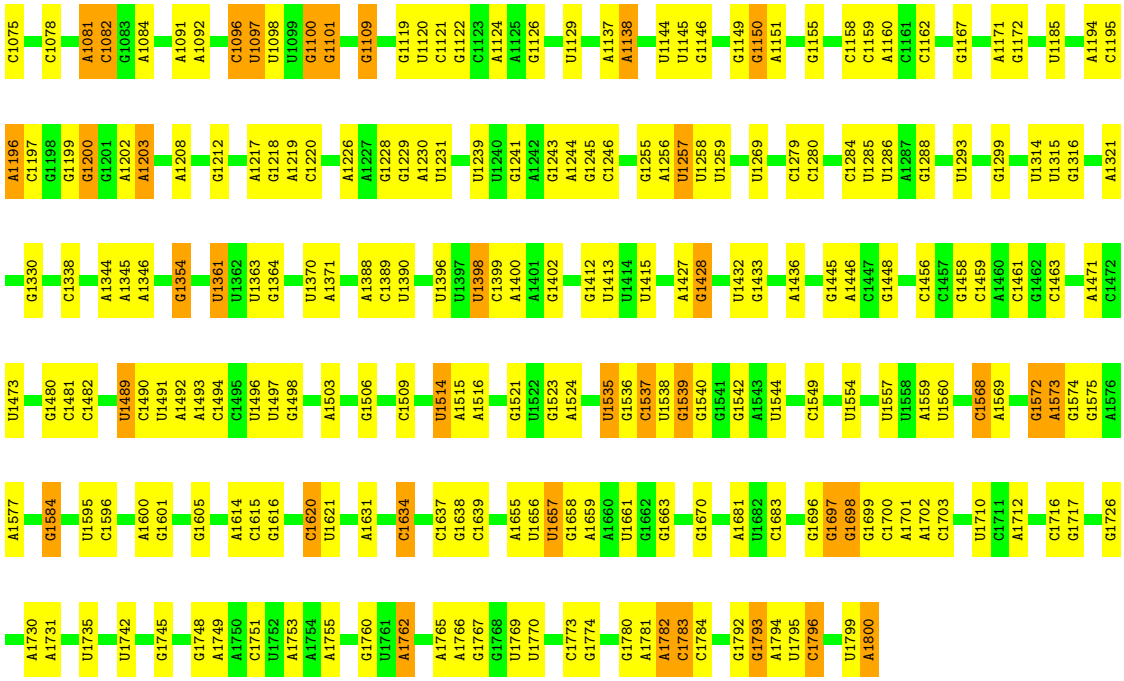
Chain 2:





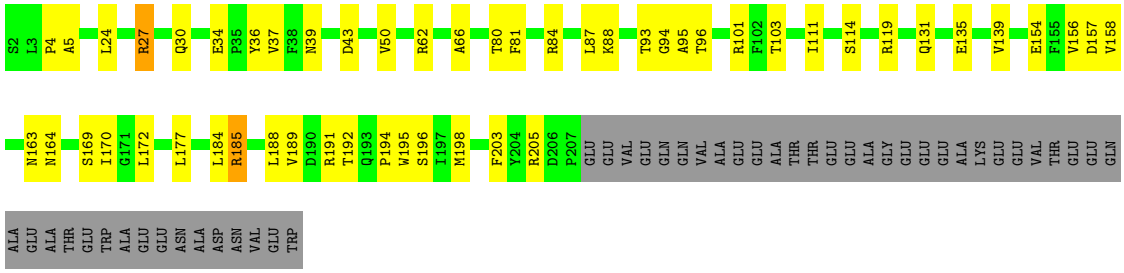
• Molecule 1: 18S ribosomal RNA

Chain 6: 65% 29% 6%



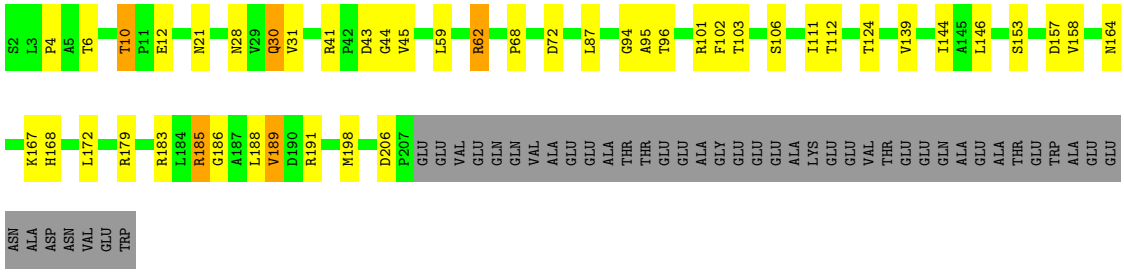
- Molecule 2: 40S ribosomal protein S0-A

Chain S0:



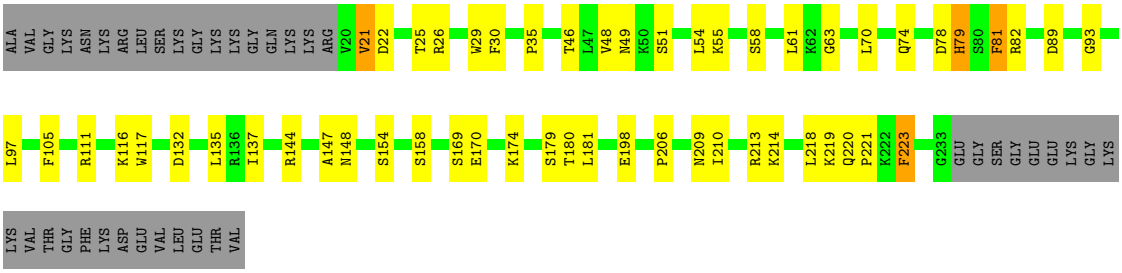
- Molecule 2: 40S ribosomal protein S0-A

Chain s0:



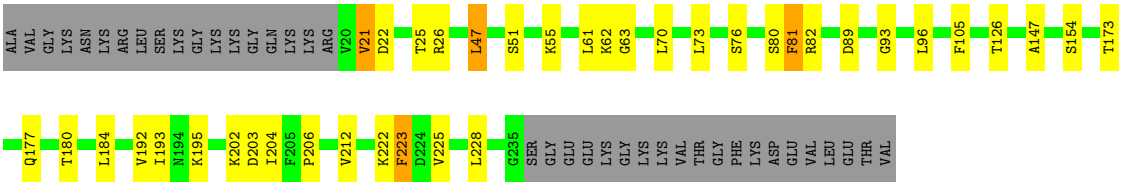
- Molecule 3: 40S ribosomal protein S1-A

Chain S1:



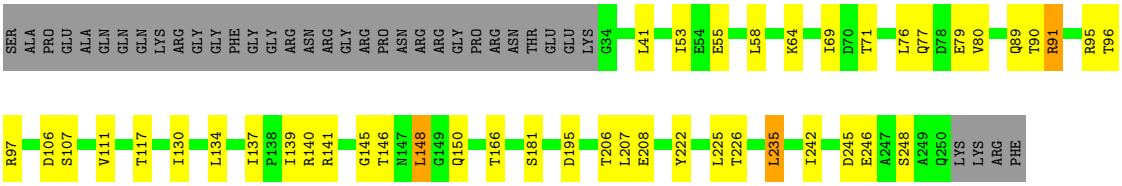
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



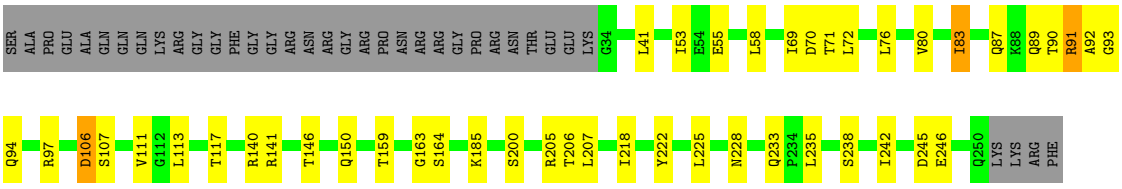
• Molecule 4: 40S ribosomal protein S2

Chain S2:



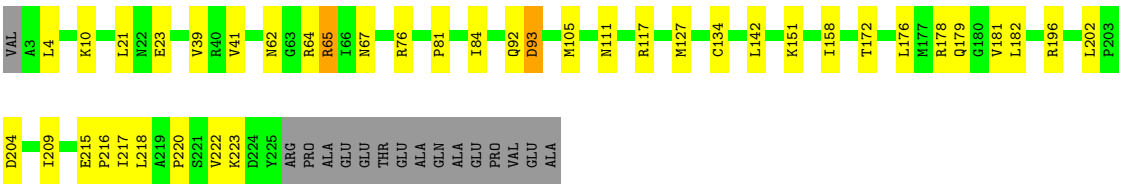
• Molecule 4: 40S ribosomal protein S2

Chain s2:



• Molecule 5: 40S ribosomal protein S3

Chain S3:



• Molecule 5: 40S ribosomal protein S3

Chain s3: 75% 17% • 7%

VAL A3 L4 K7 K8 R9 K10 V37 E38 V39 R40 L59 G60 E61 I66 L69 I84 E89 R90 Y91 Q92 D93 R94 N111 I115 R116 R117 E128 K132 L142 R143 A144 A145 R146 I158 Q162 P163 V164 D169 T172 Q179 G180 V181

R196 L202 P203 K212 P216 I217 L218 A219 P220 Y225 ARG PRO ALA GLU GLU THR GLU ALA GLN ALA GLU PRO VAL GLU ALA

• Molecule 6: 40S ribosomal protein S4-A

Chain S4: 82% 16% •

A2 K6 K7 H8 L9 L12 D21 K22 L23 C26 L38 I45 L48 K62 L65 M66 Q67 V70 K71 V72 R77 L92 V102 Y103 D104 V105 T115 D116 L123 V126 L131 G132 K133 N157 L164 L180 V181 Y182 R187

G193 T194 I195 V196 H197 K198 K211 D215 R221 L222 N223 V227 K233 K240 G241 K242 K245 I248 Q258 L261

• Molecule 6: 40S ribosomal protein S4-A

Chain s4: 83% 17% •

A2 K7 H8 L9 L12 L23 S24 R30 L38 L42 L48 R49 N50 R51 N57 Q67 V70 T78 I90 T91 T95 V102 Y103 D104 R113 D116 L123 V126 K127 K128 V129 Q130 L131 I147 R148 V160 D163 L164

K168 L180 V181 Y182 R187 I192 I195 V196 R221 L222 V227 S237 K245 R254 L261

• Molecule 7: 40S ribosomal protein S5

Chain S5: 70% 20% • 8%

SER ASP THR GLU ALA PRO VAL GLU VAL GLN GLU ASP PHE GLU VAL VAL GLU GLU F20 T21 P22 V23 V24 L25 A26 Q35 T38 E39 I40 K41 L42 F43 N44 K45 V51 E52 V53 L58 V59 D60 Q63 V64 R65 R76 N79 K84 P88 I89 L93 T94

M99 N100 G101 R112 D119 L124 Q127 N139 T146 T147 R148 V149 G150 G153 A154 A155 R156 R157 V160 D161 V162 R185 I190 T193 L194 G204 S205 S206 R225

• Molecule 7: 40S ribosomal protein S5

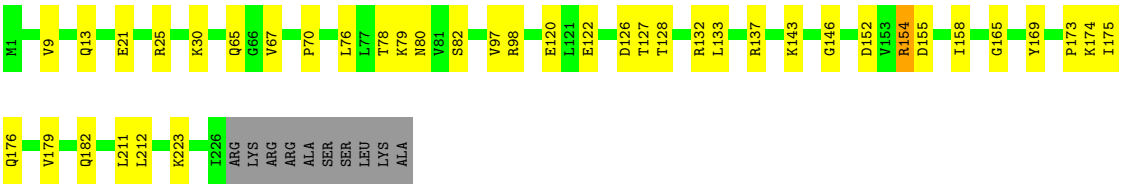
Chain s5: 70% 20% • 8%

SER ASP THR GLU ALA PRO VAL GLU VAL GLN GLU ASP PHE GLU VAL VAL GLU GLU F20 T21 P22 V23 V24 L25 A26 T27 P28 I29 E32 V33 A36 Q37 T38 E39 F43 N44 K45 K54 V59 D60 Q63 V64 I68 A71 R76 N79 R83 K84

I89 R92 L93 M99 N100 K109 I114 D119 T125 D126 Q127 T146 T147 R148 V149 G150 G151 G152 G153 R157 S163 R167 F184 I187 L194 K203 E216 R225

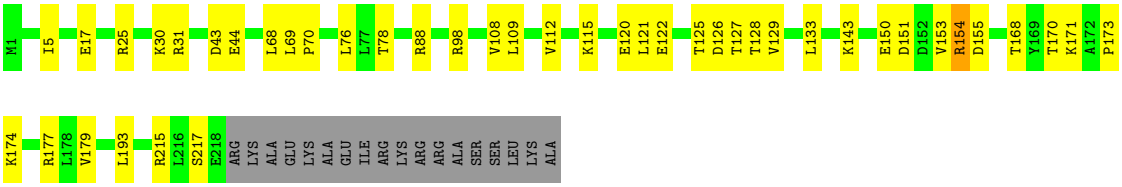
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



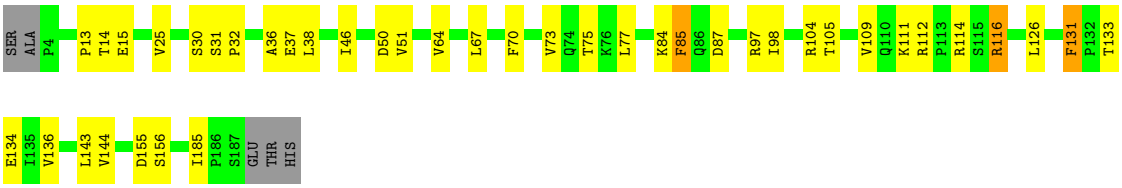
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



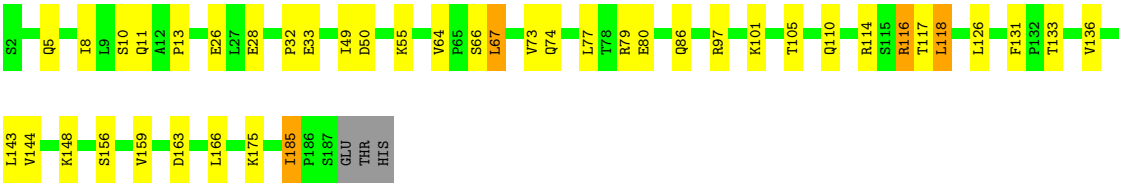
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



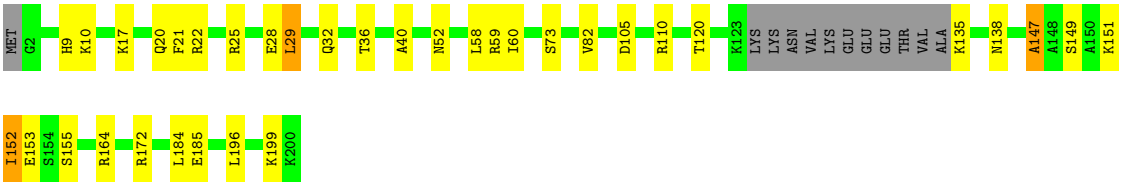
• Molecule 9: 40S ribosomal protein S7-A

Chain s7:



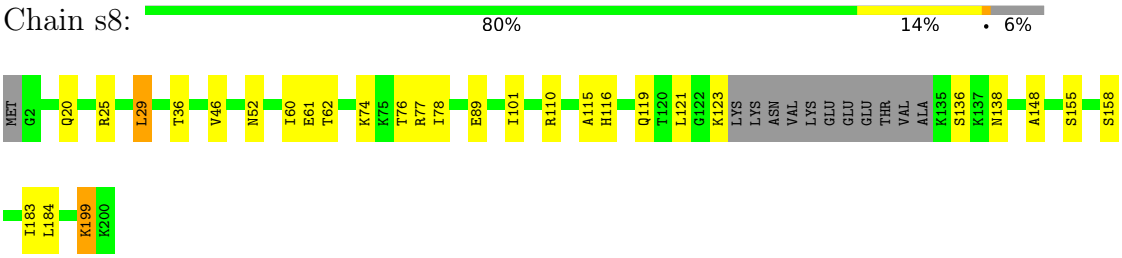
• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



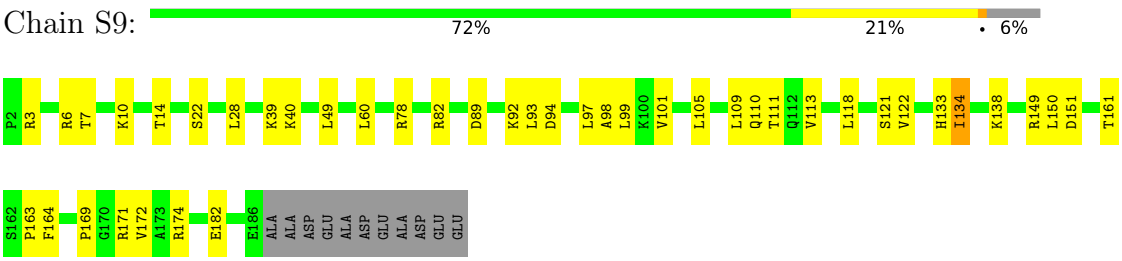
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



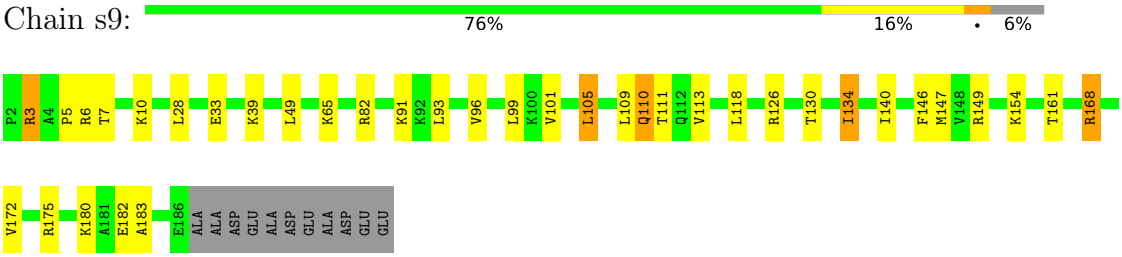
- Molecule 11: 40S ribosomal protein S9-A

Chain S9:



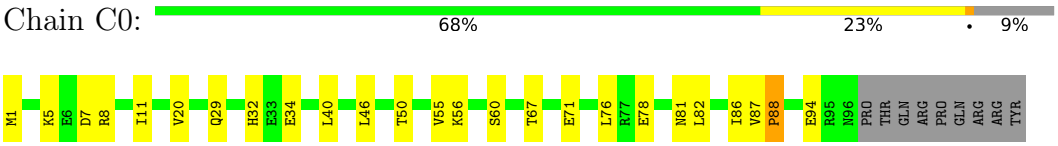
- Molecule 11: 40S ribosomal protein S9-A

Chain s9:



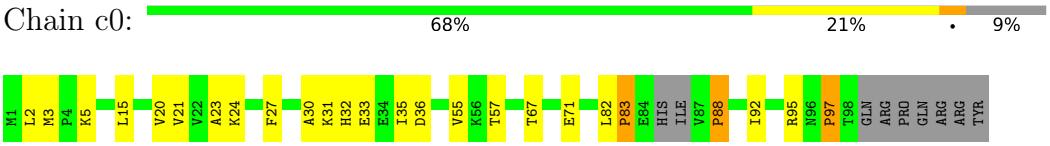
- Molecule 12: 40S ribosomal protein S10-A

Chain C0:



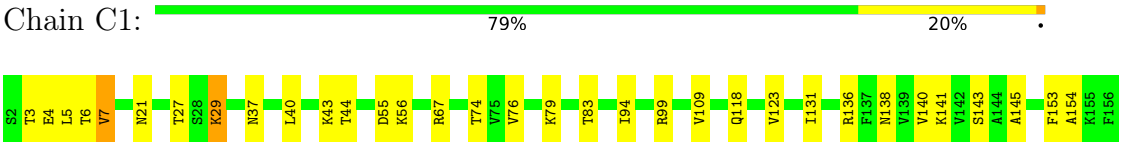
- Molecule 12: 40S ribosomal protein S10-A

Chain c0:



- Molecule 13: 40S ribosomal protein S11-A

Chain C1:



• Molecule 13: 40S ribosomal protein S11-A

Chain c1: 75% 19% • 6%

S2 L5 T6 V7 E10 N21 K26 T27 R30 T31 K32 R33 L40 T44 T47 D55 K56 F60 T61 R67 T74 M80 T83 V109 A114 V123 R129 S132 K133 V140 S143 A144 A145 A146 A147 LYS ALA ASN LYS

GLN PHE ALA LYS PHE

• Molecule 14: 40S ribosomal protein S12

Chain C2: 58% 27% • 13%

SER ASP VAL GLU GLU VAL VAL GLU VAL GLN GLU GLU THR VAL VAL GLU GLN THR A20 E21 V22 E25 L28 R33 D39 G40 R43 R46 K50 R54 G55 L59 V66 I71 I72 K73 L74 D81 V86 P87 L88 I89 K90 V91 A92 D93

L97 A101 G102 L103 I106 D107 R108 A112 V115 V116 G117 A118 S119 N125 W126 G127 A128 E129 T130 D131 E132 H139 F140 Q143

• Molecule 14: 40S ribosomal protein S12

Chain c2: 59% 25% • • 13%

SER ASP VAL GLU GLU VAL VAL GLU VAL GLN GLU GLU THR VAL VAL GLU GLN THR A20 E21 V22 E25 D26 A27 L28 V37 R43 G44 L45 T53 R54 I58 L59 V60 V61 L62 V66 I71 L74 P82 E83 N84 K85 V86 P87 L88 I89 K90 V91 A92

A101 G102 L103 I106 D107 R108 V115 V116 G117 A118 S119 V120 V121 D131 E132 M137 E138 H139 F140 Q143

• Molecule 15: 40S ribosomal protein S13

Chain C3: 81% 19% •

G2 R3 K9 G10 I11 S12 I16 A22 K27 S32 K39 R42 L45 D56 R64 V65 I66 K76 S77 E83 L88 L102 R106 R114 L115 L125 A126 R127 V134 Y141 E142 S143 A144 T145 L149 V150 N151

• Molecule 15: 40S ribosomal protein S13

Chain c3: 81% 18% •

G2 S12 I16 S19 R20 N21 A22 S29 K39 L53 V60 R64 V65 I66 T67 K70 L80 D87 L88 K93 R104 R114 L115 L125 A126 R127 P137 N138 W139 K140 S147 V150 N151

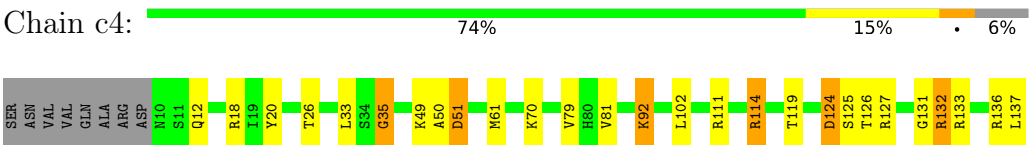
• Molecule 16: 40S ribosomal protein S14-A

Chain C4: 72% 18% • • 7%

SER ASN VAL VAL GLN ALA ARG ASP ASN S11 Q12 V13 F14 G15 V16 A17 R18 I19 Y20 H29 V30 T31 I39 A40 R41 V42 A50 D51 S55 S56 G75 T86 K92 L102 R103 R107 R114 S123 D124 S125 T126 R132 R136 L137

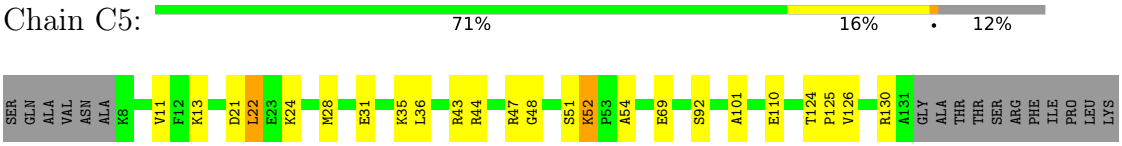
• Molecule 16: 40S ribosomal protein S14-A

Chain c4:



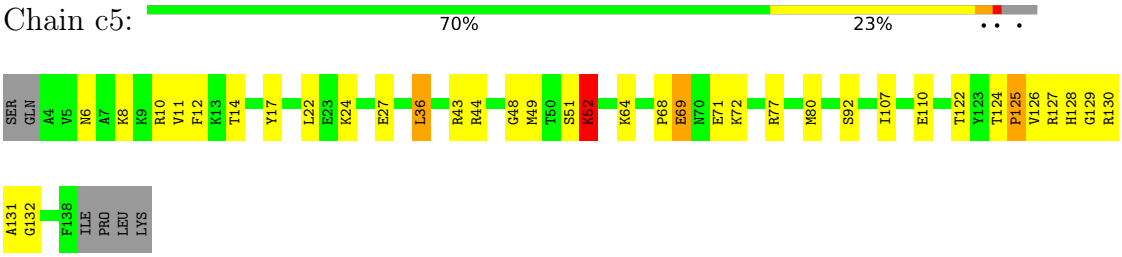
• Molecule 17: 40S ribosomal protein S15

Chain C5:



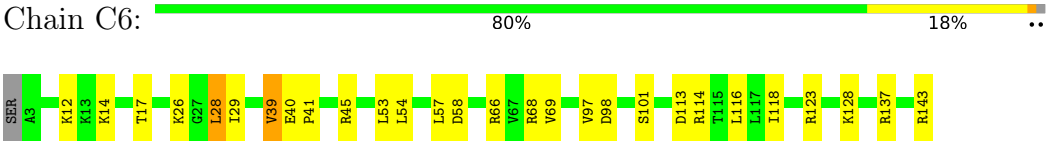
• Molecule 17: 40S ribosomal protein S15

Chain c5:



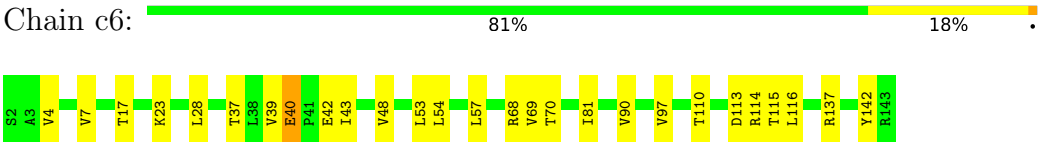
• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



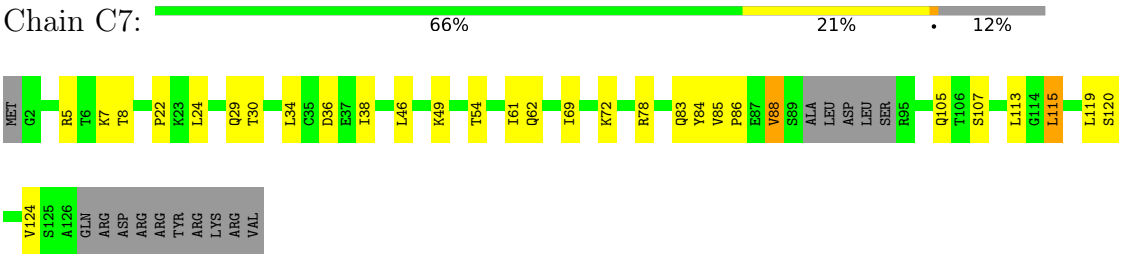
• Molecule 18: 40S ribosomal protein S16-A

Chain c6:



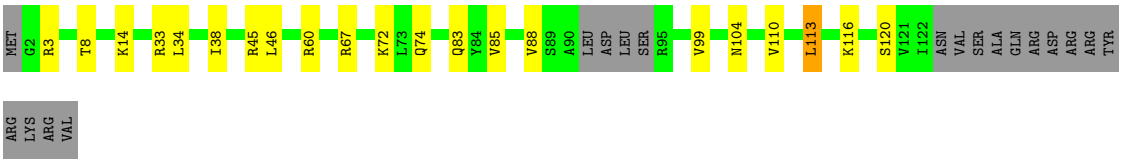
• Molecule 19: 40S ribosomal protein S17-A

Chain C7:



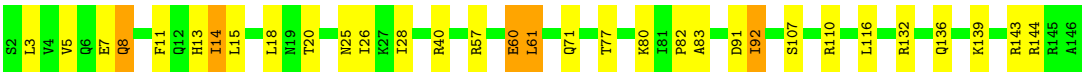
• Molecule 19: 40S ribosomal protein S17-A

Chain c7: 71% 15% • 14%



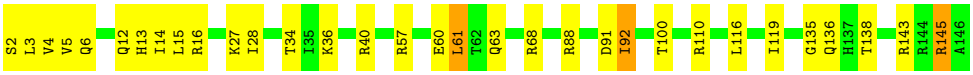
• Molecule 20: 40S ribosomal protein S18-A

Chain C8: 78% 19% •



• Molecule 20: 40S ribosomal protein S18-A

Chain c8: 78% 20% •

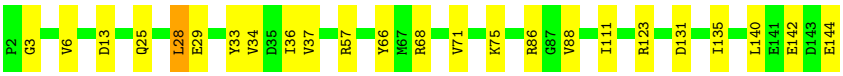


• Molecule 21: 40S ribosomal protein S19-A

Chain C9: 83% 15% •

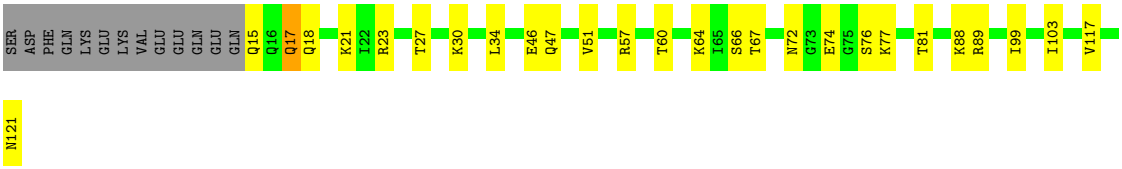
• Molecule 21: 40S ribosomal protein S19-A

Chain c9: 83% 16% •



• Molecule 22: 40S ribosomal protein S20

Chain D0: 67% 22% • 11%

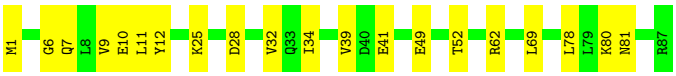


• Molecule 22: 40S ribosomal protein S20

Chain d0: 68% 22% • 8%

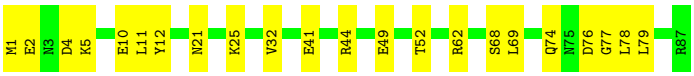
• Molecule 23: 40S ribosomal protein S21-A

Chain D1:



• Molecule 23: 40S ribosomal protein S21-A

Chain d1:



• Molecule 24: 40S ribosomal protein S22-A

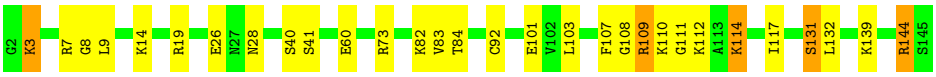
Chain D2:

• Molecule 24: 40S ribosomal protein S22-A

Chain d2:

• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



• Molecule 25: 40S ribosomal protein S23-A

Chain d3:

• Molecule 26: 40S ribosomal protein S24-A

Chain D4: 82% 16%

S2 D3 A4 V5 T6 R10 L17 R32 A33 N34 V35 S36 E51 V57 F58 G59 F60 R61 T62 V75 K84 T88 K99 K102 T121 R124 K127 K128 N133 A134 D135

• Molecule 26: 40S ribosomal protein S24-A

Chain d4: 82% 16%

S2 I13 H29 P30 A33 N34 V35 S36 E42 K43 E46 K49 A50 E51 K52 D53 F58 R61 T62 S78 T88 V100 R105 K116 V129 D135

• Molecule 27: 40S ribosomal protein S25-A

Chain D5: 42% 21% 35%

PRO PRO LYS GLN GLN LEU SER LYS ALA ALA LYS ALA ALA ALA ALA LEU ALA GLY GLY LYS LYS SER LYS LYS LYS TRP SER LYS LYS SER MET LYS ASP ARG A36 Q37 H38 A39 V40 I41 L42 D43 Q44 R49 I50 R58 Y59 V60 S63 L69 K70 I71 L75 I78

K85 I88 I92 S93 K94 H95 S96 K97 Q98 A99 I100 Y101 T102 T105 ALA SER GLU

• Molecule 27: 40S ribosomal protein S25-A

Chain d5: 52% 12% 36%

PRO PRO LYS GLN GLN LEU SER LYS ALA ALA LYS ALA ALA ALA ALA LEU ALA GLY GLY LYS LYS SER LYS LYS LYS TRP SER LYS LYS SER MET LYS ASP ARG ALA Q37 H38 D43 K46 L51 K52 E53 Y57 V60 R68 R81 H82 L83 E84 K85 E86 G87

A104 T105 ALA SER GLU

• Molecule 28: 40S ribosomal protein S26-B

Chain D6: 74% 19% 5%

P2 R10 R15 V18 I36 K37 R38 I41 V45 V50 Y59 P60 E61 Y62 A63 L64 P65 K66 T67 Y68 N69 K70 L71 R82 I83 V84 R85 V86 E90 P97 P98

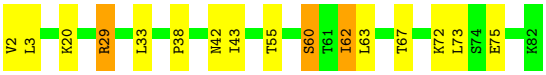
• Molecule 28: 40S ribosomal protein S26-B

Chain d6: 78% 21%

P2 N8 G9 R10 N11 V18 V24 N25 C26 K34 A35 I41 I44 V45 E46 L53 S54 E55 Y59 P60 E61 Y62 A63 R82 I83 V84 R85 E90 P98

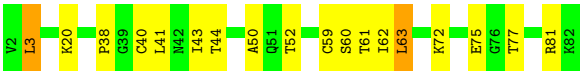
• Molecule 29: 40S ribosomal protein S27-A

Chain D7: 80% 16%



• Molecule 29: 40S ribosomal protein S27-A

Chain d7:



• Molecule 30: 40S ribosomal protein S28-A

Chain D8:

• Molecule 30: 40S ribosomal protein S28-A

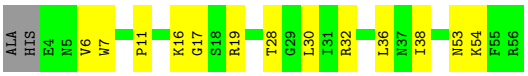
Chain d8:

• Molecule 31: 40S ribosomal protein S29-A

Chain D9:

• Molecule 31: 40S ribosomal protein S29-A

Chain d9:

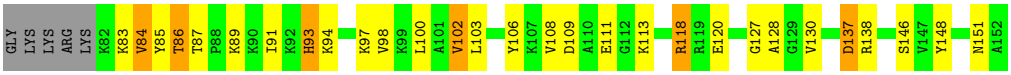


• Molecule 32: 40S ribosomal protein S30-A

Chain E0:

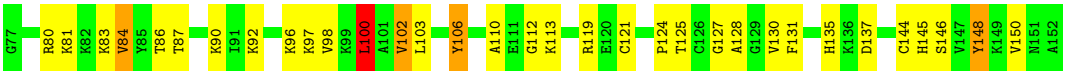
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



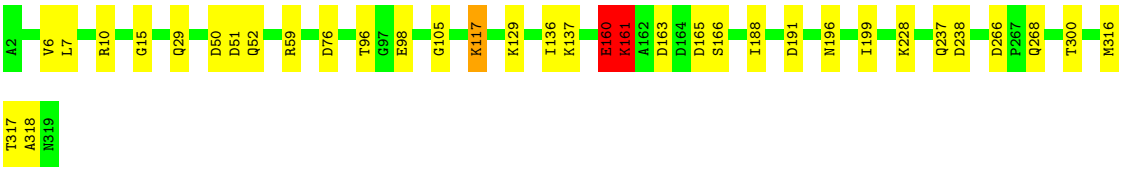
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:



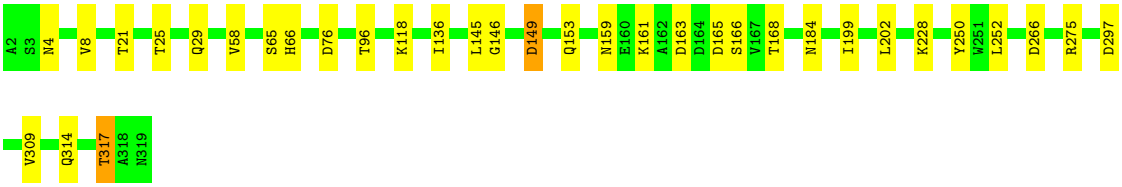
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



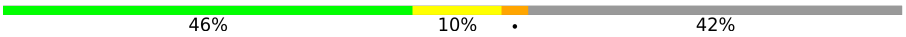
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

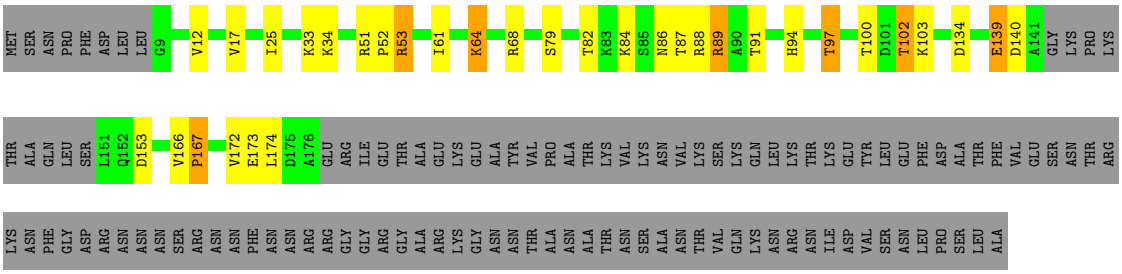
Chain sR:



• Molecule 35: Suppressor protein STM1

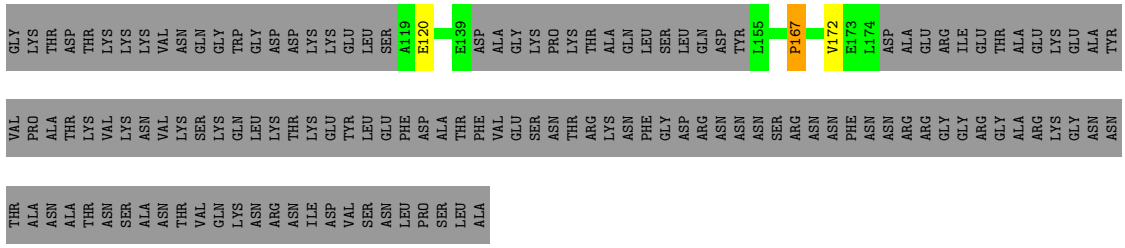
Chain SM:





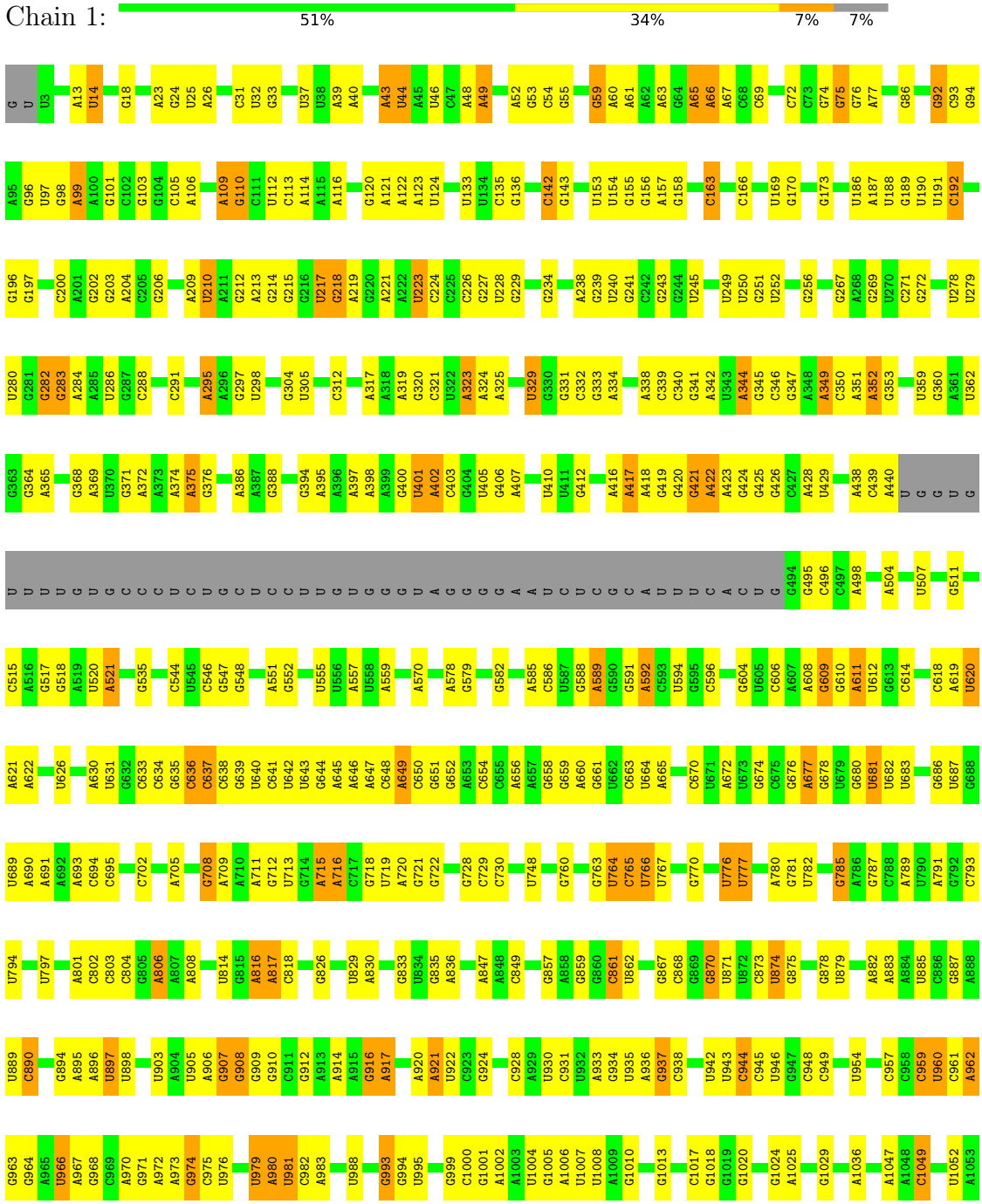
• Molecule 35: Suppressor protein STM1

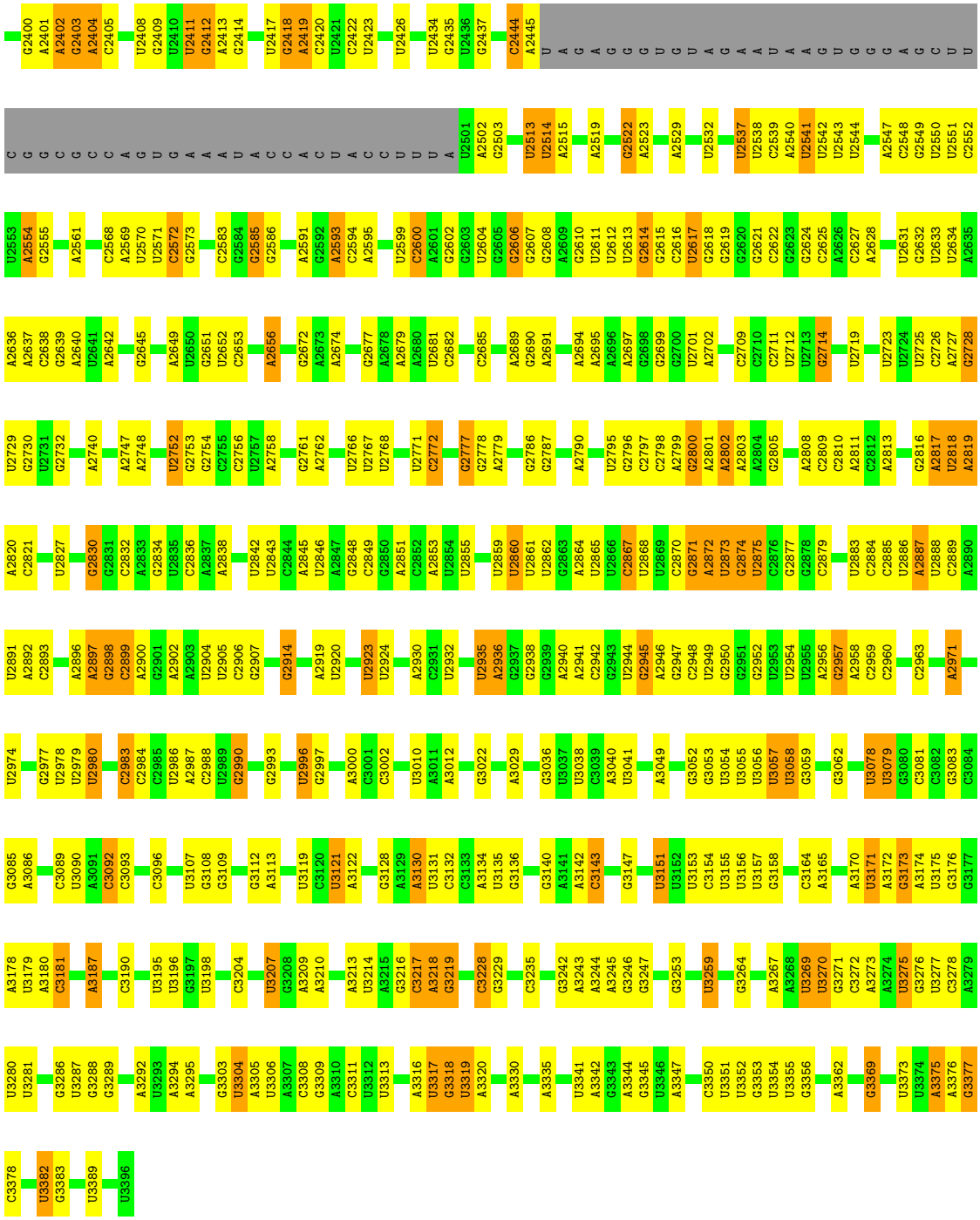
Chain sM:



• Molecule 36: 25S ribosomal RNA

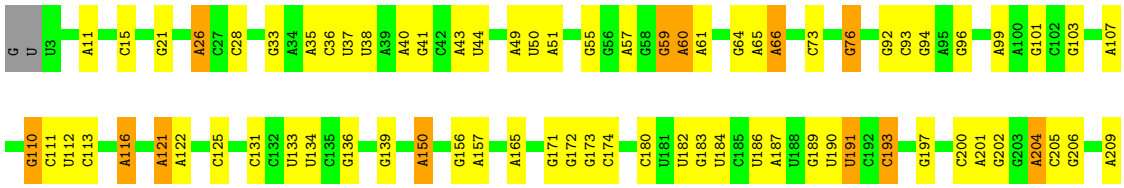
Chain 1:





• Molecule 36: 25S ribosomal RNA

Chain 5:



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C311 C312 A313 A318 A319 G320 C321 U322 A323 A324 A325 U326 U329 C339 C340 G341 G345 A348 A349 C350 A351 A352 G353 C356 U359 G360 A361 U362 G363 A366 G376 A385 A386 U393 A397 A398 A399 G400 U401 A402 C403 G404 U405 G406 U411 G412 U413
U414 G415 A416 A417 G420 G421 A422 A423 G424 G425 G426 C427 A428 A436 G437 A438 C439 A440 U441 G442 G443 U G U U U G U G C C C U C U G C U U G G G A A U C
U C G C A U U U C A C491 U492 G493 G494 G495 U506 U507 U508 U509 G513 A516 G517 U518 A519 U520 A521 A522 A532 G535 G542 C546 G547 G548 A551 U555 U556 A557 U558 A559 G560 A569 G575 C576 C577 A578 G579 C580 G583
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U681 U682 U683 G684 G685 G688 A691 A692 A693 C702 A705 G708 G712 A715 A716 C717 G718 U719 A720 G721 G722 G725 G726 A735 A736 G740 C758 C765 U766 U767 C768 G769 G770 G774 A775 U776 U777 U778 G779 A780 G781 G785 A786 G787 C788
C793 U794 G795 U796 U797 G798 A801 C802 A806 A810 U811 G812 G813 A816 A817 C818 U819 A820 C824 U825 G826 A830 G831 U834 G835 G838 G844 C851 G856 G857 C861 G867 C868 G869 U872 C873 U874 G875 A876 C877 G878 U879 A883
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C1118 C1119 A1120 U1121 U1122 U1123 U1124 U1128 A1129 A1130 G1131 C1132 A1133 G1134 C1141 U1144 G1145 C1146 G1147 G1148 G1149 G1152 A1153 A1154 G1157 A1158 A1159 C1160 G1161 U1162 A1163 G1164 A1165 G1166 U1167 U1168 A1169 A1170 G1171 G1172 U1173 G1174 C1175 C1176 G1177 G1178 A1179 A1180 U1181 A1182 C1183 G1186 C1187 U1188
C1189 C1192 A1193 C1196 C1199 A1200 C1201 A1202 A1203 U1208 G1209 U1210 U1211 A1212 U1215 C1219 G1222 A1223 C1232 U1235 G1236 G1237 C1238 C1239 A1240 U1241 G1242 A1245 G1246 C1254 U1258 A1259 G1262 A1263 G1264 U1265 G1266 C1284 G1285 A1290 A1291 C1292 C1296 C1297
C1298 U1299 G1300 A1301 A1302 A1303 A1304 U1305 G1306 G1307 A1308 U1309 G1310 G1311 C1312 G1313 C1314 U1315 C1316 G1317 A1318 G1319 U1322 G1323 C1327 C1328 U1329 U1330 U1331 A1332 C1333 U1334 C1335 U1336 A1337 G1340 G1344 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 G1362 A1363 C1364 G1365 G1370 G1371 C1372
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A2679 A2680 U2681 C2682 U2683 C2684 A2689 G2690 A2691 A2694 A2695 A2696 A2697 G2698 G2699 G2700 U2701 A2702 A2703 A2704 A2705 G2714 A2715 U2718 U2719 U2724 U2725 C2726 A2727 G2728 U2729 G2730 U2731 G2732 U2735 A2743 U2744 A2747 U2752 G2753 G2754 C2755 C2756 U2757 A2758 A2762 C2765 U2766 U2767
U2509 U2510 A2511 C2512 U2513 U2514 A2515 C2518 A2523 A2524 G2525 C2526 G2530 C2531 U2532 G2533 G2534 A2535 A2536 U2537 U2538 C2539 A2540 U2543 G2549 U2550 U2551 C2552 U2553 A2554 G2555 C2566 C2567 C2568 A2569 U2570 U2571 C2572 G2573 G2574 G2584 G2585 G2589 A2590 A2593 C2594 G2598 U2599 C2600 A2601
U2604 G2605 G2606 G2607 G2608 A2609 G2610 U2611 G2614 G2618 G2619 G2620 G2621 C2622 G2623 A2628 U2629 C2630 U2631 G2632 U2633 U2634 A2635 A2636 A2637 C2638 G2639 A2640 U2641 A2642 A2643 C2644 G2645 U2650 G2651 U2652 C2653 C2654 U2655 A2656 A2657 G2658 G2661 G2662 G2663 C2666 G2672 A2673 A2674 G2677 A2678
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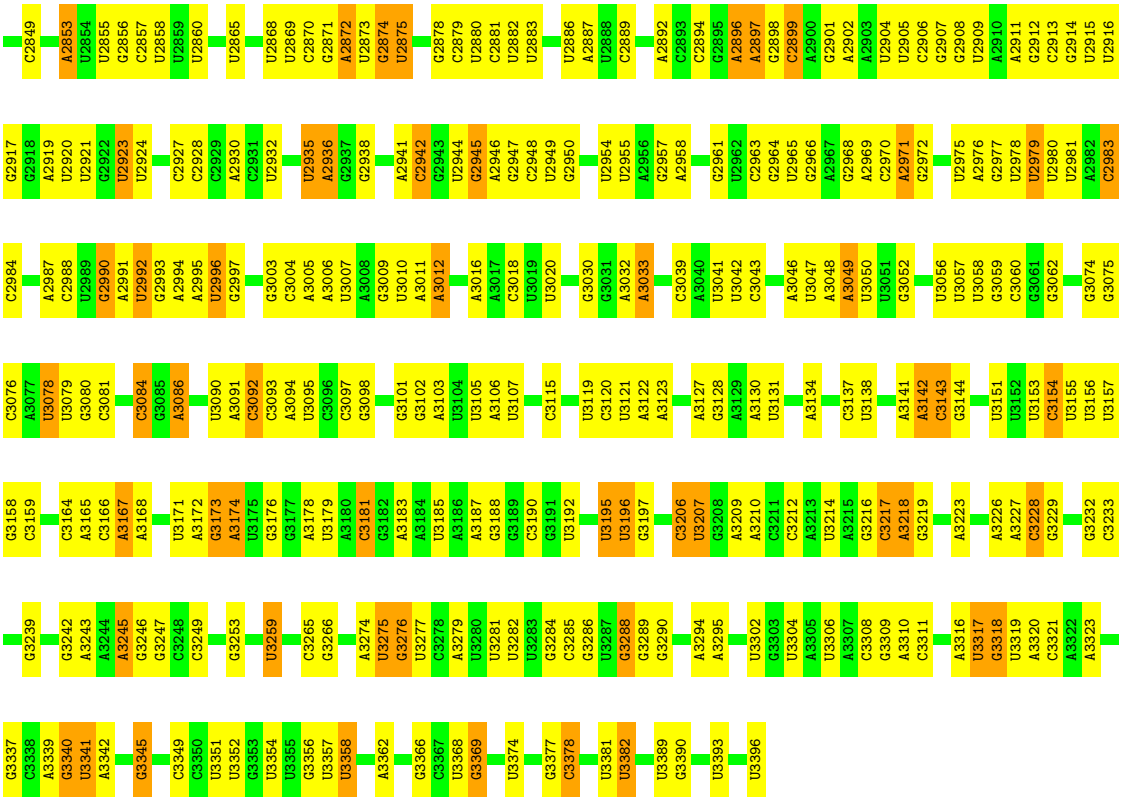
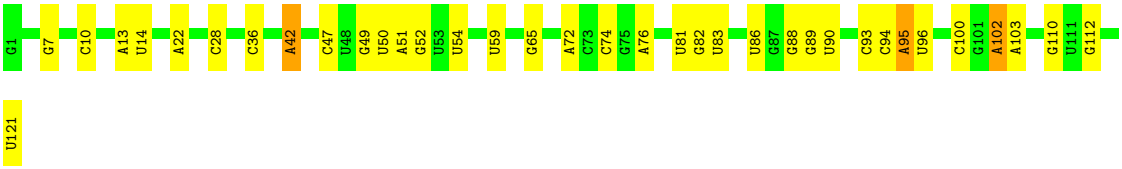


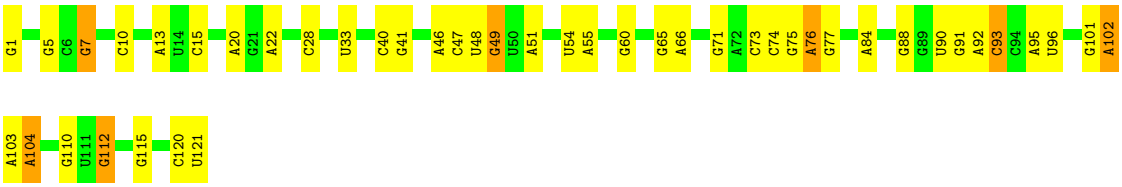
- Molecule 37: 5S ribosomal RNA

Chain 3:



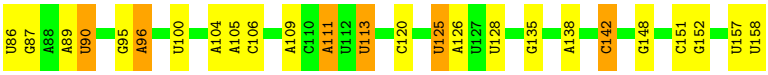
- Molecule 37: 5S ribosomal RNA

Chain 7:



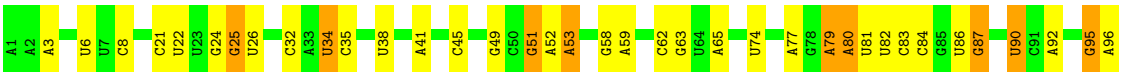
- Molecule 38: 5.8S ribosomal RNA

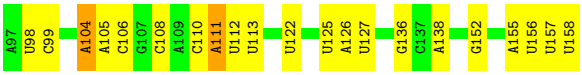
Chain 4:



• Molecule 38: 5.8S ribosomal RNA

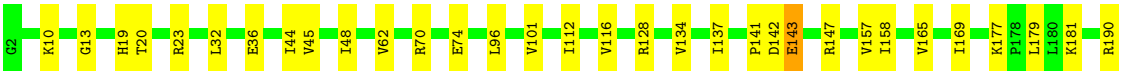
Chain 8:





• Molecule 39: 60S ribosomal protein L2-A

Chain L2:

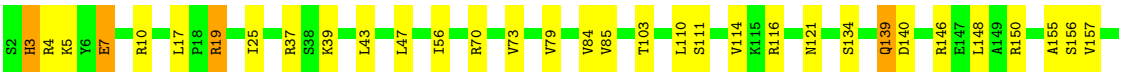


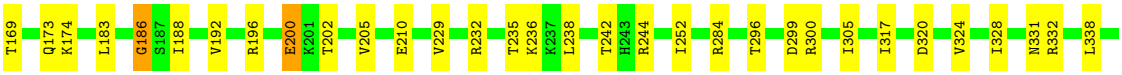
• Molecule 39: 60S ribosomal protein L2-A

Chain l2:

• Molecule 40: 60S ribosomal protein L3

Chain L3:





• Molecule 40: 60S ribosomal protein L3

Chain l3:

S2 H3 R4 R10 L17 P18 R19 K20 R21 K30 R37 S38 K39 L47 K50 I56 T77 V78 V79 D80 T81 V84 T103 V114 K120 K124 S134 A138 Q139 E145 R146 E147 L148 A149 R150 A155 S156 V157 V160 T169

L183 N184 G185 G186 S187 I188 R196 T202 V205 T221 V229 R232 T235 K236 K237 L238 T242 H243 R244 K248 V249 I252 M261 V264 A265 R266 R284 N293 T296 K302 M308 I317 V324 I328 R332 K333 R334 I335

L338 R339 K340 T346 S347 R348 K349 S355 T361 R369 T382 L387

- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 80% 18%

S2 R3 P4 Q5 E14 A15 T16 L22 V25 T40 V52 S53 T60 R69 A70 V71 I74 M93 C94 R95 E117 K118 T122 A130 V131 L136 A137 R138 G139 K144 I145 P146 E147 I148 P149 L150 V151 V152 L156 K170 A171 V172 S176

D177 L178 L179 L182 K185 R188 A189 G190 K193 Y194 R197 R198 W199 T200 R203 L206 E211 R220 N221 V222 V230 A231 S232 L233 R246 L258 S270 T283 S292 S293 T306 Q307 H311 V312 L313 P317 L318 K319 N320 V323

L327 N328 L339 K346 T349 V354 T358 L359 D362

- Molecule 41: 60S ribosomal protein L4-A

Chain l4: 81% 18%

S2 Q5 E14 V25 V52 T60 T67 R76 F90 G91 N92 M93 R98 K112 Y120 A121 T122 E143 K144 I145 P146 L150 L156 Q160 K161 V172 S176 L179 K186 L187 R188 A189 G190 K191 R198 W199 T200 R203

L206 K217 R220 N221 V222 E226 N229 V230 L233 R246 L258 V267 V272 T283 S284 T287 I295 R300 P301 A302 A305 T306 Q307 H311 V312 L313 K319 V323 L327 N328 P329 Y330 L339 K342 E345 T358 L359 K360

H361 D362

- Molecule 42: 60S ribosomal protein L5

Chain L5: 78% 20%

A2 K5 D6 A7 S10 R23 R35 K41 N57 K58 I64 T68 I69 L75 L92 T101 I105 T109 K112 L113 G114 L115 T118 V122 V125 E128 L131 D137 R140 V144 F145 L146 D147 I148 Q151 R152

T155 L163 E177 F185 E186 T187 E188 L194 L195 R196 S205 E216 E217 E221 L222 D232 A233 D234 S235 L236 A252 F253 K254 E257 K258 K259 F260 T261 K262 E263 R273 Q274 T275 K279 I290 L293 A294 G295 Q296 Q297

- Molecule 42: 60S ribosomal protein L5

Chain l5: 79% 19%

ALA PHE Q4 K5 R15 K34 R35 K41 Y44 L51 K58 I61 I65 T68 I69 T70 V73 V74 L75 T89 T93 L110 Q111 K112 L113 G114 L115 T118 Y119 K120 E124 V125 L131 T132 E133 A134 V135 E136 R140 L146 D147 I148

R152 T155 R158 F185 E186 T187 I190 L194 E210 L211 D215 E216 E217 R218 F219 S220 L227 K254 K258 K259 F260 E268 S269 K270 K271 Y272 R273 Q274 T275 R282 L293 Q297

- Molecule 43: 60S ribosomal protein L6-A

Chain L6: 76% 13% • 11%

S2 K5 A6 P7 K8 S12 T21 R31 V52 E59 L64 I65 K70 R78 V79 T89 K90 V93 E94 V98 E109 LYS LEU THR LYS LYS GLU LYS LYS GLU ALA ASN LEU PHE PRO GLU GLN GLN ASN LYS E129 R134 T152 L155

F176

- Molecule 43: 60S ribosomal protein L6-A

Chain l6: 74% 15% • 10%

S2 K8 W9 Y10 P11 S12 K20 T21 R31 A32 R46 K50 R51 V52 L64 I65 R78 V79 T89 K90 V91 S92 V93 N97 V98 E99 E109 LYS LEU THR LYS LYS GLU LYS LYS GLU ALA ASN LEU PHE PRO GLU GLN GLN ASN K128 K131 A132 E133

K143 T152 L155 K175 F176

- Molecule 44: 60S ribosomal protein L7-A

Chain L7: 80% 9% • 9%

ALA ALA GLU LYS ILE LEU THR PRO GLU SER GLN LEU LYS LYS SER LYS ALA GLN GLN LYS THR A23 E24 Q25 V26 K38 L45 R60 K82 L83 I92 K98 P99 R100 R110 K121 L124 T143 N157 K158 Q159 R160 S164 K175 I178 L179

L184 G212 F229 E234 L239 N244

- Molecule 44: 60S ribosomal protein L7-A

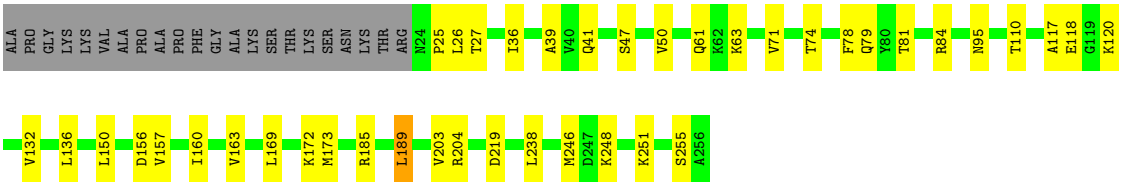
Chain l7: 79% 11% • 8%

ALA ALA GLU LYS ILE LEU THR PRO GLU SER GLN LEU LYS LYS SER LYS ALA GLN GLN LYS T22 V26 R30 R41 E54 R60 V77 L83 R88 N93 K98 P99 R100 R110 K121 L124 I130 I156 N157 K158 L173 G174 K175

I178 L179 L184 V191 G192 P193 K219 G226 G227 S228 F229 L239 N244

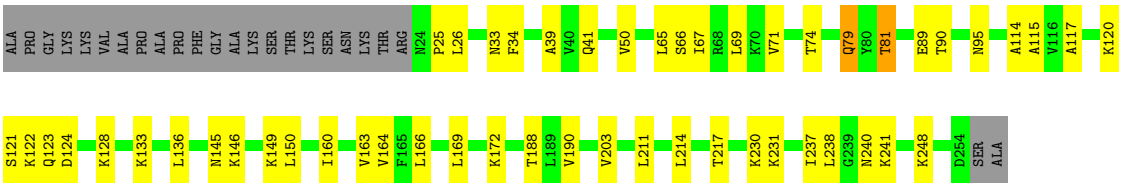
- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 75% 16% 9%



• Molecule 45: 60S ribosomal protein L8-A

Chain l8:

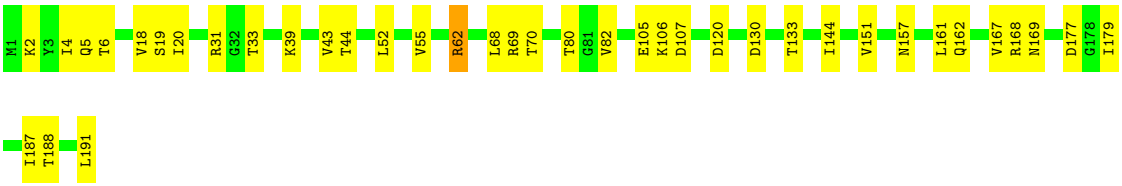


• Molecule 46: 60S ribosomal protein L9-A

Chain L9:

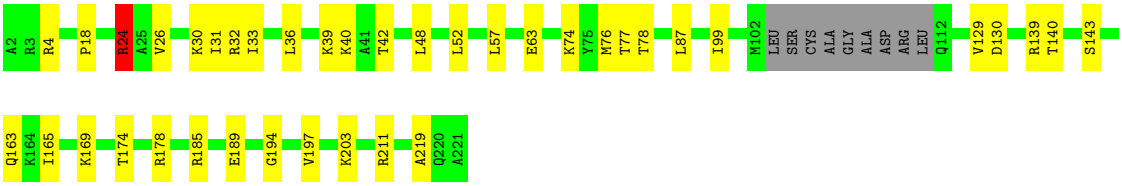
• Molecule 46: 60S ribosomal protein L9-A

Chain l9:



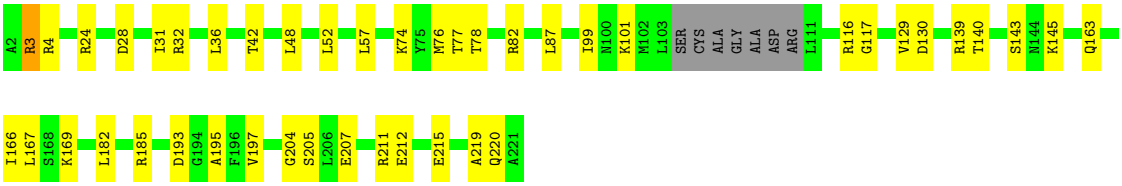
• Molecule 47: 60S ribosomal protein L10

Chain M0:



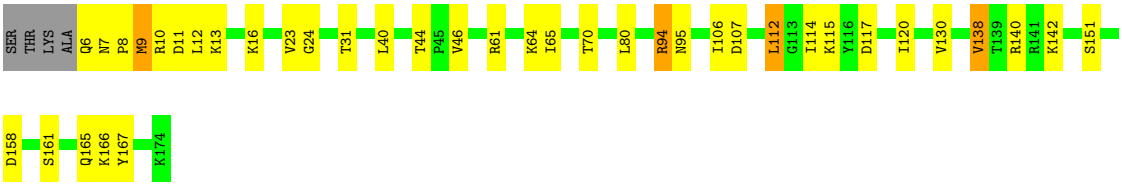
• Molecule 47: 60S ribosomal protein L10

Chain m0:



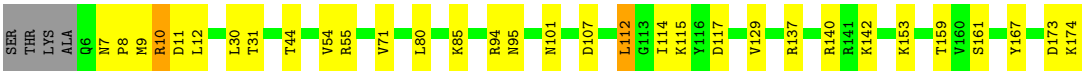
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



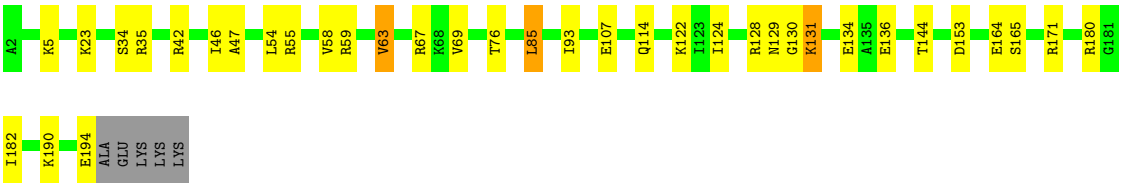
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



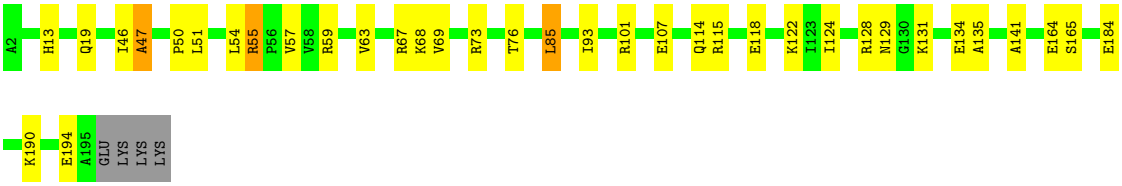
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



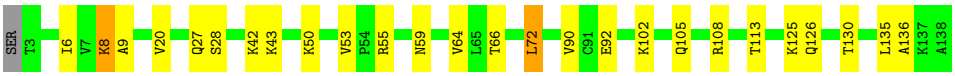
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



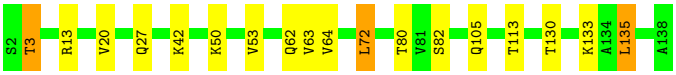
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



• Molecule 51: 60S ribosomal protein L15-A

Chain M5:

• Molecule 51: 60S ribosomal protein L15-A

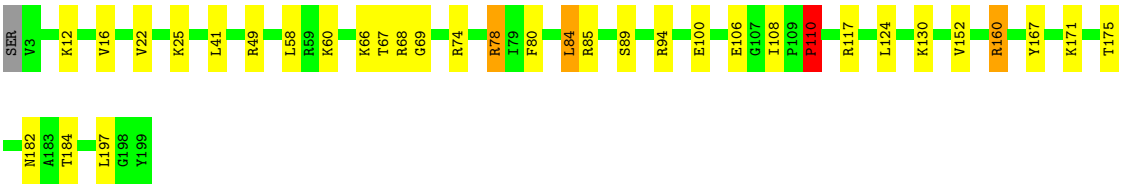
Chain m5:

• Molecule 52: 60S ribosomal protein L16-A

Chain M6:

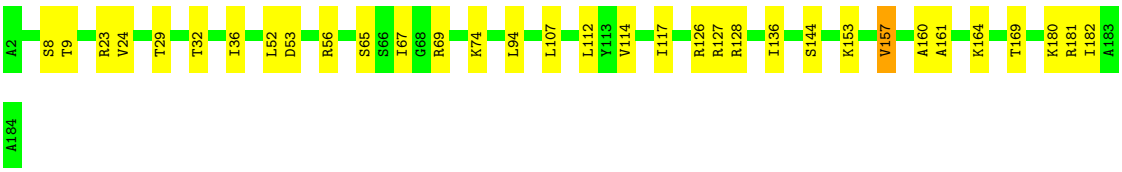
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



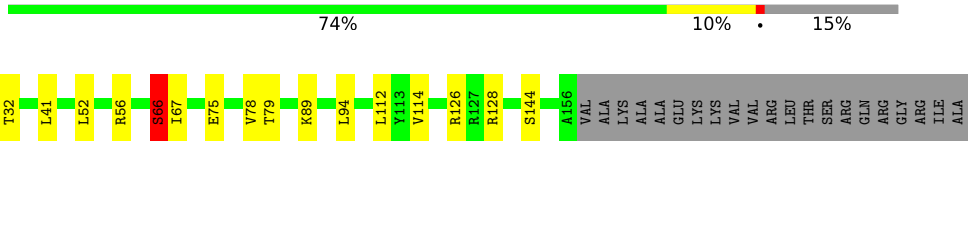
• Molecule 53: 60S ribosomal protein L17-A

Chain M7:



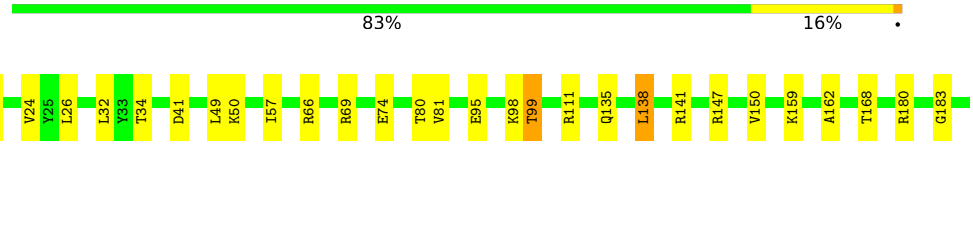
• Molecule 53: 60S ribosomal protein L17-A

Chain m7:



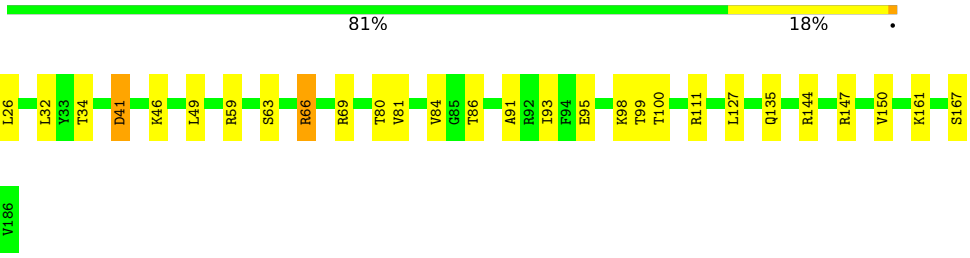
• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



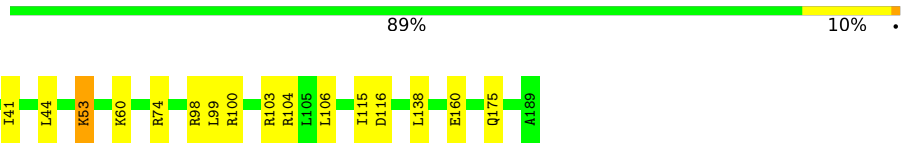
• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



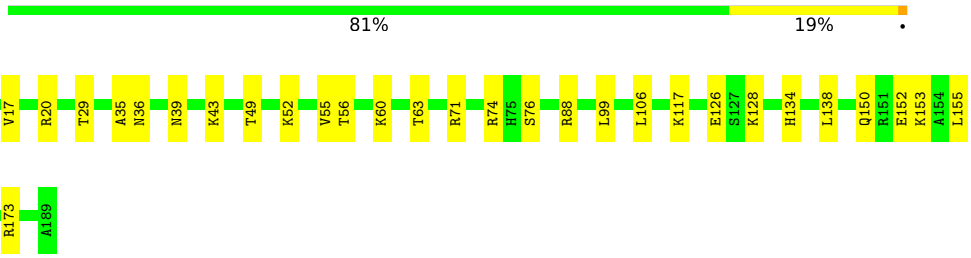
• Molecule 55: 60S ribosomal protein L19-A

Chain M9:



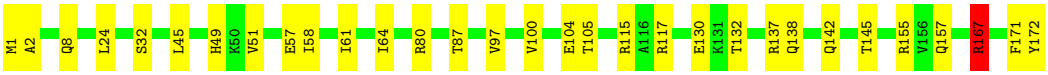
• Molecule 55: 60S ribosomal protein L19-A

Chain m9:



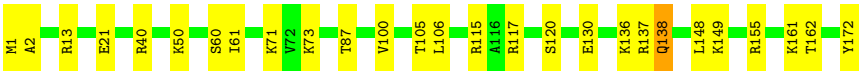
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



• Molecule 56: 60S ribosomal protein L20-A

Chain n0:

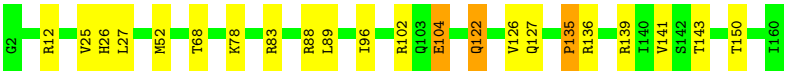


• Molecule 57: 60S ribosomal protein L21-A

Chain N1:

• Molecule 57: 60S ribosomal protein L21-A

Chain n1:

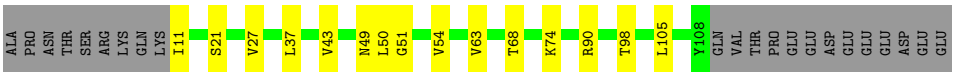


• Molecule 58: 60S ribosomal protein L22-A

Chain N2:

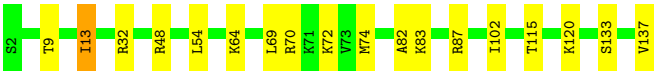
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



• Molecule 59: 60S ribosomal protein L23-A

Chain N3:

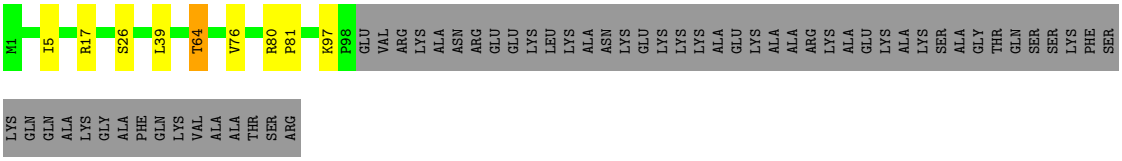


• Molecule 59: 60S ribosomal protein L23-A

Chain n3:

• Molecule 60: 60S ribosomal protein L24-A

Chain N4:

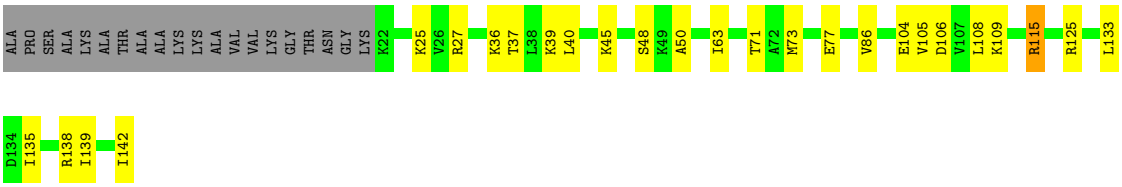


• Molecule 60: 60S ribosomal protein L24-A

Chain n4:

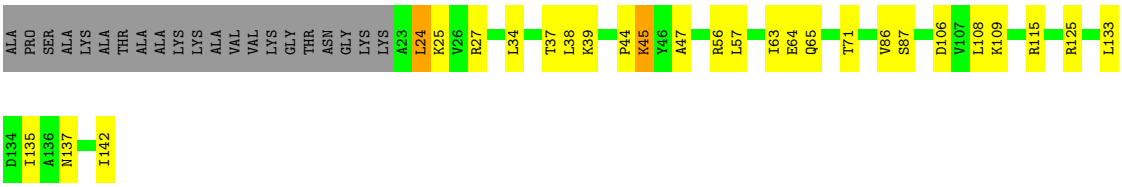
• Molecule 61: 60S ribosomal protein L25

Chain N5:



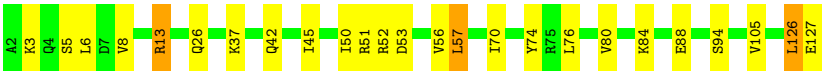
• Molecule 61: 60S ribosomal protein L25

Chain n5:



• Molecule 62: 60S ribosomal protein L26-A

Chain N6:

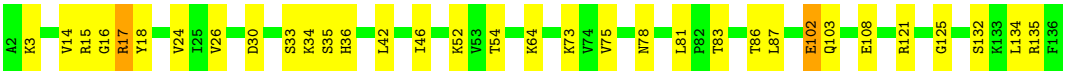


• Molecule 62: 60S ribosomal protein L26-A

Chain n6:

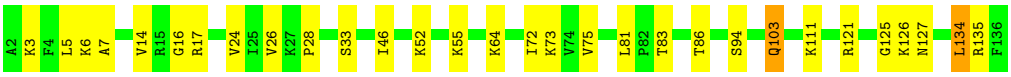
• Molecule 63: 60S ribosomal protein L27-A

Chain N7:



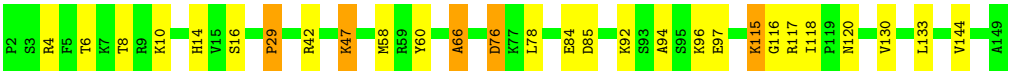
• Molecule 63: 60S ribosomal protein L27-A

Chain n7:



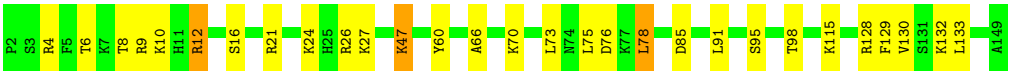
• Molecule 64: 60S ribosomal protein L28

Chain N8:



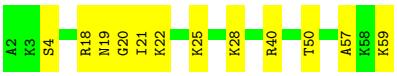
• Molecule 64: 60S ribosomal protein L28

Chain n8:



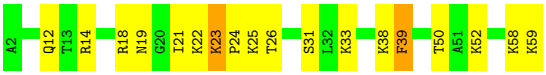
• Molecule 65: 60S ribosomal protein L29

Chain N9:



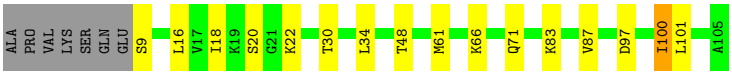
• Molecule 65: 60S ribosomal protein L29

Chain n9:



• Molecule 66: 60S ribosomal protein L30

Chain O0:

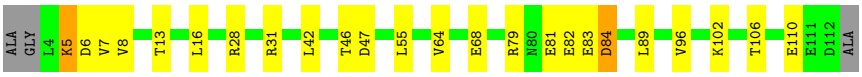


• Molecule 66: 60S ribosomal protein L30

Chain o0:

• Molecule 67: 60S ribosomal protein L31-A

Chain O1:

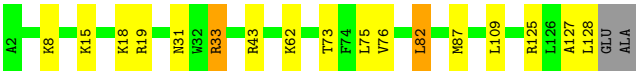


• Molecule 67: 60S ribosomal protein L31-A

Chain o1:

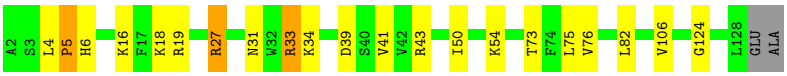
• Molecule 68: 60S ribosomal protein L32

Chain O2:



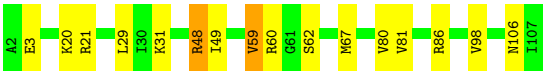
• Molecule 68: 60S ribosomal protein L32

Chain o2:



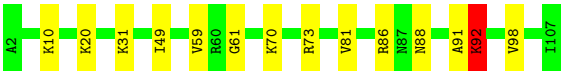
• Molecule 69: 60S ribosomal protein L33-A

Chain O3:



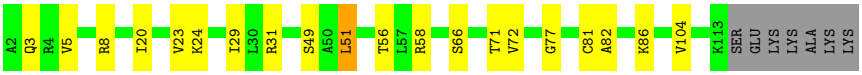
• Molecule 69: 60S ribosomal protein L33-A

Chain o3:



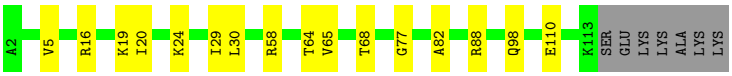
• Molecule 70: 60S ribosomal protein L34-A

Chain O4:



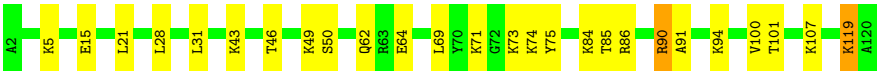
• Molecule 70: 60S ribosomal protein L34-A

Chain o4:



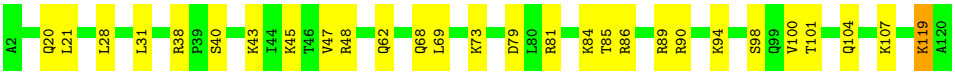
• Molecule 71: 60S ribosomal protein L35-A

Chain O5:



• Molecule 71: 60S ribosomal protein L35-A

Chain o5:

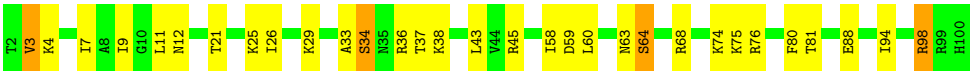


• Molecule 72: 60S ribosomal protein L36-A

Chain O6:

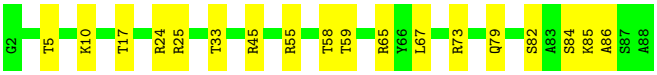
• Molecule 72: 60S ribosomal protein L36-A

Chain o6:



• Molecule 73: 60S ribosomal protein L37-A

Chain O7:



• Molecule 73: 60S ribosomal protein L37-A

Chain o7: 83% 17%

• Molecule 74: 60S ribosomal protein L38

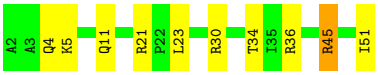
Chain O8: 79% 21%

• Molecule 74: 60S ribosomal protein L38

Chain o8: 82% 17%

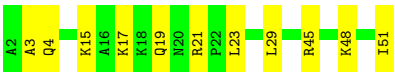
• Molecule 75: 60S ribosomal protein L39

Chain O9: 80% 18%



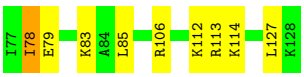
• Molecule 75: 60S ribosomal protein L39

Chain o9: 78% 22%



• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0: 83% 15%



• Molecule 76: Ubiquitin-60S ribosomal protein L40

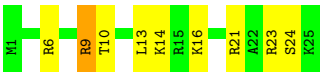
Chain q0: 85% 13%

• Molecule 77: 60S ribosomal protein L41-A

Chain Q1:

• Molecule 77: 60S ribosomal protein L41-A

Chain q1:



• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:

• Molecule 78: 60S ribosomal protein L42-A

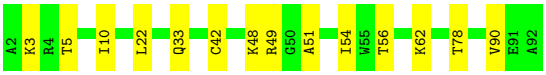
Chain q2:

• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:

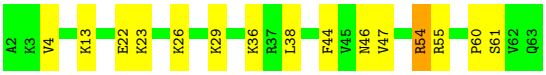
• Molecule 79: 60S ribosomal protein L43-A

Chain q3:



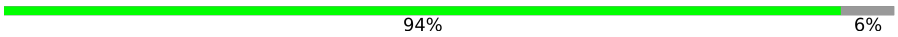
• Molecule 80: 40S ribosomal protein S30-A

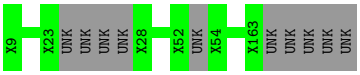
Chain e0:



• Molecule 81: Unknown protein m2

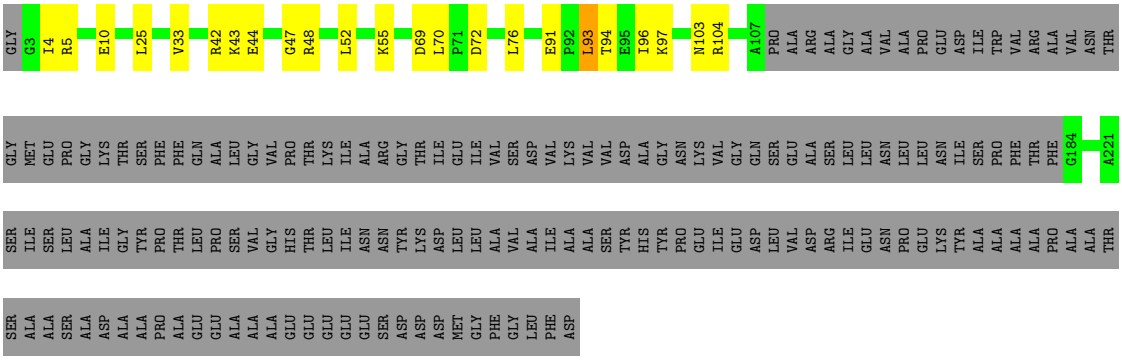
Chain m2:





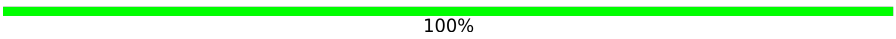
• Molecule 82: 60S acidic ribosomal protein P0

Chain p0:



• Molecule 83: Unknown protein p1

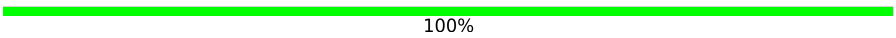
Chain p1:



There are no outlier residues recorded for this chain.

