Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 01:35 pm GMT

PDB ID	:	4U4U
Title	:	Crystal structure of Lycorine bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-24
Resolution	:	3.00 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:

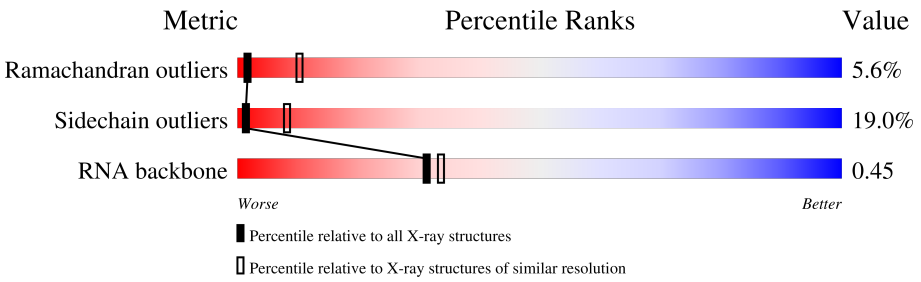
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et 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 3.00 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	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	66% 27% • •
1	6	1800	65% 28% 6%
2	S0	251	62% 19% • 18%
2	s0	251	61% 18% • 18%
3	S1	254	61% 21% • 16%
3	s1	254	70% 15% 15%
4	S2	253	69% 16% • 14%
4	s2	253	64% 21% • 14%

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Mol	Chain	Length	Quality of chain
5	S3	239	74% 18% 7%
5	s3	239	75% 16% 7%
6	S4	260	82% 16%
6	s4	260	80% 19%
7	S5	224	73% 17% 8%
7	s5	224	68% 22% 8%
8	S6	236	74% 21%
8	s6	236	74% 17% 8%
9	S7	189	75% 20%
9	s7	189	78% 17%
10	S8	200	80% 14% 6%
10	s8	200	80% 13% 6%
11	S9	196	72% 21% 6%
11	s9	196	76% 16% 6%
12	C0	105	71% 19% 9%
12	c0	105	70% 18% 9%
13	C1	155	79% 20%
13	c1	155	74% 19% 6%
14	C2	142	55% 30% 13%
14	c2	142	59% 25% 13%
15	C3	150	79% 19%
15	c3	150	78% 21%
16	C4	136	71% 18% 7%
16	c4	136	74% 18% 6%
17	C5	141	70% 16% 12%

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Mol	Chain	Length	Quality of chain
17	c5	141	72% 20%
18	C6	142	78% 20%
18	c6	142	77% 21%
19	C7	136	66% 18% 12%
19	c7	136	71% 13% 14%
20	C8	145	72% 24%
20	c8	145	77% 21%
21	C9	143	81% 19%
21	c9	143	81% 17%
22	D0	120	68% 22% 11%
22	d0	120	63% 27% 8%
23	D1	87	76% 24%
23	d1	87	75% 24%
24	D2	129	86% 12%
24	d2	129	86% 13%
25	D3	144	81% 17%
25	d3	144	86% 13%
26	D4	134	81% 18%
26	d4	134	81% 18%
27	D5	107	40% 23% 35%
27	d5	107	50% 15% 36%
28	D6	97	72% 20% 8%
28	d6	97	80% 20%
29	D7	81	86% 14%
29	d7	81	80% 19%

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Mol	Chain	Length	Quality of chain
30	D8	66	73% 21% 5%
30	d8	66	73% 21% 5%
31	D9	55	78% 16%
31	d9	55	71% 25%
32	E0	60	82% 17%
33	E1	76	53% 38% 7%
33	e1	76	59% 34% 7%
34	SR	318	85% 14%
34	sR	318	88% 12%
35	SM	273	44% 13% 42%
36	1	3396	52% 34% 7% 7%
36	5	3396	49% 37% 7% 7%
37	3	121	67% 31%
37	7	121	56% 37% 7%
38	4	158	52% 41% 7%
38	8	158	64% 31% 5%
39	L2	253	80% 18%
39	l2	253	79% 19%
40	L3	386	81% 18%
40	l3	386	79% 20%
41	L4	361	78% 21%
41	l4	361	78% 20%
42	L5	296	78% 20%
42	l5	296	81% 17%
43	L6	175	74% 14% 11%

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Mol	Chain	Length	Quality of chain
43	l6	175	74% 15% • 10%
44	L7	243	79% 10% • 9%
44	l7	243	77% 13% • 8%
45	L8	255	74% 17% 9%
45	l8	255	72% 17% • 9%
46	L9	191	77% 23% •
46	l9	191	81% 18% •
47	M0	220	76% 18% • •
47	m0	220	74% 22% • •
48	M1	173	73% 20% 5% •
48	m1	173	77% 18% • •
49	M3	198	80% 17% • •
49	m3	198	78% 18% • •
50	M4	137	80% 18% ••
50	m4	137	84% 15% •
51	M5	203	78% 22%
51	m5	203	85% 14% •
52	M6	198	83% 15% • •
52	m6	198	79% 19% •••
53	M7	183	79% 20% •
53	m7	183	72% 13% 15%
54	M8	185	85% 14% •
54	m8	185	79% 19% •
55	M9	188	88% 12%
55	m9	188	82% 16% •

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Mol	Chain	Length	Quality of chain
56	N0	172	77% 20% •
56	n0	172	80% 19% •
57	N1	159	81% 17% •
57	n1	159	80% 19% •
58	N2	120	69% 13% • 17%
58	n2	120	68% 12% • 18%
59	N3	136	86% 14%
59	n3	136	91% 8% •
60	N4	155	54% 9% • 37%
60	n4	155	71% 15% • 13%
61	N5	141	70% 15% • 14%
61	n5	141	66% 17% • 15%
62	N6	126	75% 25% •
62	n6	126	75% 25% •
63	N7	135	81% 19% •
63	n7	135	80% 16% •
64	N8	148	79% 18% •
64	n8	148	80% 18% •
65	N9	58	78% 17% 5%
65	n9	58	79% 19% •
66	O0	104	80% 12% • 7%
66	o0	104	81% 13% • •
67	O1	112	76% 19% • •
67	o1	112	74% 22% • •
68	O2	129	79% 18% • •

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Mol	Chain	Length	Quality of chain
68	o2	129	78% 18%
69	O3	106	89% 10%
69	o3	106	84% 16%
70	O4	119	76% 16% 6%
70	o4	119	73% 20% 6%
71	O5	119	79% 20%
71	o5	119	80% 19%
72	O6	99	81% 17%
72	o6	99	72% 25%
73	O7	87	84% 15%
73	o7	87	84% 15%
74	O8	77	77% 23%
74	o8	77	78% 21%
75	O9	50	86% 14%
75	o9	50	82% 16%
76	Q0	52	75% 23%
76	q0	52	75% 23%
77	Q1	25	68% 28%
77	q1	25	64% 28% 8%
78	Q2	105	73% 24%
78	q2	105	83% 16%
79	Q3	91	81% 16%
79	q3	91	90% 10%
80	e0	62	74% 24%
81	sM	273	29% 8% 62%

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Mol	Chain	Length	Quality of chain
82	m2	160	94% 6%
83	p0	311	37% 9% 54%
84	p1	47	100%
85	p2	46	100%

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 411211 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	892	562	156	172	2	0	0	0
14	c2	124	892	562	156	172	2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
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
			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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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

- 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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
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 Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
81	sM	104	681	404	140	137	0	0	0

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

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

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 84 is a protein called unknown protein chain p1.

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

- Molecule 85 is a protein called unknown protein chain p2.

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

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
86	2	123	123	123	0	0
86	S2	1	1	1	0	0
86	S8	1	1	1	0	0
86	D0	1	1	1	0	0
86	D3	1	1	1	0	0
86	D4	1	1	1	0	0
86	SM	1	1	1	0	0
86	1	477	477	477	0	0
86	3	14	14	14	0	0
86	4	21	21	21	0	0
86	L2	1	1	1	0	0
86	L3	2	2	2	0	0
86	L4	2	2	2	0	0
86	L5	2	2	2	0	0
86	L7	2	2	2	0	0
86	L8	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
86	M0	2	2	2	0	0
86	M1	1	1	1	0	0
86	M3	3	3	3	0	0
86	M5	1	1	1	0	0
86	M6	1	1	1	0	0
86	M7	6	6	6	0	0
86	M8	1	1	1	0	0
86	M9	1	1	1	0	0
86	N0	1	1	1	0	0
86	N3	3	3	3	0	0
86	N5	1	1	1	0	0
86	N8	3	3	3	0	0
86	O4	1	1	1	0	0
86	O7	1	1	1	0	0
86	O8	1	1	1	0	0
86	Q2	1	1	1	0	0
86	6	149	149	149	0	0
86	s1	1	1	1	0	0
86	s4	1	1	1	0	0
86	s8	2	2	2	0	0
86	c1	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
86	c7	1	1	1	0	0
86	d3	2	2	2	0	0
86	d4	1	1	1	0	0
86	sM	2	2	2	0	0
86	5	506	506	506	0	0
86	7	16	16	16	0	0
86	8	14	14	14	0	0
86	l2	2	2	2	0	0
86	l3	2	2	2	0	0
86	l4	1	1	1	0	0
86	l5	2	2	2	0	0
86	l7	2	2	2	0	0
86	l9	1	1	1	0	0
86	m1	1	1	1	0	0
86	m5	3	3	3	0	0
86	m6	1	1	1	0	0
86	m7	5	5	5	0	0
86	n0	1	1	1	0	0
86	n3	2	2	2	0	0
86	n6	1	1	1	0	0
86	n8	5	5	5	0	0

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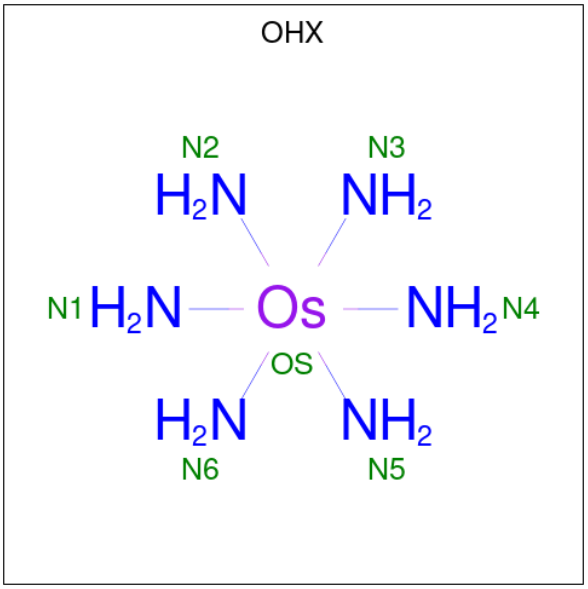
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	o1	2	Total	Mg		0	0
			2	2			
86	o3	2	Total	Mg		0	0
			2	2			
86	o4	1	Total	Mg		0	0
			1	1			
86	q0	1	Total	Mg		0	0
			1	1			
86	q1	1	Total	Mg		0	0
			1	1			
86	q3	1	Total	Mg		0	0
			1	1			

- Molecule 87 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	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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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	1	1	7	6	1	0	0
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87	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		
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87	1	1	7	6	1	0	0
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87	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		
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			Total	N	Os		
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87	1	1	7	6	1	0	0
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87	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		
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			Total	N	Os		
87	1	1	7	6	1	0	0
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			Total	N	Os		
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87	1	1	7	6	1	0	0
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87	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
87	1	1	7	6	1	0	0
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87	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	7	6	1	0	0
			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
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87	4	1	7	6	1	0	0
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87	4	1	7	6	1	0	0
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87	4	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	4	1	7	6	1	0	0
87	4	1	7	6	1	0	0
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87	4	1	7	6	1	0	0
87	4	1	7	6	1	0	0
87	4	1	7	6	1	0	0
87	L3	1	7	6	1	0	0
87	L3	1	7	6	1	0	0
87	L3	1	7	6	1	0	0
87	L4	1	7	6	1	0	0
87	M0	1	7	6	1	0	0
87	M5	1	7	6	1	0	0
87	M6	1	7	6	1	0	0
87	M7	1	7	6	1	0	0
87	M7	1	7	6	1	0	0
87	M8	1	7	6	1	0	0
87	M9	1	7	6	1	0	0
87	N1	1	7	6	1	0	0
87	N9	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	O2	1	7	6	1	0	0
87	O3	1	7	6	1	0	0
87	O7	1	7	6	1	0	0
87	O7	1	7	6	1	0	0
87	O9	1	7	6	1	0	0
87	Q2	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
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87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	7	6	1	0	0
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87	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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87	6	1	7	6	1	0	0
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87	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		
87	6	1	7	6	1	0	0
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87	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		
87	6	1	7	6	1	0	0
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87	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		
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			Total	N	Os		
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			Total	N	Os		
87	6	1	7	6	1	0	0
			Total	N	Os		
87	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		
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			Total	N	Os		
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			Total	N	Os		
87	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		
87	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		
87	6	1	7	6	1	0	0
			Total	N	Os		
87	s1	1	7	6	1	0	0
			Total	N	Os		
87	s1	1	7	6	1	0	0
			Total	N	Os		
87	s4	1	7	6	1	0	0
			Total	N	Os		
87	s8	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	c1	1	7	6	1	0	0
87	c3	1	7	6	1	0	0
87	c5	1	7	6	1	0	0
87	c8	1	7	6	1	0	0
87	d4	1	7	6	1	0	0
87	d9	1	7	6	1	0	0
87	sR	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	l3	1	7	6	1	0	0
			Total	N	Os		
87	l3	1	7	6	1	0	0
			Total	N	Os		
87	l4	1	7	6	1	0	0
			Total	N	Os		
87	l4	1	7	6	1	0	0
			Total	N	Os		
87	l5	1	7	6	1	0	0
			Total	N	Os		
87	l5	1	7	6	1	0	0
			Total	N	Os		
87	l5	1	7	6	1	0	0
			Total	N	Os		
87	l9	1	7	6	1	0	0
			Total	N	Os		
87	m0	1	7	6	1	0	0
			Total	N	Os		
87	m0	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	m1	1	7	6	1	0	0
87	m4	1	7	6	1	0	0
87	m5	1	7	6	1	0	0
87	m6	1	7	6	1	0	0
87	m7	1	7	6	1	0	0
87	m8	1	7	6	1	0	0
87	m9	1	7	6	1	0	0
87	n3	1	7	6	1	0	0
87	n6	1	7	6	1	0	0
87	n9	1	7	6	1	0	0
87	o2	1	7	6	1	0	0
87	o3	1	7	6	1	0	0
87	o7	1	7	6	1	0	0
87	o7	1	7	6	1	0	0
87	q2	1	7	6	1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
88	D6	1	1	1	0	0
88	D7	1	1	1	0	0
88	D9	1	1	1	0	0
88	E1	1	1	1	0	0

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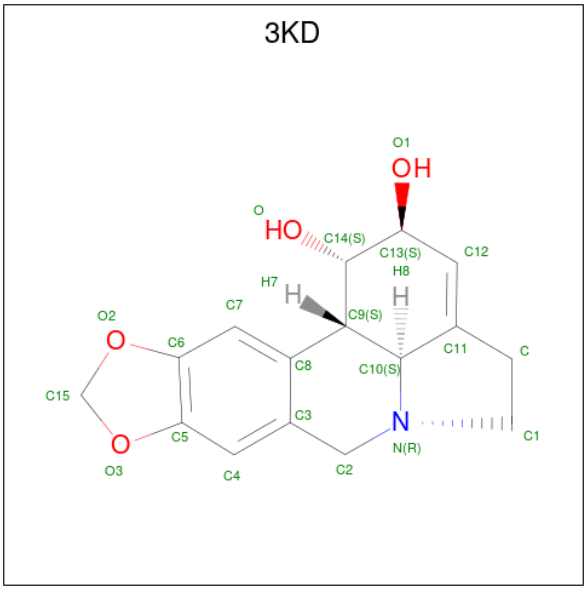
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	O7	1	Total Zn 1 1	0	0
88	Q0	1	Total Zn 1 1	0	0
88	Q2	1	Total Zn 1 1	0	0
88	Q3	1	Total Zn 1 1	0	0
88	d6	1	Total Zn 1 1	0	0
88	d7	1	Total Zn 1 1	0	0
88	d9	1	Total Zn 1 1	0	0
88	e1	1	Total Zn 1 1	0	0
88	o7	1	Total Zn 1 1	0	0
88	q0	1	Total Zn 1 1	0	0
88	q2	1	Total Zn 1 1	0	0
88	q3	1	Total Zn 1 1	0	0

- Molecule 89 is (1S,2S,12bS,12cS)-2,4,5,7,12b,12c-hexahydro-1H-[1,3]dioxolo[4,5-j]pyrrolo[3,2,1-de]phenanthridine-1,2-diol (three-letter code: 3KD) (formula: $C_{16}H_{17}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
89	1	1	21	16	1	4	0	0
			Total	C	N	O		
89	5	1	21	16	1	4	0	0

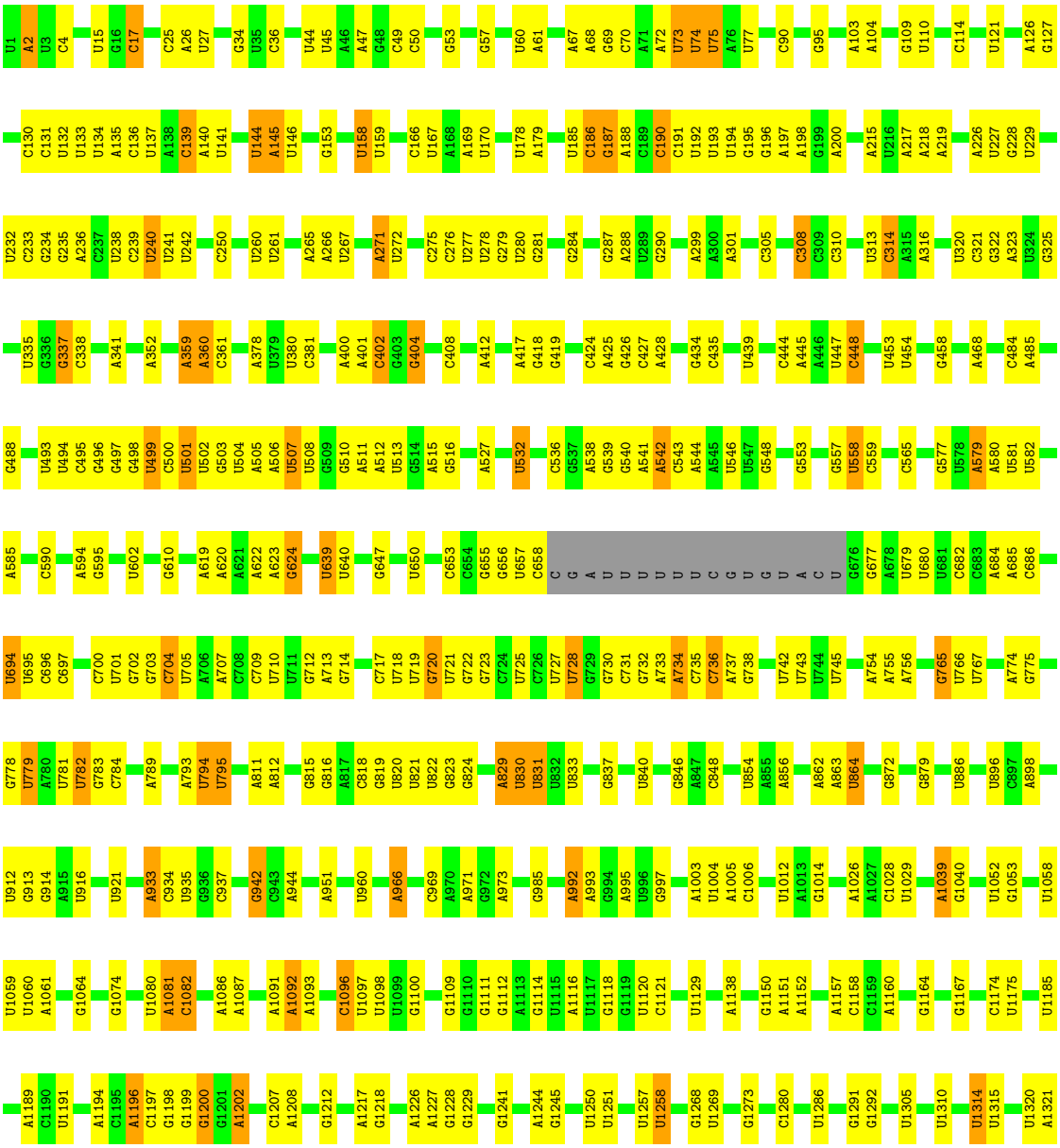
3 Residue-property plots (i)

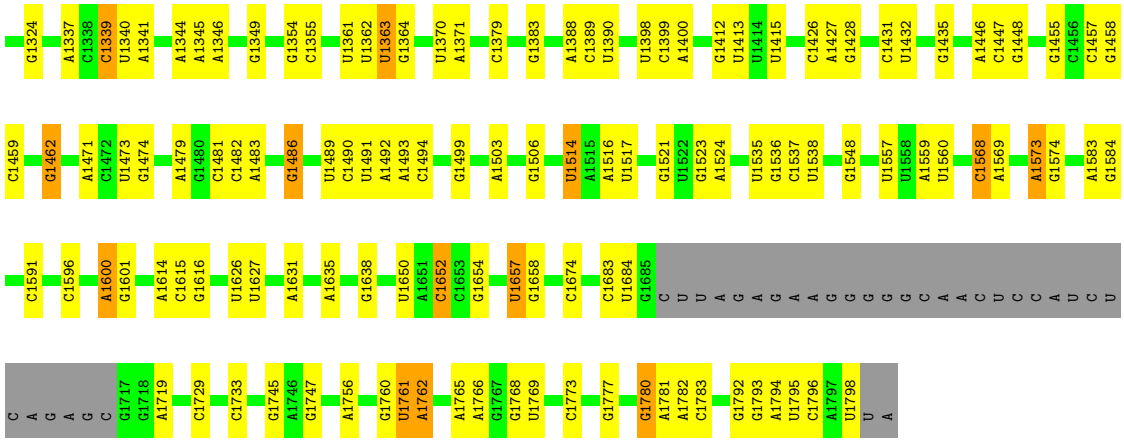
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

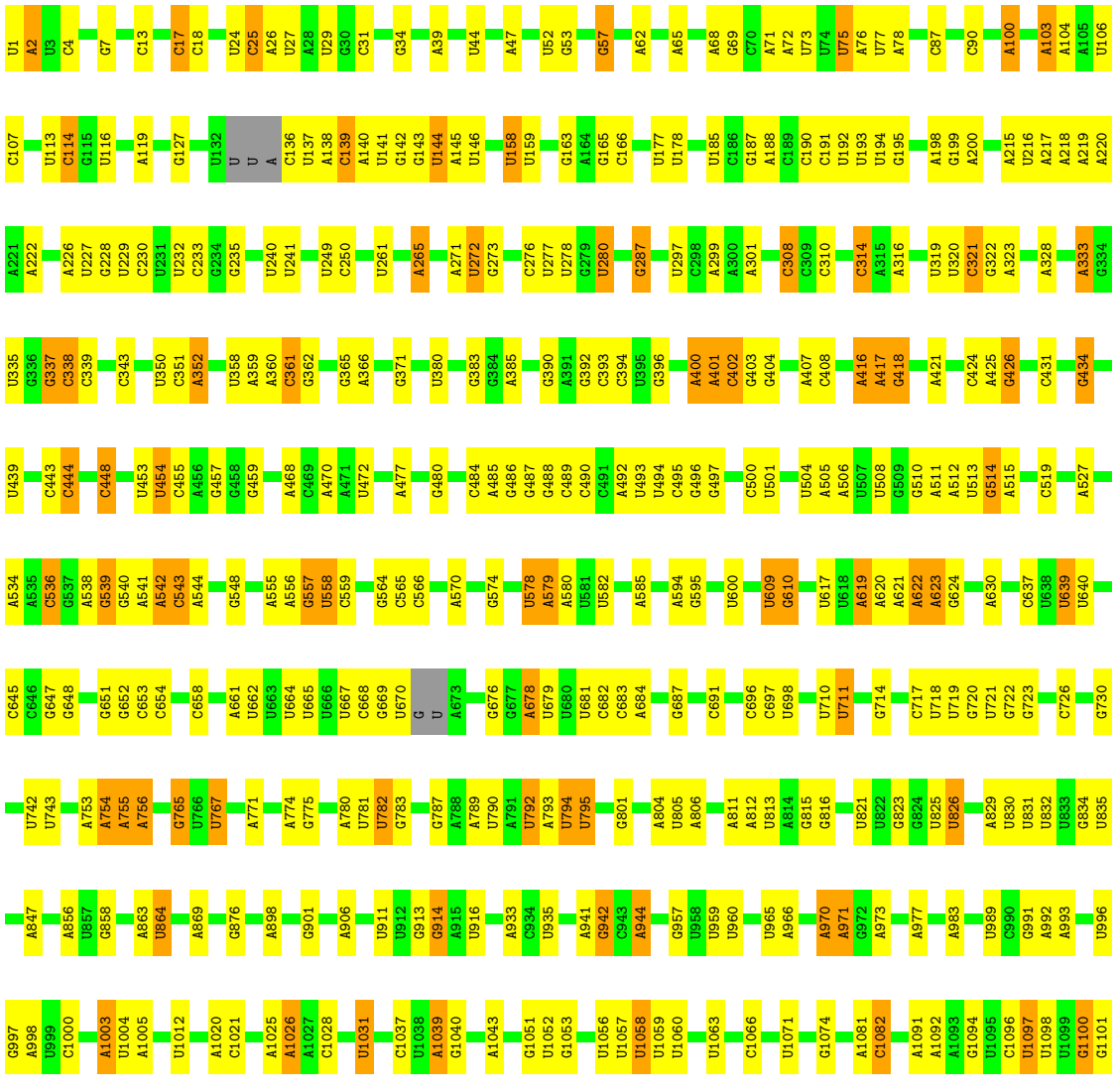
Chain 2:

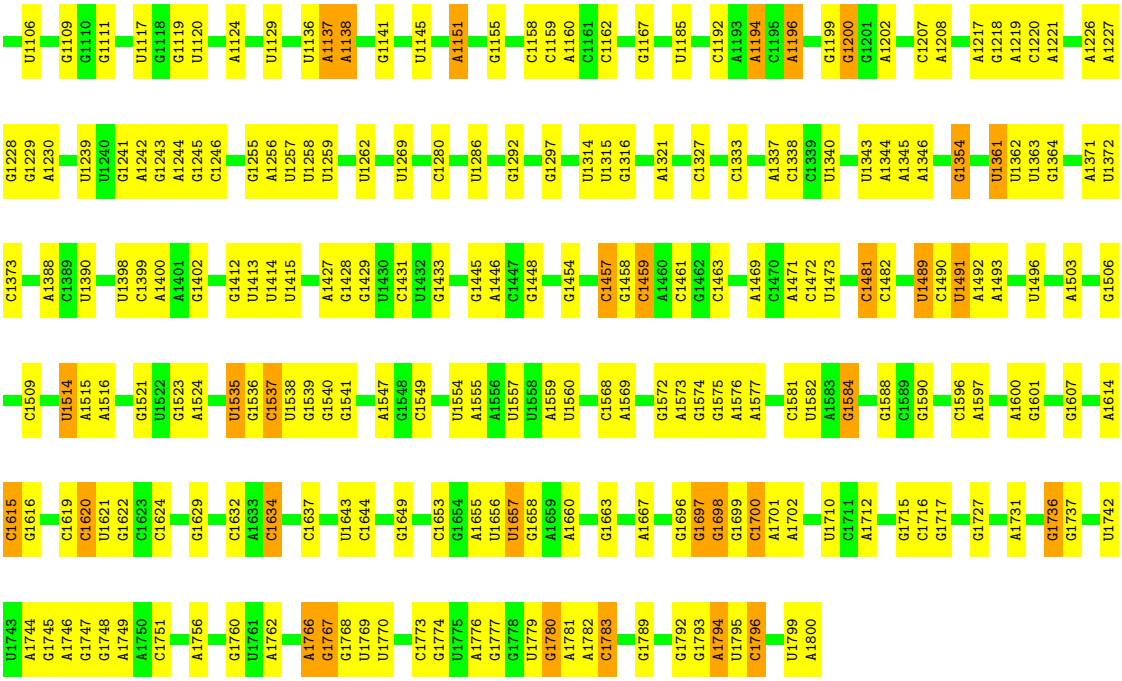




• Molecule 1: 18S ribosomal RNA

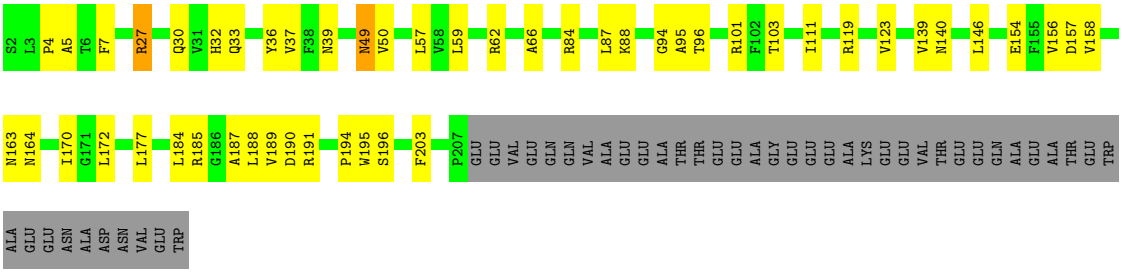
Chain 6:





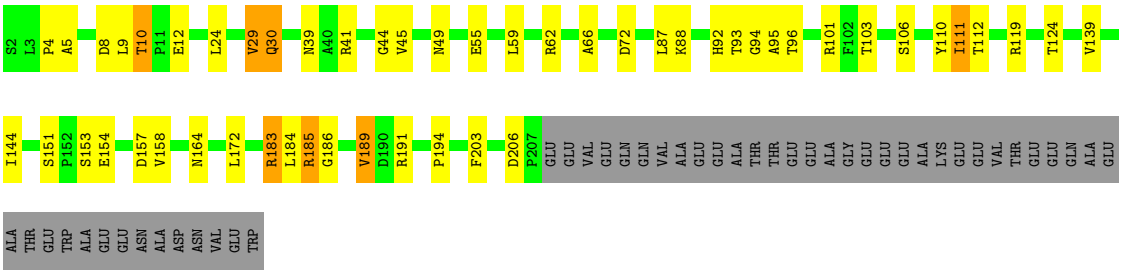
• Molecule 2: 40S ribosomal protein S0-A

Chain S0: 62% 19% • 18%



• Molecule 2: 40S ribosomal protein S0-A

Chain s0: 61% 18% • 18%



• Molecule 3: 40S ribosomal protein S1-A

Chain S1: 61% 21% • 16%

ALA VAL GLY LYS ASN LYS ARG LEU SER LYS GLY LYS LYS GLY GLN LYS LYS ARG V20 V21 T25 R26 W29 F30 P35 S36 T37 T46 N49 K50 S51 L54 S58 D59 A60 L61 K62 G63 L70 L73 E77 D78 F81 R82 D89 E90 V91

L96 L97 F105 L110 R111 S112 K116 W117 S130 D131 D132 A147 N148 S154 S158 V176 Q177 G178 S179 T180 L181 L184 I193 E198 K202 P206 N209 I210 R213 K214 L218 K219 Q220 P221 K222 F223 M229 G233 GLU GLY SER GLY

GLU GLU LYS GLY LYS LYS VAL THR GLY PHE LYS ASP GLU VAL LEU GLU THR VAL

- Molecule 3: 40S ribosomal protein S1-A

Chain s1: 70% 15% 15%

ALA VAL GLY LYS ASN LYS ARG LEU SER LYS GLY LYS LYS GLY GLN LYS LYS ARG V20 V21 D22 T25 R26 T37 F38 E39 L47 S51 K55 K62 L70 R82 K83 I84 K85 G93 F105 T126 T129 I137 A147 S154 T173

Q177 G178 S179 T180 L181 L184 K202 D203 I204 F205 P206 L207 V212 V215 K216 L217 L218 K219 K222 F223 H232 G235 SER GLY GLU GLU LYS GLY LYS LYS VAL THR GLY PHE LYS ASP GLU VAL LEU GLU THR VAL

- Molecule 4: 40S ribosomal protein S2

Chain S2: 69% 16% • 14%

SER ALA PRO GLU ALA GLN GLN GLN LYS ARG GLY GLY PHE GLY GLY ARG ASN ARG GLY ARG PRO ASN ARG ARG GLY PRO ARG ASN THR GLU GLU LYS G34 W35 V36 T39 K40 L41 I53 E54 E55 L58 I68 Q77 Q89 T90 R91 R95 T96 R97 D106 S107

V111 T117 A118 K119 I130 L134 R140 R141 G145 L148 G149 Q150 T166 S181 L187 Y222 G223 F224 L225 T226 L229 L235 P236 V237 L240 D245 E246 A247 S248 A249 Q250 LYS LYS ARG PHE

- Molecule 4: 40S ribosomal protein S2

Chain s2: 64% 21% • 14%

SER ALA PRO GLU ALA GLN GLN GLN LYS ARG GLY GLY PHE GLY GLY ARG ASN ARG GLY ARG PRO ASN ARG ARG GLY PRO ARG ASN THR GLU GLU LYS G34 T39 K40 L41 I53 E54 E55 L58 H59 S60 L61 I69 L72 L73 L76 M81 N82 I83 K84 P85 V86

Q87 K88 Q89 T90 R91 A92 G93 R97 D106 S107 V111 G112 L113 T117 I139 R140 R141 Q150 P151 H152 S153 T159 G163 S164 V165 T166 I170 P182 K185 E194 D195 T206 I218 Y222 L225 L229 Q233 P234 L235 P236 V237 S238

S244 S248 A249 Q250 LYS LYS ARG PHE

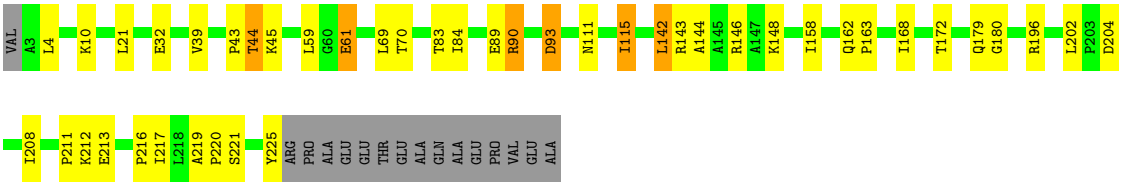
- Molecule 5: 40S ribosomal protein S3

Chain S3: 74% 18% • 7%

VAL A3 L4 I5 R9 L21 N22 E23 V37 V41 T44 L59 N62 R65 I66 N67 T70 R76 I84 E89 Q92 D93 R94 M105 N111 G112 L113 R117 V122 M127 C134 E135 V136 V137 L142 R143 K151 I158

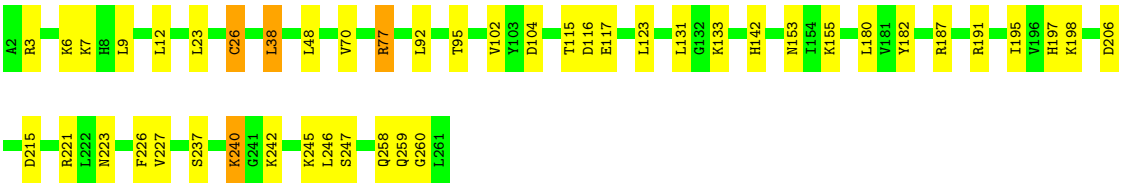
• Molecule 5: 40S ribosomal protein S3

Chain s3:



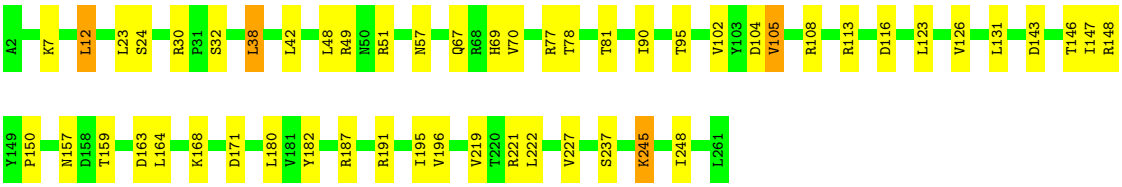
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



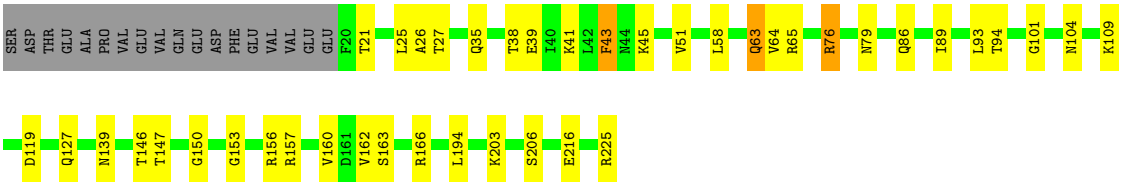
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



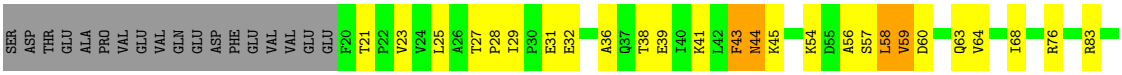
• Molecule 7: 40S ribosomal protein S5

Chain S5:



• Molecule 7: 40S ribosomal protein S5

Chain s5:



I89 L93 T94 M99 N100 G101 R102 K109 D119 N122 T125 N128 T140 T147 R148 R157 S163 R167 Q170 F184 R185 N186 L194 K203 G204 S208 K213 E216 R225

• Molecule 8: 40S ribosomal protein S6-A

Chain S6: 74% 21% • •

M1 V9 Q13 K14 R25 I32 F45 K51 K58 Q65 G66 V67 L68 L69 P70 L76 L77 T78 K79 N80 V81 S82 K93 R98 L109 E120 L121 E122 G123 L124 T125 D126 T127 T128 V129 R132 L133 K143 G146 L147 S148 K149 E150 D151

D152 V153 R154 D155 Y169 T170 P173 K174 I175 Q176 R177 R183 L211 L216 S217 K223 I226 ARG LYS ARG ARG ALA SER SER LEU LYS ALA

• Molecule 8: 40S ribosomal protein S6-A

Chain s6: 74% 17% • 8%

M1 E17 E21 R25 K30 Q34 D43 Q65 L68 L69 P70 T71 L76 L77 T78 K79 N80 V81 K93 V97 V108 L109 A110 L111 K115 E120 L121 D126 T127 T128 V129 P130 K131 K143 E150 D151 D152 V153 R154 D155 F156 G165

T170 P173 K174 L193 E203 L212 R215 E218 ARG LYS ALA GLU LYS ALA GLU ILE ARG LYS ARG ARG ALA SER SER LEU LYS ALA

• Molecule 9: 40S ribosomal protein S7-A

Chain S7: 75% 20% • •

SER ALA P4 L9 P13 N29 S30 S31 P32 L38 I46 D50 V51 V64 F70 V73 Q74 T75 K84 F85 Q86 D87 R97 I98 T105 S106 R107 K111 R112 P113 R114 S115 R116 D123 L126 V130 F131 P132 T133 E134 I135 V136 N147

D155 D158 D163 E167 N174 I185 P186 S187 GLU THR HIS

• Molecule 9: 40S ribosomal protein S7-A

Chain s7: 78% 17% • •

S2 S10 Q11 A12 P13 E28 N29 S30 E33 Q42 K55 V64 P65 S66 L67 Q74 L77 T78 R79 E80 Q86 D87 R97 S103 R104 T105 S106 R107 Q108 K111 R114 S115 R116 T117 L118 L126 F131 P132 T133 V136 R139 L143

D155 V159 I185 P186 S187 GLU THR HIS

• Molecule 10: 40S ribosomal protein S8-A

Chain S8: 80% 14% • 6%

MET G2 S7 R8 H9 K10 T14 F21 R22 K26 L29 T36 A40 V46 R49 N52 L58 S69 V82 D105 T120 K123 LYS LYS ASN VAL LYS GLU GLU GLU THR VAL ALA K135 N138 A147 A148 S149 A150 K151 I152 E153

S154 S158 S161 E187 L196 K200

• Molecule 10: 40S ribosomal protein S8-A

Chain s8: 80% 13% 6%

MET G2 Q20 R25 K26 L29 Q32 T36 V46 L58 R59 T62 K74 K75 T76 R77 I78 E89 N94 I101 Q111 T120 L121 G122 K123 LYS LYS ASN VAL LYS GLU GLU GLU THR VAL ALA K135 S136 K151 I152 S155 S158

S161 S176 I183 K200

• Molecule 11: 40S ribosomal protein S9-A

Chain S9: 72% 21% • 6%

P2 R3 T7 T14 P15 K16 L28 K40 S46 L49 R54 L60 D63 R78 R79 R82 D89 K92 L93 L97 A98 L99 L105 L109 Q110 V113 L118 S121 I134 K138 S145 R149 L150 D151 D157

P160 T161 S162 P163 F164 R168 R171 V172 A173 R174 E182 E186 ALA ALA ASP GLU ALA ASP GLU ALA ASP GLU GLU

• Molecule 11: 40S ribosomal protein S9-A

Chain s9: 76% 16% • 6%

P2 R3 T7 S22 L28 E33 K39 L49 R54 R78 R82 K90 L93 L99 K100 V101 L109 Q110 T111 K115 S121 R126 V127 T130 H133 I134 N142 R149 L150 T161 S162 P163 F164 A167 R168 V172

K180 A181 E182 A183 E186 ALA ALA ASP GLU ALA ASP GLU ALA ASP GLU GLU

• Molecule 12: 40S ribosomal protein S10-A

Chain C0: 71% 19% • 9%

M1 R8 K25 D26 F27 N28 Q29 H32 E33 E34 Y54 V55 K56 S60 Y64 E71 L76 N81 L82 I86 V87 P88 I92 Q93 E94 R95 N96 PRO THR GLN ARG PRO GLN ARG ARG TYR

• Molecule 12: 40S ribosomal protein S10-A

Chain c0: 70% 18% • 9%

M1 L2 M3 P4 K5 R8 H12 L15 V20 A23 K24 A30 K31 H32 I35 V55 K56 T57 E71 L82 P83 E84 HIS ILE V87 P88 I92 Q93 E94 R95 N96 P97 T98 GLN ARG PRO GLN ARG ARG TYR

• Molecule 13: 40S ribosomal protein S11-A

Chain C1: 79% 20% •

S2 T3 E4 L5 T6 V7 Q8 N21 T27 S28 K29 R30 N37 L40 T44 D55 L63 R67 G68 K69 T72 G73 T74 K79 T83 V109 S112 P113 Q118 V123 Q127 I131 V140 S143 A144 A145 A146 A147 A154 K155

F156

• Molecule 13: 40S ribosomal protein S11-A

Chain c1: 74% 19% • 6%

S2 T3 E4 L5 T6 V7 E10 N21 K26 T27 R30 T31 K32 R33 L40 T44 F60 T61 R67 T74 V75 V76 M80 T83 I86 A114 D121 I122 V123 R129 K133 V139 V140 A144 A145 A146 A147 LYS ALA ASN LYS GLN