• Molecule 84: Unknown protein p2

Chain p2:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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	436.64Å 287.69Å 304.39Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	300.66 – 2.80	Depositor
% Data completeness (in resolution range)	99.6 (300.66-2.80)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.208 , 0.246	Depositor
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.227	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411226	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, MG, 3H3, ZN

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	0.75	5/41698 (0.0%)	1.30	337/64972 (0.5%)
1	6	0.87	23/42765 (0.1%)	1.40	490/66634 (0.7%)
2	S0	0.47	0/1617	0.67	0/2215
2	s0	0.53	0/1623	0.76	2/2222 (0.1%)
3	S1	0.37	0/1735	0.62	0/2335
3	s1	0.52	0/1748	0.71	1/2352 (0.0%)
4	S2	0.51	0/1665	0.67	0/2263
4	s2	0.61	0/1665	0.79	0/2263
5	S3	0.50	0/1759	0.65	0/2368
5	s3	0.48	0/1759	0.62	0/2368
6	S4	0.51	0/2109	0.74	2/2839 (0.1%)
6	s4	0.57	0/2109	0.79	1/2839 (0.0%)
7	S5	0.43	0/1629	0.60	0/2202
7	s5	0.46	0/1629	0.66	1/2202 (0.0%)
8	S6	0.48	0/1823	0.65	0/2439
8	s6	0.58	0/1779	0.72	1/2379 (0.0%)
9	S7	0.46	0/1506	0.65	0/2028
9	s7	0.54	0/1516	0.70	1/2043 (0.0%)
10	S8	0.58	0/1514	0.79	3/2021 (0.1%)
10	s8	0.64	0/1514	0.77	1/2021 (0.0%)
11	S9	0.50	0/1519	0.69	0/2035
11	s9	0.59	0/1519	0.74	0/2035
12	C0	0.45	0/790	0.69	1/1069 (0.1%)
12	c0	0.40	0/777	0.63	3/1049 (0.3%)
13	C1	0.59	0/1240	0.71	0/1675
13	c1	0.66	0/1194	0.86	0/1610
14	C2	0.37	0/898	0.62	0/1220
14	c2	0.31	0/898	0.58	1/1220 (0.1%)
15	C3	0.50	0/1215	0.71	2/1638 (0.1%)
15	c3	0.61	0/1215	0.77	0/1638
16	C4	0.38	0/901	0.65	0/1217
16	c4	0.54	0/960	0.77	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.50	0/998	0.67	0/1341
17	c5	0.51	0/1060	0.68	1/1426 (0.1%)
18	C6	0.47	0/1125	0.74	3/1510 (0.2%)
18	c6	0.50	0/1131	0.69	0/1518
19	C7	0.46	0/935	0.65	0/1254
19	c7	0.50	0/914	0.70	0/1224
20	C8	0.49	0/1211	0.67	0/1628
20	c8	0.51	0/1211	0.73	1/1628 (0.1%)
21	C9	0.48	0/1130	0.68	0/1517
21	c9	0.51	0/1130	0.71	0/1517
22	D0	0.48	0/865	0.66	0/1169
22	d0	0.49	0/892	0.68	0/1205
23	D1	0.47	0/693	0.66	0/935
23	d1	0.57	0/693	0.80	0/935
24	D2	0.55	0/1038	0.75	1/1395 (0.1%)
24	d2	0.68	0/1038	0.75	0/1395
25	D3	0.63	0/1139	0.79	1/1518 (0.1%)
25	d3	0.73	0/1139	0.83	3/1518 (0.2%)
26	D4	0.48	0/1087	0.63	0/1449
26	d4	0.53	0/1087	0.72	0/1449
27	D5	0.42	0/571	0.71	0/768
27	d5	0.45	0/566	0.63	0/761
28	D6	0.47	0/782	0.67	0/1047
28	d6	0.59	0/782	0.75	0/1047
29	D7	0.46	0/620	0.68	1/838 (0.1%)
29	d7	0.52	0/620	0.73	0/838
30	D8	0.36	0/499	0.56	0/670
30	d8	0.44	0/499	0.67	0/670
31	D9	0.56	0/452	0.82	1/600 (0.2%)
31	d9	0.58	0/452	0.72	0/600
32	E0	0.49	0/483	0.65	0/643
33	E1	0.49	0/577	0.83	0/770
33	e1	0.43	0/619	0.75	1/822 (0.1%)
34	SR	1.06	2/2494 (0.1%)	1.50	6/3393 (0.2%)
34	sR	0.41	0/2495	0.58	0/3395
35	SM	0.55	0/1113	0.71	2/1502 (0.1%)
35	sM	0.51	0/683	0.68	1/923 (0.1%)
36	1	1.16	152/75394 (0.2%)	1.67	1955/117545 (1.7%)
36	5	1.20	176/75414 (0.2%)	1.69	1938/117575 (1.6%)
37	3	0.96	4/2883 (0.1%)	1.42	33/4491 (0.7%)
37	7	1.13	7/2883 (0.2%)	1.63	50/4491 (1.1%)
38	4	1.11	2/3746 (0.1%)	1.60	70/5832 (1.2%)
38	8	1.00	5/3746 (0.1%)	1.51	46/5832 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	L2	0.75	0/1948	0.87	2/2617 (0.1%)
39	l2	0.82	1/1946 (0.1%)	0.95	5/2614 (0.2%)
40	L3	0.77	2/3146 (0.1%)	0.88	2/4228 (0.0%)
40	l3	0.85	1/3146 (0.0%)	0.96	11/4228 (0.3%)
41	L4	0.86	3/2800 (0.1%)	1.02	10/3790 (0.3%)
41	l4	0.79	0/2800	0.94	6/3790 (0.2%)
42	L5	0.59	0/2425	0.72	0/3271
42	l5	0.78	0/2408	0.83	3/3248 (0.1%)
43	L6	0.77	0/1260	0.85	3/1694 (0.2%)
43	l6	0.78	0/1269	0.85	0/1705
44	L7	0.85	1/1821 (0.1%)	0.90	0/2451
44	l7	0.86	1/1828 (0.1%)	0.91	5/2461 (0.2%)
45	L8	0.59	0/1836	0.69	1/2481 (0.0%)
45	l8	0.57	0/1795	0.69	0/2429
46	L9	0.70	0/1539	0.79	0/2073
46	l9	0.80	0/1539	0.85	0/2073
47	M0	0.76	0/1741	0.88	3/2335 (0.1%)
47	m0	0.82	0/1758	0.89	0/2358
48	M1	0.55	0/1374	0.74	1/1842 (0.1%)
48	m1	0.67	0/1374	0.83	2/1842 (0.1%)
49	M3	0.77	0/1568	0.91	3/2106 (0.1%)
49	m3	0.75	0/1573	0.89	4/2113 (0.2%)
50	M4	0.79	0/1068	0.87	2/1438 (0.1%)
50	m4	0.81	0/1074	0.84	1/1446 (0.1%)
51	M5	0.78	0/1757	0.97	3/2354 (0.1%)
51	m5	0.72	0/1757	0.83	0/2354
52	M6	0.93	3/1585 (0.2%)	1.00	7/2128 (0.3%)
52	m6	1.06	2/1585 (0.1%)	1.04	9/2128 (0.4%)
53	M7	0.84	0/1443	0.87	0/1944
53	m7	0.93	1/1250 (0.1%)	0.89	0/1683
54	M8	0.84	0/1465	0.95	4/1965 (0.2%)
54	m8	0.76	0/1465	0.94	2/1965 (0.1%)
55	M9	0.58	0/1538	0.68	0/2050
55	m9	0.65	0/1538	0.72	0/2050
56	N0	0.81	0/1481	0.87	3/1990 (0.2%)
56	n0	0.84	0/1481	0.92	1/1990 (0.1%)
57	N1	0.81	0/1300	0.86	0/1743
57	n1	0.86	1/1300 (0.1%)	0.86	0/1743
58	N2	0.46	0/812	0.61	0/1099
58	n2	0.53	0/794	0.66	0/1076
59	N3	0.78	0/1018	0.94	5/1369 (0.4%)
59	n3	0.85	0/1018	0.93	4/1369 (0.3%)
60	N4	0.61	0/712	0.69	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	n4	0.68	0/1052	0.72	0/1398
61	N5	0.65	0/979	0.82	1/1321 (0.1%)
61	n5	0.68	0/974	0.84	0/1314
62	N6	0.76	0/1004	0.94	4/1341 (0.3%)
62	n6	0.68	0/1004	0.82	0/1341
63	N7	0.54	0/1118	0.72	0/1497
63	n7	0.52	0/1118	0.66	0/1497
64	N8	0.86	0/1204	0.97	4/1612 (0.2%)
64	n8	0.84	0/1204	0.97	4/1612 (0.2%)
65	N9	0.85	0/473	0.81	1/629 (0.2%)
65	n9	0.90	0/473	0.93	2/629 (0.3%)
66	O0	0.53	0/751	0.68	0/1008
66	o0	0.55	0/775	0.67	0/1040
67	O1	0.68	0/890	0.75	0/1196
67	o1	0.85	1/897 (0.1%)	0.86	0/1205
68	O2	0.87	0/1041	0.95	4/1394 (0.3%)
68	o2	0.89	0/1041	1.02	5/1394 (0.4%)
69	O3	0.92	0/868	0.90	3/1168 (0.3%)
69	o3	0.98	1/868 (0.1%)	0.92	2/1168 (0.2%)
70	O4	0.62	0/890	0.80	1/1189 (0.1%)
70	o4	0.67	0/890	0.74	0/1189
71	O5	0.71	1/978 (0.1%)	0.84	2/1301 (0.2%)
71	o5	0.62	0/974	0.71	0/1297
72	O6	0.68	0/778	0.84	0/1034
72	o6	0.60	0/777	0.74	0/1033
73	O7	0.89	1/696 (0.1%)	1.00	2/923 (0.2%)
73	o7	0.75	0/696	0.88	1/923 (0.1%)
74	O8	0.52	0/618	0.64	0/826
74	o8	0.49	0/614	0.67	0/822
75	O9	0.89	1/443 (0.2%)	0.96	1/588 (0.2%)
75	o9	0.81	0/443	0.95	0/588
76	Q0	0.73	0/423	0.90	1/562 (0.2%)
76	q0	0.89	0/423	0.92	1/562 (0.2%)
77	Q1	0.70	0/234	0.93	0/300
77	q1	0.94	0/234	1.05	1/300 (0.3%)
78	Q2	1.00	1/860 (0.1%)	0.99	2/1136 (0.2%)
78	q2	0.83	2/860 (0.2%)	0.87	0/1136
79	Q3	0.73	0/701	0.84	0/934
79	q3	0.78	0/701	0.88	0/934
80	e0	0.58	0/499	0.77	0/665
82	p0	0.46	0/1092	0.62	0/1474
All	All	0.92	400/430070 (0.1%)	1.33	5106/631356 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	S0	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	2
17	c5	0	1
19	C7	0	1
22	d0	0	1
25	D3	0	1
25	d3	0	1
26	d4	0	2
27	D5	0	1
28	D6	0	3
31	d9	0	1
33	E1	0	1
34	SR	0	2
39	L2	0	1
39	l2	0	2
40	l3	0	2
41	L4	0	2
41	l4	0	1
42	L5	0	1
42	l5	0	2
43	l6	0	1
44	L7	0	1
44	l7	0	2
51	M5	0	1
52	M6	0	2
52	m6	0	1
53	M7	0	1
53	m7	0	1
57	N1	0	1
59	n3	0	1
62	n6	0	1
63	N7	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
67	O1	0	1
67	o1	0	1
72	O6	0	1
All	All	0	57

All (400) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	SR	160	GLU	C-N	-38.52	0.45	1.34
34	SR	161	LYS	C-N	-29.42	0.66	1.34
78	Q2	17	CYS	CB-SG	16.03	2.09	1.82
36	5	1152	G	N9-C4	-13.26	1.27	1.38
39	l2	213	GLY	C-O	9.71	1.39	1.23
36	5	2899	C	N3-C4	-9.31	1.27	1.33
36	5	970	A	N9-C4	-9.17	1.32	1.37
36	5	1152	G	C2-N3	-8.92	1.25	1.32
52	m6	66	LYS	CE-NZ	8.54	1.70	1.49
36	5	2375	G	C6-N1	-8.24	1.33	1.39
36	5	2726	C	N3-C4	-8.16	1.28	1.33
1	6	1773	C	C4-N4	8.07	1.41	1.33
36	5	1152	G	N3-C4	-8.05	1.29	1.35
36	5	953	G	C5-C4	-7.92	1.32	1.38
1	6	538	A	N9-C4	7.89	1.42	1.37
36	5	2987	A	N7-C5	-7.85	1.34	1.39
1	6	163	G	N9-C4	-7.78	1.31	1.38
36	5	1152	G	N9-C8	7.74	1.43	1.37
36	1	2402	A	N9-C4	7.66	1.42	1.37
36	5	1115	G	N7-C5	-7.60	1.34	1.39
36	1	1103	A	C6-N1	7.54	1.40	1.35
1	6	337	G	C2-N2	7.54	1.42	1.34
36	5	2874	G	P-O5'	7.54	1.67	1.59
36	5	2412	G	N1-C2	-7.48	1.31	1.37
36	1	895	A	N9-C8	7.46	1.43	1.37
36	5	878	G	N7-C5	-7.32	1.34	1.39
36	1	980	A	N9-C4	7.26	1.42	1.37
36	1	2397	A	C6-N1	7.23	1.40	1.35
36	5	2635	A	N3-C4	-7.23	1.30	1.34
36	5	802	C	N1-C6	-7.21	1.32	1.37
36	5	2873	U	C2-N3	7.18	1.42	1.37
1	6	163	G	N3-C4	-7.16	1.30	1.35
69	o3	92	LYS	CE-NZ	7.09	1.66	1.49
36	5	691	A	N7-C5	-7.07	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1299	U	C4-O4	-6.98	1.18	1.23
36	5	1847	A	N9-C4	-6.97	1.33	1.37
36	1	1143	A	N9-C4	-6.95	1.33	1.37
53	m7	66	SER	C-O	6.94	1.36	1.23
36	1	895	A	N9-C4	-6.93	1.33	1.37
36	1	2726	C	N3-C4	-6.91	1.29	1.33
36	1	2403	G	N9-C4	6.89	1.43	1.38
36	1	2640	A	C6-N1	-6.87	1.30	1.35
36	1	1103	A	N9-C4	6.86	1.42	1.37
36	1	1114	U	C2-N3	-6.84	1.32	1.37
36	5	818	C	N3-C4	-6.84	1.29	1.33
36	5	1849	C	N1-C6	-6.79	1.33	1.37
36	5	1192	C	N1-C2	6.77	1.47	1.40
36	1	2977	G	C5-C4	-6.75	1.33	1.38
36	5	895	A	N9-C4	-6.74	1.33	1.37
36	5	437	G	N7-C5	6.74	1.43	1.39
36	1	96	G	N7-C5	-6.74	1.35	1.39
36	5	2371	G	C8-N7	-6.74	1.26	1.30
36	1	3181	C	N3-C4	-6.71	1.29	1.33
36	5	1332	A	N7-C5	-6.62	1.35	1.39
57	n1	104	GLU	CB-CG	6.62	1.64	1.52
36	1	2396	G	N7-C5	-6.60	1.35	1.39
78	q2	17	CYS	CB-SG	6.58	1.93	1.82
36	5	644	G	N7-C5	-6.55	1.35	1.39
36	5	795	G	N7-C5	-6.55	1.35	1.39
36	1	3209	A	C5-C4	6.53	1.43	1.38
36	5	2305	G	N7-C5	-6.50	1.35	1.39
36	5	3362	A	N9-C4	-6.49	1.33	1.37
36	5	1149	G	N9-C8	-6.45	1.33	1.37
36	5	2915	U	C2-O2	-6.43	1.16	1.22
36	1	910	G	N7-C5	-6.42	1.35	1.39
36	5	3209	A	C5-C4	6.42	1.43	1.38
36	1	2818	U	C2-O2	-6.42	1.16	1.22
36	5	2401	A	N9-C4	6.42	1.41	1.37
36	1	2617	U	N3-C4	-6.40	1.32	1.38
36	1	61	A	N7-C5	-6.40	1.35	1.39
36	1	2811	A	N3-C4	-6.39	1.31	1.34
36	5	2971	A	N9-C4	6.38	1.41	1.37
36	1	2134	G	C6-N1	-6.38	1.35	1.39
36	1	37	U	C2-O2	-6.37	1.16	1.22
36	1	921	A	N7-C5	-6.36	1.35	1.39
36	1	1112	A	N9-C4	-6.36	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2645	G	N3-C4	-6.35	1.31	1.35
36	5	1152	G	C5-C6	-6.35	1.36	1.42
36	1	2867	C	N3-C4	-6.34	1.29	1.33
36	5	2348	A	N3-C4	-6.33	1.31	1.34
36	1	637	C	C2-O2	-6.33	1.18	1.24
36	1	2867	C	C2-N3	-6.33	1.30	1.35
36	5	3245	A	N9-C4	-6.32	1.34	1.37
36	5	2385	G	N9-C4	-6.32	1.32	1.38
36	1	718	G	N9-C8	6.29	1.42	1.37
36	1	2899	C	N3-C4	-6.29	1.29	1.33
36	1	909	G	C5-C4	-6.24	1.33	1.38
40	L3	200	GLU	CG-CD	6.23	1.61	1.51
36	5	953	G	N9-C8	-6.23	1.33	1.37
36	1	2356	A	N9-C4	-6.23	1.34	1.37
36	5	872	U	C4-O4	-6.22	1.18	1.23
36	5	2954	U	C4-O4	6.22	1.28	1.23
36	5	1152	G	C8-N7	6.21	1.34	1.30
36	5	3005	A	N7-C5	-6.21	1.35	1.39
36	5	404	G	N7-C5	-6.19	1.35	1.39
36	5	2643	A	C6-N1	6.18	1.39	1.35
36	1	912	G	C5-C4	-6.16	1.34	1.38
36	5	1178	G	C2-N3	-6.16	1.27	1.32
36	5	909	G	C5-C4	-6.15	1.34	1.38
36	5	649	A	N7-C5	-6.15	1.35	1.39
36	1	2714	G	N9-C8	6.13	1.42	1.37
36	1	895	A	N3-C4	-6.12	1.31	1.34
36	5	661	G	N7-C5	-6.11	1.35	1.39
36	1	643	U	N1-C2	-6.09	1.33	1.38
36	5	2147	A	N7-C5	-6.09	1.35	1.39
38	8	80	A	N9-C4	6.08	1.41	1.37
36	1	803	C	C4-N4	-6.07	1.28	1.33
1	6	1765	A	N9-C4	-6.05	1.34	1.37
36	1	3209	A	C6-N1	6.04	1.39	1.35
36	1	938	C	C4-N4	-6.02	1.28	1.33
1	6	437	A	N3-C4	-6.02	1.31	1.34
36	1	1170	A	N9-C4	6.02	1.41	1.37
36	5	876	A	N3-C4	-6.01	1.31	1.34
36	5	1304	A	N3-C4	6.00	1.38	1.34
36	5	834	U	N1-C2	-5.99	1.33	1.38
36	5	2395	G	C5-C4	-5.97	1.34	1.38
36	5	2147	A	C5-C6	-5.96	1.35	1.41
38	8	41	A	C5-C6	-5.96	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	631	U	C2-N3	-5.95	1.33	1.37
38	8	25	G	N1-C2	-5.95	1.32	1.37
36	1	1858	A	N7-C5	-5.95	1.35	1.39
36	1	3216	G	N7-C5	-5.93	1.35	1.39
52	M6	34	VAL	CB-CG1	-5.93	1.40	1.52
36	1	1103	A	N3-C4	5.91	1.38	1.34
36	1	2800	G	C5-C4	-5.91	1.34	1.38
37	3	95	A	N7-C5	-5.91	1.35	1.39
36	1	2412	G	N7-C5	-5.91	1.35	1.39
36	5	2860	U	N3-C4	5.89	1.43	1.38
36	1	2147	A	N7-C5	-5.88	1.35	1.39
36	1	2404	A	C6-N1	5.88	1.39	1.35
36	5	1152	G	N1-C2	5.88	1.42	1.37
36	5	2975	U	C4-O4	-5.88	1.19	1.23
36	5	1311	G	C5-C4	-5.87	1.34	1.38
36	1	2836	C	N3-C4	-5.85	1.29	1.33
1	6	337	G	C2-N3	5.85	1.37	1.32
36	1	637	C	C3'-C2'	-5.83	1.46	1.52
36	5	960	U	N1-C2	5.83	1.43	1.38
36	5	2119	A	N7-C5	-5.83	1.35	1.39
36	1	2971	A	N9-C4	5.83	1.41	1.37
36	5	363	G	N3-C4	-5.82	1.31	1.35
1	6	65	A	N9-C4	-5.82	1.34	1.37
1	6	542	A	N7-C5	-5.82	1.35	1.39
36	1	368	G	N7-C5	-5.80	1.35	1.39
36	5	1103	A	N9-C4	5.80	1.41	1.37
36	1	2606	G	N7-C5	-5.79	1.35	1.39
36	1	426	G	N1-C2	-5.79	1.33	1.37
36	1	2805	G	C8-N7	-5.78	1.27	1.30
36	5	3107	U	C2-N3	-5.78	1.33	1.37
36	1	2396	G	N9-C8	-5.75	1.33	1.37
36	1	2761	G	N3-C4	-5.73	1.31	1.35
36	5	2872	A	C5-C6	5.71	1.46	1.41
36	5	426	G	C5-C4	-5.71	1.34	1.38
36	1	46	U	C2-O2	-5.70	1.17	1.22
36	1	818	C	N3-C4	-5.70	1.29	1.33
36	1	2986	U	C2-N3	-5.70	1.33	1.37
1	6	1655	A	N3-C4	-5.69	1.31	1.34
36	5	2899	C	C2-N3	-5.69	1.31	1.35
1	6	1681	A	N9-C4	-5.69	1.34	1.37
71	O5	64	GLU	CG-CD	5.68	1.60	1.51
36	5	420	G	C5-C4	-5.68	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2823	G	C5-C4	-5.67	1.34	1.38
36	5	2971	A	N7-C5	5.67	1.42	1.39
36	5	420	G	N9-C8	-5.67	1.33	1.37
36	5	94	G	C5-C4	-5.67	1.34	1.38
36	1	1164	G	N7-C5	-5.67	1.35	1.39
36	5	3052	G	N1-C2	-5.67	1.33	1.37
44	L7	234	GLU	CD-OE2	5.66	1.31	1.25
36	5	981	U	N1-C2	5.66	1.43	1.38
37	7	49	G	N9-C8	-5.65	1.33	1.37
36	5	1365	G	C6-N1	-5.63	1.35	1.39
36	1	2642	A	N7-C5	5.63	1.42	1.39
38	4	12	A	N9-C4	-5.62	1.34	1.37
36	1	960	U	C4-O4	5.62	1.28	1.23
36	1	2944	U	C4-O4	-5.62	1.19	1.23
36	5	2921	U	C4-O4	-5.62	1.19	1.23
52	m6	80	PHE	CB-CG	-5.61	1.41	1.51
36	5	2642	A	N9-C4	-5.61	1.34	1.37
36	1	2418	G	O3'-P	5.60	1.67	1.61
36	1	98	G	C6-N1	-5.59	1.35	1.39
36	5	2635	A	C6-N1	-5.59	1.31	1.35
36	5	2393	G	C8-N7	-5.58	1.27	1.30
36	1	279	U	C4-O4	-5.57	1.19	1.23
36	5	2873	U	C2-O2	5.57	1.27	1.22
36	5	1602	A	N7-C5	-5.57	1.35	1.39
36	5	2341	A	N9-C8	-5.56	1.33	1.37
36	1	1514	G	N1-C2	-5.56	1.33	1.37
36	1	2385	G	N9-C4	-5.56	1.33	1.38
36	1	2134	G	N1-C2	-5.55	1.33	1.37
36	1	2872	A	N7-C5	5.55	1.42	1.39
1	6	321	C	N1-C2	5.54	1.45	1.40
36	5	2700	G	C5-C4	-5.54	1.34	1.38
36	5	1113	G	N3-C4	-5.54	1.31	1.35
37	3	82	G	N9-C8	-5.52	1.33	1.37
36	5	877	C	C4-N4	-5.52	1.28	1.33
36	5	3106	A	N7-C5	-5.52	1.35	1.39
36	1	693	A	N7-C5	-5.52	1.35	1.39
36	5	1848	G	C5-C4	-5.52	1.34	1.38
36	1	2610	G	C8-N7	5.52	1.34	1.30
36	1	1330	A	N7-C5	-5.51	1.35	1.39
36	5	1899	G	N7-C5	-5.51	1.35	1.39
36	5	2314	U	C4-O4	5.51	1.28	1.23
41	L4	211	GLU	CG-CD	5.51	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1908	A	C6-N1	-5.50	1.31	1.35
36	1	1429	G	C2-N3	5.50	1.37	1.32
1	6	314	C	N3-C4	-5.50	1.30	1.33
36	5	2403	G	C2-N3	5.50	1.37	1.32
36	1	970	A	N9-C4	-5.49	1.34	1.37
36	1	1127	G	C5-C6	-5.49	1.36	1.42
36	5	2639	G	N7-C5	-5.49	1.35	1.39
36	5	1307	G	C3'-O3'	5.48	1.49	1.42
36	1	2397	A	N3-C4	5.48	1.38	1.34
36	1	661	G	N7-C5	-5.47	1.35	1.39
36	5	2897	A	N9-C8	-5.47	1.33	1.37
36	1	1395	G	C5-C4	-5.46	1.34	1.38
36	5	1482	A	N9-C4	-5.46	1.34	1.37
38	8	22	U	C4-O4	-5.46	1.19	1.23
36	1	2983	C	N3-C4	-5.46	1.30	1.33
36	5	2113	A	N9-C4	-5.45	1.34	1.37
36	5	1884	A	N7-C5	-5.45	1.35	1.39
36	1	2640	A	N3-C4	-5.44	1.31	1.34
36	5	2643	A	N9-C4	-5.44	1.34	1.37
36	5	2823	G	N7-C5	-5.44	1.35	1.39
36	1	968	G	C6-N1	-5.44	1.35	1.39
36	5	2899	C	N1-C6	-5.44	1.33	1.37
36	5	795	G	C5-C4	-5.43	1.34	1.38
36	5	2419	A	P-O5'	5.43	1.65	1.59
36	1	86	G	C6-N1	-5.43	1.35	1.39
36	1	278	U	C2-O2	-5.43	1.17	1.22
36	1	1103	A	N7-C5	5.43	1.42	1.39
1	2	1291	G	N3-C4	-5.42	1.31	1.35
36	1	2397	A	C5-C4	5.42	1.42	1.38
36	1	903	U	C4-O4	-5.42	1.19	1.23
36	5	2704	A	N9-C4	-5.42	1.34	1.37
36	1	2945	G	N7-C5	-5.42	1.35	1.39
36	1	94	G	N7-C5	-5.41	1.36	1.39
36	1	1305	U	C4-O4	-5.41	1.19	1.23
36	1	2371	G	C8-N7	-5.41	1.27	1.30
38	4	113	U	C2-N3	-5.39	1.33	1.37
36	5	1468	A	N9-C4	-5.39	1.34	1.37
1	2	992	A	N9-C4	-5.39	1.34	1.37
37	7	96	U	C4-O4	-5.38	1.19	1.23
36	1	1167	U	C4-O4	-5.38	1.19	1.23
36	1	637	C	C4-N4	-5.38	1.29	1.33
36	5	793	C	C4-C5	-5.38	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	3050	U	C2-N3	-5.37	1.33	1.37
36	5	2957	G	C8-N7	-5.37	1.27	1.30
36	5	3275	U	N1-C2	5.37	1.43	1.38
36	5	953	G	C5-C6	-5.36	1.36	1.42
36	5	1429	G	N9-C8	-5.36	1.34	1.37
36	5	3308	C	N3-C4	-5.36	1.30	1.33
36	1	3130	A	N7-C5	-5.33	1.36	1.39
36	5	2376	G	C6-N1	-5.33	1.35	1.39
73	O7	10	LYS	CE-NZ	5.33	1.62	1.49
1	6	607	G	C6-N1	-5.33	1.35	1.39
36	1	2761	G	N9-C4	-5.33	1.33	1.38
36	5	2164	A	N7-C5	-5.33	1.36	1.39
36	5	2272	G	C5-C4	-5.32	1.34	1.38
36	5	2971	A	C5-C4	5.32	1.42	1.38
36	1	1153	A	N3-C4	-5.31	1.31	1.34
40	L3	7	GLU	CB-CG	5.31	1.62	1.52
36	1	2988	C	C2-O2	-5.30	1.19	1.24
36	5	2813	A	N7-C5	-5.30	1.36	1.39
1	6	1537	C	N1-C6	5.30	1.40	1.37
36	1	2120	A	N7-C5	-5.29	1.36	1.39
36	5	2376	G	N9-C8	-5.28	1.34	1.37
36	5	652	G	N7-C5	-5.28	1.36	1.39
36	5	1373	A	C5-C4	-5.28	1.35	1.38
36	5	1331	U	C4-C5	-5.27	1.38	1.43
36	1	2145	A	N7-C5	-5.27	1.36	1.39
36	1	626	U	C2-N3	-5.27	1.34	1.37
36	5	2434	U	C2-N3	-5.27	1.34	1.37
36	1	1304	A	N9-C4	-5.26	1.34	1.37
36	1	1841	A	N9-C4	5.26	1.41	1.37
40	l3	349	LYS	CD-CE	5.26	1.64	1.51
38	8	79	A	N9-C4	5.26	1.41	1.37
1	6	967	A	N9-C4	5.25	1.41	1.37
1	6	1503	A	N9-C8	5.25	1.42	1.37
36	1	2945	G	C5-C4	-5.25	1.34	1.38
36	5	1902	G	C5-C4	-5.24	1.34	1.38
36	1	645	A	C2-N3	5.24	1.38	1.33
36	1	1507	G	N9-C8	-5.24	1.34	1.37
36	5	3274	A	N3-C4	-5.24	1.31	1.34
36	1	3362	A	N9-C4	-5.24	1.34	1.37
36	5	2138	A	N9-C8	-5.24	1.33	1.37
36	1	345	G	C5-C4	-5.24	1.34	1.38
36	5	937	G	C2-N3	5.23	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1173	U	C2-N3	-5.23	1.34	1.37
36	5	2403	G	N9-C4	5.23	1.42	1.38
36	1	2368	A	C5-C4	-5.23	1.35	1.38
67	o1	61	LYS	CD-CE	5.22	1.64	1.51
36	1	1592	G	N7-C5	-5.22	1.36	1.39
36	5	2412	G	C2-N3	-5.22	1.28	1.32
36	5	92	G	N1-C2	-5.22	1.33	1.37
36	1	3057	U	N3-C4	-5.22	1.33	1.38
36	5	2977	G	C6-N1	-5.21	1.35	1.39
36	1	1482	A	C5-C6	5.21	1.45	1.41
36	5	2958	A	N9-C4	-5.21	1.34	1.37
36	1	3136	G	C6-N1	-5.21	1.35	1.39
36	5	1103	A	N3-C4	5.21	1.38	1.34
36	1	2409	G	C6-N1	-5.20	1.35	1.39
36	1	2732	G	C6-N1	-5.20	1.35	1.39
36	1	2888	U	C4-O4	-5.20	1.19	1.23
36	1	3311	C	N3-C4	-5.20	1.30	1.33
1	2	1241	G	N9-C8	5.20	1.41	1.37
36	5	1103	A	C5-C4	5.20	1.42	1.38
36	5	2356	A	N3-C4	-5.20	1.31	1.34
36	1	2419	A	P-OP1	5.20	1.57	1.49
36	1	909	G	N9-C8	-5.19	1.34	1.37
36	5	818	C	N1-C2	-5.19	1.34	1.40
44	l7	158	LYS	CB-CG	5.19	1.66	1.52
36	1	2198	A	C5-C4	-5.18	1.35	1.38
36	5	2874	G	C5'-C4'	5.18	1.57	1.51
36	5	1164	G	N7-C5	-5.17	1.36	1.39
36	1	2853	A	N7-C5	-5.17	1.36	1.39
36	1	3267	A	N7-C5	-5.16	1.36	1.39
37	7	76	A	N9-C4	-5.16	1.34	1.37
37	7	92	A	C5-C4	-5.16	1.35	1.38
36	1	1380	G	C6-N1	-5.16	1.35	1.39
36	5	1117	G	C5-C4	-5.16	1.34	1.38
36	5	2724	U	C2-O2	-5.16	1.17	1.22
36	1	2808	A	C6-N6	5.15	1.38	1.33
36	1	39	A	N9-C4	-5.15	1.34	1.37
36	1	2920	U	C2-N3	-5.15	1.34	1.37
36	1	2384	A	N7-C5	-5.14	1.36	1.39
36	5	2872	A	C6-N6	5.14	1.38	1.33
1	6	1109	G	C2-N3	-5.14	1.28	1.32
36	5	2341	A	N3-C4	5.14	1.38	1.34
36	5	3006	A	N3-C4	-5.14	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2403	G	C2-N3	5.14	1.36	1.32
36	5	794	U	N3-C4	-5.13	1.33	1.38
36	5	1902	G	N7-C5	-5.12	1.36	1.39
36	1	870	G	C5-C6	-5.12	1.37	1.42
36	5	966	U	C4-C5	-5.12	1.39	1.43
36	1	2870	C	O3'-P	5.12	1.67	1.61
36	1	2714	G	N9-C4	-5.12	1.33	1.38
36	5	2824	G	N7-C5	-5.12	1.36	1.39
36	1	2873	U	N1-C2	5.11	1.43	1.38
36	1	351	A	N9-C4	-5.11	1.34	1.37
36	1	407	A	C5-C6	-5.11	1.36	1.41
36	5	3218	A	C5-C6	-5.11	1.36	1.41
36	1	945	C	N1-C6	5.10	1.40	1.37
36	1	1379	G	C6-N1	-5.09	1.35	1.39
36	1	1402	C	C2-O2	-5.09	1.19	1.24
52	M6	4	GLU	CD-OE2	5.09	1.31	1.25
41	L4	117	GLU	CD-OE2	5.08	1.31	1.25
36	5	2930	A	N3-C4	5.08	1.37	1.34
36	5	1189	C	N1-C6	-5.08	1.34	1.37
52	M6	100	GLU	CD-OE2	5.08	1.31	1.25
36	5	2434	U	N3-C4	-5.08	1.33	1.38
36	1	291	C	N3-C4	-5.08	1.30	1.33
36	1	345	G	N9-C8	-5.08	1.34	1.37
36	1	970	A	N3-C4	-5.08	1.31	1.34
36	5	838	G	C6-N1	-5.08	1.35	1.39
36	5	3084	C	N1-C6	-5.08	1.34	1.37
36	1	2940	A	C8-N7	-5.07	1.27	1.31
36	1	1459	C	N3-C4	-5.07	1.30	1.33
36	5	611	A	N9-C8	-5.07	1.33	1.37
36	5	1582	C	N1-C6	5.07	1.40	1.37
36	1	1158	A	N7-C5	-5.06	1.36	1.39
36	5	2287	C	N1-C6	5.06	1.40	1.37
36	1	3277	U	N1-C2	5.06	1.43	1.38
1	6	630	A	C5-C6	-5.06	1.36	1.41
36	5	645	A	C2-N3	5.06	1.38	1.33
37	7	84	A	N7-C5	-5.06	1.36	1.39
36	5	1123	U	C2-N3	-5.05	1.34	1.37
36	1	585	A	N7-C5	-5.05	1.36	1.39
36	5	889	U	C4-O4	-5.05	1.19	1.23
37	3	82	G	N7-C5	-5.05	1.36	1.39
36	5	953	G	N7-C5	-5.05	1.36	1.39
36	5	3050	U	N3-C4	-5.05	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2611	U	C4-O4	-5.04	1.19	1.23
41	L4	52	VAL	CB-CG2	-5.04	1.42	1.52
1	6	397	A	N9-C4	-5.04	1.34	1.37
36	1	2874	G	C5-C6	5.04	1.47	1.42
36	5	1404	G	N9-C8	-5.04	1.34	1.37
78	q2	60	LYS	CE-NZ	5.04	1.61	1.49
1	2	1100	G	N7-C5	-5.04	1.36	1.39
36	1	966	U	C4-O4	-5.03	1.19	1.23
36	5	2340	U	C4-O4	-5.03	1.19	1.23
36	5	2942	C	N1-C6	-5.02	1.34	1.37
36	5	2957	G	C5-C4	-5.02	1.34	1.38
36	1	106	A	N9-C4	-5.02	1.34	1.37
36	5	2977	G	N1-C2	-5.02	1.33	1.37
36	1	644	G	N7-C5	-5.02	1.36	1.39
36	5	2873	U	O3'-P	5.02	1.67	1.61
36	5	899	U	C4-O4	-5.02	1.19	1.23
36	5	2131	A	C5-C6	-5.02	1.36	1.41
36	5	2314	U	C2-N3	5.02	1.41	1.37
36	5	2872	A	N7-C5	5.02	1.42	1.39
36	5	283	G	C5-C6	-5.02	1.37	1.42
1	6	1800	A	N9-C4	5.01	1.40	1.37
36	1	1658	G	N7-C5	-5.01	1.36	1.39
37	3	83	U	C4-O4	-5.01	1.19	1.23
37	7	92	A	C5-C6	-5.01	1.36	1.41
36	5	2412	G	C6-N1	-5.01	1.36	1.39
1	2	1560	U	N3-C4	-5.01	1.33	1.38
75	O9	11	GLN	CG-CD	5.01	1.62	1.51
1	6	1600	A	N9-C4	-5.01	1.34	1.37
37	7	88	G	C6-N1	-5.01	1.36	1.39
36	5	2319	U	C2-N3	-5.00	1.34	1.37

All (5106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	SR	161	LYS	O-C-N	-48.73	44.74	122.70
34	SR	160	GLU	C-N-CA	-43.07	14.02	121.70
34	SR	160	GLU	CA-C-N	-38.98	31.43	117.20
36	5	1152	G	N3-C4-C5	26.73	141.96	128.60
36	5	1152	G	N3-C4-N9	-24.27	111.44	126.00
34	SR	160	GLU	O-C-N	-20.73	89.54	122.70
36	5	1152	G	C2-N3-C4	-20.72	101.54	111.90
36	1	1117	G	O5'-P-OP1	-18.27	88.78	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	N3-C2-N2	-17.50	107.65	119.90
36	5	1152	G	C5-N7-C8	-17.36	95.62	104.30
36	5	922	U	N1-C2-N3	16.97	125.08	114.90
1	6	1773	C	N3-C4-C5	-16.96	115.12	121.90
36	5	398	A	O5'-P-OP2	-16.88	90.44	110.70
1	2	553	G	N1-C6-O6	16.48	129.79	119.90
36	5	1152	G	N1-C6-O6	16.01	129.51	119.90
36	5	1152	G	C8-N9-C1'	15.19	146.75	127.00
1	6	163	G	N3-C4-N9	-15.18	116.89	126.00
36	5	922	U	C5-C6-N1	-14.62	115.39	122.70
36	1	1495	U	C5-C6-N1	-14.43	115.48	122.70
36	5	922	U	C2-N3-C4	-14.43	118.34	127.00
1	2	1200	G	N1-C6-O6	14.37	128.52	119.90
36	5	1152	G	C4-N9-C1'	-14.19	108.06	126.50
36	1	2373	A	O5'-P-OP1	-14.18	92.94	105.70
36	5	1419	A	O5'-P-OP2	-14.10	93.01	105.70
36	5	1117	G	O5'-P-OP1	-14.05	93.05	105.70
36	1	2617	U	C5-C4-O4	13.99	134.30	125.90
36	1	2714	G	N3-C4-C5	13.82	135.51	128.60
36	1	1495	U	C4-C5-C6	13.79	127.97	119.70
36	5	1879	A	O5'-P-OP1	13.78	127.24	110.70
36	1	895	A	C5-N7-C8	-13.70	97.05	103.90
36	1	1196	C	C6-N1-C2	13.63	125.75	120.30
36	5	2923	U	O5'-P-OP1	-13.58	93.47	105.70
36	5	3005	A	O5'-P-OP2	-13.50	93.55	105.70
36	5	776	U	C5-C6-N1	-13.47	115.97	122.70
36	1	2957	G	O5'-P-OP1	-13.45	93.59	105.70
36	1	2983	C	O5'-P-OP1	-13.36	93.67	105.70
36	1	2726	C	N3-C2-O2	-13.11	112.72	121.90
36	1	2938	G	O5'-P-OP1	-13.05	93.95	105.70
36	1	406	G	O4'-C1'-N9	13.04	118.64	108.20
36	5	2385	G	O5'-P-OP1	-13.01	93.99	105.70
36	1	1308	A	O5'-P-OP2	-12.98	94.02	105.70
36	5	1308	A	O5'-P-OP2	-12.95	94.05	105.70
34	SR	161	LYS	CA-C-N	12.79	145.33	117.20
36	5	1152	G	C4-C5-N7	12.79	115.91	110.80
36	5	2121	G	O5'-P-OP2	-12.76	94.22	105.70
1	6	609	U	C5-C6-N1	-12.75	116.33	122.70
36	5	3018	C	O5'-P-OP2	-12.73	94.24	105.70
36	5	2945	G	O5'-P-OP2	-12.72	94.25	105.70
36	1	218	G	O5'-P-OP2	-12.70	94.27	105.70
36	1	2978	U	O5'-P-OP2	-12.67	94.30	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2617	U	N3-C4-O4	-12.58	110.59	119.40
52	M6	78	ARG	NE-CZ-NH1	12.58	126.59	120.30
36	1	817	A	O5'-P-OP1	-12.50	94.45	105.70
36	1	2848	G	O5'-P-OP2	-12.39	94.55	105.70
40	l3	19	ARG	NE-CZ-NH2	-12.31	114.15	120.30
36	1	1400	G	O5'-P-OP2	-12.21	94.71	105.70
36	1	802	C	O5'-P-OP1	-12.17	94.75	105.70
1	6	1657	U	O5'-P-OP2	-12.14	94.78	105.70
36	5	2373	A	O5'-P-OP1	-12.06	94.85	105.70
36	1	1495	U	N1-C2-N3	12.05	122.13	114.90
36	5	3245	A	C2-N3-C4	-12.03	104.59	110.60
1	6	1773	C	N3-C4-N4	11.94	126.36	118.00
36	5	2882	U	O5'-P-OP2	-11.93	94.97	105.70
36	5	2393	G	O5'-P-OP2	-11.84	95.05	105.70
1	6	163	G	N3-C4-C5	11.83	134.51	128.60
36	5	2278	C	C6-N1-C2	-11.81	115.58	120.30
36	5	776	U	C4-C5-C6	11.78	126.77	119.70
36	1	2846	U	N3-C2-O2	-11.72	113.99	122.20
36	1	1320	C	O5'-P-OP2	-11.71	95.16	105.70
36	5	1513	G	C8-N9-C4	-11.62	101.75	106.40
36	5	2704	A	O5'-P-OP1	-11.59	95.27	105.70
36	1	2983	C	N3-C2-O2	-11.52	113.84	121.90
36	1	3362	A	C2-N3-C4	-11.50	104.85	110.60
36	5	2315	G	O5'-P-OP1	-11.47	95.37	105.70
36	1	2618	G	N1-C6-O6	-11.47	113.02	119.90
36	5	2726	C	C5-C4-N4	11.44	128.21	120.20
36	5	1551	C	O5'-P-OP1	-11.44	95.40	105.70
36	1	776	U	C4-C5-C6	11.37	126.52	119.70
36	1	2617	U	C5-C6-N1	-11.36	117.02	122.70
36	1	2714	G	N3-C4-N9	-11.27	119.24	126.00
1	6	163	G	C2-N3-C4	-11.27	106.26	111.90
36	5	3245	A	C5-N7-C8	-11.27	98.27	103.90
36	1	2631	U	N3-C4-O4	-11.25	111.53	119.40
36	1	944	C	C5-C6-N1	11.23	126.61	121.00
36	5	960	U	C2-N3-C4	-11.15	120.31	127.00
36	5	645	A	C6-N1-C2	-11.13	111.92	118.60
36	5	1152	G	C5-C6-O6	-11.13	121.92	128.60
36	1	2726	C	N3-C4-N4	-11.05	110.27	118.00
36	1	895	A	N7-C8-N9	11.04	119.32	113.80
36	1	2281	A	O5'-P-OP2	-11.04	95.76	105.70
36	5	2983	C	O5'-P-OP1	-11.03	95.77	105.70
36	5	2634	U	C2-N3-C4	-11.01	120.39	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	144	U	N3-C2-O2	-10.91	114.56	122.20
36	1	2403	G	N3-C4-C5	-10.89	123.15	128.60
1	2	553	G	C5-C6-O6	-10.85	122.09	128.60
36	5	806	A	O5'-P-OP1	-10.82	95.96	105.70
36	5	2340	U	N3-C4-O4	-10.72	111.89	119.40
36	1	954	U	O5'-P-OP2	-10.72	96.05	105.70
36	5	2289	U	N1-C2-O2	10.72	130.30	122.80
36	1	611	A	O5'-P-OP1	10.70	123.54	110.70
1	6	1773	C	C4-C5-C6	10.67	122.74	117.40
36	1	637	C	O4'-C1'-N1	10.65	116.72	108.20
1	6	1537	C	C6-N1-C2	-10.65	116.04	120.30
36	5	406	G	O4'-C1'-N9	10.64	116.71	108.20
36	5	590	G	O5'-P-OP1	-10.62	96.15	105.70
36	1	979	U	C6-N1-C2	-10.57	114.66	121.00
36	1	2412	G	C8-N9-C4	-10.56	102.17	106.40
36	1	3278	C	N3-C2-O2	-10.54	114.52	121.90
36	1	718	G	N3-C4-C5	10.53	133.87	128.60
36	5	776	U	N1-C2-N3	10.53	121.22	114.90
1	2	1291	G	N3-C4-N9	-10.52	119.69	126.00
36	5	2412	G	C8-N9-C4	-10.50	102.20	106.40
36	5	922	U	C4-C5-C6	10.50	126.00	119.70
1	6	337	G	C6-C5-N7	-10.49	124.11	130.40
36	1	2726	C	C6-N1-C2	-10.45	116.12	120.30
36	5	2800	G	N3-C2-N2	-10.44	112.59	119.90
36	5	2726	C	C6-N1-C2	-10.43	116.13	120.30
36	5	877	C	N3-C4-C5	10.39	126.06	121.90
36	5	1313	G	O5'-P-OP2	-10.38	96.36	105.70
36	1	637	C	C6-N1-C1'	10.38	133.25	120.80
36	1	2726	C	C5-C4-N4	10.37	127.46	120.20
1	2	639	U	N3-C2-O2	-10.36	114.94	122.20
38	4	113	U	C5-C4-O4	10.36	132.11	125.90
36	5	1115	G	C8-N9-C4	-10.35	102.26	106.40
36	1	3362	A	C5-N7-C8	-10.30	98.75	103.90
36	1	1381	A	O5'-P-OP2	10.30	123.06	110.70
1	2	1200	G	C5-C6-O6	-10.28	122.43	128.60
38	4	113	U	C5-C6-N1	-10.24	117.58	122.70
36	5	2632	G	C5-C6-O6	10.24	134.74	128.60
36	1	2977	G	N7-C8-N9	-10.23	107.98	113.10
37	3	10	C	O5'-P-OP2	-10.21	96.52	105.70
36	1	2860	U	N3-C2-O2	10.16	129.31	122.20
36	1	1414	G	O5'-P-OP2	-10.15	96.57	105.70
1	6	352	A	O5'-P-OP1	-10.13	96.58	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2977	G	C8-N9-C4	10.12	110.45	106.40
37	7	120	C	C6-N1-C2	10.07	124.33	120.30
36	1	3214	U	N3-C2-O2	-10.06	115.16	122.20
36	1	1555	U	C2-N1-C1'	-10.05	105.64	117.70
36	5	2899	C	N3-C2-O2	-10.04	114.87	121.90
37	3	86	U	C5-C4-O4	-10.03	119.88	125.90
36	1	2836	C	C5-C4-N4	10.00	127.20	120.20
36	1	2617	U	N1-C2-N3	10.00	120.90	114.90
36	1	979	U	N1-C2-N3	9.98	120.89	114.90
36	1	2550	U	N3-C2-O2	-9.97	115.22	122.20
36	1	608	A	N1-C6-N6	9.94	124.56	118.60
36	5	2398	A	C8-N9-C4	-9.92	101.83	105.80
1	6	1773	C	N1-C2-O2	-9.91	112.95	118.90
36	1	645	A	C6-N1-C2	-9.88	112.67	118.60
36	5	835	G	O4'-C1'-N9	9.86	116.09	108.20
36	1	2419	A	O5'-P-OP2	-9.86	96.83	105.70
36	5	2619	G	C5-C6-O6	-9.85	122.69	128.60
36	5	2865	U	N1-C2-O2	9.84	129.69	122.80
36	5	3107	U	N3-C2-O2	-9.80	115.34	122.20
36	1	2772	C	C2-N1-C1'	9.80	129.58	118.80
1	2	1200	G	N3-C2-N2	-9.79	113.05	119.90
1	6	542	A	N7-C8-N9	9.79	118.69	113.80
36	5	2836	C	C5-C4-N4	9.79	127.05	120.20
36	5	1371	G	N1-C6-O6	-9.75	114.05	119.90
36	5	3052	G	C5-C6-O6	9.75	134.45	128.60
38	8	80	A	C8-N9-C4	-9.73	101.91	105.80
36	5	2818	U	O5'-P-OP1	-9.71	96.96	105.70
36	5	922	U	N3-C2-O2	-9.63	115.46	122.20
36	1	776	U	C5-C6-N1	-9.62	117.89	122.70
36	5	3214	U	N3-C2-O2	-9.61	115.47	122.20
70	O4	51	LEU	CA-CB-CG	9.59	137.35	115.30
36	1	2867	C	N3-C4-N4	-9.57	111.30	118.00
36	1	3306	U	N1-C2-N3	9.57	120.64	114.90
36	5	2385	G	N3-C4-C5	9.55	133.38	128.60
36	1	2862	U	N3-C2-O2	-9.54	115.52	122.20
1	2	1596	C	N3-C2-O2	-9.53	115.23	121.90
36	1	909	G	N7-C8-N9	-9.52	108.34	113.10
36	1	949	C	C6-N1-C2	-9.52	116.49	120.30
36	1	2618	G	C5-C6-N1	9.51	116.26	111.50
62	N6	13	ARG	NE-CZ-NH2	-9.51	115.54	120.30
1	6	453	U	N3-C2-O2	-9.51	115.55	122.20
36	5	1152	G	N1-C2-N2	9.50	124.75	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3362	A	C2-N3-C4	-9.50	105.85	110.60
36	5	1845	G	O5'-P-OP1	-9.49	97.16	105.70
36	5	2632	G	N1-C6-O6	-9.48	114.21	119.90
36	1	3214	U	C5-C4-O4	9.47	131.58	125.90
1	2	553	G	N3-C2-N2	-9.46	113.28	119.90
36	1	280	U	C5-C4-O4	-9.45	120.23	125.90
36	5	648	C	O5'-P-OP1	-9.44	97.20	105.70
36	1	2434	U	C5-C4-O4	9.43	131.56	125.90
1	6	687	G	N3-C2-N2	-9.42	113.31	119.90
36	1	1164	G	C5-C6-O6	9.42	134.25	128.60
36	1	718	G	N3-C4-N9	-9.41	120.35	126.00
36	1	3344	A	N7-C8-N9	9.41	118.50	113.80
36	1	3306	U	N3-C4-O4	-9.40	112.82	119.40
1	6	337	G	C4-N9-C1'	9.39	138.71	126.50
36	1	2846	U	C5-C4-O4	9.39	131.53	125.90
36	1	1450	G	O5'-P-OP1	-9.39	97.25	105.70
1	6	1537	C	N3-C4-C5	-9.38	118.15	121.90
36	1	895	A	C4-C5-N7	9.37	115.38	110.70
36	1	895	A	C8-N9-C4	-9.36	102.06	105.80
1	2	1631	A	O5'-P-OP1	-9.34	97.30	105.70
38	4	74	U	O5'-P-OP1	-9.34	97.29	105.70
36	1	968	G	C8-N9-C4	-9.34	102.67	106.40
36	5	3245	A	N7-C8-N9	9.33	118.47	113.80
36	1	439	C	N1-C2-O2	9.33	124.50	118.90
1	6	1596	C	N3-C2-O2	-9.32	115.38	121.90
36	1	3362	A	N7-C8-N9	9.31	118.46	113.80
36	1	729	C	O5'-P-OP2	-9.31	97.32	105.70
1	6	1634	C	N1-C2-O2	9.29	124.48	118.90
36	1	1450	G	C8-N9-C4	9.29	110.12	106.40
36	1	909	G	C8-N9-C4	9.29	110.11	106.40
36	1	2808	A	N1-C6-N6	9.28	124.17	118.60
36	1	3214	U	N1-C2-N3	9.26	120.46	114.90
36	1	2572	C	N1-C2-O2	9.24	124.44	118.90
36	1	2550	U	C5-C4-O4	9.23	131.44	125.90
36	1	1328	C	O5'-P-OP1	-9.22	97.40	105.70
36	1	1419	A	O5'-P-OP2	-9.22	97.40	105.70
36	5	2968	G	N1-C6-O6	-9.22	114.37	119.90
36	1	2617	U	N3-C2-O2	-9.20	115.76	122.20
36	1	2944	U	N3-C4-C5	9.19	120.12	114.60
36	5	887	G	N3-C2-N2	9.19	126.33	119.90
36	1	3181	C	N3-C2-O2	-9.18	115.47	121.90
36	5	909	G	N1-C6-O6	-9.18	114.39	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D9	36	LEU	CA-CB-CG	9.17	136.39	115.30
36	1	2867	C	N3-C2-O2	-9.15	115.50	121.90
36	5	1120	A	N1-C6-N6	-9.15	113.11	118.60
36	1	2797	C	C6-N1-C2	9.14	123.96	120.30
36	5	2860	U	C5-C4-O4	-9.14	120.41	125.90
36	5	2694	A	C8-N9-C4	-9.14	102.14	105.80
36	5	1439	U	C5-C4-O4	-9.14	120.42	125.90
1	6	542	A	N1-C6-N6	9.12	124.07	118.60
1	6	337	G	C8-N9-C1'	-9.12	115.14	127.00
36	5	1314	C	N3-C4-C5	9.11	125.55	121.90
36	5	2375	G	N1-C6-O6	-9.11	114.43	119.90
1	2	1783	C	O5'-P-OP2	-9.10	97.52	105.70
36	1	2176	U	N3-C2-O2	-9.09	115.83	122.20
36	1	1189	C	N1-C2-O2	-9.08	113.45	118.90
36	1	2634	U	C2-N3-C4	-9.08	121.55	127.00
36	1	2978	U	O5'-P-OP1	9.08	121.59	110.70
40	l3	266	ARG	NE-CZ-NH2	-9.07	115.77	120.30
36	1	439	C	C2-N1-C1'	9.06	128.77	118.80
49	M3	85	LEU	CA-CB-CG	9.04	136.10	115.30
1	6	65	A	C2-N3-C4	-9.04	106.08	110.60
36	5	1501	U	C5-C6-N1	9.03	127.22	122.70
36	5	3259	U	O5'-P-OP2	-9.00	97.60	105.70
36	1	2130	G	N1-C6-O6	-9.00	114.50	119.90
36	5	1419	A	O5'-P-OP1	8.99	121.49	110.70
36	1	2945	G	O5'-P-OP2	-8.99	97.61	105.70
36	1	347	G	C5-C6-O6	-8.99	123.21	128.60
36	1	637	C	C2-N1-C1'	-8.98	108.92	118.80
1	6	1145	U	O5'-P-OP2	-8.98	97.62	105.70
36	1	960	U	C2-N3-C4	-8.97	121.62	127.00
1	6	163	G	N3-C2-N2	-8.96	113.63	119.90
38	4	113	U	N1-C2-N3	8.95	120.27	114.90
1	6	57	G	O5'-P-OP2	-8.95	97.64	105.70
36	5	1178	G	N3-C2-N2	-8.95	113.63	119.90
36	1	200	C	N1-C2-O2	8.93	124.26	118.90
36	1	967	A	N1-C6-N6	-8.93	113.24	118.60
36	5	1189	C	N3-C2-O2	8.93	128.15	121.90
1	6	542	A	C6-C5-N7	-8.93	126.05	132.30
36	1	2572	C	C2-N1-C1'	8.92	128.62	118.80
1	6	1096	C	N1-C2-O2	8.92	124.25	118.90
36	5	116	A	O4'-C1'-N9	8.91	115.33	108.20
36	5	216	G	N1-C6-O6	8.90	125.24	119.90
36	5	634	C	N3-C4-C5	8.89	125.46	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3050	U	N3-C2-O2	-8.88	115.99	122.20
36	5	637	C	C2-N1-C1'	-8.87	109.05	118.80
36	5	2415	C	O5'-P-OP2	-8.86	97.72	105.70
36	5	2836	C	N3-C4-N4	-8.86	111.80	118.00
36	1	200	C	N3-C2-O2	-8.85	115.70	121.90
1	2	553	G	C6-C5-N7	-8.85	125.09	130.40
36	5	957	C	N3-C4-C5	8.85	125.44	121.90
36	5	2119	A	N1-C6-N6	8.85	123.91	118.60
36	5	2385	G	C8-N9-C4	8.84	109.94	106.40
1	6	434	G	O5'-P-OP2	-8.83	97.75	105.70
36	1	2385	G	O5'-P-OP1	-8.83	97.75	105.70
36	1	2818	U	O5'-P-OP1	-8.83	97.76	105.70
36	5	3012	A	C8-N9-C4	8.83	109.33	105.80
36	5	2327	U	C5-C6-N1	-8.82	118.29	122.70
36	1	3306	U	N3-C2-O2	-8.82	116.03	122.20
36	5	2382	G	N1-C6-O6	-8.82	114.61	119.90
36	1	2409	G	N1-C6-O6	-8.81	114.62	119.90
36	1	2884	C	N3-C4-C5	8.80	125.42	121.90
36	5	1879	A	N1-C6-N6	8.80	123.88	118.60
36	5	960	U	N3-C4-C5	8.79	119.88	114.60
36	5	2142	A	C5-C6-N1	8.79	122.09	117.70
36	5	2978	U	O5'-P-OP2	-8.78	97.80	105.70
36	1	633	C	C6-N1-C2	8.77	123.81	120.30
36	1	3092	C	C2-N1-C1'	-8.77	109.15	118.80
1	6	1	U	O4'-C1'-N1	8.77	115.22	108.20
36	1	870	G	C5-C6-O6	-8.75	123.35	128.60
1	2	1199	G	O5'-P-OP2	-8.75	97.83	105.70
36	5	2403	G	N1-C6-O6	-8.75	114.65	119.90
36	5	3092	C	O4'-C1'-N1	8.75	115.20	108.20
36	1	59	G	O5'-P-OP2	-8.73	97.84	105.70
36	1	2860	U	N1-C2-O2	-8.73	116.69	122.80
1	6	1560	U	N3-C2-O2	-8.72	116.10	122.20
36	5	1879	A	C4-C5-N7	8.71	115.06	110.70
1	6	18	C	C6-N1-C2	-8.71	116.82	120.30
36	1	636	C	O5'-P-OP1	-8.70	97.87	105.70
36	5	2978	U	N3-C2-O2	-8.69	116.11	122.20
36	1	776	U	N1-C2-N3	8.69	120.12	114.90
36	1	967	A	N9-C4-C5	8.69	109.28	105.80
1	6	17	C	O5'-P-OP2	-8.69	97.88	105.70
1	6	1596	C	C6-N1-C2	-8.69	116.83	120.30
36	5	1181	U	C5-C6-N1	-8.69	118.36	122.70
36	1	960	U	C5-C4-O4	-8.67	120.70	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3154	C	N1-C2-O2	8.66	124.10	118.90
36	1	1411	C	N3-C2-O2	-8.66	115.84	121.90
36	5	2726	C	N3-C2-O2	-8.66	115.84	121.90
36	1	346	C	C5-C6-N1	-8.65	116.67	121.00
36	1	3207	U	C6-N1-C1'	8.65	133.32	121.20
36	5	1879	A	C5-N7-C8	-8.65	99.58	103.90
36	5	1536	G	O5'-P-OP2	-8.65	97.92	105.70
36	1	3207	U	C2-N1-C1'	-8.64	107.34	117.70
1	6	308	C	C5-C6-N1	-8.63	116.69	121.00
36	5	1406	A	O5'-P-OP1	-8.63	97.94	105.70
36	5	2340	U	N3-C4-C5	8.63	119.78	114.60
36	5	2366	C	C5-C6-N1	8.62	125.31	121.00
36	5	2289	U	N3-C2-O2	-8.61	116.17	122.20
36	1	2327	U	O5'-P-OP1	-8.61	97.95	105.70
36	5	1064	A	N1-C6-N6	8.61	123.77	118.60
36	1	2614	G	N1-C6-O6	-8.61	114.73	119.90
36	1	421	G	N3-C4-N9	8.61	131.16	126.00
36	1	1484	U	P-O3'-C3'	8.60	130.02	119.70
36	1	2340	U	N3-C4-O4	-8.60	113.38	119.40
36	1	1196	C	C5-C6-N1	-8.60	116.70	121.00
36	5	960	U	C5-C6-N1	-8.59	118.41	122.70
36	1	3278	C	N1-C2-O2	8.58	124.05	118.90
36	5	1212	A	O5'-P-OP2	-8.58	97.98	105.70
36	1	2836	C	C4-C5-C6	8.58	121.69	117.40
36	1	3055	U	C5-C4-O4	-8.58	120.75	125.90
36	5	637	C	C6-N1-C1'	8.58	131.09	120.80
36	5	2719	U	O5'-P-OP2	-8.56	97.99	105.70
1	6	1600	A	C2-N3-C4	-8.56	106.32	110.60
36	5	945	C	C6-N1-C2	8.56	123.72	120.30
36	5	776	U	C5-C4-O4	8.56	131.04	125.90
36	1	765	C	N1-C2-O2	8.55	124.03	118.90
36	1	633	C	C5-C6-N1	-8.55	116.72	121.00
36	5	110	G	O5'-P-OP2	-8.55	98.01	105.70
36	5	909	G	C4-C5-N7	-8.55	107.38	110.80
36	5	2860	U	N3-C2-O2	8.55	128.18	122.20
36	5	2638	C	N1-C2-O2	-8.54	113.77	118.90
36	1	1841	A	C2-N3-C4	8.54	114.87	110.60
36	1	2772	C	O4'-C1'-N1	8.53	115.03	108.20
36	1	2244	A	O5'-P-OP1	8.53	120.94	110.70
36	5	2865	U	C5-C6-N1	8.53	126.96	122.70
36	1	2827	U	C2-N1-C1'	-8.53	107.47	117.70
36	1	2875	U	O5'-P-OP2	-8.53	98.03	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2302	G	C5-C6-O6	8.52	133.71	128.60
36	1	3344	A	C5-N7-C8	-8.52	99.64	103.90
36	5	971	G	N7-C8-N9	-8.52	108.84	113.10
36	1	2818	U	C5-C6-N1	8.51	126.95	122.70
36	1	2679	A	C2-N3-C4	-8.50	106.35	110.60
36	5	2278	C	C5-C6-N1	8.50	125.25	121.00
36	5	2618	G	C5-C6-O6	-8.50	123.50	128.60
18	C6	40	GLU	C-N-CD	-8.49	101.91	120.60
36	5	2426	U	N3-C4-O4	-8.49	113.45	119.40
1	2	1773	C	N3-C4-C5	-8.49	118.50	121.90
36	5	2984	C	C2-N3-C4	-8.49	115.66	119.90
36	1	1082	U	C6-N1-C2	-8.47	115.92	121.00
36	5	3048	A	O5'-P-OP2	-8.46	98.09	105.70
37	3	88	G	N1-C6-O6	-8.45	114.83	119.90
36	5	662	U	O5'-P-OP1	-8.45	98.10	105.70
36	5	3245	A	C4-C5-N7	8.45	114.92	110.70
36	5	961	C	N1-C2-O2	8.45	123.97	118.90
1	6	543	C	C5-C6-N1	8.44	125.22	121.00
1	6	1039	A	O4'-C1'-N9	8.43	114.95	108.20
36	5	2978	U	N3-C4-O4	-8.43	113.50	119.40
1	6	1473	U	N3-C2-O2	-8.43	116.30	122.20
36	1	937	G	C8-N9-C4	8.41	109.77	106.40
36	1	2400	G	N1-C6-O6	8.41	124.95	119.90
36	1	2618	G	N3-C4-C5	-8.41	124.39	128.60
36	1	3209	A	N1-C6-N6	8.40	123.64	118.60
36	5	838	G	N1-C6-O6	-8.39	114.86	119.90
36	5	2572	C	N1-C2-O2	8.39	123.94	118.90
36	1	944	C	C6-N1-C2	-8.38	116.95	120.30
36	1	709	A	C8-N9-C4	8.37	109.15	105.80
38	8	80	A	N7-C8-N9	8.37	117.99	113.80
36	5	1452	A	C8-N9-C4	8.37	109.15	105.80
36	1	2298	U	C5-C6-N1	-8.37	118.52	122.70
36	1	2384	A	N1-C6-N6	8.36	123.62	118.60
68	o2	27	ARG	NE-CZ-NH2	-8.36	116.12	120.30
36	1	2249	G	N1-C6-O6	-8.36	114.88	119.90
36	1	2184	U	C5-C4-O4	-8.36	120.89	125.90
36	5	649	A	C8-N9-C4	-8.35	102.46	105.80
36	5	200	C	C2-N1-C1'	8.35	127.99	118.80
38	8	99	C	C6-N1-C2	8.35	123.64	120.30
1	2	1096	C	C2-N1-C1'	8.35	127.98	118.80
36	5	2932	U	N3-C2-O2	-8.35	116.36	122.20
36	1	342	A	O5'-P-OP2	-8.34	98.19	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	641	C	C6-N1-C2	-8.34	116.96	120.30
36	5	2634	U	N1-C2-O2	-8.34	116.97	122.80
36	5	2932	U	N1-C2-O2	8.33	128.63	122.80
38	8	98	U	C5-C4-O4	-8.33	120.90	125.90
36	5	2726	C	N3-C4-C5	-8.32	118.57	121.90
36	5	2964	G	O5'-P-OP2	-8.31	98.22	105.70
36	1	2550	U	N1-C2-N3	8.31	119.89	114.90
36	1	1331	U	C5-C4-O4	-8.31	120.92	125.90
36	1	1329	U	N1-C1'-C2'	-8.30	102.87	112.00
36	5	2412	G	N9-C4-C5	8.30	108.72	105.40
36	5	2272	G	O4'-C1'-N9	8.29	114.83	108.20
36	1	2165	G	O5'-P-OP2	-8.29	98.24	105.70
36	5	2392	C	C2-N3-C4	-8.28	115.76	119.90
36	1	2899	C	N3-C2-O2	-8.27	116.11	121.90
1	6	795	U	N3-C2-O2	-8.27	116.41	122.20
36	5	2376	G	C8-N9-C4	8.26	109.70	106.40
36	1	2883	U	C5-C6-N1	8.25	126.83	122.70
1	2	934	C	C2-N1-C1'	8.24	127.87	118.80
36	5	2913	C	O5'-P-OP1	-8.24	98.28	105.70
37	7	88	G	N1-C6-O6	-8.24	114.95	119.90
36	5	2393	G	C5-C6-O6	-8.24	123.66	128.60
1	2	1773	C	C6-N1-C2	-8.23	117.01	120.30
36	5	1902	G	C5-C6-O6	-8.23	123.66	128.60
36	5	890	C	O5'-P-OP2	-8.22	98.30	105.70
36	1	2142	A	C6-N1-C2	-8.22	113.67	118.60
36	1	2987	A	O5'-P-OP1	-8.22	98.30	105.70
36	1	14	U	O5'-P-OP2	-8.21	98.31	105.70
36	5	663	C	C2-N3-C4	-8.21	115.80	119.90
1	6	389	G	N1-C6-O6	-8.21	114.98	119.90
36	5	1327	C	N3-C4-N4	-8.21	112.26	118.00
36	1	2214	A	N1-C6-N6	8.20	123.52	118.60
36	5	2248	C	C6-N1-C2	8.20	123.58	120.30
36	1	611	A	O5'-P-OP2	-8.20	98.32	105.70
64	n8	21	ARG	NE-CZ-NH1	8.20	124.40	120.30
36	1	1555	U	C5-C6-N1	-8.20	118.60	122.70
36	1	1156	C	N3-C4-N4	-8.19	112.27	118.00
36	1	3214	U	C6-N1-C2	-8.19	116.09	121.00
36	5	909	G	C6-C5-N7	8.19	135.31	130.40
38	4	73	U	N3-C4-C5	8.18	119.51	114.60
36	1	1136	A	C5-C6-N1	8.18	121.79	117.70
36	5	637	C	N1-C2-O2	-8.18	113.99	118.90
36	5	2860	U	N1-C2-O2	-8.16	117.09	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2978	U	C5-C4-O4	8.16	130.79	125.90
36	5	2889	C	N3-C2-O2	-8.15	116.19	121.90
36	1	1589	A	O4'-C1'-N9	-8.15	101.68	108.20
36	5	2915	U	N1-C2-N3	8.14	119.79	114.90
36	1	2409	G	C5-C6-O6	8.14	133.48	128.60
36	5	2896	A	N1-C6-N6	-8.14	113.72	118.60
36	5	2730	G	N1-C6-O6	8.13	124.78	119.90
36	5	2601	A	O5'-P-OP2	-8.13	98.39	105.70
1	6	542	A	C5-N7-C8	-8.12	99.84	103.90
36	5	2800	G	N9-C4-C5	8.12	108.65	105.40
36	5	1513	G	N1-C6-O6	-8.12	115.03	119.90
36	5	3143	C	O5'-P-OP2	-8.12	98.40	105.70
36	1	980	A	C8-N9-C4	-8.11	102.56	105.80
1	6	1026	A	O5'-P-OP1	-8.11	98.40	105.70
36	5	1124	U	N3-C4-C5	8.11	119.46	114.60
36	5	2730	G	C5-C6-O6	-8.11	123.74	128.60
36	1	3362	A	N1-C6-N6	8.10	123.46	118.60
36	5	92	G	N1-C6-O6	-8.10	115.04	119.90
36	1	2395	G	N1-C6-O6	-8.10	115.04	119.90
38	4	113	U	N3-C2-O2	-8.10	116.53	122.20
38	4	79	A	C8-N9-C4	-8.09	102.56	105.80
36	1	33	G	C8-N9-C4	-8.09	103.17	106.40
36	1	960	U	N1-C2-O2	-8.08	117.14	122.80
36	1	2714	G	C2-N3-C4	-8.08	107.86	111.90
1	6	139	C	C6-N1-C2	-8.08	117.07	120.30
36	5	96	G	O5'-P-OP2	-8.08	98.43	105.70
1	2	1305	U	C5-C4-O4	8.08	130.75	125.90
1	2	1560	U	N3-C2-O2	-8.08	116.55	122.20
36	5	2813	A	C8-N9-C4	-8.08	102.57	105.80
36	1	3306	U	C5-C4-O4	8.07	130.74	125.90
36	1	360	G	N9-C4-C5	-8.07	102.17	105.40
36	5	716	A	O5'-P-OP1	-8.07	98.44	105.70
36	5	1848	G	C5-C6-O6	-8.07	123.76	128.60
36	1	2226	U	O5'-P-OP1	-8.06	98.44	105.70
36	1	1202	A	O5'-P-OP2	-8.06	98.44	105.70
36	1	3362	A	C6-C5-N7	-8.06	126.66	132.30
36	5	3107	U	N1-C2-O2	8.05	128.43	122.80
36	1	949	C	N3-C4-C5	-8.04	118.68	121.90
1	2	1560	U	C5-C4-O4	8.04	130.72	125.90
36	1	1168	U	N3-C2-O2	-8.04	116.57	122.20
36	1	3092	C	O4'-C1'-N1	8.04	114.63	108.20
36	1	2616	C	O5'-P-OP1	-8.03	98.47	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1902	G	C4-C5-N7	8.03	114.01	110.80
36	1	1405	U	N3-C4-C5	8.02	119.41	114.60
36	1	2121	G	O5'-P-OP2	-8.02	98.48	105.70
36	1	3218	A	C8-N9-C4	-8.02	102.59	105.80
36	5	437	G	N3-C4-N9	-8.02	121.19	126.00
36	5	971	G	C5-N7-C8	8.02	108.31	104.30
36	1	2758	A	C2-N3-C4	8.02	114.61	110.60
1	2	1339	C	P-O3'-C3'	8.02	129.32	119.70
36	1	371	G	O5'-P-OP2	-8.01	98.49	105.70
36	1	2867	C	N1-C2-O2	8.01	123.71	118.90
36	5	1189	C	N1-C2-O2	-8.00	114.10	118.90
37	7	110	G	O5'-P-OP2	-8.00	98.50	105.70
36	5	2360	C	C4-C5-C6	7.99	121.40	117.40
1	6	1634	C	C2-N1-C1'	7.99	127.59	118.80
36	1	3362	A	C4-C5-N7	7.99	114.69	110.70
1	6	308	C	C2-N3-C4	-7.99	115.91	119.90
36	1	2836	C	N3-C4-C5	-7.98	118.71	121.90
36	1	689	U	N1-C2-O2	7.98	128.39	122.80
36	5	1496	C	O5'-P-OP1	7.98	120.28	110.70
36	5	1152	G	N7-C8-N9	7.98	117.09	113.10
36	5	2389	C	C2-N3-C4	-7.97	115.91	119.90
36	5	2857	C	N3-C4-C5	7.97	125.09	121.90
36	5	3142	A	C8-N9-C4	7.97	108.99	105.80
36	5	2980	U	OP1-P-OP2	-7.96	107.66	119.60
1	6	687	G	N3-C4-N9	-7.96	121.23	126.00
36	5	2726	C	N1-C2-N3	7.95	124.77	119.20
36	5	671	U	C5-C4-O4	-7.94	121.13	125.90
36	1	369	A	C8-N9-C4	-7.94	102.62	105.80
38	8	25	G	N1-C6-O6	-7.94	115.14	119.90
36	5	2283	G	O5'-P-OP2	-7.94	98.56	105.70
1	6	163	G	N9-C4-C5	7.93	108.57	105.40
36	1	2215	A	C8-N9-C4	7.92	108.97	105.80
1	6	337	G	C4-C5-N7	7.92	113.97	110.80
36	1	114	A	N1-C6-N6	7.92	123.35	118.60
38	8	45	C	C6-N1-C2	-7.92	117.13	120.30
36	1	2391	G	N1-C6-O6	-7.92	115.15	119.90
1	6	1537	C	N1-C2-O2	-7.92	114.15	118.90
36	5	1308	A	C8-N9-C4	-7.91	102.64	105.80
36	5	1856	C	C6-N1-C2	-7.91	117.14	120.30
52	m6	160	ARG	NE-CZ-NH2	-7.91	116.34	120.30
36	1	3264	G	C8-N9-C4	7.91	109.56	106.40
36	5	3052	G	N1-C6-O6	-7.91	115.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	54	C	N3-C4-N4	-7.90	112.47	118.00
36	5	878	G	OP1-P-O3'	7.90	122.58	105.20
36	5	712	G	O5'-P-OP2	-7.89	98.59	105.70
36	5	816	A	C8-N9-C4	-7.89	102.64	105.80
36	1	1314	C	C6-N1-C2	-7.89	117.14	120.30
36	5	2979	U	N3-C2-O2	7.89	127.72	122.20
36	1	2936	A	O5'-P-OP2	7.89	120.17	110.70
1	2	448	C	O5'-P-OP2	-7.88	98.61	105.70
36	5	1480	G	O4'-C1'-N9	7.88	114.51	108.20
38	4	113	U	C4-C5-C6	7.88	124.43	119.70
36	1	1134	G	O5'-P-OP2	-7.88	98.61	105.70
36	1	2827	U	N1-C2-N3	7.87	119.62	114.90
1	6	543	C	C6-N1-C2	-7.86	117.15	120.30
36	5	2531	C	C2-N1-C1'	7.86	127.45	118.80
1	2	1773	C	N3-C4-N4	7.86	123.50	118.00
1	2	75	U	N1-C2-O2	7.86	128.30	122.80
36	1	116	A	O4'-C1'-N9	7.86	114.49	108.20
36	1	1201	C	O5'-P-OP1	-7.86	98.63	105.70
36	5	1004	U	N1-C2-O2	7.85	128.30	122.80
36	1	3277	U	N3-C2-O2	-7.85	116.71	122.20
36	1	2241	U	O5'-P-OP1	-7.84	98.64	105.70
36	1	770	G	O4'-C1'-N9	7.84	114.47	108.20
1	6	337	G	C5-C6-O6	-7.84	123.89	128.60
1	2	1654	G	C5-C6-O6	-7.84	123.90	128.60
36	1	1480	G	O4'-C1'-N9	7.83	114.47	108.20
36	5	1513	G	N3-C4-C5	-7.83	124.68	128.60
36	5	2142	A	C6-N1-C2	-7.82	113.91	118.60
36	5	3245	A	C6-C5-N7	-7.82	126.82	132.30
36	1	2758	A	N1-C2-N3	-7.82	125.39	129.30
36	5	2919	A	N1-C6-N6	-7.82	113.91	118.60
36	1	609	G	C5-C6-O6	-7.81	123.91	128.60
36	1	1111	U	O5'-P-OP1	-7.81	98.67	105.70
36	1	3181	C	N1-C2-N3	7.81	124.67	119.20
36	1	612	U	C2-N3-C4	-7.81	122.31	127.00
36	1	3362	A	N1-C2-N3	7.81	133.20	129.30
1	2	145	A	C8-N9-C4	-7.80	102.68	105.80
36	1	1607	U	P-O3'-C3'	7.80	129.06	119.70
36	1	2802	A	C2-N3-C4	7.80	114.50	110.60
36	5	2278	C	C4-C5-C6	-7.80	113.50	117.40
36	1	806	A	C8-N9-C4	7.80	108.92	105.80
36	1	2593	A	O5'-P-OP2	-7.80	98.68	105.70
36	1	609	G	O5'-P-OP2	-7.79	98.69	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2772	C	C6-N1-C1'	-7.79	111.45	120.80
1	6	448	C	O5'-P-OP2	-7.79	98.69	105.70
36	1	1166	G	N3-C2-N2	7.79	125.35	119.90
36	1	2886	U	C5-C4-O4	-7.79	121.23	125.90
36	5	1116	G	N1-C6-O6	-7.79	115.23	119.90
36	1	1419	A	O5'-P-OP1	7.78	120.04	110.70
36	5	2719	U	C2-N1-C1'	-7.78	108.36	117.70
36	1	905	U	N1-C2-O2	-7.78	117.36	122.80
1	2	1291	G	N3-C4-C5	7.78	132.49	128.60
64	n8	21	ARG	NE-CZ-NH2	-7.78	116.41	120.30
36	1	1389	G	C4-C5-N7	7.78	113.91	110.80
36	5	189	G	N1-C6-O6	-7.78	115.23	119.90
36	5	1064	A	N9-C4-C5	-7.77	102.69	105.80
36	1	420	G	C8-N9-C4	7.77	109.51	106.40
1	6	1514	U	C5-C4-O4	7.77	130.56	125.90
36	5	2870	C	C2-N1-C1'	-7.77	110.25	118.80
1	2	453	U	C2-N1-C1'	7.77	127.02	117.70
36	5	1513	G	C5-C6-O6	7.77	133.26	128.60
36	1	2768	U	O5'-P-OP2	-7.76	98.71	105.70
36	5	1304	A	O5'-P-OP1	-7.76	98.72	105.70
36	5	1390	A	N9-C4-C5	7.76	108.91	105.80
36	5	1434	G	O5'-P-OP2	-7.76	98.72	105.70
36	1	407	A	N1-C2-N3	-7.75	125.42	129.30
36	1	2134	G	N1-C6-O6	-7.75	115.25	119.90
36	5	1133	A	N1-C6-N6	-7.75	113.95	118.60
36	1	2726	C	N1-C2-N3	7.75	124.62	119.20
36	1	2357	A	O5'-P-OP2	-7.75	98.73	105.70
36	5	1402	C	N3-C2-O2	-7.74	116.48	121.90
36	1	1114	U	C6-N1-C2	7.74	125.64	121.00
36	1	2403	G	N3-C4-N9	7.74	130.64	126.00
36	5	1838	G	OP1-P-O3'	7.74	122.23	105.20
36	5	2341	A	C8-N9-C4	7.73	108.89	105.80
36	1	895	A	C2-N3-C4	-7.73	106.74	110.60
36	1	521	A	N1-C6-N6	7.72	123.23	118.60
36	1	217	U	OP1-P-O3'	7.71	122.17	105.20
36	1	859	G	N3-C2-N2	7.71	125.30	119.90
36	1	3143	C	C6-N1-C2	7.71	123.38	120.30
36	5	2964	G	C5-C6-N1	7.71	115.35	111.50
36	5	3185	U	O5'-P-OP2	-7.71	98.76	105.70
1	6	609	U	C5-C4-O4	7.71	130.52	125.90
36	5	1001	G	O5'-P-OP1	-7.70	98.77	105.70
36	5	1445	U	C5-C4-O4	-7.70	121.28	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3107	U	O5'-P-OP2	-7.70	98.77	105.70
36	5	2385	G	C4-N9-C1'	-7.70	116.49	126.50
36	5	2572	C	C2-N1-C1'	7.70	127.27	118.80
36	1	1082	U	C5-C6-N1	7.69	126.55	122.70
36	5	3192	U	O5'-P-OP1	-7.69	98.78	105.70
36	5	2883	U	N3-C2-O2	-7.69	116.81	122.20
38	8	38	U	C5-C6-N1	-7.69	118.85	122.70
36	5	2113	A	C8-N9-C4	7.69	108.88	105.80
36	1	504	A	N7-C8-N9	-7.68	109.96	113.80
36	5	2719	U	N1-C2-O2	-7.68	117.43	122.80
36	5	2993	G	N9-C4-C5	-7.68	102.33	105.40
36	1	2816	G	O4'-C1'-N9	7.68	114.34	108.20
36	5	3101	G	N1-C6-O6	-7.68	115.29	119.90
1	2	1282	U	N3-C2-O2	-7.67	116.83	122.20
36	1	835	G	O4'-C1'-N9	7.67	114.34	108.20
36	1	776	U	C5-C4-O4	7.67	130.50	125.90
36	5	1876	U	C5-C6-N1	7.67	126.54	122.70
36	1	2861	U	O5'-P-OP1	-7.67	98.80	105.70
36	5	1374	G	C8-N9-C4	7.67	109.47	106.40
1	6	387	A	N1-C6-N6	-7.67	114.00	118.60
36	1	797	U	C2-N3-C4	-7.67	122.40	127.00
36	5	437	G	N9-C4-C5	7.67	108.47	105.40
36	5	3197	G	N3-C4-N9	-7.67	121.40	126.00
36	1	907	G	O4'-C1'-N9	7.66	114.33	108.20
36	5	2694	A	O5'-P-OP2	-7.66	98.80	105.70
36	1	3306	U	C2-N3-C4	-7.66	122.40	127.00
36	1	716	A	O5'-P-OP1	-7.66	98.81	105.70
36	1	2873	U	N3-C2-O2	-7.66	116.84	122.20
36	1	2602	G	O5'-P-OP2	-7.65	98.81	105.70
1	2	1745	G	O5'-P-OP2	-7.65	98.81	105.70
36	1	1495	U	C2-N3-C4	-7.65	122.41	127.00
36	1	2378	C	N3-C4-C5	-7.65	118.84	121.90
36	1	1496	C	C5-C6-N1	7.65	124.82	121.00
36	1	3209	A	N9-C4-C5	-7.64	102.74	105.80
36	5	1859	A	O5'-P-OP2	-7.64	98.82	105.70
36	1	339	C	N3-C2-O2	-7.64	116.55	121.90
36	1	1170	A	C5-N7-C8	7.64	107.72	103.90
36	1	637	C	N1-C2-N3	7.64	124.55	119.20
36	1	1130	A	C2-N3-C4	7.63	114.42	110.60
36	1	2645	G	N3-C2-N2	-7.63	114.56	119.90
36	1	3022	G	O4'-C1'-N9	7.63	114.31	108.20
36	5	931	C	C2-N3-C4	-7.63	116.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2393	G	N1-C6-O6	7.63	124.48	119.90
36	5	2635	A	N9-C4-C5	7.63	108.85	105.80
36	1	2403	G	C8-N9-C4	-7.62	103.35	106.40
36	1	304	G	N1-C2-N2	7.62	123.05	116.20
1	2	1486	G	N7-C8-N9	7.61	116.91	113.10
36	5	2968	G	C5-N7-C8	7.61	108.11	104.30
1	6	194	U	C2-N1-C1'	7.61	126.83	117.70
36	5	3259	U	C5-C6-N1	7.61	126.50	122.70
36	1	1049	C	O5'-P-OP2	-7.60	98.86	105.70
36	1	2914	G	O5'-P-OP2	-7.60	98.86	105.70
36	1	3181	C	C5-C4-N4	7.60	125.52	120.20
36	1	2983	C	N3-C4-N4	-7.60	112.68	118.00
36	1	2790	A	O5'-P-OP2	-7.60	98.86	105.70
36	5	580	C	C6-N1-C2	-7.60	117.26	120.30
36	5	1513	G	N7-C8-N9	7.60	116.90	113.10
36	5	2993	G	C4-C5-N7	7.60	113.84	110.80
36	1	646	A	O5'-P-OP2	-7.59	98.86	105.70
36	1	967	A	C4-C5-N7	-7.59	106.90	110.70
36	1	2954	U	C6-N1-C2	7.59	125.56	121.00
1	2	639	U	N1-C2-O2	7.59	128.12	122.80
36	5	3362	A	O4'-C1'-N9	7.59	114.28	108.20
36	5	2211	U	N1-C2-N3	7.59	119.45	114.90
36	5	2875	U	O5'-P-OP2	-7.59	98.87	105.70
36	1	2884	C	C6-N1-C2	7.58	123.33	120.30
36	5	2524	A	O4'-C1'-N9	7.58	114.27	108.20
1	2	1600	A	C2-N3-C4	-7.58	106.81	110.60
1	2	1486	G	C5-N7-C8	-7.58	100.51	104.30
36	5	2870	C	C6-N1-C1'	7.58	129.89	120.80
36	5	1665	C	N3-C4-N4	-7.57	112.70	118.00
36	5	1493	G	O4'-C1'-N9	7.57	114.25	108.20
36	1	3362	A	O4'-C1'-N9	7.56	114.25	108.20
36	5	2975	U	N3-C4-C5	7.56	119.14	114.60
36	1	2978	U	O4'-C1'-N1	7.56	114.25	108.20
1	6	163	G	C5-N7-C8	-7.56	100.52	104.30
36	1	1308	A	N7-C8-N9	7.56	117.58	113.80
36	1	360	G	C5-C6-O6	-7.55	124.07	128.60
1	2	99	C	O5'-P-OP2	-7.55	98.91	105.70
36	1	353	G	C8-N9-C4	-7.55	103.38	106.40
36	5	2290	C	N3-C4-C5	7.55	124.92	121.90
36	5	2728	G	O4'-C1'-N9	7.55	114.24	108.20
36	1	2281	A	C2-N3-C4	-7.55	106.83	110.60
36	1	967	A	C5-C6-N6	7.54	129.73	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2827	U	C6-N1-C1'	7.54	131.76	121.20
1	6	1280	C	N3-C4-C5	-7.54	118.88	121.90
36	5	1202	A	O5'-P-OP1	-7.54	98.92	105.70
36	5	1305	U	C5-C4-O4	-7.54	121.38	125.90
1	2	453	U	N3-C2-O2	-7.53	116.93	122.20
36	1	1327	C	N3-C4-C5	7.53	124.91	121.90
36	1	2732	G	N3-C2-N2	7.53	125.17	119.90
36	1	3055	U	O5'-P-OP2	-7.53	98.92	105.70
36	5	1064	A	C5-C6-N6	-7.53	117.67	123.70
36	1	2983	C	C5-C4-N4	7.53	125.47	120.20
38	4	53	A	C2-N3-C4	7.53	114.36	110.60
36	5	2813	A	N9-C4-C5	7.53	108.81	105.80
36	5	971	G	C4-C5-N7	-7.52	107.79	110.80
1	2	543	C	N3-C2-O2	-7.52	116.64	121.90
36	5	2287	C	C6-N1-C2	-7.51	117.29	120.30
1	2	1761	U	C6-N1-C2	-7.51	116.49	121.00
36	5	2395	G	N7-C8-N9	-7.51	109.34	113.10
36	5	2915	U	C2-N3-C4	-7.51	122.49	127.00
68	o2	43	ARG	NE-CZ-NH1	7.51	124.06	120.30
36	5	201	A	OP1-P-OP2	-7.51	108.34	119.60
1	2	581	U	C2-N1-C1'	7.51	126.71	117.70
1	6	1120	U	N3-C4-O4	-7.51	114.15	119.40
1	6	163	G	C8-N9-C1'	7.50	136.75	127.00
36	5	417	A	N1-C6-N6	-7.50	114.10	118.60
36	1	3079	U	O5'-P-OP1	-7.50	98.95	105.70
36	1	2176	U	N1-C2-O2	7.50	128.05	122.80
1	2	1096	C	N1-C2-O2	7.50	123.40	118.90
36	1	2631	U	N3-C4-C5	7.50	119.10	114.60
36	1	2714	G	C5-N7-C8	-7.50	100.55	104.30
36	5	2372	A	C8-N9-C4	-7.50	102.80	105.80
36	5	3245	A	N1-C6-N6	7.50	123.10	118.60
1	6	358	U	O5'-P-OP1	-7.49	98.96	105.70
36	5	931	C	N3-C4-C5	7.49	124.90	121.90
36	1	971	G	N7-C8-N9	-7.49	109.36	113.10
36	1	2130	G	C5-C6-O6	7.49	133.09	128.60
36	1	938	C	N3-C4-C5	7.49	124.89	121.90
36	1	664	U	C2-N3-C4	-7.48	122.52	127.00
52	M6	78	ARG	NE-CZ-NH2	-7.47	116.56	120.30
36	1	46	U	N3-C2-O2	-7.47	116.97	122.20
36	1	645	A	C5-C6-N1	7.47	121.44	117.70
36	1	1103	A	C2-N3-C4	7.47	114.33	110.60
36	1	928	C	C6-N1-C2	-7.47	117.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1114	U	N3-C4-C5	7.47	119.08	114.60
36	1	99	A	O5'-P-OP2	-7.46	98.98	105.70
1	2	554	C	N3-C4-C5	-7.46	118.92	121.90
36	5	2426	U	N1-C2-O2	7.46	128.02	122.80
40	l3	4	ARG	NE-CZ-NH1	7.46	124.03	120.30
36	1	2138	A	N1-C2-N3	7.46	133.03	129.30
36	1	2178	A	N1-C6-N6	-7.45	114.13	118.60
36	5	2639	G	C5-C6-O6	-7.45	124.13	128.60
36	1	2651	G	N3-C4-C5	7.45	132.32	128.60
36	5	73	C	C6-N1-C2	7.45	123.28	120.30
36	5	1395	G	N1-C6-O6	7.45	124.37	119.90
36	5	817	A	O5'-P-OP1	-7.45	99.00	105.70
36	5	908	G	C6-C5-N7	-7.44	125.93	130.40
36	1	999	G	OP2-P-O3'	7.44	121.57	105.20
36	5	1426	C	N3-C4-C5	7.44	124.88	121.90
1	2	830	U	N3-C2-O2	-7.44	116.99	122.20
52	m6	69	GLY	N-CA-C	-7.43	94.51	113.10
36	1	935	U	C5-C6-N1	-7.43	118.98	122.70
36	5	3052	G	C4-C5-N7	-7.43	107.83	110.80
36	5	612	U	O5'-P-OP1	-7.43	99.01	105.70
36	5	2621	G	N1-C6-O6	7.43	124.36	119.90
36	1	1342	C	N3-C4-C5	7.42	124.87	121.90
36	5	641	C	N1-C2-O2	-7.42	114.44	118.90
36	1	1156	C	N3-C2-O2	-7.42	116.70	121.90
1	6	308	C	N3-C4-N4	-7.41	112.81	118.00
36	5	2799	A	O5'-P-OP2	-7.41	99.03	105.70
36	1	2632	G	N1-C6-O6	-7.41	115.45	119.90
36	5	929	A	C8-N9-C4	7.41	108.76	105.80
36	5	2718	U	O5'-P-OP2	-7.41	99.03	105.70
1	6	65	A	N1-C6-N6	7.41	123.04	118.60
36	1	2617	U	C2-N3-C4	-7.40	122.56	127.00
40	l3	19	ARG	NE-CZ-NH1	7.40	124.00	120.30
36	1	417	A	O5'-P-OP2	-7.40	99.04	105.70
36	5	1128	U	O5'-P-OP2	-7.40	99.04	105.70
36	1	2940	A	C5-N7-C8	7.40	107.60	103.90
36	1	103	G	C5-C6-O6	7.40	133.04	128.60
1	6	1036	A	N1-C6-N6	-7.40	114.16	118.60
1	2	1200	G	C6-C5-N7	-7.40	125.96	130.40
36	5	797	U	C5-C4-O4	-7.39	121.46	125.90
36	5	2404	A	N9-C1'-C2'	-7.39	103.87	112.00
36	1	2149	A	O5'-P-OP2	7.38	119.56	110.70
36	5	348	A	C8-N9-C4	7.38	108.75	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	7	121	U	N3-C2-O2	-7.38	117.03	122.20
36	1	94	G	O5'-P-OP1	-7.38	99.06	105.70
36	1	2988	C	C5-C4-N4	7.38	125.36	120.20
42	l5	35	ARG	NE-CZ-NH1	-7.38	116.61	120.30
36	5	1149	G	O5'-P-OP2	-7.38	99.06	105.70
36	1	3181	C	N3-C4-N4	-7.38	112.84	118.00
36	5	1410	U	O5'-P-OP2	-7.37	99.06	105.70
36	5	2948	C	N3-C4-N4	-7.37	112.84	118.00
36	5	2255	A	O5'-P-OP1	-7.37	99.07	105.70
36	5	2765	C	C5-C6-N1	7.37	124.68	121.00
36	1	2633	U	N3-C2-O2	-7.36	117.05	122.20
36	1	968	G	N1-C6-O6	-7.36	115.48	119.90
1	6	337	G	N3-C4-N9	7.36	130.42	126.00
36	1	33	G	O5'-P-OP2	-7.36	99.08	105.70
38	4	125	U	N1-C2-O2	7.36	127.95	122.80
36	1	359	U	C2-N3-C4	-7.36	122.59	127.00
36	1	859	G	O5'-P-OP1	-7.36	99.08	105.70
36	5	671	U	N1-C2-O2	-7.36	117.65	122.80
1	6	557	G	N1-C6-O6	-7.35	115.49	119.90
36	1	960	U	N3-C4-C5	7.35	119.01	114.60
36	1	2642	A	C8-N9-C4	7.35	108.74	105.80
36	5	2405	C	O5'-P-OP1	-7.35	99.09	105.70
36	1	25	U	C5-C4-O4	-7.35	121.49	125.90
36	5	922	U	N3-C4-O4	-7.35	114.26	119.40
36	1	2870	C	C2-N1-C1'	-7.34	110.72	118.80
36	1	1846	C	N1-C2-O2	-7.34	114.50	118.90
36	1	2411	U	N3-C4-O4	-7.34	114.26	119.40
1	6	1549	C	C6-N1-C2	-7.34	117.36	120.30
36	1	765	C	N3-C2-O2	-7.34	116.77	121.90
36	1	2617	U	C4-C5-C6	7.34	124.10	119.70
36	5	2294	U	N1-C2-N3	7.34	119.30	114.90
36	5	3106	A	N1-C2-N3	-7.34	125.63	129.30
36	1	1890	U	C5-C6-N1	-7.33	119.03	122.70
36	1	2836	C	C6-N1-C2	-7.33	117.37	120.30
36	5	1284	C	C6-N1-C2	-7.33	117.37	120.30
1	2	1454	G	N1-C6-O6	-7.32	115.51	119.90
36	5	817	A	C8-N9-C4	-7.32	102.87	105.80
36	1	1495	U	N3-C2-O2	-7.32	117.08	122.20
36	1	2278	C	C4-C5-C6	-7.32	113.74	117.40
36	5	2290	C	C2-N3-C4	-7.32	116.24	119.90
36	5	3046	A	N1-C2-N3	-7.32	125.64	129.30
40	l3	232	ARG	NE-CZ-NH2	-7.32	116.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	93	C	N1-C2-O2	-7.31	114.51	118.90
36	1	2651	G	C8-N9-C4	7.31	109.32	106.40
36	5	908	G	C4-N9-C1'	7.31	136.00	126.50
36	1	806	A	N9-C4-C5	-7.31	102.88	105.80
36	1	1060	U	C5-C6-N1	-7.30	119.05	122.70
36	1	1381	A	O5'-P-OP1	-7.30	99.13	105.70
36	1	2618	G	C6-N1-C2	-7.30	120.72	125.10
36	5	3142	A	N9-C4-C5	-7.30	102.88	105.80
36	5	931	C	C5-C6-N1	-7.30	117.35	121.00
36	5	2231	C	C2-N1-C1'	7.30	126.83	118.80
36	1	2938	G	OP1-P-OP2	7.30	130.54	119.60
36	5	1175	C	C6-N1-C2	-7.29	117.38	120.30
36	1	2418	G	OP1-P-O3'	7.29	121.25	105.20
36	5	341	G	C5-C6-O6	-7.29	124.22	128.60
36	1	664	U	C5-C6-N1	-7.29	119.05	122.70
36	5	1879	A	OP1-P-OP2	-7.29	108.66	119.60
36	5	3123	A	C8-N9-C4	7.29	108.72	105.80
1	2	1039	A	O4'-C1'-N9	7.29	114.03	108.20
36	5	702	C	C6-N1-C2	-7.29	117.39	120.30
36	5	856	G	C5-C6-O6	-7.29	124.23	128.60
36	1	2779	A	O5'-P-OP2	-7.28	99.14	105.70
36	1	2865	U	N3-C4-C5	7.28	118.97	114.60
38	8	25	G	N3-C2-N2	7.28	125.00	119.90
1	2	554	C	C2-N3-C4	7.28	123.54	119.90
36	1	2194	G	O5'-P-OP2	-7.28	99.15	105.70
36	1	2302	G	N1-C6-O6	-7.28	115.53	119.90
36	5	3127	A	N1-C6-N6	-7.28	114.23	118.60
36	1	1196	C	N3-C2-O2	7.28	127.00	121.90
36	1	1308	A	C8-N9-C4	-7.28	102.89	105.80
36	5	1331	U	N3-C2-O2	7.28	127.30	122.20
36	5	341	G	C4-C5-N7	7.28	113.71	110.80
36	5	909	G	C2-N3-C4	7.28	115.54	111.90
36	5	968	G	N3-C2-N2	7.27	124.99	119.90
36	1	766	U	O5'-P-OP1	-7.27	99.16	105.70
36	1	3029	A	C8-N9-C4	-7.27	102.89	105.80
1	6	973	A	O5'-P-OP2	-7.27	99.16	105.70
36	5	914	A	C2-N3-C4	-7.27	106.96	110.60
36	5	3218	A	C2-N3-C4	-7.27	106.96	110.60
36	1	797	U	C5-C6-N1	-7.27	119.06	122.70
36	1	2414	G	N3-C2-N2	-7.27	114.81	119.90
36	1	1160	C	O5'-P-OP1	-7.27	99.16	105.70
36	5	1496	C	OP1-P-OP2	-7.27	108.70	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	402	C	O5'-P-OP1	-7.27	99.16	105.70
36	1	53	G	O5'-P-OP2	-7.27	99.16	105.70
36	5	3197	G	N3-C4-C5	7.27	132.23	128.60
36	1	2811	A	C6-N1-C2	-7.26	114.24	118.60
36	1	2572	C	N3-C2-O2	-7.26	116.82	121.90
36	5	304	G	C2-N3-C4	7.25	115.53	111.90
36	5	922	U	C5-C4-O4	7.25	130.25	125.90
36	1	2950	G	C4-C5-N7	7.25	113.70	110.80
38	4	51	G	C5-C6-O6	-7.25	124.25	128.60
36	5	1314	C	C2-N3-C4	-7.25	116.28	119.90
1	2	1012	U	C2-N3-C4	7.24	131.35	127.00
36	5	3362	A	C5-N7-C8	-7.24	100.28	103.90
36	1	718	G	C5-N7-C8	-7.24	100.68	104.30
1	2	1535	U	C2-N1-C1'	7.24	126.39	117.70
36	5	2300	G	N1-C6-O6	-7.24	115.56	119.90
36	5	277	G	N1-C6-O6	-7.24	115.56	119.90
52	m6	94	ARG	NE-CZ-NH1	-7.23	116.68	120.30
36	1	2411	U	O5'-P-OP1	-7.23	99.19	105.70
36	1	3207	U	N1-C2-O2	-7.23	117.74	122.80
36	5	1421	G	O5'-P-OP2	-7.23	99.19	105.70
36	1	2411	U	N3-C4-C5	7.23	118.94	114.60
47	M0	57	LEU	CA-CB-CG	7.23	131.92	115.30
1	6	1537	C	C6-N1-C1'	7.23	129.47	120.80
36	5	3197	G	N3-C2-N2	-7.22	114.84	119.90
36	1	1556	C	C2-N1-C1'	7.22	126.74	118.80
1	6	1473	U	C6-N1-C2	-7.22	116.67	121.00
1	6	453	U	C2-N1-C1'	7.22	126.36	117.70
36	1	959	C	C5-C4-N4	-7.21	115.15	120.20
36	5	2899	C	N1-C2-N3	7.21	124.25	119.20
36	5	3020	U	C5-C4-O4	-7.21	121.57	125.90
36	5	2572	C	N3-C2-O2	-7.21	116.85	121.90
36	1	196	G	O5'-P-OP2	-7.21	99.21	105.70
1	2	1339	C	C6-N1-C2	-7.21	117.42	120.30
36	5	1931	U	C2-N1-C1'	-7.21	109.05	117.70
36	5	426	G	N7-C8-N9	-7.20	109.50	113.10
36	1	2719	U	N1-C2-O2	-7.20	117.76	122.80
36	1	1120	A	N1-C6-N6	-7.20	114.28	118.60
36	1	2388	U	N1-C2-O2	-7.20	117.76	122.80
34	SR	161	LYS	C-N-CA	7.20	139.69	121.70
36	1	1168	U	N1-C2-O2	7.20	127.84	122.80
36	5	2382	G	C5-C6-O6	7.20	132.92	128.60
36	1	345	G	C5-C6-N1	7.19	115.10	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1396	C	C6-N1-C2	7.19	123.18	120.30
36	5	1489	A	N1-C6-N6	7.19	122.91	118.60
36	5	2988	C	N3-C2-O2	-7.19	116.87	121.90
36	5	3047	U	N3-C4-O4	-7.19	114.37	119.40
36	1	608	A	C5-C6-N6	-7.18	117.95	123.70
36	1	401	U	C5-C4-O4	-7.18	121.59	125.90
36	1	1313	G	O5'-P-OP2	-7.18	99.24	105.70
36	5	2968	G	N7-C8-N9	-7.18	109.51	113.10
1	6	542	A	O5'-P-OP1	-7.17	99.24	105.70
1	2	287	G	O4'-C1'-N9	7.17	113.94	108.20
36	5	339	C	C6-N1-C1'	7.17	129.41	120.80
36	1	2363	A	N1-C6-N6	-7.17	114.30	118.60
36	5	2142	A	OP1-P-OP2	-7.17	108.85	119.60
36	5	2223	A	O5'-P-OP1	-7.17	99.25	105.70
36	5	1858	A	C8-N9-C4	-7.17	102.93	105.80
36	5	3006	A	C8-N9-C4	-7.17	102.93	105.80
36	1	817	A	O5'-P-OP2	7.16	119.30	110.70
36	1	2864	A	C8-N9-C4	-7.16	102.94	105.80
59	N3	87	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	6	755	A	O4'-C1'-N9	7.16	113.93	108.20
36	5	838	G	C5-C6-O6	7.16	132.90	128.60
36	1	1715	A	O4'-C1'-N9	-7.16	102.47	108.20
36	5	869	G	O5'-P-OP2	-7.16	99.26	105.70
10	s8	29	LEU	CA-CB-CG	7.15	131.75	115.30
36	5	3214	U	N3-C4-O4	-7.15	114.39	119.40
36	1	847	A	N1-C6-N6	7.15	122.89	118.60
36	5	1380	G	O5'-P-OP2	-7.15	99.26	105.70
36	5	671	U	N3-C2-O2	7.15	127.20	122.20
36	5	2356	A	C2-N3-C4	-7.15	107.03	110.60
36	5	3047	U	N3-C4-C5	7.15	118.89	114.60
36	1	3119	U	N3-C4-O4	-7.14	114.40	119.40
36	5	3052	G	C5-N7-C8	7.14	107.87	104.30
36	5	3308	C	C6-N1-C2	-7.14	117.44	120.30
36	1	439	C	C6-N1-C1'	-7.14	112.23	120.80
36	1	215	G	C8-N9-C4	-7.14	103.55	106.40
38	4	30	C	N3-C4-N4	-7.14	113.00	118.00
36	5	1307	G	P-O3'-C3'	7.14	128.26	119.70
36	1	2376	G	N3-C4-N9	7.13	130.28	126.00
36	5	2928	C	C4-C5-C6	7.13	120.97	117.40
36	5	3050	U	N1-C2-O2	7.13	127.79	122.80
36	5	2808	A	N9-C4-C5	-7.13	102.95	105.80
36	1	2827	U	C5-C4-O4	7.13	130.18	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1509	C	N1-C2-O2	7.13	123.18	118.90
36	5	92	G	C5-C6-N1	7.13	115.06	111.50
36	1	2697	A	N1-C6-N6	-7.13	114.32	118.60
36	1	3121	U	OP1-P-O3'	7.13	120.88	105.20
36	1	2408	U	O5'-P-OP1	-7.12	99.29	105.70
36	5	2278	C	N3-C4-N4	-7.12	113.02	118.00
36	5	307	A	N1-C6-N6	-7.12	114.33	118.60
36	5	2333	C	N1-C2-O2	-7.12	114.63	118.90
36	1	859	G	N3-C4-N9	7.12	130.27	126.00
36	1	721	G	C5-C6-O6	-7.12	124.33	128.60
36	5	1799	A	N1-C2-N3	-7.12	125.74	129.30
38	4	32	C	N1-C2-O2	-7.11	114.63	118.90
62	N6	13	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	2	137	U	N3-C2-O2	-7.11	117.22	122.20
36	1	2983	C	C4-C5-C6	7.11	120.95	117.40
36	5	2796	G	C5-N7-C8	-7.11	100.75	104.30
36	1	2149	A	C5-C6-N1	-7.11	114.15	117.70
36	5	1168	U	N3-C4-C5	7.11	118.86	114.60
36	1	937	G	N7-C8-N9	-7.10	109.55	113.10
36	1	1297	C	O5'-P-OP1	-7.10	99.31	105.70
36	5	934	G	C5-C6-O6	-7.10	124.34	128.60
36	1	3275	U	C5-C6-N1	7.10	126.25	122.70
36	1	643	U	N3-C2-O2	7.10	127.17	122.20
36	1	3344	A	C8-N9-C4	-7.10	102.96	105.80
1	6	868	G	C5-C6-O6	-7.10	124.34	128.60
36	5	277	G	C5-C6-O6	7.10	132.86	128.60
36	5	1129	A	C2-N3-C4	7.09	114.15	110.60
36	1	634	C	N3-C2-O2	-7.09	116.94	121.90
36	5	1513	G	N9-C4-C5	7.09	108.23	105.40
1	6	1614	A	C5-N7-C8	-7.08	100.36	103.90
36	5	339	C	N3-C4-N4	-7.08	113.04	118.00
37	7	28	C	N1-C2-O2	-7.08	114.65	118.90
1	6	1514	U	N3-C4-O4	-7.08	114.44	119.40
36	5	891	G	C5-C6-O6	7.08	132.85	128.60
38	8	110	C	C6-N1-C2	-7.08	117.47	120.30
36	1	282	G	C8-N9-C4	-7.08	103.57	106.40
36	1	1409	G	N1-C6-O6	-7.08	115.66	119.90
1	6	987	G	C5-C6-O6	-7.08	124.36	128.60
36	5	2190	U	N1-C2-N3	7.08	119.14	114.90
38	8	6	U	O5'-P-OP2	-7.08	99.33	105.70
1	6	858	G	C4-C5-N7	7.07	113.63	110.80
36	5	2743	A	C5-N7-C8	7.07	107.44	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3259	U	C6-N1-C2	-7.07	116.76	121.00
38	8	51	G	C5-C6-O6	-7.07	124.36	128.60
36	1	304	G	C2-N3-C4	7.07	115.43	111.90
36	1	2400	G	C5-C6-O6	-7.07	124.36	128.60
1	2	1096	C	C6-N1-C1'	-7.07	112.32	120.80
36	5	2412	G	C5-C6-O6	7.07	132.84	128.60
1	6	308	C	N1-C2-N3	7.07	124.15	119.20
36	1	895	A	N3-C4-C5	7.06	131.75	126.80
15	C3	22	ALA	C-N-CD	-7.06	105.06	120.60
43	L6	31	ARG	NE-CZ-NH2	-7.06	116.77	120.30
36	1	3373	U	C6-N1-C2	7.06	125.24	121.00
1	6	609	U	N3-C4-O4	-7.06	114.46	119.40
1	6	1082	C	N3-C2-O2	-7.06	116.96	121.90
36	5	2725	U	C5-C4-O4	-7.06	121.66	125.90
64	n8	73	LEU	CA-CB-CG	7.06	131.54	115.30
36	1	2885	C	C5-C6-N1	-7.06	117.47	121.00
36	5	3374	U	C6-N1-C2	7.06	125.23	121.00
1	2	1761	U	P-O3'-C3'	7.05	128.16	119.70
44	l7	229	PHE	CB-CG-CD1	7.05	125.74	120.80
1	6	315	A	C8-N9-C4	-7.05	102.98	105.80
1	6	993	A	O5'-P-OP2	-7.05	99.36	105.70
36	5	2872	A	N1-C6-N6	-7.05	114.37	118.60
36	5	2901	G	C5-C6-O6	-7.05	124.37	128.60
36	1	2808	A	C6-C5-N7	-7.04	127.37	132.30
36	5	2181	C	N1-C2-O2	-7.04	114.67	118.90
36	5	967	A	N9-C4-C5	7.04	108.62	105.80
36	5	2635	A	N1-C6-N6	-7.04	114.38	118.60
1	2	1611	A	C2-N3-C4	-7.04	107.08	110.60
36	5	73	C	N3-C4-C5	7.04	124.72	121.90
36	5	2794	G	C5-C6-O6	-7.04	124.38	128.60
1	6	321	C	N3-C2-O2	-7.03	116.98	121.90
36	5	44	U	N1-C2-O2	-7.03	117.88	122.80
36	1	708	G	O5'-P-OP1	-7.03	99.37	105.70
36	1	2983	C	N1-C2-N3	7.03	124.12	119.20
1	6	542	A	C4-N9-C1'	7.03	138.95	126.30
36	5	2160	G	N3-C2-N2	7.03	124.82	119.90
36	5	2369	G	N3-C4-N9	7.03	130.22	126.00
36	1	2242	A	C8-N9-C4	-7.03	102.99	105.80
1	6	1605	G	N1-C6-O6	-7.03	115.68	119.90
39	L2	191	LEU	CA-CB-CG	-7.02	99.14	115.30
1	2	1596	C	C6-N1-C2	-7.02	117.49	120.30
36	1	1902	G	N9-C4-C5	-7.02	102.59	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	875	G	N1-C6-O6	-7.02	115.69	119.90
36	5	1389	G	C5-C6-O6	-7.02	124.39	128.60
36	1	99	A	C5'-C4'-O4'	7.02	117.52	109.10
36	1	1142	G	C5-C6-O6	-7.01	124.39	128.60
36	1	1405	U	C6-N1-C2	7.01	125.21	121.00
36	1	1433	A	N1-C2-N3	-7.01	125.79	129.30
36	1	3178	A	N1-C6-N6	7.01	122.81	118.60
1	2	542	A	O4'-C1'-N9	7.01	113.81	108.20
36	1	2786	G	N9-C4-C5	7.01	108.20	105.40
36	1	777	U	O5'-P-OP2	-7.01	99.39	105.70
1	2	75	U	C2-N1-C1'	7.01	126.11	117.70
36	1	325	A	C5-C6-N1	7.01	121.20	117.70
36	1	2249	G	C5-C6-O6	7.00	132.80	128.60
36	1	3309	G	C6-C5-N7	-7.00	126.20	130.40
36	1	630	A	C2-N3-C4	7.00	114.10	110.60
1	6	400	A	N1-C6-N6	7.00	122.80	118.60
36	5	2299	A	C2-N3-C4	7.00	114.10	110.60
1	2	1654	G	C5-C6-N1	7.00	115.00	111.50
36	1	2957	G	O5'-P-OP2	7.00	119.10	110.70
1	2	959	U	N3-C2-O2	-7.00	117.30	122.20
1	6	1773	C	C6-N1-C2	-7.00	117.50	120.30
36	5	2211	U	C4-C5-C6	7.00	123.90	119.70
36	5	216	G	C5-C6-O6	-6.99	124.40	128.60
36	5	2375	G	C5-C6-O6	6.99	132.80	128.60
36	1	1364	C	N3-C4-C5	6.99	124.70	121.90
36	1	2830	G	N9-C4-C5	6.99	108.20	105.40
36	5	1152	G	C4-C5-C6	-6.99	114.61	118.80
36	5	189	G	C5-C6-O6	6.99	132.79	128.60
36	1	2368	A	N7-C8-N9	-6.98	110.31	113.80
36	5	282	G	C2'-C3'-O3'	6.98	124.87	113.70
68	O2	43	ARG	NE-CZ-NH1	6.97	123.79	120.30
36	1	329	U	C2-N1-C1'	-6.97	109.33	117.70
36	1	646	A	N7-C8-N9	6.97	117.29	113.80
36	5	1390	A	N1-C6-N6	-6.97	114.42	118.60
36	1	3055	U	C6-N1-C1'	-6.97	111.44	121.20
36	5	879	U	O5'-P-OP1	-6.97	99.43	105.70
36	5	2304	C	C6-N1-C2	-6.97	117.51	120.30
36	5	2908	G	C5-C6-O6	6.97	132.78	128.60
36	1	319	A	O5'-P-OP1	-6.96	99.43	105.70
36	5	427	C	OP2-P-O3'	6.96	120.52	105.20
36	5	1311	G	C2-N3-C4	6.96	115.38	111.90
36	5	3144	G	C8-N9-C4	-6.96	103.61	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	646	A	C8-N9-C4	-6.96	103.02	105.80
52	m6	94	ARG	NE-CZ-NH2	6.96	123.78	120.30
36	1	3318	G	N3-C4-C5	-6.96	125.12	128.60
1	6	638	U	N3-C2-O2	-6.96	117.33	122.20
36	5	1331	U	C5-C4-O4	-6.96	121.72	125.90
36	5	2142	A	O5'-P-OP2	6.96	119.05	110.70
36	5	935	U	C2-N3-C4	-6.95	122.83	127.00
36	1	3217	C	C2-N1-C1'	6.95	126.45	118.80
36	1	1170	A	N7-C8-N9	-6.95	110.33	113.80
1	6	10	G	C5-C6-O6	6.95	132.77	128.60
36	5	3047	U	C5-C6-N1	-6.95	119.23	122.70
1	2	728	U	C2-N1-C1'	6.94	126.03	117.70
36	5	2643	A	C5-N7-C8	-6.94	100.43	103.90
36	5	1064	A	C4-C5-N7	6.94	114.17	110.70
36	1	802	C	O5'-P-OP2	6.94	119.03	110.70
36	1	1200	A	O4'-C1'-N9	6.94	113.75	108.20
36	5	1481	A	P-O3'-C3'	6.94	128.03	119.70
36	5	1483	G	O4'-C1'-N9	6.94	113.75	108.20
36	1	2434	U	N3-C4-O4	-6.94	114.54	119.40
1	6	102	U	N1-C2-O2	-6.94	117.94	122.80
17	c5	36	LEU	CA-CB-CG	6.94	131.26	115.30
36	5	2287	C	C5-C6-N1	6.94	124.47	121.00
36	1	1307	G	N1-C6-O6	-6.93	115.74	119.90
1	6	1549	C	N3-C4-C5	-6.93	119.13	121.90
36	5	931	C	C6-N1-C2	6.93	123.07	120.30
36	5	2369	G	N9-C4-C5	-6.93	102.63	105.40
36	1	818	C	C6-N1-C2	-6.93	117.53	120.30
1	6	1389	C	N1-C2-O2	6.93	123.06	118.90
36	1	905	U	N1-C2-N3	6.93	119.06	114.90
36	1	959	C	N1-C2-O2	-6.92	114.75	118.90
36	1	203	G	N1-C6-O6	-6.92	115.75	119.90
1	2	795	U	N3-C2-O2	-6.92	117.36	122.20
36	1	591	G	C5-C6-O6	-6.92	124.45	128.60
36	1	1405	U	C2-N3-C4	-6.92	122.85	127.00
1	6	18	C	N3-C4-C5	-6.92	119.13	121.90
36	5	2141	U	OP2-P-O3'	6.92	120.42	105.20
36	1	643	U	N1-C2-O2	-6.92	117.96	122.80
36	1	1184	A	O5'-P-OP2	-6.92	99.48	105.70
1	6	163	G	C8-N9-C4	-6.92	103.63	106.40
36	5	2401	A	C2-N3-C4	6.92	114.06	110.60
36	1	1493	G	O5'-P-OP2	-6.92	99.48	105.70
36	5	857	G	C5-C6-O6	-6.91	124.45	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2374	C	C6-N1-C2	-6.91	117.54	120.30
37	3	86	U	C2-N3-C4	-6.91	122.86	127.00
36	5	3101	G	C5-C6-O6	6.91	132.75	128.60
37	7	40	C	N1-C2-O2	-6.91	114.76	118.90
36	1	1156	C	N1-C2-O2	6.91	123.04	118.90
38	4	73	U	N3-C4-O4	-6.91	114.57	119.40
36	1	652	G	N3-C2-N2	6.90	124.73	119.90
36	5	835	G	C5-C6-O6	-6.90	124.46	128.60
36	5	1163	A	O5'-P-OP2	-6.90	99.49	105.70
36	5	2308	C	N1-C2-O2	-6.90	114.76	118.90
36	1	782	U	N3-C4-O4	-6.90	114.57	119.40
1	2	453	U	N1-C2-O2	6.89	127.62	122.80
36	1	1496	C	C2-N1-C1'	6.89	126.38	118.80
36	5	2735	U	C5-C6-N1	6.89	126.15	122.70
36	5	590	G	C5-C6-O6	-6.89	124.47	128.60
36	5	2350	C	C2-N3-C4	-6.89	116.46	119.90
36	1	908	G	O4'-C1'-N9	-6.89	102.69	108.20
36	1	1495	U	C5-C4-O4	6.89	130.03	125.90
36	1	2725	U	C5-C6-N1	-6.88	119.26	122.70
36	1	968	G	N7-C8-N9	6.88	116.54	113.10
52	M6	110	PRO	C-N-CD	-6.88	105.47	120.60
36	5	950	G	C5-C6-O6	-6.88	124.47	128.60
36	1	33	G	N7-C8-N9	6.87	116.54	113.10
36	1	1489	A	N1-C6-N6	6.87	122.72	118.60
49	M3	35	ARG	NE-CZ-NH1	-6.87	116.86	120.30
36	1	1433	A	C2-N3-C4	6.87	114.03	110.60
36	1	2369	G	N3-C4-C5	-6.87	125.17	128.60
36	1	2134	G	N3-C2-N2	6.87	124.71	119.90
36	1	1586	G	O5'-P-OP2	-6.86	99.52	105.70
36	1	2899	C	N3-C4-N4	-6.86	113.19	118.00
76	Q0	127	LEU	CA-CB-CG	6.86	131.09	115.30
36	5	1855	U	C2-N3-C4	-6.86	122.88	127.00
36	1	359	U	C5-C6-N1	-6.86	119.27	122.70
36	5	3143	C	C6-N1-C2	6.86	123.05	120.30
1	2	1454	G	C5-C6-O6	6.86	132.72	128.60
1	6	778	G	N1-C6-O6	-6.86	115.78	119.90
12	C0	88	PRO	N-CA-CB	6.86	111.53	103.30
36	1	1832	C	N3-C2-O2	-6.86	117.10	121.90
36	1	2618	G	C2-N3-C4	6.86	115.33	111.90
36	5	2619	G	N1-C6-O6	6.86	124.01	119.90
1	2	1782	A	N9-C4-C5	6.85	108.54	105.80
36	5	770	G	O4'-C1'-N9	6.85	113.68	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	209	A	O5'-P-OP2	-6.85	99.53	105.70
36	1	1403	C	C2-N3-C4	-6.85	116.48	119.90
36	5	33	G	C5-C6-N1	6.85	114.92	111.50
36	5	3010	U	N3-C2-O2	-6.85	117.41	122.20
1	6	687	G	N9-C4-C5	6.85	108.14	105.40
36	5	3214	U	C5-C4-O4	6.85	130.01	125.90
36	1	1177	G	C5-C6-O6	-6.84	124.49	128.60
1	6	31	C	C6-N1-C2	-6.84	117.56	120.30
36	5	2376	G	N7-C8-N9	-6.84	109.68	113.10
36	1	2614	G	C5-C6-O6	6.84	132.71	128.60
36	5	878	G	C5-C6-O6	-6.84	124.50	128.60
36	5	909	G	C5-N7-C8	6.84	107.72	104.30
36	5	2113	A	C4-C5-C6	-6.84	113.58	117.00
36	5	3209	A	O4'-C1'-N9	6.84	113.67	108.20
36	1	280	U	N3-C4-O4	6.84	124.19	119.40
1	6	1796	C	C5-C6-N1	-6.84	117.58	121.00
36	5	28	C	C6-N1-C2	6.83	123.03	120.30
36	5	2726	C	N3-C4-N4	-6.83	113.22	118.00
37	7	101	G	N1-C6-O6	6.83	124.00	119.90
36	1	1425	U	C2-N3-C4	-6.83	122.90	127.00
36	5	2957	G	C8-N9-C4	6.83	109.13	106.40
36	1	890	C	C6-N1-C2	-6.83	117.57	120.30
36	1	2314	U	N1-C2-N3	-6.83	110.80	114.90
36	1	2362	C	N1-C2-O2	6.83	123.00	118.90
1	6	858	G	O4'-C1'-N9	6.83	113.66	108.20
36	5	1391	C	N1-C2-O2	-6.83	114.80	118.90
1	6	610	G	C8-N9-C1'	-6.83	118.13	127.00
36	1	2868	U	C5-C6-N1	-6.82	119.29	122.70
36	5	3050	U	N3-C4-O4	-6.82	114.62	119.40
1	2	142	G	N3-C4-C5	6.82	132.01	128.60
36	1	54	C	N3-C4-C5	6.82	124.63	121.90
1	6	144	U	C6-N1-C2	-6.82	116.91	121.00
1	2	158	U	P-O3'-C3'	6.82	127.88	119.70
36	1	324	A	C6-N1-C2	-6.82	114.51	118.60
36	1	2977	G	C5-N7-C8	6.82	107.71	104.30
36	1	272	G	N7-C8-N9	-6.82	109.69	113.10
36	1	2944	U	OP1-P-O3'	6.82	120.19	105.20
36	5	1481	A	N7-C8-N9	6.82	117.21	113.80
36	1	105	C	C2-N3-C4	-6.81	116.49	119.90
36	5	3120	C	C6-N1-C2	-6.81	117.57	120.30
1	2	1486	G	C8-N9-C4	-6.81	103.67	106.40
36	1	65	A	P-O3'-C3'	6.81	127.88	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	946	U	N1-C2-N3	6.81	118.99	114.90
36	5	987	U	O5'-P-OP1	-6.81	99.57	105.70
49	m3	47	ALA	C-N-CD	6.81	142.70	128.40
36	1	2148	U	N1-C2-O2	-6.81	118.03	122.80
36	5	1886	A	O5'-P-OP2	-6.81	99.57	105.70
1	2	142	G	N3-C4-N9	-6.81	121.92	126.00
36	1	272	G	C8-N9-C4	6.81	109.12	106.40
36	5	1605	A	O4'-C1'-N9	6.80	113.64	108.20
36	1	2393	G	C5-C6-O6	-6.80	124.52	128.60
36	1	2144	A	O4'-C1'-N9	6.80	113.64	108.20
36	5	1439	U	C2-N3-C4	-6.80	122.92	127.00
36	5	2314	U	N3-C4-O4	6.80	124.16	119.40
36	5	2633	U	N3-C4-O4	-6.80	114.64	119.40
36	5	1513	G	C2-N3-C4	6.80	115.30	111.90
36	5	1861	G	C8-N9-C4	-6.80	103.68	106.40
36	5	1469	C	C6-N1-C2	-6.79	117.58	120.30
36	1	2797	C	C5-C4-N4	-6.79	115.44	120.20
37	3	102	A	C8-N9-C4	6.79	108.52	105.80
36	5	2826	U	N1-C2-O2	6.79	127.56	122.80
36	1	875	G	O5'-P-OP2	-6.79	99.59	105.70
1	6	630	A	C2-N3-C4	-6.79	107.20	110.60
36	5	2643	A	N1-C6-N6	6.79	122.67	118.60
36	5	3245	A	N1-C2-N3	6.79	132.70	129.30
1	6	378	A	O5'-P-OP1	6.79	118.84	110.70
1	2	507	U	N1-C2-O2	6.78	127.55	122.80
36	1	1379	G	N3-C2-N2	6.78	124.65	119.90
36	1	521	A	C5-C6-N6	-6.78	118.28	123.70
36	1	672	A	N1-C6-N6	6.78	122.67	118.60
1	6	387	A	C2-N3-C4	6.78	113.99	110.60
1	6	1596	C	C5-C4-N4	6.78	124.95	120.20
36	5	1450	G	C6-C5-N7	6.78	134.47	130.40
36	1	1279	C	C6-N1-C2	-6.78	117.59	120.30
36	5	2231	C	O4'-C1'-N1	6.78	113.62	108.20
36	1	2952	G	C5-C6-O6	-6.78	124.53	128.60
36	5	96	G	O5'-P-OP1	6.78	118.83	110.70
36	1	2920	U	O5'-P-OP2	6.77	118.83	110.70
36	5	776	U	N3-C2-O2	-6.77	117.46	122.20
36	5	2211	U	C5-C4-O4	6.77	129.96	125.90
37	7	121	U	N1-C2-O2	6.77	127.54	122.80
36	1	1402	C	N3-C2-O2	-6.77	117.16	121.90
37	7	88	G	C5-C6-O6	6.77	132.66	128.60
36	1	806	A	O4'-C1'-N9	-6.77	102.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2830	G	N9-C4-C5	6.77	108.11	105.40
36	1	2434	U	C5-C6-N1	-6.77	119.32	122.70
36	5	883	A	N7-C8-N9	-6.77	110.42	113.80
36	5	2550	U	C5-C4-O4	6.77	129.96	125.90
36	1	1664	G	C5-C6-O6	6.77	132.66	128.60
1	2	553	G	C5-C6-N1	-6.76	108.12	111.50
36	1	421	G	N9-C4-C5	-6.76	102.70	105.40
36	5	1833	G	N1-C6-O6	-6.76	115.84	119.90
36	5	1546	A	O5'-P-OP1	-6.76	99.62	105.70
1	6	687	G	N1-C2-N2	6.76	122.28	116.20
36	1	3373	U	C5-C6-N1	-6.75	119.32	122.70
36	5	2119	A	C5-C6-N6	-6.75	118.30	123.70
36	1	424	G	N1-C6-O6	-6.75	115.85	119.90
36	1	2723	U	C5-C6-N1	-6.75	119.32	122.70
36	5	2808	A	N1-C6-N6	6.75	122.65	118.60
1	2	1096	C	N3-C2-O2	-6.75	117.17	121.90
36	1	1409	G	C5-C6-O6	6.75	132.65	128.60
1	6	389	G	C5-C6-O6	6.75	132.65	128.60
36	1	76	G	C5-C6-O6	-6.75	124.55	128.60
36	1	1847	A	OP1-P-OP2	6.75	129.72	119.60
36	5	2949	U	N3-C2-O2	-6.75	117.48	122.20
36	5	2343	C	N3-C4-N4	-6.75	113.28	118.00
36	1	288	C	C5-C4-N4	-6.74	115.48	120.20
36	5	1604	G	N3-C4-N9	6.74	130.05	126.00
36	5	2633	U	O5'-P-OP2	-6.74	99.63	105.70
36	1	2899	C	C5-C6-N1	-6.74	117.63	121.00
36	1	1931	U	N1-C2-O2	-6.74	118.08	122.80
36	1	2950	G	C5-N7-C8	-6.74	100.93	104.30
36	1	979	U	P-O3'-C3'	6.74	127.78	119.70
36	5	422	A	O5'-P-OP2	-6.74	99.64	105.70
36	5	1113	G	C2-N3-C4	-6.74	108.53	111.90
36	1	1054	A	O5'-P-OP2	-6.74	99.64	105.70
36	5	2796	G	C4-C5-N7	6.74	113.49	110.80
1	2	933	A	C8-N9-C4	-6.73	103.11	105.80
36	5	3374	U	N3-C4-C5	6.73	118.64	114.60
36	1	2936	A	O5'-P-OP1	-6.73	99.64	105.70
36	1	3207	U	C5-C4-O4	6.73	129.94	125.90
36	1	949	C	C4-C5-C6	6.73	120.76	117.40
36	1	689	U	N3-C2-O2	-6.72	117.49	122.20
36	5	2984	C	N3-C4-C5	6.72	124.59	121.90
36	5	643	U	N1-C2-O2	-6.72	118.09	122.80
36	1	895	A	N3-C4-N9	-6.72	122.02	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	647	G	N3-C4-N9	-6.72	121.97	126.00
37	3	47	C	O5'-P-OP2	-6.72	99.65	105.70
37	3	94	C	N1-C2-O2	-6.72	114.87	118.90
36	1	957	C	O5'-P-OP2	-6.72	99.66	105.70
36	1	2651	G	N7-C8-N9	-6.72	109.74	113.10
36	1	1653	G	N1-C6-O6	-6.71	115.87	119.90
36	1	1911	A	N1-C6-N6	6.71	122.63	118.60
36	1	2611	U	OP1-P-OP2	-6.71	109.53	119.60
36	5	1374	G	N7-C8-N9	-6.71	109.74	113.10
36	1	1902	G	N3-C2-N2	6.71	124.60	119.90
36	1	2422	C	N1-C2-O2	6.71	122.93	118.90
36	1	2993	G	C5-C6-N1	6.71	114.86	111.50
36	5	206	G	C5-C6-O6	-6.71	124.57	128.60
36	5	1115	G	N7-C8-N9	6.71	116.46	113.10
36	5	2797	C	N1-C2-O2	-6.71	114.87	118.90
36	5	3047	U	N3-C2-O2	-6.71	117.50	122.20
36	1	2395	G	C5-C6-O6	6.71	132.63	128.60
36	5	1176	C	C2-N3-C4	-6.71	116.55	119.90
36	1	2919	A	O5'-P-OP2	-6.71	99.66	105.70
36	1	2935	U	N1-C2-O2	6.71	127.50	122.80
1	6	610	G	C4-N9-C1'	6.71	135.22	126.50
1	6	1600	A	N1-C2-N3	6.71	132.65	129.30
36	5	793	C	C5-C6-N1	6.71	124.35	121.00
36	5	1083	G	O5'-P-OP1	-6.71	99.67	105.70
36	5	2403	G	N3-C4-C5	-6.71	125.25	128.60
36	5	427	C	N3-C4-C5	6.70	124.58	121.90
36	5	1354	G	O5'-P-OP2	-6.70	99.67	105.70
1	2	1514	U	O5'-P-OP1	-6.70	99.67	105.70
36	1	2983	C	O4'-C1'-N1	6.70	113.56	108.20
36	5	1547	G	N3-C4-C5	6.70	131.95	128.60
36	1	589	A	O5'-P-OP2	-6.70	99.67	105.70
36	1	1164	G	N1-C6-O6	-6.70	115.88	119.90
36	1	1911	A	C5-C6-N6	-6.70	118.34	123.70
36	1	2950	G	C5-C6-O6	-6.70	124.58	128.60
1	6	1361	U	C2-N1-C1'	6.70	125.74	117.70
36	1	709	A	N7-C8-N9	-6.70	110.45	113.80
36	5	3337	G	N1-C6-O6	-6.70	115.88	119.90
1	2	425	A	C8-N9-C4	-6.70	103.12	105.80
36	1	2169	G	N1-C6-O6	-6.70	115.88	119.90
36	1	2859	U	N1-C2-N3	6.69	118.92	114.90
36	1	407	A	C6-N1-C2	6.69	122.62	118.60
36	5	2979	U	N1-C2-O2	-6.69	118.11	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	830	U	N1-C2-O2	6.69	127.48	122.80
36	5	3098	G	C5-C6-O6	6.69	132.61	128.60
36	1	1639	C	O5'-P-OP2	-6.69	99.68	105.70
36	1	760	G	O4'-C1'-N9	6.69	113.55	108.20
36	1	2633	U	N1-C2-O2	6.69	127.48	122.80
36	1	271	C	N3-C2-O2	-6.68	117.22	121.90
36	1	2423	U	C5-C4-O4	-6.68	121.89	125.90
36	5	1331	U	N3-C4-C5	6.68	118.61	114.60
36	1	2426	U	N3-C4-C5	6.68	118.61	114.60
36	1	785	G	C2-N3-C4	6.68	115.24	111.90
36	5	2927	C	C6-N1-C2	-6.68	117.63	120.30
38	4	89	A	C8-N9-C4	6.68	108.47	105.80
36	5	3102	G	C5-C6-O6	6.68	132.61	128.60
36	5	3218	A	N1-C6-N6	6.68	122.61	118.60
68	o2	33	ARG	NE-CZ-NH1	6.68	123.64	120.30
36	1	2302	G	N1-C2-N2	-6.68	110.19	116.20
36	5	2429	G	C8-N9-C4	-6.68	103.73	106.40
36	1	2846	U	N1-C2-O2	6.67	127.47	122.80
36	5	938	C	C6-N1-C2	6.67	122.97	120.30
36	5	2169	G	N1-C6-O6	-6.67	115.90	119.90
36	1	229	G	N3-C2-N2	-6.67	115.23	119.90
36	1	722	G	O5'-P-OP1	-6.67	99.70	105.70
36	5	641	C	N1-C2-N3	6.67	123.87	119.20
36	5	2726	C	C4-C5-C6	6.67	120.73	117.40
36	1	360	G	C4-C5-N7	6.67	113.47	110.80
36	5	1547	G	O5'-P-OP1	-6.67	99.70	105.70
36	1	678	G	C5-C6-O6	-6.66	124.60	128.60
36	1	2786	G	O5'-P-OP2	-6.66	99.70	105.70
37	3	81	U	C6-N1-C2	6.66	125.00	121.00
36	1	641	C	C2-N1-C1'	-6.66	111.47	118.80
36	1	1494	U	N3-C4-O4	-6.66	114.74	119.40
36	5	908	G	O5'-P-OP1	6.66	118.69	110.70
78	Q2	87	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	6	1614	A	C4-C5-N7	6.66	114.03	110.70
36	5	908	G	N3-C4-N9	6.66	130.00	126.00
36	5	3137	C	N3-C4-N4	-6.66	113.34	118.00
36	5	3173	G	C5-C6-O6	-6.66	124.60	128.60
36	1	909	G	C5-N7-C8	6.66	107.63	104.30
36	5	217	U	OP1-P-O3'	6.66	119.85	105.20
36	1	344	A	N1-C6-N6	-6.66	114.61	118.60
36	1	1007	U	C5-C4-O4	-6.66	121.91	125.90
36	5	359	U	OP1-P-OP2	-6.66	109.62	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	346	C	C4-C5-C6	6.65	120.73	117.40
36	1	2846	U	N3-C4-O4	-6.65	114.74	119.40
1	6	113	U	N1-C2-O2	-6.65	118.14	122.80
1	6	1535	U	N3-C2-O2	-6.65	117.54	122.20
36	5	3009	G	O5'-P-OP1	-6.65	99.72	105.70
36	1	636	C	O5'-P-OP2	6.65	118.68	110.70
36	5	205	C	C6-N1-C2	-6.65	117.64	120.30
36	5	3003	G	N3-C4-N9	-6.65	122.01	126.00
36	1	1741	A	C2-N3-C4	-6.64	107.28	110.60
36	5	2400	G	N1-C6-O6	6.64	123.89	119.90
36	1	963	G	C8-N9-C4	6.64	109.06	106.40
1	2	1448	G	O5'-P-OP1	-6.64	99.72	105.70
36	1	2861	U	O5'-P-OP2	6.64	118.67	110.70
36	1	3344	A	C6-C5-N7	-6.64	127.65	132.30
1	6	144	U	N1-C2-N3	6.64	118.88	114.90
36	5	2188	A	C8-N9-C4	6.64	108.45	105.80
36	5	1547	G	C2-N3-C4	-6.64	108.58	111.90
36	5	3060	C	C5-C4-N4	-6.64	115.55	120.20
36	5	935	U	C5-C6-N1	-6.63	119.38	122.70
37	7	92	A	N1-C6-N6	6.63	122.58	118.60
37	3	86	U	N1-C2-O2	-6.63	118.16	122.80
36	1	3369	G	C5-C6-O6	-6.63	124.62	128.60
36	5	1192	C	N1-C2-O2	6.63	122.88	118.90
36	5	2192	C	O5'-P-OP2	-6.63	99.73	105.70
36	5	3086	A	OP1-P-OP2	-6.63	109.65	119.60
36	1	2805	G	N3-C2-N2	6.63	124.54	119.90
36	5	1284	C	P-O3'-C3'	6.63	127.65	119.70
1	6	1749	A	N1-C6-N6	6.62	122.58	118.60
37	7	101	G	C8-N9-C4	6.62	109.05	106.40
36	1	504	A	C5-N7-C8	6.62	107.21	103.90
36	5	1489	A	C5-C6-N6	-6.62	118.40	123.70
36	5	2905	U	N3-C4-C5	6.62	118.57	114.60
36	1	2384	A	C5-C6-N6	-6.62	118.41	123.70
36	1	2983	C	C2-N3-C4	-6.62	116.59	119.90
36	5	578	A	O5'-P-OP2	6.62	118.64	110.70
1	2	507	U	N3-C2-O2	-6.62	117.57	122.20
1	6	113	U	C2-N1-C1'	-6.62	109.76	117.70
36	5	2298	U	N3-C4-C5	6.61	118.57	114.60
6	s4	38	LEU	CA-CB-CG	6.61	130.51	115.30
36	5	2904	U	N1-C2-N3	6.61	118.87	114.90
36	1	283	G	O4'-C1'-N9	-6.61	102.91	108.20
36	1	1432	C	C5-C4-N4	-6.61	115.57	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3053	G	N1-C6-O6	-6.61	115.94	119.90
36	5	1461	A	N7-C8-N9	-6.61	110.50	113.80
1	6	767	U	N3-C2-O2	-6.60	117.58	122.20
37	7	90	U	C5-C4-O4	-6.60	121.94	125.90
36	1	206	G	N1-C6-O6	-6.60	115.94	119.90
1	6	308	C	C2-N1-C1'	-6.60	111.54	118.80
37	7	46	A	C8-N9-C4	-6.60	103.16	105.80
36	1	1859	A	C8-N9-C4	6.59	108.44	105.80
36	1	2137	U	O4'-C1'-N1	6.59	113.47	108.20
36	5	283	G	N1-C6-O6	6.59	123.86	119.90
36	1	1555	U	N1-C2-O2	-6.59	118.19	122.80
36	1	2572	C	C6-N1-C1'	-6.59	112.89	120.80
36	5	2803	A	O5'-P-OP2	-6.59	99.77	105.70
1	2	1585	U	O5'-P-OP2	-6.59	99.77	105.70
36	5	2920	U	C2-N3-C4	-6.59	123.05	127.00
36	5	2639	G	N3-C4-N9	6.59	129.95	126.00
1	6	430	G	O5'-P-OP1	-6.59	99.77	105.70
1	6	558	U	N1-C2-O2	6.59	127.41	122.80
36	5	1192	C	N3-C2-O2	-6.59	117.29	121.90
36	5	2968	G	C5-C6-O6	6.59	132.55	128.60
36	5	2935	U	O5'-P-OP2	-6.58	99.77	105.70
36	1	708	G	C5-C6-N1	6.58	114.79	111.50
1	6	782	U	N1-C2-O2	6.58	127.41	122.80
36	5	2968	G	C8-N9-C4	6.58	109.03	106.40
36	1	878	G	OP1-P-O3'	6.58	119.68	105.20
36	1	1144	U	C2-N3-C4	-6.58	123.05	127.00
36	5	1486	G	N1-C6-O6	-6.58	115.95	119.90
36	5	2130	G	N1-C6-O6	-6.58	115.95	119.90
37	7	51	A	C8-N9-C4	-6.58	103.17	105.80
1	2	1111	G	O5'-P-OP1	6.58	118.59	110.70
36	1	200	C	C2-N1-C1'	6.58	126.04	118.80
36	5	519	A	N1-C6-N6	6.58	122.55	118.60
36	1	972	A	C8-N9-C4	6.58	108.43	105.80
36	5	982	C	OP2-P-O3'	6.58	119.67	105.20
36	5	3018	C	O5'-P-OP1	6.58	118.59	110.70
36	5	3317	U	C5-C4-O4	6.58	129.84	125.90
36	1	1379	G	N1-C6-O6	-6.57	115.96	119.90
36	1	2514	U	O5'-P-OP2	-6.57	99.79	105.70
36	5	76	G	C8-N9-C4	6.57	109.03	106.40
36	1	2278	C	C5-C6-N1	6.57	124.28	121.00
36	5	2385	G	C5-C6-O6	-6.57	124.66	128.60
35	SM	167	PRO	N-CA-CB	6.57	111.18	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1148	G	N3-C2-N2	6.57	124.50	119.90
38	4	90	U	C6-N1-C2	6.57	124.94	121.00
36	5	682	U	C5-C4-O4	-6.57	121.96	125.90
36	1	1555	U	C6-N1-C1'	6.57	130.39	121.20
36	1	2356	A	C5-N7-C8	-6.57	100.62	103.90
36	1	2397	A	O5'-P-OP1	6.56	118.58	110.70
1	6	337	G	N1-C6-O6	6.56	123.84	119.90
36	1	186	U	OP1-P-OP2	-6.56	109.76	119.60
1	6	1560	U	C5-C4-O4	6.56	129.84	125.90
36	5	2395	G	C8-N9-C4	6.56	109.03	106.40
1	2	61	A	N7-C8-N9	6.56	117.08	113.80
36	1	2904	U	N3-C4-C5	6.56	118.53	114.60
75	O9	45	ARG	NE-CZ-NH2	-6.56	117.02	120.30
36	5	825	U	N1-C2-O2	6.56	127.39	122.80
36	1	2149	A	O5'-P-OP1	-6.56	99.80	105.70
36	5	1591	G	N1-C6-O6	-6.56	115.97	119.90
1	2	142	G	N1-C6-O6	6.55	123.83	119.90
36	1	634	C	N1-C2-O2	6.55	122.83	118.90
36	5	810	A	N1-C2-N3	-6.55	126.02	129.30
36	1	1434	G	C5-C6-O6	-6.55	124.67	128.60
36	1	2373	A	C8-N9-C4	-6.55	103.18	105.80
36	1	3318	G	C8-N9-C4	-6.55	103.78	106.40
1	6	101	U	N1-C2-O2	6.55	127.39	122.80
1	2	1339	C	OP1-P-O3'	6.55	119.61	105.20
36	1	2610	G	N1-C6-O6	-6.55	115.97	119.90
36	5	3212	C	N1-C2-O2	-6.55	114.97	118.90
36	1	980	A	N7-C8-N9	6.55	117.07	113.80
1	6	1126	G	C5-C6-O6	6.55	132.53	128.60
36	5	519	A	C8-N9-C4	6.55	108.42	105.80
36	5	974	G	N3-C4-C5	-6.55	125.33	128.60
36	5	2700	G	C8-N9-C4	-6.55	103.78	106.40
1	6	542	A	C8-N9-C4	-6.54	103.18	105.80
36	5	966	U	O5'-P-OP2	-6.54	99.81	105.70
36	5	1449	A	C5-C6-N1	-6.54	114.43	117.70
36	5	1931	U	C5-C6-N1	-6.54	119.43	122.70
36	1	2941	A	O4'-C1'-N9	-6.54	102.97	108.20
36	5	2148	U	N1-C2-O2	-6.54	118.22	122.80
36	1	423	A	C5-C6-N1	-6.54	114.43	117.70
36	1	2993	G	N9-C4-C5	-6.54	102.78	105.40
36	1	1918	C	C6-N1-C2	-6.54	117.69	120.30
36	1	1440	G	C5-C6-O6	6.53	132.52	128.60
36	1	3344	A	C4-C5-N7	6.53	113.97	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	3	102	A	N1-C2-N3	-6.53	126.03	129.30
36	5	1879	A	C6-C5-N7	-6.53	127.73	132.30
36	5	1208	U	C5-C6-N1	-6.53	119.43	122.70
36	1	631	U	C2-N3-C4	-6.53	123.08	127.00
36	1	1581	C	N3-C2-O2	-6.53	117.33	121.90
1	6	1119	G	C8-N9-C4	-6.53	103.79	106.40
36	5	2139	A	C5-C6-N1	-6.53	114.44	117.70
36	5	2139	A	C5-C6-N6	6.53	128.93	123.70
1	6	272	U	P-O3'-C3'	6.53	127.53	119.70
36	1	2924	U	C5-C6-N1	-6.53	119.44	122.70
36	5	1042	U	N3-C2-O2	-6.53	117.63	122.20
36	1	1127	G	C5-C6-O6	-6.53	124.69	128.60
36	5	2211	U	N3-C2-O2	-6.53	117.63	122.20
1	2	1241	G	C4-C5-N7	6.52	113.41	110.80
36	1	3309	G	C4-C5-N7	6.52	113.41	110.80
47	M0	24	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	6	1509	C	N3-C2-O2	-6.52	117.33	121.90
36	5	1395	G	C5-C6-O6	-6.52	124.69	128.60
36	5	2908	G	C4-C5-N7	-6.52	108.19	110.80
36	1	2905	U	N3-C2-O2	6.52	126.77	122.20
48	m1	112	LEU	CA-CB-CG	6.52	130.30	115.30
36	1	1822	C	C6-N1-C2	-6.52	117.69	120.30
36	5	2821	C	N1-C2-O2	-6.52	114.99	118.90
36	1	1548	C	N1-C2-O2	-6.52	114.99	118.90
36	5	2327	U	C2-N3-C4	-6.52	123.09	127.00
36	5	2901	G	N1-C6-O6	6.52	123.81	119.90
36	5	326	U	N3-C2-O2	6.51	126.76	122.20
52	m6	84	LEU	CB-CG-CD1	-6.51	99.93	111.00
36	1	817	A	OP1-P-O3'	6.51	119.52	105.20
36	5	2514	U	O5'-P-OP1	-6.51	99.84	105.70
36	5	3337	G	C5-C6-O6	6.51	132.50	128.60
36	1	2281	A	C8-N9-C4	6.51	108.40	105.80
25	d3	33	LEU	CA-CB-CG	-6.51	100.34	115.30
36	5	3050	U	C5-C4-O4	6.50	129.80	125.90
36	1	608	A	C6-C5-N7	-6.50	127.75	132.30
36	5	1331	U	O4'-C1'-N1	-6.50	103.00	108.20
1	2	704	C	N1-C2-O2	6.50	122.80	118.90
1	2	1486	G	C4-C5-N7	6.50	113.40	110.80
36	1	652	G	N1-C2-N2	-6.50	110.35	116.20
36	5	3012	A	N9-C4-C5	-6.50	103.20	105.80
36	1	894	G	OP1-P-O3'	6.49	119.49	105.20
36	5	950	G	C5-C6-N1	6.49	114.75	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	776	U	C2-N3-C4	-6.49	123.11	127.00
1	2	1200	G	N1-C2-N2	6.49	122.04	116.20
36	5	3123	A	N1-C2-N3	-6.49	126.06	129.30
1	6	868	G	C4-C5-N7	6.49	113.39	110.80
36	1	797	U	N3-C4-C5	6.49	118.49	114.60
36	5	2701	U	C5-C4-O4	-6.49	122.01	125.90
36	5	2843	U	N3-C2-O2	-6.49	117.66	122.20
36	5	3041	U	N3-C4-C5	6.49	118.49	114.60
49	m3	85	LEU	CA-CB-CG	6.49	130.22	115.30
36	1	69	C	O5'-P-OP2	-6.48	99.87	105.70
36	1	645	A	N3-C4-N9	6.48	132.59	127.40
38	4	30	C	C5-C4-N4	6.48	124.74	120.20
36	5	981	U	C5-C6-N1	6.48	125.94	122.70
38	4	32	C	N3-C2-O2	6.48	126.44	121.90
36	5	2337	C	N3-C4-C5	6.48	124.49	121.90
36	5	2920	U	C5-C4-O4	-6.48	122.01	125.90
1	2	1430	U	C5-C4-O4	6.48	129.79	125.90
36	1	716	A	N1-C6-N6	6.48	122.49	118.60
36	1	2897	A	C8-N9-C4	6.48	108.39	105.80
1	6	1082	C	C6-N1-C2	-6.48	117.71	120.30
36	1	988	U	C5-C6-N1	-6.48	119.46	122.70
36	5	1292	C	O5'-P-OP1	-6.48	99.87	105.70
36	1	898	U	C5-C4-O4	-6.47	122.02	125.90
38	4	96	A	O5'-P-OP1	-6.47	99.87	105.70
36	1	1113	G	C4-C5-N7	-6.47	108.21	110.80
36	1	1440	G	N3-C2-N2	6.47	124.43	119.90
36	1	2385	G	O5'-P-OP2	6.47	118.47	110.70
37	3	86	U	N3-C4-O4	6.47	123.93	119.40
36	5	116	A	O5'-P-OP1	-6.47	99.88	105.70
36	5	663	C	N1-C2-O2	-6.47	115.02	118.90
36	5	649	A	N7-C8-N9	6.47	117.04	113.80
36	5	1910	A	OP2-P-O3'	6.47	119.44	105.20
36	1	2632	G	N3-C2-N2	6.47	124.43	119.90
1	6	542	A	C4-C5-N7	6.47	113.94	110.70
36	5	1123	U	C5-C6-N1	-6.47	119.47	122.70
36	5	2654	C	OP2-P-O3'	6.47	119.43	105.20
1	2	737	A	O4'-C1'-N9	6.47	113.37	108.20
36	1	2361	A	C8-N9-C4	-6.46	103.21	105.80
36	5	3128	G	N9-C4-C5	-6.46	102.81	105.40
36	5	907	G	O5'-P-OP1	-6.46	99.89	105.70
36	5	1168	U	N3-C4-O4	-6.46	114.88	119.40
36	5	1389	G	C4-C5-N7	6.46	113.38	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	m8	178	ARG	NE-CZ-NH2	-6.46	117.07	120.30
36	1	2979	U	C2-N3-C4	-6.46	123.12	127.00
38	4	120	C	N1-C2-O2	-6.46	115.02	118.90
1	2	139	C	C6-N1-C2	-6.46	117.72	120.30
36	1	278	U	N1-C2-N3	6.46	118.77	114.90
36	1	1313	G	C5-C6-O6	-6.46	124.73	128.60
36	1	2339	C	C6-N1-C2	-6.46	117.72	120.30
36	5	361	A	N1-C6-N6	-6.46	114.73	118.60
36	5	1307	G	N3-C2-N2	6.46	124.42	119.90
36	5	2790	A	O5'-P-OP2	-6.46	99.89	105.70
36	1	649	A	OP1-P-OP2	-6.45	109.92	119.60
36	1	3002	C	N3-C4-C5	6.45	124.48	121.90
1	6	1637	C	C6-N1-C2	6.45	122.88	120.30
36	5	591	G	N1-C6-O6	6.45	123.77	119.90
36	5	1908	A	C8-N9-C4	-6.45	103.22	105.80
36	1	143	G	N1-C6-O6	-6.45	116.03	119.90
36	1	1331	U	O4'-C1'-N1	-6.45	103.04	108.20
1	6	17	C	C6-N1-C2	-6.45	117.72	120.30
36	5	200	C	OP2-P-O3'	6.45	119.38	105.20
36	5	2292	U	N3-C2-O2	-6.45	117.69	122.20
1	2	402	C	C6-N1-C2	6.45	122.88	120.30
36	5	1337	A	C8-N9-C4	-6.45	103.22	105.80
36	1	1604	G	C4-N9-C1'	6.44	134.88	126.50
36	1	645	A	N3-C4-C5	-6.44	122.29	126.80
36	1	2550	U	N3-C4-O4	-6.44	114.89	119.40
36	1	2798	C	C5-C4-N4	6.44	124.71	120.20
36	1	2802	A	N1-C6-N6	-6.44	114.73	118.60
1	6	57	G	O5'-P-OP1	6.44	118.43	110.70
36	1	1310	G	C4-C5-N7	6.44	113.38	110.80
36	1	2891	U	C5-C4-O4	-6.44	122.04	125.90
36	1	2952	G	N1-C6-O6	6.44	123.77	119.90
1	6	1634	C	N3-C2-O2	-6.44	117.39	121.90
36	5	2426	U	N3-C2-O2	-6.44	117.69	122.20
36	5	3185	U	OP1-P-O3'	6.44	119.37	105.20
36	1	637	C	C6-N1-C2	-6.44	117.72	120.30
36	5	1592	G	N3-C2-N2	6.44	124.41	119.90
1	6	1783	C	O5'-P-OP2	-6.44	99.91	105.70
36	5	2623	G	OP1-P-OP2	-6.44	109.94	119.60
36	1	936	A	C8-N9-C4	6.43	108.37	105.80
36	1	942	U	OP1-P-OP2	-6.43	109.95	119.60
36	5	1330	A	O5'-P-OP1	-6.43	99.91	105.70
36	1	2867	C	C5-C4-N4	6.43	124.70	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	L4	95	ARG	NE-CZ-NH1	6.43	123.52	120.30
36	5	93	C	N3-C4-C5	-6.43	119.33	121.90
36	5	2827	U	O4'-C1'-N1	6.43	113.35	108.20
36	1	637	C	P-O3'-C3'	6.43	127.42	119.70
36	1	1335	C	N3-C2-O2	-6.43	117.40	121.90
36	1	1931	U	C2-N1-C1'	-6.43	109.98	117.70
36	1	2305	G	C6-C5-N7	-6.43	126.54	130.40
36	1	3207	U	N1-C2-N3	6.43	118.76	114.90
64	N8	115	LYS	C-N-CA	-6.43	108.80	122.30
41	l4	90	PHE	C-N-CA	-6.43	108.80	122.30
36	5	1115	G	C4-C5-N7	6.43	113.37	110.80
36	1	2679	A	N1-C6-N6	6.43	122.45	118.60
36	1	2870	C	C6-N1-C1'	6.43	128.51	120.80
36	5	645	A	N1-C2-N3	6.43	132.51	129.30
36	5	2650	U	C2-N3-C4	-6.43	123.14	127.00
1	2	499	U	C2-N1-C1'	6.42	125.41	117.70
36	1	2380	U	C5-C4-O4	-6.42	122.05	125.90
36	5	1006	A	O5'-P-OP2	-6.42	99.92	105.70
36	1	2988	C	N3-C4-N4	-6.42	113.51	118.00
36	5	200	C	C6-N1-C1'	-6.42	113.10	120.80
36	1	3278	C	C6-N1-C2	-6.42	117.73	120.30
36	5	3078	U	C2-N1-C1'	6.42	125.40	117.70
36	5	41	G	N1-C6-O6	6.42	123.75	119.90
36	5	2814	G	N3-C2-N2	6.42	124.39	119.90
56	N0	58	ILE	CG1-CB-CG2	-6.42	97.29	111.40
36	5	2376	G	C5-C6-O6	6.41	132.45	128.60
36	1	2338	C	N1-C2-O2	6.41	122.75	118.90
36	5	1751	G	O5'-P-OP2	-6.41	99.93	105.70
36	5	949	C	N1-C2-O2	-6.41	115.06	118.90
37	7	101	G	N9-C4-C5	-6.41	102.84	105.40
36	1	2278	C	N3-C4-N4	-6.41	113.52	118.00
36	5	386	A	N1-C6-N6	6.41	122.44	118.60
36	5	1452	A	N9-C4-C5	-6.41	103.24	105.80
36	5	2881	C	C2-N3-C4	-6.41	116.70	119.90
1	2	1432	U	C6-N1-C2	6.40	124.84	121.00
1	2	1462	G	C5-C6-O6	-6.40	124.76	128.60
1	2	1652	C	C5-C6-N1	6.40	124.20	121.00
36	1	2797	C	N3-C2-O2	6.40	126.38	121.90
36	1	2836	C	N3-C2-O2	-6.40	117.42	121.90
1	6	944	A	C8-N9-C4	-6.40	103.24	105.80
36	5	2911	A	OP1-P-O3'	6.40	119.29	105.20
36	1	1605	A	O4'-C1'-N9	6.40	113.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	844	G	C8-N9-C4	6.40	108.96	106.40
36	5	1300	G	C5-C6-O6	-6.40	124.76	128.60
36	5	2816	G	O4'-C1'-N9	6.40	113.32	108.20
36	1	1904	C	C6-N1-C2	-6.40	117.74	120.30
36	5	1159	A	O5'-P-OP1	-6.40	99.94	105.70
36	1	859	G	N1-C2-N2	-6.39	110.44	116.20
1	6	194	U	N1-C2-O2	6.39	127.28	122.80
1	6	1614	A	N1-C6-N6	6.39	122.44	118.60
1	6	1663	G	C8-N9-C4	-6.39	103.84	106.40
36	1	517	G	C8-N9-C4	-6.39	103.84	106.40
36	1	871	U	N1-C2-O2	-6.39	118.33	122.80
36	5	685	G	N1-C6-O6	-6.39	116.06	119.90
36	1	2879	C	N1-C2-O2	-6.39	115.06	118.90
36	5	2993	G	N3-C4-N9	6.39	129.83	126.00
36	1	1297	C	C5-C6-N1	-6.39	117.81	121.00
36	1	2996	U	C2-N1-C1'	6.39	125.37	117.70
36	5	1178	G	N1-C2-N2	6.39	121.95	116.20
1	2	4	C	O5'-P-OP1	-6.39	99.95	105.70
36	1	49	A	C5-C6-N1	-6.39	114.51	117.70
36	5	1208	U	N3-C2-O2	-6.39	117.73	122.20
1	6	1596	C	N3-C4-N4	-6.38	113.53	118.00
36	1	329	U	N1-C2-O2	-6.38	118.33	122.80
36	1	2188	A	N1-C6-N6	-6.38	114.77	118.60
36	1	2409	G	C8-N9-C4	-6.38	103.85	106.40
36	1	59	G	O5'-P-OP1	6.38	118.36	110.70
36	5	2245	C	C6-N1-C2	-6.38	117.75	120.30
36	5	2409	G	C5-C6-O6	6.38	132.43	128.60
36	1	665	A	N1-C6-N6	-6.38	114.77	118.60
36	5	3178	A	O5'-P-OP1	-6.38	99.96	105.70
38	4	63	G	C8-N9-C4	-6.38	103.85	106.40
36	5	1793	C	N3-C4-C5	-6.38	119.35	121.90
36	5	1841	A	C8-N9-C4	-6.38	103.25	105.80
1	2	1131	A	C8-N9-C4	6.38	108.35	105.80
36	1	2104	A	C8-N9-C4	6.37	108.35	105.80
36	1	2899	C	P-O3'-C3'	6.37	127.35	119.70
36	1	2314	U	C6-N1-C1'	-6.37	112.28	121.20
36	1	2412	G	N9-C4-C5	6.37	107.95	105.40
36	1	3054	U	C5-C6-N1	-6.37	119.52	122.70
36	5	810	A	C2-N3-C4	6.37	113.78	110.60
36	5	1371	G	C5-C6-N1	6.37	114.68	111.50
36	5	1588	A	C8-N9-C4	6.37	108.35	105.80
36	1	3344	A	C2-N3-C4	-6.37	107.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1568	C	P-O3'-C3'	6.37	127.34	119.70
36	1	2758	A	C5-C6-N1	6.37	120.88	117.70
36	5	811	U	C5-C4-O4	-6.37	122.08	125.90
36	5	819	U	C5-C6-N1	-6.37	119.52	122.70
36	5	957	C	C2-N3-C4	-6.37	116.72	119.90
36	1	1454	A	O5'-P-OP1	-6.36	99.97	105.70
36	1	1493	G	O4'-C1'-N9	6.36	113.29	108.20
36	5	1878	G	C4-N9-C1'	6.36	134.77	126.50
36	5	2655	U	C5-C4-O4	6.36	129.72	125.90
38	4	125	U	C2-N1-C1'	6.36	125.33	117.70
36	5	2403	G	O5'-P-OP2	-6.36	99.98	105.70
36	1	317	A	C8-N9-C4	-6.36	103.26	105.80
36	1	2392	C	C2-N3-C4	-6.36	116.72	119.90
36	1	2795	U	O5'-P-OP1	-6.36	99.98	105.70
1	6	1774	G	N1-C6-O6	-6.36	116.09	119.90
36	5	1340	G	N1-C6-O6	-6.36	116.08	119.90
36	5	2340	U	N3-C2-O2	-6.36	117.75	122.20
36	5	3196	U	C2-N1-C1'	-6.36	110.07	117.70
1	2	142	G	N3-C2-N2	-6.36	115.45	119.90
36	1	24	G	N3-C2-N2	-6.36	115.45	119.90
36	1	360	G	N1-C6-O6	6.36	123.71	119.90
36	5	2856	G	C4-C5-N7	6.35	113.34	110.80
36	5	3016	A	OP2-P-O3'	6.35	119.18	105.20
36	1	2986	U	C5-C6-N1	-6.35	119.52	122.70
36	1	1417	G	C8-N9-C4	6.35	108.94	106.40
36	1	3078	U	N3-C2-O2	-6.35	117.75	122.20
36	1	981	U	O5'-P-OP2	-6.35	99.99	105.70
36	1	1297	C	C6-N1-C2	6.35	122.84	120.30
36	5	775	A	N1-C6-N6	-6.34	114.80	118.60
36	5	2131	A	N1-C6-N6	6.34	122.40	118.60
1	2	1455	G	C4-C5-N7	-6.34	108.27	110.80
1	6	1082	C	N1-C2-O2	6.33	122.70	118.90
37	7	102	A	C8-N9-C4	6.33	108.33	105.80
1	2	1748	G	N9-C4-C5	6.33	107.93	105.40
36	1	1379	G	C5-C6-O6	6.33	132.40	128.60
36	1	3319	U	P-O3'-C3'	6.33	127.30	119.70
52	M6	84	LEU	CB-CG-CD2	-6.33	100.23	111.00
36	5	893	C	N3-C4-C5	-6.33	119.37	121.90
38	8	90	U	C6-N1-C2	6.33	124.80	121.00
1	2	137	U	N1-C2-O2	6.33	127.23	122.80
36	1	1175	C	C2-N3-C4	-6.33	116.73	119.90
36	5	437	G	N3-C2-N2	-6.33	115.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1136	A	C6-N1-C2	-6.33	114.80	118.60
1	6	114	C	N1-C2-O2	6.33	122.70	118.90
1	6	1473	U	C2-N1-C1'	6.33	125.29	117.70
36	5	2654	C	C5-C6-N1	-6.33	117.84	121.00
36	1	637	C	OP2-P-O3'	-6.33	91.28	105.20
36	5	1118	C	O5'-P-OP1	-6.33	100.01	105.70
36	5	3275	U	N3-C2-O2	-6.33	117.77	122.20
36	1	1175	C	O5'-P-OP2	6.32	118.29	110.70
36	5	1404	G	N1-C6-O6	-6.32	116.11	119.90
36	1	67	A	O5'-P-OP1	-6.32	100.01	105.70
38	4	45	C	O5'-P-OP2	-6.32	100.01	105.70
36	5	2341	A	N7-C8-N9	-6.32	110.64	113.80
36	5	3306	U	N3-C4-C5	6.32	118.39	114.60
59	n3	48	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	2	73	U	OP1-P-O3'	6.32	119.10	105.20
36	5	2326	A	C8-N9-C4	6.32	108.33	105.80
36	1	1118	C	C6-N1-C2	-6.32	117.77	120.30
36	5	3245	A	C5-C6-N1	-6.32	114.54	117.70
36	5	2248	C	C5-C6-N1	-6.32	117.84	121.00
36	5	2833	A	N1-C6-N6	-6.32	114.81	118.60
36	5	2899	C	C5-C6-N1	-6.32	117.84	121.00
1	6	539	G	N7-C8-N9	6.31	116.26	113.10
36	5	2202	C	N3-C4-N4	6.31	122.42	118.00
36	1	2328	U	N3-C4-O4	-6.31	114.98	119.40
1	2	765	G	C5-C6-O6	-6.31	124.81	128.60
36	1	362	U	N3-C4-O4	-6.31	114.98	119.40
36	1	1450	G	O5'-P-OP2	6.31	118.27	110.70
36	1	2395	G	N3-C2-N2	6.31	124.32	119.90
10	S8	29	LEU	CA-CB-CG	6.31	129.81	115.30
1	6	1473	U	C5-C4-O4	6.31	129.69	125.90
36	1	2827	U	N1-C2-O2	-6.31	118.39	122.80
36	5	1660	C	C6-N1-C2	-6.31	117.78	120.30
1	2	359	A	C8-N9-C4	6.30	108.32	105.80
1	2	408	C	N1-C2-O2	-6.30	115.12	118.90
36	1	364	G	O5'-P-OP1	-6.30	100.03	105.70
36	1	2986	U	N1-C2-N3	6.30	118.68	114.90
36	1	2719	U	C5-C6-N1	-6.30	119.55	122.70
36	5	856	G	N1-C6-O6	6.30	123.68	119.90
36	5	3043	C	N3-C4-N4	-6.30	113.59	118.00
36	5	3181	C	O5'-P-OP2	-6.30	100.03	105.70
36	1	416	A	N1-C6-N6	-6.30	114.82	118.60
36	1	2983	C	C2-N1-C1'	6.30	125.73	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3382	U	C2-N1-C1'	6.30	125.26	117.70
36	5	426	G	N1-C6-O6	-6.30	116.12	119.90
36	5	1193	A	C8-N9-C4	-6.30	103.28	105.80
36	1	1141	C	N3-C4-C5	-6.30	119.38	121.90
36	1	1364	C	N3-C4-N4	-6.30	113.59	118.00
36	5	41	G	C5-C6-O6	-6.30	124.82	128.60
36	5	672	A	C8-N9-C4	-6.30	103.28	105.80
1	2	607	G	N1-C6-O6	6.30	123.68	119.90
36	5	1847	A	N3-C4-C5	6.30	131.21	126.80
36	5	1925	U	C5-C4-O4	-6.30	122.12	125.90
36	1	112	U	N1-C1'-C2'	-6.30	105.07	112.00
36	1	582	G	O5'-P-OP2	-6.30	100.03	105.70
36	1	716	A	N9-C4-C5	-6.30	103.28	105.80
36	1	1919	G	C8-N9-C4	-6.30	103.88	106.40
1	6	609	U	C4-C5-C6	6.30	123.48	119.70
1	6	1000	C	C2-N3-C4	-6.30	116.75	119.90
36	5	959	C	N3-C4-C5	6.30	124.42	121.90
38	4	21	C	N1-C2-O2	-6.29	115.12	118.90
1	6	1735	U	O5'-P-OP2	-6.29	100.03	105.70
36	1	2986	U	N3-C4-O4	-6.29	114.99	119.40
36	5	1307	G	OP1-P-O3'	6.29	119.04	105.20
36	5	1380	G	O5'-P-OP1	6.29	118.25	110.70
36	5	2977	G	C8-N9-C4	6.29	108.92	106.40
1	2	934	C	C6-N1-C1'	-6.29	113.25	120.80
1	6	1058	U	OP1-P-O3'	6.29	119.04	105.20
36	5	1882	G	O5'-P-OP1	-6.29	100.04	105.70
1	2	1145	U	N3-C4-O4	6.29	123.80	119.40
36	1	2385	G	N3-C4-C5	6.29	131.75	128.60
36	1	3275	U	OP1-P-O3'	6.29	119.04	105.20
36	5	1421	G	N3-C4-N9	-6.29	122.23	126.00
36	1	2366	C	C5-C6-N1	6.29	124.14	121.00
36	5	1375	G	N1-C2-N3	-6.29	120.13	123.90
36	1	346	C	C2-N3-C4	-6.29	116.76	119.90
36	5	2408	U	N1-C2-N3	6.29	118.67	114.90
1	6	1498	G	N1-C6-O6	-6.28	116.13	119.90
1	6	314	C	N3-C2-O2	-6.28	117.50	121.90
1	6	101	U	N3-C2-O2	-6.28	117.80	122.20
12	c0	97	PRO	N-CA-CB	6.28	110.84	103.30
36	5	426	G	C5-N7-C8	6.28	107.44	104.30
36	1	333	G	C5-C6-O6	6.28	132.37	128.60
36	1	2278	C	C6-N1-C2	-6.28	117.79	120.30
36	1	2278	C	N3-C4-C5	6.28	124.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2339	C	C5-C6-N1	6.28	124.14	121.00
36	1	2369	G	N3-C4-N9	6.28	129.77	126.00
36	5	3154	C	C2-N1-C1'	6.28	125.70	118.80
36	5	2346	C	C2-N3-C4	-6.27	116.76	119.90
1	2	554	C	C2-N1-C1'	6.27	125.70	118.80
36	1	97	U	N1-C2-N3	6.27	118.66	114.90
36	1	2188	A	C5-C6-N6	6.27	128.72	123.70
36	1	592	A	O5'-P-OP1	-6.27	100.06	105.70
36	5	297	G	O4'-C1'-N9	6.27	113.22	108.20
36	5	2765	C	C6-N1-C2	-6.27	117.79	120.30
1	6	158	U	P-O3'-C3'	6.27	127.22	119.70
36	1	686	G	C5-C6-O6	6.27	132.36	128.60
36	1	3055	U	C2-N1-C1'	6.27	125.22	117.70
36	5	2980	U	N1-C2-N3	6.27	118.66	114.90
36	5	339	C	C5-C4-N4	6.27	124.59	120.20
36	1	2827	U	C5-C6-N1	-6.26	119.57	122.70
36	1	3213	A	C6-C5-N7	-6.26	127.92	132.30
36	5	3216	G	O5'-P-OP2	-6.26	100.06	105.70
36	1	2714	G	C4-C5-C6	-6.26	115.04	118.80
36	5	1389	G	N1-C6-O6	6.26	123.66	119.90
36	5	1390	A	C5-C6-N6	6.26	128.71	123.70
36	1	960	U	N3-C2-O2	6.26	126.58	122.20
36	5	200	C	N1-C2-O2	6.26	122.66	118.90
36	5	2878	G	N1-C6-O6	-6.26	116.14	119.90
36	5	2883	U	N1-C2-O2	6.26	127.18	122.80
36	5	3377	G	C5-C6-O6	-6.26	124.84	128.60
1	2	1768	G	C4-C5-N7	-6.26	108.30	110.80
36	1	2800	G	N7-C8-N9	-6.26	109.97	113.10
1	6	308	C	C6-N1-C1'	6.26	128.31	120.80
1	6	801	G	N1-C6-O6	-6.26	116.14	119.90
36	5	217	U	C2-N3-C4	-6.26	123.24	127.00
36	5	2694	A	C2-N3-C4	6.26	113.73	110.60
36	1	2714	G	C6-N1-C2	6.26	128.85	125.10
36	1	3304	U	O5'-P-OP1	-6.26	100.07	105.70
38	4	32	C	C2-N1-C1'	-6.26	111.92	118.80
43	L6	31	ARG	NE-CZ-NH1	6.26	123.43	120.30
36	5	3138	U	N1-C2-N3	6.26	118.65	114.90
36	1	2726	C	N1-C2-O2	6.25	122.65	118.90
36	5	909	G	N7-C8-N9	-6.25	109.97	113.10
36	5	1049	C	N3-C4-C5	6.25	124.40	121.90
36	5	1305	U	C5-C6-N1	-6.25	119.57	122.70
1	2	1273	G	O4'-C1'-N9	6.25	113.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1659	A	C2-N3-C4	-6.25	107.47	110.60
36	5	2290	C	O5'-P-OP2	-6.25	100.07	105.70
36	5	2635	A	C5-C6-N6	6.25	128.70	123.70
36	5	2948	C	C4-C5-C6	-6.25	114.27	117.40
36	1	948	C	N1-C2-O2	-6.25	115.15	118.90
36	1	2382	G	C5-C6-O6	6.25	132.35	128.60
61	N5	115	ARG	NE-CZ-NH1	6.25	123.43	120.30
36	5	1376	C	O5'-P-OP1	-6.25	100.07	105.70
36	5	2684	C	O5'-P-OP2	-6.25	100.07	105.70
1	2	1782	A	C8-N9-C4	-6.25	103.30	105.80
36	5	2290	C	C5-C6-N1	-6.25	117.88	121.00
1	2	1731	A	O5'-P-OP2	-6.25	100.08	105.70
36	1	949	C	N3-C4-N4	6.25	122.37	118.00
36	1	3010	U	N3-C2-O2	-6.25	117.83	122.20
36	5	2719	U	C6-N1-C1'	6.25	129.94	121.20
36	1	2830	G	C4-C5-N7	-6.25	108.30	110.80
36	5	3274	A	N1-C6-N6	-6.25	114.85	118.60
36	1	1858	A	O4'-C1'-N9	6.24	113.19	108.20
1	6	387	A	C4-C5-N7	-6.24	107.58	110.70
36	5	2798	C	O5'-P-OP2	6.24	118.19	110.70
36	5	2928	C	N3-C4-C5	-6.24	119.40	121.90
36	5	3368	U	OP1-P-O3'	6.24	118.93	105.20
36	1	2818	U	C4-C5-C6	-6.24	115.95	119.70
36	5	981	U	C6-N1-C2	-6.24	117.25	121.00
1	2	1129	U	N3-C4-C5	6.24	118.34	114.60
36	1	412	G	C8-N9-C4	-6.24	103.90	106.40
36	1	637	C	C2-N3-C4	-6.24	116.78	119.90
36	1	2786	G	C8-N9-C4	-6.24	103.90	106.40
36	1	2870	C	N3-C4-N4	-6.24	113.63	118.00
52	M6	69	GLY	N-CA-C	-6.24	97.50	113.10
36	5	3123	A	N7-C8-N9	-6.24	110.68	113.80
49	m3	46	ILE	CG1-CB-CG2	-6.24	97.67	111.40
1	6	858	G	C5-N7-C8	-6.24	101.18	104.30
36	5	943	U	N3-C4-C5	6.24	118.34	114.60
39	l2	216	HIS	N-CA-C	-6.24	94.16	111.00
1	2	728	U	N1-C2-O2	6.24	127.17	122.80
1	6	1544	U	O5'-P-OP2	-6.24	100.09	105.70
36	5	506	U	C2-N3-C4	-6.24	123.26	127.00
1	2	532	U	O5'-P-OP1	-6.24	100.09	105.70
36	1	816	A	C2-N3-C4	6.24	113.72	110.60
36	1	2948	C	N3-C4-C5	6.23	124.39	121.90
36	1	3079	U	C5-C6-N1	-6.23	119.58	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	7	48	U	C5-C4-O4	-6.23	122.16	125.90
36	5	1113	G	O5'-P-OP1	-6.23	100.09	105.70
36	5	2772	C	N1-C2-O2	-6.23	115.16	118.90
36	1	910	G	C8-N9-C4	-6.23	103.91	106.40
36	5	2363	A	N9-C4-C5	6.23	108.29	105.80
36	1	365	A	N1-C6-N6	6.23	122.34	118.60
37	7	1	G	N3-C4-N9	6.22	129.74	126.00
36	1	1434	G	O5'-P-OP2	-6.22	100.10	105.70
36	1	3181	C	C4-C5-C6	6.22	120.51	117.40
36	5	1419	A	N1-C6-N6	-6.22	114.87	118.60
1	2	507	U	C2-N1-C1'	6.22	125.17	117.70
1	2	1748	G	C8-N9-C4	-6.22	103.91	106.40
36	1	3344	A	N1-C6-N6	6.22	122.33	118.60
1	6	874	C	C2-N1-C1'	6.22	125.64	118.80
36	5	2634	U	N1-C2-N3	6.22	118.63	114.90
36	1	2877	G	C5-C6-O6	6.22	132.33	128.60
36	5	1381	A	C8-N9-C4	6.22	108.29	105.80
36	5	3174	A	C5-N7-C8	-6.22	100.79	103.90
1	2	554	C	C5-C6-N1	6.21	124.11	121.00
1	2	811	A	C8-N9-C4	-6.21	103.31	105.80
1	2	966	A	C8-N9-C4	6.21	108.29	105.80
36	5	3097	C	C6-N1-C2	-6.21	117.81	120.30
36	1	2175	U	C5-C6-N1	-6.21	119.59	122.70
36	5	3091	A	N1-C6-N6	-6.21	114.87	118.60
36	1	1307	G	OP1-P-O3'	6.21	118.86	105.20
36	1	1394	A	OP2-P-O3'	6.21	118.86	105.20
1	6	174	U	O5'-P-OP2	-6.21	100.11	105.70
36	5	2919	A	C5-C6-N6	6.21	128.67	123.70
36	1	2244	A	C8-N9-C4	6.21	108.28	105.80
36	5	2412	G	N3-C4-C5	-6.21	125.50	128.60
36	5	2634	U	C5-C4-O4	-6.21	122.17	125.90
36	1	1807	G	C8-N9-C4	-6.21	103.92	106.40
36	5	908	G	C8-N9-C1'	-6.21	118.93	127.00
36	5	1589	A	O4'-C1'-N9	-6.21	103.23	108.20
1	2	1429	G	O5'-P-OP1	-6.21	100.11	105.70
36	1	215	G	N9-C4-C5	6.21	107.88	105.40
36	1	317	A	O5'-P-OP2	-6.21	100.11	105.70
36	1	2827	U	N3-C4-O4	-6.21	115.06	119.40
36	5	3060	C	N3-C4-N4	6.21	122.34	118.00
36	1	2600	C	N3-C2-O2	-6.20	117.56	121.90
36	5	3217	C	C6-N1-C2	6.20	122.78	120.30
36	5	1604	G	C8-N9-C1'	-6.20	118.94	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2714	G	C4-C5-N7	6.20	113.28	110.80
36	5	2348	A	C8-N9-C4	-6.20	103.32	105.80
36	5	2524	A	N9-C1'-C2'	6.20	122.06	114.00
36	5	1116	G	N3-C4-C5	-6.20	125.50	128.60
36	5	1327	C	N3-C4-C5	6.20	124.38	121.90
36	1	658	G	O5'-P-OP2	-6.20	100.12	105.70
36	1	2872	A	C2-N3-C4	6.20	113.70	110.60
36	5	412	G	C5-C6-O6	6.20	132.32	128.60
36	5	1170	A	C5-N7-C8	6.20	107.00	103.90
36	1	1305	U	C5-C6-N1	-6.19	119.60	122.70
36	1	874	U	C6-N1-C2	6.19	124.72	121.00
36	1	1581	C	N1-C2-O2	6.19	122.61	118.90
48	M1	112	LEU	CA-CB-CG	6.19	129.54	115.30
1	6	1539	G	N3-C4-C5	6.19	131.70	128.60
1	2	1560	U	N1-C2-N3	6.19	118.61	114.90
36	1	362	U	C2-N3-C4	-6.19	123.28	127.00
36	5	721	G	N1-C6-O6	-6.19	116.19	119.90
36	5	876	A	OP1-P-OP2	-6.19	110.31	119.60
36	1	324	A	N1-C2-N3	6.19	132.39	129.30
36	1	1447	G	O5'-P-OP2	-6.19	100.13	105.70
36	1	2868	U	C6-N1-C2	6.19	124.71	121.00
36	5	94	G	C2-N3-C4	6.19	114.99	111.90
36	5	1301	A	N1-C6-N6	6.19	122.31	118.60
36	1	910	G	N9-C4-C5	6.18	107.87	105.40
36	1	2818	U	C5'-C4'-O4'	-6.18	101.68	109.10
36	5	577	C	N1-C2-O2	-6.18	115.19	118.90
36	5	1314	C	C5-C4-N4	-6.18	115.87	120.20
36	5	1852	G	N1-C6-O6	-6.18	116.19	119.90
36	5	2663	G	C5-C6-O6	-6.18	124.89	128.60
1	2	1258	U	N3-C2-O2	-6.18	117.87	122.20
36	5	2531	C	N1-C2-O2	6.18	122.61	118.90
36	5	3317	U	N3-C2-O2	-6.18	117.87	122.20
36	1	2373	A	N7-C8-N9	6.18	116.89	113.80
36	5	2292	U	N1-C2-O2	6.18	127.13	122.80
36	1	1156	C	C5-C4-N4	6.18	124.53	120.20
36	5	2694	A	N9-C4-C5	6.18	108.27	105.80
36	5	1902	G	N3-C4-N9	6.18	129.71	126.00
36	5	107	A	N1-C6-N6	-6.18	114.89	118.60
36	5	150	A	C5-C6-N6	-6.18	118.76	123.70
36	1	694	C	N3-C4-C5	6.17	124.37	121.90
36	1	959	C	N3-C4-N4	6.17	122.32	118.00
36	5	2385	G	N9-C4-C5	-6.17	102.93	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2820	A	C8-N9-C4	-6.17	103.33	105.80
1	6	1634	C	C6-N1-C1'	-6.17	113.39	120.80
1	6	1456	C	N3-C2-O2	-6.17	117.58	121.90
36	1	2409	G	N9-C4-C5	6.17	107.87	105.40
36	1	186	U	N3-C4-C5	6.17	118.30	114.60
37	3	93	C	N3-C4-C5	6.17	124.37	121.90
36	5	2800	G	N3-C4-N9	-6.17	122.30	126.00
36	1	521	A	N9-C4-C5	-6.17	103.33	105.80
36	1	2649	A	N1-C2-N3	-6.17	126.22	129.30
36	5	645	A	C5-C6-N1	6.17	120.78	117.70
76	q0	102	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	2	75	U	N3-C2-O2	-6.16	117.89	122.20
36	5	921	A	OP1-P-OP2	-6.16	110.36	119.60
36	5	2935	U	C5-C4-O4	-6.16	122.20	125.90
1	2	1761	U	C5-C4-O4	6.16	129.60	125.90
36	1	1108	U	OP2-P-O3'	6.16	118.75	105.20
36	1	2887	A	O5'-P-OP2	-6.16	100.16	105.70
36	5	929	A	O5'-P-OP2	-6.16	100.16	105.70
36	5	2361	A	C8-N9-C4	-6.16	103.34	105.80
68	o2	33	ARG	NE-CZ-NH2	-6.16	117.22	120.30
36	1	641	C	N3-C4-C5	6.16	124.36	121.90
36	5	3197	G	C2-N3-C4	-6.16	108.82	111.90
36	1	2408	U	C2-N3-C4	-6.16	123.31	127.00
35	sM	167	PRO	N-CA-CB	6.16	110.69	103.30
36	5	801	A	O5'-P-OP2	-6.15	100.16	105.70
36	5	912	G	N1-C6-O6	-6.15	116.21	119.90
36	5	2234	G	N9-C4-C5	-6.15	102.94	105.40
1	2	144	U	N3-C2-O2	-6.15	117.89	122.20
36	1	2948	C	C6-N1-C2	6.15	122.76	120.30
1	6	970	A	P-O3'-C3'	6.15	127.08	119.70
36	5	1152	G	N1-C2-N3	6.15	127.59	123.90
36	1	1411	C	N3-C4-N4	-6.15	113.69	118.00
36	1	2366	C	O5'-P-OP1	6.15	118.08	110.70
36	1	2740	A	C8-N9-C4	-6.15	103.34	105.80
36	1	614	C	C6-N1-C2	6.15	122.76	120.30
36	1	2308	C	N1-C2-O2	-6.15	115.21	118.90
36	1	2645	G	N9-C4-C5	6.15	107.86	105.40
1	6	1082	C	O5'-P-OP2	-6.15	100.17	105.70
36	5	1113	G	N7-C8-N9	-6.15	110.03	113.10
36	5	2955	U	N3-C2-O2	-6.15	117.90	122.20
36	5	2400	G	C6-C5-N7	-6.14	126.71	130.40
36	5	2404	A	O5'-P-OP2	6.14	118.07	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2979	U	O4'-C1'-N1	-6.14	103.28	108.20
36	1	2719	U	N1-C2-N3	6.14	118.59	114.90
36	1	3147	G	N1-C6-O6	-6.14	116.21	119.90
36	5	2639	G	C6-C5-N7	-6.14	126.72	130.40
36	1	3181	C	C2-N3-C4	-6.14	116.83	119.90
1	6	400	A	OP2-P-O3'	6.14	118.71	105.20
36	5	1839	A	N1-C6-N6	-6.14	114.92	118.60
36	1	120	G	C8-N9-C4	6.14	108.86	106.40
1	6	754	A	N1-C6-N6	6.14	122.28	118.60
36	1	1371	G	N7-C8-N9	-6.14	110.03	113.10
36	5	942	U	O5'-P-OP1	6.14	118.07	110.70
36	5	1159	A	N1-C2-N3	-6.14	126.23	129.30
37	3	100	C	N3-C4-C5	-6.14	119.44	121.90
1	6	44	U	N1-C2-O2	-6.14	118.50	122.80
36	5	2289	U	C2-N1-C1'	6.14	125.06	117.70
36	1	32	U	C2-N3-C4	-6.13	123.32	127.00
36	1	329	U	C6-N1-C1'	6.13	129.79	121.20
36	5	820	A	C8-N9-C4	-6.13	103.35	105.80
36	5	1942	U	N1-C2-O2	-6.13	118.51	122.80
1	2	728	U	N3-C2-O2	-6.13	117.91	122.20
36	1	2302	G	N3-C2-N2	6.13	124.19	119.90
1	2	1572	G	C4-C5-N7	6.13	113.25	110.80
37	3	82	G	C5-C6-O6	6.13	132.28	128.60
1	6	315	A	N9-C4-C5	6.13	108.25	105.80
36	5	1130	A	C5-N7-C8	6.13	106.97	103.90
36	5	1290	A	OP2-P-O3'	6.13	118.69	105.20
56	n0	40	ARG	NE-CZ-NH1	6.13	123.37	120.30
36	1	1444	G	N9-C4-C5	-6.13	102.95	105.40
36	1	1656	A	C8-N9-C4	6.13	108.25	105.80
36	5	2630	C	C2-N3-C4	-6.13	116.83	119.90
36	5	2872	A	C5-C6-N6	6.13	128.60	123.70
36	1	882	A	O5'-P-OP1	-6.13	100.19	105.70
36	1	1843	C	O5'-P-OP2	-6.13	100.19	105.70
36	1	1852	G	C6-N1-C2	6.13	128.78	125.10
36	1	1931	U	C5-C6-N1	-6.13	119.64	122.70
36	1	3214	U	N3-C4-O4	-6.13	115.11	119.40
36	1	1536	G	O5'-P-OP2	-6.12	100.19	105.70
36	5	994	G	N1-C6-O6	-6.12	116.22	119.90
1	2	400	A	O4'-C1'-N9	6.12	113.10	108.20
1	2	1748	G	C5-C6-O6	6.12	132.27	128.60
1	6	380	U	N3-C2-O2	-6.12	117.91	122.20
36	5	3382	U	C2-N1-C1'	6.12	125.05	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	369	A	N9-C4-C5	6.12	108.25	105.80
36	1	3172	A	C8-N9-C4	6.12	108.25	105.80
36	5	640	U	OP1-P-OP2	-6.12	110.42	119.60
36	5	3217	C	C2-N1-C1'	-6.12	112.07	118.80
36	1	606	C	N3-C2-O2	-6.12	117.62	121.90
36	1	806	A	C5-C6-N6	-6.12	118.81	123.70
37	3	90	U	C5-C4-O4	-6.12	122.23	125.90
36	5	644	G	C8-N9-C4	-6.12	103.95	106.40
40	L3	186	GLY	N-CA-C	6.12	128.39	113.10
36	1	609	G	C4-C5-N7	6.12	113.25	110.80
36	1	650	C	N1-C2-O2	-6.12	115.23	118.90
36	1	970	A	C5-N7-C8	-6.12	100.84	103.90
36	1	2343	C	N3-C4-C5	6.12	124.35	121.90
36	1	2372	A	C2-N3-C4	6.12	113.66	110.60
36	5	1899	G	C8-N9-C4	-6.12	103.95	106.40
36	5	2295	A	N9-C4-C5	-6.11	103.36	105.80
36	5	2744	U	N3-C2-O2	-6.11	117.92	122.20
1	6	387	A	C5-N7-C8	6.11	106.96	103.90
36	5	1461	A	C8-N9-C4	6.11	108.25	105.80
1	2	553	G	N1-C2-N2	6.11	121.70	116.20
36	1	3143	C	O5'-P-OP2	-6.11	100.20	105.70
36	5	2151	C	C4-C5-C6	6.11	120.45	117.40
36	1	155	G	N3-C4-C5	-6.11	125.55	128.60
1	6	337	G	N9-C4-C5	-6.11	102.96	105.40
36	5	2281	A	C8-N9-C4	6.11	108.24	105.80
36	1	362	U	N3-C4-C5	6.11	118.26	114.60
36	1	1313	G	C4-C5-N7	6.11	113.24	110.80
36	1	1501	U	O5'-P-OP2	-6.11	100.20	105.70
36	1	2215	A	N9-C4-C5	-6.11	103.36	105.80
36	5	2290	C	C6-N1-C2	6.11	122.74	120.30
36	1	2604	U	N1-C2-O2	6.10	127.07	122.80
36	5	329	U	C2-N1-C1'	-6.10	110.38	117.70
36	1	1143	A	O5'-P-OP1	-6.10	100.21	105.70
36	1	1898	G	C5-C6-O6	-6.10	124.94	128.60
1	6	1121	C	C6-N1-C2	-6.10	117.86	120.30
36	1	284	A	O4'-C1'-N9	6.10	113.08	108.20
36	1	648	C	C6-N1-C2	-6.10	117.86	120.30
36	1	718	G	C4-C5-N7	6.10	113.24	110.80
36	1	1425	U	C5-C6-N1	-6.10	119.65	122.70
36	5	2366	C	C2-N1-C1'	6.10	125.51	118.80
36	5	2905	U	C2-N3-C4	-6.10	123.34	127.00
36	1	922	U	N3-C4-O4	-6.10	115.13	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2632	G	C5-C6-O6	6.10	132.26	128.60
1	6	314	C	O5'-P-OP1	-6.10	100.21	105.70
36	1	709	A	N9-C4-C5	-6.10	103.36	105.80
36	1	2159	U	O5'-P-OP1	-6.10	100.21	105.70
36	5	2118	C	N3-C2-O2	-6.10	117.63	121.90
36	1	1114	U	N1-C2-N3	-6.09	111.24	114.90
36	5	2385	G	C4-C5-N7	6.09	113.24	110.80
36	1	153	U	C6-N1-C2	-6.09	117.34	121.00
36	1	3309	G	C5-N7-C8	-6.09	101.25	104.30
36	5	951	A	O5'-P-OP2	-6.09	100.22	105.70
36	1	1294	A	O4'-C1'-N9	6.09	113.07	108.20
36	5	2838	A	O5'-P-OP1	6.09	118.01	110.70
36	1	971	G	C8-N9-C4	6.09	108.83	106.40
37	3	36	C	N3-C2-O2	-6.09	117.64	121.90
1	6	453	U	C5-C4-O4	6.09	129.55	125.90
36	5	2744	U	N1-C2-O2	6.09	127.06	122.80
1	6	1600	A	N9-C1'-C2'	6.08	121.91	114.00
36	5	640	U	C4-C5-C6	6.08	123.35	119.70
36	5	125	C	N3-C4-N4	-6.08	113.74	118.00
36	5	794	U	C6-N1-C2	-6.08	117.35	121.00
36	5	1421	G	N3-C4-C5	6.08	131.64	128.60
36	5	3195	U	P-O3'-C3'	6.08	127.00	119.70
36	1	1196	C	C2-N1-C1'	-6.08	112.11	118.80
36	1	2188	A	C5-N7-C8	6.08	106.94	103.90
36	1	1168	U	O5'-P-OP1	6.08	117.99	110.70
1	6	571	G	N3-C2-N2	-6.08	115.64	119.90
36	5	933	A	N1-C2-N3	6.08	132.34	129.30
36	5	2990	G	N3-C4-N9	6.08	129.65	126.00
36	5	2849	C	OP1-P-OP2	6.08	128.72	119.60
36	1	295	A	C8-N9-C4	-6.08	103.37	105.80
36	1	1405	U	C5-C6-N1	-6.08	119.66	122.70
36	1	2805	G	N1-C6-O6	-6.08	116.25	119.90
36	5	1388	U	N3-C4-C5	-6.08	110.95	114.60
36	5	2305	G	O4'-C1'-N9	6.08	113.06	108.20
36	1	2636	A	C8-N9-C4	-6.07	103.37	105.80
36	5	652	G	OP2-P-O3'	6.07	118.56	105.20
36	1	439	C	C5-C6-N1	6.07	124.04	121.00
37	3	83	U	C2-N3-C4	-6.07	123.36	127.00
38	4	39	G	N1-C6-O6	-6.07	116.26	119.90
36	5	767	U	O4'-C1'-N1	6.07	113.06	108.20
36	5	2341	A	C5-N7-C8	6.07	106.94	103.90
36	1	2699	G	O5'-P-OP2	-6.07	100.24	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2719	U	C2-N3-C4	-6.07	123.36	127.00
36	1	3375	A	C8-N9-C4	-6.07	103.37	105.80
36	5	339	C	C6-N1-C2	-6.07	117.87	120.30
36	1	63	A	C2-N3-C4	6.06	113.63	110.60
36	1	1192	C	C5-C6-N1	6.06	124.03	121.00
36	1	1919	G	N9-C4-C5	6.06	107.83	105.40
1	2	554	C	N1-C2-O2	6.06	122.54	118.90
36	1	1820	U	P-O3'-C3'	6.06	126.97	119.70
36	1	2846	U	N1-C2-N3	6.06	118.53	114.90
1	6	1781	A	C4-C5-C6	6.06	120.03	117.00
36	5	2340	U	C2-N3-C4	-6.06	123.36	127.00
1	2	18	C	C5-C6-N1	6.06	124.03	121.00
36	1	46	U	C5-C4-O4	6.06	129.53	125.90
36	1	859	G	C8-N9-C1'	-6.06	119.13	127.00
36	1	1192	C	C2-N1-C1'	6.06	125.46	118.80
1	6	647	G	N3-C4-N9	-6.06	122.36	126.00
36	5	2655	U	N3-C4-O4	-6.06	115.16	119.40
36	5	3128	G	N3-C4-N9	6.06	129.63	126.00
36	1	402	A	O5'-P-OP1	-6.06	100.25	105.70
36	1	2945	G	O5'-P-OP1	6.06	117.97	110.70
1	2	334	G	C2-N3-C4	-6.05	108.87	111.90
1	2	1291	G	N9-C4-C5	6.05	107.82	105.40
1	6	363	G	C5-C6-O6	-6.05	124.97	128.60
36	5	1894	U	OP1-P-OP2	6.05	128.68	119.60
36	5	2421	U	C5-C6-N1	-6.05	119.67	122.70
36	5	2697	A	O5'-P-OP1	-6.05	100.25	105.70
36	5	2865	U	C4-C5-C6	-6.05	116.07	119.70
1	6	2	A	O5'-P-OP1	-6.05	100.25	105.70
1	6	1726	G	OP2-P-O3'	6.05	118.51	105.20
36	5	2362	C	C6-N1-C2	-6.05	117.88	120.30
36	1	1411	C	N1-C2-O2	6.05	122.53	118.90
1	2	1200	G	C4-C5-C6	6.05	122.43	118.80
36	5	2361	A	N9-C4-C5	6.05	108.22	105.80
36	1	2653	C	N3-C2-O2	-6.05	117.67	121.90
36	1	3344	A	O4'-C1'-N9	6.05	113.04	108.20
37	3	88	G	C5-C6-O6	6.05	132.23	128.60
41	L4	206	LEU	CA-CB-CG	6.05	129.21	115.30
1	6	87	C	C6-N1-C2	-6.05	117.88	120.30
1	6	1514	U	N3-C2-O2	-6.05	117.97	122.20
36	5	2598	G	C5-C6-O6	-6.04	124.97	128.60
36	1	1869	C	N1-C2-O2	6.04	122.53	118.90
36	1	2817	A	OP1-P-OP2	-6.04	110.53	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2897	A	N7-C8-N9	-6.04	110.78	113.80
1	6	987	G	N1-C6-O6	6.04	123.53	119.90
36	5	1296	C	C6-N1-C2	-6.04	117.88	120.30
36	5	1430	U	C5-C6-N1	-6.04	119.68	122.70
1	2	1000	C	N3-C2-O2	-6.04	117.67	121.90
36	1	640	U	C4-C5-C6	6.04	123.33	119.70
1	6	558	U	C2-N1-C1'	6.04	124.95	117.70
36	1	1898	G	O4'-C1'-N9	6.04	113.03	108.20
36	1	2347	U	C4-C5-C6	-6.04	116.08	119.70
36	5	915	A	N3-C4-C5	-6.04	122.57	126.80
36	1	2679	A	N1-C2-N3	6.04	132.32	129.30
38	4	135	G	N9-C4-C5	6.04	107.81	105.40
36	5	960	U	N3-C2-O2	-6.04	117.97	122.20
36	1	1118	C	C4-C5-C6	6.03	120.42	117.40
36	1	2188	A	C4-C5-N7	-6.03	107.68	110.70
36	1	2397	A	O5'-P-OP2	-6.03	100.27	105.70
1	6	1631	A	C8-N9-C4	6.03	108.21	105.80
36	5	1308	A	N7-C8-N9	6.03	116.82	113.80
36	5	2176	U	N3-C2-O2	-6.03	117.98	122.20
36	5	2917	G	C5-C6-O6	-6.03	124.98	128.60
1	2	704	C	O4'-C1'-N1	6.03	113.02	108.20
36	1	407	A	O5'-P-OP1	6.03	117.94	110.70
36	5	633	C	C5-C6-N1	-6.03	117.98	121.00
36	1	2595	A	C4-C5-N7	6.03	113.72	110.70
1	6	1097	U	P-O3'-C3'	6.03	126.94	119.70
62	N6	57	LEU	CA-CB-CG	6.03	129.16	115.30
36	1	92	G	O5'-P-OP1	-6.03	100.28	105.70
36	5	953	G	O4'-C1'-N9	6.02	113.02	108.20
36	1	1838	G	OP1-P-O3'	6.02	118.45	105.20
36	1	2685	C	N3-C4-C5	-6.02	119.49	121.90
36	5	1113	G	N3-C4-C5	6.02	131.61	128.60
36	5	1544	G	N3-C2-N2	6.02	124.12	119.90
36	5	1884	A	C8-N9-C4	-6.02	103.39	105.80
36	1	153	U	N3-C4-C5	-6.02	110.99	114.60
36	1	143	G	N3-C4-C5	-6.02	125.59	128.60
36	1	818	C	N3-C2-O2	-6.02	117.69	121.90
36	1	974	G	N3-C4-C5	-6.02	125.59	128.60
36	1	1426	C	C5-C4-N4	6.02	124.41	120.20
36	5	1397	C	O5'-P-OP1	-6.02	100.28	105.70
36	5	2618	G	C5-C6-N1	6.02	114.51	111.50
36	5	386	A	C6-C5-N7	-6.02	128.09	132.30
36	5	2897	A	N1-C6-N6	-6.02	114.99	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
65	n9	18	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	2	1462	G	N9-C4-C5	-6.01	102.99	105.40
36	1	1325	U	N1-C2-O2	-6.01	118.59	122.80
36	1	2323	G	N3-C2-N2	6.01	124.11	119.90
36	1	2950	G	N7-C8-N9	6.01	116.11	113.10
36	1	1703	U	C5-C6-N1	6.01	125.71	122.70
36	1	2426	U	N3-C4-O4	-6.01	115.19	119.40
36	1	2899	C	C2-N3-C4	-6.01	116.89	119.90
1	6	1	U	N3-C2-O2	-6.01	117.99	122.20
1	6	542	A	C4-C5-C6	6.01	120.01	117.00
36	5	682	U	C6-N1-C2	6.01	124.61	121.00
1	2	1428	G	N3-C4-N9	-6.01	122.39	126.00
36	5	1908	A	N9-C4-C5	6.01	108.20	105.80
36	5	2234	G	C5-C6-O6	-6.01	124.99	128.60
36	1	93	C	C6-N1-C1'	6.01	128.01	120.80
36	1	2766	U	O5'-P-OP2	-6.01	100.29	105.70
36	1	2945	G	C5-C6-O6	-6.01	125.00	128.60
1	6	1129	U	N3-C4-O4	-6.01	115.19	119.40
36	5	1112	A	N1-C6-N6	6.01	122.20	118.60
36	5	1311	G	C5-C6-N1	6.01	114.50	111.50
36	5	1725	C	C5'-C4'-O4'	6.01	116.31	109.10
10	S8	172	ARG	NE-CZ-NH1	6.01	123.30	120.30
36	1	1095	U	C2-N1-C1'	-6.00	110.49	117.70
36	1	663	C	N1-C2-O2	-6.00	115.30	118.90
36	1	2307	G	C8-N9-C4	6.00	108.80	106.40
38	4	151	C	C5-C6-N1	6.00	124.00	121.00
36	1	2795	U	N3-C4-O4	-6.00	115.20	119.40
1	6	25	C	P-O3'-C3'	6.00	126.90	119.70
1	6	1568	C	C2-N1-C1'	6.00	125.40	118.80
36	5	872	U	N3-C4-C5	6.00	118.20	114.60
36	5	2371	G	C2-N3-C4	-6.00	108.90	111.90
36	5	2703	A	C8-N9-C4	-6.00	103.40	105.80
36	1	1412	G	N1-C6-O6	-6.00	116.30	119.90
1	2	543	C	N1-C2-O2	6.00	122.50	118.90
36	1	2756	C	C6-N1-C2	-6.00	117.90	120.30
36	5	1371	G	C4-C5-N7	-6.00	108.40	110.80
36	5	2400	G	C5-C6-O6	-6.00	125.00	128.60
36	5	3245	A	C8-N9-C4	-6.00	103.40	105.80
37	7	93	C	O5'-P-OP2	-6.00	100.30	105.70
36	5	793	C	C6-N1-C2	-6.00	117.90	120.30
36	5	915	A	N3-C4-N9	6.00	132.20	127.40
38	8	22	U	N3-C4-C5	6.00	118.20	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1891	A	C8-N9-C4	6.00	108.20	105.80
1	6	767	U	C5-C4-O4	6.00	129.50	125.90
1	6	1100	G	N3-C4-N9	6.00	129.60	126.00
36	5	2188	A	N7-C8-N9	-6.00	110.80	113.80
36	1	422	A	C2-N3-C4	5.99	113.60	110.60
1	6	10	G	C4-C5-N7	-5.99	108.40	110.80
1	6	595	G	O5'-P-OP2	-5.99	100.31	105.70
36	1	2291	A	OP1-P-O3'	5.99	118.38	105.20
36	5	1938	U	C5-C6-N1	-5.99	119.70	122.70
36	5	2979	U	OP1-P-O3'	5.99	118.38	105.20
36	5	1044	U	N3-C4-O4	-5.99	115.21	119.40
36	5	3105	U	N1-C2-O2	-5.99	118.61	122.80
37	7	48	U	C2-N3-C4	-5.99	123.41	127.00
1	2	767	U	N3-C2-O2	-5.99	118.01	122.20
36	1	1852	G	C8-N9-C4	5.99	108.80	106.40
36	1	69	C	C4-C5-C6	5.98	120.39	117.40
36	1	689	U	C2-N1-C1'	5.98	124.88	117.70
36	1	2314	U	N1-C2-O2	5.98	126.99	122.80
36	5	1802	C	N3-C4-N4	5.98	122.19	118.00
36	5	2800	G	N1-C2-N2	5.98	121.58	116.20
36	1	375	A	O5'-P-OP2	-5.98	100.31	105.70
36	1	1308	A	O5'-P-OP1	5.98	117.88	110.70
36	5	844	G	N7-C8-N9	-5.98	110.11	113.10
36	5	1115	G	C4-N9-C1'	5.98	134.28	126.50
36	5	2315	G	N3-C4-C5	5.98	131.59	128.60
37	7	96	U	OP2-P-O3'	5.98	118.36	105.20
36	1	2817	A	C6-N1-C2	-5.98	115.01	118.60
36	1	3210	A	N1-C6-N6	-5.98	115.01	118.60
36	1	2645	G	C4-C5-N7	-5.98	108.41	110.80
36	1	2280	A	N1-C6-N6	5.98	122.19	118.60
36	1	2298	U	C2-N3-C4	-5.98	123.41	127.00
1	6	75	U	O4'-C1'-N1	5.98	112.98	108.20
36	5	92	G	N3-C4-C5	-5.98	125.61	128.60
36	5	3009	G	C5-C6-O6	5.98	132.19	128.60
36	1	143	G	N9-C4-C5	5.98	107.79	105.40
36	1	1425	U	N1-C2-N3	5.98	118.49	114.90
20	c8	15	LEU	CA-CB-CG	5.98	129.04	115.30
36	5	2912	G	O5'-P-OP1	-5.98	100.32	105.70
36	5	3101	G	N3-C2-N2	5.98	124.08	119.90
36	1	702	C	C2-N3-C4	-5.97	116.91	119.90
36	1	1481	A	C6-C5-N7	-5.97	128.12	132.30
36	1	2877	G	N1-C6-O6	-5.97	116.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	740	G	N1-C6-O6	-5.97	116.31	119.90
36	5	1846	C	C5-C6-N1	-5.97	118.01	121.00
36	1	2392	C	C5-C4-N4	-5.97	116.02	120.20
36	5	2140	U	C5-C4-O4	5.97	129.48	125.90
1	6	14	C	C6-N1-C2	-5.97	117.91	120.30
36	5	3010	U	N1-C2-O2	5.97	126.98	122.80
36	5	971	G	OP2-P-O3'	5.97	118.33	105.20
36	1	789	A	N1-C2-N3	5.97	132.28	129.30
36	1	1841	A	C5-C6-N1	5.97	120.68	117.70
36	5	230	U	N1-C2-O2	-5.97	118.62	122.80
36	5	2260	U	O5'-P-OP1	-5.97	100.33	105.70
36	1	2370	G	O5'-P-OP2	-5.96	100.33	105.70
36	5	507	U	N1-C2-O2	5.96	126.97	122.80
36	5	2298	U	C2-N1-C1'	-5.96	110.54	117.70
36	5	2402	A	N1-C2-N3	5.96	132.28	129.30
36	5	2434	U	C5-C6-N1	-5.96	119.72	122.70
36	1	369	A	C2-N3-C4	5.96	113.58	110.60
1	6	355	G	OP2-P-O3'	5.96	118.32	105.20
36	5	1115	G	C6-C5-N7	-5.96	126.82	130.40
36	5	1604	G	C4-N9-C1'	5.96	134.25	126.50
1	6	322	G	O5'-P-OP1	-5.96	100.34	105.70
36	1	2851	A	C8-N9-C4	5.96	108.18	105.80
36	5	205	C	N3-C2-O2	-5.96	117.73	121.90
36	5	1883	A	N1-C6-N6	-5.96	115.03	118.60
36	1	1114	U	C4-C5-C6	-5.96	116.13	119.70
36	1	1797	A	O5'-P-OP1	-5.96	100.34	105.70
36	5	575	G	C8-N9-C4	-5.96	104.02	106.40
36	5	1496	C	C2-N1-C1'	5.96	125.35	118.80
36	5	1907	C	N3-C4-C5	-5.96	119.52	121.90
36	5	2364	G	N9-C4-C5	5.96	107.78	105.40
36	1	2871	G	C8-N9-C1'	5.96	134.74	127.00
36	5	412	G	C8-N9-C4	-5.96	104.02	106.40
36	5	1201	C	C6-N1-C1'	5.96	127.95	120.80
36	5	2968	G	C4-C5-N7	-5.96	108.42	110.80
1	2	1565	C	N1-C2-O2	-5.95	115.33	118.90
36	1	364	G	C5-C6-N1	5.95	114.48	111.50
36	1	922	U	C5-C6-N1	5.95	125.68	122.70
36	5	2857	C	C5-C4-N4	-5.95	116.03	120.20
36	1	406	G	N1-C6-O6	-5.95	116.33	119.90
36	1	1196	C	N1-C2-O2	-5.95	115.33	118.90
37	3	96	U	C6-N1-C2	5.95	124.57	121.00
1	6	359	A	C6-N1-C2	5.95	122.17	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3009	G	N1-C6-O6	-5.95	116.33	119.90
36	1	1520	G	C5-N7-C8	5.95	107.27	104.30
36	5	96	G	N3-C4-N9	-5.95	122.43	126.00
36	1	2165	G	C8-N9-C4	-5.95	104.02	106.40
41	L4	327	LEU	CA-CB-CG	5.95	128.97	115.30
36	5	2144	A	O4'-C1'-N9	5.95	112.96	108.20
41	l4	98	ARG	NE-CZ-NH2	-5.95	117.33	120.30
36	1	2754	G	O5'-P-OP2	-5.94	100.35	105.70
1	6	687	G	C6-C5-N7	5.94	133.97	130.40
36	5	326	U	C5-C4-O4	-5.94	122.33	125.90
36	5	2724	U	N1-C2-N3	5.94	118.47	114.90
36	1	2608	G	N7-C8-N9	-5.94	110.13	113.10
36	5	416	A	N9-C4-C5	5.94	108.18	105.80
36	5	3214	U	N1-C2-N3	5.94	118.47	114.90
38	8	32	C	N1-C2-O2	-5.94	115.33	118.90
36	1	1940	G	N1-C6-O6	-5.94	116.34	119.90
36	1	2356	A	C4-C5-N7	5.94	113.67	110.70
36	1	2403	G	C2-N3-C4	5.94	114.87	111.90
36	5	2630	C	N1-C2-O2	-5.94	115.34	118.90
36	1	1392	G	N1-C6-O6	5.94	123.46	119.90
36	1	2871	G	C4-N9-C1'	-5.94	118.78	126.50
36	5	1159	A	N9-C4-C5	-5.94	103.42	105.80
36	5	1314	C	C6-N1-C1'	-5.94	113.67	120.80
36	5	3049	A	C6-N1-C2	5.94	122.16	118.60
36	5	1863	G	C5-C6-N1	5.94	114.47	111.50
1	2	736	C	C2-N1-C1'	5.93	125.33	118.80
36	1	278	U	C6-N1-C2	-5.93	117.44	121.00
36	1	2389	C	C5-C6-N1	-5.93	118.03	121.00
36	5	3047	U	N1-C2-O2	5.93	126.95	122.80
36	5	1448	U	C5-C6-N1	-5.93	119.73	122.70
1	6	402	C	C5-C4-N4	-5.93	116.05	120.20
36	5	2366	C	N3-C4-N4	5.93	122.15	118.00
1	2	416	A	O5'-P-OP1	-5.92	100.37	105.70
1	2	1119	G	N1-C6-O6	-5.92	116.35	119.90
36	1	971	G	C5-N7-C8	5.92	107.26	104.30
36	5	922	U	C6-N1-C1'	5.92	129.49	121.20
36	5	44	U	C2-N3-C4	-5.92	123.45	127.00
1	2	779	U	O4'-C1'-N1	5.92	112.94	108.20
36	5	2882	U	N1-C2-N3	5.92	118.45	114.90
36	1	2811	A	C5-C6-N1	5.92	120.66	117.70
36	1	2874	G	C5-C6-O6	5.92	132.15	128.60
36	5	2376	G	N1-C6-O6	-5.92	116.35	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	618	C	N1-C2-O2	-5.92	115.35	118.90
36	5	2874	G	O5'-P-OP2	5.92	117.80	110.70
36	5	945	C	N3-C4-C5	5.92	124.27	121.90
36	1	610	G	N9-C4-C5	-5.92	103.03	105.40
36	1	2798	C	N3-C4-C5	-5.91	119.53	121.90
36	5	3128	G	C5-C6-O6	-5.91	125.05	128.60
36	1	1507	G	C5-N7-C8	5.91	107.26	104.30
36	1	686	G	N1-C6-O6	-5.91	116.35	119.90
36	1	3269	U	N1-C2-N3	5.91	118.45	114.90
1	6	16	G	N1-C6-O6	-5.91	116.35	119.90
36	5	662	U	C5-C4-O4	5.91	129.45	125.90
36	1	25	U	N3-C4-O4	5.91	123.54	119.40
36	5	401	U	O5'-P-OP2	-5.91	100.38	105.70
36	5	3020	U	N3-C4-O4	5.91	123.54	119.40
36	1	962	A	C6-N1-C2	-5.91	115.06	118.60
36	1	2846	U	O5'-P-OP1	-5.91	100.38	105.70
36	1	1122	U	N3-C4-C5	5.91	118.14	114.60
36	1	2821	C	N1-C2-O2	-5.91	115.36	118.90
64	N8	66	ALA	N-CA-C	-5.91	95.06	111.00
1	6	901	G	C4-C5-N7	5.91	113.16	110.80
36	5	1192	C	N3-C4-C5	5.91	124.26	121.90
36	5	1907	C	N1-C2-O2	-5.91	115.36	118.90
36	1	2380	U	N3-C4-C5	5.90	118.14	114.60
36	1	2892	A	N1-C6-N6	-5.90	115.06	118.60
36	5	1189	C	C6-N1-C2	5.90	122.66	120.30
36	5	2621	G	N3-C2-N2	-5.90	115.77	119.90
36	5	2758	A	C2-N3-C4	5.90	113.55	110.60
36	1	1113	G	C5-N7-C8	5.90	107.25	104.30
36	1	1481	A	O4'-C1'-N9	5.90	112.92	108.20
36	1	2787	G	C8-N9-C4	-5.90	104.04	106.40
36	5	2899	C	N3-C4-N4	-5.90	113.87	118.00
36	1	641	C	OP1-P-O3'	5.90	118.18	105.20
37	3	28	C	C6-N1-C2	-5.90	117.94	120.30
1	6	1560	U	N1-C2-O2	5.90	126.93	122.80
36	5	861	C	O5'-P-OP1	5.90	117.78	110.70
36	5	1592	G	C4-C5-N7	5.90	113.16	110.80
36	5	3003	G	C5-N7-C8	-5.90	101.35	104.30
36	1	1115	G	N3-C4-N9	5.90	129.54	126.00
36	1	1304	A	O5'-P-OP1	-5.90	100.39	105.70
36	1	2701	U	C5-C6-N1	-5.90	119.75	122.70
36	1	3318	G	C4-N9-C1'	5.90	134.17	126.50
36	5	1305	U	C2-N3-C4	-5.90	123.46	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2899	C	C2-N3-C4	-5.90	116.95	119.90
38	8	111	A	O5'-P-OP1	5.90	117.78	110.70
36	1	3173	G	N7-C8-N9	5.90	116.05	113.10
25	d3	73	ARG	NE-CZ-NH1	-5.90	117.35	120.30
36	1	2870	C	O4'-C1'-N1	5.89	112.92	108.20
36	5	386	A	N9-C4-C5	-5.89	103.44	105.80
36	5	998	A	OP2-P-O3'	5.89	118.17	105.20
36	1	86	G	O5'-P-OP2	-5.89	100.40	105.70
36	1	1931	U	C6-N1-C2	5.89	124.54	121.00
12	c0	83	PRO	N-CA-CB	5.89	110.37	103.30
36	5	1152	G	C5-C6-N1	-5.89	108.55	111.50
36	5	1833	G	C5-C6-N1	5.89	114.45	111.50
36	5	1863	G	N9-C1'-C2'	-5.89	105.52	112.00
1	2	610	G	C5-C6-O6	-5.89	125.06	128.60
36	1	1387	G	C5-C6-O6	5.89	132.13	128.60
36	5	813	G	N3-C4-C5	-5.89	125.66	128.60
36	1	1909	A	C2-N3-C4	-5.89	107.66	110.60
1	6	523	G	C8-N9-C4	5.89	108.76	106.40
36	5	2363	A	C8-N9-C4	-5.89	103.44	105.80
36	5	3047	U	C2-N3-C4	-5.89	123.47	127.00
1	2	74	U	O5'-P-OP1	-5.89	100.40	105.70
36	1	971	G	C5-C6-N1	5.89	114.44	111.50
36	1	1167	U	N3-C4-O4	-5.89	115.28	119.40
36	1	3053	G	C5-C6-O6	5.89	132.13	128.60
1	6	1096	C	N3-C2-O2	-5.89	117.78	121.90
36	1	214	G	N9-C4-C5	5.89	107.75	105.40
36	1	1431	G	N1-C6-O6	-5.89	116.37	119.90
36	1	2365	C	N1-C2-O2	5.88	122.43	118.90
36	1	2403	G	C4-N9-C1'	5.88	134.15	126.50
54	M8	99	THR	N-CA-C	5.88	126.89	111.00
36	5	1120	A	C4-C5-N7	-5.88	107.76	110.70
36	5	1655	G	C8-N9-C4	-5.88	104.05	106.40
36	5	1902	G	C5-C6-N1	5.88	114.44	111.50
1	2	1535	U	C6-N1-C1'	-5.88	112.97	121.20
36	5	648	C	C6-N1-C2	-5.88	117.95	120.30
36	5	646	A	N7-C8-N9	5.88	116.74	113.80
1	2	1416	G	N1-C6-O6	5.88	123.43	119.90
36	1	61	A	N1-C6-N6	5.88	122.13	118.60
36	5	963	G	C5-C6-N1	5.88	114.44	111.50
36	5	1316	C	N1-C2-O2	-5.88	115.37	118.90
36	1	1433	A	C5-C6-N1	5.88	120.64	117.70
36	1	1546	A	C2-N3-C4	5.88	113.54	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1693	C	N1-C2-O2	-5.88	115.38	118.90
36	5	2244	A	O5'-P-OP1	5.88	117.75	110.70
36	5	2754	G	N3-C4-C5	-5.88	125.66	128.60
36	5	2814	G	C4-C5-N7	5.88	113.15	110.80
36	1	44	U	N3-C4-C5	5.88	118.12	114.60
36	1	979	U	N3-C2-O2	-5.88	118.09	122.20
36	5	661	G	C8-N9-C4	-5.88	104.05	106.40
36	1	1476	G	N1-C6-O6	-5.87	116.38	119.90
1	6	879	G	N1-C6-O6	-5.87	116.38	119.90
36	5	2393	G	O5'-P-OP1	5.87	117.75	110.70
36	1	2389	C	C2-N3-C4	-5.87	116.96	119.90
36	1	2821	C	N3-C2-O2	5.87	126.01	121.90
1	6	422	G	C8-N9-C4	-5.87	104.05	106.40
36	5	909	G	C5-C6-O6	5.87	132.12	128.60
36	1	1305	U	N1-C2-O2	5.87	126.91	122.80
36	1	2621	G	N9-C4-C5	5.87	107.75	105.40
36	1	2871	G	N3-C4-N9	-5.87	122.48	126.00
36	1	2944	U	N1-C2-O2	5.87	126.91	122.80
36	5	150	A	N1-C6-N6	5.87	122.12	118.60
36	5	1420	C	OP2-P-O3'	5.87	118.11	105.20
36	1	2305	G	N1-C6-O6	5.87	123.42	119.90
36	1	2996	U	C6-N1-C1'	-5.87	112.99	121.20
36	5	283	G	C4-C5-N7	5.87	113.15	110.80
1	2	1560	U	C6-N1-C2	-5.87	117.48	121.00
36	1	1392	G	C5-C6-O6	-5.87	125.08	128.60
36	1	2679	A	O4'-C1'-N9	5.87	112.89	108.20
1	6	306	U	C5-C6-N1	-5.87	119.77	122.70
36	5	3075	G	OP1-P-O3'	5.87	118.11	105.20
36	1	114	A	C4-C5-N7	5.86	113.63	110.70
36	1	2123	G	N7-C8-N9	-5.86	110.17	113.10
36	5	877	C	C4-C5-C6	-5.86	114.47	117.40
36	5	908	G	N7-C8-N9	5.86	116.03	113.10
36	5	3218	A	C5-C6-N1	-5.86	114.77	117.70
36	5	3309	G	N3-C4-C5	-5.86	125.67	128.60
1	2	1559	A	O4'-C1'-N9	5.86	112.89	108.20
36	1	304	G	N1-C2-N3	-5.86	120.38	123.90
36	1	944	C	C4-C5-C6	-5.86	114.47	117.40
62	N6	6	LEU	CA-CB-CG	-5.86	101.82	115.30
36	5	2598	G	N1-C6-O6	5.86	123.42	119.90
1	2	1339	C	C5-C6-N1	5.86	123.93	121.00
36	1	931	C	N3-C4-C5	5.86	124.24	121.90
36	1	2634	U	C5-C6-N1	-5.86	119.77	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1040	G	N1-C6-O6	-5.86	116.38	119.90
36	5	2376	G	C8-N9-C1'	-5.86	119.38	127.00
1	6	1656	U	OP2-P-O3'	5.86	118.09	105.20
36	5	1849	C	N1-C2-O2	5.86	122.42	118.90
36	1	1103	A	C5-C6-N1	5.86	120.63	117.70
36	1	1336	U	C5-C4-O4	5.86	129.41	125.90
36	1	1371	G	C8-N9-C4	5.86	108.74	106.40
36	5	779	G	O5'-P-OP2	-5.86	100.43	105.70
36	5	914	A	C8-N9-C4	5.86	108.14	105.80
36	1	946	U	C2-N3-C4	-5.86	123.49	127.00
36	1	1307	G	P-O3'-C3'	5.86	126.73	119.70
36	1	2862	U	N1-C2-O2	5.86	126.90	122.80
36	5	1450	G	N1-C6-O6	-5.86	116.39	119.90
36	5	3217	C	C5-C6-N1	-5.86	118.07	121.00
36	1	2298	U	O4'-C1'-N1	5.85	112.88	108.20
36	5	777	U	O5'-P-OP2	-5.85	100.43	105.70
36	5	1121	U	N1-C2-O2	-5.85	118.70	122.80
36	5	1124	U	C4-C5-C6	-5.85	116.19	119.70
36	5	2160	G	N1-C2-N2	-5.85	110.93	116.20
1	6	90	C	N3-C2-O2	-5.85	117.81	121.90
36	5	110	G	O5'-P-OP1	5.85	117.72	110.70
36	5	929	A	N7-C8-N9	-5.85	110.88	113.80
36	5	941	G	N1-C6-O6	-5.85	116.39	119.90
36	1	1396	C	N3-C4-C5	5.85	124.24	121.90
36	5	1202	A	N7-C8-N9	5.85	116.72	113.80
36	5	2245	C	N3-C4-C5	-5.85	119.56	121.90
36	5	2894	C	C6-N1-C2	-5.85	117.96	120.30
36	5	2964	G	N1-C6-O6	-5.85	116.39	119.90