PHE ALA LYS PHE

• Molecule 14: 40S ribosomal protein S12

Chain C2: 55% 30% • 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 V37 H38 D39 R43 R46 K50 A51 L52 I53 R54 G55 L58 V61 V66 A69 N70 I71 L74 D81 P82 E83 V86

P87 L88 I89 K90 V91 A92 D93 A101 G102 L103 I106 D107 A112 R113 K114 V115 S119 V120 V121 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 L28 L36 D39 G40 R43 G44 L45 L52 L58 L59 L62 V63 V66 I71 L74 P82 E83 N84 K85 V86 P87 L88 I89 K90 V91 L97

A101 G102 L103 I106 D107 R108 E109 A110 V115 V116 G117 A118 S119 V120 V121 G127 A128 E129 T130 D131 E132 I136 F140 Q143

• Molecule 15: 40S ribosomal protein S13

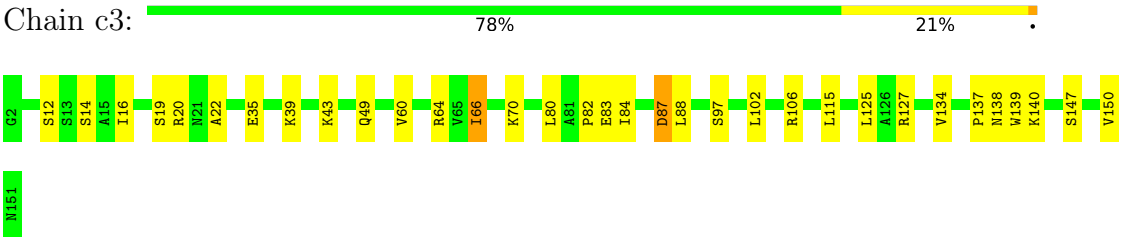
Chain C3: 79% 19% •

G2 R3 K9 G10 I11 S12 S13 I16 S19 A22 K27 S32 K39 R42 L45 I50 D56 A57 H58 R64 V65 I66 T67 G68 K76 E83 L88 L102 D110 R114 L115 L125 V134 P137 N138 E142 T145

N151

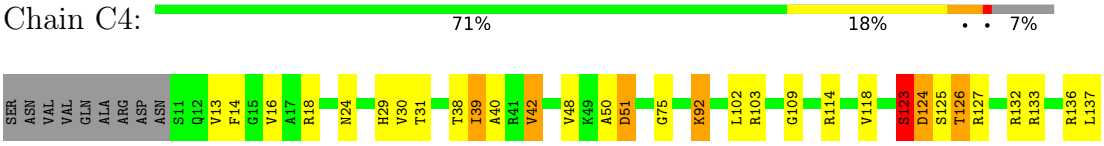
• Molecule 15: 40S ribosomal protein S13

Chain c3:



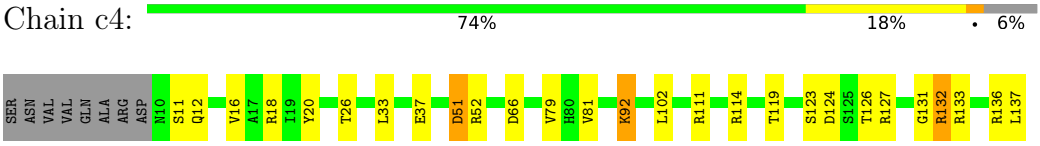
• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



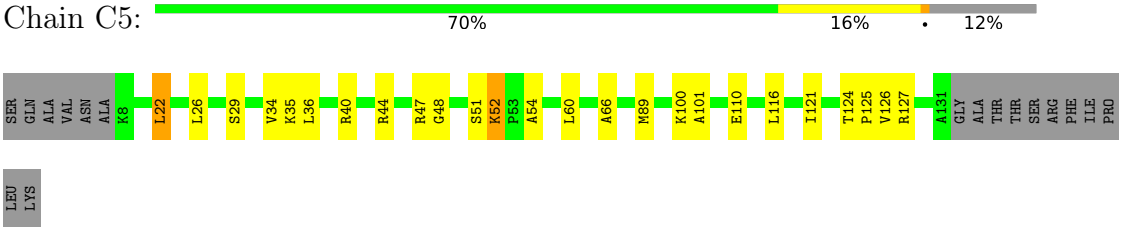
• Molecule 16: 40S ribosomal protein S14-A

Chain c4:



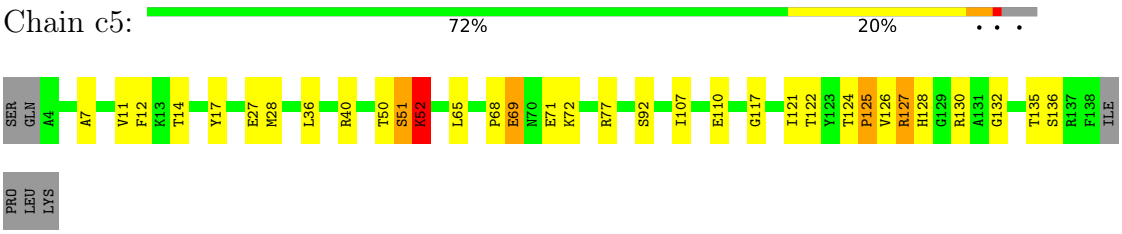
• Molecule 17: 40S ribosomal protein S15

Chain C5:



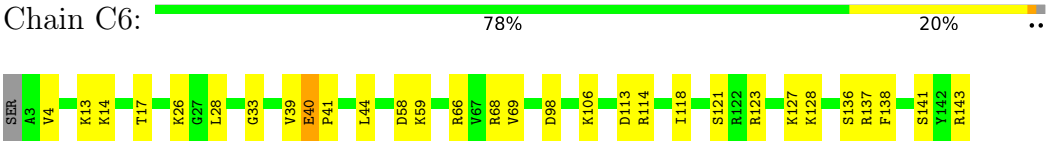
• Molecule 17: 40S ribosomal protein S15

Chain c5:



• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



• Molecule 18: 40S ribosomal protein S16-A

Chain c6: 77% 21% •

S2 A3 V4 T17 K23 L28 T37 L38 V39 E40 P41 E42 I43 V48 L53 L54 L57 R66 V67 R68 V69 T70 I81 Q94 V97 D98 K106 T110 D113 R114 T115 L116 R123 R137 Y142 R143

• Molecule 19: 40S ribosomal protein S17-A

Chain C7: 66% 18% • 12%

MET G2 R5 T6 P22 K23 L24 T25 Q29 T30 L34 I38 L46 K49 T54 I69 S70 F71 K72 R78 Q83 Y84 V85 P86 E87 V88 S89 ALA LEU ASP LEU SER R95 N104 Q105 T106 S107 L113 G114 L115 L119 N123 V124 S125 A126

GLN ARG ASP ARG ARG TYR ARG LYS ARG VAL

• Molecule 19: 40S ribosomal protein S17-A

Chain c7: 71% 13% • 14%

MET G2 R3 T8 Q29 L34 L46 K49 I50 R60 I61 Q62 K63 I69 V85 V88 S89 A90 LEU ASP LEU SER R95 G98 V99 N104 V110 L113 K116 S120 V121 I122 ASN VAL SER ALA GLN ARG ASP ARG ARG TYR ARG LYS ARG

VAL

• Molecule 20: 40S ribosomal protein S18-A

Chain C8: 72% 24% •

S2 L3 V4 V5 Q6 E7 Q8 F11 Q12 H13 I14 L17 L18 N19 T20 N25 I26 K27 I28 L32 R40 D53 L54 E60 L61 Q71 K80 I81 P82 A83 Q89 N90 D91 I92 D97 K108 R115 L116 R120 T125 R132 Q136

K139 T140 T141 G142 R143 R144 R145 A146

• Molecule 20: 40S ribosomal protein S18-A

Chain c8: 77% 21% •

S2 L3 V4 V5 Q6 S10 H13 I14 L15 L18 N25 I26 K27 I28 T33 V38 G39 R40 E60 L61 T62 Q63 L66 E67 R68 D91 I92 A102 L116 I119 R120 V133 R134 G135 T138 K139 R143 R144 R145 A146

• Molecule 21: 40S ribosomal protein S19-A

Chain C9: 81% 19%

P2 G3 V4 S5 V6 Y18 L22 L28 E29 V30 P31 G32 Y33 V34 D35 I36 V37 A50 W53 R57 M67 R68 K69 Q70 K84 I94 I111 I116 S117 R130 D131 R134 L140 E144

• Molecule 21: 40S ribosomal protein S19-A

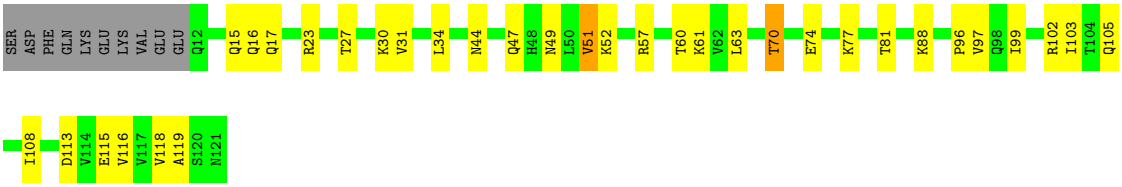
Chain c9:

• Molecule 22: 40S ribosomal protein S20

Chain D0:

• Molecule 22: 40S ribosomal protein S20

Chain d0:



• Molecule 23: 40S ribosomal protein S21-A

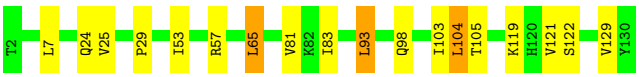
Chain D1:

• Molecule 23: 40S ribosomal protein S21-A

Chain d1:

• Molecule 24: 40S ribosomal protein S22-A

Chain D2:

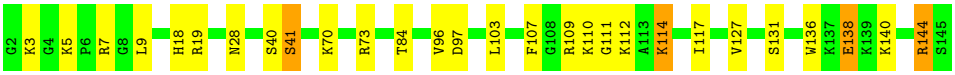


• Molecule 24: 40S ribosomal protein S22-A

Chain d2:

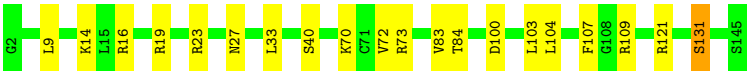
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



• Molecule 25: 40S ribosomal protein S23-A

Chain d3:

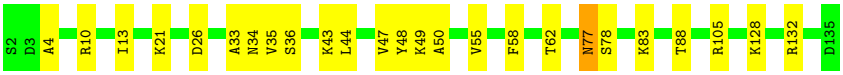


• Molecule 26: 40S ribosomal protein S24-A

Chain D4:

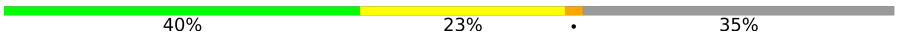
• Molecule 26: 40S ribosomal protein S24-A

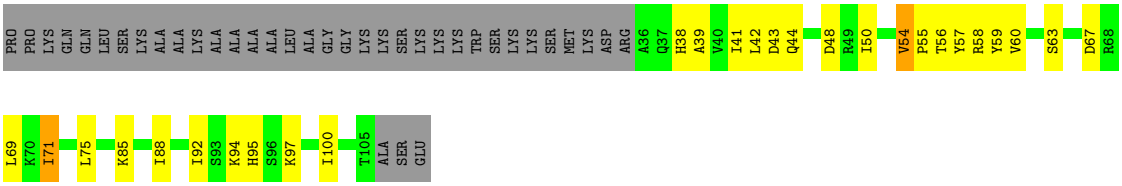
Chain d4:



• Molecule 27: 40S ribosomal protein S25-A

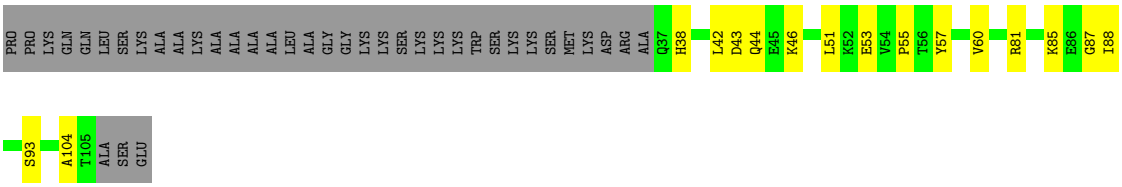
Chain D5:





• Molecule 27: 40S ribosomal protein S25-A

Chain d5:

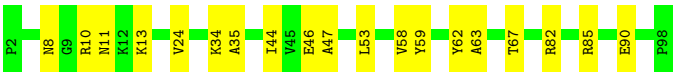


• Molecule 28: 40S ribosomal protein S26-B

Chain D6: 72% 20% 8%

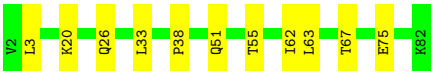
• Molecule 28: 40S ribosomal protein S26-B

Chain d6: 80% 20%



• Molecule 29: 40S ribosomal protein S27-A

Chain D7: 86% 14%



• Molecule 29: 40S ribosomal protein S27-A

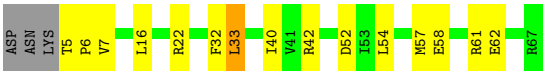
Chain d7: 80% 19%

• Molecule 30: 40S ribosomal protein S28-A

Chain D8: 73% 21% 5%

• Molecule 30: 40S ribosomal protein S28-A

Chain d8: 73% 21% 5%

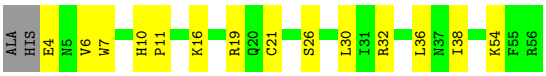


• Molecule 31: 40S ribosomal protein S29-A

Chain D9: 78% 16%

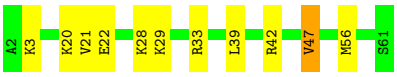
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



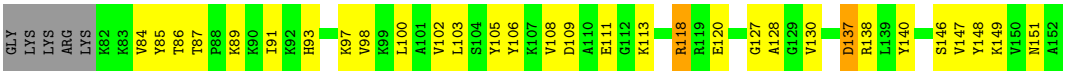
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



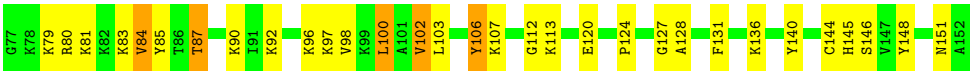
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



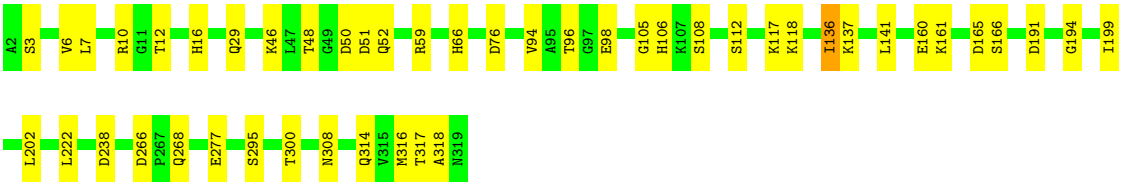
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:



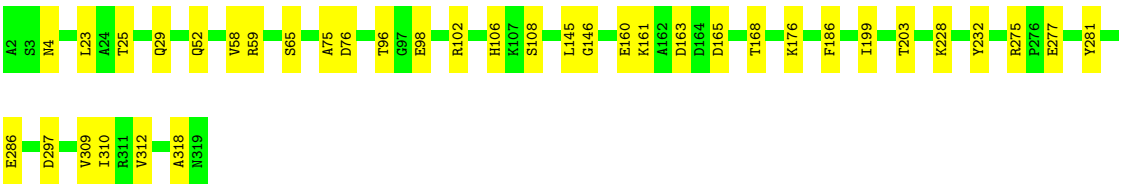
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



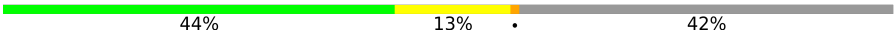
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

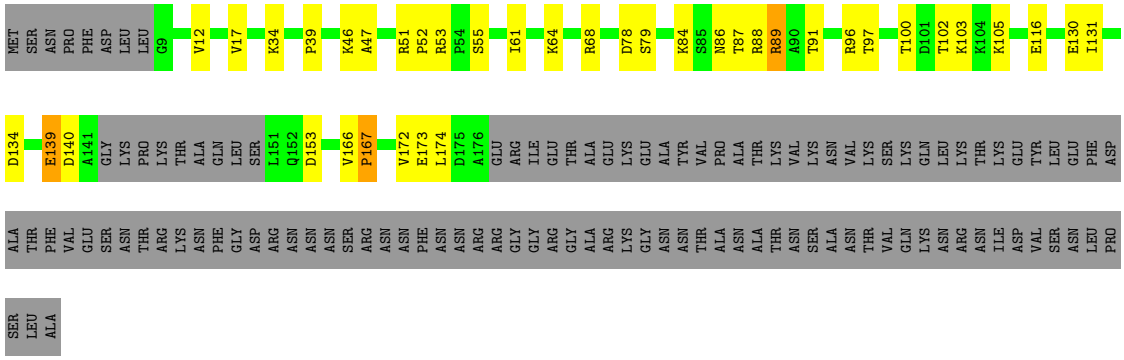
Chain sR:



• Molecule 35: Suppressor protein STM1

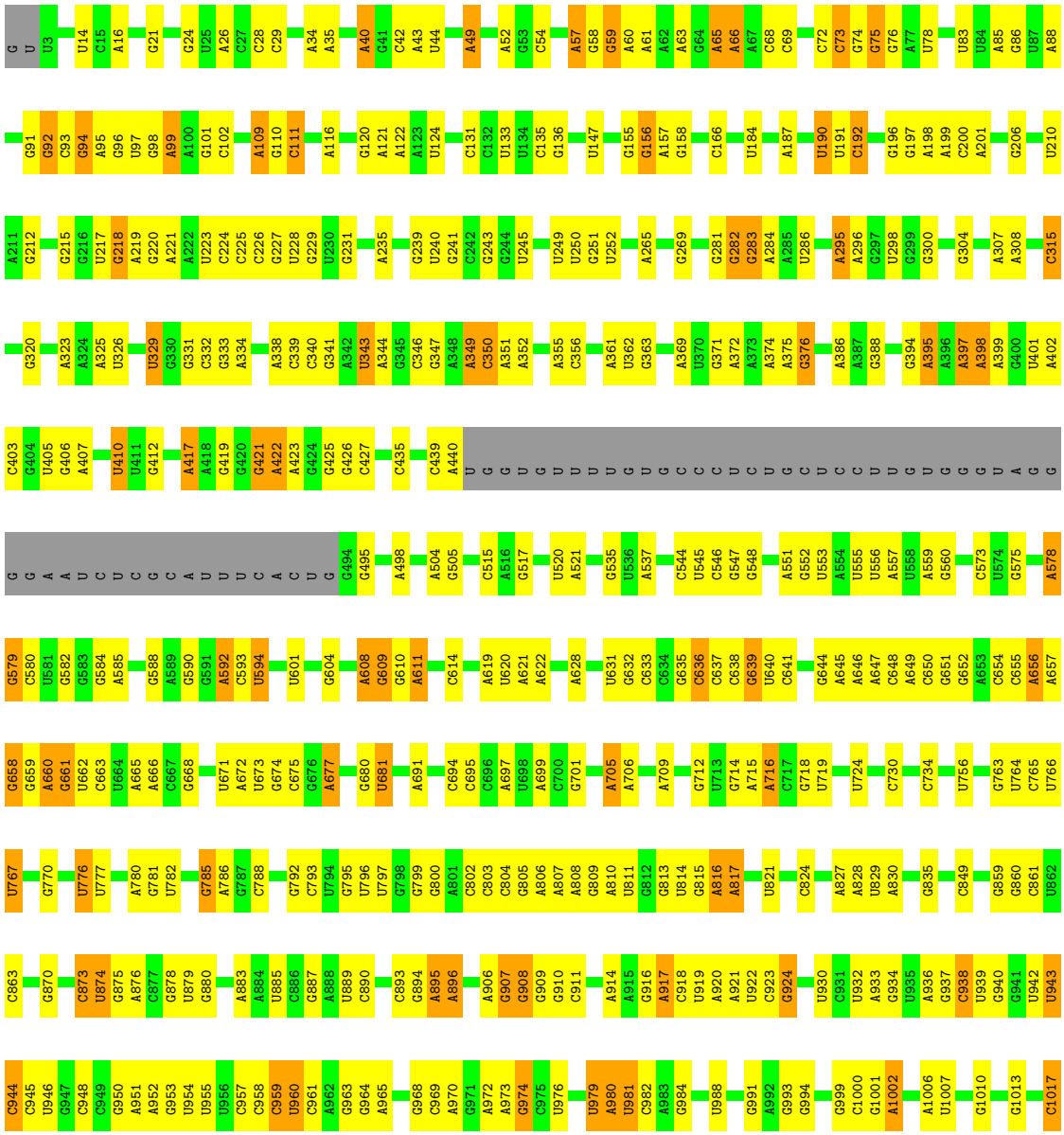
Chain SM:





• Molecule 36: 25S ribosomal RNA

Chain 1:



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A2188 U2189 U2190 U2191 C2192 U2193 G2194 A2198 G2199 U2200 G2201 C2202 U2205 G2206 A2207 A2208 U2209 G2210 U2211 C2212 A2215 G2216 A2222 A2223 C2227 A2228 C2237 G2238 G2239 G2240 U2241 A2242 A2243 A2244 C2245 G2246 G2247 C2248 G2249 G2250 A2255 A2256 C2257 G2272 G2273 C2278 A2279 A2280 A2281 U2282 G2283
C2094 C2101 U2102 A2106 A2107 G2111 U2112 A2113 C2114 G2115 G2116 A2120 G2121 G2122 G2123 A2126 U2129 G2130 A2131 C2132 U2133 G2134 A2138 A2139 U2140 U2141 A2142 A2143 A2144 A2147 U2148 A2152 A2158 U2159 C2163 A2164 G2165 G2169 U2170 U2173 U2176 G2177 C2181 G2187
C G U G C C U U G G U U C G G U U G A U U G U U G G U G G U C A G A C U U G G C U U C C C U C C U G G U G G C C U U G G C U U A A C U U A A C U U A G A2093
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C1866 A1867 C1870 U1871 G1878 A1879 U1880 A1886 U1890 A1891 G1892 A1893 A1896 A1901 G1902 U1903 C1904 G1905 G1906 A1909 U1920 C1923 C1926 G1948 G1949 U1950 C1951 G1952 G1953 G1954 U1955 A G U G G A A G G C C U1834 A1835 C1836 U1837 G1838 A1839 U1840 A1841 A1842 C1843 C1844 G1845 C1846 A1847 G1848 C1849 A1858
C1761 C1762 U1765 G1766 C1767 G1770 G1780 C1781 U1782 U1783 G1790 C1791 C1792 C1793 G1794 U1795 G1796 A1797 C1802 G1807 A1810 G1811 G1812 A1813 A1814 U1815 A1816 G1817 U1818 U1819 U1820 U1821 C1822 U1834 A1835 C1836 U1837 G1838 A1839 U1840 A1841 A1842 C1843 C1844 G1845 C1846 A1847 G1848 C1849 A1858
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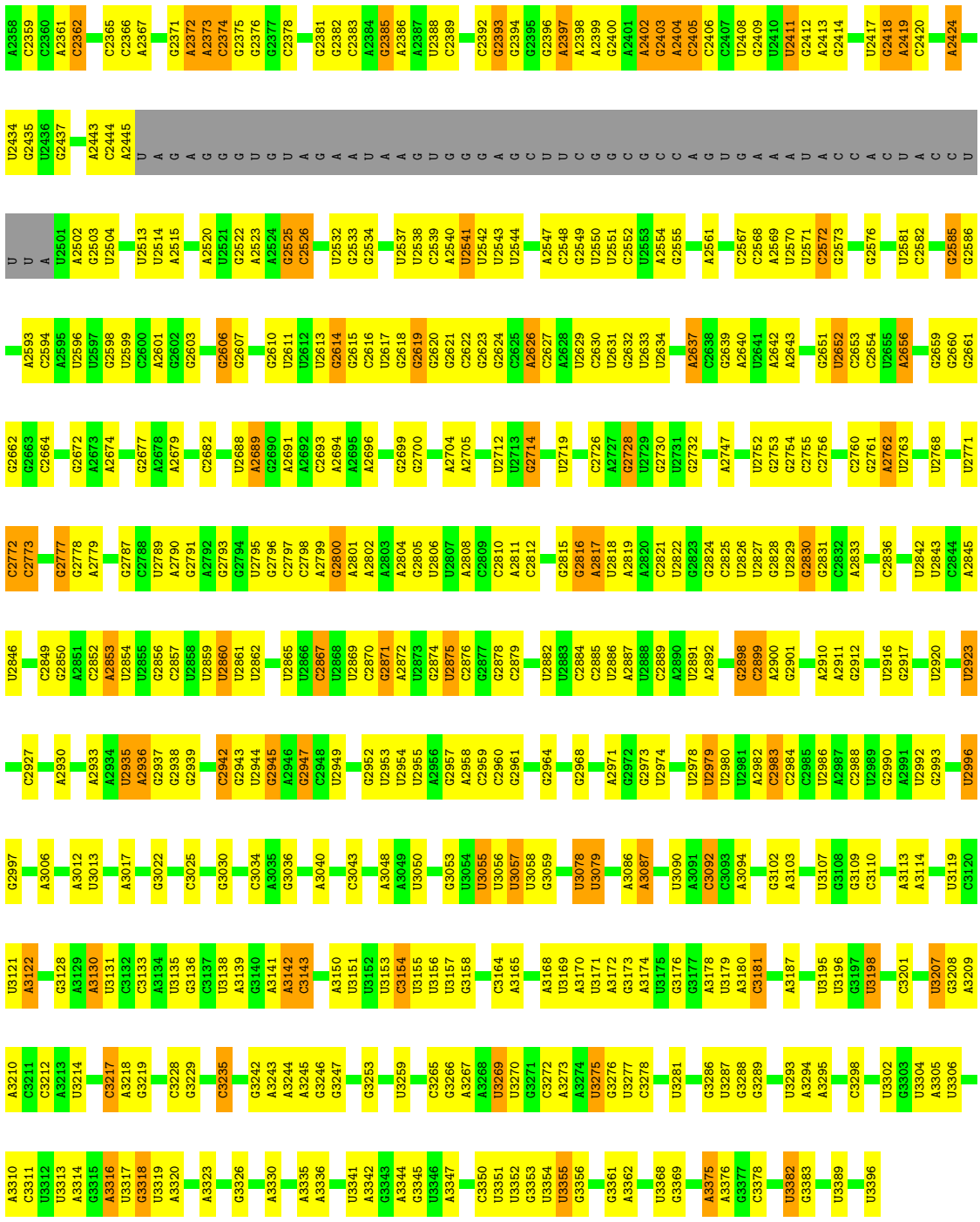
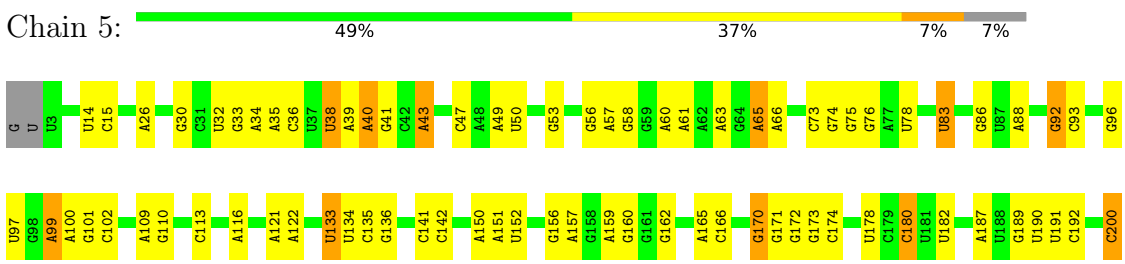


• Molecule 36: 25S ribosomal RNA

Chain 5:



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U C U G C U C C U U G G U G G U A G G G G A A U C U U C C A U U U C A C491 U492 G495 C496 C497 C500 A501 U502 C503 A504 G505 U506 U509 G513 G514 C515 A516 A519 U520 A521
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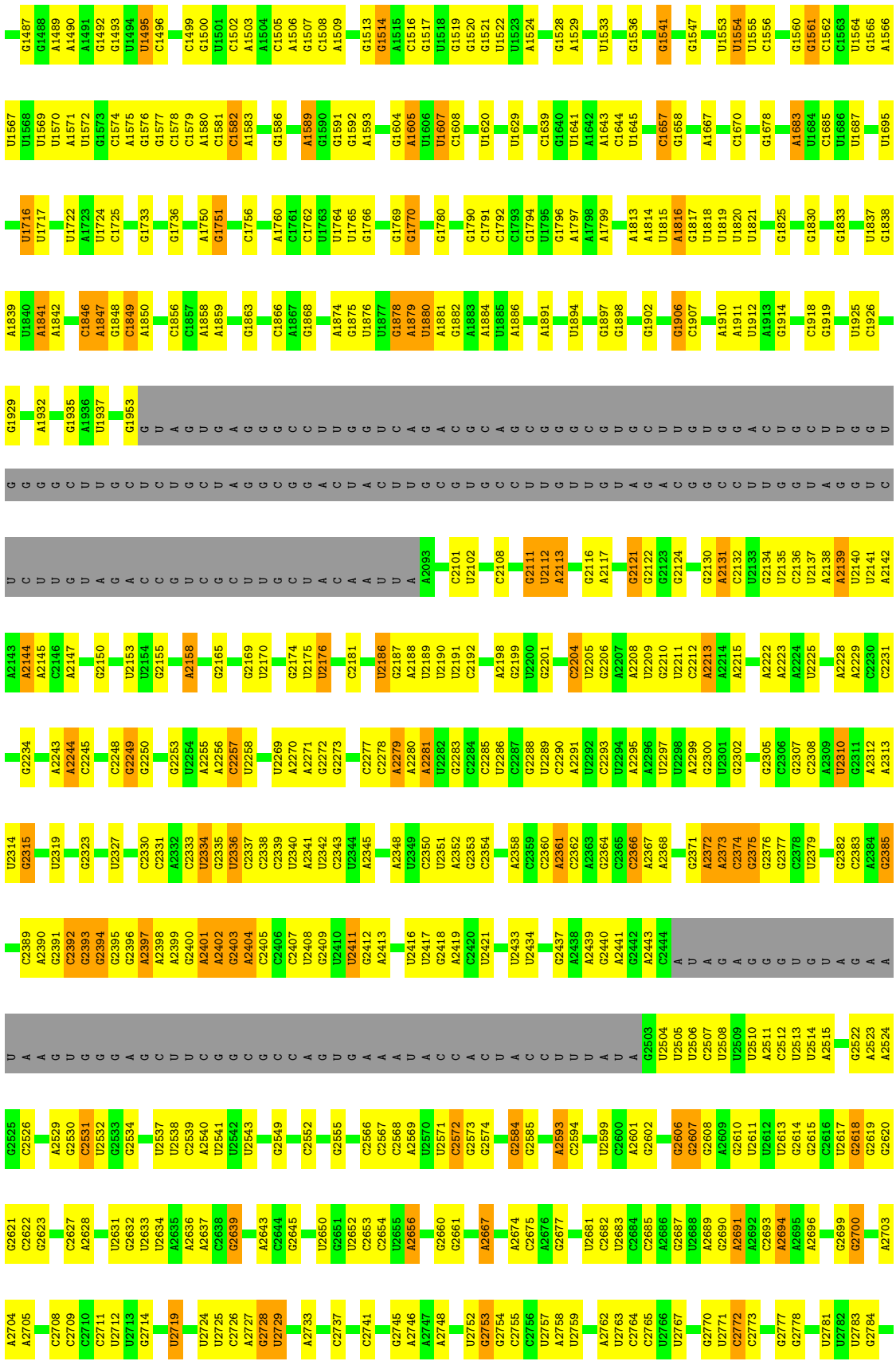
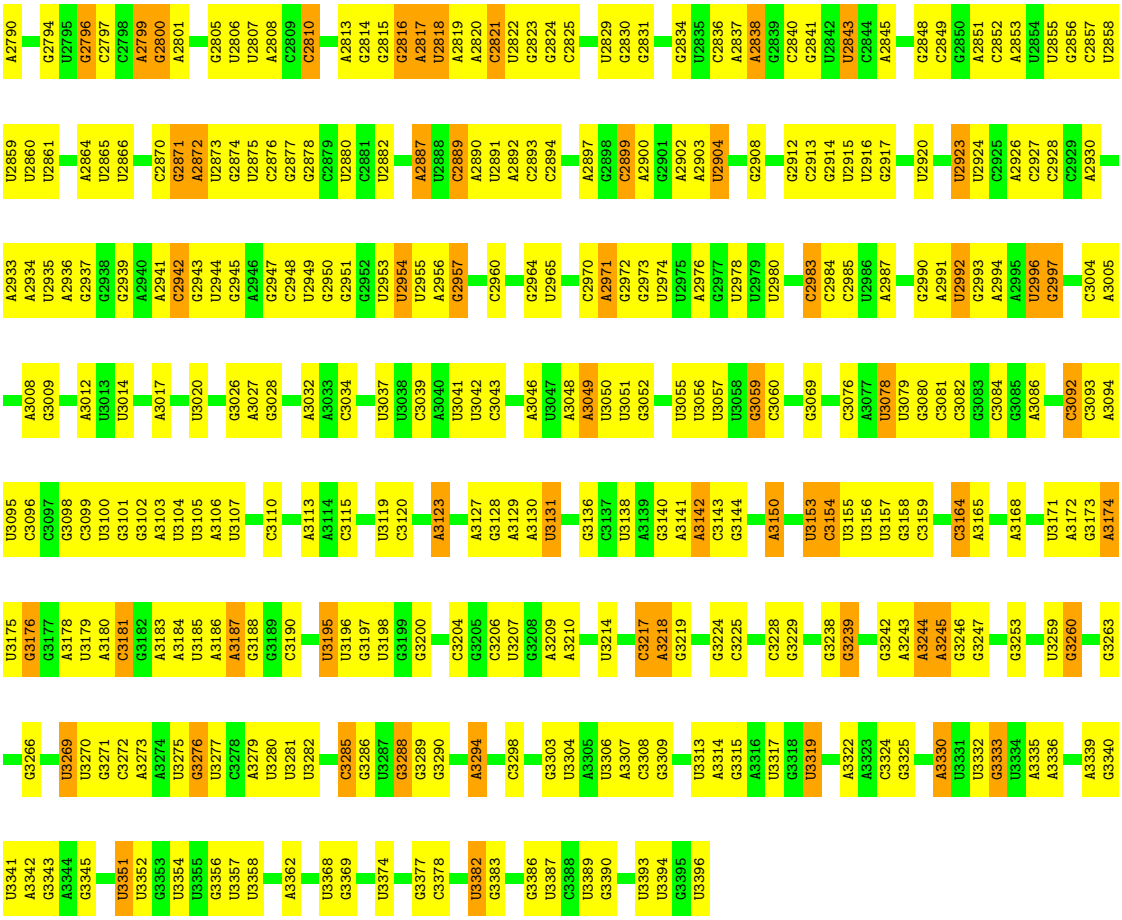
A1130 G1131 C1132 A1133 G1134 A1135 U1138 A1143 G1147 G1148 G1149 A1150 U1151 G1152 A1153 A1154 C1155 C1156 G1157 A1158 A1159 C1160 G1161 U1162 G1166 U1167 U1168 A1169 A1170 G1171 C1175 C1176 A1180 U1181 A1182 C1183 A1184 C1187 U1188 C1189 A1190 U1191 C1192 A1193 G1194 A1197 C1198 C1199 A1200 C1201 A1202 A1203
A1204 A1205 U1208 G1209 A1212 G1213 G1222 G1226 C1232 G1236 G1237 C1238 C1239 A1240 U1241 G1242 G1243 A1244 A1245 G1246 A1252 U1253 C1254 U1258 G1262 A1263 G1264 U1265 G1266 G1295 C1296 C1297 C1298 U1299 G1300 A1301 A1302 A1303 A1304 U1305 G1306 G1307 A1308 U1309 G1310 G1311 C1312 G1313 C1314 U1315
C1316 A1317 A1318 G1319 C1320 G1321 U1322 G1323 U1329 A1330 U1331 A1332 C1335 U1336 A1337 C1338 C1339 G1340 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 C1358 C1359 G1362 A1363 C1364 G1365 A1366 A1369 G1370 G1371 C1372 A1373 G1374 G1375 C1376 G1380 C1385 A1386 G1387 A1390 C1391 G1392 A1393 A1394 G1395
U1398 A1399 G1400 A1406 A1407 U1410 C1411 G1412 C1416 A1419 G1422 C1423 C1424 G1429 U1430 G1431 C1432 A1433 G1434 A1435 U1436 C1437 G1440 U1445 A1446 G1447 U1448 A1449 G1450 C1451 A1452 U1455 A1456 A1460 A1461 G1464 A1465 A1468 G1473 G1476 G1480 A1481 A1482 G1483



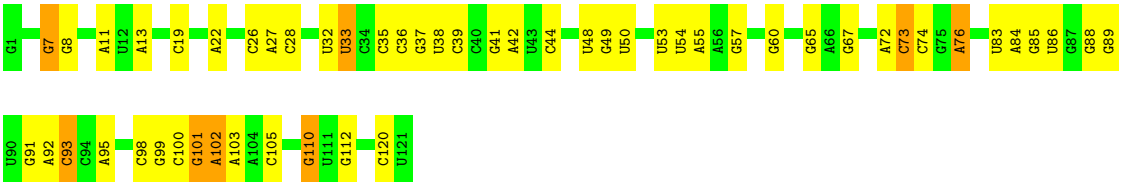


- Molecule 37: 5S ribosomal RNA

Chain 3:

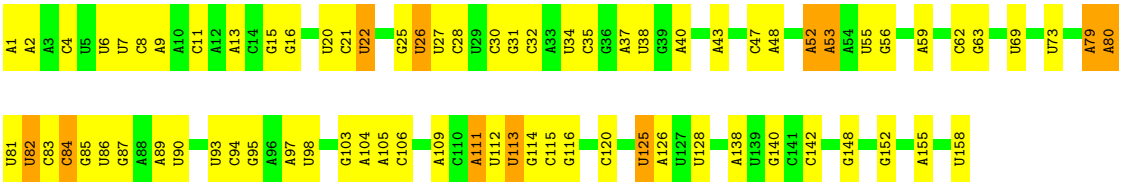
- Molecule 37: 5S ribosomal RNA

Chain 7:



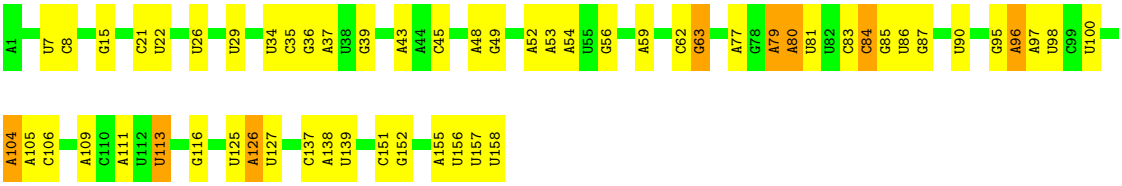
- Molecule 38: 5.8S ribosomal RNA

Chain 4:



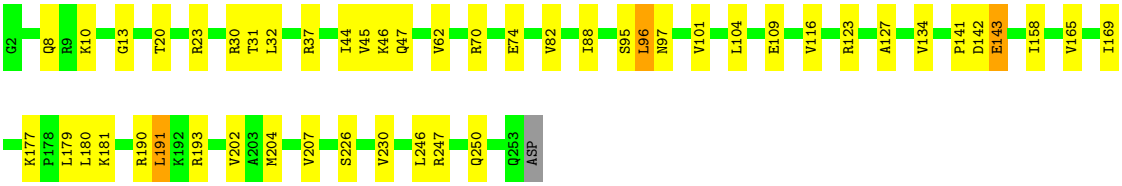
- Molecule 38: 5.8S ribosomal RNA

Chain 8:



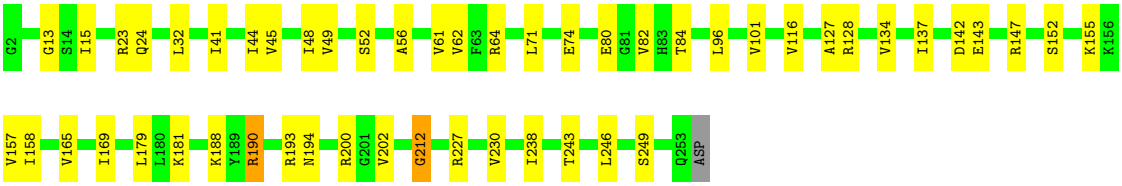
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



- Molecule 39: 60S ribosomal protein L2-A

Chain l2:

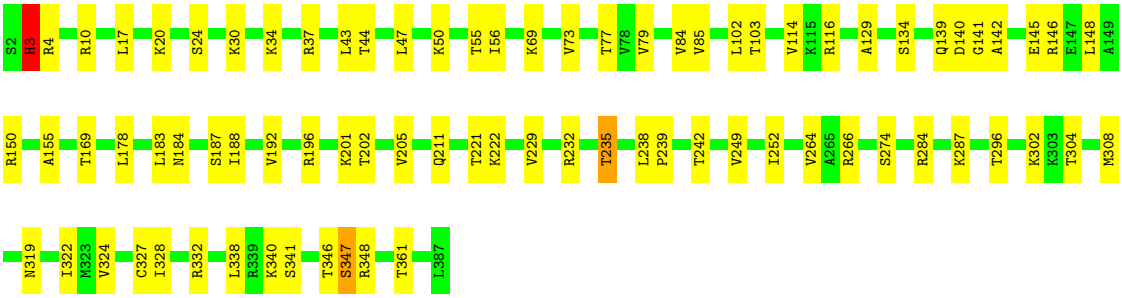


- Molecule 40: 60S ribosomal protein L3

Chain L3:

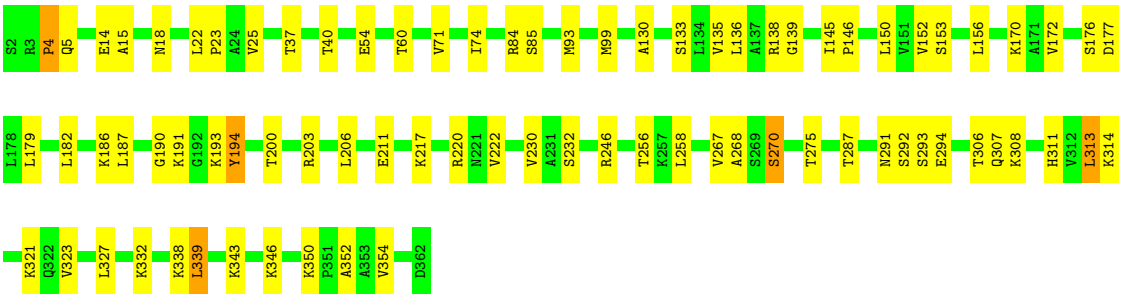
- Molecule 40: 60S ribosomal protein L3

Chain l3: 79% 20%



- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 78% 21%

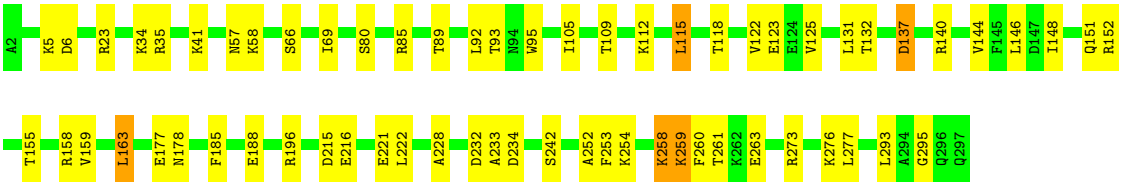


- Molecule 41: 60S ribosomal protein L4-A

Chain l4: 78% 20%

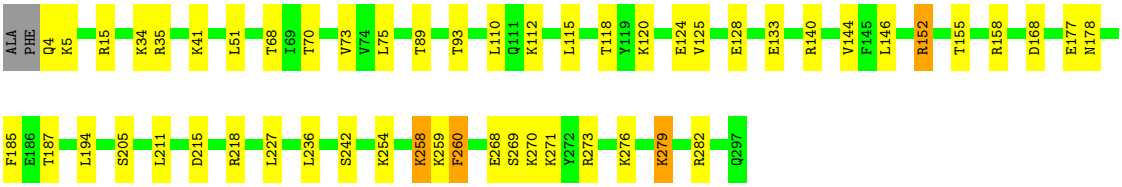
- Molecule 42: 60S ribosomal protein L5

Chain L5: 78% 20%



• Molecule 42: 60S ribosomal protein L5

Chain l5:

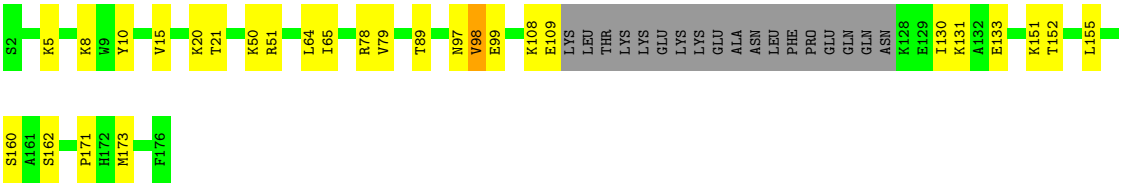


• Molecule 43: 60S ribosomal protein L6-A

Chain L6:

• Molecule 43: 60S ribosomal protein L6-A

Chain l6:

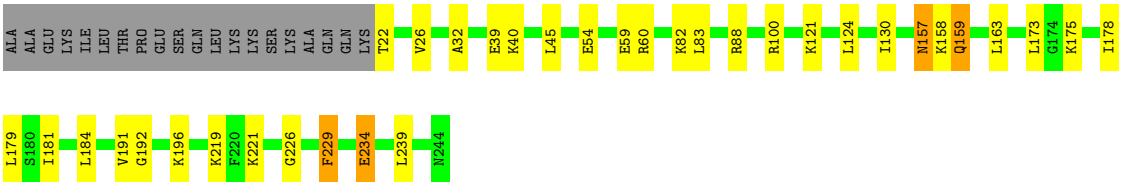


• Molecule 44: 60S ribosomal protein L7-A

Chain L7:

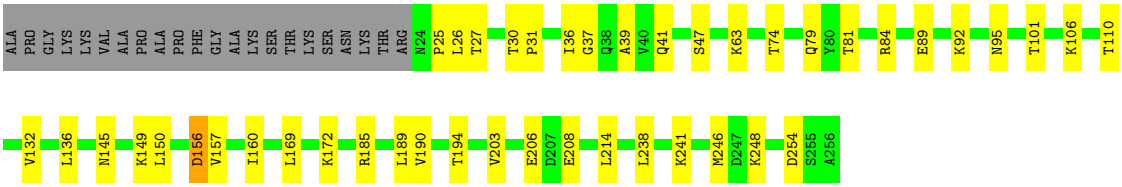
• Molecule 44: 60S ribosomal protein L7-A

Chain l7:



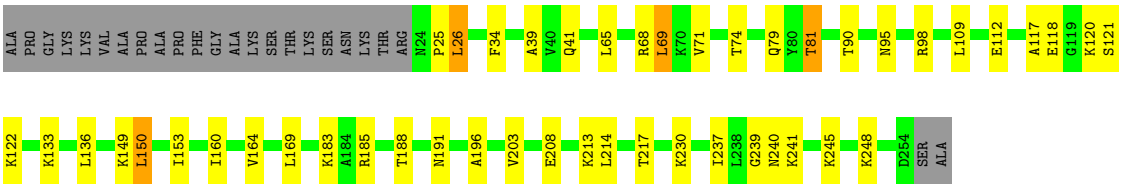
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



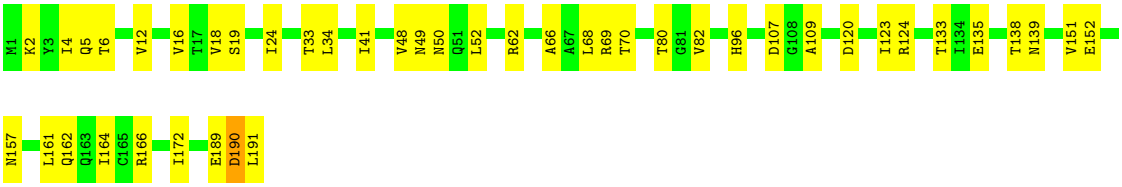
• Molecule 45: 60S ribosomal protein L8-A

Chain l8:



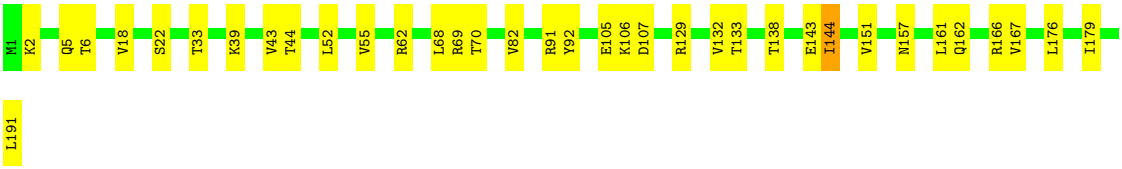
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



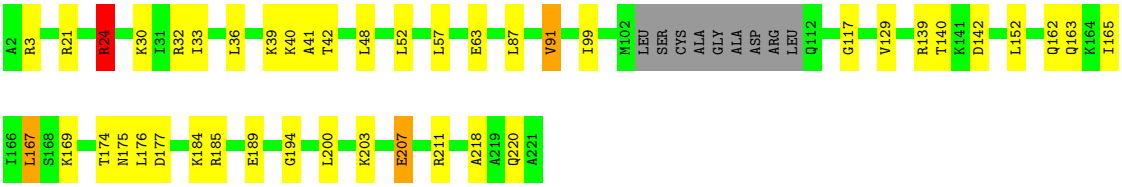
• Molecule 46: 60S ribosomal protein L9-A

Chain l9:



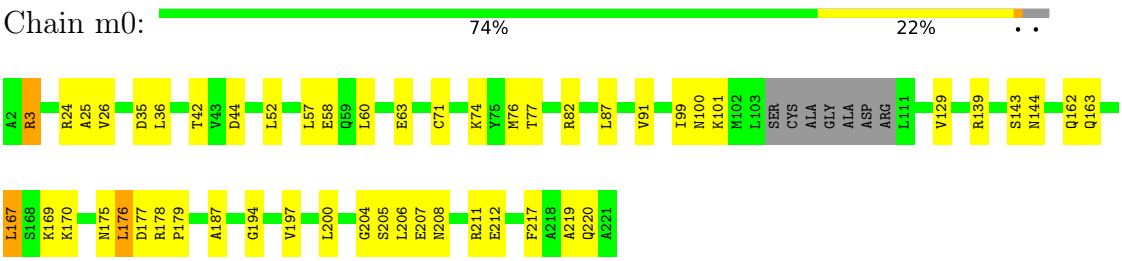
• Molecule 47: 60S ribosomal protein L10

Chain M0:



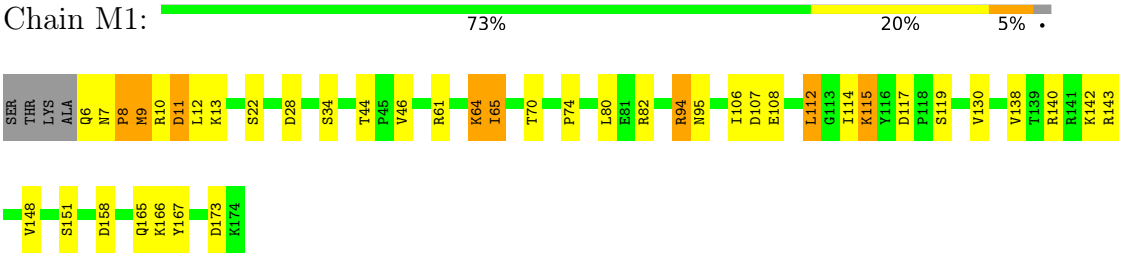
• Molecule 47: 60S ribosomal protein L10

Chain m0:



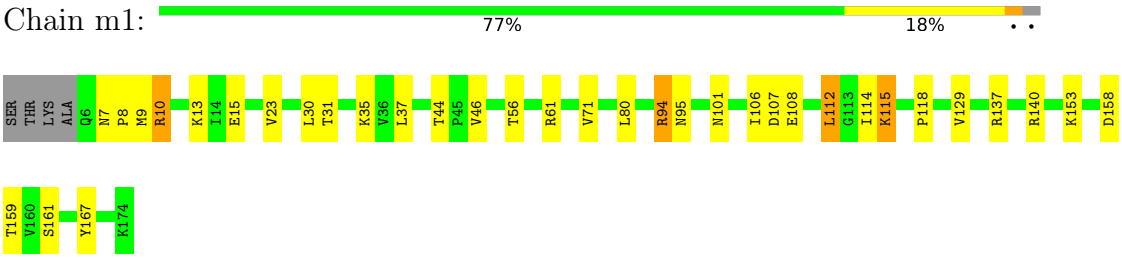
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



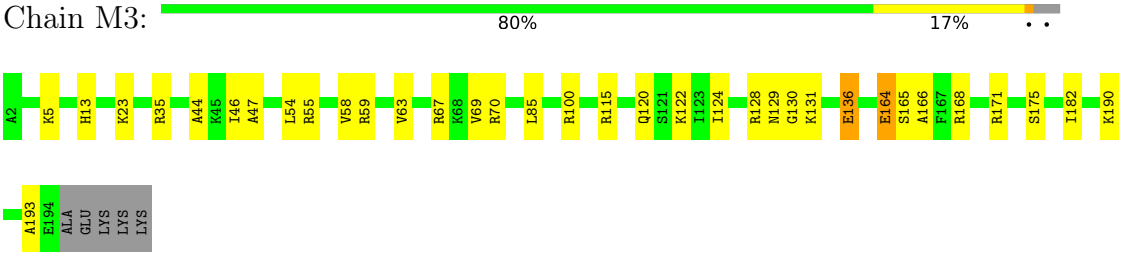
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



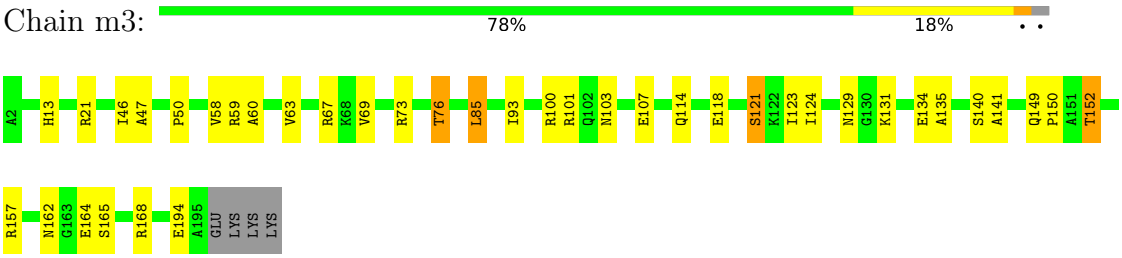
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



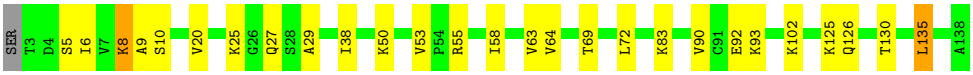
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



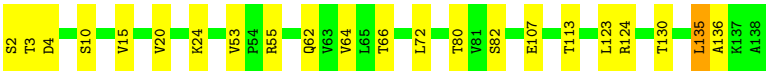
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



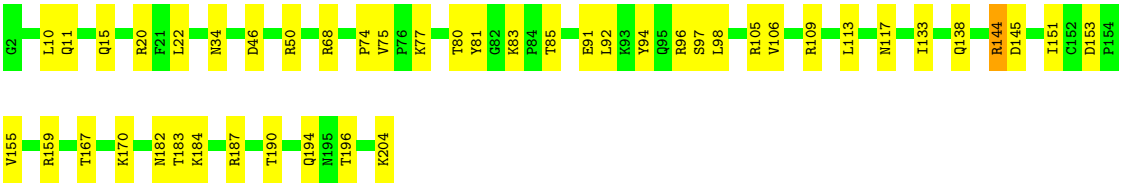
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



• Molecule 51: 60S ribosomal protein L15-A

Chain M5:

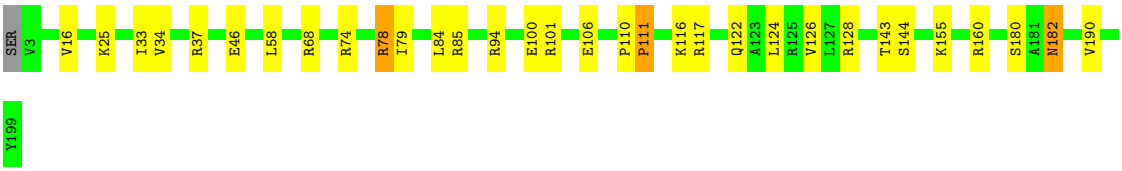


• Molecule 51: 60S ribosomal protein L15-A

Chain m5:

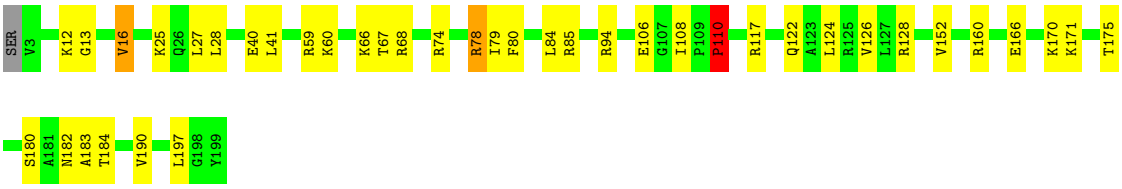
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



• Molecule 53: 60S ribosomal protein L17-A

Chain M7: 79% 20%

A2 S8 T9 G19 R23 V24 T29 T32 A33 Q34 A35 I36 L41 V51 L52 D53 S65 S66 I67 G68 R69 E75 V78 T79 L107 L112 Q118 V119 P123 R126 R127 I136 N137 K138 S142 P143 S144 V157 A160 A161 E162

K163 K164 L168 R171 K180 R181 A184

• Molecule 53: 60S ribosomal protein L17-A

Chain m7: 72% 13% 15%

A2 T9 V24 T29 T32 L41 L52 R56 S66 E75 T79 K80 K86 L94 L107 V114 Q118 V119 N120 R126 R127 I136 N137 K138 S144 E155 A156 VAL ALA LYS ALA ALA GLU LYS LYS VAL VAL ARG LEU THR SER

ARG GLN ARG GLY ARG ILE ALA ALA GLN LYS ARG ILE ALA ALA

• Molecule 54: 60S ribosomal protein L18-A

Chain M8: 85% 14%

G2 I3 D4 T17 V24 Y25 L26 L32 Y33 T34 D41 K46 L49 I57 V64 Q73 E95 T99 R111 A112 K113 E120 Q135 L138 R141 V150 A162 P163 R164 R170 R178 R179 R180 V186

• Molecule 54: 60S ribosomal protein L18-A

Chain m8: 79% 19%

G2 I3 S7 R12 T17 K20 L26 K31 L32 Y33 T34 D41 L49 I57 S63 V64 S65 R66 R69 T80 T86 A91 R92 I93 K98 T99 T100 A112 K113 L127 Q135 L138 R147 V150 R151 K159 G160 K161

I165 R170 R176 G177 R178 R179 R180 V186

• Molecule 55: 60S ribosomal protein L19-A

Chain M9: 88% 12%

A2 T29 L44 V45 K46 V51 K52 K53 A54 V55 R71 R74 S91 R98 L99 R103 R104 L105 L106 I115 D116 K135 L138 K146 L164 R173 D182 A189

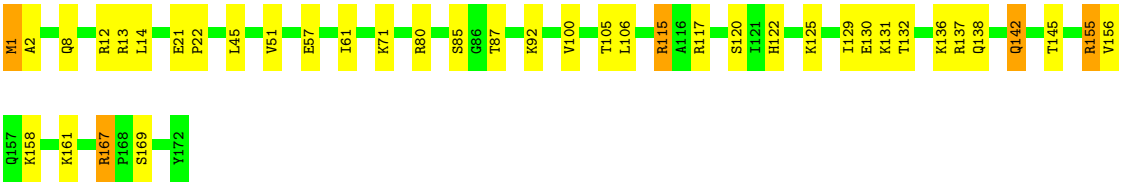
• Molecule 55: 60S ribosomal protein L19-A

Chain m9: 82% 16%

A2 Q7 K8 R9 L10 V17 R20 T29 S30 N36 K43 T49 K52 V55 T56 T63 R71 R74 H75 S76 R88 S91 L99 D116 K117 E126 L138 E152 K153 R162 R163 L164 R167 R170 R173 K180

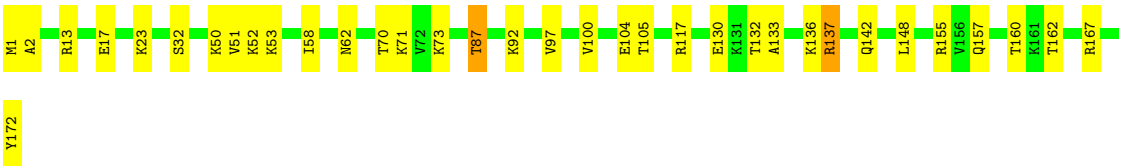
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



• Molecule 56: 60S ribosomal protein L20-A

Chain n0:

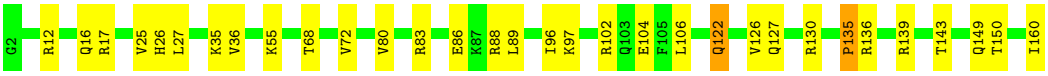


• Molecule 57: 60S ribosomal protein L21-A

Chain N1:

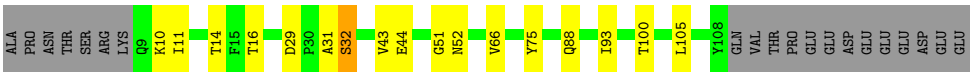
• Molecule 57: 60S ribosomal protein L21-A

Chain n1:



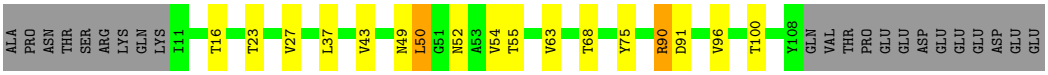
• Molecule 58: 60S ribosomal protein L22-A

Chain N2:



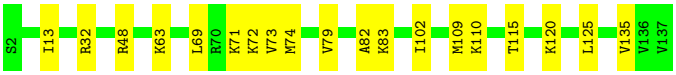
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



• Molecule 59: 60S ribosomal protein L23-A

Chain N3:

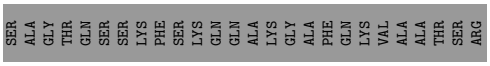


• Molecule 59: 60S ribosomal protein L23-A

Chain n3:

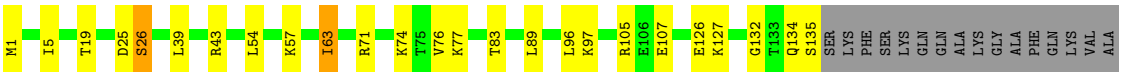
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



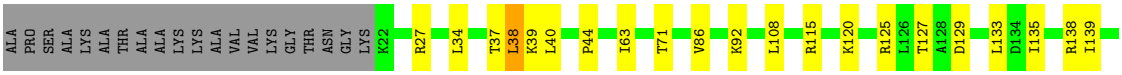
• Molecule 60: 60S ribosomal protein L24-A

Chain n4:



• Molecule 61: 60S ribosomal protein L25

Chain N5:



• Molecule 61: 60S ribosomal protein L25

Chain n5:

ALA PRO SER ALA LYS ALA THR ALA ALA LYS LYS LYS ALA VAL VAL LYS GLY THR ASN GLY LYS LYS A23 L24 K25 V26 R27 L34 T37 L38 K39 L40 P44 K45 Y46 A47 S48 R56 L57 I63 T71 K74 V86 V105 L108 K109 R115 R125 L126

T127 I135 A136 N137 I142

• Molecule 62: 60S ribosomal protein L26-A

Chain N6: 75% 25%

A2 K3 Q4 S5 R13 K17 S36 K37 E38 L39 Q42 I45 I50 R51 R52 D53 D54 E55 V56 L57 R60 K64 I70 Y74 R75 L76 V80 D83 K84 E88 K89 G92 A93 S94 V105 R115 K125 L126 E127