36	1	3303	G	O4'-C1'-N9	5.85	112.88	108.20
16	c4	35	GLY	N-CA-C	5.85	127.72	113.10
36	5	659	G	C5-C6-N1	5.85	114.42	111.50
36	1	76	G	N3-C4-C5	-5.84	125.68	128.60
36	1	1451	C	C5-C6-N1	-5.84	118.08	121.00
36	1	2811	A	N9-C4-C5	5.84	108.14	105.80
36	1	3057	U	C5-C6-N1	-5.84	119.78	122.70
38	4	6	U	C5-C4-O4	-5.84	122.39	125.90
36	1	3213	A	N1-C6-N6	5.84	122.11	118.60
36	5	1047	A	O5'-P-OP1	-5.84	100.44	105.70
36	5	2990	G	C5-C6-O6	-5.84	125.09	128.60
1	2	1596	C	N1-C2-O2	5.84	122.41	118.90
36	1	59	G	N3-C2-N2	5.84	123.99	119.90
36	1	1440	G	C6-N1-C2	5.84	128.60	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1536	G	C5-C6-O6	-5.84	125.09	128.60
1	6	1048	G	N9-C4-C5	-5.84	103.06	105.40
36	5	1466	G	O5'-P-OP1	-5.84	100.44	105.70
36	5	1902	G	O5'-P-OP1	-5.84	100.44	105.70
36	5	2314	U	C5-C4-O4	-5.84	122.39	125.90
36	1	1326	A	N9-C4-C5	5.84	108.14	105.80
36	1	2305	G	C5-C6-O6	-5.84	125.10	128.60
36	1	2634	U	N1-C2-N3	5.84	118.40	114.90
36	5	2666	C	N1-C2-O2	-5.84	115.40	118.90
36	1	421	G	C5-C6-O6	-5.84	125.10	128.60
1	6	453	U	N1-C2-O2	5.84	126.89	122.80
36	5	2991	A	C8-N9-C4	-5.84	103.47	105.80
1	6	874	C	N1-C2-O2	5.84	122.40	118.90
1	6	1149	G	N1-C6-O6	-5.84	116.40	119.90
36	5	2634	U	C5-C6-N1	-5.84	119.78	122.70
1	6	48	G	O5'-P-OP2	-5.83	100.45	105.70
1	6	630	A	N1-C6-N6	5.83	122.10	118.60
38	8	22	U	O4'-C1'-N1	5.83	112.87	108.20
36	1	1440	G	N1-C2-N3	-5.83	120.40	123.90
36	1	2768	U	C5-C6-N1	-5.83	119.78	122.70
36	5	1495	U	N3-C4-C5	-5.83	111.10	114.60
1	6	1010	C	C6-N1-C2	-5.83	117.97	120.30
1	6	1028	C	O5'-P-OP1	-5.83	100.45	105.70
36	5	1931	U	C6-N1-C2	5.83	124.50	121.00
36	5	2858	U	C2-N1-C1'	5.83	124.70	117.70
36	5	3154	C	N3-C2-O2	-5.83	117.82	121.90
36	1	1366	A	N1-C2-N3	-5.83	126.39	129.30
36	1	2883	U	C4-C5-C6	-5.83	116.20	119.70
1	6	633	U	C6-N1-C2	5.83	124.50	121.00
36	5	2148	U	C2-N3-C4	-5.83	123.50	127.00
36	5	2377	G	C2-N3-C4	5.83	114.81	111.90
36	1	2123	G	C8-N9-C4	5.83	108.73	106.40
1	6	142	G	C8-N9-C1'	-5.83	119.42	127.00
36	5	110	G	O4'-C1'-N9	5.83	112.86	108.20
36	5	2747	A	N1-C6-N6	-5.83	115.10	118.60
36	5	2981	U	N3-C4-C5	5.83	118.10	114.60
36	1	339	C	C5-C4-N4	5.83	124.28	120.20
12	c0	88	PRO	N-CA-CB	5.83	110.29	103.30
36	1	43	A	N1-C2-N3	-5.83	126.39	129.30
36	1	282	G	C2'-C3'-O3'	5.83	123.02	113.70
36	1	968	G	C5-C6-O6	5.83	132.09	128.60
36	5	3173	G	N7-C8-N9	5.83	116.01	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3183	A	C8-N9-C4	-5.83	103.47	105.80
40	l3	232	ARG	NE-CZ-NH1	5.83	123.21	120.30
36	1	39	A	C5-N7-C8	-5.82	100.99	103.90
36	1	407	A	O5'-P-OP2	-5.82	100.46	105.70
36	1	1846	C	O5'-P-OP1	-5.82	100.46	105.70
36	1	3151	U	O5'-P-OP2	-5.82	100.46	105.70
1	6	1144	U	OP2-P-O3'	5.82	118.01	105.20
36	1	862	U	C5-C6-N1	5.82	125.61	122.70
36	1	1368	U	C5-C6-N1	-5.82	119.79	122.70
36	1	2184	U	N3-C4-O4	5.82	123.48	119.40
36	1	2187	G	N1-C6-O6	5.82	123.39	119.90
36	1	2986	U	C2-N3-C4	-5.82	123.51	127.00
1	6	390	G	N3-C4-C5	-5.82	125.69	128.60
1	6	597	G	O5'-P-OP2	-5.82	100.46	105.70
36	5	967	A	N1-C6-N6	-5.82	115.11	118.60
36	5	1847	A	C8-N9-C4	5.82	108.13	105.80
1	2	992	A	C2-N3-C4	-5.82	107.69	110.60
36	1	163	C	C6-N1-C2	-5.82	117.97	120.30
36	1	3078	U	C5-C4-O4	5.82	129.39	125.90
36	5	1888	U	C5-C6-N1	-5.82	119.79	122.70
36	5	911	C	N3-C4-N4	5.82	122.07	118.00
38	8	108	C	C6-N1-C2	-5.82	117.97	120.30
36	5	959	C	C5-C4-N4	-5.82	116.13	120.20
37	7	41	G	N9-C4-C5	-5.82	103.07	105.40
51	M5	105	ARG	NE-CZ-NH1	5.81	123.21	120.30
36	5	2302	G	C5-C6-O6	5.81	132.09	128.60
36	5	2377	G	N1-C6-O6	-5.81	116.41	119.90
36	1	2283	G	N1-C6-O6	5.81	123.39	119.90
36	1	2608	G	C8-N9-C4	5.81	108.72	106.40
45	L8	189	LEU	CA-CB-CG	5.81	128.66	115.30
1	6	144	U	O4'-C1'-N1	5.81	112.85	108.20
36	5	1872	C	C4-C5-C6	5.81	120.31	117.40
36	1	53	G	N3-C4-N9	5.81	129.49	126.00
36	1	645	A	C5-N7-C8	5.81	106.81	103.90
36	1	2323	G	N1-C6-O6	-5.81	116.41	119.90
36	5	1120	A	OP2-P-O3'	5.81	117.98	105.20
36	5	2800	G	C4-C5-N7	-5.81	108.48	110.80
36	5	2909	U	C5-C4-O4	-5.81	122.41	125.90
36	1	964	G	OP2-P-O3'	5.81	117.98	105.20
1	6	102	U	O5'-P-OP1	-5.81	100.47	105.70
1	6	194	U	N3-C2-O2	-5.81	118.14	122.20
36	5	2772	C	N3-C2-O2	5.81	125.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2141	U	N3-C2-O2	-5.81	118.14	122.20
36	1	2306	C	N1-C2-O2	-5.81	115.42	118.90
1	2	113	U	N1-C2-O2	-5.80	118.74	122.80
1	2	1241	G	C5-N7-C8	-5.80	101.40	104.30
36	5	2816	G	N9-C4-C5	5.80	107.72	105.40
36	5	2996	U	O5'-P-OP1	5.80	117.67	110.70
36	5	3339	A	N1-C6-N6	5.80	122.08	118.60
1	2	1324	G	N3-C2-N2	-5.80	115.84	119.90
36	1	346	C	OP2-P-O3'	5.80	117.97	105.20
36	1	49	A	N1-C6-N6	5.80	122.08	118.60
36	1	2727	A	O4'-C1'-N9	-5.80	103.56	108.20
1	6	1489	U	N3-C2-O2	-5.80	118.14	122.20
36	5	376	G	C5-C6-N1	5.80	114.40	111.50
36	1	1839	A	N1-C6-N6	-5.80	115.12	118.60
1	6	2	A	C8-N9-C4	5.80	108.12	105.80
36	5	692	A	O5'-P-OP1	-5.80	100.48	105.70
36	5	1044	U	C5-C6-N1	-5.80	119.80	122.70
38	8	112	U	C2-N1-C1'	-5.80	110.74	117.70
36	5	1303	A	O5'-P-OP1	-5.80	100.48	105.70
36	1	1319	G	N1-C6-O6	-5.80	116.42	119.90
36	1	2133	U	O4'-C1'-N1	5.80	112.84	108.20
36	1	2935	U	C2-N3-C4	5.80	130.48	127.00
36	5	2350	C	N1-C2-N3	5.80	123.26	119.20
36	1	885	U	C5-C6-N1	-5.79	119.80	122.70
36	1	2412	G	OP1-P-O3'	5.79	117.95	105.20
36	1	2800	G	C5-N7-C8	5.79	107.20	104.30
1	6	874	C	N3-C2-O2	-5.79	117.84	121.90
36	5	341	G	OP1-P-O3'	5.79	117.95	105.20
36	5	643	U	N3-C2-O2	5.79	126.26	122.20
36	5	2388	U	C5-C6-N1	-5.79	119.80	122.70
36	1	1437	C	C6-N1-C2	-5.79	117.98	120.30
36	1	2640	A	N1-C6-N6	-5.79	115.12	118.60
1	6	782	U	C2-N1-C1'	5.79	124.65	117.70
36	5	2889	C	N1-C2-O2	5.79	122.38	118.90
36	5	3094	A	N1-C6-N6	-5.79	115.12	118.60
1	2	1535	U	N1-C2-O2	5.79	126.86	122.80
38	4	32	C	C6-N1-C1'	5.79	127.75	120.80
1	2	1611	A	N1-C2-N3	5.79	132.19	129.30
36	1	2275	A	O5'-P-OP1	-5.79	100.49	105.70
36	1	2950	G	C5-C6-N1	5.79	114.39	111.50
69	O3	67	MET	CG-SD-CE	-5.79	90.94	100.20
1	6	1	U	N1-C2-O2	5.79	126.85	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1784	C	O5'-P-OP1	-5.79	100.49	105.70
36	5	437	G	C8-N9-C4	-5.79	104.08	106.40
36	5	878	G	N1-C6-O6	5.79	123.37	119.90
36	5	922	U	C2-N1-C1'	-5.79	110.75	117.70
36	5	1404	G	C5-C6-O6	5.79	132.07	128.60
38	4	17	A	OP1-P-OP2	-5.78	110.92	119.60
36	5	636	C	C2-N3-C4	-5.78	117.01	119.90
37	7	120	C	C5-C6-N1	-5.78	118.11	121.00
36	1	3270	U	O5'-P-OP1	-5.78	100.50	105.70
1	6	1082	C	C2-N1-C1'	5.78	125.16	118.80
36	5	908	G	N3-C4-C5	-5.78	125.71	128.60
36	1	2920	U	N3-C2-O2	-5.78	118.15	122.20
38	4	23	U	C5-C6-N1	-5.78	119.81	122.70
36	5	1426	C	N1-C2-O2	-5.78	115.43	118.90
36	5	2976	A	C5-C6-N1	5.78	120.59	117.70
36	1	189	G	N3-C2-N2	5.78	123.94	119.90
36	1	2376	G	C5-C6-N1	5.78	114.39	111.50
36	1	2732	G	N1-C2-N2	-5.78	111.00	116.20
1	6	1036	A	N9-C4-C5	5.78	108.11	105.80
36	5	1520	G	OP2-P-O3'	5.78	117.91	105.20
1	2	553	G	C4-C5-C6	5.78	122.27	118.80
1	2	1218	G	N1-C6-O6	5.78	123.37	119.90
36	1	24	G	C5-C6-O6	-5.78	125.13	128.60
36	1	424	G	C8-N9-C4	5.78	108.71	106.40
36	1	829	U	N3-C2-O2	-5.78	118.16	122.20
36	1	1132	C	N3-C2-O2	-5.78	117.86	121.90
36	5	1419	A	N7-C8-N9	-5.78	110.91	113.80
36	5	1607	U	N3-C4-O4	-5.78	115.36	119.40
36	5	2370	G	C5-C6-N1	5.78	114.39	111.50
36	1	1178	G	N1-C6-O6	-5.78	116.44	119.90
36	5	2190	U	N3-C2-O2	-5.78	118.16	122.20
1	2	1595	U	N1-C2-O2	-5.77	118.76	122.80
36	5	1855	U	C5-C6-N1	-5.77	119.81	122.70
1	6	1172	G	O5'-P-OP1	-5.77	100.51	105.70
1	2	1731	A	N1-C2-N3	-5.77	126.42	129.30
36	1	674	G	C4-C5-N7	-5.77	108.49	110.80
1	6	1584	G	OP1-P-O3'	5.77	117.89	105.20
36	5	1203	A	O5'-P-OP1	-5.77	100.51	105.70
36	5	2113	A	C4-N9-C1'	-5.77	115.92	126.30
36	5	2643	A	C4-C5-N7	5.77	113.58	110.70
36	1	826	G	O5'-P-OP1	-5.77	100.51	105.70
36	1	670	C	C2-N3-C4	-5.77	117.02	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2711	C	C6-N1-C2	-5.77	117.99	120.30
36	1	1724	U	O4'-C1'-N1	5.76	112.81	108.20
36	1	2314	U	C5-C4-O4	-5.76	122.44	125.90
36	1	2631	U	C5-C4-O4	5.76	129.36	125.90
38	4	90	U	C5-C6-N1	-5.76	119.82	122.70
1	6	297	U	N3-C4-O4	5.76	123.43	119.40
36	5	2421	U	N1-C2-N3	5.76	118.36	114.90
36	1	802	C	C4-C5-C6	5.76	120.28	117.40
38	4	47	C	O5'-P-OP1	5.76	117.61	110.70
1	6	402	C	N3-C4-C5	5.76	124.20	121.90
36	5	2880	U	C6-N1-C2	-5.76	117.55	121.00
1	2	1596	C	N3-C4-N4	-5.76	113.97	118.00
1	6	1101	G	C5-C6-O6	5.76	132.05	128.60
36	1	223	U	N1-C2-O2	-5.75	118.77	122.80
36	5	404	G	O5'-P-OP2	-5.75	100.52	105.70
36	5	989	A	OP2-P-O3'	5.75	117.86	105.20
36	1	806	A	O5'-P-OP1	-5.75	100.52	105.70
36	1	2945	G	N1-C6-O6	5.75	123.35	119.90
36	1	3092	C	C6-N1-C1'	5.75	127.70	120.80
36	5	1445	U	N3-C2-O2	5.75	126.23	122.20
36	5	2330	C	N1-C2-O2	-5.75	115.45	118.90
77	q1	9	ARG	NE-CZ-NH2	-5.75	117.42	120.30
36	1	972	A	N7-C8-N9	-5.75	110.92	113.80
1	6	1748	G	O5'-P-OP2	5.75	117.60	110.70
36	5	693	A	N1-C6-N6	-5.75	115.15	118.60
36	5	1188	U	C5-C4-O4	-5.75	122.45	125.90
36	5	1592	G	N1-C2-N2	-5.75	111.02	116.20
36	5	1848	G	N1-C6-O6	5.75	123.35	119.90
36	5	423	A	C2-N3-C4	5.75	113.47	110.60
36	1	271	C	N1-C2-O2	5.75	122.35	118.90
36	1	360	G	C6-C5-N7	-5.75	126.95	130.40
36	1	887	G	N1-C6-O6	5.75	123.35	119.90
36	1	2396	G	C4-C5-C6	5.75	122.25	118.80
36	1	2599	U	C6-N1-C2	-5.75	117.55	121.00
36	1	2624	G	C5-C6-O6	-5.75	125.15	128.60
36	1	2868	U	C2-N3-C4	-5.75	123.55	127.00
1	6	1000	C	C2-N1-C1'	5.75	125.12	118.80
36	5	1330	A	OP1-P-OP2	5.75	128.22	119.60
36	5	1387	G	O5'-P-OP1	-5.75	100.53	105.70
36	1	817	A	N9-C1'-C2'	5.75	121.47	114.00
38	4	109	A	C5-C6-N6	-5.75	119.10	123.70
36	5	2298	U	N3-C4-O4	-5.75	115.38	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2808	A	C4-C5-N7	5.75	113.57	110.70
36	1	648	C	O5'-P-OP1	-5.75	100.53	105.70
36	1	1167	U	N3-C4-C5	5.75	118.05	114.60
38	4	46	G	C4-C5-N7	-5.75	108.50	110.80
36	5	426	G	C8-N9-C4	5.75	108.70	106.40
36	1	916	G	C5-C6-O6	5.74	132.05	128.60
36	5	2777	G	C5-C6-O6	5.74	132.05	128.60
36	1	63	A	N1-C2-N3	-5.74	126.43	129.30
36	1	2142	A	O5'-P-OP2	5.74	117.59	110.70
1	6	431	C	O5'-P-OP1	-5.74	100.53	105.70
1	6	594	A	OP1-P-O3'	5.74	117.83	105.20
36	5	3016	A	OP1-P-O3'	-5.74	92.57	105.20
36	1	66	A	O5'-P-OP1	-5.74	100.53	105.70
36	1	186	U	N1-C2-O2	5.74	126.82	122.80
36	1	1450	G	N9-C4-C5	-5.74	103.11	105.40
36	1	2363	A	C5-C6-N6	5.74	128.29	123.70
36	1	2865	U	OP2-P-O3'	5.74	117.83	105.20
1	6	403	G	N9-C4-C5	-5.74	103.10	105.40
36	5	661	G	N1-C2-N3	-5.74	120.46	123.90
36	1	2227	C	P-O3'-C3'	5.74	126.58	119.70
37	7	5	G	N9-C4-C5	-5.74	103.11	105.40
6	S4	164	LEU	CA-CB-CG	5.74	128.49	115.30
18	C6	40	GLU	C-N-CA	5.74	146.09	122.00
36	1	620	U	N1-C1'-C2'	5.74	121.46	114.00
36	1	1122	U	C2-N3-C4	-5.74	123.56	127.00
36	1	1131	G	O5'-P-OP2	-5.74	100.54	105.70
36	1	2201	G	N3-C2-N2	5.74	123.91	119.90
36	5	895	A	C5'-C4'-O4'	5.74	115.98	109.10
36	5	3245	A	N3-C4-C5	5.74	130.82	126.80
52	m6	78	ARG	NE-CZ-NH2	-5.74	117.43	120.30
36	1	410	U	N1-C2-O2	-5.73	118.79	122.80
36	1	1305	U	N3-C4-C5	5.73	118.04	114.60
36	5	2335	G	C5-C6-O6	-5.73	125.16	128.60
41	l4	300	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	2	720	G	OP1-P-O3'	5.73	117.81	105.20
36	1	1476	G	C8-N9-C4	5.73	108.69	106.40
1	6	308	C	N3-C2-O2	-5.73	117.89	121.90
36	5	61	A	C2-N3-C4	-5.73	107.73	110.60
36	5	1475	A	O5'-P-OP2	-5.73	100.54	105.70
36	5	2144	A	N1-C6-N6	5.73	122.04	118.60
36	5	1297	C	C2-N3-C4	-5.73	117.03	119.90
36	1	1552	G	C5-C6-O6	-5.73	125.16	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2870	C	N3-C4-C5	5.73	124.19	121.90
1	2	1517	U	O5'-P-OP2	-5.73	100.55	105.70
36	1	221	A	N1-C2-N3	5.73	132.16	129.30
36	1	304	G	N9-C4-C5	5.73	107.69	105.40
36	1	674	G	N9-C4-C5	5.73	107.69	105.40
36	1	1888	U	C2-N3-C4	-5.73	123.56	127.00
1	6	287	G	C5-C6-O6	-5.73	125.16	128.60
36	5	3138	U	N1-C2-O2	-5.73	118.79	122.80
36	1	609	G	N3-C4-N9	5.73	129.44	126.00
36	1	801	A	O5'-P-OP1	5.73	117.57	110.70
36	1	973	A	C8-N9-C4	-5.73	103.51	105.80
36	1	2281	A	N9-C4-C5	-5.73	103.51	105.80
1	2	810	G	C6-C5-N7	-5.72	126.97	130.40
1	2	1119	G	C5-C6-O6	5.72	132.03	128.60
36	1	2368	A	C8-N9-C4	5.72	108.09	105.80
36	5	1133	A	C5-N7-C8	5.72	106.76	103.90
36	5	1391	C	C5-C4-N4	-5.72	116.19	120.20
1	6	1078	C	N3-C4-N4	-5.72	114.00	118.00
36	5	37	U	C6-N1-C2	-5.72	117.57	121.00
1	2	810	G	C4-C5-N7	5.72	113.09	110.80
36	5	96	G	C5-C6-O6	5.72	132.03	128.60
36	5	186	U	N1-C2-O2	5.72	126.80	122.80
36	5	218	G	O5'-P-OP1	-5.72	100.55	105.70
36	5	1878	G	C8-N9-C1'	-5.72	119.56	127.00
36	5	2412	G	N1-C6-O6	-5.72	116.47	119.90
36	5	3115	C	C6-N1-C2	-5.72	118.01	120.30
36	5	1219	C	N3-C4-C5	5.72	124.19	121.90
36	1	1124	U	OP2-P-O3'	5.72	117.78	105.20
36	1	2434	U	N3-C2-O2	-5.72	118.20	122.20
41	L4	139	GLY	N-CA-C	-5.72	98.81	113.10
36	5	1107	C	OP2-P-O3'	5.72	117.78	105.20
36	5	2249	G	C8-N9-C4	-5.72	104.11	106.40
36	1	23	A	C5-C6-N6	-5.71	119.13	123.70
36	1	1123	U	C5-C6-N1	-5.71	119.84	122.70
1	6	1535	U	P-O3'-C3'	5.71	126.56	119.70
36	5	1154	A	C5-C6-N1	5.71	120.56	117.70
36	5	2250	G	N1-C6-O6	-5.71	116.47	119.90
36	1	371	G	N3-C2-N2	5.71	123.90	119.90
36	1	1664	G	N1-C6-O6	-5.71	116.47	119.90
36	1	2827	U	O4'-C1'-N1	5.71	112.77	108.20
1	6	554	C	N3-C2-O2	-5.71	117.90	121.90
36	5	2287	C	C4-C5-C6	-5.71	114.54	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2968	G	C6-C5-N7	5.71	133.83	130.40
1	2	1455	G	N3-C2-N2	-5.71	115.90	119.90
36	1	2893	C	OP1-P-OP2	5.71	128.17	119.60
37	3	96	U	C5-C6-N1	-5.71	119.84	122.70
1	6	362	G	N3-C4-N9	5.71	129.43	126.00
36	5	436	A	N7-C8-N9	5.71	116.66	113.80
36	1	1592	G	N3-C2-N2	5.71	123.90	119.90
36	1	2391	G	C5-C6-O6	5.71	132.03	128.60
36	5	1487	G	C8-N9-C4	-5.71	104.12	106.40
36	5	2593	A	P-O3'-C3'	5.71	126.55	119.70
36	1	975	C	OP1-P-OP2	5.71	128.16	119.60
36	1	1906	G	N3-C4-C5	-5.71	125.75	128.60
36	1	2813	A	C4-C5-N7	-5.71	107.85	110.70
36	5	775	A	C8-N9-C4	-5.71	103.52	105.80
36	5	953	G	C5-C6-O6	-5.71	125.18	128.60
1	2	380	U	N1-C2-O2	5.71	126.79	122.80
36	1	661	G	C4-N9-C1'	5.71	133.92	126.50
36	1	2800	G	C6-N1-C2	-5.71	121.68	125.10
36	1	2960	C	N3-C4-C5	5.71	124.18	121.90
1	6	174	U	C5-C4-O4	-5.71	122.48	125.90
37	3	102	A	N9-C4-C5	-5.70	103.52	105.80
1	6	66	U	P-O3'-C3'	5.70	126.54	119.70
36	5	1189	C	C5-C4-N4	-5.70	116.21	120.20
36	5	1487	G	N1-C6-O6	-5.70	116.48	119.90
1	2	1196	A	P-O3'-C3'	5.70	126.54	119.70
36	1	507	U	O5'-P-OP1	5.70	117.54	110.70
36	5	1481	A	C8-N9-C4	-5.70	103.52	105.80
38	4	125	U	N3-C2-O2	-5.70	118.21	122.20
1	6	425	A	O5'-P-OP1	5.70	117.54	110.70
36	5	1931	U	N3-C4-O4	-5.70	115.41	119.40
37	7	7	G	O5'-P-OP1	5.70	117.54	110.70
38	8	8	C	C6-N1-C2	-5.70	118.02	120.30
36	1	2621	G	N3-C2-N2	-5.70	115.91	119.90
36	5	213	A	O5'-P-OP2	-5.70	100.57	105.70
36	1	3271	G	N1-C6-O6	5.70	123.32	119.90
36	5	2402	A	OP2-P-O3'	5.70	117.73	105.20
36	5	2944	U	C2-N3-C4	-5.70	123.58	127.00
36	5	3062	G	C8-N9-C4	-5.70	104.12	106.40
36	1	2819	A	C2-N3-C4	5.70	113.45	110.60
36	1	3305	A	O5'-P-OP2	-5.70	100.58	105.70
1	6	1269	U	N3-C2-O2	-5.70	118.21	122.20
36	5	513	G	N1-C6-O6	-5.70	116.48	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	112	U	O4'-C1'-N1	5.69	112.75	108.20
36	1	1189	C	C2-N3-C4	-5.69	117.05	119.90
36	5	509	U	O5'-P-OP1	-5.69	100.58	105.70
36	1	297	G	O4'-C1'-N9	5.69	112.75	108.20
36	5	26	A	C8-N9-C4	5.69	108.08	105.80
36	5	2335	G	C6-N1-C2	-5.69	121.68	125.10
36	1	718	G	C4-C5-C6	-5.69	115.39	118.80
36	1	764	U	P-O3'-C3'	5.69	126.53	119.70
36	1	1365	G	N3-C2-N2	5.69	123.88	119.90
36	1	1389	G	N9-C4-C5	-5.69	103.12	105.40
36	1	1888	U	C5-C6-N1	-5.69	119.86	122.70
36	1	2305	G	N9-C4-C5	-5.69	103.12	105.40
36	5	518	G	O4'-C1'-N9	5.69	112.75	108.20
36	5	2836	C	C5-C6-N1	-5.69	118.16	121.00
36	5	3004	C	N1-C2-O2	-5.69	115.49	118.90
69	o3	73	ARG	NE-CZ-NH1	-5.69	117.45	120.30
36	1	53	G	C5-C6-N1	5.69	114.34	111.50
36	1	2362	C	O5'-P-OP2	-5.69	100.58	105.70
36	5	202	G	N1-C2-N2	-5.69	111.08	116.20
36	5	339	C	C2-N1-C1'	-5.69	112.54	118.80
36	5	1161	G	C5-C6-N1	5.69	114.34	111.50
36	1	1366	A	C6-N1-C2	5.69	122.01	118.60
36	1	1661	G	O5'-P-OP2	-5.69	100.58	105.70
36	1	2226	U	O5'-P-OP2	5.69	117.53	110.70
1	6	390	G	N3-C4-N9	5.69	129.41	126.00
1	6	1124	A	N9-C4-C5	-5.69	103.53	105.80
36	5	1048	A	OP1-P-O3'	5.69	117.71	105.20
36	5	2656	A	C8-N9-C4	-5.69	103.53	105.80
1	2	734	A	P-O3'-C3'	5.69	126.52	119.70
36	1	1841	A	N3-C4-C5	-5.69	122.82	126.80
36	1	2198	A	N7-C8-N9	-5.69	110.96	113.80
36	1	2651	G	N3-C4-N9	-5.69	122.59	126.00
1	6	65	A	C4-C5-N7	5.69	113.54	110.70
1	2	992	A	N3-C4-C5	5.68	130.78	126.80
36	1	143	G	C2-N3-C4	5.68	114.74	111.90
36	1	2790	A	N1-C6-N6	-5.68	115.19	118.60
36	1	3209	A	C4-C5-N7	5.68	113.54	110.70
36	1	2632	G	N1-C2-N2	-5.68	111.08	116.20
36	1	2818	U	O5'-P-OP2	-5.68	100.59	105.70
36	5	1186	G	C8-N9-C4	-5.68	104.13	106.40
36	5	2403	G	C5-C6-O6	5.68	132.01	128.60
36	5	2743	A	N7-C8-N9	-5.68	110.96	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	320	U	N3-C2-O2	5.68	126.18	122.20
36	5	437	G	C6-C5-N7	5.68	133.81	130.40
36	1	1513	G	C5-C6-N1	5.68	114.34	111.50
1	6	4	C	O5'-P-OP1	-5.68	100.59	105.70
1	6	542	A	P-O3'-C3'	5.68	126.52	119.70
36	5	780	A	N1-C2-N3	-5.68	126.46	129.30
36	5	903	U	N3-C4-C5	5.68	118.01	114.60
36	5	1833	G	C8-N9-C4	5.68	108.67	106.40
36	1	422	A	C5-C6-N1	5.68	120.54	117.70
36	1	903	U	N3-C2-O2	-5.68	118.23	122.20
1	6	321	C	N1-C2-O2	5.68	122.31	118.90
1	6	1620	C	C6-N1-C2	-5.68	118.03	120.30
36	1	1859	A	N7-C8-N9	-5.68	110.96	113.80
36	1	2867	C	C4-C5-C6	-5.68	114.56	117.40
36	5	778	U	N1-C2-O2	5.68	126.77	122.80
36	1	1420	C	C5-C4-N4	5.67	124.17	120.20
36	1	1857	C	N1-C2-O2	-5.67	115.50	118.90
36	5	1116	G	C5-C6-O6	5.67	132.00	128.60
36	5	2639	G	N3-C4-C5	-5.67	125.76	128.60
36	5	2913	C	N1-C2-O2	-5.67	115.50	118.90
36	1	2367	A	O5'-P-OP1	-5.67	100.59	105.70
36	1	3204	C	N3-C4-C5	5.67	124.17	121.90
1	6	313	U	C2-N3-C4	-5.67	123.60	127.00
36	1	420	G	O5'-P-OP2	-5.67	100.60	105.70
36	5	1412	G	C8-N9-C4	-5.67	104.13	106.40
36	1	765	C	C6-N1-C2	-5.67	118.03	120.30
38	4	9	A	C8-N9-C4	-5.67	103.53	105.80
36	5	926	A	C5-C6-N6	-5.67	119.17	123.70
36	5	2531	C	C6-N1-C1'	-5.67	114.00	120.80
36	5	2894	C	C5-C6-N1	5.67	123.83	121.00
1	2	432	G	C2-N3-C4	5.67	114.73	111.90
1	2	1634	C	C6-N1-C2	5.67	122.57	120.30
36	1	272	G	C5-N7-C8	5.67	107.13	104.30
36	1	2148	U	N3-C2-O2	5.67	126.17	122.20
36	1	2983	C	C5-C6-N1	-5.67	118.17	121.00
36	5	1302	A	OP2-P-O3'	5.67	117.66	105.20
36	1	963	G	O5'-P-OP1	5.67	117.50	110.70
36	5	3032	A	C2-N3-C4	5.67	113.43	110.60
36	1	2297	U	N3-C4-C5	5.66	118.00	114.60
38	4	25	G	O5'-P-OP1	5.66	117.50	110.70
36	5	2426	U	C5-C4-O4	5.66	129.30	125.90
36	1	204	A	C2-N3-C4	5.66	113.43	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2651	G	C6-C5-N7	5.66	133.80	130.40
36	5	3223	A	N1-C6-N6	-5.66	115.20	118.60
36	5	2127	U	O5'-P-OP1	-5.66	100.61	105.70
36	1	1442	U	C5-C6-N1	5.66	125.53	122.70
1	6	1781	A	C5-C6-N1	-5.66	114.87	117.70
36	5	887	G	N1-C2-N2	-5.66	111.11	116.20
36	5	2857	C	C6-N1-C2	5.66	122.56	120.30
37	7	5	G	C8-N9-C4	5.66	108.66	106.40
37	7	112	G	C8-N9-C4	-5.66	104.14	106.40
36	1	2180	G	N9-C4-C5	5.66	107.66	105.40
37	3	81	U	N1-C2-O2	5.66	126.76	122.80
1	6	163	G	N7-C8-N9	5.66	115.93	113.10
1	2	542	A	C4-N9-C1'	5.66	136.48	126.30
1	6	76	A	O4'-C1'-N9	5.66	112.72	108.20
36	5	216	G	C4-C5-N7	5.66	113.06	110.80
36	5	1065	A	O5'-P-OP1	-5.66	100.61	105.70
36	1	1476	G	N7-C8-N9	-5.65	110.27	113.10
36	1	2409	G	N3-C4-C5	-5.65	125.77	128.60
38	4	151	C	N3-C4-N4	5.65	121.96	118.00
1	2	1564	U	N1-C2-O2	-5.65	118.84	122.80
36	1	2160	G	N3-C2-N2	5.65	123.86	119.90
36	1	3136	G	N1-C6-O6	-5.65	116.51	119.90
36	5	1371	G	C6-C5-N7	5.65	133.79	130.40
36	5	2820	A	N9-C4-C5	5.65	108.06	105.80
38	8	38	U	N3-C4-O4	-5.65	115.44	119.40
36	5	2604	U	N3-C2-O2	-5.65	118.25	122.20
36	1	916	G	C5-C6-N1	-5.65	108.68	111.50
36	1	2827	U	C2-N3-C4	-5.65	123.61	127.00
54	M8	138	LEU	CA-CB-CG	5.65	128.29	115.30
36	5	629	U	C5-C4-O4	-5.65	122.51	125.90
36	5	931	C	C5-C4-N4	-5.65	116.25	120.20
36	5	2792	A	C8-N9-C4	-5.65	103.54	105.80
36	5	3218	A	P-O3'-C3'	5.65	126.48	119.70
1	2	1559	A	C2-N3-C4	-5.65	107.78	110.60
36	5	1178	G	C8-N9-C4	-5.65	104.14	106.40
1	2	320	U	C5-C4-O4	-5.64	122.51	125.90
36	1	124	U	N3-C2-O2	-5.64	118.25	122.20
36	1	2522	G	C4-N9-C1'	5.64	133.84	126.50
1	6	634	G	O5'-P-OP2	-5.64	100.62	105.70
36	5	516	A	N1-C6-N6	5.64	121.99	118.60
36	5	715	A	O4'-C1'-N9	5.64	112.72	108.20
36	5	1162	U	C2-N3-C4	-5.64	123.61	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3217	C	C6-N1-C1'	-5.64	114.03	120.80
1	6	144	U	C2-N1-C1'	5.64	124.47	117.70
36	5	35	A	C2-N3-C4	-5.64	107.78	110.60
36	5	2119	A	C6-C5-N7	-5.64	128.35	132.30
36	5	2994	A	N1-C6-N6	5.64	121.98	118.60
1	2	1361	U	N1-C2-O2	5.64	126.75	122.80
36	1	957	C	N3-C2-O2	5.64	125.85	121.90
36	1	2257	C	C6-N1-C2	-5.64	118.04	120.30
36	5	1323	G	N1-C6-O6	-5.64	116.52	119.90
36	5	2874	G	C5-C6-O6	5.64	131.98	128.60
36	5	946	U	C5-C4-O4	5.64	129.28	125.90
36	1	1114	U	N3-C4-O4	-5.64	115.45	119.40
1	6	795	U	OP1-P-OP2	-5.64	111.14	119.60
1	2	1432	U	C5-C4-O4	-5.63	122.52	125.90
36	1	2142	A	N1-C2-N3	5.63	132.12	129.30
36	1	3181	C	C5-C6-N1	-5.63	118.18	121.00
36	5	3076	C	N1-C2-O2	5.63	122.28	118.90
1	2	1675	C	N3-C2-O2	-5.63	117.96	121.90
36	5	202	G	N3-C2-N2	5.63	123.84	119.90
36	5	925	A	C2-N3-C4	5.63	113.42	110.60
36	1	890	C	O5'-P-OP2	-5.63	100.63	105.70
36	1	907	G	N3-C4-C5	-5.63	125.78	128.60
51	M5	38	ARG	NE-CZ-NH1	5.63	123.11	120.30
36	5	1879	A	O5'-P-OP2	-5.63	100.63	105.70
36	5	2398	A	N9-C4-C5	5.63	108.05	105.80
36	5	2966	G	C5-C6-O6	-5.63	125.22	128.60
36	1	995	U	C4-C5-C6	-5.63	116.32	119.70
36	1	2980	U	OP1-P-OP2	-5.63	111.16	119.60
36	5	301	G	C8-N9-C4	5.63	108.65	106.40
52	m6	160	ARG	NE-CZ-NH1	5.63	123.11	120.30
36	1	24	G	C6-N1-C2	-5.63	121.72	125.10
36	1	425	G	N1-C6-O6	-5.63	116.53	119.90
36	1	2423	U	C2-N1-C1'	5.63	124.45	117.70
36	5	1375	G	C2-N3-C4	5.63	114.71	111.90
36	5	1506	A	N9-C4-C5	5.63	108.05	105.80
36	5	2907	G	OP2-P-O3'	5.63	117.58	105.20
36	5	3302	U	C5-C4-O4	-5.63	122.52	125.90
36	1	1598	G	N1-C6-O6	-5.62	116.53	119.90
37	3	72	A	C8-N9-C4	-5.62	103.55	105.80
78	Q2	93	LEU	CA-CB-CG	5.62	128.24	115.30
36	5	1313	G	O5'-P-OP1	5.62	117.45	110.70
36	5	1446	A	C8-N9-C4	5.62	108.05	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2339	C	O4'-C1'-N1	-5.62	103.70	108.20
1	2	1441	C	C5-C6-N1	-5.62	118.19	121.00
36	1	192	C	O5'-P-OP1	-5.62	100.64	105.70
36	1	1419	A	C5'-C4'-O4'	5.62	115.85	109.10
36	5	1588	A	N9-C4-C5	-5.62	103.55	105.80
36	1	388	G	C8-N9-C4	-5.62	104.15	106.40
36	1	859	G	N9-C4-C5	-5.62	103.15	105.40
36	5	101	G	O4'-C1'-N9	5.62	112.70	108.20
36	5	2373	A	OP1-P-O3'	5.62	117.57	105.20
36	5	2949	U	N1-C2-O2	5.62	126.73	122.80
36	1	338	A	N9-C4-C5	5.62	108.05	105.80
36	1	967	A	C6-C5-N7	5.62	136.23	132.30
1	6	119	A	C2-N3-C4	-5.62	107.79	110.60
36	1	2612	U	O5'-P-OP1	-5.62	100.64	105.70
1	6	1257	U	N3-C2-O2	-5.62	118.27	122.20
1	6	1498	G	C5-C6-O6	5.62	131.97	128.60
64	n8	12	ARG	NE-CZ-NH2	-5.62	117.49	120.30
36	1	3278	C	C5-C4-N4	5.62	124.13	120.20
37	3	102	A	C4-C5-C6	-5.62	114.19	117.00
1	6	401	A	N1-C6-N6	5.62	121.97	118.60
1	6	1100	G	N3-C4-C5	-5.62	125.79	128.60
1	6	1749	A	C6-C5-N7	-5.62	128.37	132.30
36	5	682	U	C2-N3-C4	-5.62	123.63	127.00
36	5	3218	A	C5-N7-C8	-5.62	101.09	103.90
37	7	20	A	N1-C6-N6	5.62	121.97	118.60
36	1	210	U	N3-C2-O2	-5.61	118.27	122.20
1	2	1766	A	C8-N9-C4	5.61	108.05	105.80
36	1	1713	G	C8-N9-C4	5.61	108.64	106.40
36	5	2969	A	C8-N9-C4	5.61	108.05	105.80
36	1	226	C	C5-C4-N4	-5.61	116.27	120.20
36	1	420	G	N9-C4-C5	-5.61	103.16	105.40
36	1	2313	A	N1-C6-N6	5.61	121.97	118.60
36	5	437	G	C8-N9-C1'	5.61	134.29	127.00
36	5	1210	U	N1-C2-O2	5.61	126.73	122.80
36	5	1340	G	N3-C2-N2	5.61	123.83	119.90
73	o7	45	ARG	NE-CZ-NH2	-5.61	117.50	120.30
36	1	641	C	O4'-C1'-N1	5.61	112.69	108.20
36	1	895	A	C5-C6-N1	-5.61	114.89	117.70
38	4	81	U	N3-C2-O2	-5.61	118.27	122.20
1	6	17	C	N3-C2-O2	-5.61	117.97	121.90
1	6	1572	G	N3-C2-N2	-5.61	115.97	119.90
36	5	2963	C	OP2-P-O3'	5.61	117.54	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1539	G	N3-C4-N9	-5.61	122.64	126.00
36	5	2892	A	C6-N1-C2	5.61	121.96	118.60
36	5	1433	A	O4'-C1'-N9	-5.61	103.72	108.20
38	8	99	C	N3-C4-C5	5.61	124.14	121.90
1	2	992	A	N3-C4-N9	-5.60	122.92	127.40
36	1	1426	C	N3-C4-N4	-5.60	114.08	118.00
36	1	730	C	N3-C4-C5	5.60	124.14	121.90
36	1	1412	G	C5-C6-O6	5.60	131.96	128.60
36	1	2656	A	C2-N3-C4	5.60	113.40	110.60
36	5	93	C	C6-N1-C2	-5.60	118.06	120.30
1	6	542	A	C5-C6-N6	-5.60	119.22	123.70
36	5	1495	U	C6-N1-C2	-5.60	117.64	121.00
36	1	25	U	C2-N3-C4	-5.60	123.64	127.00
1	6	1745	G	C5-C6-O6	-5.60	125.24	128.60
25	d3	23	ARG	CG-CD-NE	5.60	123.56	111.80
36	5	819	U	OP2-P-O3'	5.60	117.52	105.20
36	1	2956	A	O5'-P-OP1	-5.60	100.66	105.70
36	5	1686	U	N1-C2-O2	-5.60	118.88	122.80
37	7	92	A	N9-C4-C5	-5.60	103.56	105.80
36	1	3057	U	N3-C2-O2	-5.60	118.28	122.20
36	1	3089	C	N3-C4-C5	5.60	124.14	121.90
37	7	48	U	N3-C4-C5	5.60	117.96	114.60
36	1	340	C	N3-C2-O2	-5.59	117.98	121.90
36	1	1536	G	N1-C6-O6	5.59	123.26	119.90
36	1	2642	A	C4-C5-C6	-5.59	114.20	117.00
36	1	2697	A	N9-C4-C5	5.59	108.04	105.80
1	2	720	G	P-O3'-C3'	5.59	126.41	119.70
24	D2	65	LEU	CA-CB-CG	5.59	128.16	115.30
36	1	386	A	C4-C5-C6	5.59	119.80	117.00
36	1	1329	U	C3'-C2'-C1'	5.59	105.97	101.50
36	1	2178	A	C5-C6-N6	5.59	128.17	123.70
1	6	93	A	N1-C6-N6	5.59	121.95	118.60
36	5	50	U	O5'-P-OP1	-5.59	100.67	105.70
1	2	1456	C	N3-C2-O2	-5.59	117.99	121.90
36	1	1379	G	N1-C2-N2	-5.59	111.17	116.20
36	5	629	U	N3-C4-C5	5.59	117.95	114.60
36	5	2651	G	OP2-P-O3'	5.59	117.50	105.20
36	5	3052	G	N9-C4-C5	5.59	107.64	105.40
1	2	610	G	C8-N9-C1'	-5.59	119.74	127.00
36	5	630	A	C5-C6-N1	-5.59	114.91	117.70
36	5	2157	G	C8-N9-C4	5.59	108.64	106.40
36	5	2352	A	C5-C6-N1	-5.59	114.91	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2618	G	C6-N1-C2	-5.59	121.75	125.10
1	2	1524	A	N9-C4-C5	5.59	108.03	105.80
36	1	374	A	O4'-C1'-N9	5.59	112.67	108.20
1	6	687	G	C8-N9-C1'	5.59	134.26	127.00
36	5	693	A	N9-C4-C5	5.59	108.03	105.80
36	5	1336	U	O5'-P-OP2	-5.59	100.67	105.70
36	5	1589	A	N1-C2-N3	-5.59	126.51	129.30
36	5	2371	G	N3-C4-C5	5.59	131.39	128.60
36	5	2830	G	C4-C5-N7	-5.59	108.56	110.80
36	1	2787	G	C2-N3-C4	5.58	114.69	111.90
36	1	2836	C	N3-C4-N4	-5.58	114.09	118.00
38	4	56	G	N3-C2-N2	5.58	123.81	119.90
36	5	2139	A	O4'-C1'-N9	-5.58	103.73	108.20
36	5	2153	U	C5-C6-N1	-5.58	119.91	122.70
36	1	123	A	C8-N9-C4	-5.58	103.57	105.80
36	1	212	G	O4'-C1'-N9	5.58	112.67	108.20
36	1	2639	G	OP2-P-O3'	5.58	117.49	105.20
36	5	1124	U	C6-N1-C2	5.58	124.35	121.00
36	1	3054	U	C2-N3-C4	-5.58	123.65	127.00
36	1	3090	U	O5'-P-OP2	-5.58	100.68	105.70
37	3	86	U	OP1-P-O3'	5.58	117.48	105.20
36	1	364	G	C5-C6-O6	-5.58	125.25	128.60
36	1	1178	G	N9-C4-C5	5.58	107.63	105.40
36	1	1342	C	C5-C4-N4	-5.58	116.29	120.20
36	5	1057	A	N1-C6-N6	5.58	121.95	118.60
36	5	3074	G	N3-C2-N2	5.58	123.81	119.90
36	1	2382	G	N3-C2-N2	5.58	123.80	119.90
1	6	1361	U	C6-N1-C1'	-5.58	113.39	121.20
36	5	2814	G	C6-C5-N7	-5.58	127.05	130.40
1	2	1365	C	C6-N1-C2	-5.58	118.07	120.30
1	2	1462	G	C8-N9-C4	5.58	108.63	106.40
36	5	2398	A	N7-C8-N9	5.58	116.59	113.80
36	5	2860	U	N3-C4-O4	5.58	123.30	119.40
1	2	704	C	C2-N1-C1'	5.57	124.93	118.80
36	1	369	A	N1-C6-N6	-5.57	115.26	118.60
36	5	1517	G	O5'-P-OP2	-5.57	100.69	105.70
38	4	85	G	N1-C6-O6	5.57	123.24	119.90
52	M6	189	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	6	782	U	N3-C2-O2	-5.57	118.30	122.20
36	5	2735	U	C6-N1-C2	-5.57	117.66	121.00
36	1	609	G	C5-C6-N1	5.57	114.28	111.50
36	1	862	U	C6-N1-C2	-5.57	117.66	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	920	A	OP1-P-O3'	5.57	117.45	105.20
38	4	100	U	N1-C2-O2	5.57	126.70	122.80
59	n3	45	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	2	75	U	C6-N1-C1'	-5.57	113.41	121.20
1	2	1455	G	C5-C6-N1	-5.57	108.72	111.50
36	1	110	G	C5'-C4'-O4'	5.57	115.78	109.10
36	1	344	A	C6-C5-N7	5.57	136.20	132.30
36	1	801	A	N7-C8-N9	5.57	116.58	113.80
36	1	967	A	C5-N7-C8	5.57	106.68	103.90
36	1	2305	G	N3-C4-N9	5.57	129.34	126.00
38	4	19	C	C5-C4-N4	5.57	124.10	120.20
38	4	23	U	N3-C2-O2	5.57	126.09	122.20
36	5	221	A	N9-C4-C5	-5.57	103.57	105.80
36	5	1370	G	N1-C6-O6	-5.57	116.56	119.90
1	6	542	A	O4'-C1'-N9	5.56	112.65	108.20
36	5	2725	U	O5'-P-OP1	-5.56	100.69	105.70
36	5	2990	G	N3-C4-C5	-5.56	125.82	128.60
18	C6	28	LEU	CA-CB-CG	5.56	128.09	115.30
36	1	1444	G	C8-N9-C4	5.56	108.62	106.40
36	1	2376	G	N9-C4-C5	-5.56	103.17	105.40
36	1	2619	G	OP1-P-OP2	5.56	127.94	119.60
38	4	15	G	C5-C6-O6	-5.56	125.26	128.60
36	5	532	A	C8-N9-C4	-5.56	103.58	105.80
36	5	2408	U	N3-C4-O4	-5.56	115.51	119.40
38	8	104	A	C8-N9-C4	5.56	108.03	105.80
36	1	186	U	N3-C2-O2	-5.56	118.31	122.20
36	1	410	U	C4-C5-C6	5.56	123.04	119.70
36	1	429	U	N1-C2-O2	5.56	126.69	122.80
36	1	2871	G	N3-C2-N2	-5.56	116.01	119.90
36	5	2637	A	N1-C6-N6	5.56	121.94	118.60
1	2	780	A	C2-N3-C4	-5.56	107.82	110.60
36	1	1180	A	OP1-P-O3'	5.56	117.43	105.20
36	1	1931	U	N3-C2-O2	5.56	126.09	122.20
1	6	1432	U	O4'-C1'-N1	5.56	112.65	108.20
1	2	554	C	C6-N1-C2	-5.56	118.08	120.30
1	2	1243	G	O4'-C1'-N9	5.56	112.64	108.20
1	2	1473	U	N3-C2-O2	-5.56	118.31	122.20
68	O2	43	ARG	NE-CZ-NH2	-5.56	117.52	120.30
36	5	625	G	N9-C4-C5	5.56	107.62	105.40
36	5	1337	A	N9-C4-C5	5.56	108.02	105.80
36	5	2808	A	C6-C5-N7	-5.56	128.41	132.30
36	5	3266	G	C5-C6-O6	5.56	131.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1047	A	C5-N7-C8	-5.56	101.12	103.90
40	l3	19	ARG	CG-CD-NE	-5.56	100.13	111.80
36	1	3010	U	N1-C2-O2	5.55	126.69	122.80
36	5	1159	A	C4-C5-N7	5.55	113.48	110.70
37	7	104	A	N1-C6-N6	5.55	121.93	118.60
38	8	111	A	O5'-P-OP2	-5.55	100.70	105.70
1	2	1761	U	N3-C2-O2	-5.55	118.31	122.20
36	1	267	G	O4'-C1'-N9	-5.55	103.76	108.20
36	1	419	G	N3-C2-N2	5.55	123.78	119.90
1	6	331	A	C2-N3-C4	-5.55	107.82	110.60
1	6	623	A	O4'-C1'-N9	5.55	112.64	108.20
36	5	415	G	C5-N7-C8	5.55	107.08	104.30
36	5	2231	C	C6-N1-C1'	-5.55	114.14	120.80
36	5	2715	A	C2-N3-C4	5.55	113.38	110.60
36	5	2946	A	N1-C6-N6	-5.55	115.27	118.60
36	1	288	C	N1-C2-O2	-5.55	115.57	118.90
36	1	2376	G	C8-N9-C1'	-5.55	119.78	127.00
36	5	648	C	C5-C6-N1	5.55	123.78	121.00
36	5	2384	A	N1-C6-N6	5.55	121.93	118.60
36	1	959	C	N3-C2-O2	5.55	125.78	121.90
36	1	3259	U	N1-C2-O2	-5.55	118.92	122.80
36	5	1319	G	N1-C6-O6	-5.55	116.57	119.90
36	1	1411	C	C5-C4-N4	5.55	124.08	120.20
36	1	1665	C	N3-C4-C5	5.55	124.12	121.90
1	6	1269	U	N1-C2-N3	5.55	118.23	114.90
36	5	907	G	N3-C4-N9	5.55	129.33	126.00
36	5	1379	G	N3-C2-N2	5.55	123.78	119.90
36	5	2180	G	C8-N9-C4	5.55	108.62	106.40
1	6	1751	C	N1-C2-O2	5.54	122.23	118.90
36	5	301	G	N7-C8-N9	-5.54	110.33	113.10
36	5	1047	A	C5-C6-N6	-5.54	119.26	123.70
36	5	1489	A	N9-C4-C5	-5.54	103.58	105.80
36	5	2897	A	C4-C5-N7	-5.54	107.93	110.70
36	5	2917	G	C2-N3-C4	5.54	114.67	111.90
36	1	1005	G	N1-C6-O6	-5.54	116.57	119.90
36	1	1369	A	C5-N7-C8	5.54	106.67	103.90
1	6	260	U	C6-N1-C2	5.54	124.33	121.00
1	2	145	A	N9-C4-C5	5.54	108.02	105.80
1	2	380	U	O5'-P-OP1	-5.54	100.71	105.70
1	6	1573	A	P-O3'-C3'	5.54	126.35	119.70
36	5	1858	A	N7-C8-N9	5.54	116.57	113.80
36	5	2836	C	C4-C5-C6	5.54	120.17	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3052	G	C6-C5-N7	5.54	133.72	130.40
36	1	859	G	C6-C5-N7	-5.54	127.08	130.40
36	1	2513	U	N1-C1'-C2'	-5.54	105.91	112.00
36	5	997	A	OP2-P-O3'	5.54	117.38	105.20
36	5	2631	U	N1-C2-N3	5.54	118.22	114.90
36	1	321	C	C6-N1-C2	-5.54	118.08	120.30
37	7	75	G	C5-C6-N1	-5.54	108.73	111.50
1	2	142	G	C5-C6-N1	-5.54	108.73	111.50
36	1	66	A	O5'-P-OP2	5.54	117.34	110.70
36	1	1402	C	N3-C4-N4	-5.54	114.13	118.00
36	1	2198	A	C8-N9-C4	5.54	108.02	105.80
38	4	79	A	N7-C8-N9	5.54	116.57	113.80
36	5	2772	C	P-O3'-C3'	5.54	126.34	119.70
36	5	2831	G	C8-N9-C4	-5.54	104.19	106.40
36	5	3341	U	C6-N1-C2	-5.54	117.68	121.00
1	2	401	A	OP2-P-O3'	5.53	117.37	105.20
47	M0	4	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	6	1600	A	C5-N7-C8	-5.53	101.13	103.90
36	5	1482	A	O5'-P-OP2	-5.53	100.72	105.70
36	5	2349	U	N3-C4-O4	-5.53	115.53	119.40
36	5	3206	C	C6-N1-C1'	5.53	127.44	120.80
1	6	864	U	C2-N3-C4	-5.53	123.68	127.00
36	1	76	G	N3-C4-N9	5.53	129.32	126.00
36	1	1389	G	C5-C6-O6	-5.53	125.28	128.60
36	1	1482	A	C2-N3-C4	5.53	113.36	110.60
36	5	1141	C	N1-C2-O2	-5.53	115.58	118.90
36	1	1163	A	O5'-P-OP2	-5.53	100.72	105.70
38	4	30	C	O5'-P-OP1	-5.53	100.72	105.70
36	5	1192	C	C2-N3-C4	-5.53	117.14	119.90
36	1	945	C	N3-C4-C5	5.53	124.11	121.90
36	1	1858	A	N3-C4-C5	-5.53	122.93	126.80
36	1	3081	C	N3-C4-N4	-5.53	114.13	118.00
36	5	318	A	N1-C6-N6	5.53	121.92	118.60
36	5	1402	C	N1-C2-O2	5.53	122.22	118.90
36	5	2805	G	C5-C6-O6	-5.53	125.28	128.60
38	8	79	A	O5'-P-OP2	-5.53	100.73	105.70
36	1	2169	G	C6-C5-N7	5.53	133.72	130.40
51	M5	105	ARG	NE-CZ-NH2	-5.53	117.54	120.30
36	5	2654	C	C6-N1-C2	5.53	122.51	120.30
64	N8	116	GLY	N-CA-C	5.52	126.91	113.10
1	2	610	G	C4-N9-C1'	5.52	133.68	126.50
36	5	1049	C	C4-C5-C6	-5.52	114.64	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2323	G	C8-N9-C4	-5.52	104.19	106.40
36	5	2360	C	N3-C4-C5	-5.52	119.69	121.90
36	5	2966	G	C5-C6-N1	5.52	114.26	111.50
39	l2	246	LEU	CA-CB-CG	5.52	128.00	115.30
36	1	2156	C	C5-C6-N1	-5.52	118.24	121.00
36	1	2227	C	C6-N1-C2	-5.52	118.09	120.30
1	6	1697	G	N3-C4-C5	-5.52	125.84	128.60
36	1	2817	A	OP2-P-O3'	5.52	117.34	105.20
36	5	313	A	C8-N9-C4	-5.52	103.59	105.80
36	5	1846	C	OP2-P-O3'	5.52	117.34	105.20
36	5	1942	U	N3-C4-O4	5.52	123.26	119.40
36	5	3137	C	C5-C4-N4	5.52	124.06	120.20
36	5	3228	C	N3-C2-O2	-5.52	118.04	121.90
1	2	73	U	N3-C2-O2	-5.52	118.34	122.20
1	2	1776	A	N1-C6-N6	-5.52	115.29	118.60
36	5	1116	G	C4-C5-N7	-5.52	108.59	110.80
36	5	2927	C	N3-C2-O2	-5.52	118.04	121.90
1	2	359	A	C4-C5-C6	-5.51	114.24	117.00
1	2	1490	C	OP1-P-O3'	5.51	117.33	105.20
36	1	341	G	C4-C5-N7	5.51	113.01	110.80
36	1	2131	A	N1-C6-N6	5.51	121.91	118.60
37	3	42	A	C2-N3-C4	-5.51	107.84	110.60
1	6	489	C	C2-N1-C1'	5.51	124.87	118.80
36	5	59	G	O5'-P-OP1	5.51	117.32	110.70
36	5	927	C	N3-C4-C5	5.51	124.11	121.90
36	5	995	U	C5-C6-N1	-5.51	119.94	122.70
36	5	1158	A	N1-C6-N6	5.51	121.91	118.60
36	5	1391	C	N3-C2-O2	5.51	125.76	121.90
36	5	2904	U	C5-C6-N1	-5.51	119.94	122.70
1	2	499	U	C6-N1-C1'	-5.51	113.48	121.20
50	M4	72	LEU	CA-CB-CG	5.51	127.97	115.30
36	5	437	G	C5-C6-O6	5.51	131.91	128.60
36	5	1592	G	C6-C5-N7	-5.51	127.09	130.40
36	5	2643	A	N1-C2-N3	-5.51	126.55	129.30
36	5	1655	G	O5'-P-OP1	-5.51	100.74	105.70
36	5	3317	U	C6-N1-C2	-5.51	117.69	121.00
36	5	2818	U	C5'-C4'-O4'	-5.51	102.49	109.10
36	5	2966	G	N3-C4-N9	5.51	129.31	126.00
36	5	2971	A	C2-N3-C4	5.51	113.35	110.60
1	2	536	C	C5-C6-N1	5.51	123.75	121.00
36	1	2171	G	N3-C4-N9	5.51	129.30	126.00
36	5	201	A	C5-C6-N1	-5.51	114.95	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	691	A	C8-N9-C4	-5.51	103.60	105.80
36	5	2643	A	O5'-P-OP2	-5.50	100.75	105.70
36	5	1159	A	N1-C6-N6	5.50	121.90	118.60
36	5	1873	U	N1-C2-N3	5.50	118.20	114.90
36	1	109	A	C8-N9-C4	-5.50	103.60	105.80
59	N3	70	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	6	103	A	N7-C8-N9	5.50	116.55	113.80
36	5	1169	A	C5-C6-N1	-5.50	114.95	117.70
36	5	2634	U	N3-C4-C5	5.50	117.90	114.60
36	1	1178	G	C5-C6-O6	5.50	131.90	128.60
36	1	930	U	C2-N3-C4	-5.50	123.70	127.00
36	1	1374	G	N3-C2-N2	5.50	123.75	119.90
36	1	2422	C	N3-C2-O2	-5.50	118.05	121.90
1	6	114	C	C2-N1-C1'	5.50	124.85	118.80
36	5	963	G	C8-N9-C4	5.50	108.60	106.40
36	5	2618	G	C2-N3-C4	5.50	114.65	111.90
1	6	638	U	N1-C2-O2	5.50	126.65	122.80
37	7	95	A	N1-C2-N3	-5.50	126.55	129.30
36	1	1646	G	O4'-C1'-N9	5.50	112.60	108.20
36	1	2551	U	N1-C2-N3	5.50	118.20	114.90
36	1	2585	G	N3-C4-N9	5.50	129.30	126.00
36	1	94	G	N1-C2-N3	-5.49	120.60	123.90
36	1	394	G	C5-C6-O6	5.49	131.90	128.60
1	6	1473	U	N1-C2-N3	5.49	118.20	114.90
36	5	972	A	OP2-P-O3'	5.49	117.28	105.20
36	1	835	G	C5-C6-O6	-5.49	125.31	128.60
1	6	1783	C	N1-C2-O2	5.49	122.19	118.90
36	5	1432	C	N3-C2-O2	-5.49	118.06	121.90
36	5	2908	G	N9-C4-C5	5.49	107.60	105.40
36	5	3101	G	N1-C2-N2	-5.49	111.26	116.20
1	2	398	G	C4-C5-N7	5.49	113.00	110.80
36	1	3369	G	N1-C6-O6	5.49	123.19	119.90
1	6	1	U	N1-C1'-C2'	5.49	121.14	114.00
36	5	51	A	N1-C6-N6	5.49	121.89	118.60
36	5	3369	G	C5-C6-O6	-5.49	125.31	128.60
1	2	1000	C	N3-C4-N4	-5.49	114.16	118.00
36	1	711	A	N1-C6-N6	-5.49	115.31	118.60
36	1	728	G	OP2-P-O3'	5.49	117.27	105.20
36	1	2317	A	O5'-P-OP1	-5.49	100.76	105.70
33	e1	100	LEU	CA-CB-CG	5.49	127.92	115.30
36	5	2798	C	C6-N1-C2	5.49	122.50	120.30
36	1	3175	U	C6-N1-C2	5.49	124.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2355	G	C4-C5-N7	5.49	112.99	110.80
36	5	3323	A	C2-N3-C4	-5.49	107.86	110.60
36	1	2340	U	C5-C4-O4	5.48	129.19	125.90
36	1	3079	U	C2-N1-C1'	-5.48	111.12	117.70
36	5	911	C	O5'-P-OP2	5.48	117.28	110.70
36	1	2139	A	N1-C6-N6	-5.48	115.31	118.60
36	1	2871	G	N3-C4-C5	5.48	131.34	128.60
1	6	542	A	C8-N9-C1'	-5.48	117.83	127.70
36	5	1308	A	O5'-P-OP1	5.48	117.28	110.70
36	5	1376	C	OP1-P-OP2	5.48	127.82	119.60
1	2	440	U	N3-C4-O4	-5.48	115.56	119.40
36	1	406	G	O5'-P-OP2	-5.48	100.77	105.70
36	1	645	A	C2-N3-C4	5.48	113.34	110.60
36	1	1555	U	O4'-C1'-N1	5.48	112.58	108.20
36	1	2777	G	C5-C6-O6	5.48	131.89	128.60
68	O2	82	LEU	CA-CB-CG	5.48	127.90	115.30
36	5	494	G	N3-C4-C5	-5.48	125.86	128.60
1	2	1441	C	C6-N1-C2	5.48	122.49	120.30
36	5	363	G	N9-C4-C5	5.48	107.59	105.40
36	1	1148	G	C8-N9-C4	5.48	108.59	106.40
1	6	53	G	N1-C6-O6	-5.48	116.61	119.90
1	6	1681	A	O4'-C1'-N9	5.48	112.58	108.20
14	c2	58	LEU	CA-CB-CG	5.48	127.90	115.30
36	5	92	G	O5'-P-OP2	5.48	117.27	110.70
36	5	2278	C	C5-C4-N4	5.48	124.03	120.20
36	5	3091	A	N9-C4-C5	5.48	107.99	105.80
36	5	413	U	C2-N3-C4	-5.48	123.71	127.00
36	1	2809	C	N3-C2-O2	-5.47	118.07	121.90
36	1	2907	G	OP2-P-O3'	5.47	117.25	105.20
38	4	53	A	N3-C4-C5	-5.47	122.97	126.80
36	5	795	G	N1-C2-N3	-5.47	120.62	123.90
36	1	209	A	C5-C6-N1	-5.47	114.96	117.70
36	1	908	G	C8-N9-C1'	-5.47	119.89	127.00
36	1	1144	U	N1-C2-N3	5.47	118.18	114.90
36	1	1437	C	C2-N1-C1'	5.47	124.82	118.80
9	s7	118	LEU	CA-CB-CG	5.47	127.89	115.30
36	5	1130	A	C4-C5-N7	-5.47	107.96	110.70
36	5	2993	G	C5-C6-O6	-5.47	125.32	128.60
36	1	412	G	N9-C4-C5	5.47	107.59	105.40
36	1	661	G	C8-N9-C4	-5.47	104.21	106.40
36	1	1323	G	N1-C6-O6	-5.47	116.62	119.90
36	1	1507	G	O4'-C1'-N9	-5.47	103.83	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	294	U	C5-C4-O4	-5.47	122.62	125.90
36	5	999	G	N1-C6-O6	-5.47	116.62	119.90
36	5	3062	G	N3-C4-C5	-5.47	125.86	128.60
36	1	3375	A	P-O3'-C3'	5.47	126.26	119.70
36	1	1201	C	C6-N1-C2	-5.47	118.11	120.30
38	4	113	U	N3-C4-O4	-5.47	115.57	119.40
36	5	522	A	O5'-P-OP1	-5.47	100.78	105.70
36	5	2271	A	N1-C6-N6	-5.47	115.32	118.60
36	5	2632	G	N3-C2-N2	5.47	123.73	119.90
36	1	295	A	N7-C8-N9	5.46	116.53	113.80
36	1	2622	C	C6-N1-C2	-5.46	118.11	120.30
36	1	2740	A	C2-N3-C4	5.46	113.33	110.60
1	6	421	A	N1-C6-N6	5.46	121.88	118.60
36	5	1083	G	OP1-P-OP2	5.46	127.80	119.60
36	5	1397	C	OP1-P-O3'	5.46	117.22	105.20
36	5	2945	G	C8-N9-C4	5.46	108.59	106.40
38	8	74	U	C5-C4-O4	-5.46	122.62	125.90
1	2	396	G	C5-C6-O6	-5.46	125.32	128.60
36	5	304	G	O4'-C1'-N9	-5.46	103.83	108.20
36	1	52	A	OP1-P-OP2	5.46	127.79	119.60
36	1	1201	C	N1-C2-O2	-5.46	115.62	118.90
36	1	3093	C	C6-N1-C2	5.46	122.48	120.30
1	6	387	A	N9-C4-C5	5.46	107.98	105.80
36	5	932	U	C5-C4-O4	-5.46	122.62	125.90
36	5	1847	A	C2-N3-C4	-5.46	107.87	110.60
36	1	949	C	N1-C2-O2	-5.46	115.62	118.90
36	1	2748	A	N1-C6-N6	5.46	121.88	118.60
38	4	56	G	N1-C2-N2	-5.46	111.29	116.20
1	6	696	C	O4'-C1'-N1	5.46	112.57	108.20
36	5	426	G	C4-C5-N7	-5.46	108.62	110.80
36	5	902	G	O5'-P-OP1	-5.46	100.79	105.70
36	5	982	C	N1-C2-O2	5.46	122.17	118.90
36	5	986	U	N1-C2-O2	5.46	126.62	122.80
36	5	1073	U	O5'-P-OP1	-5.46	100.79	105.70
36	5	1087	G	C5-C6-O6	-5.46	125.33	128.60
36	5	2402	A	C2-N3-C4	-5.46	107.87	110.60
1	2	385	A	C8-N9-C4	5.46	107.98	105.80
1	2	1052	U	C2-N1-C1'	5.46	124.25	117.70
1	2	1428	G	N3-C2-N2	-5.46	116.08	119.90
36	1	651	G	N1-C6-O6	-5.46	116.63	119.90
36	1	1556	C	C6-N1-C2	-5.46	118.12	120.30
36	1	3244	A	O4'-C1'-N9	-5.46	103.83	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1539	G	O4'-C1'-N9	-5.46	103.83	108.20
36	5	2142	A	C2-N3-C4	5.46	113.33	110.60
1	2	453	U	C6-N1-C1'	-5.46	113.56	121.20
36	1	2923	U	O5'-P-OP1	-5.46	100.79	105.70
37	3	36	C	N1-C2-O2	5.46	122.17	118.90
1	6	389	G	N1-C2-N2	-5.46	111.29	116.20
36	5	1014	U	C2-N1-C1'	5.46	124.25	117.70
36	1	405	U	C2-N3-C4	-5.45	123.73	127.00
36	1	868	C	N1-C2-O2	5.45	122.17	118.90
36	1	2125	A	C8-N9-C4	5.45	107.98	105.80
36	1	2192	C	O5'-P-OP2	-5.45	100.79	105.70
36	1	3112	G	C5-C6-O6	-5.45	125.33	128.60
36	5	193	C	OP1-P-O3'	5.45	117.20	105.20
36	5	345	G	N1-C2-N2	-5.45	111.29	116.20
36	5	2380	U	N1-C2-N3	5.45	118.17	114.90
1	2	18	C	C6-N1-C2	-5.45	118.12	120.30
1	2	570	A	C2-N3-C4	5.45	113.33	110.60
36	1	74	G	N1-C2-N3	5.45	127.17	123.90
36	1	817	A	C2-N3-C4	5.45	113.33	110.60
36	1	2550	U	C6-N1-C2	-5.45	117.73	121.00
38	4	26	U	N3-C4-O4	-5.45	115.58	119.40
1	6	466	U	C6-N1-C2	-5.45	117.73	121.00
36	5	1170	A	N7-C8-N9	-5.45	111.08	113.80
1	2	973	A	C2-N3-C4	-5.45	107.88	110.60
36	1	1507	G	N3-C4-C5	-5.45	125.88	128.60
36	1	2196	C	C6-N1-C2	-5.45	118.12	120.30
36	1	2747	A	N1-C6-N6	-5.45	115.33	118.60
36	5	57	A	OP2-P-O3'	5.45	117.19	105.20
36	5	2271	A	C2-N3-C4	5.45	113.32	110.60
36	5	3098	G	N3-C2-N2	5.45	123.71	119.90
1	6	433	C	N1-C2-O2	-5.45	115.63	118.90
36	5	2287	C	N3-C4-C5	5.45	124.08	121.90
36	1	53	G	N1-C6-O6	-5.45	116.63	119.90
36	1	218	G	N9-C4-C5	5.45	107.58	105.40
36	1	2522	G	C8-N9-C1'	-5.45	119.92	127.00
1	6	3	U	C6-N1-C2	5.45	124.27	121.00
36	5	3340	G	P-O3'-C3'	5.45	126.23	119.70
37	7	10	C	N1-C2-O2	5.45	122.17	118.90
36	1	1130	A	N1-C2-N3	-5.44	126.58	129.30
36	1	2551	U	N3-C2-O2	-5.44	118.39	122.20
36	1	3375	A	N9-C4-C5	5.44	107.98	105.80
36	5	197	G	C8-N9-C4	-5.44	104.22	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	581	U	C6-N1-C1'	-5.44	113.58	121.20
1	2	973	A	O5'-P-OP2	-5.44	100.80	105.70
36	1	1178	G	C2-N3-C4	5.44	114.62	111.90
36	5	718	G	OP2-P-O3'	5.44	117.17	105.20
36	5	2286	U	N3-C2-O2	-5.44	118.39	122.20
36	5	3046	A	C2-N3-C4	5.44	113.32	110.60
36	5	3120	C	C5-C6-N1	5.44	123.72	121.00
1	2	1573	A	P-O3'-C3'	5.44	126.23	119.70
36	1	642	U	C5-C4-O4	-5.44	122.64	125.90
36	1	2298	U	N1-C2-N3	5.44	118.17	114.90
36	1	2885	C	C6-N1-C2	5.44	122.48	120.30
36	5	715	A	C2-N3-C4	5.44	113.32	110.60
36	5	3012	A	N7-C8-N9	-5.44	111.08	113.80
36	5	3295	A	OP2-P-O3'	5.44	117.17	105.20
1	2	1399	C	C5-C6-N1	5.44	123.72	121.00
36	1	1890	U	C6-N1-C2	5.44	124.26	121.00
36	1	2389	C	OP2-P-O3'	5.44	117.17	105.20
1	6	308	C	C5-C4-N4	5.44	124.01	120.20
36	5	2404	A	OP1-P-OP2	-5.44	111.44	119.60
36	1	226	C	N3-C4-N4	5.44	121.81	118.00
36	1	861	C	O5'-P-OP1	5.44	117.22	110.70
36	1	1212	A	O5'-P-OP2	-5.44	100.81	105.70
36	1	2121	G	N1-C6-O6	-5.44	116.64	119.90
36	1	2811	A	N1-C6-N6	-5.44	115.34	118.60
36	5	2288	G	C5-C6-N1	5.44	114.22	111.50
36	5	2364	G	C8-N9-C4	-5.44	104.22	106.40
36	5	2365	C	OP1-P-OP2	5.44	127.76	119.60
36	5	2424	A	N1-C6-N6	5.44	121.86	118.60
36	5	2572	C	C6-N1-C2	-5.44	118.12	120.30
36	5	2599	U	N1-C2-O2	-5.44	118.99	122.80
36	5	3107	U	C2-N1-C1'	5.44	124.22	117.70
36	1	916	G	P-O3'-C3'	5.44	126.22	119.70
36	1	2615	G	C8-N9-C4	-5.44	104.23	106.40
36	1	702	C	N1-C2-O2	-5.43	115.64	118.90
36	1	2400	G	N3-C2-N2	-5.43	116.10	119.90
36	1	3112	G	N1-C6-O6	5.43	123.16	119.90
41	L4	194	TYR	CA-CB-CG	5.43	123.73	113.40
1	6	1299	G	N3-C4-C5	-5.43	125.88	128.60
36	5	673	U	C2-N3-C4	-5.43	123.74	127.00
36	5	1817	G	O4'-C1'-N9	5.43	112.55	108.20
36	5	3141	A	O4'-C1'-N9	-5.43	103.85	108.20
38	8	53	A	OP1-P-OP2	-5.43	111.45	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	m6	66	LYS	CD-CE-NZ	5.43	124.20	111.70
36	1	206	G	N1-C2-N3	-5.43	120.64	123.90
36	5	1487	G	C5-C6-O6	5.43	131.86	128.60
36	5	2246	G	OP1-P-OP2	-5.43	111.45	119.60
36	5	3196	U	O5'-P-OP1	-5.43	100.81	105.70
1	6	1101	G	N1-C6-O6	-5.43	116.64	119.90
36	5	569	A	C5-N7-C8	5.43	106.61	103.90
36	5	2167	A	C8-N9-C4	-5.43	103.63	105.80
1	2	1134	C	N3-C4-C5	5.43	124.07	121.90
36	1	101	G	O4'-C1'-N9	5.43	112.54	108.20
36	1	713	U	C2-N3-C4	-5.43	123.74	127.00
36	1	2214	A	C6-C5-N7	-5.43	128.50	132.30
1	6	455	C	N1-C2-O2	-5.43	115.64	118.90
1	6	1793	G	C4-C5-N7	-5.43	108.63	110.80
36	5	267	G	O4'-C1'-N9	-5.43	103.86	108.20
36	5	3210	A	C2-N3-C4	-5.43	107.89	110.60
36	5	3321	C	C4-C5-C6	5.43	120.11	117.40
1	6	39	A	O4'-C1'-N9	5.43	112.54	108.20
1	6	1109	G	O5'-P-OP2	-5.43	100.82	105.70
36	5	356	C	N3-C4-N4	5.43	121.80	118.00
36	5	1929	G	C2-N3-C4	-5.43	109.19	111.90
36	5	2404	A	C8-N9-C4	5.43	107.97	105.80
36	5	2896	A	N9-C4-C5	5.43	107.97	105.80
42	l5	147	ASP	CB-CG-OD1	5.43	123.18	118.30
36	1	2554	A	P-O3'-C3'	5.42	126.21	119.70
1	6	1354	G	C8-N9-C4	-5.42	104.23	106.40
36	5	893	C	C2-N3-C4	5.42	122.61	119.90
36	5	908	G	C4-C5-N7	5.42	112.97	110.80
36	1	683	U	C5-C6-N1	-5.42	119.99	122.70
1	6	1596	C	N1-C2-N3	5.42	123.00	119.20
36	1	721	G	C4-C5-N7	5.42	112.97	110.80
36	1	1269	U	C2-N1-C1'	5.42	124.21	117.70
36	1	1937	U	N3-C4-C5	5.42	117.85	114.60
1	6	794	U	N3-C2-O2	-5.42	118.41	122.20
36	5	1466	G	O5'-P-OP2	5.42	117.21	110.70
36	5	1879	A	N7-C8-N9	5.42	116.51	113.80
36	5	2865	U	N3-C2-O2	-5.42	118.41	122.20
1	2	501	U	OP1-P-O3'	5.42	117.12	105.20
36	1	1119	C	N3-C4-C5	5.42	124.07	121.90
36	5	44	U	C5-C4-O4	-5.42	122.65	125.90
36	5	283	G	C6-C5-N7	-5.42	127.15	130.40
36	5	1655	G	N7-C8-N9	5.42	115.81	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2289	U	C6-N1-C1'	-5.42	113.61	121.20
36	1	515	C	C6-N1-C2	-5.42	118.13	120.30
36	1	680	G	OP1-P-OP2	5.42	127.73	119.60
36	1	2728	G	N3-C4-C5	-5.42	125.89	128.60
38	4	111	A	C8-N9-C4	-5.42	103.63	105.80
36	5	2719	U	C5-C6-N1	-5.42	119.99	122.70
1	2	1462	G	N1-C6-O6	5.42	123.15	119.90
36	1	3135	U	C2-N3-C4	-5.42	123.75	127.00
36	5	366	A	N1-C6-N6	5.42	121.85	118.60
36	5	1044	U	C5-C4-O4	5.42	129.15	125.90
36	5	2142	A	OP1-P-O3'	5.42	117.11	105.20
36	5	3288	G	C5-C6-N1	5.42	114.21	111.50
36	1	2305	G	C8-N9-C1'	-5.42	119.96	127.00
36	5	1322	U	N3-C4-C5	5.42	117.85	114.60
36	1	320	G	N3-C2-N2	-5.41	116.11	119.90
36	1	847	A	C6-C5-N7	-5.41	128.51	132.30
36	1	1141	C	N3-C4-N4	5.41	121.79	118.00
1	6	1428	G	C8-N9-C4	-5.41	104.23	106.40
36	5	1054	A	C8-N9-C4	5.41	107.97	105.80
36	5	2584	G	C5-C6-O6	-5.41	125.35	128.60
36	5	914	A	O5'-P-OP1	-5.41	100.83	105.70
36	5	1215	U	C5-C4-O4	-5.41	122.65	125.90
36	5	2369	G	C8-N9-C1'	-5.41	119.96	127.00
41	l4	76	ARG	NE-CZ-NH2	-5.41	117.59	120.30
36	1	496	C	OP2-P-O3'	5.41	117.10	105.20
36	5	1888	U	C4-C5-C6	5.41	122.95	119.70
36	5	2856	G	C5-N7-C8	-5.41	101.59	104.30
36	5	2906	C	C6-N1-C2	-5.41	118.14	120.30
36	1	331	G	N9-C4-C5	5.41	107.56	105.40
36	1	410	U	N3-C4-O4	5.41	123.19	119.40
36	1	1117	G	C5-C6-O6	-5.41	125.36	128.60
36	1	1296	C	C6-N1-C2	-5.41	118.14	120.30
36	1	1349	G	N3-C4-C5	-5.41	125.90	128.60
36	1	2404	A	N9-C1'-C2'	-5.41	106.05	112.00
36	1	2756	C	C2-N1-C1'	5.41	124.75	118.80
36	1	2932	U	O5'-P-OP2	-5.41	100.83	105.70
36	1	2952	G	C4-C5-N7	5.41	112.96	110.80
36	1	3209	A	C6-C5-N7	-5.41	128.51	132.30
1	6	1171	A	C8-N9-C4	-5.41	103.64	105.80
36	5	989	A	N1-C6-N6	-5.41	115.36	118.60
36	5	1917	C	C2-N3-C4	-5.41	117.20	119.90
36	5	2190	U	C6-N1-C2	-5.41	117.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2874	G	N1-C6-O6	-5.41	116.66	119.90
36	1	917	A	C5-C6-N6	5.41	128.02	123.70
36	1	1904	C	C5-C6-N1	5.41	123.70	121.00
36	1	2984	C	C6-N1-C2	-5.41	118.14	120.30
1	6	577	G	N7-C8-N9	5.41	115.80	113.10
36	1	3147	G	C5-C6-O6	5.40	131.84	128.60
36	5	1297	C	C5-C6-N1	-5.40	118.30	121.00
1	2	17	C	O5'-P-OP2	-5.40	100.84	105.70
36	1	228	U	N3-C2-O2	-5.40	118.42	122.20
36	1	802	C	N3-C2-O2	-5.40	118.12	121.90
36	1	1596	C	N3-C4-N4	-5.40	114.22	118.00
1	6	333	A	N7-C8-N9	-5.40	111.10	113.80
1	6	1398	U	C2-N1-C1'	5.40	124.18	117.70
36	5	1172	G	C5-C6-O6	5.40	131.84	128.60
36	5	2178	A	C8-N9-C4	5.40	107.96	105.80
38	8	26	U	N3-C2-O2	-5.40	118.42	122.20
36	1	1158	A	C8-N9-C4	-5.40	103.64	105.80
1	6	1753	A	N9-C4-C5	5.40	107.96	105.80
36	5	3043	C	O5'-P-OP2	-5.40	100.84	105.70
36	5	3362	A	N3-C4-C5	5.40	130.58	126.80
36	1	1127	G	C4-C5-N7	5.40	112.96	110.80
37	7	10	C	O5'-P-OP2	-5.40	100.84	105.70
36	1	1157	G	OP2-P-O3'	5.40	117.07	105.20
36	1	2834	G	OP1-P-OP2	5.40	127.70	119.60
36	5	1201	C	N1-C2-O2	-5.40	115.66	118.90
36	5	1854	C	C5-C4-N4	5.40	123.98	120.20
36	5	2681	U	C5-C6-N1	-5.40	120.00	122.70
54	m8	66	ARG	NE-CZ-NH2	-5.40	117.60	120.30
36	1	682	U	C5-C4-O4	-5.40	122.66	125.90
36	1	2811	A	N1-C2-N3	5.40	132.00	129.30
36	1	2855	U	N3-C4-C5	5.39	117.84	114.60
36	5	960	U	N3-C4-O4	-5.39	115.62	119.40
36	5	3134	A	C8-N9-C4	-5.39	103.64	105.80
1	2	607	G	C4-C5-N7	5.39	112.96	110.80
36	1	2924	U	C2-N1-C1'	-5.39	111.23	117.70
36	5	2234	G	C8-N9-C4	5.39	108.56	106.40
36	1	428	A	OP2-P-O3'	5.39	117.06	105.20
36	1	612	U	C5-C4-O4	-5.39	122.67	125.90
36	1	993	G	O4'-C1'-N9	5.39	112.51	108.20
64	N8	14	HIS	C-N-CA	-5.39	108.23	121.70
36	5	3078	U	C6-N1-C1'	-5.39	113.66	121.20
36	1	406	G	N3-C2-N2	5.39	123.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3036	G	N3-C4-C5	-5.39	125.91	128.60
38	8	34	U	C5-C6-N1	-5.39	120.01	122.70
36	1	227	G	C5-C6-O6	-5.39	125.37	128.60
36	1	2959	C	N1-C2-O2	-5.39	115.67	118.90
1	6	754	A	C5-C6-N6	-5.39	119.39	123.70
36	5	1858	A	O4'-C1'-N9	5.39	112.51	108.20
36	5	2210	G	C5-C6-O6	-5.39	125.37	128.60
36	5	283	G	C5-C6-O6	-5.38	125.37	128.60
36	5	824	C	C6-N1-C2	-5.38	118.15	120.30
36	5	2637	A	N9-C4-C5	-5.38	103.65	105.80
36	1	3280	U	O4'-C1'-N1	5.38	112.51	108.20
36	1	2121	G	N3-C2-N2	5.38	123.67	119.90
36	1	2145	A	C2-N3-C4	5.38	113.29	110.60
36	1	3306	U	C5-C6-N1	-5.38	120.01	122.70
1	6	310	C	C4-C5-C6	5.38	120.09	117.40
7	s5	92	ARG	NE-CZ-NH1	5.38	122.99	120.30
36	5	191	U	C2-N1-C1'	-5.38	111.24	117.70
36	5	1157	G	N7-C8-N9	-5.38	110.41	113.10
36	5	1833	G	C2-N3-C4	5.38	114.59	111.90
36	5	2385	G	C2-N3-C4	-5.38	109.21	111.90
36	5	2912	G	C5-N7-C8	5.38	106.99	104.30
36	5	2988	C	N1-C2-O2	5.38	122.13	118.90
36	5	3115	C	N1-C2-N3	5.38	122.97	119.20
37	7	77	G	O5'-P-OP1	5.38	117.16	110.70
36	5	416	A	OP2-P-O3'	5.38	117.04	105.20
36	1	963	G	N7-C8-N9	-5.38	110.41	113.10
36	1	2382	G	N1-C6-O6	-5.38	116.67	119.90
36	1	2958	A	C5-C6-N1	5.38	120.39	117.70
36	1	2963	C	N1-C2-O2	5.38	122.13	118.90
1	6	114	C	C6-N1-C1'	-5.38	114.35	120.80
36	5	2753	G	N3-C2-N2	-5.38	116.14	119.90
36	1	1135	A	N1-C2-N3	-5.38	126.61	129.30
36	1	1329	U	O4'-C1'-N1	5.38	112.50	108.20
1	6	995	A	C8-N9-C4	-5.38	103.65	105.80
1	6	1196	A	P-O3'-C3'	5.38	126.15	119.70
1	6	1656	U	N1-C1'-C2'	-5.38	106.09	112.00
36	5	1302	A	C8-N9-C4	-5.38	103.65	105.80
36	5	2798	C	C2-N1-C1'	-5.38	112.89	118.80
36	1	2802	A	OP2-P-O3'	5.38	117.02	105.20
36	5	2245	C	N3-C2-O2	-5.38	118.14	121.90
36	5	2320	A	C5-C6-N1	-5.38	115.01	117.70
36	5	3127	A	C6-C5-N7	5.38	136.06	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	720	A	C8-N9-C4	-5.37	103.65	105.80
36	1	1305	U	N3-C2-O2	-5.37	118.44	122.20
1	6	362	G	C4-N9-C1'	5.37	133.48	126.50
36	5	57	A	N1-C6-N6	5.37	121.82	118.60
36	5	324	A	N9-C4-C5	5.37	107.95	105.80
36	5	867	G	N1-C6-O6	5.37	123.12	119.90
36	5	1603	A	N1-C2-N3	5.37	131.99	129.30
36	1	933	A	O5'-P-OP2	-5.37	100.87	105.70
36	1	1118	C	N3-C4-C5	-5.37	119.75	121.90
36	1	1420	C	OP2-P-O3'	5.37	117.02	105.20
56	N0	24	LEU	CA-CB-CG	5.37	127.65	115.30
36	5	282	G	P-O3'-C3'	5.37	126.14	119.70
36	5	341	G	C5-N7-C8	-5.37	101.61	104.30
36	5	2160	G	C5-C6-O6	5.37	131.82	128.60
36	5	2948	C	C5-C4-N4	5.37	123.96	120.20
36	1	2142	A	OP1-P-OP2	-5.37	111.55	119.60
36	1	3317	U	C5-C4-O4	5.37	129.12	125.90
36	5	1319	G	C5-C6-O6	5.37	131.82	128.60
36	5	2623	G	C8-N9-C4	5.37	108.55	106.40
1	2	1024	U	N1-C2-O2	5.37	126.56	122.80
36	1	25	U	N1-C2-O2	-5.37	119.04	122.80
36	1	280	U	N3-C2-O2	5.37	125.96	122.20
38	4	148	G	N1-C6-O6	-5.37	116.68	119.90
1	6	142	G	C4-N9-C1'	5.37	133.48	126.50
36	5	1520	G	C5-C6-N1	5.37	114.19	111.50
36	5	2672	G	C8-N9-C4	5.37	108.55	106.40
36	5	3090	U	C2-N3-C4	-5.37	123.78	127.00
38	8	51	G	N1-C6-O6	5.37	123.12	119.90
1	2	406	U	C6-N1-C2	5.37	124.22	121.00
36	1	1507	G	C4-C5-N7	-5.37	108.65	110.80
36	5	1157	G	C8-N9-C4	5.37	108.55	106.40
36	1	39	A	N3-C4-N9	-5.37	123.11	127.40
36	1	641	C	C6-N1-C1'	5.37	127.24	120.80
38	4	29	U	C2-N3-C4	-5.37	123.78	127.00
36	5	1430	U	C6-N1-C2	5.37	124.22	121.00
36	5	2346	C	N3-C4-C5	5.37	124.05	121.90
36	5	2704	A	OP1-P-OP2	5.37	127.65	119.60
38	8	3	A	N1-C6-N6	-5.37	115.38	118.60
1	2	355	G	N3-C4-C5	-5.36	125.92	128.60
36	1	631	U	N1-C2-N3	5.36	118.12	114.90
36	1	976	U	O5'-P-OP2	-5.36	100.87	105.70
36	1	3096	C	O5'-P-OP1	-5.36	100.87	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3264	G	N7-C8-N9	-5.36	110.42	113.10
1	6	1480	G	C8-N9-C4	-5.36	104.25	106.40
36	5	1724	U	O4'-C1'-N1	5.36	112.49	108.20
37	7	92	A	C4-C5-N7	5.36	113.38	110.70
38	8	25	G	C5-C6-O6	5.36	131.82	128.60
1	2	542	A	N7-C8-N9	5.36	116.48	113.80
38	4	64	U	N3-C4-O4	-5.36	115.65	119.40
65	N9	20	GLY	N-CA-C	5.36	126.50	113.10
36	5	1110	U	N1-C2-O2	5.36	126.55	122.80
36	1	2390	A	C8-N9-C4	5.36	107.94	105.80
36	1	2767	U	O5'-P-OP2	-5.36	100.88	105.70
1	6	328	A	O5'-P-OP2	-5.36	100.88	105.70
1	6	1638	G	N1-C6-O6	-5.36	116.68	119.90
36	5	221	A	C8-N9-C4	5.36	107.94	105.80
36	5	1892	G	N1-C6-O6	-5.36	116.68	119.90
36	1	677	A	C5-C6-N6	-5.36	119.41	123.70
36	1	970	A	N7-C8-N9	5.36	116.48	113.80
36	1	1403	C	N1-C2-O2	-5.36	115.69	118.90
36	1	1753	G	C5-C6-O6	-5.36	125.39	128.60
36	1	2787	G	C5-C6-N1	5.36	114.18	111.50
71	O5	69	LEU	CA-CB-CG	5.36	127.62	115.30
1	6	858	G	N7-C8-N9	5.36	115.78	113.10
36	5	1161	G	C8-N9-C4	5.36	108.54	106.40
36	5	2920	U	N1-C2-N3	5.36	118.11	114.90
36	5	2938	G	O5'-P-OP1	-5.36	100.88	105.70
36	5	2941	A	C6-N1-C2	-5.36	115.39	118.60
36	1	351	A	OP1-P-OP2	5.36	127.63	119.60
36	1	808	A	C4-C5-N7	-5.36	108.02	110.70
36	1	1513	G	C5-C6-O6	-5.36	125.39	128.60
36	1	2368	A	N1-C6-N6	-5.36	115.39	118.60
36	1	3000	A	C8-N9-C4	5.36	107.94	105.80
1	6	1657	U	C2-N1-C1'	5.36	124.13	117.70
36	5	103	G	C5-C6-O6	5.36	131.81	128.60
36	5	1183	C	N3-C4-N4	-5.36	114.25	118.00
36	5	1881	A	N1-C6-N6	5.36	121.81	118.60
36	5	2386	A	C8-N9-C4	-5.36	103.66	105.80
36	5	3276	G	OP1-P-O3'	5.36	116.98	105.20
36	1	1741	A	N1-C2-N3	5.35	131.98	129.30
36	1	2194	G	O5'-P-OP1	5.35	117.12	110.70
1	6	1782	A	O5'-P-OP1	-5.35	100.88	105.70
36	5	1087	G	N3-C2-N2	-5.35	116.15	119.90
36	1	2624	G	N1-C6-O6	5.35	123.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2797	C	N1-C2-O2	-5.35	115.69	118.90
1	6	163	G	C4-N9-C1'	-5.35	119.54	126.50
36	5	341	G	N1-C6-O6	5.35	123.11	119.90
36	5	1242	G	C4-N9-C1'	5.35	133.46	126.50
36	5	2131	A	N9-C1'-C2'	-5.35	106.11	112.00
36	5	2393	G	N1-C2-N2	5.35	121.02	116.20
65	n9	39	PHE	N-CA-CB	5.35	120.24	110.60
1	2	497	G	P-O3'-C3'	5.35	126.12	119.70
36	1	1445	U	N1-C2-O2	-5.35	119.05	122.80
36	1	2365	C	C5-C4-N4	5.35	123.95	120.20
36	1	608	A	N9-C4-C5	-5.35	103.66	105.80
36	1	1468	A	OP1-P-OP2	5.35	127.62	119.60
36	1	1483	G	O4'-C1'-N9	5.35	112.48	108.20
36	1	2300	G	OP2-P-O3'	5.35	116.97	105.20
36	5	307	A	N9-C4-C5	5.35	107.94	105.80
36	5	1725	C	O4'-C1'-N1	5.35	112.48	108.20
1	2	1297	G	C4-N9-C1'	-5.35	119.55	126.50
36	1	229	G	N1-C2-N2	5.35	121.01	116.20
36	1	1434	G	N3-C4-C5	-5.35	125.93	128.60
36	1	2283	G	N3-C2-N2	-5.35	116.16	119.90
38	4	9	A	N1-C6-N6	-5.35	115.39	118.60
36	5	2211	U	C6-N1-C2	-5.35	117.79	121.00
1	2	1796	C	C4-C5-C6	5.35	120.07	117.40
36	1	1795	U	C2-N3-C4	-5.35	123.79	127.00
36	5	92	G	N3-C2-N2	5.35	123.64	119.90
36	5	1396	C	OP2-P-O3'	5.35	116.96	105.20
36	1	963	G	N9-C4-C5	-5.34	103.26	105.40
36	1	1581	C	C6-N1-C2	-5.34	118.16	120.30
36	1	2977	G	C5-C6-N1	5.34	114.17	111.50
1	6	163	G	N1-C2-N3	5.34	127.11	123.90
36	5	3058	U	C2-N3-C4	-5.34	123.79	127.00
36	1	2282	U	N3-C4-C5	5.34	117.81	114.60
36	1	2613	U	C6-N1-C2	-5.34	117.79	121.00
36	5	2889	C	N3-C4-N4	-5.34	114.26	118.00
36	5	3218	A	C4-C5-N7	5.34	113.37	110.70
36	1	1435	A	C8-N9-C4	-5.34	103.66	105.80
36	5	423	A	OP2-P-O3'	5.34	116.95	105.20
36	5	2833	A	OP1-P-OP2	5.34	127.61	119.60
36	5	2878	G	C5-C6-N1	5.34	114.17	111.50
36	5	3151	U	C6-N1-C2	5.34	124.20	121.00
36	1	1181	U	O5'-P-OP1	-5.34	100.89	105.70
36	1	1395	G	C5-C6-N1	5.34	114.17	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2990	G	C4-C5-N7	-5.34	108.66	110.80
59	N3	13	ILE	CG1-CB-CG2	-5.34	99.65	111.40
1	6	280	U	C2-N1-C1'	5.34	124.11	117.70
36	5	660	A	C2-N3-C4	-5.34	107.93	110.60
36	5	2868	U	N3-C4-C5	5.34	117.80	114.60
38	4	16	G	C8-N9-C4	5.34	108.53	106.40
36	5	3011	A	C2-N3-C4	5.34	113.27	110.60
1	2	1657	U	C5-C6-N1	-5.34	120.03	122.70
1	2	1658	G	N9-C4-C5	-5.34	103.27	105.40
36	1	401	U	N3-C4-O4	5.34	123.14	119.40
36	1	659	G	OP1-P-O3'	5.34	116.94	105.20
36	1	3143	C	N3-C2-O2	5.34	125.64	121.90
1	6	17	C	N1-C2-O2	5.34	122.10	118.90
1	6	402	C	C6-N1-C2	5.34	122.44	120.30
36	1	637	C	N3-C4-N4	-5.33	114.27	118.00
1	6	260	U	C5-C6-N1	-5.33	120.03	122.70
36	5	2147	A	N1-C6-N6	5.33	121.80	118.60
36	5	2392	C	N1-C2-O2	-5.33	115.70	118.90
36	1	333	G	N1-C6-O6	-5.33	116.70	119.90
36	1	2347	U	N3-C4-C5	5.33	117.80	114.60
36	1	2381	G	O5'-P-OP1	-5.33	100.90	105.70
1	6	536	C	N3-C4-C5	-5.33	119.77	121.90
36	5	439	C	C4-C5-C6	5.33	120.07	117.40
36	5	646	A	OP1-P-OP2	-5.33	111.60	119.60
36	5	1116	G	O5'-P-OP1	-5.33	100.90	105.70
36	5	2932	U	N3-C4-O4	-5.33	115.67	119.40
1	2	1138	A	O5'-P-OP1	-5.33	100.90	105.70
36	1	1313	G	C8-N9-C4	-5.33	104.27	106.40
36	1	1494	U	C5-C6-N1	-5.33	120.03	122.70
36	1	2628	A	C8-N9-C4	-5.33	103.67	105.80
1	6	957	G	N1-C6-O6	5.33	123.10	119.90
1	6	1031	U	N3-C4-C5	5.33	117.80	114.60
36	5	2981	U	C2-N3-C4	-5.33	123.80	127.00
1	6	31	C	C5-C4-N4	5.33	123.93	120.20
1	6	1022	C	O5'-P-OP2	5.33	117.10	110.70
36	5	204	A	N1-C6-N6	-5.33	115.40	118.60
36	5	2825	C	C5-C4-N4	-5.33	116.47	120.20
36	5	1487	G	N9-C4-C5	5.33	107.53	105.40
36	5	3228	C	C6-N1-C2	-5.33	118.17	120.30
36	1	716	A	C4-C5-N7	5.33	113.36	110.70
36	1	1556	C	N3-C2-O2	-5.33	118.17	121.90
36	1	2236	G	N1-C6-O6	5.33	123.10	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3140	G	N1-C6-O6	5.33	123.10	119.90
36	5	2141	U	OP1-P-O3'	-5.33	93.48	105.20
36	5	3309	G	N3-C4-N9	5.33	129.20	126.00
36	1	1507	G	C4-C5-C6	5.33	122.00	118.80
36	1	1815	U	P-O3'-C3'	5.33	126.09	119.70
36	1	3311	C	C6-N1-C2	5.33	122.43	120.30
38	4	23	U	N3-C4-C5	5.33	117.80	114.60
36	5	300	G	N3-C4-N9	-5.33	122.80	126.00
36	5	688	G	N3-C2-N2	-5.33	116.17	119.90
36	5	1115	G	P-O3'-C3'	5.33	126.09	119.70
36	5	1506	A	C8-N9-C4	-5.33	103.67	105.80
36	5	2996	U	C6-N1-C2	5.33	124.20	121.00
38	8	136	G	C5-C6-O6	5.33	131.79	128.60
1	2	18	C	N3-C4-C5	-5.32	119.77	121.90
1	2	1748	G	C4-C5-N7	-5.32	108.67	110.80
36	1	730	C	C2-N3-C4	-5.32	117.24	119.90
36	1	1119	C	N3-C4-N4	-5.32	114.27	118.00
36	1	1598	G	C5-C6-O6	5.32	131.79	128.60
36	1	2411	U	C4-C5-C6	-5.32	116.51	119.70
36	1	2883	U	C5-C4-O4	5.32	129.09	125.90
36	1	3218	A	N9-C4-C5	5.32	107.93	105.80
1	6	1762	A	N1-C2-N3	-5.32	126.64	129.30
36	5	999	G	OP1-P-OP2	-5.32	111.61	119.60
36	5	1839	A	N9-C4-C5	5.32	107.93	105.80
36	5	2247	G	N1-C6-O6	-5.32	116.70	119.90
36	1	3181	C	C6-N1-C2	-5.32	118.17	120.30
10	S8	172	ARG	NE-CZ-NH2	-5.32	117.64	120.30
36	1	2186	U	N1-C2-O2	5.32	126.52	122.80
36	5	1101	G	N3-C2-N2	5.32	123.62	119.90
36	1	620	U	C2-N1-C1'	-5.32	111.32	117.70
36	1	1340	G	N3-C2-N2	5.32	123.62	119.90
36	1	690	A	C2-N3-C4	5.32	113.26	110.60
36	1	2363	A	C6-C5-N7	5.32	136.02	132.30
36	1	2954	U	N3-C2-O2	5.32	125.92	122.20
1	6	65	A	N3-C4-C5	5.32	130.52	126.80
1	6	399	A	C8-N9-C4	5.32	107.93	105.80
36	5	583	G	C8-N9-C4	5.32	108.53	106.40
36	5	811	U	C2-N3-C4	-5.32	123.81	127.00
36	5	2119	A	N9-C4-C5	-5.32	103.67	105.80
36	5	2178	A	N1-C6-N6	5.32	121.79	118.60
1	2	1486	G	O4'-C1'-N9	5.32	112.45	108.20
36	1	332	C	O5'-P-OP1	-5.32	100.92	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1005	G	N1-C2-N2	-5.32	111.42	116.20
1	6	583	C	C2-N1-C1'	5.32	124.65	118.80
36	5	353	G	O4'-C1'-N9	5.32	112.45	108.20
36	5	2970	C	C2-N1-C1'	-5.32	112.95	118.80
36	1	155	G	N3-C4-N9	5.31	129.19	126.00
36	1	695	C	C5-C6-N1	-5.31	118.34	121.00
36	1	196	G	C5-C6-O6	-5.31	125.41	128.60
36	1	906	A	C5-C6-N1	5.31	120.36	117.70
36	1	2384	A	C6-C5-N7	-5.31	128.58	132.30
1	6	377	G	N1-C6-O6	-5.31	116.71	119.90
1	6	1122	G	N3-C4-C5	5.31	131.26	128.60
36	5	1370	G	C5-C6-O6	5.31	131.79	128.60
36	1	424	G	C5-C6-N1	5.31	114.16	111.50
37	3	81	U	N3-C4-C5	5.31	117.79	114.60
36	5	2930	A	N9-C4-C5	5.31	107.92	105.80
36	1	1852	G	C5-C6-N1	-5.31	108.84	111.50
36	1	2318	U	N1-C2-N3	5.31	118.09	114.90
36	1	3151	U	O5'-P-OP1	5.31	117.07	110.70
36	5	908	G	C5-N7-C8	-5.31	101.64	104.30
36	5	2641	U	N3-C2-O2	5.31	125.92	122.20
36	1	323	A	O5'-P-OP1	-5.31	100.92	105.70
36	1	439	C	N3-C2-O2	-5.31	118.19	121.90
36	1	635	G	C5-C6-O6	-5.31	125.42	128.60
1	6	362	G	C8-N9-C1'	-5.31	120.10	127.00
36	5	2207	A	O4'-C1'-N9	5.31	112.44	108.20
36	5	2680	A	OP2-P-O3'	5.31	116.88	105.20
36	5	2756	C	OP2-P-O3'	5.31	116.88	105.20
36	5	3058	U	N3-C4-C5	5.31	117.78	114.60
36	1	202	G	N1-C6-O6	-5.31	116.72	119.90
36	5	1180	A	C2-N3-C4	-5.31	107.95	110.60
1	2	1486	G	C6-C5-N7	-5.30	127.22	130.40
36	1	92	G	O5'-C5'-C4'	-5.30	101.62	111.70
36	1	401	U	C2-N3-C4	-5.30	123.82	127.00
36	1	944	C	N3-C4-N4	5.30	121.71	118.00
36	1	1430	U	N1-C2-O2	-5.30	119.09	122.80
36	1	1450	G	N7-C8-N9	-5.30	110.45	113.10
36	1	1604	G	C8-N9-C1'	-5.30	120.10	127.00
36	1	1671	C	C6-N1-C2	-5.30	118.18	120.30
36	1	1786	G	O5'-P-OP1	-5.30	100.93	105.70
36	1	2541	U	P-O3'-C3'	5.30	126.06	119.70
36	5	216	G	C6-C5-N7	-5.30	127.22	130.40
36	5	393	U	N1-C2-N3	5.30	118.08	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	652	G	N3-C4-C5	-5.30	125.95	128.60
36	5	1042	U	N1-C2-O2	5.30	126.51	122.80
36	5	2856	G	C5-C6-O6	-5.30	125.42	128.60
37	7	92	A	C5-C6-N6	-5.30	119.46	123.70
36	1	936	A	C5-C6-N6	-5.30	119.46	123.70
54	M8	12	ARG	NE-CZ-NH1	-5.30	117.65	120.30
36	1	630	A	N9-C4-C5	5.30	107.92	105.80
38	4	23	U	C6-N1-C2	5.30	124.18	121.00
1	6	453	U	C6-N1-C2	-5.30	117.82	121.00
1	6	639	U	O4'-C1'-N1	5.30	112.44	108.20
36	5	1419	A	C8-N9-C4	5.30	107.92	105.80
36	5	1656	A	O5'-P-OP2	-5.30	100.93	105.70
36	5	2600	C	O5'-P-OP1	-5.30	100.93	105.70
36	1	715	A	O4'-C1'-N9	5.30	112.44	108.20
36	1	2752	U	N3-C4-O4	-5.30	115.69	119.40
36	1	2797	C	O5'-P-OP1	-5.30	100.93	105.70
36	1	3175	U	C5-C6-N1	-5.30	120.05	122.70
1	6	1058	U	P-O3'-C3'	5.30	126.06	119.70
36	5	349	A	O5'-P-OP1	-5.30	100.93	105.70
36	5	718	G	O4'-C1'-N9	5.30	112.44	108.20
36	5	2375	G	N3-C2-N2	5.30	123.61	119.90
36	5	2833	A	C8-N9-C4	5.30	107.92	105.80
36	1	75	G	N3-C4-N9	5.30	129.18	126.00
36	5	878	G	C6-C5-N7	-5.30	127.22	130.40
36	5	3107	U	OP2-P-O3'	5.30	116.86	105.20
68	o2	39	ASP	CB-CG-OD1	-5.30	113.53	118.30
36	1	659	G	N3-C2-N2	5.30	123.61	119.90
3	s1	47	LEU	CA-CB-CG	5.30	127.48	115.30
36	5	1371	G	N7-C8-N9	-5.30	110.45	113.10
36	5	3032	A	N1-C2-N3	-5.30	126.65	129.30
36	1	674	G	C2-N3-C4	5.29	114.55	111.90
36	1	1163	A	OP1-P-OP2	5.29	127.54	119.60
36	5	2302	G	N1-C6-O6	-5.29	116.72	119.90
36	5	3181	C	O5'-P-OP1	5.29	117.05	110.70
36	1	1349	G	N3-C4-N9	5.29	129.18	126.00
1	6	95	G	C8-N9-C4	-5.29	104.28	106.40
1	6	102	U	N1-C2-N3	5.29	118.08	114.90
36	5	826	G	N3-C4-N9	-5.29	122.82	126.00
36	5	851	C	N1-C2-O2	-5.29	115.72	118.90
36	5	2369	G	C8-N9-C4	5.29	108.52	106.40
36	5	2658	G	N7-C8-N9	-5.29	110.45	113.10
36	1	3135	U	C5-C6-N1	-5.29	120.06	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	144	U	N1-C2-O2	5.29	126.50	122.80
36	5	2298	U	C5-C6-N1	-5.29	120.05	122.70
36	1	1395	G	N1-C2-N3	-5.29	120.73	123.90
1	6	864	U	O4'-C1'-N1	5.29	112.43	108.20
1	6	1773	C	N3-C2-O2	5.29	125.60	121.90
36	5	619	A	N1-C6-N6	-5.29	115.43	118.60
1	2	139	C	P-O3'-C3'	5.29	126.05	119.70
36	1	515	C	N3-C4-C5	-5.29	119.78	121.90
36	1	1859	A	N9-C4-C5	-5.29	103.69	105.80
36	1	2725	U	C6-N1-C2	5.29	124.17	121.00
36	5	26	A	N7-C8-N9	-5.29	111.16	113.80
36	5	1376	C	N1-C2-O2	5.29	122.07	118.90
40	l3	47	LEU	CA-CB-CG	5.29	127.46	115.30
1	2	543	C	C4-C5-C6	5.29	120.04	117.40
36	1	2808	A	N9-C4-C5	-5.29	103.69	105.80
36	5	73	C	C5-C6-N1	-5.29	118.36	121.00
1	2	499	U	P-O3'-C3'	5.29	126.04	119.70
36	1	3269	U	N3-C2-O2	-5.29	118.50	122.20
1	6	609	U	N1-C2-N3	5.29	118.07	114.90
36	5	2145	A	C2-N3-C4	5.29	113.24	110.60
36	5	2817	A	OP2-P-O3'	5.29	116.83	105.20
36	5	3311	C	C5-C4-N4	5.29	123.90	120.20
36	1	124	U	N1-C2-O2	5.28	126.50	122.80
36	1	288	C	N3-C2-O2	5.28	125.60	121.90
36	1	791	A	N9-C4-C5	5.28	107.91	105.80
36	1	2129	U	N3-C4-C5	5.28	117.77	114.60
36	1	2811	A	C8-N9-C4	-5.28	103.69	105.80
36	5	60	A	O5'-P-OP2	-5.28	100.95	105.70
36	5	963	G	C4-C5-C6	-5.28	115.63	118.80
36	5	2869	U	N1-C2-N3	5.28	118.07	114.90
1	6	1535	U	C5-C6-N1	-5.28	120.06	122.70
36	5	363	G	OP1-P-O3'	5.28	116.82	105.20
1	2	1762	A	O5'-P-OP1	-5.28	100.95	105.70
15	C3	22	ALA	C-N-CA	5.28	144.18	122.00
36	1	143	G	C4-C5-N7	-5.28	108.69	110.80
36	1	372	A	N9-C4-C5	-5.28	103.69	105.80
36	1	418	A	C2-N3-C4	-5.28	107.96	110.60
36	1	2142	A	N3-C4-C5	-5.28	123.10	126.80
1	6	1279	C	C6-N1-C2	-5.28	118.19	120.30
36	5	2732	G	N3-C4-N9	5.28	129.17	126.00
36	5	2935	U	OP1-P-O3'	5.28	116.82	105.20
36	5	3033	A	C8-N9-C4	5.28	107.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1190	C	C6-N1-C2	5.28	122.41	120.30
36	1	3121	U	P-O3'-C3'	5.28	126.03	119.70
36	5	916	G	P-O3'-C3'	5.28	126.03	119.70
36	5	961	C	C6-N1-C1'	-5.28	114.47	120.80
1	2	402	C	N3-C2-O2	5.28	125.59	121.90
1	2	527	A	C8-N9-C4	-5.28	103.69	105.80
36	1	1546	A	C4-C5-N7	-5.28	108.06	110.70
36	1	2583	C	O5'-P-OP2	-5.28	100.95	105.70
1	6	543	C	C4-C5-C6	-5.28	114.76	117.40
1	6	795	U	N1-C2-O2	5.28	126.49	122.80
36	5	1452	A	C5-C6-N6	-5.28	119.48	123.70
36	5	2369	G	N3-C2-N2	5.28	123.59	119.90
36	5	2724	U	OP1-P-O3'	5.28	116.81	105.20
36	5	3311	C	N3-C4-N4	-5.28	114.31	118.00
1	6	470	A	C8-N9-C4	-5.28	103.69	105.80
36	5	1311	G	OP1-P-OP2	-5.28	111.69	119.60
36	5	1322	U	C6-N1-C2	5.28	124.17	121.00
36	5	1517	G	C5-C6-O6	5.28	131.76	128.60
36	5	2643	A	C5-C6-N6	-5.28	119.48	123.70
36	5	2747	A	N9-C4-C5	5.28	107.91	105.80
36	5	2855	U	N1-C2-N3	-5.28	111.73	114.90
38	8	38	U	C2-N3-C4	-5.28	123.83	127.00
36	1	345	G	C6-N1-C2	-5.27	121.94	125.10
36	1	609	G	N9-C4-C5	-5.27	103.29	105.40
36	1	895	A	C6-N1-C2	5.27	121.76	118.60
36	1	2417	U	N1-C2-N3	5.27	118.06	114.90
36	5	986	U	N3-C2-O2	-5.27	118.51	122.20
1	2	1524	A	N1-C6-N6	-5.27	115.44	118.60
36	1	109	A	N1-C6-N6	-5.27	115.44	118.60
36	1	765	C	C2-N1-C1'	5.27	124.60	118.80
36	1	1400	G	C5-C6-O6	5.27	131.76	128.60
36	1	1907	C	N3-C4-C5	-5.27	119.79	121.90
36	5	424	G	C5-C6-O6	-5.27	125.44	128.60
36	5	1113	G	C8-N9-C4	5.27	108.51	106.40
36	5	2130	G	N3-C2-N2	5.27	123.59	119.90
37	7	93	C	N3-C4-N4	-5.27	114.31	118.00
36	5	2641	U	N1-C2-O2	-5.27	119.11	122.80
36	1	648	C	OP1-P-O3'	5.27	116.79	105.20
36	1	652	G	N1-C6-O6	-5.27	116.74	119.90
36	1	1408	G	C5-C6-O6	5.27	131.76	128.60
36	1	1500	G	OP2-P-O3'	5.27	116.79	105.20
1	2	624	G	N1-C6-O6	-5.27	116.74	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	504	A	C4-C5-N7	-5.27	108.07	110.70
1	6	410	A	N1-C6-N6	-5.27	115.44	118.60
37	7	47	C	C2-N3-C4	-5.27	117.27	119.90
40	l3	266	ARG	NE-CZ-NH1	5.27	122.93	120.30
36	5	21	G	N3-C2-N2	5.27	123.59	119.90
36	5	2611	U	C5-C6-N1	-5.27	120.07	122.70
36	1	2255	A	O5'-P-OP1	-5.26	100.96	105.70
36	5	2392	C	N3-C4-C5	5.26	124.00	121.90
37	7	115	G	C8-N9-C4	-5.26	104.29	106.40
36	5	671	U	C2-N3-C4	-5.26	123.84	127.00
36	5	1591	G	C8-N9-C4	-5.26	104.30	106.40
36	1	596	C	N3-C2-O2	-5.26	118.22	121.90
1	6	390	G	C4-N9-C1'	5.26	133.34	126.50
1	6	416	A	O5'-P-OP2	-5.26	100.97	105.70
36	5	937	G	N3-C4-C5	-5.26	125.97	128.60
36	5	2869	U	C5-C4-O4	5.26	129.06	125.90
36	1	31	C	C2-N3-C4	-5.26	117.27	119.90
36	1	39	A	O5'-P-OP2	-5.26	100.97	105.70
36	5	2409	G	C8-N9-C4	-5.26	104.30	106.40
36	5	3004	C	C5-C4-N4	-5.26	116.52	120.20
37	7	49	G	O4'-C1'-N9	5.26	112.41	108.20
36	1	664	U	C5-C4-O4	-5.26	122.75	125.90
1	6	1048	G	C8-N9-C4	5.26	108.50	106.40
36	5	393	U	C6-N1-C2	-5.26	117.84	121.00
36	5	2909	U	C2-N3-C4	-5.26	123.84	127.00
1	2	61	A	C5-N7-C8	-5.26	101.27	103.90
36	1	1169	A	OP2-P-O3'	5.26	116.77	105.20
36	1	2625	C	C2-N3-C4	-5.26	117.27	119.90
1	6	299	A	O5'-P-OP1	5.26	117.01	110.70
36	5	41	G	C5-N7-C8	-5.26	101.67	104.30
36	5	1242	G	N3-C4-C5	-5.26	125.97	128.60
36	5	1308	A	C5'-C4'-C3'	-5.26	107.59	116.00
36	5	2645	G	C5-C6-N1	5.26	114.13	111.50
36	1	857	G	N1-C6-O6	5.25	123.05	119.90
36	5	708	G	C4-C5-N7	5.25	112.90	110.80
36	5	2289	U	C5-C4-O4	5.25	129.05	125.90
36	5	3039	C	N1-C2-O2	5.25	122.05	118.90
1	2	647	G	N3-C2-N2	-5.25	116.22	119.90
36	1	94	G	N3-C2-N2	5.25	123.58	119.90
36	1	98	G	N1-C6-O6	-5.25	116.75	119.90
36	1	2613	U	C5-C6-N1	5.25	125.33	122.70
36	5	1552	G	C5-C6-O6	-5.25	125.45	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2970	C	C6-N1-C2	5.25	122.40	120.30
44	l7	88	ARG	NE-CZ-NH2	-5.25	117.67	120.30
36	1	188	U	C5-C4-O4	5.25	129.05	125.90
36	1	1339	C	C4-C5-C6	5.25	120.03	117.40
36	5	509	U	C2-N3-C4	-5.25	123.85	127.00
36	5	1435	A	P-O3'-C3'	5.25	126.00	119.70
36	5	1901	A	C4-C5-C6	5.25	119.63	117.00
36	1	2242	A	N1-C2-N3	5.25	131.93	129.30
36	1	65	A	C8-N9-C4	-5.25	103.70	105.80
36	1	419	G	N1-C2-N2	-5.25	111.48	116.20
36	1	1474	A	OP2-P-O3'	5.25	116.75	105.20
1	6	416	A	N1-C6-N6	5.25	121.75	118.60
36	5	726	G	N1-C6-O6	5.25	123.05	119.90
36	5	802	C	C4-C5-C6	5.25	120.03	117.40
36	5	1921	A	OP2-P-O3'	5.25	116.75	105.20
36	1	347	G	N1-C6-O6	5.25	123.05	119.90
36	1	2813	A	N9-C4-C5	5.25	107.90	105.80
36	5	1149	G	O4'-C1'-N9	5.25	112.40	108.20
1	2	323	A	C8-N9-C4	-5.25	103.70	105.80
36	1	96	G	N3-C2-N2	5.25	123.57	119.90
36	1	349	A	N9-C4-C5	5.25	107.90	105.80
36	1	504	A	C5-C6-N6	5.25	127.90	123.70
36	1	1446	A	O5'-P-OP1	-5.25	100.98	105.70
54	M8	159	LYS	CD-CE-NZ	5.25	123.76	111.70
36	5	33	G	N1-C6-O6	-5.25	116.75	119.90
36	5	110	G	N1-C6-O6	-5.25	116.75	119.90
1	2	1200	G	C8-N9-C4	-5.24	104.30	106.40
36	1	304	G	C6-C5-N7	5.24	133.55	130.40
36	1	345	G	C2-N3-C4	5.24	114.52	111.90
36	1	1398	U	OP2-P-O3'	5.24	116.73	105.20
36	1	1405	U	C5-C4-O4	-5.24	122.75	125.90
36	1	2836	C	N1-C2-N3	5.24	122.87	119.20
36	5	911	C	C5-C4-N4	-5.24	116.53	120.20
36	5	1340	G	N1-C2-N2	-5.24	111.48	116.20
39	l2	238	ILE	C-N-CA	-5.24	108.59	121.70
36	1	1788	C	C5-C4-N4	-5.24	116.53	120.20
1	2	403	G	N3-C4-N9	5.24	129.15	126.00
36	1	608	A	C4-C5-N7	5.24	113.32	110.70
36	1	1008	U	C2-N1-C1'	-5.24	111.41	117.70
36	1	2808	A	C4-C5-C6	5.24	119.62	117.00
38	4	23	U	C2-N1-C1'	-5.24	111.41	117.70
36	5	649	A	OP2-P-O3'	5.24	116.73	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	929	A	N1-C2-N3	-5.24	126.68	129.30
36	5	1408	G	C5-C6-O6	5.24	131.75	128.60
36	5	3076	C	N3-C2-O2	-5.24	118.23	121.90
36	5	3218	A	C6-C5-N7	-5.24	128.63	132.30
1	2	1196	A	C8-N9-C4	-5.24	103.70	105.80
1	6	607	G	N1-C6-O6	-5.24	116.76	119.90
36	5	1166	G	N3-C2-N2	5.24	123.57	119.90
1	2	580	A	C8-N9-C4	-5.24	103.70	105.80
36	1	1110	U	OP1-P-OP2	5.24	127.45	119.60
36	5	3007	U	N3-C2-O2	-5.24	118.53	122.20
36	5	3232	G	O5'-P-OP2	-5.24	100.99	105.70
36	1	630	A	C8-N9-C4	-5.24	103.71	105.80
36	1	1140	G	N3-C4-N9	5.24	129.14	126.00
36	1	1931	U	C2-N3-C4	-5.24	123.86	127.00
36	1	3055	U	OP1-P-OP2	5.24	127.45	119.60
36	5	1484	U	C5-C6-N1	-5.24	120.08	122.70
36	5	2572	C	C6-N1-C1'	-5.24	114.52	120.80
36	1	72	C	C2-N3-C4	-5.23	117.28	119.90
36	1	114	A	C6-C5-N7	-5.23	128.64	132.30
36	5	2661	G	OP1-P-O3'	5.23	116.72	105.20
1	2	1596	C	C5-C4-N4	5.23	123.86	120.20
36	1	2242	A	N7-C8-N9	5.23	116.42	113.80
37	3	103	A	OP2-P-O3'	5.23	116.71	105.20
1	6	1071	U	OP1-P-O3'	5.23	116.71	105.20
36	5	708	G	C8-N9-C4	-5.23	104.31	106.40
36	5	1890	U	C5-C6-N1	-5.23	120.08	122.70
36	5	2139	A	C6-N1-C2	5.23	121.74	118.60
36	1	1408	G	O5'-P-OP1	-5.23	100.99	105.70
69	O3	48	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	6	113	U	N3-C2-O2	5.23	125.86	122.20
36	5	590	G	O5'-P-OP2	5.23	116.98	110.70
36	5	2349	U	OP1-P-O3'	5.23	116.71	105.20
36	5	2609	A	N1-C6-N6	-5.23	115.46	118.60
36	5	2841	G	N3-C2-N2	5.23	123.56	119.90
36	5	2944	U	N3-C4-C5	5.23	117.74	114.60
36	1	1338	C	N3-C4-C5	-5.23	119.81	121.90
36	5	645	A	OP1-P-O3'	5.23	116.70	105.20
36	5	2334	U	O5'-P-OP2	-5.23	100.99	105.70
1	2	1773	C	C2-N1-C1'	5.23	124.55	118.80
36	1	206	G	C2-N3-C4	5.23	114.51	111.90
36	1	1307	G	OP2-P-O3'	-5.23	93.70	105.20
36	1	2906	C	N3-C2-O2	-5.23	118.24	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3090	U	N1-C2-O2	-5.23	119.14	122.80
1	6	429	G	C4-C5-N7	-5.23	108.71	110.80
2	s0	62	ARG	NE-CZ-NH1	5.23	122.91	120.30
36	5	121	A	C8-N9-C4	5.23	107.89	105.80
36	5	1538	G	O5'-P-OP1	-5.23	101.00	105.70
37	3	89	G	OP2-P-O3'	5.23	116.70	105.20
36	5	1308	A	N9-C4-C5	5.23	107.89	105.80
1	2	1671	A	C6-N1-C2	5.22	121.73	118.60
36	1	53	G	N3-C2-N2	5.22	123.56	119.90
36	1	334	A	C8-N9-C4	-5.22	103.71	105.80
36	1	416	A	C6-C5-N7	5.22	135.96	132.30
36	1	802	C	C2-N1-C1'	5.22	124.55	118.80
1	6	904	G	N3-C4-C5	-5.22	125.99	128.60
36	5	278	U	C5-C6-N1	5.22	125.31	122.70
36	5	1789	G	C4-N9-C1'	-5.22	119.71	126.50
36	5	2796	G	C5-C6-O6	-5.22	125.47	128.60
1	2	1324	G	N9-C4-C5	5.22	107.49	105.40
36	1	2879	C	N3-C4-C5	-5.22	119.81	121.90
1	6	945	U	N3-C2-O2	-5.22	118.55	122.20
1	2	1768	G	C5-C6-O6	5.22	131.73	128.60
56	N0	167	ARG	NE-CZ-NH1	5.22	122.91	120.30
36	5	2794	G	C5-C6-N1	5.22	114.11	111.50
36	5	2992	U	C6-N1-C1'	-5.22	113.89	121.20
35	SM	134	ASP	CB-CG-OD2	5.22	123.00	118.30
36	1	368	G	N1-C2-N3	5.22	127.03	123.90
36	1	421	G	C4-C5-N7	5.22	112.89	110.80
36	1	498	A	N1-C6-N6	-5.22	115.47	118.60
36	1	1653	G	C5-C6-O6	5.22	131.73	128.60
36	1	2403	G	N7-C8-N9	5.22	115.71	113.10
36	1	2728	G	C2-N3-C4	5.22	114.51	111.90
36	1	2889	C	C4-C5-C6	5.22	120.01	117.40
1	6	747	C	C2-N3-C4	-5.22	117.29	119.90
1	6	1150	G	C8-N9-C4	5.22	108.49	106.40
36	5	1918	C	C6-N1-C2	-5.22	118.21	120.30
36	5	2683	U	N1-C2-O2	5.22	126.45	122.80
36	5	3142	A	N1-C6-N6	5.22	121.73	118.60
36	1	859	G	C4-N9-C1'	5.22	133.28	126.50
36	1	2946	A	C6-N1-C2	5.22	121.73	118.60
1	6	4	C	N3-C2-O2	5.22	125.55	121.90
36	5	1514	G	C5-N7-C8	5.22	106.91	104.30
1	2	1733	C	N3-C4-C5	-5.22	119.81	121.90
36	1	794	U	N1-C2-N3	5.22	118.03	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	870	G	N1-C6-O6	5.22	123.03	119.90
36	1	3140	G	C5-C6-O6	-5.22	125.47	128.60
37	7	1	G	N1-C2-N2	-5.22	111.50	116.20
36	1	154	U	O4'-C1'-N1	5.21	112.37	108.20
36	1	2638	C	N1-C2-O2	-5.21	115.77	118.90
36	1	3040	A	C2-N3-C4	5.21	113.21	110.60
1	6	306	U	C6-N1-C2	5.21	124.13	121.00
36	5	2142	A	C5-C6-N6	-5.21	119.53	123.70
1	2	268	C	C6-N1-C2	-5.21	118.22	120.30
36	1	1871	U	OP2-P-O3'	5.21	116.67	105.20
36	1	2422	C	C5-C4-N4	5.21	123.85	120.20
36	1	2513	U	O4'-C1'-N1	5.21	112.37	108.20
36	5	994	G	N3-C2-N2	5.21	123.55	119.90
36	5	3197	G	N1-C6-O6	5.21	123.03	119.90
41	l4	76	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	2	783	G	O4'-C1'-N9	5.21	112.37	108.20
1	2	1129	U	N3-C4-O4	-5.21	115.75	119.40
1	6	194	U	C5-C6-N1	5.21	125.31	122.70
1	6	945	U	N1-C2-O2	5.21	126.45	122.80
36	5	921	A	O4'-C1'-N9	-5.21	104.03	108.20
50	m4	72	LEU	CA-CB-CG	5.21	127.29	115.30
36	1	619	A	N9-C4-C5	-5.21	103.72	105.80
36	1	2283	G	C5-C6-O6	-5.21	125.47	128.60
36	1	2702	A	C8-N9-C4	-5.21	103.72	105.80
73	O7	65	ARG	NE-CZ-NH1	5.21	122.91	120.30
36	1	2355	G	N1-C6-O6	5.21	123.03	119.90
36	1	2682	C	O5'-P-OP2	-5.21	101.01	105.70
36	1	2832	C	OP2-P-O3'	5.21	116.66	105.20
36	1	2867	C	N3-C4-C5	5.21	123.98	121.90
36	1	2983	C	N1-C2-O2	5.21	122.03	118.90
1	6	1121	C	C5-C4-N4	5.21	123.85	120.20
36	5	2191	U	N3-C4-O4	-5.21	115.75	119.40
36	5	2869	U	C6-N1-C1'	5.21	128.49	121.20
36	5	2913	C	C2-N3-C4	-5.21	117.30	119.90
1	2	334	G	N1-C2-N2	-5.21	111.51	116.20
1	2	1658	G	C4-C5-N7	5.21	112.88	110.80
36	1	2188	A	N7-C8-N9	-5.21	111.20	113.80
36	1	2730	G	C2-N3-C4	-5.21	109.30	111.90
1	6	572	C	C5-C4-N4	-5.21	116.56	120.20
36	5	1307	G	C2'-C3'-O3'	5.21	122.03	113.70
36	5	2992	U	N1-C2-O2	5.21	126.44	122.80
36	5	2830	G	N1-C2-N3	5.21	127.02	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	213	A	N1-C2-N3	-5.20	126.70	129.30
36	1	517	G	N9-C4-C5	5.20	107.48	105.40
36	1	661	G	OP2-P-O3'	5.20	116.65	105.20
36	1	720	A	C2-N3-C4	5.20	113.20	110.60
36	5	1331	U	N1-C2-N3	-5.20	111.78	114.90
36	5	2300	G	N3-C2-N2	5.20	123.54	119.90
36	5	2614	G	C5-C6-O6	5.20	131.72	128.60
36	1	2949	U	N3-C4-O4	-5.20	115.76	119.40
36	1	3052	G	N9-C4-C5	5.20	107.48	105.40
1	6	359	A	C4-C5-C6	-5.20	114.40	117.00
36	5	3081	C	N3-C4-N4	-5.20	114.36	118.00
36	1	197	G	N3-C2-N2	-5.20	116.26	119.90
36	1	1718	G	N1-C2-N2	5.20	120.88	116.20
36	1	1902	G	N3-C4-N9	5.20	129.12	126.00
41	L4	197	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	6	337	G	C4-C5-C6	5.20	121.92	118.80
1	6	1120	U	C5-C4-O4	5.20	129.02	125.90
36	5	971	G	C6-C5-N7	5.20	133.52	130.40
36	5	1120	A	C6-C5-N7	5.20	135.94	132.30
36	5	1141	C	O5'-P-OP1	-5.20	101.02	105.70
36	5	1451	C	C6-N1-C2	5.20	122.38	120.30
36	5	2898	G	O4'-C1'-N9	-5.20	104.04	108.20
1	2	1762	A	C8-N9-C4	5.20	107.88	105.80
36	1	847	A	C5-C6-N6	-5.20	119.54	123.70
37	3	52	G	N1-C6-O6	-5.20	116.78	119.90
36	5	1436	U	C5-C4-O4	-5.20	122.78	125.90
36	5	2249	G	C2'-C3'-O3'	5.20	122.02	113.70
36	1	212	G	N3-C4-N9	5.20	129.12	126.00
36	1	504	A	N1-C6-N6	-5.20	115.48	118.60
36	1	643	U	C2-N1-C1'	-5.20	111.47	117.70
36	1	867	G	N3-C2-N2	-5.20	116.26	119.90
36	1	1005	G	C5-C6-O6	5.20	131.72	128.60
36	1	3085	G	N1-C6-O6	5.20	123.02	119.90
1	6	978	A	C8-N9-C4	-5.20	103.72	105.80
36	5	205	C	N1-C2-O2	5.20	122.02	118.90
36	5	2955	U	N1-C2-N3	5.20	118.02	114.90
36	5	2957	G	N7-C8-N9	-5.20	110.50	113.10
36	5	3006	A	N9-C4-C5	5.20	107.88	105.80
38	8	95	G	N3-C4-N9	-5.20	122.88	126.00
1	2	17	C	C6-N1-C2	-5.19	118.22	120.30
36	1	1484	U	N3-C2-O2	-5.19	118.56	122.20
36	1	2393	G	O5'-P-OP2	-5.19	101.03	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	o3	86	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	2	55	A	C8-N9-C4	-5.19	103.72	105.80
36	1	344	A	C4-C5-N7	-5.19	108.10	110.70
36	1	836	A	C5-C6-N6	-5.19	119.55	123.70
36	1	1881	A	C8-N9-C4	5.19	107.88	105.80
36	1	3377	G	C5-C6-O6	-5.19	125.48	128.60
1	6	557	G	C5-C6-O6	5.19	131.72	128.60
36	5	831	G	C5-C6-O6	-5.19	125.48	128.60
36	5	1942	U	N1-C2-N3	5.19	118.02	114.90
36	5	2584	G	OP2-P-O3'	5.19	116.62	105.20
36	5	2836	C	OP2-P-O3'	5.19	116.62	105.20
36	1	360	G	N3-C4-N9	5.19	129.11	126.00
36	1	1133	A	C8-N9-C4	5.19	107.88	105.80
36	5	295	A	O5'-P-OP1	-5.19	101.03	105.70
36	5	1901	A	C4-N9-C1'	5.19	135.64	126.30
36	5	2754	G	N3-C4-N9	5.19	129.12	126.00
36	5	2881	C	N3-C4-C5	5.19	123.98	121.90
36	5	3154	C	C5-C6-N1	5.19	123.59	121.00
40	l3	10	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	2	1537	C	C5-C4-N4	-5.19	116.57	120.20
36	1	103	G	N1-C6-O6	-5.19	116.79	119.90
36	1	2980	U	O5'-P-OP2	5.19	116.93	110.70
1	6	139	C	N3-C2-O2	-5.19	118.27	121.90
39	l2	241	ARG	NE-CZ-NH2	-5.19	117.71	120.30
36	1	2873	U	N1-C2-O2	5.19	126.43	122.80
36	1	2945	G	C8-N9-C4	5.19	108.47	106.40
36	1	3058	U	C2-N1-C1'	5.19	123.93	117.70
1	6	118	U	N3-C4-C5	5.19	117.71	114.60
36	5	385	A	N1-C6-N6	5.19	121.71	118.60
1	6	1354	G	N7-C8-N9	5.19	115.69	113.10
36	5	2992	U	C2-N1-C1'	5.19	123.92	117.70
1	2	794	U	P-O3'-C3'	5.18	125.92	119.70
1	2	934	C	N3-C4-N4	5.18	121.63	118.00
36	1	405	U	O5'-P-OP1	-5.18	101.03	105.70
36	1	1115	G	C8-N9-C1'	-5.18	120.26	127.00
36	1	3058	U	C6-N1-C1'	-5.18	113.94	121.20
36	5	1327	C	N1-C2-O2	5.18	122.01	118.90
36	5	2167	A	N9-C4-C5	5.18	107.87	105.80
36	5	2818	U	N3-C4-C5	5.18	117.71	114.60
36	5	2928	C	O5'-P-OP2	-5.18	101.03	105.70
38	8	3	A	C2-N3-C4	5.18	113.19	110.60
36	1	33	G	C5-N7-C8	-5.18	101.71	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	223	U	C2-N3-C4	-5.18	123.89	127.00
36	1	780	A	N1-C6-N6	-5.18	115.49	118.60
36	1	2830	G	N3-C2-N2	-5.18	116.27	119.90
36	1	3271	G	C8-N9-C4	5.18	108.47	106.40
38	4	47	C	OP2-P-O3'	5.18	116.60	105.20
1	6	394	C	C5-C6-N1	-5.18	118.41	121.00
36	5	611	A	O5'-P-OP1	5.18	116.92	110.70
36	5	2379	U	C2-N3-C4	-5.18	123.89	127.00
36	5	2724	U	C5-C4-O4	5.18	129.01	125.90
37	7	74	C	N1-C2-O2	-5.18	115.79	118.90
52	m6	49	ARG	NE-CZ-NH1	-5.18	117.71	120.30
36	1	1117	G	C8-N9-C4	5.18	108.47	106.40
1	6	31	C	N3-C4-C5	-5.18	119.83	121.90
36	5	37	U	N1-C2-N3	5.18	118.01	114.90
36	1	2585	G	N3-C4-C5	-5.18	126.01	128.60
1	2	1458	G	C8-N9-C1'	-5.18	120.27	127.00
36	1	96	G	C2-N3-C4	-5.18	109.31	111.90
36	1	158	G	N3-C4-N9	-5.18	122.89	126.00
36	1	1838	G	C5-C6-O6	-5.18	125.49	128.60
36	1	2145	A	C8-N9-C4	-5.18	103.73	105.80
36	1	2286	U	O5'-P-OP2	-5.18	101.04	105.70
52	M6	33	ILE	CG1-CB-CG2	-5.18	100.01	111.40
1	6	794	U	C2-N1-C1'	5.18	123.91	117.70
1	6	1661	U	N1-C2-O2	-5.18	119.18	122.80
8	s6	133	LEU	CA-CB-CG	5.18	127.20	115.30
36	5	1134	G	O5'-P-OP2	-5.18	101.04	105.70
36	5	1464	G	C8-N9-C4	5.18	108.47	106.40
36	5	2234	G	C4-C5-N7	5.18	112.87	110.80
36	5	2995	A	C8-N9-C4	5.18	107.87	105.80
1	2	1739	C	N3-C4-C5	5.17	123.97	121.90
36	5	1154	A	C2-N3-C4	5.17	113.19	110.60
36	5	1199	C	C2-N3-C4	-5.17	117.31	119.90
36	5	1858	A	C2-N3-C4	5.17	113.19	110.60
36	5	2924	U	O5'-P-OP1	-5.17	101.04	105.70
38	4	63	G	N9-C4-C5	5.17	107.47	105.40
40	L3	19	ARG	NE-CZ-NH2	-5.17	117.71	120.30
36	5	1889	G	C5-C6-O6	5.17	131.70	128.60
36	5	2202	C	C5-C4-N4	-5.17	116.58	120.20
36	5	2294	U	C2-N3-C4	-5.17	123.90	127.00
1	2	758	U	N3-C2-O2	-5.17	118.58	122.20
1	6	417	A	C6-C5-N7	-5.17	128.68	132.30
36	5	411	U	N1-C2-N3	5.17	118.00	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2371	G	C6-N1-C2	5.17	128.20	125.10
29	D7	29	ARG	NE-CZ-NH1	5.17	122.89	120.30
36	1	340	C	N3-C4-C5	5.17	123.97	121.90
36	1	3173	G	C6-N1-C2	-5.17	122.00	125.10
68	O2	33	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	2	1678	A	C8-N9-C4	-5.17	103.73	105.80
36	1	793	C	N1-C2-O2	-5.17	115.80	118.90
36	1	897	U	C5-C6-N1	5.17	125.28	122.70
36	1	1112	A	N1-C6-N6	5.17	121.70	118.60
36	1	2157	G	C2-N3-C4	5.17	114.48	111.90
1	6	1084	A	N1-C6-N6	-5.17	115.50	118.60
36	5	914	A	N7-C8-N9	-5.17	111.22	113.80
36	1	400	G	C5-C6-O6	-5.17	125.50	128.60
1	6	65	A	C5-N7-C8	-5.17	101.32	103.90
1	6	1031	U	C2-N1-C1'	-5.17	111.50	117.70
36	5	428	A	OP2-P-O3'	5.17	116.57	105.20
38	8	65	A	C5-C6-N6	-5.17	119.57	123.70
36	1	291	C	N1-C2-N3	5.16	122.81	119.20
36	1	2883	U	C6-N1-C2	-5.16	117.90	121.00
36	1	2958	A	N7-C8-N9	-5.16	111.22	113.80
36	1	3108	G	C2-N3-C4	5.16	114.48	111.90
36	5	1305	U	N3-C4-O4	5.16	123.01	119.40
36	5	1390	A	C8-N9-C4	-5.16	103.73	105.80
36	5	2955	U	C6-N1-C2	-5.16	117.90	121.00
1	2	1768	G	N9-C4-C5	5.16	107.47	105.40
36	1	1370	G	N1-C2-N2	-5.16	111.55	116.20
1	6	1101	G	N9-C4-C5	5.16	107.47	105.40
36	1	352	A	O4'-C1'-N9	5.16	112.33	108.20
36	1	1153	A	O5'-P-OP1	-5.16	101.06	105.70
1	6	320	U	O5'-P-OP2	5.16	116.89	110.70
1	6	697	C	N3-C2-O2	-5.16	118.29	121.90
1	6	1670	G	O5'-P-OP2	-5.16	101.06	105.70
36	5	649	A	C5-N7-C8	-5.16	101.32	103.90
36	5	1604	G	N3-C4-C5	-5.16	126.02	128.60
36	5	3358	U	N3-C2-O2	-5.16	118.59	122.20
1	2	73	U	P-O3'-C3'	5.16	125.89	119.70
1	2	1206	U	N3-C4-O4	5.16	123.01	119.40
36	1	885	U	N3-C4-O4	-5.16	115.79	119.40
36	1	963	G	C5-C6-O6	-5.16	125.50	128.60
36	1	1908	A	C8-N9-C4	5.16	107.86	105.80
36	1	2714	G	O5'-P-OP2	5.16	116.89	110.70
1	6	539	G	C8-N9-C4	-5.16	104.34	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1605	G	C5-C6-O6	5.16	131.69	128.60
36	5	2607	G	N9-C4-C5	5.16	107.46	105.40
36	5	2836	C	N1-C2-N3	5.16	122.81	119.20
36	5	2917	G	N3-C4-N9	5.16	129.09	126.00
59	n3	42	SER	N-CA-C	5.16	124.93	111.00
36	1	37	U	C5-C6-N1	-5.16	120.12	122.70
36	1	1125	U	OP2-P-O3'	5.16	116.55	105.20
1	2	1792	G	N9-C4-C5	-5.16	103.34	105.40
36	1	930	U	N3-C4-C5	5.16	117.69	114.60
36	1	2138	A	C2-N3-C4	-5.16	108.02	110.60
36	5	640	U	C5-C6-N1	-5.16	120.12	122.70
36	5	2260	U	OP2-P-O3'	5.16	116.54	105.20
36	1	72	C	N3-C4-C5	5.15	123.96	121.90
36	1	142	C	C6-N1-C2	-5.15	118.24	120.30
36	5	793	C	C4-C5-C6	-5.15	114.82	117.40
36	5	1679	A	N1-C6-N6	-5.15	115.51	118.60
36	5	2961	G	N1-C6-O6	-5.15	116.81	119.90
1	2	447	U	C6-N1-C2	-5.15	117.91	121.00
36	1	1310	G	N3-C2-N2	5.15	123.51	119.90
36	1	2853	A	C8-N9-C4	-5.15	103.74	105.80
1	6	1006	C	C6-N1-C2	-5.15	118.24	120.30
1	6	1697	G	N3-C4-N9	5.15	129.09	126.00
36	5	94	G	N1-C2-N3	-5.15	120.81	123.90
36	5	2378	C	C2-N3-C4	5.15	122.48	119.90
36	5	2630	C	N1-C2-N3	5.15	122.81	119.20
36	5	3310	A	N1-C6-N6	-5.15	115.51	118.60
1	2	61	A	O4'-C1'-N9	5.15	112.32	108.20
36	1	2695	A	O4'-C1'-N9	5.15	112.32	108.20
59	N3	87	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	6	448	C	OP1-P-O3'	5.15	116.53	105.20
36	5	708	G	C5-N7-C8	-5.15	101.72	104.30
36	5	722	G	N9-C4-C5	5.15	107.46	105.40
36	5	1208	U	C5-C4-O4	5.15	128.99	125.90
36	5	217	U	C5-C6-N1	-5.15	120.13	122.70
36	5	1146	C	C6-N1-C2	-5.15	118.24	120.30
36	1	349	A	N1-C6-N6	-5.15	115.51	118.60
36	1	1060	U	C6-N1-C2	5.15	124.09	121.00
36	5	1371	G	C5-N7-C8	5.15	106.87	104.30
36	5	1908	A	N3-C4-C5	-5.15	123.20	126.80
36	5	2366	C	C6-N1-C2	-5.15	118.24	120.30
36	5	2608	G	N1-C2-N2	-5.15	111.57	116.20
36	1	93	C	C2-N1-C1'	-5.15	113.14	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2314	U	C2-N1-C1'	5.15	123.88	117.70
36	1	3187	A	C2-N3-C4	5.15	113.17	110.60
1	2	938	G	OP2-P-O3'	5.14	116.52	105.20
1	2	1051	G	P-O3'-C3'	5.14	125.87	119.70
36	1	971	G	N1-C6-O6	-5.14	116.81	119.90
36	1	1082	U	C2-N1-C1'	5.14	123.87	117.70
36	1	2392	C	N3-C4-N4	5.14	121.60	118.00
36	5	640	U	N1-C2-N3	5.14	117.99	114.90
36	5	1382	G	N1-C6-O6	-5.14	116.81	119.90
36	5	1468	A	OP1-P-OP2	5.14	127.32	119.60
36	5	2180	G	N7-C8-N9	-5.14	110.53	113.10
36	5	3362	A	C4-C5-N7	5.14	113.27	110.70
36	1	1152	G	C4-C5-N7	5.14	112.86	110.80
36	1	2365	C	N3-C4-N4	-5.14	114.40	118.00
36	1	2402	A	C4-C5-C6	5.14	119.57	117.00
36	1	2627	C	O4'-C1'-N1	5.14	112.31	108.20
69	O3	29	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	6	1535	U	C4-C5-C6	5.14	122.79	119.70
36	5	906	A	N1-C6-N6	-5.14	115.51	118.60
36	5	3042	U	N3-C4-C5	5.14	117.69	114.60
36	5	348	A	N7-C8-N9	-5.14	111.23	113.80
36	5	1439	U	N3-C4-C5	5.14	117.69	114.60
36	1	2236	G	C5-C6-O6	-5.14	125.52	128.60
36	1	2343	C	N3-C2-O2	-5.14	118.30	121.90
36	1	3171	U	N1-C2-O2	-5.14	119.20	122.80
1	6	1149	G	C5-C6-O6	5.14	131.68	128.60
36	5	653	A	OP2-P-O3'	5.14	116.51	105.20
36	5	2965	U	N1-C2-O2	-5.14	119.20	122.80
36	5	3093	C	N1-C2-O2	-5.14	115.82	118.90
1	2	142	G	C2-N3-C4	-5.14	109.33	111.90
1	6	90	C	N3-C4-N4	-5.14	114.40	118.00
1	6	417	A	C4-C5-C6	5.14	119.57	117.00
1	6	1203	A	O5'-P-OP1	-5.14	101.08	105.70
36	5	1133	A	N9-C4-C5	5.14	107.86	105.80
36	5	1634	G	N1-C6-O6	5.14	122.98	119.90
36	5	2794	G	N9-C4-C5	-5.14	103.34	105.40
1	2	1490	C	C6-N1-C2	-5.14	118.25	120.30
36	1	518	G	O4'-C1'-N9	5.14	112.31	108.20
36	1	1124	U	C4-C5-C6	-5.14	116.62	119.70
36	1	1150	A	C2-N3-C4	-5.14	108.03	110.60
43	L6	64	LEU	CA-CB-CG	5.14	127.11	115.30
1	6	350	U	N1-C2-N3	5.14	117.98	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1681	A	C2-N3-C4	-5.14	108.03	110.60
36	5	288	C	C6-N1-C2	5.14	122.36	120.30
36	5	2524	A	C3'-C2'-C1'	-5.14	97.39	101.50
1	2	1516	A	N1-C6-N6	5.13	121.68	118.60
36	1	48	A	O4'-C1'-N9	5.13	112.31	108.20
36	1	416	A	C5-C6-N6	5.13	127.81	123.70
36	5	509	U	N1-C2-N3	5.13	117.98	114.90
36	5	1096	U	N1-C2-O2	-5.13	119.21	122.80
36	5	1168	U	C4-C5-C6	-5.13	116.62	119.70
36	1	1419	A	N9-C1'-C2'	-5.13	106.35	112.00
1	6	1781	A	C8-N9-C4	-5.13	103.75	105.80
36	1	645	A	C5-C6-N6	-5.13	119.59	123.70
36	1	2320	A	OP1-P-OP2	-5.13	111.90	119.60
36	1	3083	G	N3-C4-C5	-5.13	126.03	128.60
36	1	3219	G	N3-C4-N9	5.13	129.08	126.00
36	5	1211	U	N3-C4-O4	-5.13	115.81	119.40
36	5	2639	G	N1-C6-O6	5.13	122.98	119.90
36	5	2886	U	N1-C2-N3	5.13	117.98	114.90
36	5	3226	A	N9-C4-C5	-5.13	103.75	105.80
36	5	3378	C	C2-N3-C4	-5.13	117.33	119.90
36	1	2300	G	C5-C6-O6	5.13	131.68	128.60
1	6	1081	A	O4'-C1'-N9	5.13	112.30	108.20
36	5	1145	G	N9-C4-C5	5.13	107.45	105.40
36	1	962	A	C5-C6-N1	5.13	120.26	117.70
36	1	2444	C	C2-N1-C1'	5.13	124.44	118.80
36	1	3038	U	N3-C2-O2	-5.13	118.61	122.20
38	4	9	A	N9-C4-C5	5.13	107.85	105.80
36	5	66	A	C8-N9-C4	5.13	107.85	105.80
36	5	1108	U	O5'-P-OP2	-5.13	101.08	105.70
1	2	734	A	OP1-P-O3'	5.13	116.48	105.20
1	2	765	G	O4'-C1'-N9	-5.13	104.10	108.20
36	1	291	C	OP2-P-O3'	5.13	116.48	105.20
36	1	347	G	C4-C5-N7	5.13	112.85	110.80
36	1	2627	C	C6-N1-C2	5.13	122.35	120.30
36	1	2820	A	C2-N3-C4	5.13	113.16	110.60
1	6	1138	A	N1-C2-N3	-5.13	126.74	129.30
1	6	1396	U	C6-N1-C2	-5.13	117.92	121.00
36	5	191	U	N3-C2-O2	5.13	125.79	122.20
36	5	594	U	O5'-P-OP2	-5.13	101.09	105.70
36	5	2341	A	N9-C4-C5	-5.13	103.75	105.80
36	5	3188	G	N1-C6-O6	-5.13	116.82	119.90
44	l7	88	ARG	NE-CZ-NH1	5.13	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3308	C	C6-N1-C2	5.12	122.35	120.30
1	6	1600	A	C4-C5-N7	5.12	113.26	110.70
36	5	908	G	C5-C6-O6	-5.12	125.53	128.60
36	5	1242	G	N3-C4-N9	5.12	129.07	126.00
36	1	351	A	C8-N9-C4	5.12	107.85	105.80
36	1	966	U	N3-C2-O2	-5.12	118.61	122.20
36	1	3083	G	C2-N3-C4	5.12	114.46	111.90
1	6	60	U	N1-C2-O2	5.12	126.39	122.80
1	6	151	G	N9-C4-C5	5.12	107.45	105.40
1	6	577	G	C5-N7-C8	-5.12	101.74	104.30
36	5	1201	C	C2-N1-C1'	-5.12	113.16	118.80
36	5	1942	U	C5-C4-O4	-5.12	122.83	125.90
1	2	1491	U	O5'-P-OP1	-5.12	101.09	105.70
36	1	709	A	N1-C6-N6	5.12	121.67	118.60
36	1	3228	C	P-O3'-C3'	5.12	125.85	119.70
36	1	3275	U	P-O3'-C3'	5.12	125.84	119.70
1	6	187	G	P-O3'-C3'	5.12	125.84	119.70
36	5	1313	G	C6-N1-C2	5.12	128.17	125.10
36	5	1481	A	C5-N7-C8	-5.12	101.34	103.90
36	5	2886	U	O4'-C1'-N1	5.12	112.30	108.20
36	5	3030	G	N7-C8-N9	-5.12	110.54	113.10
1	2	1458	G	C4-N9-C1'	5.12	133.16	126.50
36	1	959	C	C2-N3-C4	-5.12	117.34	119.90
36	1	1305	U	N3-C4-O4	-5.12	115.82	119.40
36	1	2952	G	C2-N3-C4	-5.12	109.34	111.90
36	5	2699	G	C2-N3-C4	5.12	114.46	111.90
36	5	2834	G	OP1-P-OP2	5.12	127.28	119.60
37	7	96	U	C2-N3-C4	-5.12	123.93	127.00
1	2	829	A	P-O3'-C3'	5.12	125.84	119.70
36	1	748	U	N3-C4-C5	5.12	117.67	114.60
36	5	1507	G	O4'-C1'-N9	-5.12	104.11	108.20
1	2	959	U	N1-C2-O2	5.12	126.38	122.80
36	5	112	U	O4'-C1'-N1	5.12	112.29	108.20
36	5	2112	U	O5'-P-OP2	-5.12	101.10	105.70
36	5	2610	G	O4'-C1'-N9	5.12	112.29	108.20
36	5	3003	G	N3-C4-C5	5.12	131.16	128.60
38	8	92	A	N1-C6-N6	5.12	121.67	118.60
36	5	437	G	C4-C5-N7	-5.11	108.75	110.80
36	5	629	U	C2-N3-C4	-5.11	123.93	127.00
36	5	1178	G	C5-C6-O6	-5.11	125.53	128.60
36	5	2222	A	OP2-P-O3'	5.11	116.45	105.20
36	5	2767	U	O5'-P-OP2	-5.11	101.10	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2936	A	N1-C6-N6	5.11	121.67	118.60
44	l7	227	GLY	N-CA-C	5.11	125.89	113.10
36	5	3369	G	C6-N1-C2	-5.11	122.03	125.10
36	1	74	G	N1-C2-N2	-5.11	111.60	116.20
36	1	1116	G	O5'-P-OP1	-5.11	101.10	105.70
36	1	1177	G	N3-C2-N2	-5.11	116.32	119.90
36	1	1287	A	O5'-P-OP1	-5.11	101.10	105.70
36	1	1482	A	N1-C6-N6	-5.11	115.53	118.60
36	1	3275	U	C6-N1-C2	-5.11	117.93	121.00
38	4	113	U	C2-N1-C1'	-5.11	111.57	117.70
36	5	1112	A	O5'-P-OP1	-5.11	101.10	105.70
36	5	1606	U	OP1-P-OP2	5.11	127.27	119.60
36	5	2611	U	C4-C5-C6	5.11	122.77	119.70
36	5	2955	U	O5'-P-OP2	-5.11	101.10	105.70
36	1	814	U	O5'-P-OP2	5.11	116.83	110.70
36	5	688	G	N3-C4-N9	-5.11	122.94	126.00
37	7	13	A	C2-N3-C4	5.11	113.15	110.60
36	1	1418	A	O5'-P-OP1	5.11	116.83	110.70
36	1	2606	G	N3-C4-N9	5.11	129.06	126.00
36	1	2787	G	N3-C4-C5	-5.11	126.05	128.60
36	1	3041	U	N1-C2-O2	-5.11	119.22	122.80
39	L2	207	VAL	CB-CA-C	-5.11	101.70	111.40
36	5	2808	A	O5'-P-OP2	-5.11	101.10	105.70
36	5	2860	U	C6-N1-C2	5.11	124.06	121.00
36	5	2995	A	N7-C8-N9	-5.11	111.25	113.80
1	2	1654	G	O5'-P-OP2	-5.11	101.11	105.70
36	1	681	U	O5'-P-OP2	-5.11	101.11	105.70
36	1	2946	A	N1-C2-N3	-5.11	126.75	129.30
1	6	1698	G	P-O3'-C3'	5.11	125.83	119.70
36	5	798	G	OP1-P-OP2	-5.11	111.94	119.60
36	5	2257	C	C6-N1-C2	-5.11	118.26	120.30
36	5	3249	C	OP1-P-OP2	5.11	127.26	119.60
36	1	1161	G	N1-C6-O6	-5.10	116.84	119.90
36	1	2385	G	C2-N3-C4	-5.10	109.35	111.90
36	1	2993	G	N3-C4-N9	5.10	129.06	126.00
36	5	1555	U	O4'-C1'-N1	5.10	112.28	108.20
1	2	391	A	C4-C5-C6	-5.10	114.45	117.00
36	1	2338	C	N3-C2-O2	-5.10	118.33	121.90
1	6	1389	C	C2-N1-C1'	5.10	124.41	118.80
2	s0	62	ARG	NE-CZ-NH2	-5.10	117.75	120.30
36	5	646	A	C8-N9-C4	-5.10	103.76	105.80
36	5	659	G	N3-C2-N2	5.10	123.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1334	U	N3-C4-O4	5.10	122.97	119.40
39	l2	214	GLY	N-CA-C	5.10	125.85	113.10
36	1	351	A	N7-C8-N9	-5.10	111.25	113.80
36	1	2870	C	C4-C5-C6	-5.10	114.85	117.40
36	1	3109	G	C2-N3-C4	5.10	114.45	111.90
1	6	550	A	O5'-P-OP2	-5.10	101.11	105.70
44	l7	191	VAL	C-N-CA	-5.10	111.59	122.30
1	2	1145	U	N1-C2-O2	-5.10	119.23	122.80
1	2	1277	G	N3-C4-N9	-5.10	122.94	126.00
36	1	959	C	C6-N1-C2	5.10	122.34	120.30
1	6	980	G	N1-C6-O6	-5.10	116.84	119.90
36	5	1373	A	C5-N7-C8	5.10	106.45	103.90
36	5	2409	G	N9-C4-C5	5.10	107.44	105.40
1	2	1354	G	C8-N9-C4	-5.10	104.36	106.40
36	1	3190	C	N3-C4-C5	5.10	123.94	121.90
38	4	23	U	C2-N3-C4	-5.10	123.94	127.00
1	6	352	A	N1-C6-N6	-5.10	115.54	118.60
1	6	1436	A	C8-N9-C4	-5.10	103.76	105.80
36	5	2610	G	C5-C6-O6	5.10	131.66	128.60
36	1	804	C	N1-C2-O2	-5.10	115.84	118.90
36	5	2938	G	OP1-P-OP2	5.10	127.25	119.60
1	2	1776	A	N9-C4-C5	5.09	107.84	105.80
36	1	24	G	N1-C6-O6	5.09	122.96	119.90
36	1	1897	G	OP2-P-O3'	5.09	116.41	105.20
36	1	2376	G	C4-C5-N7	5.09	112.84	110.80
36	1	2883	U	N3-C4-O4	-5.09	115.83	119.40
1	6	879	G	C5-C6-O6	5.09	131.66	128.60
36	5	101	G	C8-N9-C1'	-5.09	120.38	127.00
36	5	874	U	O5'-P-OP1	-5.09	101.12	105.70
36	5	1445	U	C2-N3-C4	-5.09	123.94	127.00
36	5	2950	G	O4'-C1'-N9	5.09	112.28	108.20
36	5	3060	C	N1-C2-O2	-5.09	115.84	118.90
37	7	71	G	OP2-P-O3'	5.09	116.41	105.20
36	1	678	G	N1-C6-O6	5.09	122.96	119.90
36	5	1162	U	C5-C6-N1	-5.09	120.15	122.70
36	1	55	G	C8-N9-C4	5.09	108.44	106.40
36	1	371	G	N9-C1'-C2'	-5.09	106.40	112.00
36	1	582	G	C5-C6-N1	5.09	114.05	111.50
36	1	2413	A	N1-C6-N6	-5.09	115.55	118.60
1	6	1084	A	C5-C6-N6	5.09	127.77	123.70
36	5	3041	U	C5-C4-O4	-5.09	122.84	125.90
36	5	3095	U	N3-C4-C5	5.09	117.66	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	7	66	A	N1-C2-N3	-5.09	126.75	129.30
1	2	704	C	N3-C2-O2	-5.09	118.34	121.90
25	D3	111	GLY	N-CA-C	-5.09	100.37	113.10
36	1	1724	U	N3-C2-O2	-5.09	118.64	122.20
36	1	2123	G	C5-N7-C8	5.09	106.84	104.30
41	L4	198	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	6	1782	A	P-O3'-C3'	5.09	125.81	119.70
36	5	1181	U	C6-N1-C2	5.09	124.05	121.00
36	5	1429	G	N3-C2-N2	5.09	123.46	119.90
36	5	2333	C	OP2-P-O3'	5.09	116.40	105.20
36	5	3144	G	N9-C4-C5	5.09	107.44	105.40
36	1	1138	U	N3-C2-O2	-5.09	118.64	122.20
36	1	1720	U	N1-C2-N3	5.09	117.95	114.90
36	1	2396	G	C5-C6-N1	-5.09	108.96	111.50
1	2	1280	C	N3-C4-C5	-5.09	119.86	121.90
36	1	93	C	C6-N1-C2	-5.09	118.27	120.30
36	1	112	U	C5-C6-N1	5.09	125.24	122.70
38	4	142	C	C6-N1-C2	-5.09	118.27	120.30
1	6	313	U	C5-C6-N1	-5.09	120.16	122.70
36	5	914	A	N3-C4-C5	5.09	130.36	126.80
36	5	2912	G	N1-C6-O6	-5.09	116.85	119.90
36	5	3309	G	C4-N9-C1'	5.09	133.11	126.50
38	8	79	A	C8-N9-C4	-5.09	103.77	105.80
1	2	425	A	N7-C8-N9	5.08	116.34	113.80
1	2	1600	A	P-O3'-C3'	5.08	125.80	119.70
36	1	2550	U	C4-C5-C6	5.08	122.75	119.70
49	M3	63	VAL	CB-CA-C	-5.08	101.74	111.40
1	6	1048	G	C4-C5-N7	5.08	112.83	110.80
1	6	1796	C	N3-C4-N4	-5.08	114.44	118.00
36	5	1858	A	N3-C4-C5	-5.08	123.24	126.80
36	5	1863	G	C5-C6-O6	-5.08	125.55	128.60
1	2	934	C	C5-C6-N1	5.08	123.54	121.00
36	1	895	A	C6-C5-N7	-5.08	128.74	132.30
36	1	934	G	C8-N9-C4	5.08	108.43	106.40
36	1	1413	G	N1-C6-O6	-5.08	116.85	119.90
36	1	1807	G	N3-C4-C5	-5.08	126.06	128.60
36	1	2883	U	N1-C2-O2	5.08	126.36	122.80
36	5	883	A	C8-N9-C4	5.08	107.83	105.80
36	5	1305	U	N1-C2-O2	-5.08	119.24	122.80
36	5	2644	C	N1-C2-O2	-5.08	115.85	118.90
49	m3	55	ARG	CG-CD-NE	5.08	122.47	111.80
1	6	1101	G	C4-C5-N7	-5.08	108.77	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1730	A	OP1-P-O3'	5.08	116.38	105.20
36	5	1307	G	C5-C6-N1	5.08	114.04	111.50
1	2	736	C	C5-C6-N1	5.08	123.54	121.00
36	1	1467	A	C8-N9-C4	-5.08	103.77	105.80
36	1	2636	A	N9-C4-C5	5.08	107.83	105.80
36	5	775	A	C5-C6-N1	5.08	120.24	117.70
36	5	788	C	OP2-P-O3'	5.08	116.38	105.20
36	5	810	A	N1-C6-N6	-5.08	115.55	118.60
36	5	2160	G	N1-C6-O6	-5.08	116.85	119.90
36	5	708	G	N7-C8-N9	5.08	115.64	113.10
36	5	1014	U	C6-N1-C1'	-5.08	114.09	121.20
36	5	1147	G	OP2-P-O3'	5.08	116.37	105.20
36	5	2833	A	C2-N3-C4	5.08	113.14	110.60
37	7	15	C	N3-C4-C5	5.08	123.93	121.90
36	1	686	G	N9-C4-C5	5.08	107.43	105.40
36	1	1906	G	N3-C4-N9	5.08	129.05	126.00
37	3	95	A	C6-C5-N7	-5.08	128.75	132.30
59	N3	54	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	6	359	A	N1-C2-N3	-5.08	126.76	129.30
36	5	64	G	OP2-P-O3'	5.08	116.37	105.20
36	5	1064	A	O4'-C1'-N9	-5.08	104.14	108.20
36	5	1362	G	N1-C6-O6	-5.08	116.85	119.90
36	5	2362	C	N1-C2-O2	5.08	121.95	118.90
37	7	92	A	OP1-P-O3'	5.08	116.36	105.20
36	1	3178	A	C2-N3-C4	-5.07	108.06	110.60
41	L4	194	TYR	CB-CG-CD1	-5.07	117.96	121.00
36	5	2808	A	C2-N3-C4	-5.07	108.06	110.60
36	5	3049	A	N1-C2-N3	-5.07	126.76	129.30
36	5	3052	G	N7-C8-N9	-5.07	110.56	113.10
36	1	511	G	N1-C6-O6	-5.07	116.86	119.90
36	1	1004	U	N3-C2-O2	-5.07	118.65	122.20
36	1	1397	C	C6-N1-C2	5.07	122.33	120.30
36	1	1556	C	N1-C2-O2	5.07	121.94	118.90
36	1	2142	A	OP1-P-O3'	5.07	116.35	105.20
36	1	2314	U	C4-C5-C6	-5.07	116.66	119.70
36	1	2339	C	OP1-P-O3'	5.07	116.35	105.20
1	6	351	C	C4-C5-C6	5.07	119.94	117.40
36	5	286	U	OP2-P-O3'	5.07	116.36	105.20
36	5	386	A	C4-C5-N7	5.07	113.23	110.70
36	5	1445	U	N1-C2-O2	-5.07	119.25	122.80
36	5	2326	A	N7-C8-N9	-5.07	111.27	113.80
36	5	2420	C	C5-C4-N4	-5.07	116.65	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2817	A	C2-N3-C4	5.07	113.14	110.60
36	5	2853	A	OP1-P-OP2	-5.07	111.99	119.60
36	1	787	G	N1-C6-O6	-5.07	116.86	119.90
36	1	2388	U	N3-C2-O2	5.07	125.75	122.20
1	6	951	A	C2-N3-C4	-5.07	108.06	110.60
36	5	1863	G	N9-C4-C5	-5.07	103.37	105.40
36	1	721	G	N1-C6-O6	5.07	122.94	119.90
36	1	1893	A	N9-C4-C5	5.07	107.83	105.80
36	1	2979	U	C5-C6-N1	-5.07	120.17	122.70
36	5	3317	U	N3-C4-O4	-5.07	115.85	119.40
36	1	374	A	N1-C2-N3	-5.07	126.77	129.30
36	1	2180	G	C5-C6-O6	5.07	131.64	128.60
1	6	162	A	O5'-P-OP2	-5.07	101.14	105.70
1	6	1595	U	O4'-C1'-N1	5.07	112.25	108.20
36	5	1464	G	N3-C2-N2	5.07	123.45	119.90
36	5	3340	G	N9-C4-C5	5.07	107.43	105.40
36	1	1129	A	C5-C6-N6	-5.06	119.65	123.70
36	1	2945	G	OP1-P-OP2	-5.06	112.00	119.60
36	1	3092	C	C6-N1-C2	5.06	122.33	120.30
1	6	308	C	C4-C5-C6	5.06	119.93	117.40
36	5	2314	U	O5'-P-OP1	-5.06	101.14	105.70
48	m1	9	MET	N-CA-C	-5.06	97.33	111.00
36	1	2420	C	C2-N3-C4	-5.06	117.37	119.90
36	5	1130	A	N9-C4-C5	5.06	107.83	105.80
36	5	1876	U	C4-C5-C6	-5.06	116.66	119.70
36	5	362	U	N1-C2-N3	5.06	117.94	114.90
1	2	1782	A	C5-C6-N6	5.06	127.75	123.70
36	1	213	A	C6-N1-C2	5.06	121.64	118.60
36	1	1858	A	C4-N9-C1'	5.06	135.41	126.30
1	6	1121	C	N3-C2-O2	-5.06	118.36	121.90
36	5	2349	U	O5'-P-OP1	5.06	116.77	110.70
36	5	2404	A	N9-C4-C5	-5.06	103.78	105.80
36	5	2882	U	OP1-P-OP2	5.06	127.19	119.60
1	2	1654	G	C6-N1-C2	-5.06	122.06	125.10
36	1	1415	U	N3-C4-O4	-5.06	115.86	119.40
36	1	1870	C	C2-N3-C4	-5.06	117.37	119.90
38	4	13	A	C8-N9-C4	-5.06	103.78	105.80
1	6	1195	C	OP1-P-O3'	5.06	116.33	105.20
36	5	412	G	N1-C6-O6	-5.06	116.87	119.90
36	5	2113	A	N7-C8-N9	-5.06	111.27	113.80
36	5	2298	U	O4'-C1'-N1	5.06	112.25	108.20
36	5	2914	G	N1-C6-O6	-5.06	116.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3093	C	C4-C5-C6	5.06	119.93	117.40
36	1	46	U	N1-C2-N3	5.06	117.93	114.90
36	5	2841	G	OP1-P-O3'	5.06	116.32	105.20
36	5	3366	G	N1-C6-O6	-5.06	116.87	119.90
1	2	1585	U	C5-C4-O4	5.05	128.93	125.90
1	6	114	C	O5'-P-OP1	-5.05	101.15	105.70
36	5	111	C	C6-N1-C2	5.05	122.32	120.30
36	5	927	C	N1-C2-O2	-5.05	115.87	118.90
36	5	948	C	OP1-P-OP2	-5.05	112.02	119.60
36	5	2258	U	N1-C2-O2	5.05	126.34	122.80
36	5	2628	A	C6-N1-C2	-5.05	115.57	118.60
1	2	582	U	O5'-P-OP1	-5.05	101.15	105.70
36	1	2595	A	N1-C6-N6	5.05	121.63	118.60
36	5	1439	U	C6-N1-C2	5.05	124.03	121.00
36	5	2970	C	C5-C6-N1	-5.05	118.47	121.00
42	l5	152	ARG	NE-CZ-NH1	5.05	122.83	120.30
36	1	687	U	OP2-P-O3'	5.05	116.31	105.20
36	1	2423	U	C6-N1-C1'	-5.05	114.13	121.20
36	5	94	G	C5-C6-N1	5.05	114.03	111.50
36	5	320	G	C4-C5-N7	-5.05	108.78	110.80
36	5	2805	G	N3-C4-N9	5.05	129.03	126.00
6	S4	38	LEU	CA-CB-CG	5.05	126.92	115.30
36	1	421	G	N3-C2-N2	5.05	123.43	119.90
1	6	1783	C	O5'-P-OP1	5.05	116.76	110.70
36	5	416	A	C8-N9-C4	-5.05	103.78	105.80
36	5	2385	G	C8-N9-C1'	5.05	133.56	127.00
36	5	2964	G	C2-N3-C4	5.05	114.42	111.90
36	5	3190	C	C6-N1-C2	-5.05	118.28	120.30
36	5	3318	G	C5-C6-O6	5.05	131.63	128.60
36	1	983	A	C8-N9-C4	5.05	107.82	105.80
36	1	1845	G	N1-C6-O6	-5.05	116.87	119.90
1	6	541	A	P-O3'-C3'	-5.05	113.64	119.70
36	5	1475	A	C8-N9-C4	-5.05	103.78	105.80
36	1	1456	A	OP1-P-O3'	5.05	116.30	105.20
36	1	2131	A	C5-C6-N1	-5.05	115.18	117.70
36	5	110	G	N3-C4-C5	-5.05	126.08	128.60
36	5	125	C	N3-C2-O2	-5.05	118.37	121.90
36	5	813	G	C8-N9-C4	-5.05	104.38	106.40
36	5	2350	C	O5'-P-OP2	-5.05	101.16	105.70
36	5	2821	C	N3-C2-O2	5.05	125.43	121.90
36	1	1310	G	N1-C2-N2	-5.04	111.66	116.20
36	5	2390	A	OP2-P-O3'	5.04	116.30	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3103	A	C5-C6-N1	5.04	120.22	117.70
36	1	312	C	C6-N1-C2	5.04	122.32	120.30
50	M4	135	LEU	CA-CB-CG	5.04	126.90	115.30
1	6	314	C	N1-C2-O2	5.04	121.93	118.90
36	5	895	A	OP2-P-O3'	5.04	116.30	105.20
36	5	1481	A	O5'-P-OP2	-5.04	101.16	105.70
36	5	2743	A	C4-C5-N7	-5.04	108.18	110.70
36	5	2872	A	C4-C5-N7	-5.04	108.18	110.70
36	5	2916	U	O5'-P-OP2	-5.04	101.16	105.70
36	1	112	U	C2-N1-C1'	5.04	123.75	117.70
36	1	340	C	C6-N1-C2	-5.04	118.28	120.30
36	1	608	A	N3-C4-N9	5.04	131.43	127.40
36	1	690	A	OP1-P-O3'	5.04	116.29	105.20
36	1	1155	C	C5-C6-N1	5.04	123.52	121.00
36	1	1323	G	OP2-P-O3'	5.04	116.29	105.20
36	1	1708	C	O5'-P-OP2	-5.04	101.16	105.70
36	1	2752	U	C5-C6-N1	-5.04	120.18	122.70
1	6	1783	C	N3-C2-O2	-5.04	118.37	121.90
36	5	2941	A	C4-C5-C6	5.04	119.52	117.00
1	2	570	A	N3-C4-C5	-5.04	123.27	126.80
1	2	1765	A	O4'-C1'-N9	5.04	112.23	108.20
36	1	2867	C	C5'-C4'-O4'	-5.04	103.05	109.10
1	6	1082	C	OP1-P-OP2	5.04	127.16	119.60
36	5	413	U	C5-C4-O4	-5.04	122.88	125.90
36	5	436	A	C5-N7-C8	-5.04	101.38	103.90
36	5	941	G	C4-C5-N7	-5.04	108.78	110.80
1	2	608	U	O5'-P-OP1	-5.04	101.17	105.70
36	1	829	U	N1-C2-N3	5.04	117.92	114.90
36	1	1151	U	N1-C2-N3	5.04	117.92	114.90
36	1	1395	G	C2-N3-C4	5.04	114.42	111.90
36	1	2537	U	P-O3'-C3'	5.04	125.75	119.70
36	1	3062	G	N1-C6-O6	-5.04	116.88	119.90
36	5	36	C	OP2-P-O3'	5.04	116.28	105.20
36	5	986	U	C4-C5-C6	-5.04	116.68	119.70
36	5	1450	G	OP2-P-O3'	5.04	116.28	105.20
36	1	2279	A	N9-C4-C5	-5.04	103.78	105.80
1	6	1119	G	N3-C4-C5	-5.04	126.08	128.60
36	5	900	G	C8-N9-C4	-5.04	104.39	106.40
38	8	87	G	O4'-C1'-N9	5.04	112.23	108.20
1	2	822	U	C5-C6-N1	5.04	125.22	122.70
36	1	806	A	N1-C6-N6	5.04	121.62	118.60
36	1	1492	G	C2-N3-C4	5.04	114.42	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2147	A	O5'-P-OP2	5.04	116.74	110.70
36	1	2813	A	C5-N7-C8	5.04	106.42	103.90
36	1	2819	A	N1-C2-N3	-5.04	126.78	129.30
36	1	2930	A	O4'-C1'-N9	5.04	112.23	108.20
71	O5	86	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	6	170	U	OP2-P-O3'	5.04	116.28	105.20
1	6	1200	G	C4-N9-C1'	-5.04	119.95	126.50
36	5	1131	G	N3-C2-N2	-5.04	116.38	119.90
36	5	2896	A	C6-C5-N7	5.04	135.82	132.30
36	5	2965	U	N3-C4-O4	5.04	122.92	119.40
36	5	3042	U	N3-C4-O4	-5.04	115.88	119.40
1	2	1057	U	C5-C6-N1	5.03	125.22	122.70
36	1	2786	G	C2-N3-C4	5.03	114.42	111.90
41	L4	190	GLY	N-CA-C	5.03	125.68	113.10
36	5	2790	A	C8-N9-C4	-5.03	103.79	105.80
1	2	1000	C	N1-C2-O2	5.03	121.92	118.90
38	8	95	G	N3-C4-C5	5.03	131.12	128.60
36	1	570	A	C8-N9-C4	-5.03	103.79	105.80
38	4	51	G	N1-C6-O6	5.03	122.92	119.90
41	L4	194	TYR	CB-CG-CD2	5.03	124.02	121.00
1	6	31	C	N3-C2-O2	-5.03	118.38	121.90
36	5	1115	G	C5-N7-C8	-5.03	101.78	104.30
36	5	2142	A	N3-C4-N9	5.03	131.42	127.40
36	5	2273	G	C4-C5-N7	-5.03	108.79	110.80
38	8	104	A	N9-C4-C5	-5.03	103.79	105.80
36	1	639	G	N9-C1'-C2'	-5.03	106.47	112.00
36	1	2920	U	C2-N3-C4	-5.03	123.98	127.00
36	5	301	G	C6-C5-N7	5.03	133.42	130.40
36	5	721	G	C5-C6-O6	5.03	131.62	128.60
36	1	835	G	C5-C6-N1	5.03	114.01	111.50
36	1	908	G	C4-N9-C1'	5.03	133.04	126.50
36	1	2444	C	O4'-C1'-N1	5.03	112.22	108.20
36	5	813	G	C4-N9-C1'	5.03	133.04	126.50
1	2	1782	A	N1-C6-N6	-5.03	115.58	118.60
36	1	515	C	N3-C4-N4	5.03	121.52	118.00
36	1	1695	U	C6-N1-C2	5.03	124.02	121.00
36	5	630	A	C5-C6-N6	5.03	127.72	123.70
36	5	1544	G	C5-C6-O6	5.03	131.62	128.60
36	5	2207	A	N1-C6-N6	5.03	121.61	118.60
36	5	2590	A	OP2-P-O3'	5.03	116.26	105.20
36	1	833	G	N1-C6-O6	-5.02	116.89	119.90
73	O7	73	ARG	NE-CZ-NH1	5.02	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1178	G	OP2-P-O3'	5.02	116.25	105.20
36	5	1908	A	N1-C6-N6	-5.02	115.59	118.60
36	5	2553	U	C5-C6-N1	-5.02	120.19	122.70
1	2	113	U	N3-C2-O2	5.02	125.72	122.20
1	2	1537	C	C5-C6-N1	5.02	123.51	121.00
36	1	44	U	C2-N3-C4	-5.02	123.99	127.00
36	1	94	G	N1-C6-O6	-5.02	116.89	119.90
36	1	676	G	N3-C4-C5	-5.02	126.09	128.60
36	1	1716	U	P-O3'-C3'	5.02	125.73	119.70
36	1	1940	G	C5-C6-O6	5.02	131.61	128.60
36	1	2340	U	N1-C2-O2	5.02	126.32	122.80
36	5	1379	G	C5-N7-C8	5.02	106.81	104.30
36	5	2879	C	N3-C4-C5	5.02	123.91	121.90
36	5	3006	A	N7-C8-N9	5.02	116.31	113.80
38	8	110	C	OP2-P-O3'	5.02	116.25	105.20
36	1	1000	C	C5-C4-N4	-5.02	116.69	120.20
36	1	1495	U	N3-C4-C5	-5.02	111.59	114.60
1	6	1542	G	N9-C4-C5	5.02	107.41	105.40
36	5	1223	A	O5'-P-OP1	-5.02	101.18	105.70
36	1	344	A	C5-C6-N6	5.02	127.72	123.70
36	1	586	C	N3-C4-N4	5.02	121.51	118.00
36	1	1146	C	OP1-P-O3'	5.02	116.24	105.20
36	1	1365	G	N3-C4-N9	5.02	129.01	126.00
36	1	2898	G	C5-C6-O6	-5.02	125.59	128.60
36	5	1064	A	C6-C5-N7	-5.02	128.79	132.30
36	5	1364	C	C6-N1-C2	5.02	122.31	120.30
36	5	2825	C	C2-N3-C4	-5.02	117.39	119.90
36	5	3345	G	N3-C2-N2	-5.02	116.39	119.90
36	1	394	G	O5'-P-OP2	-5.02	101.18	105.70
36	1	1906	G	OP1-P-O3'	5.02	116.24	105.20
36	1	2393	G	N1-C6-O6	5.02	122.91	119.90
1	6	362	G	N3-C4-C5	-5.02	126.09	128.60
1	6	1782	A	O5'-P-OP2	5.02	116.72	110.70
36	5	55	G	N3-C2-N2	5.02	123.41	119.90
1	2	795	U	O5'-P-OP1	-5.01	101.19	105.70
36	1	282	G	P-O3'-C3'	5.01	125.72	119.70
36	1	907	G	N3-C2-N2	5.01	123.41	119.90
36	1	1103	A	OP2-P-O3'	5.01	116.23	105.20
36	1	2600	C	N1-C2-O2	5.01	121.91	118.90
36	1	2889	C	N3-C2-O2	-5.01	118.39	121.90
36	5	326	U	N1-C2-O2	-5.01	119.29	122.80
36	5	1344	G	OP2-P-O3'	5.01	116.23	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2896	A	C4-C5-N7	-5.01	108.19	110.70
36	5	2964	G	N9-C1'-C2'	-5.01	106.48	112.00
36	1	1049	C	C4-C5-C6	-5.01	114.89	117.40
36	1	1661	G	N3-C4-N9	5.01	129.01	126.00
1	6	1257	U	N1-C2-O2	5.01	126.31	122.80
36	5	2299	A	N1-C2-N3	-5.01	126.79	129.30
36	1	1140	G	N3-C2-N2	5.01	123.41	119.90
36	1	2642	A	C6-N1-C2	5.01	121.61	118.60
1	6	1293	U	C5-C6-N1	-5.01	120.19	122.70
36	5	1365	G	N3-C2-N2	5.01	123.41	119.90
36	5	1373	A	N7-C8-N9	-5.01	111.29	113.80
36	5	2366	C	C2-N3-C4	5.01	122.41	119.90
36	5	2966	G	C4-C5-N7	5.01	112.80	110.80
36	5	3206	C	N3-C2-O2	-5.01	118.39	121.90
1	2	570	A	N3-C4-N9	5.01	131.41	127.40
1	2	605	A	C8-N9-C4	5.01	107.80	105.80
1	2	1773	C	C5-C6-N1	5.01	123.50	121.00
36	1	1426	C	N1-C2-O2	5.01	121.91	118.90
36	1	2193	U	OP2-P-O3'	5.01	116.22	105.20
36	5	2211	U	N3-C4-C5	-5.01	111.59	114.60
36	5	2732	G	N3-C2-N2	5.01	123.41	119.90
41	l4	190	GLY	N-CA-C	5.01	125.62	113.10
1	2	1486	G	C4-N9-C1'	5.01	133.01	126.50
36	1	1140	G	N1-C2-N2	-5.01	111.69	116.20
36	5	1120	A	C5-N7-C8	5.01	106.40	103.90
36	5	3207	U	N1-C2-N3	5.01	117.91	114.90
38	8	6	U	C5-C4-O4	-5.01	122.89	125.90
38	8	77	A	C2-N3-C4	-5.01	108.10	110.60
36	1	1192	C	C6-N1-C2	-5.01	118.30	120.30
36	1	1313	G	N1-C6-O6	5.01	122.90	119.90
36	1	1796	G	C8-N9-C4	-5.01	104.40	106.40
36	1	2960	C	C6-N1-C2	5.01	122.30	120.30
36	1	2993	G	C8-N9-C4	5.01	108.40	106.40
1	6	314	C	C6-N1-C2	-5.01	118.30	120.30
1	6	815	G	N9-C4-C5	-5.01	103.40	105.40
1	6	1200	G	C8-N9-C1'	5.01	133.51	127.00
1	6	1463	C	C6-N1-C2	5.01	122.30	120.30
36	5	248	U	C2-N1-C1'	5.01	123.71	117.70
36	5	296	A	C8-N9-C4	-5.01	103.80	105.80
36	5	867	G	C5-C6-N1	-5.01	109.00	111.50
36	5	945	C	C5-C6-N1	-5.01	118.50	121.00
36	5	1117	G	N7-C8-N9	-5.01	110.60	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1545	A	O5'-P-OP2	-5.01	101.19	105.70
40	l3	184	ASN	C-N-CA	-5.01	111.79	122.30
59	n3	87	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	6	86	A	OP2-P-O3'	5.00	116.21	105.20
1	6	314	C	C5'-C4'-O4'	5.00	115.11	109.10
36	5	658	G	C5-C6-O6	-5.00	125.60	128.60
36	5	3167	A	C8-N9-C4	-5.00	103.80	105.80
36	5	3382	U	N1-C2-O2	5.00	126.30	122.80
36	1	1336	U	OP2-P-O3'	5.00	116.21	105.20
36	1	3078	U	C6-N1-C2	-5.00	118.00	121.00
36	5	1607	U	N3-C4-C5	5.00	117.60	114.60
38	8	21	C	O4'-C1'-N1	5.00	112.20	108.20
38	8	24	G	C8-N9-C4	5.00	108.40	106.40
1	2	1241	G	O4'-C1'-N9	5.00	112.20	108.20
36	1	2215	A	C4-C5-C6	-5.00	114.50	117.00
36	1	3132	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
19	C7	22	PRO	Peptide
25	D3	3	LYS	Peptide
27	D5	94	LYS	Peptide
28	D6	84	VAL	Peptide
28	D6	85	ARG	Peptide
28	D6	97	PRO	Peptide
33	E1	137	ASP	Peptide
39	L2	19	HIS	Peptide
41	L4	190	GLY	Peptide
41	L4	318	LEU	Peptide
42	L5	257	GLU	Peptide
44	L7	157	ASN	Peptide
51	M5	182	ASN	Peptide
52	M6	110	PRO	Peptide
52	M6	111	PRO	Peptide
53	M7	8	SER	Peptide
57	N1	16	GLN	Peptide
63	N7	3	LYS	Peptide
65	N9	19	ASN	Peptide

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Mol	Chain	Res	Type	Group
67	O1	5	LYS	Peptide
72	O6	2	THR	Peptide
2	S0	188	LEU	Peptide
9	S7	131	PHE	Peptide
10	S8	147	ALA	Peptide
34	SR	160	GLU	Mainchain
34	SR	161	LYS	Mainchain
17	c5	52	LYS	Peptide
22	d0	70	THR	Peptide
25	d3	44	GLY	Peptide
26	d4	29	HIS	Peptide
26	d4	50	ALA	Peptide
31	d9	17	GLY	Peptide
39	l2	143	GLU	Peptide
39	l2	171	GLY	Peptide
40	l3	139	GLN	Peptide
40	l3	185	GLY	Peptide
41	l4	91	GLY	Peptide
42	l5	270	LYS	Peptide
42	l5	271	LYS	Peptide
43	l6	51	ARG	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
52	m6	110	PRO	Peptide
53	m7	66	SER	Peptide
59	n3	41	GLY	Peptide
62	n6	111	LEU	Peptide
63	n7	6	LYS	Peptide
64	n8	66	ALA	Peptide
64	n8	75	LEU	Peptide
65	n9	19	ASN	Peptide
65	n9	23	LYS	Peptide
65	n9	24	PRO	Peptide
67	o1	64	VAL	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	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%)	154 (76%)	27 (13%)	23 (11%)	0	1
2	s0	204/251 (81%)	161 (79%)	27 (13%)	16 (8%)	1	2
3	S1	212/254 (84%)	152 (72%)	31 (15%)	29 (14%)	0	0
3	s1	214/254 (84%)	179 (84%)	23 (11%)	12 (6%)	2	5
4	S2	215/253 (85%)	181 (84%)	25 (12%)	9 (4%)	3	9
4	s2	215/253 (85%)	187 (87%)	16 (7%)	12 (6%)	2	5
5	S3	221/239 (92%)	198 (90%)	14 (6%)	9 (4%)	3	9
5	s3	221/239 (92%)	193 (87%)	15 (7%)	13 (6%)	1	4
6	S4	258/260 (99%)	219 (85%)	27 (10%)	12 (5%)	2	7
6	s4	258/260 (99%)	223 (86%)	23 (9%)	12 (5%)	2	7
7	S5	204/224 (91%)	162 (79%)	21 (10%)	21 (10%)	0	1
7	s5	204/224 (91%)	164 (80%)	23 (11%)	17 (8%)	1	2
8	S6	224/236 (95%)	195 (87%)	21 (9%)	8 (4%)	3	11
8	s6	216/236 (92%)	194 (90%)	14 (6%)	8 (4%)	3	11
9	S7	182/189 (96%)	143 (79%)	21 (12%)	18 (10%)	0	1
9	s7	184/189 (97%)	148 (80%)	22 (12%)	14 (8%)	1	2
10	S8	184/200 (92%)	159 (86%)	12 (6%)	13 (7%)	1	2
10	s8	184/200 (92%)	164 (89%)	11 (6%)	9 (5%)	2	7
11	S9	183/196 (93%)	159 (87%)	15 (8%)	9 (5%)	2	7
11	s9	183/196 (93%)	148 (81%)	23 (13%)	12 (7%)	1	3
12	C0	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	1	3
12	c0	92/105 (88%)	63 (68%)	16 (17%)	13 (14%)	0	0
13	C1	153/155 (99%)	125 (82%)	18 (12%)	10 (6%)	1	3
13	c1	144/155 (93%)	117 (81%)	18 (12%)	9 (6%)	1	3
14	C2	122/142 (86%)	70 (57%)	26 (21%)	26 (21%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/142 (86%)	71 (58%)	29 (24%)	22 (18%)	0	0
15	C3	148/150 (99%)	132 (89%)	13 (9%)	3 (2%)	7	24
15	c3	148/150 (99%)	123 (83%)	16 (11%)	9 (6%)	1	4
16	C4	125/136 (92%)	97 (78%)	16 (13%)	12 (10%)	0	1
16	c4	126/136 (93%)	101 (80%)	15 (12%)	10 (8%)	1	2
17	C5	122/141 (86%)	95 (78%)	16 (13%)	11 (9%)	1	1
17	c5	133/141 (94%)	97 (73%)	16 (12%)	20 (15%)	0	0
18	C6	139/142 (98%)	121 (87%)	13 (9%)	5 (4%)	3	11
18	c6	140/142 (99%)	121 (86%)	11 (8%)	8 (6%)	1	5
19	C7	116/136 (85%)	87 (75%)	22 (19%)	7 (6%)	1	4
19	c7	113/136 (83%)	96 (85%)	11 (10%)	6 (5%)	2	6
20	C8	143/145 (99%)	121 (85%)	11 (8%)	11 (8%)	1	2
20	c8	143/145 (99%)	115 (80%)	21 (15%)	7 (5%)	2	7
21	C9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	3	12
21	c9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	3	12
22	D0	105/120 (88%)	88 (84%)	15 (14%)	2 (2%)	8	26
22	d0	108/120 (90%)	85 (79%)	15 (14%)	8 (7%)	1	2
23	D1	85/87 (98%)	69 (81%)	10 (12%)	6 (7%)	1	2
23	d1	85/87 (98%)	75 (88%)	5 (6%)	5 (6%)	1	4
24	D2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	19	49
24	d2	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	19	49
25	D3	142/144 (99%)	117 (82%)	14 (10%)	11 (8%)	1	2
25	d3	142/144 (99%)	131 (92%)	10 (7%)	1 (1%)	22	53
26	D4	132/134 (98%)	110 (83%)	14 (11%)	8 (6%)	1	4
26	d4	132/134 (98%)	106 (80%)	15 (11%)	11 (8%)	1	2
27	D5	68/107 (64%)	51 (75%)	9 (13%)	8 (12%)	0	1
27	d5	67/107 (63%)	48 (72%)	13 (19%)	6 (9%)	1	1
28	D6	95/97 (98%)	69 (73%)	12 (13%)	14 (15%)	0	0
28	d6	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	1	2
29	D7	79/81 (98%)	62 (78%)	12 (15%)	5 (6%)	1	3
29	d7	79/81 (98%)	60 (76%)	10 (13%)	9 (11%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D8	61/66 (92%)	51 (84%)	7 (12%)	3 (5%)	2	7
30	d8	61/66 (92%)	46 (75%)	10 (16%)	5 (8%)	1	2
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	1	4
31	d9	51/55 (93%)	42 (82%)	5 (10%)	4 (8%)	1	2
32	E0	58/60 (97%)	45 (78%)	12 (21%)	1 (2%)	9	29
33	E1	69/76 (91%)	36 (52%)	14 (20%)	19 (28%)	0	0
33	e1	74/76 (97%)	38 (51%)	16 (22%)	20 (27%)	0	0
34	SR	316/318 (99%)	274 (87%)	29 (9%)	13 (4%)	3	9
34	sR	316/318 (99%)	268 (85%)	40 (13%)	8 (2%)	5	19
35	SM	155/273 (57%)	109 (70%)	26 (17%)	20 (13%)	0	1
35	sM	98/273 (36%)	61 (62%)	24 (24%)	13 (13%)	0	0
39	L2	250/253 (99%)	226 (90%)	20 (8%)	4 (2%)	9	31
39	l2	250/253 (99%)	214 (86%)	27 (11%)	9 (4%)	3	11
40	L3	384/386 (100%)	340 (88%)	31 (8%)	13 (3%)	3	13
40	l3	384/386 (100%)	350 (91%)	25 (6%)	9 (2%)	6	21
41	L4	359/361 (99%)	315 (88%)	23 (6%)	21 (6%)	1	4
41	l4	359/361 (99%)	308 (86%)	38 (11%)	13 (4%)	3	11
42	L5	294/296 (99%)	253 (86%)	23 (8%)	18 (6%)	1	4
42	l5	292/296 (99%)	262 (90%)	21 (7%)	9 (3%)	4	14
43	L6	152/175 (87%)	141 (93%)	8 (5%)	3 (2%)	7	24
43	l6	153/175 (87%)	132 (86%)	17 (11%)	4 (3%)	5	18
44	L7	220/243 (90%)	205 (93%)	6 (3%)	9 (4%)	3	9
44	l7	221/243 (91%)	203 (92%)	15 (7%)	3 (1%)	11	34
45	L8	231/255 (91%)	193 (84%)	30 (13%)	8 (4%)	3	12
45	l8	229/255 (90%)	184 (80%)	25 (11%)	20 (9%)	1	1
46	L9	189/191 (99%)	170 (90%)	14 (7%)	5 (3%)	5	18
46	l9	189/191 (99%)	173 (92%)	10 (5%)	6 (3%)	4	13
47	M0	207/220 (94%)	185 (89%)	17 (8%)	5 (2%)	6	20
47	m0	209/220 (95%)	181 (87%)	20 (10%)	8 (4%)	3	10
48	M1	167/173 (96%)	133 (80%)	20 (12%)	14 (8%)	1	2
48	m1	167/173 (96%)	146 (87%)	11 (7%)	10 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	164 (86%)	19 (10%)	8 (4%)	3	9
49	m3	192/198 (97%)	164 (85%)	17 (9%)	11 (6%)	1	5
50	M4	134/137 (98%)	118 (88%)	11 (8%)	5 (4%)	3	11
50	m4	135/137 (98%)	127 (94%)	6 (4%)	2 (2%)	10	33
51	M5	201/203 (99%)	188 (94%)	7 (4%)	6 (3%)	4	15
51	m5	201/203 (99%)	180 (90%)	14 (7%)	7 (4%)	3	12
52	M6	195/198 (98%)	185 (95%)	6 (3%)	4 (2%)	7	23
52	m6	195/198 (98%)	185 (95%)	8 (4%)	2 (1%)	15	44
53	M7	181/183 (99%)	159 (88%)	16 (9%)	6 (3%)	4	13
53	m7	153/183 (84%)	140 (92%)	10 (6%)	3 (2%)	7	24
54	M8	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	6	22
54	m8	183/185 (99%)	165 (90%)	11 (6%)	7 (4%)	3	10
55	M9	186/188 (99%)	173 (93%)	12 (6%)	1 (0%)	29	61
55	m9	186/188 (99%)	175 (94%)	8 (4%)	3 (2%)	9	31
56	N0	170/172 (99%)	157 (92%)	11 (6%)	2 (1%)	13	39
56	n0	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	8	28
57	N1	157/159 (99%)	138 (88%)	14 (9%)	5 (3%)	4	13
57	n1	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	5	19
58	N2	98/120 (82%)	79 (81%)	15 (15%)	4 (4%)	3	9
58	n2	96/120 (80%)	84 (88%)	9 (9%)	3 (3%)	4	14
59	N3	134/136 (98%)	126 (94%)	7 (5%)	1 (1%)	22	53
59	n3	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	22	53
60	N4	96/155 (62%)	77 (80%)	14 (15%)	5 (5%)	2	6
60	n4	133/155 (86%)	113 (85%)	12 (9%)	8 (6%)	1	4
61	N5	119/141 (84%)	110 (92%)	8 (7%)	1 (1%)	19	49
61	n5	118/141 (84%)	100 (85%)	13 (11%)	5 (4%)	3	9
62	N6	124/126 (98%)	114 (92%)	6 (5%)	4 (3%)	4	13
62	n6	124/126 (98%)	113 (91%)	6 (5%)	5 (4%)	3	9
63	N7	133/135 (98%)	111 (84%)	12 (9%)	10 (8%)	1	2
63	n7	133/135 (98%)	111 (84%)	14 (10%)	8 (6%)	1	4
64	N8	146/148 (99%)	122 (84%)	16 (11%)	8 (6%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	n8	146/148 (99%)	126 (86%)	16 (11%)	4 (3%)	5	17
65	N9	56/58 (97%)	49 (88%)	5 (9%)	2 (4%)	3	11
65	n9	56/58 (97%)	43 (77%)	9 (16%)	4 (7%)	1	2
66	O0	95/104 (91%)	87 (92%)	6 (6%)	2 (2%)	7	23
66	o0	98/104 (94%)	89 (91%)	7 (7%)	2 (2%)	7	24
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	2	7
67	o1	107/112 (96%)	98 (92%)	5 (5%)	4 (4%)	3	11
68	O2	125/129 (97%)	116 (93%)	8 (6%)	1 (1%)	19	49
68	o2	125/129 (97%)	111 (89%)	11 (9%)	3 (2%)	6	20
69	O3	104/106 (98%)	101 (97%)	2 (2%)	1 (1%)	15	44
69	o3	104/106 (98%)	92 (88%)	7 (7%)	5 (5%)	2	7
70	O4	110/119 (92%)	103 (94%)	4 (4%)	3 (3%)	5	17
70	o4	110/119 (92%)	100 (91%)	8 (7%)	2 (2%)	8	28
71	O5	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	3	13
71	o5	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	9	29
72	O6	97/99 (98%)	78 (80%)	11 (11%)	8 (8%)	1	2
72	o6	97/99 (98%)	81 (84%)	9 (9%)	7 (7%)	1	2
73	O7	85/87 (98%)	76 (89%)	6 (7%)	3 (4%)	3	12
73	o7	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	3	12
74	O8	75/77 (97%)	62 (83%)	10 (13%)	3 (4%)	3	9
74	o8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	3	9
75	O9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	7	23
76	Q0	50/52 (96%)	48 (96%)	0	2 (4%)	3	9
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	7	24
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100
78	Q2	103/105 (98%)	90 (87%)	10 (10%)	3 (3%)	4	15
78	q2	103/105 (98%)	92 (89%)	8 (8%)	3 (3%)	4	15
79	Q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	6	22
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	14	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
80	e0	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	1 3
82	p0	139/311 (45%)	117 (84%)	19 (14%)	3 (2%)	6 22
All	All	22333/24141 (92%)	19119 (86%)	2092 (9%)	1122 (5%)	2 6