• Molecule 62: 60S ribosomal protein L26-A

Chain n6: 75% 25%

A2 S9 S10 D11 R12 R13 K14 K17 K37 E38 L39 R40 I45 I50 R51 E55 V56 L57 S62 Q66 I70 Y74 R75 L76 V80 D83 K84 K89 S94 V95 V105 K108 L111 Q120 K125 L126 E127

• Molecule 63: 60S ribosomal protein L27-A

Chain N7: 81% 19%

A2 V14 R17 K21 V24 D30 K34 S35 H36 I46 T54 K60 K64 N78 L81 P82 T83 T86 E90 S97 E102 Q103 E108 E109 E120 R121 G125 L134 R135 F136

• Molecule 63: 60S ribosomal protein L27-A

Chain n7: 80% 16%

A2 L5 V14 R15 G16 R17 V24 K34 I46 K52 K56 R65 I72 K73 Y74 V75 L81 P82 T83 T86 T98 E99 T100 F101 E102 Q103 R121 G125 K126 N127 Q128 W129 L134 R135 F136

• Molecule 64: 60S ribosomal protein L28

Chain N8: 79% 18%

P2 S3 R4 F5 T6 K7 T8 R9 K10 V15 K19 K24 R32 G33 M34 R42 D46 K47 G57 Y60 A66 K70 D76 K77 L78 D85 L91 K92 K96 K115 G116 R117 N120 V130 L133 A134 E135 R139 I148 A149

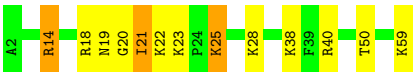
• Molecule 64: 60S ribosomal protein L28

Chain n8: 80% 18%

P2 S3 R4 F5 T6 K7 T8 R9 K10 K24 H25 R26 K27 H28 R42 D46 K47 V56 Y60 A66 D76 K77 L78 I82 D85 K86 R87 L91 E97 T98 K115 V123 R128 F129 K132 L133 R139 A149

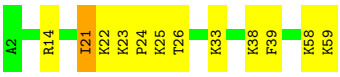
• Molecule 65: 60S ribosomal protein L29

Chain N9:



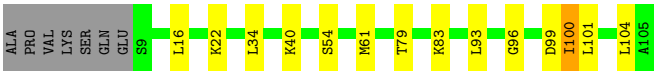
• Molecule 65: 60S ribosomal protein L29

Chain n9:



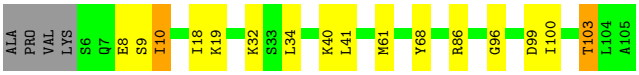
• Molecule 66: 60S ribosomal protein L30

Chain O0:



• Molecule 66: 60S ribosomal protein L30

Chain o0:

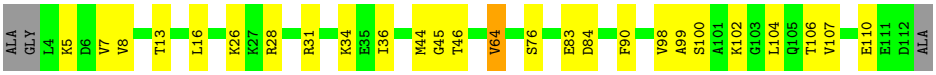


• Molecule 67: 60S ribosomal protein L31-A

Chain O1:

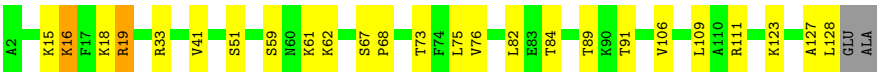
• Molecule 67: 60S ribosomal protein L31-A

Chain o1:



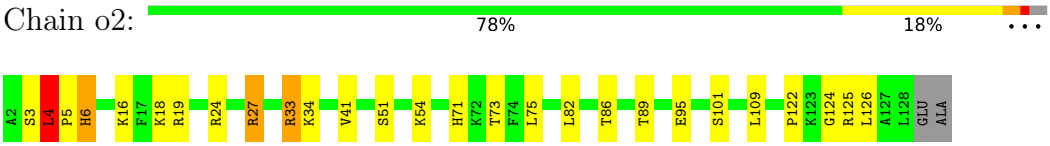
• Molecule 68: 60S ribosomal protein L32

Chain O2:



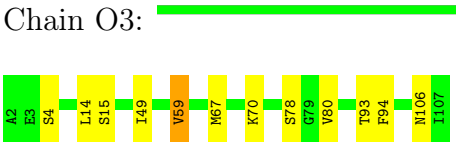
• Molecule 68: 60S ribosomal protein L32

Chain o2:



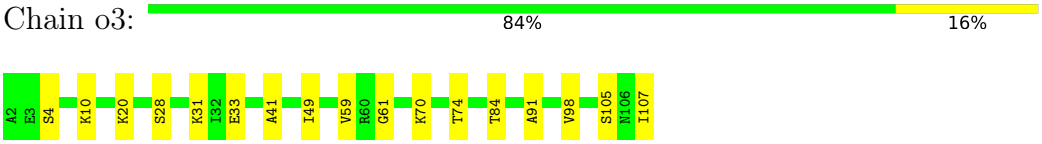
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



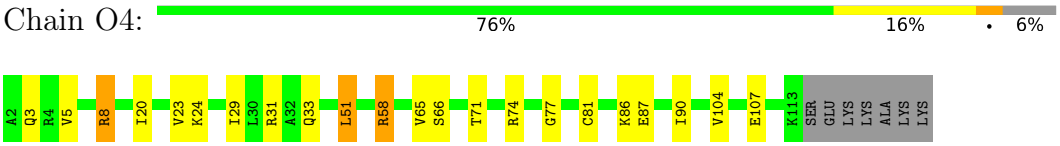
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



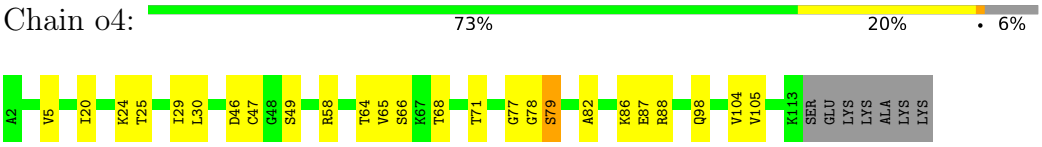
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



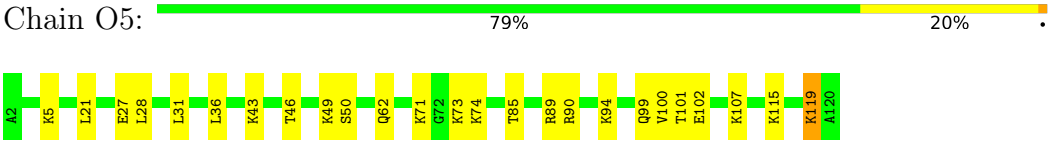
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:



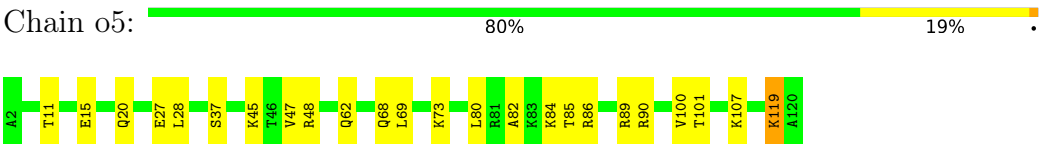
- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



- Molecule 71: 60S ribosomal protein L35-A

Chain o5:

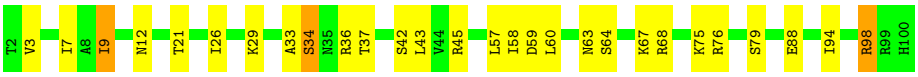


- Molecule 72: 60S ribosomal protein L36-A

Chain O6: 81% 17%

• Molecule 72: 60S ribosomal protein L36-A

Chain o6: 72% 25%

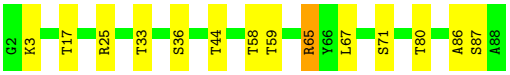


• Molecule 73: 60S ribosomal protein L37-A

Chain O7: 84% 15%

• Molecule 73: 60S ribosomal protein L37-A

Chain o7: 84% 15%



• Molecule 74: 60S ribosomal protein L38

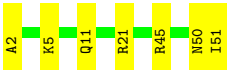
Chain O8: 77% 23%

• Molecule 74: 60S ribosomal protein L38

Chain o8: 78% 21%

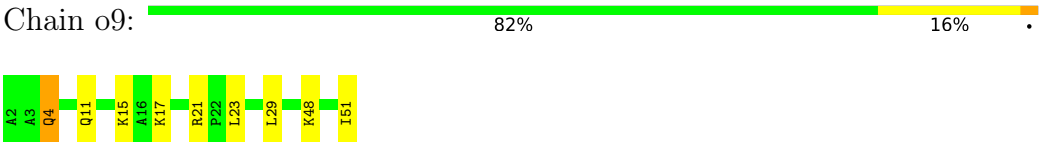
• Molecule 75: 60S ribosomal protein L39

Chain O9: 86% 14%



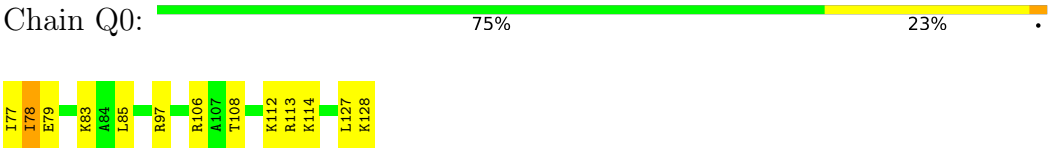
• Molecule 75: 60S ribosomal protein L39

Chain o9:



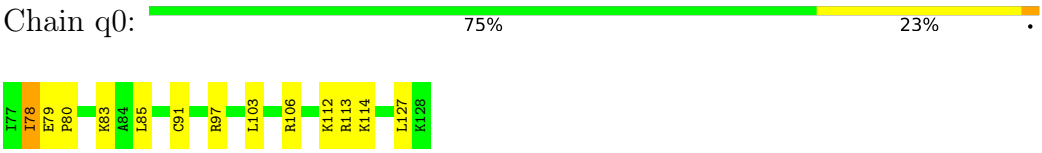
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



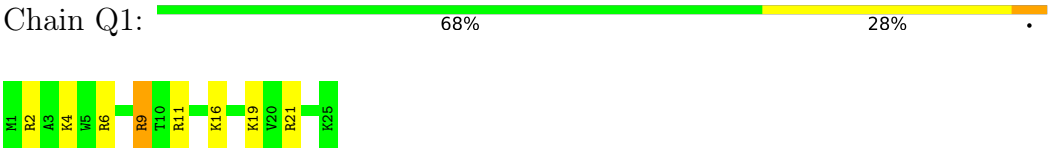
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



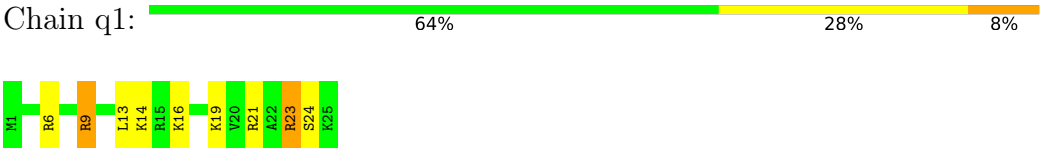
• Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



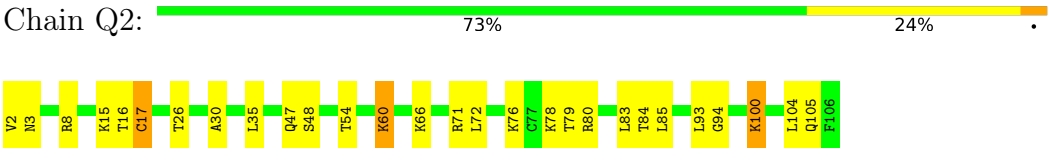
• Molecule 77: 60S ribosomal protein L41-A

Chain q1:



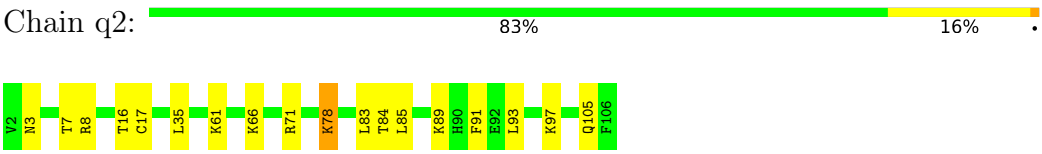
• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



• Molecule 78: 60S ribosomal protein L42-A

Chain q2:



• Molecule 79: 60S ribosomal protein L43-A

Chain Q3: 81% 16% •

A2 K7 T11 Q25 K45 T46 R49 G50 A51 T56 C57 S58 C59 C60 V64 T73 T78 T82 I83 R84 V90 E91 A92

• Molecule 79: 60S ribosomal protein L43-A

Chain q3: 90% 10%

A2 K3 R4 S20 R24 S40 F41 C42 I54 W55 T56 T70 V71 S72 A92

• Molecule 80: 40S ribosomal protein S30-A

Chain e0: 74% 24% •

A2 K13 E22 K23 K26 K29 L38 T41 R42 R43 F44 V47 T48 L49 V50 N51 R54 R55 P60 S61 V62 Q63

• Molecule 81: Suppressor protein STM1

Chain sM: 29% 8% • 62%

MET SER ASN PRO PHE ASP LEU LEU ALA ASN ASP VAL GLU ASP ALA ASP VAL VAL VAL LEU PRO PRO K23 T30 K33 A42 D43 P44 S45 K46 A47 R48 K49 N50 R51 P52 R53 P54 S55 I61 R62 D63 K64 T65 A66 G67 R68 K74 D75 V76 T77 D78 T82

S85 ASN THR ARG ARG ALA THR ASP ARG HIS SER ARG THR GLY LYS THR ASP THR LYS LYS LYS VAL ASN GLN GLY TRP GLY ASP ASP LYS LYS GLU LEU SER A119 E139 ASP ALA GLY LYS PRO LYS THR ALA GLN LEU SER LEU GLN ASP TYR L155 P167 V172 E173 L174 ASP

ALA GLU ARG ILE GLU THR ALA GLU LYS GLU ALA TYR VAL PRO ALA THR LYS VAL LYS ASN VAL LYS SER LYS GLN LEU LYS THR LYS GLU TYR LEU GLU PHE ASP ALA THR PHE VAL GLU SER ASN THR ARG LYS ASN PHE GLY ASP ARG ASN ASN ASN SER ARG ASN ASN PHE ASN ASN

ARG ARG GLY GLY ARG GLY ALA ARG LYS GLY ASN ASN THR ALA ASN ALA THR ASN SER ALA ASN THR VAL GLN LYS ASN ARG ASN ILE ASP VAL SER ASN LEU PRO SER LEU ALA

• Molecule 82: unknown protein chain m2

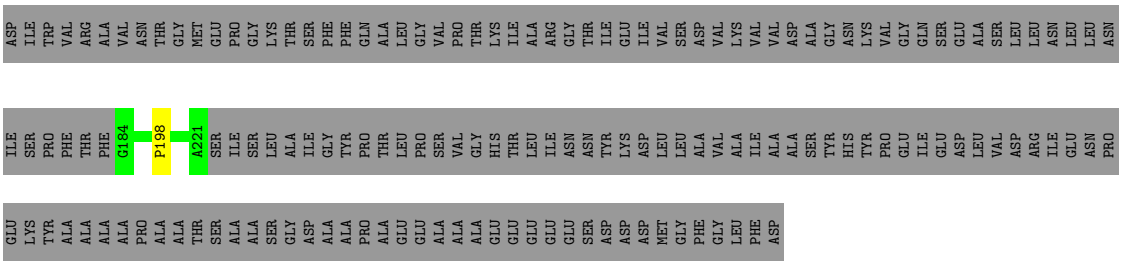
Chain m2: 94% 6%

X9 X23 UNK UNK UNK UNK X28 X52 UNK X54 X163 UNK UNK UNK UNK UNK

• Molecule 83: 60S acidic ribosomal protein P0

Chain p0: 37% 9% 54%

GLY G3 I4 R5 E6 K7 E10 K14 L15 L25 V33 H39 R42 K43 E44 R48 V51 L52 K55 L67 S68 D69 L70 E74 K75 L76 V80 K81 V84 L93 K97 R104 A107 PRO ALA ARG ALA GLY ALA VAL ALA PRO GLU



• Molecule 84: unknown protein chain p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

• Molecule 85: unknown protein chain p2

Chain p2: 100%

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	435.26Å 287.54Å 304.02Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	73.99 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (73.99-3.00)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.211 , 0.259	Depositor
Wilson B-factor (Å^2)	64.9	Xtriage
Anisotropy	0.199	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411211	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: ZN, 3KD, OHX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	2	0.71	1/41698 (0.0%)	1.27	275/64972 (0.4%)
1	6	0.88	13/42765 (0.0%)	1.38	436/66634 (0.7%)
2	S0	0.43	0/1617	0.66	0/2215
2	s0	0.49	0/1623	0.71	0/2222
3	S1	0.35	0/1735	0.63	1/2335 (0.0%)
3	s1	0.48	0/1748	0.66	0/2352
4	S2	0.49	0/1665	0.67	0/2263
4	s2	0.57	0/1665	0.75	2/2263 (0.1%)
5	S3	0.48	0/1759	0.66	1/2368 (0.0%)
5	s3	0.42	0/1759	0.60	0/2368
6	S4	0.46	0/2109	0.73	1/2839 (0.0%)
6	s4	0.55	0/2109	0.78	1/2839 (0.0%)
7	S5	0.36	0/1629	0.58	0/2202
7	s5	0.44	0/1629	0.64	0/2202
8	S6	0.44	0/1823	0.64	0/2439
8	s6	0.54	0/1779	0.70	0/2379
9	S7	0.42	0/1506	0.65	0/2028
9	s7	0.45	0/1516	0.67	1/2043 (0.0%)
10	S8	0.54	0/1514	0.72	1/2021 (0.0%)
10	s8	0.60	0/1514	0.76	1/2021 (0.0%)
11	S9	0.47	0/1519	0.64	0/2035
11	s9	0.55	0/1519	0.76	2/2035 (0.1%)
12	C0	0.42	0/790	0.70	1/1069 (0.1%)
12	c0	0.36	0/777	0.63	3/1049 (0.3%)
13	C1	0.55	0/1240	0.66	0/1675
13	c1	0.61	0/1194	0.77	0/1610
14	C2	0.38	0/900	0.62	0/1224
14	c2	0.28	0/900	0.56	0/1224
15	C3	0.47	0/1215	0.68	2/1638 (0.1%)
15	c3	0.56	0/1215	0.73	0/1638
16	C4	0.36	0/901	0.63	0/1217
16	c4	0.52	0/960	0.72	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.44	0/998	0.68	0/1341
17	c5	0.45	0/1060	0.66	0/1426
18	C6	0.41	0/1125	0.69	2/1510 (0.1%)
18	c6	0.49	0/1131	0.69	0/1518
19	C7	0.41	0/935	0.62	0/1254
19	c7	0.48	0/914	0.71	0/1224
20	C8	0.42	0/1211	0.63	0/1628
20	c8	0.49	0/1211	0.71	2/1628 (0.1%)
21	C9	0.41	0/1130	0.63	0/1517
21	c9	0.50	0/1130	0.70	2/1517 (0.1%)
22	D0	0.45	0/865	0.64	0/1169
22	d0	0.46	0/892	0.65	0/1205
23	D1	0.44	0/693	0.62	0/935
23	d1	0.54	0/693	0.71	0/935
24	D2	0.48	0/1038	0.73	3/1395 (0.2%)
24	d2	0.59	0/1038	0.74	1/1395 (0.1%)
25	D3	0.60	0/1139	0.77	1/1518 (0.1%)
25	d3	0.70	0/1139	0.89	3/1518 (0.2%)
26	D4	0.44	0/1087	0.63	0/1449
26	d4	0.53	0/1087	0.73	0/1449
27	D5	0.39	0/571	0.68	0/768
27	d5	0.41	0/566	0.63	0/761
28	D6	0.43	0/782	0.67	0/1047
28	d6	0.56	0/782	0.71	0/1047
29	D7	0.42	0/620	0.66	0/838
29	d7	0.46	0/620	0.66	0/838
30	D8	0.35	0/499	0.57	0/670
30	d8	0.44	0/499	0.64	0/670
31	D9	0.50	0/452	0.70	1/600 (0.2%)
31	d9	0.50	0/452	0.64	0/600
32	E0	0.46	0/483	0.63	0/643
33	E1	0.42	0/577	0.78	0/770
33	e1	0.39	0/619	0.72	0/822
34	SR	0.37	0/2494	0.57	0/3393
34	sR	0.38	0/2495	0.56	0/3395
35	SM	0.48	0/1113	0.70	2/1502 (0.1%)
36	1	1.16	153/75394 (0.2%)	1.66	1837/117545 (1.6%)
36	5	1.20	178/75414 (0.2%)	1.67	1863/117575 (1.6%)
37	3	0.95	2/2883 (0.1%)	1.47	39/4491 (0.9%)
37	7	1.16	5/2883 (0.2%)	1.62	57/4491 (1.3%)
38	4	1.13	5/3746 (0.1%)	1.66	86/5832 (1.5%)
38	8	0.98	2/3746 (0.1%)	1.48	42/5832 (0.7%)
39	L2	0.74	0/1948	0.84	3/2617 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	l2	0.71	0/1946	0.86	2/2614 (0.1%)
40	L3	0.74	1/3146 (0.0%)	0.82	1/4228 (0.0%)
40	l3	0.88	1/3146 (0.0%)	0.89	2/4228 (0.0%)
41	L4	0.84	1/2800 (0.0%)	0.94	7/3790 (0.2%)
41	l4	0.74	1/2800 (0.0%)	0.90	6/3790 (0.2%)
42	L5	0.57	0/2425	0.69	1/3271 (0.0%)
42	l5	0.73	0/2408	0.82	1/3248 (0.0%)
43	L6	0.76	0/1260	0.84	0/1694
43	l6	0.78	0/1269	0.84	1/1705 (0.1%)
44	L7	0.78	1/1821 (0.1%)	0.90	2/2451 (0.1%)
44	l7	0.85	1/1828 (0.1%)	0.90	4/2461 (0.2%)
45	L8	0.55	0/1836	0.70	1/2481 (0.0%)
45	l8	0.51	0/1795	0.65	1/2429 (0.0%)
46	L9	0.65	0/1539	0.77	1/2073 (0.0%)
46	l9	0.77	0/1539	0.85	0/2073
47	M0	0.71	0/1741	0.84	3/2335 (0.1%)
47	m0	0.75	0/1758	0.87	2/2358 (0.1%)
48	M1	0.54	0/1374	0.73	1/1842 (0.1%)
48	m1	0.65	0/1374	0.82	2/1842 (0.1%)
49	M3	0.75	0/1568	0.86	0/2106
49	m3	0.69	0/1573	0.85	3/2113 (0.1%)
50	M4	0.73	0/1068	0.80	1/1438 (0.1%)
50	m4	0.82	0/1074	0.85	0/1446
51	M5	0.77	0/1757	0.85	0/2354
51	m5	0.66	0/1757	0.79	0/2354
52	M6	0.86	1/1585 (0.1%)	0.92	3/2128 (0.1%)
52	m6	1.02	5/1585 (0.3%)	0.98	7/2128 (0.3%)
53	M7	0.80	0/1443	0.85	2/1944 (0.1%)
53	m7	0.89	0/1250	0.89	0/1683
54	M8	0.79	0/1465	0.92	3/1965 (0.2%)
54	m8	0.73	0/1465	0.95	2/1965 (0.1%)
55	M9	0.57	0/1538	0.69	0/2050
55	m9	0.61	0/1538	0.70	0/2050
56	N0	0.78	0/1481	0.87	4/1990 (0.2%)
56	n0	0.87	0/1481	0.91	2/1990 (0.1%)
57	N1	0.78	0/1300	0.82	0/1743
57	n1	0.85	1/1300 (0.1%)	0.86	1/1743 (0.1%)
58	N2	0.42	0/812	0.62	0/1099
58	n2	0.51	0/794	0.65	0/1076
59	N3	0.70	0/1018	0.81	0/1369
59	n3	0.87	0/1018	0.98	1/1369 (0.1%)
60	N4	0.56	0/712	0.68	0/958
60	n4	0.69	0/1052	0.75	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
61	N5	0.63	0/979	0.80	2/1321 (0.2%)
61	n5	0.65	0/974	0.77	0/1314
62	N6	0.68	0/1004	0.90	1/1341 (0.1%)
62	n6	0.71	1/1004 (0.1%)	0.84	0/1341
63	N7	0.52	0/1118	0.66	0/1497
63	n7	0.46	0/1118	0.63	0/1497
64	N8	0.82	0/1204	0.92	2/1612 (0.1%)
64	n8	0.79	0/1204	0.90	0/1612
65	N9	0.67	0/473	0.83	2/629 (0.3%)
65	n9	0.80	0/473	0.97	0/629
66	O0	0.48	0/751	0.66	0/1008
66	o0	0.49	0/775	0.65	0/1040
67	O1	0.60	0/890	0.72	0/1196
67	o1	0.76	0/897	0.86	0/1205
68	O2	0.85	0/1041	0.89	2/1394 (0.1%)
68	o2	0.82	0/1041	0.94	2/1394 (0.1%)
69	O3	0.95	0/868	0.91	1/1168 (0.1%)
69	o3	0.92	0/868	0.84	0/1168
70	O4	0.58	0/890	0.82	4/1189 (0.3%)
70	o4	0.59	0/890	0.78	0/1189
71	O5	0.70	0/978	0.81	1/1301 (0.1%)
71	o5	0.59	0/974	0.72	0/1297
72	O6	0.64	0/778	0.79	0/1034
72	o6	0.54	0/777	0.73	0/1033
73	O7	0.78	0/696	0.90	1/923 (0.1%)
73	o7	0.75	0/696	0.85	1/923 (0.1%)
74	O8	0.51	0/618	0.64	0/826
74	o8	0.42	0/614	0.61	0/822
75	O9	0.83	1/443 (0.2%)	0.90	0/588
75	o9	0.76	0/443	0.83	0/588
76	Q0	0.73	0/423	0.84	0/562
76	q0	0.95	0/423	1.03	1/562 (0.2%)
77	Q1	0.72	0/234	0.96	1/300 (0.3%)
77	q1	0.82	0/234	1.05	2/300 (0.7%)
78	Q2	0.93	1/860 (0.1%)	0.85	1/1136 (0.1%)
78	q2	0.82	1/860 (0.1%)	0.83	0/1136
79	Q3	0.74	0/701	0.85	0/934
79	q3	0.72	0/701	0.81	0/934
80	e0	0.56	0/499	0.74	0/665
81	sM	0.50	0/684	0.69	1/925 (0.1%)
83	p0	0.46	0/1092	0.61	0/1474
All	All	0.90	376/430075 (0.1%)	1.30	4764/631366 (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
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	2
17	c5	0	1
18	c6	0	1
19	C7	0	2
22	d0	0	1
27	D5	0	2
28	D6	0	1
33	E1	0	1
39	l2	0	1
42	l5	0	2
43	L6	0	1
43	l6	0	1
44	l7	0	2
45	L8	0	1
48	M1	0	2
51	M5	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
55	m9	0	1
56	N0	0	2
56	n0	0	2
57	N1	0	1
62	n6	0	1
64	N8	0	1
64	n8	0	2
65	N9	0	1
67	O1	0	1
67	o1	0	2
All	All	0	43

All (376) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	15.91	2.09	1.82
36	5	1152	G	N9-C4	-12.55	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	11.87	2.02	1.82
36	1	3181	C	N3-C4	-9.25	1.27	1.33
36	5	2138	A	N7-C5	-8.87	1.33	1.39
36	5	953	G	C5-C4	-8.69	1.32	1.38
36	5	1152	G	N3-C4	-8.53	1.29	1.35
36	5	2980	U	C2-O2	-8.15	1.15	1.22
36	5	953	G	N7-C5	-7.97	1.34	1.39
36	5	2987	A	N7-C5	-7.84	1.34	1.39
36	5	647	A	N9-C4	-7.81	1.33	1.37
36	5	953	G	C5-C6	-7.58	1.34	1.42
36	5	642	U	C2-N3	-7.47	1.32	1.37
36	1	200	C	N1-C6	-7.42	1.32	1.37
36	1	1394	A	N9-C4	-7.29	1.33	1.37
36	1	637	C	N1-C6	-7.28	1.32	1.37
36	5	1332	A	N3-C4	-7.17	1.30	1.34
36	1	1103	A	N9-C4	7.17	1.42	1.37
36	1	1452	A	N9-C4	-7.15	1.33	1.37
36	5	1847	A	N9-C4	-7.12	1.33	1.37
36	1	34	A	N9-C4	-7.09	1.33	1.37
36	5	1152	G	N1-C2	7.04	1.43	1.37
36	1	1547	G	C5-C4	-7.04	1.33	1.38
36	1	2281	A	N9-C4	-7.04	1.33	1.37
36	5	895	A	N9-C4	-7.03	1.33	1.37
36	5	924	G	C2-N3	-7.01	1.27	1.32
57	n1	104	GLU	CB-CG	6.99	1.65	1.52
36	5	2335	G	N3-C4	-6.96	1.30	1.35
36	5	631	U	C2-N3	-6.94	1.32	1.37
41	l4	94	CYS	CB-SG	-6.91	1.70	1.82
36	5	523	A	N9-C4	-6.90	1.33	1.37
36	1	1143	A	N9-C4	-6.88	1.33	1.37
36	5	2280	A	N9-C4	-6.83	1.33	1.37
36	5	2636	A	C6-N1	-6.81	1.30	1.35
36	1	1116	G	N7-C5	-6.81	1.35	1.39
36	5	1332	A	C5-C4	-6.81	1.33	1.38
52	m6	16	VAL	CB-CG2	-6.80	1.38	1.52
36	5	1199	C	N1-C6	-6.78	1.33	1.37
36	5	2704	A	N9-C4	-6.77	1.33	1.37
36	1	1114	U	C2-N3	-6.72	1.33	1.37
36	5	2830	G	N3-C4	-6.71	1.30	1.35
36	5	960	U	N1-C2	6.70	1.44	1.38
36	5	2726	C	N3-C4	-6.70	1.29	1.33
36	1	1103	A	N3-C4	6.67	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	644	G	N7-C5	-6.66	1.35	1.39
36	1	2396	G	N9-C8	-6.62	1.33	1.37
36	5	1304	A	N3-C4	6.61	1.38	1.34
36	5	3008	A	N9-C4	-6.59	1.33	1.37
36	5	2335	G	C5-C4	-6.58	1.33	1.38
40	L3	200	GLU	CG-CD	6.56	1.61	1.51
36	5	40	A	N7-C5	-6.55	1.35	1.39
36	5	2147	A	C5-C6	-6.53	1.35	1.41
36	5	2943	G	N7-C5	-6.53	1.35	1.39
36	5	3106	A	N7-C5	-6.51	1.35	1.39
36	1	1132	C	N3-C4	-6.51	1.29	1.33
36	5	1841	A	N7-C5	-6.50	1.35	1.39
36	1	2911	A	N9-C4	-6.47	1.33	1.37
36	5	416	A	N7-C5	-6.42	1.35	1.39
36	1	49	A	N9-C4	-6.42	1.34	1.37
36	1	2356	A	N9-C4	-6.39	1.34	1.37
1	6	163	G	N9-C4	-6.39	1.32	1.38
36	1	343	U	N3-C4	-6.38	1.32	1.38
36	1	970	A	N3-C4	-6.38	1.31	1.34
36	5	367	A	N9-C4	-6.35	1.34	1.37
36	5	1149	G	N9-C8	-6.34	1.33	1.37
36	1	2406	C	N1-C6	-6.33	1.33	1.37
36	1	3209	A	C5-C4	6.31	1.43	1.38
36	5	1143	A	N9-C4	-6.28	1.34	1.37
36	5	802	C	N1-C6	-6.27	1.33	1.37
36	5	2944	U	C2-N3	-6.27	1.33	1.37
36	1	2800	G	C5-C4	-6.26	1.33	1.38
75	O9	2	ALA	CA-CB	-6.23	1.39	1.52
36	5	2894	C	C4-C5	-6.23	1.38	1.43
36	5	1152	G	C5-C6	-6.21	1.36	1.42
52	m6	80	PHE	CB-CG	-6.20	1.40	1.51
36	1	1143	A	N3-C4	-6.18	1.31	1.34
36	1	1159	A	C6-N1	-6.18	1.31	1.35
36	1	2147	A	N9-C4	-6.17	1.34	1.37
36	1	338	A	N7-C5	-6.17	1.35	1.39
36	1	1116	G	N1-C2	-6.16	1.32	1.37
36	5	1304	A	N7-C5	-6.15	1.35	1.39
36	1	2147	A	N3-C4	-6.13	1.31	1.34
36	1	2169	G	C5-C6	6.12	1.48	1.42
38	4	52	A	N3-C4	-6.11	1.31	1.34
36	5	883	A	C5-C4	-6.10	1.34	1.38
36	5	634	C	C4-C5	-6.10	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2915	U	C2-N3	-6.09	1.33	1.37
36	1	876	A	N3-C4	6.08	1.38	1.34
36	1	1154	A	N7-C5	-6.08	1.35	1.39
36	1	2762	A	N3-C4	-6.08	1.31	1.34
36	1	1382	G	C5-C4	-6.08	1.34	1.38
36	1	2419	A	N9-C4	-6.08	1.34	1.37
36	5	699	A	N9-C4	-6.05	1.34	1.37
36	5	1476	G	N9-C4	-6.05	1.33	1.38
36	5	1311	G	C5-C4	-6.04	1.34	1.38
36	5	1149	G	N7-C5	-6.04	1.35	1.39
36	1	3278	C	N3-C4	-6.03	1.29	1.33
62	n6	55	GLU	CG-CD	6.03	1.60	1.51
36	5	36	C	C4-C5	-6.01	1.38	1.43
36	1	1308	A	N3-C4	-6.01	1.31	1.34
36	1	1392	G	C5-C4	-6.00	1.34	1.38
36	5	2727	A	N7-C5	-6.00	1.35	1.39
36	1	638	C	N1-C6	-6.00	1.33	1.37
36	5	1849	C	N3-C4	-5.99	1.29	1.33
1	6	623	A	N9-C4	-5.98	1.34	1.37
36	1	960	U	N3-C4	5.97	1.43	1.38
36	1	1133	A	C5-C4	-5.96	1.34	1.38
36	5	3004	C	N1-C6	-5.96	1.33	1.37
36	1	3142	A	N3-C4	-5.95	1.31	1.34
36	1	1159	A	N3-C4	-5.93	1.31	1.34
36	1	1367	G	C5-C6	-5.93	1.36	1.42
1	6	163	G	N3-C4	-5.93	1.31	1.35
36	5	426	G	C5-C4	-5.91	1.34	1.38
36	5	1152	G	C2-N3	-5.90	1.28	1.32
36	1	2910	A	N9-C4	-5.90	1.34	1.37
36	1	661	G	N7-C5	-5.89	1.35	1.39
36	1	895	A	C5-C6	-5.89	1.35	1.41
36	1	1164	G	N7-C5	-5.89	1.35	1.39
36	1	2867	C	N3-C4	-5.89	1.29	1.33
36	5	1863	G	C5-C4	-5.89	1.34	1.38
36	5	1370	G	C6-N1	-5.89	1.35	1.39
36	5	2860	U	C4-O4	5.87	1.28	1.23
36	1	1492	G	C8-N7	-5.87	1.27	1.30
36	5	2953	U	C2-N3	5.87	1.41	1.37
36	5	3095	U	C2-N3	-5.86	1.33	1.37
36	5	1134	G	N3-C4	-5.86	1.31	1.35
36	1	92	G	C5-C4	-5.84	1.34	1.38
36	5	2903	A	N9-C4	-5.84	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	426	G	N9-C8	-5.83	1.33	1.37
36	5	2813	A	N7-C5	-5.82	1.35	1.39
36	5	1103	A	N9-C4	5.81	1.41	1.37
36	1	2917	G	C5-C4	-5.80	1.34	1.38
36	5	2799	A	C6-N1	-5.80	1.31	1.35
36	5	36	C	N1-C2	-5.79	1.34	1.40
1	2	992	A	N9-C4	-5.79	1.34	1.37
36	5	1307	G	P-O5'	-5.79	1.53	1.59
36	5	2419	A	P-O5'	5.79	1.65	1.59
36	5	1320	C	C4-C5	-5.78	1.38	1.43
36	1	895	A	N7-C5	-5.78	1.35	1.39
36	1	979	U	N1-C2	5.77	1.43	1.38
36	1	659	G	N7-C5	-5.77	1.35	1.39
36	5	895	A	N3-C4	-5.75	1.31	1.34
36	1	2617	U	N3-C4	-5.74	1.33	1.38
36	5	872	U	C4-O4	-5.73	1.19	1.23
36	5	970	A	N9-C4	-5.73	1.34	1.37
37	7	102	A	N9-C4	-5.72	1.34	1.37
36	1	980	A	N9-C4	5.72	1.41	1.37
36	5	1169	A	N3-C4	-5.71	1.31	1.34
36	1	1153	A	N7-C5	-5.71	1.35	1.39
36	5	2899	C	N3-C4	-5.70	1.29	1.33
36	1	2714	G	N9-C4	-5.69	1.33	1.38
36	5	1476	G	C5-C4	-5.69	1.34	1.38
36	1	2761	G	N9-C8	-5.68	1.33	1.37
36	5	2291	A	N9-C4	-5.68	1.34	1.37
36	5	2871	G	C6-N1	-5.68	1.35	1.39
36	5	2993	G	C5-C4	-5.66	1.34	1.38
36	1	407	A	C5-C6	-5.66	1.35	1.41
36	5	924	G	C5-C4	-5.65	1.34	1.38
36	5	1103	A	N3-C4	5.65	1.38	1.34
36	1	2802	A	C8-N7	5.63	1.35	1.31
36	1	2917	G	N7-C5	-5.63	1.35	1.39
36	1	1310	G	C6-N1	-5.61	1.35	1.39
36	5	1311	G	C8-N7	-5.61	1.27	1.30
1	6	17	C	N3-C4	-5.61	1.30	1.33
36	5	3042	U	C4-O4	-5.60	1.19	1.23
1	6	1137	A	C5-C4	-5.60	1.34	1.38
36	1	952	A	N3-C4	-5.59	1.31	1.34
36	1	407	A	N7-C5	-5.59	1.35	1.39
36	1	1129	A	C5-C6	-5.59	1.36	1.41
36	5	2823	G	N7-C5	-5.58	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2620	G	N1-C2	-5.58	1.33	1.37
36	1	1468	A	N7-C5	-5.57	1.35	1.39
36	5	2411	U	C2-N3	-5.57	1.33	1.37
36	5	2342	U	C2-N3	-5.57	1.33	1.37
36	1	1495	U	N3-C4	-5.56	1.33	1.38
36	1	942	U	C5-C6	-5.55	1.29	1.34
36	5	3210	A	N9-C4	-5.54	1.34	1.37
36	1	2411	U	C2-O2	-5.54	1.17	1.22
52	m6	40	GLU	CG-CD	5.54	1.60	1.51
36	5	639	G	N9-C4	-5.54	1.33	1.38
36	1	1377	G	N1-C2	-5.53	1.33	1.37
36	1	1127	G	C5-C6	-5.53	1.36	1.42
36	1	1308	A	N7-C5	-5.53	1.35	1.39
36	5	2643	A	N9-C4	-5.52	1.34	1.37
36	1	2598	G	C5-C4	-5.51	1.34	1.38
36	1	505	G	N3-C4	-5.51	1.31	1.35
36	5	649	A	C5-C6	-5.50	1.36	1.41
1	6	1119	G	N7-C5	-5.49	1.35	1.39
36	1	369	A	N3-C4	-5.49	1.31	1.34
36	1	1436	U	C4-C5	-5.48	1.38	1.43
38	4	28	C	N1-C6	-5.48	1.33	1.37
1	6	1746	A	N7-C5	-5.47	1.35	1.39
36	1	3130	A	N7-C5	-5.47	1.35	1.39
36	5	1451	C	N1-C6	-5.47	1.33	1.37
36	1	1141	C	N1-C6	-5.47	1.33	1.37
52	M6	100	GLU	CD-OE1	5.46	1.31	1.25
36	5	1338	C	N1-C6	-5.46	1.33	1.37
36	5	1132	C	N3-C4	-5.46	1.30	1.33
36	5	2808	A	N7-C5	-5.46	1.35	1.39
36	1	645	A	N7-C5	-5.46	1.35	1.39
36	1	2147	A	C5-C4	-5.45	1.34	1.38
36	5	101	G	C6-N1	-5.45	1.35	1.39
36	1	3087	A	N3-C4	-5.45	1.31	1.34
36	5	1331	U	C5-C6	-5.43	1.29	1.34
36	1	957	C	N1-C6	-5.43	1.33	1.37
36	1	1492	G	N7-C5	-5.43	1.35	1.39
36	1	1416	C	N3-C4	-5.43	1.30	1.33
37	3	83	U	C2-N3	-5.42	1.33	1.37
36	1	1330	A	C5-C4	-5.42	1.34	1.38
36	5	407	A	N7-C5	-5.42	1.35	1.39
36	1	1179	A	C6-N1	-5.42	1.31	1.35
36	1	910	G	N7-C5	-5.41	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2335	G	N1-C2	-5.41	1.33	1.37
52	m6	40	GLU	CD-OE1	5.41	1.31	1.25
36	5	1301	A	C5-C6	-5.40	1.36	1.41
36	5	2639	G	N7-C5	-5.40	1.36	1.39
36	5	2871	G	N7-C5	5.40	1.42	1.39
36	1	2714	G	N9-C8	5.40	1.41	1.37
1	6	1744	A	N9-C4	-5.40	1.34	1.37
36	5	2924	U	N1-C2	-5.40	1.33	1.38
36	1	699	A	N9-C4	-5.39	1.34	1.37
1	6	542	A	N7-C5	-5.39	1.36	1.39
36	1	2652	U	N3-C4	-5.38	1.33	1.38
36	1	1102	A	N9-C4	-5.38	1.34	1.37
36	1	1556	C	N1-C2	5.38	1.45	1.40
36	1	2386	A	N7-C5	-5.38	1.36	1.39
36	5	810	A	N3-C4	5.38	1.38	1.34
36	1	2819	A	C5-C4	-5.38	1.34	1.38
36	5	2899	C	C2-N3	-5.38	1.31	1.35
36	1	2138	A	N7-C5	-5.37	1.36	1.39
36	5	2954	U	N1-C2	5.36	1.43	1.38
36	1	2333	C	N3-C4	-5.36	1.30	1.33
36	1	504	A	N3-C4	-5.35	1.31	1.34
36	5	3042	U	N3-C4	-5.35	1.33	1.38
36	1	1132	C	N1-C6	-5.35	1.33	1.37
36	5	1152	G	N9-C8	5.35	1.41	1.37
36	5	795	G	C5-C4	-5.34	1.34	1.38
36	5	2934	A	C6-N1	-5.34	1.31	1.35
36	5	889	U	C4-O4	-5.33	1.19	1.23
36	1	2619	G	C5-C4	-5.33	1.34	1.38
36	5	509	U	N1-C2	-5.33	1.33	1.38
36	1	1495	U	N1-C6	-5.32	1.33	1.38
36	1	952	A	N7-C5	-5.31	1.36	1.39
36	1	2793	G	C2-N3	-5.30	1.28	1.32
36	1	1330	A	N9-C4	-5.30	1.34	1.37
36	1	658	G	C8-N7	-5.30	1.27	1.30
36	1	61	A	N3-C4	-5.29	1.31	1.34
41	L4	211	GLU	CG-CD	5.29	1.59	1.51
36	5	980	A	N7-C5	5.29	1.42	1.39
36	1	652	G	C6-N1	-5.29	1.35	1.39
36	5	1303	A	C5-C4	-5.29	1.35	1.38
36	5	2728	G	C5-C4	-5.29	1.34	1.38
37	7	88	G	N1-C2	-5.29	1.33	1.37
36	5	3005	A	N7-C5	-5.28	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	l3	327	CYS	CB-SG	-5.28	1.73	1.81
36	1	1103	A	N7-C5	5.28	1.42	1.39
36	5	1152	G	C8-N7	5.28	1.34	1.30
36	1	343	U	N1-C6	-5.28	1.33	1.38
36	1	919	U	C2-N3	-5.28	1.34	1.37
36	1	296	A	N9-C4	5.27	1.41	1.37
36	5	925	A	N7-C5	-5.27	1.36	1.39
36	1	1137	C	N1-C6	-5.27	1.33	1.37
36	1	2614	G	N9-C8	-5.27	1.34	1.37
36	1	716	A	N9-C4	-5.27	1.34	1.37
36	1	951	A	N9-C4	-5.27	1.34	1.37
36	1	2402	A	C5-C4	-5.26	1.35	1.38
36	5	2943	G	N9-C8	-5.25	1.34	1.37
44	L7	234	GLU	CD-OE2	5.24	1.31	1.25
36	5	1370	G	N1-C2	-5.24	1.33	1.37
36	5	1902	G	C5-C4	-5.23	1.34	1.38
36	5	1151	U	C2-N3	5.23	1.41	1.37
36	1	1099	A	N7-C5	-5.23	1.36	1.39
38	4	79	A	N9-C4	5.23	1.41	1.37
36	1	655	C	C2-O2	-5.22	1.19	1.24
36	1	2115	G	N7-C5	-5.22	1.36	1.39
36	5	1433	A	N7-C5	-5.22	1.36	1.39
36	5	2348	A	N3-C4	-5.22	1.31	1.34
36	5	924	G	N1-C2	-5.22	1.33	1.37
36	5	2302	G	N1-C2	-5.22	1.33	1.37
36	1	1310	G	N3-C4	-5.22	1.31	1.35
36	1	2326	A	N9-C4	-5.22	1.34	1.37
36	5	642	U	N3-C4	-5.22	1.33	1.38
36	5	1476	G	N3-C4	-5.20	1.31	1.35
36	1	92	G	P-O5'	-5.20	1.54	1.59
37	3	82	G	C6-N1	-5.20	1.35	1.39
36	5	1306	G	C8-N7	-5.20	1.27	1.30
36	1	919	U	C4-O4	-5.19	1.19	1.23
36	5	2358	A	N9-C4	-5.17	1.34	1.37
36	1	1126	G	N7-C5	-5.17	1.36	1.39
36	5	63	A	N7-C5	-5.16	1.36	1.39
36	5	1113	G	N3-C4	-5.16	1.31	1.35
1	6	1748	G	C5-C4	-5.16	1.34	1.38
36	5	425	G	C5-C6	-5.15	1.37	1.42
36	5	2302	G	C6-N1	-5.15	1.35	1.39
36	5	278	U	N1-C2	-5.15	1.33	1.38
36	5	2375	G	C5-C4	-5.14	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1049	C	C4-C5	-5.14	1.38	1.43
36	5	2362	C	N3-C4	-5.14	1.30	1.33
36	1	654	C	N1-C6	-5.14	1.34	1.37
36	1	657	A	C5-C4	-5.13	1.35	1.38
36	1	1660	C	N1-C6	-5.13	1.34	1.37
36	5	1429	G	N9-C4	-5.13	1.33	1.38
36	5	2912	G	C5-C4	-5.13	1.34	1.38
37	7	11	A	C5-C6	-5.13	1.36	1.41
36	1	40	A	C8-N7	-5.13	1.27	1.31
36	5	2877	G	N1-C2	-5.13	1.33	1.37
36	5	2334	U	C4-O4	-5.12	1.19	1.23
38	4	13	A	N7-C5	-5.12	1.36	1.39
36	5	2138	A	N3-C4	-5.12	1.31	1.34
36	1	3006	A	N9-C4	-5.12	1.34	1.37
1	6	366	A	N9-C4	-5.12	1.34	1.37
36	5	1170	A	N7-C5	-5.12	1.36	1.39
36	5	2372	A	N7-C5	-5.12	1.36	1.39
36	1	1369	A	N9-C4	-5.12	1.34	1.37
38	8	15	G	C8-N7	-5.12	1.27	1.30
36	1	3209	A	N7-C5	5.11	1.42	1.39
36	5	950	G	C5-C4	-5.11	1.34	1.38
36	5	2897	A	C5-C4	-5.11	1.35	1.38
1	6	754	A	N9-C4	5.11	1.41	1.37
36	5	3218	A	C5-C6	-5.11	1.36	1.41
36	1	584	G	C5-C4	-5.10	1.34	1.38
36	5	848	A	N3-C4	-5.10	1.31	1.34
36	5	1432	C	N1-C6	-5.10	1.34	1.37
36	5	1189	C	N1-C6	-5.10	1.34	1.37
36	5	1434	G	C5-C4	-5.10	1.34	1.38
36	5	895	A	C5-C4	-5.09	1.35	1.38
36	5	214	G	C8-N7	-5.09	1.27	1.30
36	5	1203	A	C5-C6	-5.09	1.36	1.41
36	1	40	A	N9-C8	-5.08	1.33	1.37
36	1	1429	G	N9-C8	-5.08	1.34	1.37
36	5	356	C	N1-C6	-5.08	1.34	1.37
36	5	1157	G	N9-C8	-5.08	1.34	1.37
36	1	2945	G	N7-C5	-5.08	1.36	1.39
37	7	11	A	N7-C5	-5.08	1.36	1.39
36	5	2286	U	C2-N3	-5.08	1.34	1.37
36	5	2942	C	N1-C6	-5.08	1.34	1.37
36	5	3174	A	N9-C8	5.07	1.41	1.37
36	1	2797	C	N1-C2	-5.07	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1902	G	N7-C5	-5.07	1.36	1.39
36	5	2145	A	C6-N1	-5.07	1.32	1.35
36	5	962	A	N7-C5	-5.06	1.36	1.39
36	5	1049	C	N3-C4	-5.06	1.30	1.33
44	l7	234	GLU	CD-OE1	5.06	1.31	1.25
36	1	1905	G	N1-C2	-5.06	1.33	1.37
36	1	92	G	C5-C6	-5.06	1.37	1.42
36	1	2817	A	C6-N6	-5.06	1.29	1.33
36	5	2860	U	N3-C4	5.06	1.43	1.38
36	5	3174	A	C5-C4	5.06	1.42	1.38
36	1	423	A	N7-C5	-5.05	1.36	1.39
36	1	716	A	C5-C6	-5.05	1.36	1.41
36	1	2335	G	C5-C4	-5.05	1.34	1.38
36	5	1175	C	N3-C4	-5.05	1.30	1.33
36	1	1417	G	N9-C4	-5.05	1.33	1.38
36	1	1330	A	C5-C6	-5.05	1.36	1.41
36	5	430	U	N1-C2	-5.05	1.34	1.38
36	5	635	G	N3-C4	-5.05	1.31	1.35
36	5	1499	C	N3-C4	-5.05	1.30	1.33
38	8	79	A	C5-C4	5.04	1.42	1.38
36	5	1049	C	C4-N4	-5.04	1.29	1.33
1	6	343	C	N1-C6	-5.03	1.34	1.37
36	1	792	G	N9-C4	-5.03	1.33	1.38
36	5	2243	A	N3-C4	-5.02	1.31	1.34
36	1	1133	A	N9-C4	-5.02	1.34	1.37
37	7	95	A	N7-C5	-5.02	1.36	1.39
36	1	2968	G	C6-N1	-5.02	1.36	1.39
36	5	2970	C	N1-C6	-5.02	1.34	1.37
36	5	1874	A	N9-C4	-5.01	1.34	1.37
36	1	953	G	C5-C4	-5.01	1.34	1.38
52	m6	80	PHE	CD1-CE1	-5.01	1.29	1.39
36	1	426	G	N1-C2	-5.01	1.33	1.37
36	1	1127	G	C5-C4	-5.01	1.34	1.38
36	5	2351	U	N3-C4	-5.01	1.33	1.38
38	4	20	U	C4-O4	-5.01	1.19	1.23
36	1	1307	G	C3'-O3'	5.01	1.49	1.42
36	5	1175	C	C4-N4	-5.01	1.29	1.33
36	5	2971	A	N9-C4	5.00	1.40	1.37