All (1122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	39	ASN
2	S0	66	ALA
2	S0	103	THR
2	S0	158	VAL
2	S0	163	ASN
2	S0	191	ARG
2	S0	203	PHE
3	S1	49	ASN
3	S1	79	HIS
3	S1	117	TRP
3	S1	132	ASP
3	S1	148	ASN
3	S1	179	SER
3	S1	206	PRO
3	S1	221	PRO
4	S2	148	LEU
5	S3	62	ASN
5	S3	64	ARG
5	S3	65	ARG
5	S3	93	ASP
5	S3	216	PRO
5	S3	220	PRO
6	S4	104	ASP
6	S4	164	LEU
6	S4	195	ILE
6	S4	223	ASN
7	S5	26	ALA
7	S5	35	GLN
7	S5	39	GLU
7	S5	43	PHE
7	S5	58	LEU
7	S5	60	ASP
7	S5	63	GLN
7	S5	101	GLY

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Mol	Chain	Res	Type
8	S6	122	GLU
8	S6	173	PRO
9	S7	32	PRO
9	S7	64	VAL
9	S7	111	LYS
9	S7	112	ARG
9	S7	116	ARG
9	S7	131	PHE
9	S7	133	THR
9	S7	134	GLU
9	S7	155	ASP
10	S8	22	ARG
10	S8	152	ILE
10	S8	153	GLU
11	S9	98	ALA
11	S9	121	SER
11	S9	134	ILE
11	S9	150	LEU
12	C0	60	SER
12	C0	87	VAL
12	C0	88	PRO
13	C1	7	VAL
13	C1	29	LYS
14	C2	25	GLU
14	C2	93	ASP
14	C2	101	ALA
14	C2	119	SER
14	C2	127	GLY
15	C3	22	ALA
16	C4	50	ALA
16	C4	124	ASP
16	C4	125	SER
16	C4	126	THR
17	C5	54	ALA
17	C5	125	PRO
17	C5	130	ARG
18	C6	39	VAL
18	C6	58	ASP
18	C6	97	VAL
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL

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Mol	Chain	Res	Type
19	C7	124	VAL
20	C8	14	ILE
20	C8	61	LEU
20	C8	83	ALA
20	C8	91	ASP
20	C8	92	ILE
21	C9	53	TRP
22	D0	17	GLN
24	D2	83	ILE
25	D3	3	LYS
25	D3	92	CYS
25	D3	109	ARG
25	D3	144	ARG
26	D4	6	THR
27	D5	39	ALA
27	D5	43	ASP
27	D5	44	GLN
27	D5	71	ILE
28	D6	45	VAL
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
29	D7	62	ILE
31	D9	8	PHE
32	E0	47	VAL
33	E1	102	VAL
33	E1	103	LEU
33	E1	106	TYR
33	E1	128	ALA
33	E1	138	ARG
34	SR	160	GLU
35	SM	52	PRO
35	SM	86	ASN
35	SM	87	THR
35	SM	102	THR
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
40	L3	3	HIS
40	L3	4	ARG
40	L3	5	LYS
40	L3	139	GLN

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Mol	Chain	Res	Type
40	L3	140	ASP
40	L3	174	LYS
40	L3	186	GLY
41	L4	4	PRO
41	L4	292	SER
41	L4	293	SER
41	L4	311	HIS
41	L4	317	PRO
41	L4	320	ASN
42	L5	57	ASN
42	L5	233	ALA
42	L5	234	ASP
42	L5	258	LYS
43	L6	6	ALA
43	L6	98	VAL
44	L7	26	VAL
44	L7	160	ARG
45	L8	25	PRO
45	L8	39	ALA
46	L9	190	ASP
47	M0	189	GLU
47	M0	219	ALA
48	M1	8	PRO
48	M1	9	MET
48	M1	11	ASP
48	M1	94	ARG
48	M1	115	LYS
48	M1	165	GLN
49	M3	47	ALA
49	M3	129	ASN
49	M3	134	GLU
50	M4	8	LYS
50	M4	9	ALA
51	M5	74	PRO
51	M5	144	ARG
52	M6	16	VAL
52	M6	111	PRO
53	M7	157	VAL
53	M7	182	ILE
54	M8	98	LYS
54	M8	99	THR
56	N0	2	ALA

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Mol	Chain	Res	Type
56	N0	167	ARG
57	N1	124	VAL
57	N1	159	PHE
58	N2	31	ALA
60	N4	80	ARG
60	N4	81	PRO
60	N4	97	LYS
62	N6	52	ARG
62	N6	53	ASP
62	N6	84	LYS
63	N7	35	SER
64	N8	29	PRO
64	N8	76	ASP
64	N8	96	LYS
67	O1	5	LYS
67	O1	6	ASP
67	O1	84	ASP
68	O2	127	ALA
71	O5	119	LYS
72	O6	33	ALA
72	O6	34	SER
74	O8	33	LYS
76	Q0	78	ILE
78	Q2	15	LYS
78	Q2	100	LYS
2	s0	4	PRO
2	s0	44	GLY
2	s0	103	THR
2	s0	158	VAL
2	s0	164	ASN
2	s0	186	GLY
2	s0	189	VAL
2	s0	206	ASP
3	s1	62	LYS
3	s1	63	GLY
3	s1	81	PHE
3	s1	82	ARG
3	s1	147	ALA
3	s1	206	PRO
3	s1	223	PHE
4	s2	91	ARG
4	s2	92	ALA

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Mol	Chain	Res	Type
4	s2	163	GLY
5	s3	61	GLU
5	s3	90	ARG
5	s3	115	ILE
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	104	ASP
6	s4	163	ASP
6	s4	164	LEU
7	s5	184	PHE
8	s6	153	VAL
8	s6	154	ARG
8	s6	173	PRO
8	s6	174	LYS
9	s7	10	SER
9	s7	64	VAL
9	s7	66	SER
9	s7	74	GLN
9	s7	116	ARG
9	s7	131	PHE
9	s7	163	ASP
9	s7	185	ILE
10	s8	115	ALA
10	s8	116	HIS
12	c0	32	HIS
12	c0	82	LEU
12	c0	83	PRO
12	c0	88	PRO
12	c0	92	ILE
12	c0	97	PRO
13	c1	114	ALA
13	c1	133	LYS
13	c1	144	ALA
14	c2	22	VAL
14	c2	89	ILE
15	c3	19	SER
15	c3	66	ILE
15	c3	87	ASP
15	c3	137	PRO
15	c3	139	TRP
16	c4	35	GLY

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Mol	Chain	Res	Type
16	c4	126	THR
16	c4	132	ARG
17	c5	11	VAL
17	c5	51	SER
17	c5	52	LYS
17	c5	125	PRO
17	c5	126	VAL
17	c5	127	ARG
18	c6	42	GLU
18	c6	116	LEU
19	c7	67	ARG
19	c7	88	VAL
19	c7	99	VAL
19	c7	116	LYS
20	c8	92	ILE
20	c8	145	ARG
21	c9	28	LEU
21	c9	29	GLU
21	c9	33	TYR
22	d0	15	GLN
22	d0	49	ASN
22	d0	52	LYS
26	d4	30	PRO
26	d4	78	SER
27	d5	85	LYS
27	d5	104	ALA
29	d7	38	PRO
29	d7	60	SER
29	d7	62	ILE
29	d7	63	LEU
30	d8	33	LEU
30	d8	61	ARG
31	d9	6	VAL
80	e0	47	VAL
80	e0	60	PRO
33	e1	83	LYS
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	103	LEU
33	e1	106	TYR
34	sR	4	ASN

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Mol	Chain	Res	Type
34	sR	163	ASP
34	sR	165	ASP
34	sR	250	TYR
35	sM	47	ALA
35	sM	50	ASN
35	sM	64	LYS
35	sM	65	THR
39	l2	15	ILE
40	l3	3	HIS
40	l3	139	GLN
40	l3	293	ASN
40	l3	347	SER
41	l4	90	PHE
41	l4	272	VAL
41	l4	311	HIS
41	l4	329	PRO
41	l4	339	LEU
42	l5	260	PHE
43	l6	98	VAL
45	l8	25	PRO
45	l8	34	PHE
45	l8	117	ALA
45	l8	122	LYS
46	l9	144	ILE
46	l9	188	THR
47	m0	220	GLN
48	m1	8	PRO
48	m1	10	ARG
48	m1	94	ARG
49	m3	47	ALA
49	m3	51	LEU
49	m3	134	GLU
51	m5	48	ALA
51	m5	49	ARG
51	m5	76	PRO
52	m6	16	VAL
52	m6	110	PRO
53	m7	67	ILE
54	m8	98	LYS
54	m8	99	THR
56	n0	2	ALA
57	n1	122	GLN

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Mol	Chain	Res	Type
57	n1	136	ARG
60	n4	76	VAL
61	n5	24	LEU
61	n5	25	LYS
61	n5	44	PRO
61	n5	45	LYS
62	n6	83	ASP
62	n6	84	LYS
62	n6	126	LEU
63	n7	5	LEU
63	n7	7	ALA
63	n7	125	GLY
64	n8	76	ASP
65	n9	21	ILE
65	n9	23	LYS
65	n9	39	PHE
66	o0	100	ILE
67	o1	83	GLU
67	o1	86	LYS
69	o3	88	ASN
71	o5	119	LYS
72	o6	33	ALA
72	o6	63	ASN
72	o6	98	ARG
73	o7	85	LYS
74	o8	18	ALA
82	p0	93	LEU
2	S0	5	ALA
2	S0	27	ARG
2	S0	30	GLN
2	S0	94	GLY
2	S0	95	ALA
2	S0	139	VAL
2	S0	185	ARG
2	S0	189	VAL
2	S0	192	THR
2	S0	194	PRO
2	S0	195	TRP
3	S1	35	PRO
3	S1	51	SER
3	S1	63	GLY
3	S1	93	GLY

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Mol	Chain	Res	Type
3	S1	116	LYS
3	S1	213	ARG
3	S1	223	PHE
4	S2	145	GLY
5	S3	218	LEU
6	S4	12	LEU
6	S4	26	CYS
6	S4	222	LEU
7	S5	156	ARG
7	S5	204	GLY
7	S5	206	SER
8	S6	154	ARG
8	S6	174	LYS
9	S7	30	SER
9	S7	31	SER
9	S7	73	VAL
9	S7	85	PHE
9	S7	98	ILE
9	S7	156	SER
10	S8	59	ARG
10	S8	105	ASP
10	S8	120	THR
11	S9	169	PRO
12	C0	86	ILE
13	C1	4	GLU
13	C1	145	ALA
13	C1	154	ALA
14	C2	55	GLY
14	C2	91	VAL
14	C2	115	VAL
14	C2	125	ASN
14	C2	130	THR
15	C3	12	SER
16	C4	42	VAL
16	C4	51	ASP
16	C4	123	SER
17	C5	48	GLY
17	C5	101	ALA
18	C6	113	ASP
20	C8	7	GLU
20	C8	8	GLN
20	C8	82	PRO

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Mol	Chain	Res	Type
20	C8	139	LYS
21	C9	69	LYS
23	D1	49	GLU
25	D3	8	GLY
25	D3	41	SER
25	D3	114	LYS
25	D3	131	SER
26	D4	4	ALA
26	D4	36	SER
26	D4	60	PHE
28	D6	18	VAL
28	D6	63	ALA
28	D6	86	VAL
28	D6	97	PRO
29	D7	60	SER
29	D7	75	GLU
30	D8	36	THR
33	E1	84	VAL
33	E1	85	TYR
33	E1	98	VAL
33	E1	127	GLY
34	SR	98	GLU
34	SR	318	ALA
35	SM	82	THR
35	SM	88	ARG
35	SM	139	GLU
39	L2	250	GLN
39	L2	251	LYS
40	L3	351	LEU
41	L4	15	ALA
41	L4	190	GLY
41	L4	232	SER
41	L4	270	SER
41	L4	318	LEU
41	L4	339	LEU
42	L5	6	ASP
42	L5	137	ASP
42	L5	187	THR
42	L5	253	PHE
42	L5	260	PHE
42	L5	295	GLY
44	L7	24	GLU

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Mol	Chain	Res	Type
44	L7	164	SER
44	L7	175	LYS
45	L8	157	VAL
47	M0	24	ARG
47	M0	194	GLY
48	M1	24	GLY
48	M1	167	TYR
51	M5	184	LYS
52	M6	182	ASN
53	M7	67	ILE
53	M7	160	ALA
53	M7	161	ALA
58	N2	11	ILE
59	N3	82	ALA
60	N4	64	THR
62	N6	126	LEU
63	N7	17	ARG
63	N7	18	TYR
64	N8	47	LYS
64	N8	66	ALA
67	O1	83	GLU
70	O4	77	GLY
70	O4	82	ALA
71	O5	90	ARG
71	O5	91	ALA
72	O6	28	TYR
73	O7	79	GLN
78	Q2	94	GLY
79	Q3	51	ALA
2	s0	30	GLN
2	s0	94	GLY
2	s0	95	ALA
2	s0	185	ARG
3	s1	93	GLY
4	s2	107	SER
4	s2	164	SER
4	s2	228	ASN
6	s4	12	LEU
6	s4	24	SER
6	s4	195	ILE
6	s4	196	VAL
7	s5	28	PRO

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Mol	Chain	Res	Type
7	s5	36	ALA
7	s5	43	PHE
7	s5	54	LYS
7	s5	151	GLY
8	s6	68	LEU
8	s6	122	GLU
10	s8	62	THR
10	s8	101	ILE
11	s9	110	GLN
11	s9	134	ILE
11	s9	183	ALA
12	c0	23	ALA
12	c0	31	LYS
12	c0	35	ILE
13	c1	55	ASP
14	c2	58	LEU
14	c2	101	ALA
14	c2	119	SER
14	c2	131	ASP
15	c3	140	LYS
16	c4	50	ALA
16	c4	51	ASP
16	c4	124	ASP
16	c4	131	GLY
17	c5	17	TYR
17	c5	132	GLY
19	c7	113	LEU
20	c8	61	LEU
20	c8	135	GLY
22	d0	17	GLN
23	d1	4	ASP
23	d1	77	GLY
25	d3	131	SER
26	d4	33	ALA
26	d4	35	VAL
26	d4	53	ASP
27	d5	38	HIS
27	d5	83	LEU
28	d6	62	TYR
29	d7	20	LYS
29	d7	50	ALA
29	d7	75	GLU

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Mol	Chain	Res	Type
31	d9	7	TRP
31	d9	19	ARG
80	e0	61	SER
33	e1	84	VAL
33	e1	97	LYS
33	e1	102	VAL
33	e1	127	GLY
39	l2	215	ASN
39	l2	238	ILE
39	l2	249	SER
40	l3	138	ALA
41	l4	302	ALA
42	l5	135	VAL
42	l5	258	LYS
42	l5	270	LYS
43	l6	97	ASN
45	l8	39	ALA
45	l8	79	GLN
45	l8	114	ALA
45	l8	121	SER
45	l8	188	THR
45	l8	190	VAL
45	l8	203	VAL
47	m0	204	GLY
47	m0	207	GLU
48	m1	7	ASN
49	m3	129	ASN
49	m3	141	ALA
50	m4	3	THR
50	m4	135	LEU
51	m5	183	THR
51	m5	184	LYS
54	m8	41	ASP
54	m8	167	SER
54	m8	171	LYS
55	m9	35	ALA
55	m9	155	LEU
55	m9	156	ASN
56	n0	50	LYS
57	n1	127	GLN
58	n2	51	GLY
60	n4	63	ILE

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Mol	Chain	Res	Type
60	n4	71	ARG
60	n4	77	LYS
62	n6	92	GLY
62	n6	125	LYS
63	n7	16	GLY
64	n8	47	LYS
64	n8	129	PHE
67	o1	84	ASP
68	o2	124	GLY
70	o4	77	GLY
72	o6	12	ASN
72	o6	64	SER
74	o8	15	THR
82	p0	47	GLY
3	S1	26	ARG
3	S1	58	SER
3	S1	78	ASP
3	S1	147	ALA
4	S2	79	GLU
4	S2	91	ARG
4	S2	107	SER
4	S2	235	LEU
4	S2	248	SER
6	S4	77	ARG
6	S4	245	LYS
7	S5	127	GLN
7	S5	150	GLY
8	S6	70	PRO
8	S6	152	ASP
9	S7	84	LYS
10	S8	9	HIS
10	S8	40	ALA
10	S8	149	SER
10	S8	199	LYS
11	S9	118	LEU
11	S9	164	PHE
12	C0	94	GLU
13	C1	3	THR
13	C1	55	ASP
13	C1	153	PHE
14	C2	21	GLU
14	C2	22	VAL

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Mol	Chain	Res	Type
14	C2	39	ASP
16	C4	40	ALA
16	C4	75	GLY
17	C5	51	SER
17	C5	69	GLU
17	C5	126	VAL
19	C7	120	SER
20	C8	60	GLU
25	D3	112	LYS
26	D4	34	ASN
26	D4	58	PHE
26	D4	133	ASN
28	D6	10	ARG
28	D6	62	TYR
28	D6	65	PRO
29	D7	38	PRO
33	E1	83	LYS
33	E1	86	THR
33	E1	87	THR
33	E1	118	ARG
34	SR	50	ASP
34	SR	161	LYS
34	SR	228	LYS
35	SM	53	ARG
35	SM	89	ARG
35	SM	153	ASP
35	SM	174	LEU
40	L3	155	ALA
40	L3	300	ARG
41	L4	5	GLN
41	L4	16	THR
42	L5	58	LYS
42	L5	188	GLU
42	L5	252	ALA
42	L5	259	LYS
44	L7	25	GLN
44	L7	212	GLY
45	L8	117	ALA
45	L8	255	SER
46	L9	2	LYS
47	M0	211	ARG
48	M1	7	ASN

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Mol	Chain	Res	Type
49	M3	76	THR
49	M3	130	GLY
49	M3	131	LYS
50	M4	28	SER
50	M4	136	ALA
53	M7	164	LYS
54	M8	183	GLY
57	N1	125	ALA
58	N2	91	ASP
63	N7	33	SER
63	N7	78	ASN
65	N9	57	ALA
72	O6	3	VAL
72	O6	21	THR
72	O6	95	ALA
72	O6	98	ARG
73	O7	85	LYS
2	s0	68	PRO
2	s0	102	PHE
3	s1	26	ARG
3	s1	154	SER
4	s2	238	SER
5	s3	93	ASP
6	s4	57	ASN
6	s4	245	LYS
7	s5	100	ASN
7	s5	127	GLN
7	s5	153	GLY
10	s8	199	LYS
11	s9	5	PRO
11	s9	105	LEU
11	s9	147	MET
12	c0	30	ALA
13	c1	61	THR
13	c1	132	SER
13	c1	146	ALA
14	c2	26	ASP
14	c2	59	LEU
14	c2	87	PRO
14	c2	103	LEU
14	c2	106	ILE
14	c2	107	ASP

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Mol	Chain	Res	Type
14	c2	108	ARG
14	c2	118	ALA
16	c4	12	GLN
16	c4	92	LYS
17	c5	8	LYS
17	c5	49	MET
17	c5	68	PRO
17	c5	80	MET
17	c5	128	HIS
17	c5	129	GLY
18	c6	39	VAL
18	c6	97	VAL
18	c6	142	TYR
19	c7	120	SER
20	c8	91	ASP
23	d1	44	ARG
23	d1	78	LEU
24	d2	68	ARG
26	d4	51	GLU
26	d4	58	PHE
28	d6	46	GLU
28	d6	63	ALA
29	d7	3	LEU
30	d8	62	GLU
80	e0	54	ARG
33	e1	81	LYS
33	e1	110	ALA
33	e1	128	ALA
33	e1	148	TYR
34	sR	146	GLY
34	sR	161	LYS
35	sM	48	ARG
35	sM	66	ALA
35	sM	78	ASP
35	sM	167	PRO
39	l2	96	LEU
39	l2	142	ASP
41	l4	145	ILE
43	l6	32	ALA
45	l8	26	LEU
45	l8	120	LYS
45	l8	123	GLN

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Mol	Chain	Res	Type
45	l8	124	ASP
45	l8	133	LYS
45	l8	237	ILE
46	l9	107	ASP
47	m0	3	ARG
47	m0	195	ALA
47	m0	219	ALA
48	m1	95	ASN
48	m1	173	ASP
49	m3	19	GLN
49	m3	135	ALA
53	m7	66	SER
54	m8	91	ALA
56	n0	138	GLN
57	n1	135	PRO
60	n4	83	THR
60	n4	127	LYS
61	n5	47	ALA
63	n7	127	ASN
64	n8	78	LEU
68	o2	6	HIS
69	o3	91	ALA
69	o3	92	LYS
70	o4	82	ALA
71	o5	40	SER
72	o6	34	SER
73	o7	86	ALA
74	o8	17	ARG
75	o9	3	ALA
76	q0	78	ILE
2	S0	4	PRO
2	S0	36	TYR
3	S1	54	LEU
3	S1	55	LYS
3	S1	82	ARG
3	S1	158	SER
3	S1	209	ASN
4	S2	150	GLN
5	S3	217	ILE
6	S4	157	ASN
6	S4	193	GLY
7	S5	21	THR

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Mol	Chain	Res	Type
7	S5	45	LYS
7	S5	64	VAL
7	S5	79	ASN
7	S5	154	ALA
8	S6	165	GLY
10	S8	10	LYS
10	S8	52	ASN
12	C0	34	GLU
14	C2	89	ILE
14	C2	106	ILE
14	C2	107	ASP
14	C2	108	ARG
14	C2	112	ALA
14	C2	131	ASP
15	C3	106	ARG
16	C4	18	ARG
16	C4	86	THR
16	C4	114	ARG
17	C5	24	LYS
17	C5	52	LYS
18	C6	41	PRO
21	C9	29	GLU
21	C9	130	ARG
23	D1	10	GLU
23	D1	28	ASP
23	D1	81	ASN
25	D3	40	SER
26	D4	5	VAL
27	D5	41	ILE
28	D6	36	ILE
28	D6	64	LEU
29	D7	63	LEU
30	D8	61	ARG
31	D9	34	TYR
33	E1	94	LYS
33	E1	100	LEU
33	E1	137	ASP
33	E1	148	TYR
34	SR	51	ASP
34	SR	117	LYS
34	SR	163	ASP
34	SR	237	GLN

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Mol	Chain	Res	Type
35	SM	97	THR
35	SM	172	VAL
35	SM	173	GLU
40	L3	385	LYS
41	L4	182	LEU
41	L4	233	LEU
42	L5	7	ALA
42	L5	115	LEU
42	L5	125	VAL
43	L6	5	LYS
45	L8	120	LYS
46	L9	66	ALA
46	L9	189	GLU
48	M1	64	LYS
48	M1	114	ILE
49	M3	136	GLU
51	M5	75	VAL
54	M8	162	ALA
55	M9	53	LYS
60	N4	76	VAL
64	N8	94	ALA
73	O7	86	ALA
4	s2	235	LEU
6	s4	90	ILE
7	s5	29	ILE
7	s5	39	GLU
7	s5	60	ASP
7	s5	125	THR
9	s7	11	GLN
9	s7	133	THR
10	s8	52	ASN
11	s9	3	ARG
11	s9	65	LYS
11	s9	168	ARG
14	c2	54	ARG
14	c2	115	VAL
15	c3	29	SER
15	c3	60	VAL
16	c4	114	ARG
17	c5	14	THR
17	c5	69	GLU
17	c5	130	ARG

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Mol	Chain	Res	Type
18	c6	115	THR
20	c8	60	GLU
22	d0	51	VAL
22	d0	118	VAL
23	d1	21	ASN
27	d5	53	GLU
28	d6	11	ASN
28	d6	59	TYR
29	d7	59	CYS
33	e1	100	LEU
33	e1	131	PHE
33	e1	144	CYS
34	sR	149	ASP
34	sR	317	THR
35	sM	63	ASP
35	sM	120	GLU
39	l2	24	GLN
39	l2	56	ALA
40	l3	155	ALA
40	l3	333	LYS
41	l4	305	ALA
41	l4	330	TYR
42	l5	44	TYR
42	l5	158	ARG
43	l6	10	TYR
44	l7	191	VAL
45	l8	240	ASN
46	l9	62	ARG
46	l9	167	VAL
48	m1	117	ASP
48	m1	167	TYR
49	m3	93	ILE
49	m3	101	ARG
53	m7	75	GLU
58	n2	49	ASN
58	n2	50	LEU
59	n3	46	LEU
60	n4	72	SER
60	n4	132	GLY
63	n7	103	GLN
68	o2	5	PRO
73	o7	84	SER

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Mol	Chain	Res	Type
78	q2	32	LYS
2	S0	81	PHE
2	S0	164	ASN
2	S0	205	ARG
3	S1	81	PHE
5	S3	196	ARG
7	S5	51	VAL
7	S5	65	ARG
11	S9	99	LEU
11	S9	163	PRO
14	C2	66	VAL
14	C2	87	PRO
14	C2	129	GLU
17	C5	22	LEU
19	C7	115	LEU
20	C8	144	ARG
22	D0	21	LYS
23	D1	12	TYR
27	D5	38	HIS
27	D5	42	LEU
33	E1	93	HIS
35	SM	12	VAL
35	SM	64	LYS
39	L2	143	GLU
40	L3	317	ILE
41	L4	14	GLU
41	L4	130	ALA
44	L7	158	LYS
45	L8	36	ILE
45	L8	78	PHE
48	M1	151	SER
49	M3	153	ASP
50	M4	6	ILE
57	N1	18	ASP
57	N1	123	GLY
58	N2	10	LYS
61	N5	50	ALA
63	N7	36	HIS
63	N7	102	GLU
63	N7	103	GLN
64	N8	117	ARG
66	O0	71	GLN

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Mol	Chain	Res	Type
67	O1	7	VAL
69	O3	59	VAL
70	O4	3	GLN
71	O5	75	TYR
76	Q0	79	GLU
79	Q3	7	LYS
2	s0	10	THR
4	s2	106	ASP
4	s2	150	GLN
5	s3	145	ALA
5	s3	179	GLN
5	s3	196	ARG
5	s3	219	ALA
7	s5	71	ALA
9	s7	67	LEU
10	s8	136	SER
10	s8	148	ALA
11	s9	91	LYS
11	s9	146	PHE
12	c0	24	LYS
12	c0	95	ARG
13	c1	129	ARG
14	c2	82	PRO
14	c2	92	ALA
15	c3	22	ALA
17	c5	6	ASN
17	c5	131	ALA
18	c6	40	GLU
26	d4	34	ASN
26	d4	50	ALA
28	d6	8	ASN
28	d6	35	ALA
28	d6	60	PRO
30	d8	64	ARG
31	d9	11	PRO
35	sM	43	ASP
35	sM	83	LYS
39	l2	247	ARG
40	l3	37	ARG
40	l3	187	SER
41	l4	5	GLN
41	l4	146	PRO

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Mol	Chain	Res	Type
41	l4	233	LEU
42	l5	125	VAL
42	l5	216	GLU
44	l7	229	PHE
45	l8	81	THR
45	l8	115	ALA
47	m0	193	ASP
48	m1	114	ILE
48	m1	115	LYS
49	m3	50	PRO
49	m3	76	THR
51	m5	68	ARG
51	m5	81	TYR
63	n7	28	PRO
63	n7	134	LEU
65	n9	25	LYS
78	q2	33	ALA
82	p0	33	VAL
3	S1	210	ILE
4	S2	106	ASP
6	S4	233	LYS
8	S6	146	GLY
9	S7	36	ALA
10	S8	147	ALA
13	C1	5	LEU
13	C1	6	THR
14	C2	126	TRP
19	C7	24	LEU
21	C9	35	ASP
27	D5	88	ILE
28	D6	59	TYR
30	D8	34	GLU
33	E1	111	GLU
34	SR	105	GLY
39	L2	13	GLY
40	L3	299	ASP
42	L5	221	GLU
44	L7	178	ILE
48	M1	117	ASP
48	M1	138	VAL
51	M5	94	TYR
63	N7	125	GLY

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Mol	Chain	Res	Type
64	N8	97	GLU
65	N9	21	ILE
72	O6	78	GLY
74	O8	35	GLY
2	s0	139	VAL
3	s1	21	VAL
3	s1	22	ASP
5	s3	180	GLY
6	s4	30	ARG
6	s4	168	LYS
7	s5	21	THR
7	s5	59	VAL
10	s8	78	ILE
11	s9	126	ARG
12	c0	3	MET
14	c2	25	GLU
14	c2	66	VAL
21	c9	66	TYR
26	d4	52	LYS
27	d5	87	GLY
30	d8	32	PHE
33	e1	145	HIS
41	l4	328	ASN
42	l5	215	ASP
69	o3	59	VAL
72	o6	3	VAL
78	q2	31	GLY
79	q3	51	ALA
9	S7	13	PRO
14	C2	117	GLY
34	SR	15	GLY
34	SR	188	ILE
63	N7	16	GLY
4	s2	93	GLY
7	s5	33	VAL
9	s7	13	PRO
22	d0	96	PRO
26	d4	129	VAL
33	e1	124	PRO
47	m0	117	GLY
66	o0	10	ILE
14	C2	40	GLY

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Mol	Chain	Res	Type
41	L4	328	ASN
4	s2	83	ILE
8	s6	69	LEU
8	s6	70	PRO
9	s7	32	PRO
13	c1	7	VAL
69	o3	61	GLY
3	S1	48	VAL
7	S5	153	GLY
14	C2	81	ASP
23	D1	6	GLY
41	L4	131	VAL
41	L4	146	PRO
46	L9	13	PRO
66	O0	100	ILE
74	O8	37	PRO
9	s7	73	VAL
18	c6	4	VAL
20	c8	14	ILE
21	c9	3	GLY
22	d0	97	VAL
33	e1	112	GLY
44	l7	178	ILE
3	S1	21	VAL
25	D3	108	GLY
31	D9	6	VAL
35	SM	17	VAL
51	M5	89	VAL
52	M6	110	PRO
5	s3	203	PRO
14	c2	91	VAL
14	c2	121	VAL
17	c5	48	GLY
35	sM	172	VAL
67	o1	45	GLY
3	S1	22	ASP
46	l9	187	ILE
54	m8	84	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	134 (82%)	30 (18%)	1	5
2	s0	165/209 (79%)	131 (79%)	34 (21%)	1	3
3	S1	191/223 (86%)	162 (85%)	29 (15%)	3	8
3	s1	192/223 (86%)	162 (84%)	30 (16%)	2	8
4	S2	176/204 (86%)	137 (78%)	39 (22%)	1	2
4	s2	176/204 (86%)	139 (79%)	37 (21%)	1	3
5	S3	182/194 (94%)	149 (82%)	33 (18%)	1	5
5	s3	182/194 (94%)	149 (82%)	33 (18%)	1	5
6	S4	221/221 (100%)	182 (82%)	39 (18%)	2	5
6	s4	221/221 (100%)	187 (85%)	34 (15%)	2	8
7	S5	173/190 (91%)	140 (81%)	33 (19%)	1	4
7	s5	173/190 (91%)	138 (80%)	35 (20%)	1	4
8	S6	188/201 (94%)	155 (82%)	33 (18%)	2	5
8	s6	187/201 (93%)	152 (81%)	35 (19%)	1	5
9	S7	165/169 (98%)	140 (85%)	25 (15%)	3	8
9	s7	165/169 (98%)	134 (81%)	31 (19%)	1	5
10	S8	150/161 (93%)	128 (85%)	22 (15%)	3	9
10	s8	150/161 (93%)	129 (86%)	21 (14%)	3	11
11	S9	158/165 (96%)	123 (78%)	35 (22%)	1	2
11	s9	158/165 (96%)	128 (81%)	30 (19%)	1	4
12	C0	77/98 (79%)	58 (75%)	19 (25%)	0	2
12	c0	73/98 (74%)	61 (84%)	12 (16%)	2	7
13	C1	129/136 (95%)	104 (81%)	25 (19%)	1	4
13	c1	129/136 (95%)	107 (83%)	22 (17%)	2	6
14	C2	88/118 (75%)	68 (77%)	20 (23%)	1	2
14	c2	88/118 (75%)	65 (74%)	23 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	3
15	c3	127/127 (100%)	105 (83%)	22 (17%)	2	6
16	C4	81/104 (78%)	61 (75%)	20 (25%)	0	2
16	c4	97/104 (93%)	75 (77%)	22 (23%)	1	2
17	C5	101/117 (86%)	86 (85%)	15 (15%)	3	9
17	c5	103/117 (88%)	83 (81%)	20 (19%)	1	4
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1	4
18	c6	118/118 (100%)	98 (83%)	20 (17%)	2	6
19	C7	94/124 (76%)	70 (74%)	24 (26%)	0	1
19	c7	92/124 (74%)	76 (83%)	16 (17%)	2	6
20	C8	128/128 (100%)	102 (80%)	26 (20%)	1	4
20	c8	128/128 (100%)	101 (79%)	27 (21%)	1	3
21	C9	115/115 (100%)	93 (81%)	22 (19%)	1	4
21	c9	115/115 (100%)	95 (83%)	20 (17%)	2	6
22	D0	100/113 (88%)	74 (74%)	26 (26%)	0	1
22	d0	103/113 (91%)	80 (78%)	23 (22%)	1	2
23	D1	74/74 (100%)	60 (81%)	14 (19%)	1	5
23	d1	74/74 (100%)	57 (77%)	17 (23%)	1	2
24	D2	110/110 (100%)	94 (86%)	16 (14%)	3	9
24	d2	110/110 (100%)	96 (87%)	14 (13%)	4	14
25	D3	119/119 (100%)	97 (82%)	22 (18%)	1	5
25	d3	119/119 (100%)	104 (87%)	15 (13%)	4	14
26	D4	112/112 (100%)	93 (83%)	19 (17%)	2	6
26	d4	112/112 (100%)	99 (88%)	13 (12%)	5	17
27	D5	61/88 (69%)	43 (70%)	18 (30%)	0	1
27	d5	61/88 (69%)	54 (88%)	7 (12%)	5	17
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1	3
28	d6	83/83 (100%)	69 (83%)	14 (17%)	2	6
29	D7	70/70 (100%)	57 (81%)	13 (19%)	1	5
29	d7	70/70 (100%)	59 (84%)	11 (16%)	2	8
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d8	56/59 (95%)	48 (86%)	8 (14%)	3	10
31	D9	47/48 (98%)	38 (81%)	9 (19%)	1	4
31	d9	47/48 (98%)	39 (83%)	8 (17%)	2	6
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1	4
33	E1	62/66 (94%)	47 (76%)	15 (24%)	0	2
33	e1	66/66 (100%)	48 (73%)	18 (27%)	0	1
34	SR	260/261 (100%)	237 (91%)	23 (9%)	10	29
34	sR	260/261 (100%)	232 (89%)	28 (11%)	6	19
35	SM	97/228 (42%)	79 (81%)	18 (19%)	1	5
35	sM	54/228 (24%)	47 (87%)	7 (13%)	4	13
39	L2	193/195 (99%)	157 (81%)	36 (19%)	1	5
39	l2	192/195 (98%)	155 (81%)	37 (19%)	1	4
40	L3	321/322 (100%)	258 (80%)	63 (20%)	1	4
40	l3	320/322 (99%)	255 (80%)	65 (20%)	1	4
41	L4	288/288 (100%)	239 (83%)	49 (17%)	2	6
41	l4	288/288 (100%)	235 (82%)	53 (18%)	1	5
42	L5	244/244 (100%)	194 (80%)	50 (20%)	1	3
42	l5	243/244 (100%)	192 (79%)	51 (21%)	1	3
43	L6	134/152 (88%)	115 (86%)	19 (14%)	3	10
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	5
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4	13
44	l7	187/204 (92%)	159 (85%)	28 (15%)	3	9
45	L8	187/207 (90%)	154 (82%)	33 (18%)	2	5
45	l8	177/207 (86%)	143 (81%)	34 (19%)	1	4
46	L9	171/171 (100%)	139 (81%)	32 (19%)	1	5
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1	4
47	M0	177/186 (95%)	144 (81%)	33 (19%)	1	5
47	m0	179/186 (96%)	142 (79%)	37 (21%)	1	3
48	M1	147/150 (98%)	119 (81%)	28 (19%)	1	4
48	m1	147/150 (98%)	125 (85%)	22 (15%)	3	9
49	M3	154/158 (98%)	126 (82%)	28 (18%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	m3	154/158 (98%)	130 (84%)	24 (16%)	2	8
50	M4	107/108 (99%)	86 (80%)	21 (20%)	1	4
50	m4	108/108 (100%)	90 (83%)	18 (17%)	2	6
51	M5	175/175 (100%)	146 (83%)	29 (17%)	2	7
51	m5	175/175 (100%)	148 (85%)	27 (15%)	2	8
52	M6	160/161 (99%)	137 (86%)	23 (14%)	3	10
52	m6	160/161 (99%)	132 (82%)	28 (18%)	2	6
53	M7	140/145 (97%)	113 (81%)	27 (19%)	1	4
53	m7	125/145 (86%)	108 (86%)	17 (14%)	3	11
54	M8	150/150 (100%)	125 (83%)	25 (17%)	2	6
54	m8	150/150 (100%)	122 (81%)	28 (19%)	1	5
55	M9	153/153 (100%)	133 (87%)	20 (13%)	4	12
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	2
56	N0	156/156 (100%)	128 (82%)	28 (18%)	2	5
56	n0	156/156 (100%)	132 (85%)	24 (15%)	2	8
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1	3
57	n1	136/136 (100%)	116 (85%)	20 (15%)	3	9
58	N2	87/106 (82%)	76 (87%)	11 (13%)	4	14
58	n2	85/106 (80%)	73 (86%)	12 (14%)	3	10
59	N3	104/104 (100%)	90 (86%)	14 (14%)	4	11
59	n3	104/104 (100%)	95 (91%)	9 (9%)	10	30
60	N4	57/129 (44%)	52 (91%)	5 (9%)	10	29
60	n4	100/129 (78%)	88 (88%)	12 (12%)	5	15
61	N5	104/117 (89%)	79 (76%)	25 (24%)	0	2
61	n5	104/117 (89%)	80 (77%)	24 (23%)	1	2
62	N6	109/109 (100%)	88 (81%)	21 (19%)	1	4
62	n6	109/109 (100%)	84 (77%)	25 (23%)	1	2
63	N7	115/115 (100%)	91 (79%)	24 (21%)	1	3
63	n7	115/115 (100%)	92 (80%)	23 (20%)	1	4
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	5
64	n8	118/118 (100%)	95 (80%)	23 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2	6
65	n9	46/46 (100%)	35 (76%)	11 (24%)	0	2
66	O0	81/87 (93%)	66 (82%)	15 (18%)	1	5
66	o0	84/87 (97%)	68 (81%)	16 (19%)	1	4
67	O1	92/96 (96%)	72 (78%)	20 (22%)	1	3
67	o1	94/96 (98%)	77 (82%)	17 (18%)	1	5
68	O2	109/110 (99%)	94 (86%)	15 (14%)	3	11
68	o2	109/110 (99%)	92 (84%)	17 (16%)	2	8
69	O3	90/90 (100%)	76 (84%)	14 (16%)	2	8
69	o3	90/90 (100%)	82 (91%)	8 (9%)	9	28
70	O4	95/101 (94%)	78 (82%)	17 (18%)	2	5
70	o4	95/101 (94%)	81 (85%)	14 (15%)	3	9
71	O5	104/104 (100%)	83 (80%)	21 (20%)	1	4
71	o5	103/104 (99%)	76 (74%)	27 (26%)	0	1
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0	1
72	o6	80/81 (99%)	52 (65%)	28 (35%)	0	0
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	6
73	o7	70/70 (100%)	59 (84%)	11 (16%)	2	8
74	O8	68/68 (100%)	55 (81%)	13 (19%)	1	4
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	5
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1	4
75	o9	45/45 (100%)	35 (78%)	10 (22%)	1	2
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	3	9
76	q0	47/47 (100%)	40 (85%)	7 (15%)	3	9
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	76 (84%)	14 (16%)	2	8
78	q2	90/90 (100%)	73 (81%)	17 (19%)	1	5
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	3	10
79	q3	71/71 (100%)	58 (82%)	13 (18%)	1	5
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
82	p0	105/253 (42%)	84 (80%)	21 (20%)	1 4
All	All	18729/20239 (92%)	15348 (82%)	3381 (18%)	1 5

All (3381) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	24	LEU
2	S0	27	ARG
2	S0	34	GLU
2	S0	37	VAL
2	S0	43	ASP
2	S0	50	VAL
2	S0	62	ARG
2	S0	80	THR
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	93	THR
2	S0	96	THR
2	S0	101	ARG
2	S0	111	ILE
2	S0	114	SER
2	S0	119	ARG
2	S0	131	GLN
2	S0	135	GLU
2	S0	154	GLU
2	S0	156	VAL
2	S0	157	ASP
2	S0	169	SER
2	S0	170	ILE
2	S0	172	LEU
2	S0	177	LEU
2	S0	184	LEU
2	S0	185	ARG
2	S0	196	SER
2	S0	198	MET
3	S1	21	VAL
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	46	THR
3	S1	61	LEU

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Mol	Chain	Res	Type
3	S1	70	LEU
3	S1	74	GLN
3	S1	79	HIS
3	S1	81	PHE
3	S1	89	ASP
3	S1	97	LEU
3	S1	105	PHE
3	S1	111	ARG
3	S1	135	LEU
3	S1	137	ILE
3	S1	144	ARG
3	S1	154	SER
3	S1	169	SER
3	S1	170	GLU
3	S1	174	LYS
3	S1	180	THR
3	S1	181	LEU
3	S1	198	GLU
3	S1	214	LYS
3	S1	218	LEU
3	S1	219	LYS
3	S1	220	GLN
3	S1	223	PHE
4	S2	41	LEU
4	S2	53	ILE
4	S2	55	GLU
4	S2	58	LEU
4	S2	64	LYS
4	S2	69	ILE
4	S2	71	THR
4	S2	76	LEU
4	S2	77	GLN
4	S2	80	VAL
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	111	VAL
4	S2	117	THR
4	S2	130	ILE

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Mol	Chain	Res	Type
4	S2	134	LEU
4	S2	137	ILE
4	S2	139	ILE
4	S2	140	ARG
4	S2	141	ARG
4	S2	146	THR
4	S2	148	LEU
4	S2	166	THR
4	S2	181	SER
4	S2	195	ASP
4	S2	206	THR
4	S2	207	LEU
4	S2	208	GLU
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	235	LEU
4	S2	242	ILE
4	S2	245	ASP
4	S2	246	GLU
5	S3	4	LEU
5	S3	10	LYS
5	S3	21	LEU
5	S3	23	GLU
5	S3	39	VAL
5	S3	41	VAL
5	S3	65	ARG
5	S3	67	ASN
5	S3	76	ARG
5	S3	81	PRO
5	S3	84	ILE
5	S3	92	GLN
5	S3	93	ASP
5	S3	105	MET
5	S3	111	ASN
5	S3	117	ARG
5	S3	127	MET
5	S3	134	CYS
5	S3	142	LEU
5	S3	151	LYS
5	S3	158	ILE
5	S3	172	THR

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Mol	Chain	Res	Type
5	S3	176	LEU
5	S3	178	ARG
5	S3	179	GLN
5	S3	181	VAL
5	S3	182	LEU
5	S3	202	LEU
5	S3	204	ASP
5	S3	209	ILE
5	S3	215	GLU
5	S3	222	VAL
5	S3	223	LYS
6	S4	6	LYS
6	S4	7	LYS
6	S4	9	LEU
6	S4	12	LEU
6	S4	21	ASP
6	S4	23	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	45	ILE
6	S4	48	LEU
6	S4	62	LYS
6	S4	65	LEU
6	S4	67	GLN
6	S4	70	VAL
6	S4	72	VAL
6	S4	77	ARG
6	S4	92	LEU
6	S4	102	VAL
6	S4	105	VAL
6	S4	115	THR
6	S4	116	ASP
6	S4	123	LEU
6	S4	126	VAL
6	S4	131	LEU
6	S4	133	LYS
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	197	HIS
6	S4	198	LYS
6	S4	211	LYS

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Mol	Chain	Res	Type
6	S4	215	ASP
6	S4	221	ARG
6	S4	222	LEU
6	S4	227	VAL
6	S4	240	LYS
6	S4	242	LYS
6	S4	248	ILE
6	S4	258	GLN
7	S5	23	VAL
7	S5	25	LEU
7	S5	38	THR
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS
7	S5	53	VAL
7	S5	65	ARG
7	S5	76	ARG
7	S5	79	ASN
7	S5	84	LYS
7	S5	88	PRO
7	S5	89	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	99	MET
7	S5	112	ARG
7	S5	119	ASP
7	S5	124	LEU
7	S5	139	ASN
7	S5	146	THR
7	S5	147	THR
7	S5	148	ARG
7	S5	149	VAL
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	162	VAL
7	S5	185	ARG
7	S5	190	ILE
7	S5	193	THR
7	S5	194	LEU
7	S5	225	ARG
8	S6	9	VAL

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Mol	Chain	Res	Type
8	S6	13	GLN
8	S6	21	GLU
8	S6	25	ARG
8	S6	30	LYS
8	S6	65	GLN
8	S6	67	VAL
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	80	ASN
8	S6	82	SER
8	S6	97	VAL
8	S6	98	ARG
8	S6	120	GLU
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	132	ARG
8	S6	133	LEU
8	S6	137	ARG
8	S6	143	LYS
8	S6	154	ARG
8	S6	155	ASP
8	S6	158	ILE
8	S6	169	TYR
8	S6	175	ILE
8	S6	176	GLN
8	S6	179	VAL
8	S6	182	GLN
8	S6	211	LEU
8	S6	212	LEU
8	S6	223	LYS
9	S7	14	THR
9	S7	15	GLU
9	S7	25	VAL
9	S7	37	GLU
9	S7	38	LEU
9	S7	46	ILE
9	S7	50	ASP
9	S7	51	VAL
9	S7	67	LEU
9	S7	70	PHE

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Mol	Chain	Res	Type
9	S7	75	THR
9	S7	77	LEU
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG
9	S7	104	ARG
9	S7	105	THR
9	S7	109	VAL
9	S7	114	ARG
9	S7	116	ARG
9	S7	126	LEU
9	S7	136	VAL
9	S7	143	LEU
9	S7	144	VAL
9	S7	185	ILE
10	S8	17	LYS
10	S8	20	GLN
10	S8	21	PHE
10	S8	25	ARG
10	S8	28	GLU
10	S8	29	LEU
10	S8	32	GLN
10	S8	36	THR
10	S8	58	LEU
10	S8	60	ILE
10	S8	73	SER
10	S8	82	VAL
10	S8	110	ARG
10	S8	135	LYS
10	S8	138	ASN
10	S8	151	LYS
10	S8	152	ILE
10	S8	155	SER
10	S8	164	ARG
10	S8	184	LEU
10	S8	185	GLU
10	S8	196	LEU
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR
11	S9	10	LYS
11	S9	14	THR

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Mol	Chain	Res	Type
11	S9	22	SER
11	S9	28	LEU
11	S9	39	LYS
11	S9	40	LYS
11	S9	49	LEU
11	S9	60	LEU
11	S9	78	ARG
11	S9	82	ARG
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	97	LEU
11	S9	101	VAL
11	S9	105	LEU
11	S9	109	LEU
11	S9	110	GLN
11	S9	111	THR
11	S9	113	VAL
11	S9	122	VAL
11	S9	133	HIS
11	S9	134	ILE
11	S9	138	LYS
11	S9	149	ARG
11	S9	151	ASP
11	S9	161	THR
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	182	GLU
12	C0	1	MET
12	C0	5	LYS
12	C0	7	ASP
12	C0	8	ARG
12	C0	11	ILE
12	C0	20	VAL
12	C0	29	GLN
12	C0	32	HIS
12	C0	40	LEU
12	C0	46	LEU
12	C0	50	THR
12	C0	55	VAL

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Mol	Chain	Res	Type
12	C0	56	LYS
12	C0	67	THR
12	C0	71	GLU
12	C0	76	LEU
12	C0	78	GLU
12	C0	81	ASN
12	C0	82	LEU
13	C1	7	VAL
13	C1	21	ASN
13	C1	27	THR
13	C1	29	LYS
13	C1	37	ASN
13	C1	40	LEU
13	C1	43	LYS
13	C1	44	THR
13	C1	56	LYS
13	C1	67	ARG
13	C1	74	THR
13	C1	76	VAL
13	C1	79	LYS
13	C1	83	THR
13	C1	94	ILE
13	C1	99	ARG
13	C1	109	VAL
13	C1	118	GLN
13	C1	123	VAL
13	C1	131	ILE
13	C1	136	ARG
13	C1	138	ASN
13	C1	140	VAL
13	C1	141	LYS
13	C1	143	SER
14	C2	28	LEU
14	C2	33	ARG
14	C2	43	ARG
14	C2	46	ARG
14	C2	50	LYS
14	C2	54	ARG
14	C2	59	LEU
14	C2	66	VAL
14	C2	71	ILE
14	C2	73	LYS

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Mol	Chain	Res	Type
14	C2	74	LEU
14	C2	86	VAL
14	C2	89	ILE
14	C2	97	LEU
14	C2	103	LEU
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	139	HIS
14	C2	140	PHE
15	C3	3	ARG
15	C3	9	LYS
15	C3	11	ILE
15	C3	16	ILE
15	C3	27	LYS
15	C3	32	SER
15	C3	39	LYS
15	C3	42	ARG
15	C3	45	LEU
15	C3	56	ASP
15	C3	64	ARG
15	C3	66	ILE
15	C3	76	LYS
15	C3	77	SER
15	C3	83	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	141	TYR
15	C3	143	SER
15	C3	145	THR
15	C3	149	LEU
16	C4	13	VAL
16	C4	14	PHE
16	C4	16	VAL
16	C4	20	TYR
16	C4	29	HIS
16	C4	30	VAL

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Mol	Chain	Res	Type
16	C4	31	THR
16	C4	39	ILE
16	C4	42	VAL
16	C4	51	ASP
16	C4	55	SER
16	C4	56	SER
16	C4	92	LYS
16	C4	102	LEU
16	C4	103	ARG
16	C4	107	ARG
16	C4	123	SER
16	C4	132	ARG
16	C4	136	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	13	LYS
17	C5	21	ASP
17	C5	22	LEU
17	C5	28	MET
17	C5	31	GLU
17	C5	35	LYS
17	C5	36	LEU
17	C5	43	ARG
17	C5	44	ARG
17	C5	47	ARG
17	C5	52	LYS
17	C5	92	SER
17	C5	110	GLU
17	C5	124	THR
18	C6	12	LYS
18	C6	14	LYS
18	C6	17	THR
18	C6	26	LYS
18	C6	28	LEU
18	C6	29	ILE
18	C6	39	VAL
18	C6	45	ARG
18	C6	53	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	66	ARG
18	C6	68	ARG

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Mol	Chain	Res	Type
18	C6	69	VAL
18	C6	98	ASP
18	C6	101	SER
18	C6	114	ARG
18	C6	116	LEU
18	C6	118	ILE
18	C6	123	ARG
18	C6	128	LYS
18	C6	137	ARG
18	C6	143	ARG
19	C7	5	ARG
19	C7	7	LYS
19	C7	8	THR
19	C7	29	GLN
19	C7	30	THR
19	C7	34	LEU
19	C7	36	ASP
19	C7	38	ILE
19	C7	46	LEU
19	C7	49	LYS
19	C7	54	THR
19	C7	61	ILE
19	C7	62	GLN
19	C7	69	ILE
19	C7	72	LYS
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	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	8	GLN
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	18	LEU

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Mol	Chain	Res	Type
20	C8	20	THR
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	40	ARG
20	C8	57	ARG
20	C8	60	GLU
20	C8	61	LEU
20	C8	71	GLN
20	C8	77	THR
20	C8	80	LYS
20	C8	92	ILE
20	C8	107	SER
20	C8	110	ARG
20	C8	116	LEU
20	C8	132	ARG
20	C8	136	GLN
20	C8	143	ARG
21	C9	4	VAL
21	C9	22	LEU
21	C9	28	LEU
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	53	TRP
21	C9	57	ARG
21	C9	63	ARG
21	C9	67	MET
21	C9	68	ARG
21	C9	84	LYS
21	C9	86	ARG
21	C9	88	VAL
21	C9	94	ILE
21	C9	117	SER
21	C9	126	GLU
21	C9	130	ARG
21	C9	131	ASP
21	C9	134	ARG
21	C9	144	GLU
22	D0	15	GLN
22	D0	17	GLN

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Mol	Chain	Res	Type
22	D0	18	GLN
22	D0	23	ARG
22	D0	27	THR
22	D0	30	LYS
22	D0	34	LEU
22	D0	46	GLU
22	D0	47	GLN
22	D0	51	VAL
22	D0	57	ARG
22	D0	60	THR
22	D0	64	LYS
22	D0	66	SER
22	D0	67	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	117	VAL
22	D0	121	ASN
23	D1	1	MET
23	D1	7	GLN
23	D1	9	VAL
23	D1	11	LEU
23	D1	25	LYS
23	D1	32	VAL
23	D1	34	ILE
23	D1	39	VAL
23	D1	41	GLU
23	D1	52	THR
23	D1	62	ARG
23	D1	69	LEU
23	D1	78	LEU
23	D1	80	LYS
24	D2	3	ARG
24	D2	4	SER
24	D2	7	LEU
24	D2	12	ASN

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Mol	Chain	Res	Type
24	D2	22	LYS
24	D2	24	GLN
24	D2	25	VAL
24	D2	29	PRO
24	D2	49	GLU
24	D2	53	ILE
24	D2	65	LEU
24	D2	93	LEU
24	D2	98	GLN
24	D2	103	ILE
24	D2	105	THR
24	D2	129	VAL
25	D3	7	ARG
25	D3	9	LEU
25	D3	14	LYS
25	D3	19	ARG
25	D3	26	GLU
25	D3	28	ASN
25	D3	60	GLU
25	D3	73	ARG
25	D3	82	LYS
25	D3	83	VAL
25	D3	84	THR
25	D3	101	GLU
25	D3	103	LEU
25	D3	107	PHE
25	D3	109	ARG
25	D3	110	LYS
25	D3	114	LYS
25	D3	117	ILE
25	D3	131	SER
25	D3	132	LEU
25	D3	139	LYS
25	D3	144	ARG
26	D4	10	ARG
26	D4	17	LEU
26	D4	32	ARG
26	D4	34	ASN
26	D4	36	SER
26	D4	51	GLU
26	D4	57	VAL
26	D4	61	ARG

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Mol	Chain	Res	Type
26	D4	62	THR
26	D4	75	VAL
26	D4	84	LYS
26	D4	88	THR
26	D4	99	LYS
26	D4	102	LYS
26	D4	121	THR
26	D4	124	ARG
26	D4	127	LYS
26	D4	128	LYS
26	D4	133	ASN
27	D5	42	LEU
27	D5	49	ARG
27	D5	50	ILE
27	D5	58	ARG
27	D5	59	TYR
27	D5	60	VAL
27	D5	63	SER
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	78	ILE
27	D5	85	LYS
27	D5	92	ILE
27	D5	95	HIS
27	D5	97	LYS
27	D5	98	GLN
27	D5	100	ILE
27	D5	102	THR
28	D6	10	ARG
28	D6	15	ARG
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	45	VAL
28	D6	50	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	67	THR
28	D6	68	TYR
28	D6	69	ASN
28	D6	71	LEU

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Mol	Chain	Res	Type
28	D6	83	ILE
28	D6	84	VAL
28	D6	85	ARG
28	D6	90	GLU
29	D7	2	VAL
29	D7	3	LEU
29	D7	20	LYS
29	D7	29	ARG
29	D7	33	LEU
29	D7	42	ASN
29	D7	43	ILE
29	D7	55	THR
29	D7	60	SER
29	D7	62	ILE
29	D7	67	THR
29	D7	72	LYS
29	D7	73	LEU
30	D8	14	LYS
30	D8	19	THR
30	D8	28	VAL
30	D8	35	ASP
30	D8	36	THR
30	D8	39	THR
30	D8	44	VAL
30	D8	49	ARG
30	D8	52	ASP
30	D8	59	SER
30	D8	64	ARG
30	D8	65	ARG
31	D9	5	ASN
31	D9	6	VAL
31	D9	12	ARG
31	D9	19	ARG
31	D9	22	ARG
31	D9	28	THR
31	D9	30	LEU
31	D9	32	ARG
31	D9	39	CYS
32	E0	3	LYS
32	E0	21	VAL
32	E0	25	GLU
32	E0	28	LYS

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Mol	Chain	Res	Type
32	E0	29	LYS
32	E0	39	LEU
32	E0	42	ARG
32	E0	43	ARG
32	E0	47	VAL
32	E0	49	LEU
33	E1	84	VAL
33	E1	86	THR
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
33	E1	102	VAL
33	E1	108	VAL
33	E1	109	ASP
33	E1	113	LYS
33	E1	118	ARG
33	E1	120	GLU
33	E1	130	VAL
33	E1	146	SER
33	E1	151	ASN
34	SR	6	VAL
34	SR	7	LEU
34	SR	10	ARG
34	SR	29	GLN
34	SR	52	GLN
34	SR	59	ARG
34	SR	76	ASP
34	SR	96	THR
34	SR	117	LYS
34	SR	129	LYS
34	SR	136	ILE
34	SR	137	LYS
34	SR	165	ASP
34	SR	166	SER
34	SR	191	ASP
34	SR	196	ASN
34	SR	199	ILE
34	SR	238	ASP
34	SR	266	ASP
34	SR	268	GLN
34	SR	300	THR

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Mol	Chain	Res	Type
34	SR	316	MET
34	SR	317	THR
35	SM	25	ILE
35	SM	33	LYS
35	SM	34	LYS
35	SM	51	ARG
35	SM	53	ARG
35	SM	61	ILE
35	SM	64	LYS
35	SM	68	ARG
35	SM	79	SER
35	SM	84	LYS
35	SM	89	ARG
35	SM	91	THR
35	SM	94	HIS
35	SM	97	THR
35	SM	100	THR
35	SM	102	THR
35	SM	103	LYS
35	SM	139	GLU
39	L2	10	LYS
39	L2	20	THR
39	L2	23	ARG
39	L2	32	LEU
39	L2	36	GLU
39	L2	44	ILE
39	L2	45	VAL
39	L2	48	ILE
39	L2	62	VAL
39	L2	70	ARG
39	L2	74	GLU
39	L2	96	LEU
39	L2	101	VAL
39	L2	112	ILE
39	L2	116	VAL
39	L2	128	ARG
39	L2	134	VAL
39	L2	137	ILE
39	L2	141	PRO
39	L2	142	ASP
39	L2	143	GLU
39	L2	147	ARG

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Mol	Chain	Res	Type
39	L2	157	VAL
39	L2	158	ILE
39	L2	165	VAL
39	L2	169	ILE
39	L2	177	LYS
39	L2	179	LEU
39	L2	181	LYS
39	L2	190	ARG
39	L2	191	LEU
39	L2	204	MET
39	L2	207	VAL
39	L2	227	ARG
39	L2	230	VAL
39	L2	247	ARG
40	L3	3	HIS
40	L3	7	GLU
40	L3	10	ARG
40	L3	17	LEU
40	L3	19	ARG
40	L3	25	ILE
40	L3	37	ARG
40	L3	39	LYS
40	L3	43	LEU
40	L3	47	LEU
40	L3	56	ILE
40	L3	70	ARG
40	L3	73	VAL
40	L3	79	VAL
40	L3	84	VAL
40	L3	85	VAL
40	L3	103	THR
40	L3	110	LEU
40	L3	111	SER
40	L3	114	VAL
40	L3	116	ARG
40	L3	121	ASN
40	L3	134	SER
40	L3	139	GLN
40	L3	146	ARG
40	L3	148	LEU
40	L3	150	ARG
40	L3	156	SER

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Mol	Chain	Res	Type
40	L3	157	VAL
40	L3	169	THR
40	L3	173	GLN
40	L3	183	LEU
40	L3	188	ILE
40	L3	192	VAL
40	L3	196	ARG
40	L3	200	GLU
40	L3	202	THR
40	L3	205	VAL
40	L3	210	GLU
40	L3	229	VAL
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	238	LEU
40	L3	242	THR
40	L3	244	ARG
40	L3	252	ILE
40	L3	284	ARG
40	L3	296	THR
40	L3	305	ILE
40	L3	320	ASP
40	L3	324	VAL
40	L3	328	ILE
40	L3	331	ASN
40	L3	332	ARG
40	L3	338	LEU
40	L3	344	THR
40	L3	346	THR
40	L3	347	SER
40	L3	355	SER
40	L3	361	THR
40	L3	364	LYS
40	L3	380	MET
41	L4	4	PRO
41	L4	22	LEU
41	L4	25	VAL
41	L4	40	THR
41	L4	52	VAL
41	L4	53	SER
41	L4	60	THR

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Mol	Chain	Res	Type
41	L4	69	ARG
41	L4	71	VAL
41	L4	74	ILE
41	L4	93	MET
41	L4	118	LYS
41	L4	122	THR
41	L4	136	LEU
41	L4	138	ARG
41	L4	144	LYS
41	L4	148	ILE
41	L4	150	LEU
41	L4	152	VAL
41	L4	156	LEU
41	L4	170	LYS
41	L4	172	VAL
41	L4	176	SER
41	L4	177	ASP
41	L4	179	LEU
41	L4	182	LEU
41	L4	185	LYS
41	L4	188	ARG
41	L4	193	LYS
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	206	LEU
41	L4	220	ARG
41	L4	222	VAL
41	L4	230	VAL
41	L4	246	ARG
41	L4	258	LEU
41	L4	283	THR
41	L4	306	THR
41	L4	307	GLN
41	L4	313	LEU
41	L4	323	VAL
41	L4	327	LEU
41	L4	346	LYS
41	L4	349	THR
41	L4	354	VAL
41	L4	358	THR
41	L4	359	LEU

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Mol	Chain	Res	Type
42	L5	5	LYS
42	L5	10	SER
42	L5	23	ARG
42	L5	35	ARG
42	L5	41	LYS
42	L5	64	ILE
42	L5	68	THR
42	L5	69	ILE
42	L5	75	LEU
42	L5	92	LEU
42	L5	101	THR
42	L5	105	ILE
42	L5	109	THR
42	L5	112	LYS
42	L5	113	LEU
42	L5	115	LEU
42	L5	118	THR
42	L5	122	VAL
42	L5	128	GLU
42	L5	131	LEU
42	L5	137	ASP
42	L5	140	ARG
42	L5	144	VAL
42	L5	146	LEU
42	L5	148	ILE
42	L5	151	GLN
42	L5	152	ARG
42	L5	155	THR
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE
42	L5	194	LEU
42	L5	196	ARG
42	L5	205	SER
42	L5	216	GLU
42	L5	217	GLU
42	L5	222	LEU
42	L5	232	ASP
42	L5	234	ASP
42	L5	236	LEU
42	L5	254	LYS
42	L5	257	GLU

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Mol	Chain	Res	Type
42	L5	259	LYS
42	L5	261	THR
42	L5	263	GLU
42	L5	273	ARG
42	L5	275	THR
42	L5	279	LYS
42	L5	290	ILE
42	L5	293	LEU
43	L6	2	SER
43	L6	5	LYS
43	L6	8	LYS
43	L6	12	SER
43	L6	21	THR
43	L6	52	VAL
43	L6	59	GLU
43	L6	65	ILE
43	L6	70	LYS
43	L6	78	ARG
43	L6	79	VAL
43	L6	89	THR
43	L6	90	LYS
43	L6	93	VAL
43	L6	94	GLU
43	L6	129	GLU
43	L6	134	ARG
43	L6	152	THR
43	L6	155	LEU
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	38	LYS
44	L7	45	LEU
44	L7	60	ARG
44	L7	82	LYS
44	L7	83	LEU
44	L7	92	ILE
44	L7	98	LYS
44	L7	100	ARG
44	L7	110	ARG
44	L7	121	LYS
44	L7	124	LEU
44	L7	143	THR

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Mol	Chain	Res	Type
44	L7	157	ASN
44	L7	158	LYS
44	L7	164	SER
44	L7	175	LYS
44	L7	179	LEU
44	L7	184	LEU
44	L7	229	PHE
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	27	THR
45	L8	41	GLN
45	L8	47	SER
45	L8	50	VAL
45	L8	61	GLN
45	L8	63	LYS
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	81	THR
45	L8	84	ARG
45	L8	95	ASN
45	L8	110	THR
45	L8	118	GLU
45	L8	132	VAL
45	L8	136	LEU
45	L8	150	LEU
45	L8	156	ASP
45	L8	160	ILE
45	L8	163	VAL
45	L8	169	LEU
45	L8	172	LYS
45	L8	173	MET
45	L8	185	ARG
45	L8	189	LEU
45	L8	203	VAL
45	L8	204	ARG
45	L8	219	ASP
45	L8	238	LEU
45	L8	246	MET
45	L8	248	LYS
45	L8	251	LYS

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Mol	Chain	Res	Type
46	L9	4	ILE
46	L9	5	GLN
46	L9	9	GLN
46	L9	14	GLU
46	L9	18	VAL
46	L9	22	SER
46	L9	33	THR
46	L9	41	ILE
46	L9	48	VAL
46	L9	52	LEU
46	L9	62	ARG
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	80	THR
46	L9	82	VAL
46	L9	124	ARG
46	L9	132	VAL
46	L9	135	GLU
46	L9	137	SER
46	L9	138	THR
46	L9	139	ASN
46	L9	150	SER
46	L9	151	VAL
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	173	ARG
46	L9	177	ASP
46	L9	188	THR
46	L9	189	GLU
46	L9	190	ASP
47	M0	18	PRO
47	M0	24	ARG
47	M0	26	VAL
47	M0	30	LYS
47	M0	31	ILE
47	M0	32	ARG
47	M0	33	ILE
47	M0	36	LEU
47	M0	39	LYS
47	M0	40	LYS

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Mol	Chain	Res	Type
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	63	GLU
47	M0	74	LYS
47	M0	76	MET
47	M0	77	THR
47	M0	78	THR
47	M0	87	LEU
47	M0	99	ILE
47	M0	129	VAL
47	M0	130	ASP
47	M0	139	ARG
47	M0	140	THR
47	M0	143	SER
47	M0	163	GLN
47	M0	165	ILE
47	M0	169	LYS
47	M0	174	THR
47	M0	178	ARG
47	M0	185	ARG
47	M0	197	VAL
47	M0	203	LYS
48	M1	6	GLN
48	M1	9	MET
48	M1	10	ARG
48	M1	12	LEU
48	M1	13	LYS
48	M1	16	LYS
48	M1	23	VAL
48	M1	31	THR
48	M1	40	LEU
48	M1	44	THR
48	M1	46	VAL
48	M1	61	ARG
48	M1	65	ILE
48	M1	70	THR
48	M1	80	LEU
48	M1	94	ARG
48	M1	95	ASN
48	M1	106	ILE
48	M1	107	ASP

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Mol	Chain	Res	Type
48	M1	112	LEU
48	M1	120	ILE
48	M1	130	VAL
48	M1	138	VAL
48	M1	140	ARG
48	M1	142	LYS
48	M1	158	ASP
48	M1	161	SER
48	M1	166	LYS
49	M3	5	LYS
49	M3	23	LYS
49	M3	34	SER
49	M3	42	ARG
49	M3	46	ILE
49	M3	54	LEU
49	M3	55	ARG
49	M3	58	VAL
49	M3	59	ARG
49	M3	63	VAL
49	M3	67	ARG
49	M3	69	VAL
49	M3	85	LEU
49	M3	93	ILE
49	M3	107	GLU
49	M3	114	GLN
49	M3	122	LYS
49	M3	124	ILE
49	M3	128	ARG
49	M3	131	LYS
49	M3	144	THR
49	M3	164	GLU
49	M3	165	SER
49	M3	171	ARG
49	M3	180	ARG
49	M3	182	ILE
49	M3	190	LYS
49	M3	194	GLU
50	M4	8	LYS
50	M4	20	VAL
50	M4	27	GLN
50	M4	42	LYS
50	M4	43	LYS

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Mol	Chain	Res	Type
50	M4	50	LYS
50	M4	53	VAL
50	M4	55	ARG
50	M4	59	ASN
50	M4	64	VAL
50	M4	66	THR
50	M4	72	LEU
50	M4	90	VAL
50	M4	92	GLU
50	M4	102	LYS
50	M4	105	GLN
50	M4	108	ARG
50	M4	113	THR
50	M4	125	LYS
50	M4	126	GLN
50	M4	130	THR
51	M5	10	LEU
51	M5	15	GLN
51	M5	20	ARG
51	M5	22	LEU
51	M5	38	ARG
51	M5	49	ARG
51	M5	50	ARG
51	M5	56	LYS
51	M5	68	ARG
51	M5	80	THR
51	M5	83	LYS
51	M5	85	THR
51	M5	92	LEU
51	M5	96	ARG
51	M5	97	SER
51	M5	98	LEU
51	M5	105	ARG
51	M5	106	VAL
51	M5	109	ARG
51	M5	113	LEU
51	M5	133	ILE
51	M5	134	LEU
51	M5	138	GLN
51	M5	151	ILE
51	M5	155	VAL
51	M5	182	ASN

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Mol	Chain	Res	Type
51	M5	183	THR
51	M5	187	ARG
51	M5	190	THR
52	M6	25	LYS
52	M6	33	ILE
52	M6	34	VAL
52	M6	41	LEU
52	M6	46	GLU
52	M6	66	LYS
52	M6	67	THR
52	M6	78	ARG
52	M6	82	LYS
52	M6	84	LEU
52	M6	85	ARG
52	M6	106	GLU
52	M6	115	LYS
52	M6	116	LYS
52	M6	117	ARG
52	M6	124	LEU
52	M6	126	VAL
52	M6	128	ARG
52	M6	160	ARG
52	M6	166	GLU
52	M6	180	SER
52	M6	189	ASP
52	M6	190	VAL
53	M7	9	THR
53	M7	23	ARG
53	M7	24	VAL
53	M7	29	THR
53	M7	32	THR
53	M7	36	ILE
53	M7	52	LEU
53	M7	53	ASP
53	M7	56	ARG
53	M7	65	SER
53	M7	69	ARG
53	M7	74	LYS
53	M7	94	LEU
53	M7	107	LEU
53	M7	112	LEU
53	M7	114	VAL

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Mol	Chain	Res	Type
53	M7	117	ILE
53	M7	126	ARG
53	M7	127	ARG
53	M7	128	ARG
53	M7	136	ILE
53	M7	144	SER
53	M7	153	LYS
53	M7	157	VAL
53	M7	169	THR
53	M7	180	LYS
53	M7	181	ARG
54	M8	3	ILE
54	M8	8	LYS
54	M8	17	THR
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	34	THR
54	M8	41	ASP
54	M8	49	LEU
54	M8	50	LYS
54	M8	57	ILE
54	M8	66	ARG
54	M8	69	ARG
54	M8	74	GLU
54	M8	80	THR
54	M8	81	VAL
54	M8	95	GLU
54	M8	111	ARG
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	147	ARG
54	M8	150	VAL
54	M8	168	THR
54	M8	180	ARG
55	M9	22	VAL
55	M9	29	THR
55	M9	30	SER
55	M9	31	GLU
55	M9	41	ILE
55	M9	44	LEU

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Mol	Chain	Res	Type
55	M9	53	LYS
55	M9	60	LYS
55	M9	74	ARG
55	M9	98	ARG
55	M9	99	LEU
55	M9	100	ARG
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	115	ILE
55	M9	116	ASP
55	M9	138	LEU
55	M9	160	GLU
55	M9	175	GLN
56	N0	1	MET
56	N0	8	GLN
56	N0	32	SER
56	N0	45	LEU
56	N0	49	HIS
56	N0	51	VAL
56	N0	57	GLU
56	N0	61	ILE
56	N0	64	ILE
56	N0	80	ARG
56	N0	87	THR
56	N0	97	VAL
56	N0	100	VAL
56	N0	104	GLU
56	N0	105	THR
56	N0	115	ARG
56	N0	117	ARG
56	N0	130	GLU
56	N0	132	THR
56	N0	137	ARG
56	N0	138	GLN
56	N0	142	GLN
56	N0	145	THR
56	N0	155	ARG
56	N0	157	GLN
56	N0	167	ARG
56	N0	171	PHE
56	N0	172	TYR

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Mol	Chain	Res	Type
57	N1	25	VAL
57	N1	26	HIS
57	N1	27	LEU
57	N1	43	LYS
57	N1	55	LYS
57	N1	68	THR
57	N1	71	SER
57	N1	78	LYS
57	N1	79	MET
57	N1	83	ARG
57	N1	88	ARG
57	N1	96	ILE
57	N1	102	ARG
57	N1	104	GLU
57	N1	106	LEU
57	N1	118	GLU
57	N1	124	VAL
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	139	ARG
57	N1	141	VAL
57	N1	143	THR
57	N1	146	ASN
57	N1	149	GLN
57	N1	158	THR
57	N1	159	PHE
57	N1	160	ILE
58	N2	10	LYS
58	N2	39	ASP
58	N2	43	VAL
58	N2	52	ASN
58	N2	54	VAL
58	N2	61	THR
58	N2	66	VAL
58	N2	87	ASN
58	N2	88	GLN
58	N2	93	ILE
58	N2	100	THR
59	N3	9	THR
59	N3	13	ILE
59	N3	32	ARG

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Mol	Chain	Res	Type
59	N3	48	ARG
59	N3	64	LYS
59	N3	69	LEU
59	N3	72	LYS
59	N3	74	MET
59	N3	83	LYS
59	N3	102	ILE
59	N3	115	THR
59	N3	120	LYS
59	N3	133	SER
59	N3	137	VAL
60	N4	5	ILE
60	N4	17	ARG
60	N4	26	SER
60	N4	39	LEU
60	N4	64	THR
61	N5	25	LYS
61	N5	27	ARG
61	N5	36	LYS
61	N5	37	THR
61	N5	39	LYS
61	N5	40	LEU
61	N5	45	LYS
61	N5	48	SER
61	N5	63	ILE
61	N5	71	THR
61	N5	73	MET
61	N5	77	GLU
61	N5	86	VAL
61	N5	104	GLU
61	N5	105	VAL
61	N5	106	ASP
61	N5	108	LEU
61	N5	109	LYS
61	N5	115	ARG
61	N5	125	ARG
61	N5	133	LEU
61	N5	135	ILE
61	N5	138	ARG
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS

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Mol	Chain	Res	Type
62	N6	5	SER
62	N6	8	VAL
62	N6	13	ARG
62	N6	26	GLN
62	N6	37	LYS
62	N6	42	GLN
62	N6	45	ILE
62	N6	50	ILE
62	N6	51	ARG
62	N6	56	VAL
62	N6	57	LEU
62	N6	70	ILE
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	88	GLU
62	N6	94	SER
62	N6	105	VAL
62	N6	126	LEU
62	N6	127	GLU
63	N7	14	VAL
63	N7	15	ARG
63	N7	17	ARG
63	N7	24	VAL
63	N7	26	VAL
63	N7	30	ASP
63	N7	34	LYS
63	N7	42	LEU
63	N7	46	ILE
63	N7	52	LYS
63	N7	54	THR
63	N7	64	LYS
63	N7	73	LYS
63	N7	75	VAL
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	87	LEU
63	N7	102	GLU
63	N7	108	GLU
63	N7	121	ARG
63	N7	132	SER

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Mol	Chain	Res	Type
63	N7	134	LEU
63	N7	135	ARG
64	N8	4	ARG
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	16	SER
64	N8	29	PRO
64	N8	42	ARG
64	N8	47	LYS
64	N8	58	MET
64	N8	60	TYR
64	N8	76	ASP
64	N8	78	LEU
64	N8	84	GLU
64	N8	85	ASP
64	N8	92	LYS
64	N8	115	LYS
64	N8	118	ILE
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
64	N8	144	VAL
65	N9	4	SER
65	N9	18	ARG
65	N9	22	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	40	ARG
65	N9	50	THR
65	N9	59	LYS
66	O0	9	SER
66	O0	16	LEU
66	O0	18	ILE
66	O0	20	SER
66	O0	22	LYS
66	O0	30	THR
66	O0	34	LEU
66	O0	48	THR
66	O0	61	MET
66	O0	66	LYS
66	O0	83	LYS

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Mol	Chain	Res	Type
66	O0	87	VAL
66	O0	97	ASP
66	O0	100	ILE
66	O0	101	LEU
67	O1	8	VAL
67	O1	13	THR
67	O1	16	LEU
67	O1	28	ARG
67	O1	31	ARG
67	O1	42	LEU
67	O1	46	THR
67	O1	47	ASP
67	O1	55	LEU
67	O1	64	VAL
67	O1	68	GLU
67	O1	79	ARG
67	O1	81	GLU
67	O1	82	GLU
67	O1	84	ASP
67	O1	89	LEU
67	O1	96	VAL
67	O1	102	LYS
67	O1	106	THR
67	O1	110	GLU
68	O2	8	LYS
68	O2	15	LYS
68	O2	18	LYS
68	O2	19	ARG
68	O2	31	ASN
68	O2	33	ARG
68	O2	62	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	76	VAL
68	O2	82	LEU
68	O2	87	MET
68	O2	109	LEU
68	O2	125	ARG
68	O2	128	LEU
69	O3	3	GLU
69	O3	20	LYS
69	O3	21	ARG

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Mol	Chain	Res	Type
69	O3	31	LYS
69	O3	48	ARG
69	O3	49	ILE
69	O3	59	VAL
69	O3	60	ARG
69	O3	62	SER
69	O3	80	VAL
69	O3	81	VAL
69	O3	86	ARG
69	O3	98	VAL
69	O3	106	ASN
70	O4	5	VAL
70	O4	8	ARG
70	O4	20	ILE
70	O4	23	VAL
70	O4	24	LYS
70	O4	29	ILE
70	O4	31	ARG
70	O4	49	SER
70	O4	51	LEU
70	O4	56	THR
70	O4	58	ARG
70	O4	66	SER
70	O4	71	THR
70	O4	72	VAL
70	O4	81	CYS
70	O4	86	LYS
70	O4	104	VAL
71	O5	5	LYS
71	O5	15	GLU
71	O5	21	LEU
71	O5	28	LEU
71	O5	31	LEU
71	O5	43	LYS
71	O5	46	THR
71	O5	49	LYS
71	O5	50	SER
71	O5	62	GLN
71	O5	71	LYS
71	O5	73	LYS
71	O5	74	LYS
71	O5	84	LYS

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Mol	Chain	Res	Type
71	O5	85	THR
71	O5	90	ARG
71	O5	94	LYS
71	O5	100	VAL
71	O5	101	THR
71	O5	107	LYS
71	O5	119	LYS
72	O6	11	LEU
72	O6	17	VAL
72	O6	18	THR
72	O6	21	THR
72	O6	26	ILE
72	O6	36	ARG
72	O6	45	ARG
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	64	SER
72	O6	68	ARG
72	O6	70	ARG
72	O6	72	VAL
72	O6	75	LYS
72	O6	76	ARG
72	O6	81	THR
72	O6	88	GLU
72	O6	89	GLU
72	O6	90	MET
72	O6	99	ARG
73	O7	5	THR
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	45	ARG
73	O7	55	ARG
73	O7	58	THR
73	O7	59	THR
73	O7	67	LEU
73	O7	82	SER
73	O7	84	SER
74	O8	5	ILE
74	O8	8	ILE

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Mol	Chain	Res	Type
74	O8	24	THR
74	O8	32	ASN
74	O8	45	VAL
74	O8	46	ARG
74	O8	48	SER
74	O8	53	THR
74	O8	61	LYS
74	O8	65	LEU
74	O8	67	GLN
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	30	ARG
75	O9	34	THR
75	O9	36	ARG
75	O9	45	ARG
75	O9	51	ILE
76	Q0	78	ILE
76	Q0	83	LYS
76	Q0	85	LEU
76	Q0	106	ARG
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	114	LYS
77	Q1	6	ARG
77	Q1	9	ARG
77	Q1	10	THR
77	Q1	11	ARG
77	Q1	13	LEU
77	Q1	15	ARG
77	Q1	19	LYS
77	Q1	21	ARG
78	Q2	3	ASN
78	Q2	4	VAL
78	Q2	8	ARG
78	Q2	29	LYS
78	Q2	35	LEU
78	Q2	47	GLN
78	Q2	60	LYS

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Mol	Chain	Res	Type
78	Q2	78	LYS
78	Q2	79	THR
78	Q2	80	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	93	LEU
78	Q2	104	LEU
79	Q3	11	THR
79	Q3	25	GLN
79	Q3	45	LYS
79	Q3	46	THR
79	Q3	48	LYS
79	Q3	49	ARG
79	Q3	56	THR
79	Q3	60	CYS
79	Q3	78	THR
79	Q3	80	ARG
2	s0	6	THR
2	s0	10	THR
2	s0	12	GLU
2	s0	21	ASN
2	s0	28	ASN
2	s0	30	GLN
2	s0	31	VAL
2	s0	41	ARG
2	s0	43	ASP
2	s0	45	VAL
2	s0	59	LEU
2	s0	62	ARG
2	s0	72	ASP
2	s0	87	LEU
2	s0	96	THR
2	s0	101	ARG
2	s0	106	SER
2	s0	111	ILE
2	s0	112	THR
2	s0	124	THR
2	s0	144	ILE
2	s0	146	LEU
2	s0	153	SER
2	s0	157	ASP
2	s0	167	LYS

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Mol	Chain	Res	Type
2	s0	168	HIS
2	s0	172	LEU
2	s0	179	ARG
2	s0	183	ARG
2	s0	185	ARG
2	s0	188	LEU
2	s0	189	VAL
2	s0	191	ARG
2	s0	198	MET
3	s1	21	VAL
3	s1	25	THR
3	s1	47	LEU
3	s1	51	SER
3	s1	55	LYS
3	s1	61	LEU
3	s1	70	LEU
3	s1	73	LEU
3	s1	76	SER
3	s1	80	SER
3	s1	81	PHE
3	s1	89	ASP
3	s1	96	LEU
3	s1	105	PHE
3	s1	126	THR
3	s1	173	THR
3	s1	177	GLN
3	s1	180	THR
3	s1	184	LEU
3	s1	192	VAL
3	s1	193	ILE
3	s1	195	LYS
3	s1	202	LYS
3	s1	203	ASP
3	s1	204	ILE
3	s1	212	VAL
3	s1	222	LYS
3	s1	223	PHE
3	s1	225	VAL
3	s1	228	LEU
4	s2	41	LEU
4	s2	53	ILE
4	s2	55	GLU

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Mol	Chain	Res	Type
4	s2	58	LEU
4	s2	69	ILE
4	s2	70	ASP
4	s2	71	THR
4	s2	72	LEU
4	s2	76	LEU
4	s2	80	VAL
4	s2	83	ILE
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	94	GLN
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	113	LEU
4	s2	117	THR
4	s2	140	ARG
4	s2	141	ARG
4	s2	146	THR
4	s2	159	THR
4	s2	185	LYS
4	s2	200	SER
4	s2	205	ARG
4	s2	206	THR
4	s2	207	LEU
4	s2	218	ILE
4	s2	222	TYR
4	s2	225	LEU
4	s2	233	GLN
4	s2	242	ILE
4	s2	245	ASP
4	s2	246	GLU
5	s3	4	LEU
5	s3	7	LYS
5	s3	9	ARG
5	s3	10	LYS
5	s3	37	VAL
5	s3	39	VAL
5	s3	40	ARG
5	s3	59	LEU

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Mol	Chain	Res	Type
5	s3	66	ILE
5	s3	69	LEU
5	s3	84	ILE
5	s3	89	GLU
5	s3	90	ARG
5	s3	92	GLN
5	s3	93	ASP
5	s3	94	ARG
5	s3	111	ASN
5	s3	115	ILE
5	s3	117	ARG
5	s3	128	GLU
5	s3	132	LYS
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	169	ASP
5	s3	172	THR
5	s3	181	VAL
5	s3	202	LEU
5	s3	212	LYS
5	s3	225	TYR
6	s4	7	LYS
6	s4	9	LEU
6	s4	23	LEU
6	s4	30	ARG
6	s4	38	LEU
6	s4	42	LEU
6	s4	48	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	67	GLN
6	s4	70	VAL
6	s4	78	THR
6	s4	91	THR
6	s4	95	THR
6	s4	102	VAL
6	s4	113	ARG
6	s4	116	ASP

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Mol	Chain	Res	Type
6	s4	123	LEU
6	s4	126	VAL
6	s4	127	LYS
6	s4	129	VAL
6	s4	131	LEU
6	s4	147	ILE
6	s4	148	ARG
6	s4	160	VAL
6	s4	180	LEU
6	s4	182	TYR
6	s4	187	ARG
6	s4	192	ILE
6	s4	221	ARG
6	s4	222	LEU
6	s4	227	VAL
6	s4	237	SER
6	s4	254	ARG
7	s5	23	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	32	GLU
7	s5	38	THR
7	s5	39	GLU
7	s5	45	LYS
7	s5	59	VAL
7	s5	63	GLN
7	s5	64	VAL
7	s5	68	ILE
7	s5	76	ARG
7	s5	79	ASN
7	s5	83	ARG
7	s5	84	LYS
7	s5	89	ILE
7	s5	92	ARG
7	s5	93	LEU
7	s5	99	MET
7	s5	109	LYS
7	s5	114	ILE
7	s5	119	ASP
7	s5	125	THR
7	s5	146	THR
7	s5	147	THR

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Mol	Chain	Res	Type
7	s5	148	ARG
7	s5	149	VAL
7	s5	157	ARG
7	s5	163	SER
7	s5	167	ARG
7	s5	187	ILE
7	s5	194	LEU
7	s5	203	LYS
7	s5	216	GLU
7	s5	225	ARG
8	s6	5	ILE
8	s6	17	GLU
8	s6	25	ARG
8	s6	30	LYS
8	s6	31	ARG
8	s6	43	ASP
8	s6	44	GLU
8	s6	76	LEU
8	s6	78	THR
8	s6	88	ARG
8	s6	98	ARG
8	s6	108	VAL
8	s6	109	LEU
8	s6	112	VAL
8	s6	115	LYS
8	s6	120	GLU
8	s6	121	LEU
8	s6	125	THR
8	s6	126	ASP
8	s6	127	THR
8	s6	128	THR
8	s6	129	VAL
8	s6	143	LYS
8	s6	150	GLU
8	s6	151	ASP
8	s6	154	ARG
8	s6	155	ASP
8	s6	168	THR
8	s6	170	THR
8	s6	171	LYS
8	s6	177	ARG
8	s6	179	VAL

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Mol	Chain	Res	Type
8	s6	193	LEU
8	s6	215	ARG
8	s6	217	SER
9	s7	5	GLN
9	s7	8	ILE
9	s7	26	GLU
9	s7	28	GLU
9	s7	33	GLU
9	s7	49	ILE
9	s7	50	ASP
9	s7	55	LYS
9	s7	67	LEU
9	s7	77	LEU
9	s7	79	ARG
9	s7	80	GLU
9	s7	86	GLN
9	s7	97	ARG
9	s7	101	LYS
9	s7	105	THR
9	s7	110	GLN
9	s7	114	ARG
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	126	LEU
9	s7	136	VAL
9	s7	143	LEU
9	s7	144	VAL
9	s7	148	LYS
9	s7	156	SER
9	s7	159	VAL
9	s7	166	LEU
9	s7	175	LYS
9	s7	185	ILE
10	s8	20	GLN
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	46	VAL
10	s8	60	ILE
10	s8	61	GLU
10	s8	74	LYS

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Mol	Chain	Res	Type
10	s8	76	THR
10	s8	77	ARG
10	s8	89	GLU
10	s8	110	ARG
10	s8	119	GLN
10	s8	121	LEU
10	s8	123	LYS
10	s8	138	ASN
10	s8	155	SER
10	s8	158	SER
10	s8	183	ILE
10	s8	184	LEU
10	s8	199	LYS
11	s9	3	ARG
11	s9	6	ARG
11	s9	7	THR
11	s9	10	LYS
11	s9	28	LEU
11	s9	33	GLU
11	s9	39	LYS
11	s9	49	LEU
11	s9	82	ARG
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	110	GLN
11	s9	111	THR
11	s9	113	VAL
11	s9	118	LEU
11	s9	130	THR
11	s9	134	ILE
11	s9	140	ILE
11	s9	149	ARG
11	s9	154	LYS
11	s9	161	THR
11	s9	168	ARG
11	s9	172	VAL
11	s9	175	ARG
11	s9	180	LYS

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Mol	Chain	Res	Type
11	s9	182	GLU
12	c0	2	LEU
12	c0	5	LYS
12	c0	15	LEU
12	c0	20	VAL
12	c0	21	VAL
12	c0	27	PHE
12	c0	33	GLU
12	c0	36	ASP
12	c0	55	VAL
12	c0	57	THR
12	c0	67	THR
12	c0	71	GLU
13	c1	5	LEU
13	c1	10	GLU
13	c1	21	ASN
13	c1	26	LYS
13	c1	27	THR
13	c1	30	ARG
13	c1	32	LYS
13	c1	33	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	47	THR
13	c1	56	LYS
13	c1	60	PHE
13	c1	67	ARG
13	c1	74	THR
13	c1	80	MET
13	c1	83	THR
13	c1	109	VAL
13	c1	123	VAL
13	c1	129	ARG
13	c1	140	VAL
13	c1	143	SER
14	c2	28	LEU
14	c2	37	VAL
14	c2	43	ARG
14	c2	45	LEU
14	c2	53	THR
14	c2	58	LEU
14	c2	59	LEU

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Mol	Chain	Res	Type
14	c2	61	VAL
14	c2	62	LEU
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	86	VAL
14	c2	89	ILE
14	c2	103	LEU
14	c2	116	VAL
14	c2	120	VAL
14	c2	121	VAL
14	c2	132	GLU
14	c2	137	MET
14	c2	138	GLU
14	c2	140	PHE
15	c3	12	SER
15	c3	16	ILE
15	c3	20	ARG
15	c3	21	ASN
15	c3	39	LYS
15	c3	53	LEU
15	c3	64	ARG
15	c3	66	ILE
15	c3	67	THR
15	c3	70	LYS
15	c3	80	LEU
15	c3	87	ASP
15	c3	88	LEU
15	c3	93	LYS
15	c3	104	ARG
15	c3	114	ARG
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	138	ASN
15	c3	147	SER
15	c3	150	VAL
16	c4	18	ARG
16	c4	20	TYR
16	c4	26	THR
16	c4	33	LEU

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Mol	Chain	Res	Type
16	c4	49	LYS
16	c4	51	ASP
16	c4	61	MET
16	c4	70	LYS
16	c4	79	VAL
16	c4	81	VAL
16	c4	92	LYS
16	c4	102	LEU
16	c4	111	ARG
16	c4	114	ARG
16	c4	119	THR
16	c4	124	ASP
16	c4	125	SER
16	c4	127	ARG
16	c4	132	ARG
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
17	c5	10	ARG
17	c5	12	PHE
17	c5	22	LEU
17	c5	24	LYS
17	c5	27	GLU
17	c5	36	LEU
17	c5	43	ARG
17	c5	44	ARG
17	c5	52	LYS
17	c5	64	LYS
17	c5	69	GLU
17	c5	71	GLU
17	c5	72	LYS
17	c5	77	ARG
17	c5	92	SER
17	c5	107	ILE
17	c5	110	GLU
17	c5	122	THR
17	c5	124	THR
17	c5	125	PRO
18	c6	7	VAL
18	c6	17	THR
18	c6	23	LYS
18	c6	28	LEU

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Mol	Chain	Res	Type
18	c6	37	THR
18	c6	40	GLU
18	c6	43	ILE
18	c6	48	VAL
18	c6	53	LEU
18	c6	54	LEU
18	c6	57	LEU
18	c6	68	ARG
18	c6	69	VAL
18	c6	70	THR
18	c6	81	ILE
18	c6	90	VAL
18	c6	110	THR
18	c6	113	ASP
18	c6	114	ARG
18	c6	137	ARG
19	c7	3	ARG
19	c7	8	THR
19	c7	14	LYS
19	c7	33	ARG
19	c7	34	LEU
19	c7	38	ILE
19	c7	45	ARG
19	c7	46	LEU
19	c7	60	ARG
19	c7	72	LYS
19	c7	74	GLN
19	c7	83	GLN
19	c7	85	VAL
19	c7	104	ASN
19	c7	110	VAL
19	c7	113	LEU
20	c8	2	SER
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	12	GLN
20	c8	13	HIS
20	c8	16	ARG
20	c8	27	LYS
20	c8	28	ILE

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Mol	Chain	Res	Type
20	c8	34	THR
20	c8	36	LYS
20	c8	40	ARG
20	c8	57	ARG
20	c8	61	LEU
20	c8	63	GLN
20	c8	68	ARG
20	c8	88	ARG
20	c8	92	ILE
20	c8	100	THR
20	c8	110	ARG
20	c8	116	LEU
20	c8	119	ILE
20	c8	136	GLN
20	c8	138	THR
20	c8	143	ARG
20	c8	145	ARG
21	c9	6	VAL
21	c9	13	ASP
21	c9	25	GLN
21	c9	28	LEU
21	c9	34	VAL
21	c9	36	ILE
21	c9	37	VAL
21	c9	57	ARG
21	c9	68	ARG
21	c9	71	VAL
21	c9	75	LYS
21	c9	86	ARG
21	c9	88	VAL
21	c9	111	ILE
21	c9	123	ARG
21	c9	131	ASP
21	c9	135	ILE
21	c9	140	LEU
21	c9	142	GLU
21	c9	144	GLU
22	d0	12	GLN
22	d0	20	ILE
22	d0	23	ARG
22	d0	27	THR
22	d0	30	LYS

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Mol	Chain	Res	Type
22	d0	44	ASN
22	d0	47	GLN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	67	THR
22	d0	70	THR
22	d0	72	ASN
22	d0	74	GLU
22	d0	81	THR
22	d0	88	LYS
22	d0	89	ARG
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	107	THR
22	d0	108	ILE
22	d0	118	VAL
23	d1	1	MET
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	41	GLU
23	d1	49	GLU
23	d1	52	THR
23	d1	62	ARG
23	d1	68	SER
23	d1	69	LEU
23	d1	74	GLN
23	d1	76	ASP
23	d1	79	LEU
24	d2	6	VAL
24	d2	7	LEU
24	d2	22	LYS
24	d2	23	ARG
24	d2	25	VAL
24	d2	26	LEU
24	d2	43	LYS

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Mol	Chain	Res	Type
24	d2	65	LEU
24	d2	74	VAL
24	d2	88	LYS
24	d2	93	LEU
24	d2	103	ILE
24	d2	105	THR
24	d2	129	VAL
25	d3	9	LEU
25	d3	16	ARG
25	d3	19	ARG
25	d3	23	ARG
25	d3	40	SER
25	d3	69	ARG
25	d3	73	ARG
25	d3	83	VAL
25	d3	84	THR
25	d3	98	GLU
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	114	LYS
25	d3	131	SER
26	d4	13	ILE
26	d4	36	SER
26	d4	42	GLU
26	d4	43	LYS
26	d4	46	GLU
26	d4	49	LYS
26	d4	51	GLU
26	d4	61	ARG
26	d4	62	THR
26	d4	88	THR
26	d4	100	VAL
26	d4	105	ARG
26	d4	116	LYS
27	d5	43	ASP
27	d5	46	LYS
27	d5	51	LEU
27	d5	57	TYR
27	d5	60	VAL
27	d5	68	ARG
27	d5	81	ARG

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Mol	Chain	Res	Type
28	d6	10	ARG
28	d6	11	ASN
28	d6	18	VAL
28	d6	24	VAL
28	d6	26	CYS
28	d6	34	LYS
28	d6	41	ILE
28	d6	44	ILE
28	d6	53	LEU
28	d6	55	GLU
28	d6	82	ARG
28	d6	83	ILE
28	d6	85	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	40	CYS
29	d7	41	LEU
29	d7	43	ILE
29	d7	44	THR
29	d7	52	THR
29	d7	61	THR
29	d7	63	LEU
29	d7	72	LYS
29	d7	77	THR
29	d7	81	ARG
30	d8	8	THR
30	d8	22	ARG
30	d8	32	PHE
30	d8	33	LEU
30	d8	36	THR
30	d8	48	VAL
30	d8	49	ARG
30	d8	54	LEU
31	d9	16	LYS
31	d9	28	THR
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	38	ILE
31	d9	53	ASN
31	d9	54	LYS
80	e0	4	VAL

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Mol	Chain	Res	Type
80	e0	13	LYS
80	e0	22	GLU
80	e0	23	LYS
80	e0	26	LYS
80	e0	29	LYS
80	e0	36	LYS
80	e0	38	LEU
80	e0	44	PHE
80	e0	46	ASN
80	e0	54	ARG
80	e0	55	ARG
33	e1	80	ARG
33	e1	84	VAL
33	e1	86	THR
33	e1	90	LYS
33	e1	96	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	113	LYS
33	e1	119	ARG
33	e1	121	CYS
33	e1	125	THR
33	e1	130	VAL
33	e1	135	HIS
33	e1	137	ASP
33	e1	146	SER
33	e1	148	TYR
33	e1	150	VAL
34	sR	8	VAL
34	sR	21	THR
34	sR	25	THR
34	sR	29	GLN
34	sR	58	VAL
34	sR	65	SER
34	sR	66	HIS
34	sR	76	ASP
34	sR	96	THR
34	sR	118	LYS
34	sR	136	ILE
34	sR	145	LEU
34	sR	149	ASP

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Mol	Chain	Res	Type
34	sR	153	GLN
34	sR	159	ASN
34	sR	166	SER
34	sR	168	THR
34	sR	184	ASN
34	sR	199	ILE
34	sR	202	LEU
34	sR	228	LYS
34	sR	252	LEU
34	sR	266	ASP
34	sR	275	ARG
34	sR	297	ASP
34	sR	309	VAL
34	sR	314	GLN
34	sR	317	THR
35	sM	23	LYS
35	sM	33	LYS
35	sM	43	ASP
35	sM	45	SER
35	sM	64	LYS
35	sM	74	LYS
35	sM	75	ASP
39	l2	15	ILE
39	l2	23	ARG
39	l2	32	LEU
39	l2	41	ILE
39	l2	44	ILE
39	l2	45	VAL
39	l2	46	LYS
39	l2	48	ILE
39	l2	61	VAL
39	l2	62	VAL
39	l2	70	ARG
39	l2	71	LEU
39	l2	74	GLU
39	l2	101	VAL
39	l2	112	ILE
39	l2	116	VAL
39	l2	119	LYS
39	l2	137	ILE
39	l2	142	ASP
39	l2	155	LYS

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Mol	Chain	Res	Type
39	l2	157	VAL
39	l2	158	ILE
39	l2	165	VAL
39	l2	179	LEU
39	l2	180	LEU
39	l2	181	LYS
39	l2	193	ARG
39	l2	194	ASN
39	l2	202	VAL
39	l2	207	VAL
39	l2	215	ASN
39	l2	224	THR
39	l2	225	ILE
39	l2	230	VAL
39	l2	241	ARG
39	l2	246	LEU
39	l2	249	SER
40	l3	3	HIS
40	l3	4	ARG
40	l3	10	ARG
40	l3	17	LEU
40	l3	19	ARG
40	l3	21	ARG
40	l3	30	LYS
40	l3	39	LYS
40	l3	47	LEU
40	l3	50	LYS
40	l3	56	ILE
40	l3	77	THR
40	l3	79	VAL
40	l3	81	THR
40	l3	84	VAL
40	l3	103	THR
40	l3	114	VAL
40	l3	120	LYS
40	l3	124	LYS
40	l3	134	SER
40	l3	145	GLU
40	l3	146	ARG
40	l3	148	LEU
40	l3	150	ARG
40	l3	157	VAL

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Mol	Chain	Res	Type
40	l3	160	VAL
40	l3	169	THR
40	l3	183	LEU
40	l3	187	SER
40	l3	188	ILE
40	l3	196	ARG
40	l3	202	THR
40	l3	205	VAL
40	l3	221	THR
40	l3	229	VAL
40	l3	232	ARG
40	l3	235	THR
40	l3	236	LYS
40	l3	238	LEU
40	l3	242	THR
40	l3	244	ARG
40	l3	248	LYS
40	l3	249	VAL
40	l3	252	ILE
40	l3	261	MET
40	l3	264	VAL
40	l3	284	ARG
40	l3	296	THR
40	l3	302	LYS
40	l3	308	MET
40	l3	317	ILE
40	l3	324	VAL
40	l3	328	ILE
40	l3	332	ARG
40	l3	335	ILE
40	l3	338	LEU
40	l3	340	LYS
40	l3	346	THR
40	l3	347	SER
40	l3	348	ARG
40	l3	349	LYS
40	l3	355	SER
40	l3	361	THR
40	l3	369	ARG
40	l3	382	THR
41	l4	2	SER
41	l4	14	GLU

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Mol	Chain	Res	Type
41	l4	25	VAL
41	l4	52	VAL
41	l4	60	THR
41	l4	67	THR
41	l4	93	MET
41	l4	112	LYS
41	l4	120	TYR
41	l4	122	THR
41	l4	143	GLU
41	l4	144	LYS
41	l4	145	ILE
41	l4	150	LEU
41	l4	156	LEU
41	l4	160	GLN
41	l4	161	LYS
41	l4	172	VAL
41	l4	176	SER
41	l4	179	LEU
41	l4	186	LYS
41	l4	187	LEU
41	l4	188	ARG
41	l4	191	LYS
41	l4	198	ARG
41	l4	200	THR
41	l4	203	ARG
41	l4	206	LEU
41	l4	217	LYS
41	l4	220	ARG
41	l4	222	VAL
41	l4	226	GLU
41	l4	229	ASN
41	l4	230	VAL
41	l4	246	ARG
41	l4	258	LEU
41	l4	267	VAL
41	l4	283	THR
41	l4	284	SER
41	l4	287	THR
41	l4	295	ILE
41	l4	300	ARG
41	l4	306	THR
41	l4	307	GLN

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Mol	Chain	Res	Type
41	l4	313	LEU
41	l4	319	LYS
41	l4	323	VAL
41	l4	327	LEU
41	l4	342	LYS
41	l4	345	GLU
41	l4	358	THR
41	l4	359	LEU
41	l4	360	LYS
42	l5	4	GLN
42	l5	5	LYS
42	l5	15	ARG
42	l5	34	LYS
42	l5	41	LYS
42	l5	51	LEU
42	l5	58	LYS
42	l5	61	ILE
42	l5	65	ILE
42	l5	68	THR
42	l5	70	THR
42	l5	73	VAL
42	l5	74	VAL
42	l5	75	LEU
42	l5	89	THR
42	l5	93	THR
42	l5	110	LEU
42	l5	112	LYS
42	l5	113	LEU
42	l5	115	LEU
42	l5	118	THR
42	l5	120	LYS
42	l5	124	GLU
42	l5	131	LEU
42	l5	132	THR
42	l5	133	GLU
42	l5	135	VAL
42	l5	136	GLU
42	l5	140	ARG
42	l5	146	LEU
42	l5	148	ILE
42	l5	152	ARG
42	l5	155	THR

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Mol	Chain	Res	Type
42	l5	185	PHE
42	l5	187	THR
42	l5	190	ILE
42	l5	194	LEU
42	l5	210	GLU
42	l5	211	LEU
42	l5	218	ARG
42	l5	220	SER
42	l5	227	LEU
42	l5	254	LYS
42	l5	258	LYS
42	l5	259	LYS
42	l5	268	GLU
42	l5	269	SER
42	l5	273	ARG
42	l5	275	THR
42	l5	282	ARG
42	l5	293	LEU
43	l6	8	LYS
43	l6	12	SER
43	l6	20	LYS
43	l6	21	THR
43	l6	31	ARG
43	l6	46	ARG
43	l6	50	LYS
43	l6	52	VAL
43	l6	64	LEU
43	l6	65	ILE
43	l6	78	ARG
43	l6	79	VAL
43	l6	89	THR
43	l6	91	VAL
43	l6	93	VAL
43	l6	98	VAL
43	l6	99	GLU
43	l6	109	GLU
43	l6	131	LYS
43	l6	133	GLU
43	l6	143	LYS
43	l6	152	THR
43	l6	155	LEU
43	l6	175	LYS

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Mol	Chain	Res	Type
44	l7	22	THR
44	l7	26	VAL
44	l7	30	ARG
44	l7	41	ARG
44	l7	54	GLU
44	l7	60	ARG
44	l7	77	VAL
44	l7	83	LEU
44	l7	88	ARG
44	l7	93	ASN
44	l7	98	LYS
44	l7	100	ARG
44	l7	110	ARG
44	l7	121	LYS
44	l7	124	LEU
44	l7	130	ILE
44	l7	156	ILE
44	l7	158	LYS
44	l7	173	LEU
44	l7	175	LYS
44	l7	178	ILE
44	l7	179	LEU
44	l7	184	LEU
44	l7	193	PRO
44	l7	219	LYS
44	l7	228	SER
44	l7	229	PHE
44	l7	239	LEU
45	l8	33	ASN
45	l8	41	GLN
45	l8	50	VAL
45	l8	65	LEU
45	l8	66	SER
45	l8	67	ILE
45	l8	69	LEU
45	l8	71	VAL
45	l8	74	THR
45	l8	79	GLN
45	l8	81	THR
45	l8	89	GLU
45	l8	90	THR
45	l8	95	ASN

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Mol	Chain	Res	Type
45	l8	128	LYS
45	l8	136	LEU
45	l8	145	ASN
45	l8	146	LYS
45	l8	149	LYS
45	l8	150	LEU
45	l8	160	ILE
45	l8	163	VAL
45	l8	164	VAL
45	l8	166	LEU
45	l8	169	LEU
45	l8	172	LYS
45	l8	211	LEU
45	l8	214	LEU
45	l8	217	THR
45	l8	230	LYS
45	l8	231	LYS
45	l8	238	LEU
45	l8	241	LYS
45	l8	248	LYS
46	l9	2	LYS
46	l9	4	ILE
46	l9	5	GLN
46	l9	6	THR
46	l9	18	VAL
46	l9	19	SER
46	l9	20	ILE
46	l9	31	ARG
46	l9	33	THR
46	l9	39	LYS
46	l9	43	VAL
46	l9	44	THR
46	l9	52	LEU
46	l9	55	VAL
46	l9	62	ARG
46	l9	68	LEU
46	l9	69	ARG
46	l9	70	THR
46	l9	80	THR
46	l9	82	VAL
46	l9	105	GLU
46	l9	106	LYS

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Mol	Chain	Res	Type
46	l9	120	ASP
46	l9	130	ASP
46	l9	133	THR
46	l9	151	VAL
46	l9	157	ASN
46	l9	161	LEU
46	l9	162	GLN
46	l9	168	ARG
46	l9	169	ASN
46	l9	177	ASP
46	l9	179	ILE
46	l9	191	LEU
47	m0	3	ARG
47	m0	4	ARG
47	m0	24	ARG
47	m0	28	ASP
47	m0	31	ILE
47	m0	32	ARG
47	m0	36	LEU
47	m0	42	THR
47	m0	48	LEU
47	m0	52	LEU
47	m0	57	LEU
47	m0	74	LYS
47	m0	76	MET
47	m0	77	THR
47	m0	78	THR
47	m0	82	ARG
47	m0	87	LEU
47	m0	99	ILE
47	m0	101	LYS
47	m0	116	ARG
47	m0	129	VAL
47	m0	130	ASP
47	m0	139	ARG
47	m0	140	THR
47	m0	143	SER
47	m0	145	LYS
47	m0	163	GLN
47	m0	166	ILE
47	m0	167	LEU
47	m0	169	LYS

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Mol	Chain	Res	Type
47	m0	182	LEU
47	m0	185	ARG
47	m0	197	VAL
47	m0	205	SER
47	m0	211	ARG
47	m0	212	GLU
47	m0	215	GLU
48	m1	10	ARG
48	m1	11	ASP
48	m1	12	LEU
48	m1	30	LEU
48	m1	31	THR
48	m1	44	THR
48	m1	54	VAL
48	m1	55	ARG
48	m1	71	VAL
48	m1	80	LEU
48	m1	85	LYS
48	m1	101	ASN
48	m1	107	ASP
48	m1	112	LEU
48	m1	129	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	142	LYS
48	m1	153	LYS
48	m1	159	THR
48	m1	161	SER
48	m1	174	LYS
49	m3	13	HIS
49	m3	54	LEU
49	m3	55	ARG
49	m3	57	VAL
49	m3	59	ARG
49	m3	63	VAL
49	m3	67	ARG
49	m3	68	LYS
49	m3	69	VAL
49	m3	73	ARG
49	m3	85	LEU
49	m3	107	GLU
49	m3	114	GLN

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Mol	Chain	Res	Type
49	m3	115	ARG
49	m3	118	GLU
49	m3	122	LYS
49	m3	124	ILE
49	m3	128	ARG
49	m3	131	LYS
49	m3	164	GLU
49	m3	165	SER
49	m3	184	GLU
49	m3	190	LYS
49	m3	194	GLU
50	m4	3	THR
50	m4	13	ARG
50	m4	20	VAL
50	m4	27	GLN
50	m4	42	LYS
50	m4	50	LYS
50	m4	53	VAL
50	m4	62	GLN
50	m4	63	VAL
50	m4	64	VAL
50	m4	72	LEU
50	m4	80	THR
50	m4	82	SER
50	m4	105	GLN
50	m4	113	THR
50	m4	130	THR
50	m4	133	LYS
50	m4	135	LEU
51	m5	5	LYS
51	m5	10	LEU
51	m5	12	ARG
51	m5	22	LEU
51	m5	24	ARG
51	m5	49	ARG
51	m5	68	ARG
51	m5	76	PRO
51	m5	80	THR
51	m5	83	LYS
51	m5	85	THR
51	m5	92	LEU
51	m5	96	ARG

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Mol	Chain	Res	Type
51	m5	97	SER
51	m5	98	LEU
51	m5	105	ARG
51	m5	106	VAL
51	m5	125	SER
51	m5	138	GLN
51	m5	153	ASP
51	m5	155	VAL
51	m5	159	ARG
51	m5	170	LYS
51	m5	188	ARG
51	m5	190	THR
51	m5	194	GLN
51	m5	196	THR
52	m6	12	LYS
52	m6	22	VAL
52	m6	25	LYS
52	m6	41	LEU
52	m6	58	LEU
52	m6	60	LYS
52	m6	67	THR
52	m6	68	ARG
52	m6	74	ARG
52	m6	78	ARG
52	m6	84	LEU
52	m6	85	ARG
52	m6	89	SER
52	m6	100	GLU
52	m6	106	GLU
52	m6	108	ILE
52	m6	110	PRO
52	m6	117	ARG
52	m6	124	LEU
52	m6	130	LYS
52	m6	152	VAL
52	m6	160	ARG
52	m6	167	TYR
52	m6	171	LYS
52	m6	175	THR
52	m6	182	ASN
52	m6	184	THR
52	m6	197	LEU

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Mol	Chain	Res	Type
53	m7	9	THR
53	m7	23	ARG
53	m7	24	VAL
53	m7	31	GLU
53	m7	32	THR
53	m7	41	LEU
53	m7	52	LEU
53	m7	56	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	126	ARG
53	m7	128	ARG
53	m7	144	SER
54	m8	7	SER
54	m8	17	THR
54	m8	24	VAL
54	m8	26	LEU
54	m8	32	LEU
54	m8	34	THR
54	m8	41	ASP
54	m8	46	LYS
54	m8	49	LEU
54	m8	59	ARG
54	m8	63	SER
54	m8	66	ARG
54	m8	69	ARG
54	m8	80	THR
54	m8	81	VAL
54	m8	86	THR
54	m8	93	ILE
54	m8	95	GLU
54	m8	100	THR
54	m8	111	ARG
54	m8	127	LEU
54	m8	135	GLN
54	m8	144	ARG
54	m8	147	ARG
54	m8	150	VAL

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Mol	Chain	Res	Type
54	m8	161	LYS
54	m8	170	ARG
54	m8	180	ARG
55	m9	5	ARG
55	m9	7	GLN
55	m9	10	LEU
55	m9	17	VAL
55	m9	20	ARG
55	m9	29	THR
55	m9	36	ASN
55	m9	39	ASN
55	m9	43	LYS
55	m9	49	THR
55	m9	52	LYS
55	m9	55	VAL
55	m9	56	THR
55	m9	60	LYS
55	m9	63	THR
55	m9	71	ARG
55	m9	74	ARG
55	m9	76	SER
55	m9	88	ARG
55	m9	99	LEU
55	m9	106	LEU
55	m9	117	LYS
55	m9	126	GLU
55	m9	128	LYS
55	m9	134	HIS
55	m9	138	LEU
55	m9	150	GLN
55	m9	152	GLU
55	m9	153	LYS
55	m9	156	ASN
55	m9	158	GLU
55	m9	164	LEU
55	m9	170	ARG
55	m9	173	ARG
56	n0	1	MET
56	n0	13	ARG
56	n0	21	GLU
56	n0	60	SER
56	n0	61	ILE

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Mol	Chain	Res	Type
56	n0	71	LYS
56	n0	73	LYS
56	n0	87	THR
56	n0	100	VAL
56	n0	105	THR
56	n0	106	LEU
56	n0	115	ARG
56	n0	117	ARG
56	n0	120	SER
56	n0	130	GLU
56	n0	136	LYS
56	n0	137	ARG
56	n0	138	GLN
56	n0	148	LEU
56	n0	149	LYS
56	n0	155	ARG
56	n0	161	LYS
56	n0	162	THR
56	n0	172	TYR
57	n1	12	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	52	MET
57	n1	68	THR
57	n1	78	LYS
57	n1	83	ARG
57	n1	88	ARG
57	n1	89	LEU
57	n1	96	ILE
57	n1	102	ARG
57	n1	104	GLU
57	n1	122	GLN
57	n1	126	VAL
57	n1	135	PRO
57	n1	139	ARG
57	n1	141	VAL
57	n1	143	THR
57	n1	150	THR
58	n2	11	ILE
58	n2	21	SER
58	n2	27	VAL

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Mol	Chain	Res	Type
58	n2	37	LEU
58	n2	43	VAL
58	n2	54	VAL
58	n2	63	VAL
58	n2	68	THR
58	n2	74	LYS
58	n2	90	ARG
58	n2	98	THR
58	n2	105	LEU
59	n3	13	ILE
59	n3	14	SER
59	n3	45	ARG
59	n3	48	ARG
59	n3	73	VAL
59	n3	91	VAL
59	n3	110	LYS
59	n3	115	THR
59	n3	120	LYS
60	n4	1	MET
60	n4	2	LYS
60	n4	5	ILE
60	n4	26	SER
60	n4	39	LEU
60	n4	43	ARG
60	n4	54	LEU
60	n4	63	ILE
60	n4	96	LEU
60	n4	99	GLU
60	n4	100	VAL
60	n4	127	LYS
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	38	LEU
61	n5	39	LYS
61	n5	45	LYS
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	64	GLU
61	n5	65	GLN

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Mol	Chain	Res	Type
61	n5	71	THR
61	n5	86	VAL
61	n5	87	SER
61	n5	106	ASP
61	n5	108	LEU
61	n5	109	LYS
61	n5	115	ARG
61	n5	125	ARG
61	n5	133	LEU
61	n5	135	ILE
61	n5	137	ASN
61	n5	142	ILE
62	n6	12	ARG
62	n6	13	ARG
62	n6	37	LYS
62	n6	39	LEU
62	n6	40	ARG
62	n6	45	ILE
62	n6	50	ILE
62	n6	51	ARG
62	n6	55	GLU
62	n6	56	VAL
62	n6	57	LEU
62	n6	62	SER
62	n6	66	GLN
62	n6	71	SER
62	n6	74	TYR
62	n6	76	LEU
62	n6	80	VAL
62	n6	83	ASP
62	n6	94	SER
62	n6	97	ILE
62	n6	108	LYS
62	n6	113	LYS
62	n6	115	ARG
62	n6	120	GLN
62	n6	127	GLU
63	n7	3	LYS
63	n7	14	VAL
63	n7	17	ARG
63	n7	24	VAL
63	n7	26	VAL

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Mol	Chain	Res	Type
63	n7	33	SER
63	n7	46	ILE
63	n7	52	LYS
63	n7	55	LYS
63	n7	64	LYS
63	n7	72	ILE
63	n7	73	LYS
63	n7	75	VAL
63	n7	81	LEU
63	n7	83	THR
63	n7	86	THR
63	n7	94	SER
63	n7	103	GLN
63	n7	111	LYS
63	n7	121	ARG
63	n7	126	LYS
63	n7	134	LEU
63	n7	135	ARG
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	9	ARG
64	n8	10	LYS
64	n8	12	ARG
64	n8	16	SER
64	n8	24	LYS
64	n8	26	ARG
64	n8	27	LYS
64	n8	47	LYS
64	n8	60	TYR
64	n8	70	LYS
64	n8	78	LEU
64	n8	85	ASP
64	n8	91	LEU
64	n8	95	SER
64	n8	98	THR
64	n8	115	LYS
64	n8	128	ARG
64	n8	130	VAL
64	n8	132	LYS
64	n8	133	LEU
65	n9	12	GLN

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Mol	Chain	Res	Type
65	n9	14	ARG
65	n9	22	LYS
65	n9	26	THR
65	n9	31	SER
65	n9	33	LYS
65	n9	38	LYS
65	n9	50	THR
65	n9	52	LYS
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	9	SER
66	o0	18	ILE
66	o0	33	SER
66	o0	34	LEU
66	o0	40	LYS
66	o0	41	LEU
66	o0	61	MET
66	o0	66	LYS
66	o0	68	TYR
66	o0	81	VAL
66	o0	86	ARG
66	o0	87	VAL
66	o0	97	ASP
66	o0	101	LEU
66	o0	103	THR
67	o1	6	ASP
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	31	ARG
67	o1	34	LYS
67	o1	47	ASP
67	o1	50	ARG
67	o1	64	VAL
67	o1	83	GLU
67	o1	90	PHE
67	o1	96	VAL
67	o1	102	LYS
67	o1	106	THR
67	o1	107	VAL

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Mol	Chain	Res	Type
67	o1	110	GLU
68	o2	4	LEU
68	o2	5	PRO
68	o2	16	LYS
68	o2	18	LYS
68	o2	19	ARG
68	o2	27	ARG
68	o2	31	ASN
68	o2	33	ARG
68	o2	34	LYS
68	o2	41	VAL
68	o2	50	ILE
68	o2	54	LYS
68	o2	73	THR
68	o2	75	LEU
68	o2	76	VAL
68	o2	82	LEU
68	o2	106	VAL
69	o3	10	LYS
69	o3	20	LYS
69	o3	31	LYS
69	o3	49	ILE
69	o3	70	LYS
69	o3	81	VAL
69	o3	92	LYS
69	o3	98	VAL
70	o4	5	VAL
70	o4	16	ARG
70	o4	19	LYS
70	o4	20	ILE
70	o4	24	LYS
70	o4	29	ILE
70	o4	30	LEU
70	o4	58	ARG
70	o4	64	THR
70	o4	65	VAL
70	o4	68	THR
70	o4	88	ARG
70	o4	98	GLN
70	o4	110	GLU
71	o5	20	GLN
71	o5	21	LEU

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Mol	Chain	Res	Type
71	o5	28	LEU
71	o5	31	LEU
71	o5	38	ARG
71	o5	43	LYS
71	o5	45	LYS
71	o5	47	VAL
71	o5	48	ARG
71	o5	62	GLN
71	o5	68	GLN
71	o5	69	LEU
71	o5	73	LYS
71	o5	79	ASP
71	o5	81	ARG
71	o5	84	LYS
71	o5	85	THR
71	o5	86	ARG
71	o5	89	ARG
71	o5	90	ARG
71	o5	94	LYS
71	o5	98	SER
71	o5	100	VAL
71	o5	101	THR
71	o5	104	GLN
71	o5	107	LYS
71	o5	119	LYS
72	o6	3	VAL
72	o6	4	LYS
72	o6	7	ILE
72	o6	9	ILE
72	o6	11	LEU
72	o6	21	THR
72	o6	25	LYS
72	o6	26	ILE
72	o6	29	LYS
72	o6	34	SER
72	o6	36	ARG
72	o6	37	THR
72	o6	38	LYS
72	o6	43	LEU
72	o6	45	ARG
72	o6	58	ILE
72	o6	59	ASP

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Mol	Chain	Res	Type
72	o6	60	LEU
72	o6	64	SER
72	o6	68	ARG
72	o6	74	LYS
72	o6	75	LYS
72	o6	76	ARG
72	o6	80	PHE
72	o6	81	THR
72	o6	88	GLU
72	o6	94	ILE
72	o6	98	ARG
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	58	THR
73	o7	67	LEU
73	o7	68	LYS
73	o7	80	THR
74	o8	5	ILE
74	o8	12	LEU
74	o8	17	ARG
74	o8	31	LEU
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	68	SER
74	o8	72	THR
75	o9	4	GLN
75	o9	15	LYS
75	o9	17	LYS
75	o9	19	GLN
75	o9	21	ARG
75	o9	23	LEU
75	o9	29	LEU
75	o9	45	ARG

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Mol	Chain	Res	Type
75	o9	48	LYS
75	o9	51	ILE
76	q0	78	ILE
76	q0	85	LEU
76	q0	93	LYS
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	127	LEU
77	q1	6	ARG
77	q1	9	ARG
77	q1	10	THR
77	q1	13	LEU
77	q1	14	LYS
77	q1	16	LYS
77	q1	21	ARG
77	q1	23	ARG
77	q1	24	SER
78	q2	7	THR
78	q2	8	ARG
78	q2	16	THR
78	q2	22	GLN
78	q2	46	LYS
78	q2	47	GLN
78	q2	48	SER
78	q2	61	LYS
78	q2	71	ARG
78	q2	78	LYS
78	q2	79	THR
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	93	LEU
78	q2	100	LYS
78	q2	104	LEU
79	q3	3	LYS
79	q3	5	THR
79	q3	10	ILE
79	q3	22	LEU
79	q3	33	GLN
79	q3	42	CYS
79	q3	48	LYS

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Mol	Chain	Res	Type
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	62	LYS
79	q3	78	THR
79	q3	90	VAL
82	p0	4	ILE
82	p0	5	ARG
82	p0	10	GLU
82	p0	25	LEU
82	p0	42	ARG
82	p0	43	LYS
82	p0	44	GLU
82	p0	48	ARG
82	p0	52	LEU
82	p0	55	LYS
82	p0	69	ASP
82	p0	70	LEU
82	p0	72	ASP
82	p0	76	LEU
82	p0	91	GLU
82	p0	93	LEU
82	p0	94	THR
82	p0	96	ILE
82	p0	97	LYS
82	p0	103	ASN
82	p0	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
2	S0	163	ASN
2	S0	168	HIS
3	S1	79	HIS
5	S3	159	HIS
7	S5	103	ASN
9	S7	71	HIS
11	S9	110	GLN
13	C1	110	HIS
15	C3	105	ASN
20	C8	6	GLN
23	D1	74	GLN

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Mol	Chain	Res	Type
24	D2	70	ASN
26	D4	63	GLN
27	D5	44	GLN
27	D5	95	HIS
39	L2	83	HIS
39	L2	209	HIS
40	L3	121	ASN
42	L5	40	HIS
42	L5	81	HIS
44	L7	244	ASN
48	M1	95	ASN
53	M7	125	GLN
54	M8	73	GLN
59	N3	81	GLN
59	N3	98	ASN
61	N5	80	ASN
68	O2	104	ASN
69	O3	42	GLN
2	s0	140	ASN
9	s7	71	HIS
11	s9	110	GLN
12	c0	29	GLN
12	c0	32	HIS
15	c3	49	GLN
15	c3	62	GLN
23	d1	21	ASN
24	d2	56	HIS
26	d4	22	GLN
33	e1	93	HIS
34	sR	184	ASN
42	l5	264	GLN
45	l8	33	ASN
56	n0	108	GLN
61	n5	111	ASN
62	n6	120	GLN
64	n8	28	HIS
75	o9	19	GLN

5.3.3 RNA (i)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	449 (25%)	63 (3%)
1	6	1794/1800 (99%)	430 (23%)	59 (3%)
36	1	3145/3396 (92%)	609 (19%)	99 (3%)
36	5	3145/3396 (92%)	613 (19%)	101 (3%)
37	3	120/121 (99%)	17 (14%)	2 (1%)
37	7	120/121 (99%)	15 (12%)	1 (0%)
38	4	157/158 (99%)	35 (22%)	3 (1%)
38	8	157/158 (99%)	37 (23%)	2 (1%)
All	All	10385/10950 (94%)	2205 (21%)	330 (3%)

All (2205) 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	45	U
1	2	46	A
1	2	47	A
1	2	57	G
1	2	60	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	100	A
1	2	103	A
1	2	104	A
1	2	114	C
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U

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Mol	Chain	Res	Type
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	175	G
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	226	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	231	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U

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Mol	Chain	Res	Type
1	2	250	C
1	2	251	A
1	2	260	U
1	2	261	U
1	2	265	A
1	2	266	A
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	309	C
1	2	314	C
1	2	316	A
1	2	319	U
1	2	320	U
1	2	321	C
1	2	322	G
1	2	337	G
1	2	338	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	390	G
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	418	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A

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Mol	Chain	Res	Type
1	2	434	G
1	2	439	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	460	A
1	2	470	A
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	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	527	A
1	2	528	U
1	2	532	U
1	2	536	C
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A

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Mol	Chain	Res	Type
1	2	543	C
1	2	544	A
1	2	548	G
1	2	555	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	570	A
1	2	578	U
1	2	579	A
1	2	580	A
1	2	582	U
1	2	585	A
1	2	594	A
1	2	595	G
1	2	609	U
1	2	611	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	639	U
1	2	640	U
1	2	645	C
1	2	650	U
1	2	653	C
1	2	654	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	693	U
1	2	694	U

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Mol	Chain	Res	Type
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
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	754	A
1	2	755	A
1	2	756	A
1	2	758	U
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	778	G

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Mol	Chain	Res	Type
1	2	779	U
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	789	A
1	2	794	U
1	2	795	U
1	2	811	A
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	833	U
1	2	837	G
1	2	840	U
1	2	846	G
1	2	856	A
1	2	860	U
1	2	862	A
1	2	863	A
1	2	864	U
1	2	876	G
1	2	886	U
1	2	898	A
1	2	912	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	916	U
1	2	933	A
1	2	935	U
1	2	942	G

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Mol	Chain	Res	Type
1	2	959	U
1	2	960	U
1	2	961	U
1	2	966	A
1	2	974	A
1	2	992	A
1	2	993	A
1	2	995	A
1	2	997	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1021	C
1	2	1026	A
1	2	1028	C
1	2	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	1074	G
1	2	1079	U
1	2	1080	U
1	2	1082	C
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1111	G
1	2	1138	A
1	2	1139	A
1	2	1146	G
1	2	1151	A
1	2	1155	G
1	2	1157	A
1	2	1158	C

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Mol	Chain	Res	Type
1	2	1160	A
1	2	1161	C
1	2	1167	G
1	2	1176	G
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1203	A
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G
1	2	1219	A
1	2	1226	A
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1235	C
1	2	1241	G
1	2	1242	A
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	1310	U
1	2	1314	U
1	2	1315	U
1	2	1320	U
1	2	1321	A
1	2	1337	A
1	2	1339	C
1	2	1340	U
1	2	1341	A

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Mol	Chain	Res	Type
1	2	1344	A
1	2	1345	A
1	2	1354	G
1	2	1361	U
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1370	U
1	2	1371	A
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1412	G
1	2	1413	U
1	2	1414	U
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1446	A
1	2	1448	G
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1462	G
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1477	G
1	2	1478	G
1	2	1482	C
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1499	G
1	2	1506	G
1	2	1514	U
1	2	1515	A
1	2	1516	A

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Mol	Chain	Res	Type
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	1569	A
1	2	1573	A
1	2	1574	G
1	2	1584	G
1	2	1590	G
1	2	1601	G
1	2	1616	G
1	2	1631	A
1	2	1657	U
1	2	1658	G
1	2	1663	G
1	2	1681	A
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1731	A
1	2	1751	C
1	2	1756	A
1	2	1759	C
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	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

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Mol	Chain	Res	Type
1	2	1796	C
36	1	13	A
36	1	14	U
36	1	18	G
36	1	26	A
36	1	40	A
36	1	43	A
36	1	44	U
36	1	49	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	75	G
36	1	77	A
36	1	92	G
36	1	99	A
36	1	109	A
36	1	110	G
36	1	113	C
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	142	C
36	1	156	G
36	1	157	A
36	1	163	C
36	1	166	C
36	1	169	U
36	1	170	G
36	1	173	G
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	210	U
36	1	218	G
36	1	219	A
36	1	224	C
36	1	234	G

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Mol	Chain	Res	Type
36	1	238	A
36	1	240	U
36	1	241	G
36	1	243	G
36	1	245	U
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	256	G
36	1	269	G
36	1	282	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	305	U
36	1	323	A
36	1	329	U
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	395	A
36	1	398	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	417	A
36	1	421	G
36	1	422	A
36	1	438	A
36	1	440	A
36	1	495	G
36	1	520	U
36	1	521	A
36	1	535	G
36	1	544	C
36	1	546	C
36	1	547	G

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Mol	Chain	Res	Type
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	578	A
36	1	579	G
36	1	588	G
36	1	589	A
36	1	592	A
36	1	604	G
36	1	609	G
36	1	611	A
36	1	620	U
36	1	621	A
36	1	622	A
36	1	636	C
36	1	637	C
36	1	638	C
36	1	649	A
36	1	654	C
36	1	656	A
36	1	660	A
36	1	677	A
36	1	681	U
36	1	691	A
36	1	705	A
36	1	708	G
36	1	712	G
36	1	715	A
36	1	716	A
36	1	763	G
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	781	G
36	1	785	G
36	1	806	A

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Mol	Chain	Res	Type
36	1	817	A
36	1	830	A
36	1	849	C
36	1	861	C
36	1	870	G
36	1	874	U
36	1	879	U
36	1	883	A
36	1	889	U
36	1	890	C
36	1	896	A
36	1	897	U
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	924	G
36	1	937	G
36	1	943	U
36	1	944	C
36	1	959	C
36	1	960	U
36	1	961	C
36	1	962	A
36	1	966	U
36	1	974	G
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	994	G
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1013	G
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1024	G

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Mol	Chain	Res	Type
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1064	A
36	1	1065	A
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	1093	A
36	1	1094	U
36	1	1095	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1121	U
36	1	1131	G
36	1	1153	A
36	1	1159	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1191	U
36	1	1192	C
36	1	1201	C
36	1	1202	A
36	1	1209	G
36	1	1217	A
36	1	1218	U
36	1	1222	G
36	1	1225	A
36	1	1226	G
36	1	1227	C
36	1	1232	C
36	1	1233	G

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Mol	Chain	Res	Type
36	1	1235	U
36	1	1236	G
36	1	1237	G
36	1	1239	C
36	1	1241	U
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
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	1287	A
36	1	1292	C
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1329	U
36	1	1330	A
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	1380	G

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Mol	Chain	Res	Type
36	1	1386	A
36	1	1399	A
36	1	1400	G
36	1	1419	A
36	1	1422	G
36	1	1434	G
36	1	1437	C
36	1	1445	U
36	1	1446	A
36	1	1449	A
36	1	1450	G
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1489	A
36	1	1496	C
36	1	1503	A
36	1	1508	C
36	1	1526	U
36	1	1527	C
36	1	1555	U
36	1	1556	C
36	1	1557	A
36	1	1560	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1576	G
36	1	1578	C
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	1605	A

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Mol	Chain	Res	Type
36	1	1607	U
36	1	1608	C
36	1	1612	A
36	1	1620	U
36	1	1629	U
36	1	1633	C
36	1	1643	A
36	1	1657	C
36	1	1658	G
36	1	1683	A
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1725	C
36	1	1741	A
36	1	1742	U
36	1	1750	A
36	1	1751	G
36	1	1760	A
36	1	1761	C
36	1	1762	C
36	1	1764	U
36	1	1765	U
36	1	1767	C
36	1	1768	U
36	1	1770	G
36	1	1780	G
36	1	1781	C
36	1	1797	A
36	1	1809	A
36	1	1810	A
36	1	1812	G
36	1	1814	A
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1835	A
36	1	1839	A
36	1	1841	A
36	1	1842	A

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Mol	Chain	Res	Type
36	1	1846	C
36	1	1849	C
36	1	1855	U
36	1	1879	A
36	1	1880	U
36	1	1901	A
36	1	1906	G
36	1	1951	C
36	1	1952	G
36	1	1954	G
36	1	2094	C
36	1	2101	C
36	1	2102	U
36	1	2106	A
36	1	2107	A
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2121	G
36	1	2122	G
36	1	2125	A
36	1	2130	G
36	1	2131	A
36	1	2140	U
36	1	2158	A
36	1	2169	G
36	1	2201	G
36	1	2205	U
36	1	2208	A
36	1	2210	G
36	1	2223	A
36	1	2228	A
36	1	2244	A
36	1	2249	G
36	1	2250	G
36	1	2255	A
36	1	2256	A
36	1	2272	G
36	1	2273	G
36	1	2279	A
36	1	2281	A
36	1	2282	U

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Mol	Chain	Res	Type
36	1	2284	C
36	1	2288	G
36	1	2298	U
36	1	2299	A
36	1	2307	G
36	1	2308	C
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2319	U
36	1	2334	U
36	1	2336	U
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	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2405	C
36	1	2411	U
36	1	2412	G
36	1	2418	G
36	1	2419	A
36	1	2435	G
36	1	2437	G
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2513	U
36	1	2514	U
36	1	2515	A
36	1	2519	A
36	1	2522	G
36	1	2523	A
36	1	2529	A

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Mol	Chain	Res	Type
36	1	2532	U
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2544	U
36	1	2547	A
36	1	2548	C
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2561	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2585	G
36	1	2586	G
36	1	2591	A
36	1	2593	A
36	1	2594	C
36	1	2600	C
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2617	U
36	1	2637	A
36	1	2652	U
36	1	2656	A
36	1	2672	G
36	1	2674	A
36	1	2677	G
36	1	2681	U
36	1	2689	A
36	1	2690	G
36	1	2691	A

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Mol	Chain	Res	Type
36	1	2694	A
36	1	2709	C
36	1	2712	U
36	1	2714	G
36	1	2728	G
36	1	2729	U
36	1	2752	U
36	1	2753	G
36	1	2762	A
36	1	2771	U
36	1	2772	C
36	1	2777	G
36	1	2778	G
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2803	A
36	1	2810	C
36	1	2817	A
36	1	2818	U
36	1	2819	A
36	1	2830	G
36	1	2838	A
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2849	C
36	1	2860	U
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2873	U
36	1	2874	G
36	1	2875	U
36	1	2887	A
36	1	2896	A
36	1	2897	A
36	1	2898	G
36	1	2899	C
36	1	2900	A

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Mol	Chain	Res	Type
36	1	2902	A
36	1	2914	G
36	1	2923	U
36	1	2935	U
36	1	2936	A
36	1	2942	C
36	1	2945	G
36	1	2947	G
36	1	2957	G
36	1	2971	A
36	1	2974	U
36	1	2980	U
36	1	2983	C
36	1	2990	G
36	1	2996	U
36	1	2997	G
36	1	3012	A
36	1	3049	A
36	1	3056	U
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3086	A
36	1	3092	C
36	1	3113	A
36	1	3122	A
36	1	3128	G
36	1	3130	A
36	1	3131	U
36	1	3134	A
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3158	G
36	1	3164	C

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Mol	Chain	Res	Type
36	1	3165	A
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3180	A
36	1	3181	C
36	1	3187	A
36	1	3196	U
36	1	3198	U
36	1	3207	U
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3229	G
36	1	3235	C
36	1	3243	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3270	U
36	1	3272	C
36	1	3273	A
36	1	3276	G
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3288	G
36	1	3289	G
36	1	3292	A
36	1	3294	A
36	1	3295	A
36	1	3304	U
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U

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Mol	Chain	Res	Type
36	1	3320	A
36	1	3330	A
36	1	3335	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	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	3377	G
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
37	3	7	G
37	3	13	A
37	3	14	U
37	3	22	A
37	3	42	A
37	3	50	U
37	3	51	A
37	3	54	U
37	3	59	U
37	3	65	G
37	3	74	C
37	3	76	A
37	3	95	A
37	3	102	A
37	3	110	G
37	3	112	G
37	3	121	U
38	4	2	A
38	4	11	C
38	4	22	U

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Mol	Chain	Res	Type
38	4	34	U
38	4	35	C
38	4	52	A
38	4	53	A
38	4	59	A
38	4	62	C
38	4	63	G
38	4	79	A
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	96	A
38	4	104	A
38	4	105	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	125	U
38	4	126	A
38	4	128	U
38	4	138	A
38	4	142	C
38	4	152	G
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	13	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	42	G
1	6	44	U
1	6	46	A

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Mol	Chain	Res	Type
1	6	47	A
1	6	49	C
1	6	50	C
1	6	57	G
1	6	60	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	78	A
1	6	100	A
1	6	104	A
1	6	114	C
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	144	U
1	6	145	A
1	6	146	U
1	6	153	G
1	6	158	U
1	6	159	U
1	6	166	C
1	6	178	U
1	6	179	A
1	6	185	U
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	195	G
1	6	197	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U

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Mol	Chain	Res	Type
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	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	261	U
1	6	262	U
1	6	265	A
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	299	A
1	6	308	C
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	370	A
1	6	393	C
1	6	400	A
1	6	401	A
1	6	402	C

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Mol	Chain	Res	Type
1	6	404	G
1	6	416	A
1	6	417	A
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	439	U
1	6	444	C
1	6	445	A
1	6	448	C
1	6	454	U
1	6	469	C
1	6	470	A
1	6	475	A
1	6	477	A
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	495	C
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	507	U
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	514	G
1	6	519	C

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Mol	Chain	Res	Type
1	6	527	A
1	6	534	A
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	555	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	565	C
1	6	570	A
1	6	574	G
1	6	579	A
1	6	580	A
1	6	582	U
1	6	594	A
1	6	595	G
1	6	606	A
1	6	609	U
1	6	610	G
1	6	617	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	630	A
1	6	637	C
1	6	639	U
1	6	640	U
1	6	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

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Mol	Chain	Res	Type
1	6	668	C
1	6	670	U
1	6	676	G
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	687	G
1	6	689	G
1	6	691	C
1	6	696	C
1	6	710	U
1	6	711	U
1	6	714	G
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	723	G
1	6	730	G
1	6	733	A
1	6	742	U
1	6	753	A
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	789	A
1	6	793	A
1	6	794	U
1	6	795	U
1	6	806	A
1	6	807	A

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Mol	Chain	Res	Type
1	6	811	A
1	6	812	A
1	6	815	G
1	6	821	U
1	6	823	G
1	6	825	U
1	6	826	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	856	A
1	6	863	A
1	6	864	U
1	6	873	U
1	6	898	A
1	6	906	A
1	6	910	C
1	6	912	U
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	959	U
1	6	960	U
1	6	966	A
1	6	969	C
1	6	970	A
1	6	971	A
1	6	991	G
1	6	992	A
1	6	993	A
1	6	996	U
1	6	997	G
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1026	A

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Mol	Chain	Res	Type
1	6	1028	C
1	6	1039	A
1	6	1040	G
1	6	1046	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	1075	C
1	6	1082	C
1	6	1091	A
1	6	1092	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1101	G
1	6	1109	G
1	6	1138	A
1	6	1146	G
1	6	1150	G
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1162	C
1	6	1167	G
1	6	1185	U
1	6	1194	A
1	6	1196	A
1	6	1197	C
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1203	A
1	6	1208	A
1	6	1212	G
1	6	1217	A
1	6	1218	G

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Mol	Chain	Res	Type
1	6	1219	A
1	6	1220	C
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1231	U
1	6	1239	U
1	6	1241	G
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1259	U
1	6	1284	C
1	6	1285	U
1	6	1286	U
1	6	1288	G
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1330	G
1	6	1338	C
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	1361	U
1	6	1363	U
1	6	1364	G
1	6	1370	U
1	6	1371	A
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A

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Mol	Chain	Res	Type
1	6	1402	G
1	6	1412	G
1	6	1413	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1433	G
1	6	1445	G
1	6	1446	A
1	6	1448	G
1	6	1458	G
1	6	1459	C
1	6	1461	C
1	6	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	1494	C
1	6	1496	U
1	6	1497	U
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	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	1569	A
1	6	1573	A

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Mol	Chain	Res	Type
1	6	1574	G
1	6	1575	G
1	6	1577	A
1	6	1584	G
1	6	1601	G
1	6	1616	G
1	6	1621	U
1	6	1634	C
1	6	1639	C
1	6	1657	U
1	6	1658	G
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	1703	C
1	6	1710	U
1	6	1712	A
1	6	1716	C
1	6	1717	G
1	6	1731	A
1	6	1742	U
1	6	1755	A
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	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

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Mol	Chain	Res	Type
36	5	11	A
36	5	15	C
36	5	26	A
36	5	38	U
36	5	40	A
36	5	49	A
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	76	G
36	5	99	A
36	5	110	G
36	5	113	C
36	5	116	A
36	5	121	A
36	5	122	A
36	5	131	C
36	5	133	U
36	5	134	U
36	5	136	G
36	5	139	G
36	5	150	A
36	5	156	G
36	5	157	A
36	5	165	A
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	184	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	193	C
36	5	204	A
36	5	210	U
36	5	218	G
36	5	219	A
36	5	221	A

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Mol	Chain	Res	Type
36	5	236	G
36	5	237	G
36	5	238	A
36	5	239	G
36	5	240	U
36	5	244	G
36	5	247	C
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	259	C
36	5	269	G
36	5	282	G
36	5	283	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	298	U
36	5	311	C
36	5	322	U
36	5	323	A
36	5	329	U
36	5	349	A
36	5	350	C
36	5	352	A
36	5	376	G
36	5	397	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	421	G
36	5	422	A
36	5	436	A
36	5	437	G
36	5	438	A
36	5	439	C

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Mol	Chain	Res	Type
36	5	440	A
36	5	441	U
36	5	442	G
36	5	443	G
36	5	492	U
36	5	495	G
36	5	520	U
36	5	521	A
36	5	535	G
36	5	542	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	551	A
36	5	555	U
36	5	557	A
36	5	559	A
36	5	560	G
36	5	578	A
36	5	579	G
36	5	592	A
36	5	600	G
36	5	604	G
36	5	609	G
36	5	611	A
36	5	619	A
36	5	620	U
36	5	621	A
36	5	630	A
36	5	636	C
36	5	649	A
36	5	660	A
36	5	677	A
36	5	681	U
36	5	683	U
36	5	684	G
36	5	705	A
36	5	708	G
36	5	712	G
36	5	715	A
36	5	716	A
36	5	719	U

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Mol	Chain	Res	Type
36	5	720	A
36	5	725	G
36	5	726	G
36	5	735	A
36	5	736	A
36	5	758	C
36	5	766	U
36	5	767	U
36	5	768	C
36	5	774	G
36	5	776	U
36	5	777	U
36	5	781	G
36	5	785	G
36	5	786	A
36	5	806	A
36	5	817	A
36	5	830	A
36	5	861	C
36	5	874	U
36	5	876	A
36	5	879	U
36	5	891	G
36	5	895	A
36	5	896	A
36	5	897	U
36	5	907	G
36	5	908	G
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	923	C
36	5	937	G
36	5	944	C
36	5	959	C
36	5	960	U
36	5	963	G
36	5	974	G
36	5	979	U
36	5	980	A
36	5	983	A

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Mol	Chain	Res	Type
36	5	994	G
36	5	1001	G
36	5	1002	A
36	5	1003	A
36	5	1010	G
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1028	U
36	5	1029	G
36	5	1032	C
36	5	1034	U
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1071	U
36	5	1072	G
36	5	1075	A
36	5	1081	U
36	5	1082	U
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1117	G
36	5	1131	G
36	5	1144	U
36	5	1153	A
36	5	1159	A
36	5	1166	G
36	5	1180	A

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Mol	Chain	Res	Type
36	5	1181	U
36	5	1182	A
36	5	1192	C
36	5	1193	A
36	5	1196	C
36	5	1201	C
36	5	1202	A
36	5	1222	G
36	5	1232	C
36	5	1235	U
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	1245	A
36	5	1246	G
36	5	1254	C
36	5	1258	U
36	5	1259	A
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1285	G
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1312	C
36	5	1314	C
36	5	1329	U
36	5	1330	A
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

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Mol	Chain	Res	Type
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1428	A
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1481	A
36	5	1482	A
36	5	1490	A
36	5	1500	G
36	5	1502	C
36	5	1503	A
36	5	1508	C
36	5	1522	U
36	5	1536	G
36	5	1553	U
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1564	U
36	5	1565	G
36	5	1566	A
36	5	1567	U
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C

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Mol	Chain	Res	Type
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1593	A
36	5	1605	A
36	5	1620	U
36	5	1629	U
36	5	1638	A
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1655	G
36	5	1657	C
36	5	1658	G
36	5	1683	A
36	5	1685	C
36	5	1686	U
36	5	1687	U
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1725	C
36	5	1741	A
36	5	1750	A
36	5	1751	G
36	5	1762	C
36	5	1765	U
36	5	1766	G
36	5	1770	G
36	5	1779	C
36	5	1780	G
36	5	1797	A
36	5	1810	A
36	5	1814	A
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1821	U
36	5	1839	A

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Mol	Chain	Res	Type
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	1876	U
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1893	A
36	5	1906	G
36	5	1935	G
36	5	1940	G
36	5	1952	G
36	5	1953	G
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2112	U
36	5	2113	A
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2158	A
36	5	2169	G
36	5	2170	U
36	5	2179	C
36	5	2201	G
36	5	2205	U
36	5	2206	G
36	5	2210	G
36	5	2223	A
36	5	2228	A
36	5	2244	A
36	5	2250	G
36	5	2251	G
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2258	U

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Mol	Chain	Res	Type
36	5	2269	U
36	5	2273	G
36	5	2279	A
36	5	2281	A
36	5	2288	G
36	5	2306	C
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2360	C
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2393	G
36	5	2394	G
36	5	2396	G
36	5	2397	A
36	5	2398	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	2419	A
36	5	2435	G
36	5	2436	U
36	5	2438	A
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

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Mol	Chain	Res	Type
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2512	C
36	5	2514	U
36	5	2515	A
36	5	2518	C
36	5	2523	A
36	5	2526	C
36	5	2530	G
36	5	2531	C
36	5	2532	U
36	5	2534	G
36	5	2536	A
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2549	G
36	5	2550	U
36	5	2552	C
36	5	2555	G
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2589	G
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2610	G
36	5	2614	G
36	5	2622	C
36	5	2637	A
36	5	2639	G

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Mol	Chain	Res	Type
36	5	2652	U
36	5	2656	A
36	5	2674	A
36	5	2677	G
36	5	2678	A
36	5	2681	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
36	5	2728	G
36	5	2729	U
36	5	2752	U
36	5	2753	G
36	5	2755	C
36	5	2762	A
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2796	G
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2810	C
36	5	2817	A
36	5	2818	U
36	5	2819	A
36	5	2822	U
36	5	2843	U
36	5	2845	A
36	5	2853	A
36	5	2871	G
36	5	2872	A
36	5	2874	G
36	5	2875	U
36	5	2887	A
36	5	2896	A

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Mol	Chain	Res	Type
36	5	2897	A
36	5	2899	C
36	5	2902	A
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2945	G
36	5	2947	G
36	5	2971	A
36	5	2972	G
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2992	U
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3033	A
36	5	3049	A
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3080	G
36	5	3084	C
36	5	3086	A
36	5	3092	C
36	5	3119	U
36	5	3122	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	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

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Mol	Chain	Res	Type
36	5	3165	A
36	5	3166	C
36	5	3167	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	3179	U
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3206	C
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3227	A
36	5	3228	C
36	5	3229	G
36	5	3233	C
36	5	3239	G
36	5	3243	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3265	C
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

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Mol	Chain	Res	Type
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3316	A
36	5	3317	U
36	5	3318	G
36	5	3319	U
36	5	3320	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3349	C
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3356	G
36	5	3358	U
36	5	3369	G
36	5	3378	C
36	5	3381	U
36	5	3382	U
36	5	3389	U
36	5	3390	G
36	5	3393	U
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	33	U
37	7	54	U
37	7	55	A
37	7	60	G
37	7	65	G
37	7	73	C
37	7	76	A
37	7	91	G
37	7	93	C
37	7	102	A
37	7	103	A
37	7	104	A
37	7	112	G
38	8	25	G
38	8	34	U

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Mol	Chain	Res	Type
38	8	35	C
38	8	49	G
38	8	51	G
38	8	52	A
38	8	53	A
38	8	58	G
38	8	59	A
38	8	62	C
38	8	63	G
38	8	79	A
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	86	U
38	8	87	G
38	8	90	U
38	8	95	G
38	8	96	A
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	122	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	138	A
38	8	152	G
38	8	155	A
38	8	156	U
38	8	157	U
38	8	158	U

All (330) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A

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Mol	Chain	Res	Type
1	2	73	U
1	2	74	U
1	2	93	A
1	2	103	A
1	2	130	C
1	2	131	C
1	2	132	U
1	2	139	C
1	2	144	U
1	2	158	U
1	2	218	A
1	2	240	U
1	2	278	U
1	2	280	U
1	2	352	A
1	2	400	A
1	2	417	A
1	2	468	A
1	2	497	G
1	2	498	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	510	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	782	U
1	2	794	U
1	2	811	A
1	2	829	A
1	2	1051	G
1	2	1058	U
1	2	1081	A
1	2	1137	A
1	2	1157	A

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Mol	Chain	Res	Type
1	2	1196	A
1	2	1207	C
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1339	C
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1489	U
1	2	1490	C
1	2	1568	C
1	2	1572	G
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	99	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	397	A
36	1	398	A
36	1	547	G
36	1	588	G
36	1	594	U
36	1	620	U
36	1	637	C
36	1	647	A
36	1	715	A
36	1	719	U
36	1	763	G
36	1	764	U
36	1	816	A
36	1	873	C
36	1	896	A

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Mol	Chain	Res	Type
36	1	916	G
36	1	979	U
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1196	C
36	1	1273	A
36	1	1307	G
36	1	1317	A
36	1	1329	U
36	1	1352	A
36	1	1355	A
36	1	1481	A
36	1	1484	U
36	1	1507	G
36	1	1514	G
36	1	1554	U
36	1	1562	C
36	1	1607	U
36	1	1643	A
36	1	1716	U
36	1	1751	G
36	1	1815	U
36	1	1816	A
36	1	1820	U
36	1	1841	A
36	1	1849	C
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2227	C
36	1	2249	G
36	1	2281	A
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2385	G
36	1	2403	G
36	1	2418	G

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Mol	Chain	Res	Type
36	1	2513	U
36	1	2522	G
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2677	G
36	1	2689	A
36	1	2728	G
36	1	2752	U
36	1	2801	A
36	1	2817	A
36	1	2818	U
36	1	2867	C
36	1	2896	A
36	1	2996	U
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3157	U
36	1	3195	U
36	1	3217	C
36	1	3218	A
36	1	3228	C
36	1	3242	G
36	1	3269	U
36	1	3275	U
36	1	3316	A
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
37	3	13	A
37	3	49	G
38	4	85	G
38	4	111	A
38	4	125	U
1	6	1	U
1	6	25	C
1	6	66	U
1	6	103	A

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Mol	Chain	Res	Type
1	6	114	C
1	6	136	C
1	6	139	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	249	U
1	6	272	U
1	6	277	U
1	6	352	A
1	6	400	A
1	6	417	A
1	6	434	G
1	6	468	A
1	6	512	A
1	6	541	A
1	6	542	A
1	6	557	G
1	6	558	U
1	6	651	G
1	6	667	U
1	6	678	A
1	6	717	C
1	6	755	A
1	6	794	U
1	6	815	G
1	6	829	A
1	6	834	G
1	6	1004	U
1	6	1051	G
1	6	1058	U
1	6	1081	A
1	6	1097	U
1	6	1098	U
1	6	1137	A
1	6	1196	A
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1481	C

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Mol	Chain	Res	Type
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1535	U
1	6	1568	C
1	6	1572	G
1	6	1573	A
1	6	1584	G
1	6	1615	C
1	6	1620	C
1	6	1657	U
1	6	1696	G
1	6	1698	G
36	5	43	A
36	5	65	A
36	5	110	G
36	5	183	G
36	5	210	U
36	5	217	U
36	5	221	A
36	5	238	A
36	5	282	G
36	5	397	A
36	5	588	G
36	5	594	U
36	5	647	A
36	5	715	A
36	5	719	U
36	5	726	G
36	5	735	A
36	5	765	C
36	5	786	A
36	5	816	A
36	5	873	C
36	5	895	A
36	5	896	A
36	5	916	G
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G

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Mol	Chain	Res	Type
36	5	1181	U
36	5	1192	C
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1317	A
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1434	G
36	5	1481	A
36	5	1507	G
36	5	1514	G
36	5	1554	U
36	5	1560	G
36	5	1589	A
36	5	1716	U
36	5	1725	C
36	5	1815	U
36	5	1816	A
36	5	1841	A
36	5	1846	C
36	5	1849	C
36	5	2101	C
36	5	2112	U
36	5	2116	G
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2385	G
36	5	2398	A
36	5	2440	G
36	5	2507	C
36	5	2513	U

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Mol	Chain	Res	Type
36	5	2531	C
36	5	2539	C
36	5	2584	G
36	5	2585	G
36	5	2593	A
36	5	2704	A
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	3049	A
36	5	3056	U
36	5	3078	U
36	5	3121	U
36	5	3154	C
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3242	G
36	5	3259	U
36	5	3275	U
36	5	3289	G
36	5	3317	U
36	5	3340	G
36	5	3341	U
36	5	3357	U
37	7	49	G
38	8	59	A
38	8	111	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2559 ligands modelled in this entry, 1424 are monoatomic - leaving 1135 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4181	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	1	4213	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	7	217	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	7	216	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	L6	202	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	1	4116	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	m1	203	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	C1	201	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	l3	404	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	1	4210	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	6	2201	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	1	4204	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	2	2180	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	O2	201	-	0,6,6	-	-	-		
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	7	227	-	0,6,6	-	-	-		
86	OHX	5	4179	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	l3	402	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	3	225	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	O7	103	-	0,6,6	-	-	-		
86	OHX	5	4248	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	1	4176	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4194	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	1	4208	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	1	4150	-	0,6,6	-	-	-		
86	OHX	O3	202	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	c1	202	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	5	4246	-	0,6,6	-	-	-		
86	OHX	8	215	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	3	226	-	0,6,6	-	-	-		
86	OHX	m5	302	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	5	3899	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	2	2179	-	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	m7	206	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	5	4232	86	0,6,6	-	-	-		
86	OHX	4	222	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4191	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	6	2202	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	M6	202	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	m0	301	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	1	4211	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	5	4218	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
88	3H3	5	4251	-	33,34,34	0.97	2 (6%)	34,45,45	1.42	4 (11%)
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		
86	OHX	l5	306	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	5	4226	-	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
88	3H3	1	4216	-	33,34,34	1.01	3 (9%)	34,45,45	1.65	7 (20%)
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	1	4161	-	0,6,6	-	-	-		
86	OHX	l9	600	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	2	2032	86	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	m6	202	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	l4	402	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	Q2	503	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	5	4216	-	0,6,6	-	-	-		
86	OHX	5	4230	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	1	4197	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	5	4197	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	S8	302	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	O7	104	-	0,6,6	-	-	-		
86	OHX	6	2187	-	0,6,6	-	-	-		
86	OHX	1	4170	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	1	4168	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	8	214	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	2	2181	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	5	3942	86	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	5	4249	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	C3	202	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	1	4194	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	1	4215	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	1	4130	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	M5	304	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	5	3943	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	l5	304	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		
86	OHX	2	2168	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	5	4223	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	5	4238	-	0,6,6	-	-	-		
86	OHX	m4	202	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	l3	403	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	6	2204	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	l4	403	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	5	4178	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	1	4179	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	l5	305	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	2	2158	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	n3	203	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	7	225	-	0,6,6	-	-	-		
86	OHX	5	4228	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	6	2203	-	0,6,6	-	-	-		
86	OHX	1	4200	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	M7	208	-	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	5	4233	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	o4	203	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	n9	3803	-	0,6,6	-	-	-		
86	OHX	1	4188	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	4250	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	M9	202	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	o2	201	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	6	2190	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	o3	203	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	1	4214	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	M7	207	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	1	4117	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	1	4209	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	2	2178	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	2	2147	86	0,6,6	-	-	-		
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	3	224	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	L4	404	-	0,6,6	-	-	-		
86	OHX	O9	101	-	0,6,6	-	-	-		
86	OHX	5	3898	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	5	4195	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	5	4175	-	0,6,6	-	-	-		
86	OHX	1	4212	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	1	4119	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	3H3	5	4251	-	-	7/39/51/51	0/1/2/2
88	3H3	1	4216	-	-	7/39/51/51	0/1/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4216	3H3	C3-C2	3.57	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	5	4251	3H3	C14-C16	3.36	1.56	1.53
88	5	4251	3H3	C15-C14	-2.77	1.50	1.54
88	1	4216	3H3	C15-C14	-2.77	1.50	1.54
88	1	4216	3H3	C14-C13	2.16	1.54	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	5	4251	3H3	C15-C14-C16	4.81	116.50	109.19
88	1	4216	3H3	C15-C14-C16	4.77	116.44	109.19
88	1	4216	3H3	C1-C11-C12	4.38	122.64	113.89
88	5	4251	3H3	C1-C11-C12	3.40	120.67	113.89
88	1	4216	3H3	C-C1-C2	-3.30	102.02	109.99
88	1	4216	3H3	O1-C11-C12	-2.71	103.55	109.60
88	1	4216	3H3	C6-C7-C8	-2.27	106.97	112.92
88	5	4251	3H3	O2-C16-C17	2.21	124.38	121.41
88	1	4216	3H3	O2-C16-C17	2.15	124.30	121.41
88	5	4251	3H3	C6-C7-C8	-2.14	107.32	112.92
88	1	4216	3H3	C8-C9-C10	-2.13	117.49	122.92

There are no chirality outliers.

All (14) torsion outliers are listed below:

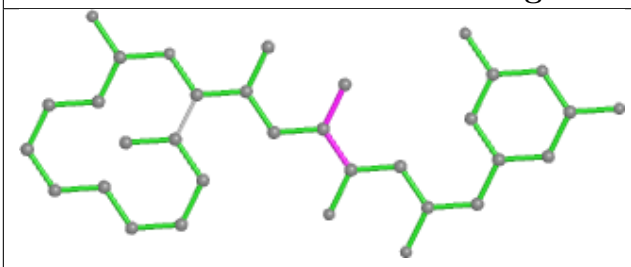
Mol	Chain	Res	Type	Atoms
88	1	4216	3H3	C2-C1-C11-O1
88	1	4216	3H3	C2-C1-C11-C12
88	1	4216	3H3	C-C1-C11-O1
88	1	4216	3H3	C-C1-C11-C12
88	1	4216	3H3	C12-C13-C14-C16
88	5	4251	3H3	C12-C11-O1-C10
88	5	4251	3H3	C1-C11-O1-C10
88	5	4251	3H3	C1-C2-C3-C4
88	5	4251	3H3	C9-C10-O1-C11
88	1	4216	3H3	C2-C3-C4-C5
88	5	4251	3H3	O-C10-O1-C11
88	5	4251	3H3	C6-C7-C8-C9
88	5	4251	3H3	C2-C3-C4-C5
88	1	4216	3H3	C6-C7-C8-C9

There are no ring outliers.

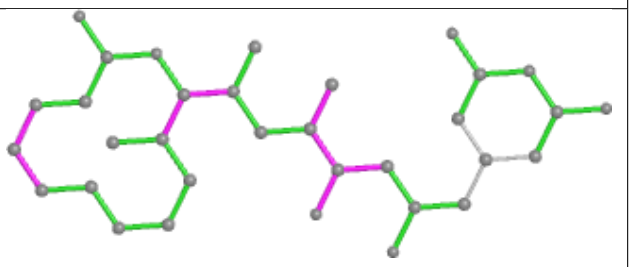
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

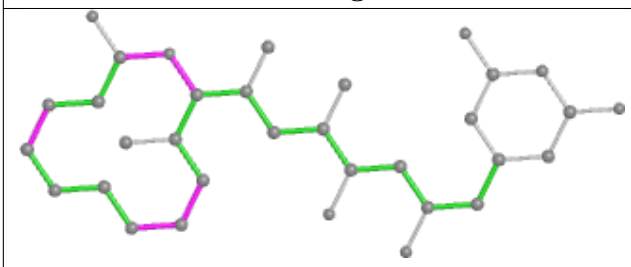
Ligand 3H3 5 4251



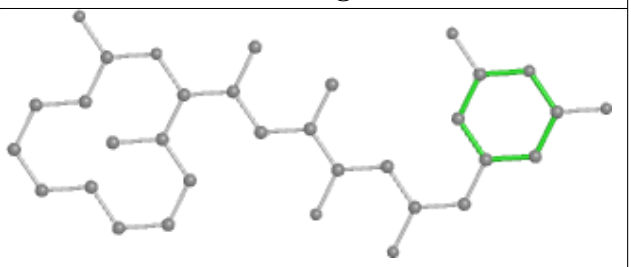
Bond lengths



Bond angles

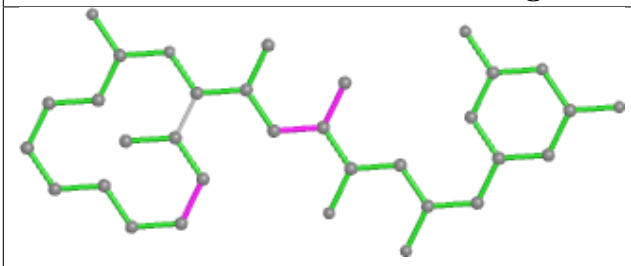


Torsions

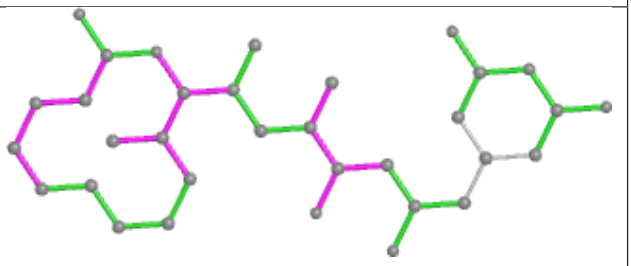


Rings

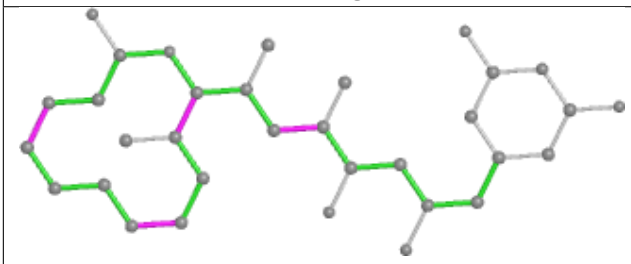
Ligand 3H3 1 4216



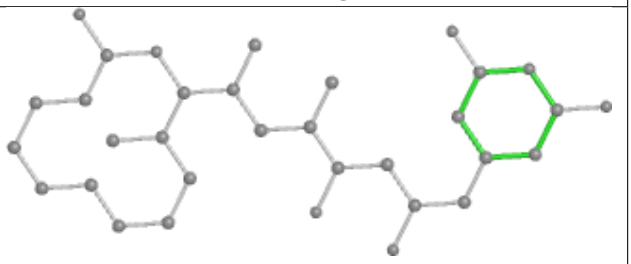
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	SR	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SR	161:LYS	C	162:ALA	N	0.66
1	SR	160:GLU	C	161:LYS	N	0.45

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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