All (4764) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	N3-C4-C5	24.25	140.73	128.60
36	5	1152	G	N3-C4-N9	-22.33	112.60	126.00
36	5	1152	G	C2-N3-C4	-20.90	101.45	111.90
36	1	2945	G	O5'-P-OP2	-17.25	90.00	110.70
36	1	1308	A	O5'-P-OP2	-17.00	90.30	110.70
36	5	2385	G	O5'-P-OP1	-16.30	91.03	105.70
36	5	1152	G	N1-C6-O6	15.87	129.42	119.90
36	5	1152	G	N3-C2-N2	-15.79	108.85	119.90
36	1	1450	G	O5'-P-OP1	-15.75	91.53	105.70
36	5	642	U	O5'-P-OP2	-14.86	92.33	105.70
36	5	1308	A	O5'-P-OP1	-14.52	92.63	105.70
36	1	960	U	C5-C4-O4	-13.69	117.69	125.90
36	5	2875	U	C5-C6-N1	-13.69	115.86	122.70
36	1	2714	G	N3-C4-C5	13.65	135.42	128.60
36	5	1152	G	C5-N7-C8	-13.47	97.57	104.30
1	6	163	G	N3-C4-N9	-13.39	117.97	126.00
36	1	979	U	N3-C2-O2	-13.39	112.83	122.20
36	1	2371	G	O5'-P-OP2	-13.37	93.66	105.70
36	1	1495	U	C5-C6-N1	-13.32	116.04	122.70
36	1	2617	U	C5-C6-N1	-13.17	116.12	122.70
36	1	406	G	O4'-C1'-N9	12.84	118.47	108.20
1	2	553	G	N1-C6-O6	12.78	127.57	119.90
36	1	1304	A	O5'-P-OP1	-12.70	94.27	105.70
36	1	636	C	O5'-P-OP1	-12.60	94.36	105.70
36	1	1160	C	O5'-P-OP1	-12.53	94.42	105.70
36	5	2875	U	C2-N3-C4	-12.52	119.49	127.00
36	1	2831	G	N1-C6-O6	12.44	127.36	119.90
36	5	3005	A	O5'-P-OP2	-12.36	94.57	105.70
36	1	960	U	N3-C2-O2	12.12	130.68	122.20
36	1	958	C	N3-C4-C5	12.10	126.74	121.90
36	1	2617	U	N1-C2-N3	12.06	122.14	114.90
36	1	979	U	C6-N1-C2	-11.99	113.80	121.00
1	6	1773	C	N3-C4-C5	-11.86	117.16	121.90
36	5	3245	A	C2-N3-C4	-11.85	104.68	110.60
37	7	101	G	N1-C6-O6	11.70	126.92	119.90
36	1	2808	A	N1-C6-N6	11.67	125.60	118.60
1	2	1200	G	N1-C6-O6	11.67	126.90	119.90
36	1	2617	U	C5-C4-O4	11.55	132.83	125.90
36	5	877	C	N3-C4-C5	11.53	126.51	121.90
36	1	1308	A	C8-N9-C4	-11.49	101.20	105.80
36	1	2953	U	N1-C2-O2	-11.47	114.77	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	639	U	N3-C2-O2	-11.38	114.24	122.20
36	5	662	U	O5'-P-OP1	-11.30	95.53	105.70
36	5	2403	G	O5'-P-OP2	-11.25	95.58	105.70
36	1	1495	U	C4-C5-C6	11.24	126.45	119.70
36	1	2404	A	N1-C6-N6	11.22	125.33	118.60
36	1	2281	A	O5'-P-OP2	-11.19	95.63	105.70
36	1	1838	G	N1-C6-O6	11.15	126.59	119.90
36	5	776	U	C5-C6-N1	-11.12	117.14	122.70
36	1	1381	A	O5'-P-OP2	11.10	124.02	110.70
36	1	2797	C	O5'-P-OP1	-11.10	95.71	105.70
36	1	422	A	N1-C6-N6	-11.05	111.97	118.60
36	5	2704	A	O5'-P-OP1	-11.01	95.79	105.70
36	5	2923	U	O5'-P-OP1	-11.01	95.79	105.70
36	1	1381	A	O5'-P-OP1	-11.00	95.80	105.70
36	1	960	U	N1-C2-O2	-10.98	115.12	122.80
36	5	1152	G	C8-N9-C1'	10.96	141.24	127.00
36	1	1346	G	O5'-P-OP2	-10.93	95.87	105.70
36	1	1858	A	C2-N3-C4	10.90	116.05	110.60
36	1	1308	A	N7-C8-N9	10.90	119.25	113.80
36	1	2798	C	C6-N1-C2	-10.88	115.95	120.30
36	1	2846	U	N3-C2-O2	-10.87	114.59	122.20
36	5	3245	A	C5-N7-C8	-10.87	98.47	103.90
36	5	922	U	N3-C2-O2	-10.86	114.60	122.20
36	1	2714	G	N3-C4-N9	-10.83	119.50	126.00
36	1	636	C	N3-C4-C5	10.76	126.20	121.90
36	5	2875	U	C2-N1-C1'	-10.76	104.79	117.70
36	1	3172	A	C8-N9-C4	10.74	110.10	105.80
36	5	426	G	C8-N9-C4	10.73	110.69	106.40
36	1	2871	G	O5'-P-OP2	-10.73	96.05	105.70
36	1	2996	U	C2-N1-C1'	10.72	130.57	117.70
1	6	453	U	N3-C2-O2	-10.72	114.69	122.20
36	1	957	C	O5'-P-OP2	-10.68	96.09	105.70
1	6	163	G	N3-C4-C5	10.67	133.94	128.60
36	5	641	C	N1-C2-O2	-10.66	112.50	118.90
36	5	806	A	O5'-P-OP1	-10.62	96.14	105.70
36	1	2621	G	N3-C2-N2	-10.61	112.47	119.90
1	6	901	G	C4-C5-N7	10.61	115.04	110.80
36	1	1367	G	N1-C6-O6	10.57	126.25	119.90
36	1	2622	C	C6-N1-C2	-10.57	116.07	120.30
36	1	2870	C	C2-N1-C1'	-10.57	107.17	118.80
36	1	2617	U	N3-C2-O2	-10.56	114.81	122.20
1	6	901	G	C5-C6-O6	-10.55	122.27	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3278	C	N3-C2-O2	-10.54	114.52	121.90
36	1	2314	U	C5-C4-O4	-10.53	119.58	125.90
36	5	1307	G	P-O3'-C3'	10.52	132.32	119.70
36	1	2860	U	C5-C6-N1	10.51	127.95	122.70
36	1	1433	A	C5-C6-N6	-10.48	115.32	123.70
36	5	2374	C	N1-C2-O2	-10.46	112.62	118.90
38	8	80	A	C8-N9-C4	-10.42	101.63	105.80
36	1	1127	G	C5-C6-O6	-10.41	122.35	128.60
36	5	1116	G	O5'-P-OP1	-10.41	96.33	105.70
36	1	3181	C	C5-C4-N4	10.41	127.49	120.20
36	5	2617	U	O5'-P-OP2	-10.35	96.39	105.70
36	1	2165	G	O5'-P-OP2	-10.34	96.39	105.70
36	1	716	A	N9-C4-C5	-10.33	101.67	105.80
36	5	1152	G	C4-N9-C1'	-10.30	113.11	126.50
36	1	639	G	N1-C6-O6	10.29	126.07	119.90
36	1	2945	G	O5'-P-OP1	10.29	123.04	110.70
36	1	2617	U	C4-C5-C6	10.28	125.87	119.70
36	5	2393	G	O5'-P-OP2	-10.27	96.46	105.70
36	5	1127	G	C5-C6-N1	10.17	116.58	111.50
36	1	958	C	C2-N3-C4	-10.13	114.83	119.90
36	1	608	A	N1-C6-N6	10.13	124.68	118.60
36	1	1132	C	O5'-P-OP1	-10.12	96.59	105.70
36	5	1390	A	N9-C4-C5	10.08	109.83	105.80
36	1	2279	A	N9-C4-C5	-10.06	101.78	105.80
36	1	895	A	C2-N3-C4	-10.05	105.57	110.60
36	5	3218	A	N1-C6-N6	10.05	124.63	118.60
36	5	3377	G	N1-C6-O6	10.04	125.92	119.90
36	1	218	G	O5'-P-OP2	-10.03	96.67	105.70
36	5	953	G	C5-C6-O6	-10.03	122.58	128.60
36	1	3181	C	N3-C4-N4	-10.02	110.98	118.00
36	5	1370	G	N1-C2-N2	-9.99	107.21	116.20
36	1	1405	U	C2-N3-C4	-9.95	121.03	127.00
36	1	1450	G	O5'-P-OP2	9.94	122.63	110.70
36	5	3244	A	O5'-P-OP1	-9.93	96.76	105.70
36	1	282	G	C8-N9-C4	-9.91	102.44	106.40
36	5	406	G	O4'-C1'-N9	9.91	116.13	108.20
36	1	2831	G	C5-C6-O6	-9.82	122.71	128.60
1	2	558	U	N1-C2-O2	9.81	129.67	122.80
36	1	776	U	C4-C5-C6	9.80	125.58	119.70
36	1	2169	G	N1-C6-O6	-9.80	114.02	119.90
36	5	1308	A	O5'-P-OP2	9.79	122.45	110.70
36	1	646	A	O5'-P-OP2	-9.78	96.90	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1047	A	N1-C6-N6	9.78	124.47	118.60
36	5	2389	C	N3-C4-C5	9.77	125.81	121.90
36	5	2392	C	N3-C4-C5	9.75	125.80	121.90
36	1	2247	G	N1-C6-O6	9.75	125.75	119.90
36	5	1152	G	C5-C6-O6	-9.73	122.76	128.60
36	1	2798	C	N3-C4-C5	-9.73	118.01	121.90
36	1	439	C	N1-C2-O2	9.72	124.73	118.90
36	5	2953	U	N3-C4-O4	9.71	126.20	119.40
36	5	1301	A	N1-C6-N6	9.71	124.42	118.60
36	1	369	A	O5'-P-OP2	-9.70	96.97	105.70
36	5	3154	C	N1-C2-O2	9.69	124.72	118.90
36	1	677	A	O5'-P-OP1	-9.68	96.99	105.70
36	1	3306	U	N3-C4-O4	-9.67	112.63	119.40
36	1	2870	C	N3-C4-C5	9.65	125.76	121.90
36	1	86	G	O5'-P-OP2	-9.64	97.03	105.70
36	5	2815	G	C8-N9-C4	9.64	110.25	106.40
36	5	2954	U	C2-N1-C1'	9.62	129.24	117.70
36	1	3278	C	N1-C2-O2	9.61	124.67	118.90
36	5	2816	G	C5-C6-O6	-9.58	122.85	128.60
36	5	2408	U	C5-C6-N1	-9.56	117.92	122.70
36	5	2297	U	O5'-P-OP2	-9.55	97.10	105.70
36	5	3377	G	C5-C6-O6	-9.55	122.87	128.60
37	7	101	G	C5-C6-O6	-9.54	122.87	128.60
36	1	201	A	O5'-P-OP2	-9.54	97.12	105.70
36	5	2383	C	N1-C2-O2	-9.53	113.18	118.90
1	6	901	G	N1-C6-O6	9.51	125.61	119.90
36	5	437	G	C8-N9-C4	-9.51	102.60	106.40
36	1	1367	G	C5-C6-O6	-9.51	122.90	128.60
36	1	1405	U	N3-C4-C5	9.50	120.30	114.60
38	8	8	C	C6-N1-C2	-9.49	116.50	120.30
36	1	1495	U	N1-C2-N3	9.49	120.59	114.90
36	1	2349	U	O5'-P-OP2	-9.49	97.16	105.70
36	5	2830	G	N9-C4-C5	9.49	109.19	105.40
38	4	31	G	O5'-P-OP2	-9.49	97.16	105.70
36	5	2572	C	N1-C2-O2	9.47	124.58	118.90
59	n3	45	ARG	NE-CZ-NH1	-9.45	115.58	120.30
36	1	805	G	C8-N9-C4	9.44	110.18	106.40
36	1	1197	A	N1-C6-N6	9.44	124.26	118.60
36	1	2409	G	C2-N3-C4	9.43	116.62	111.90
36	5	2726	C	C5-C4-N4	9.41	126.79	120.20
36	5	2726	C	C6-N1-C2	-9.40	116.54	120.30
36	5	2913	C	C6-N1-C2	-9.39	116.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3245	A	N7-C8-N9	9.39	118.49	113.80
36	1	2875	U	N3-C4-O4	9.38	125.97	119.40
36	1	876	A	N9-C4-C5	-9.38	102.05	105.80
1	2	639	U	N1-C2-O2	9.36	129.35	122.80
38	4	103	G	C8-N9-C4	-9.35	102.66	106.40
36	5	2402	A	N9-C4-C5	9.35	109.54	105.80
36	5	2980	U	N1-C2-N3	9.34	120.50	114.90
36	5	1412	G	C8-N9-C4	-9.34	102.67	106.40
36	5	636	C	C6-N1-C2	9.33	124.03	120.30
38	8	80	A	N7-C8-N9	9.32	118.46	113.80
36	1	1127	G	N1-C6-O6	9.31	125.48	119.90
36	1	2617	U	C2-N3-C4	-9.29	121.42	127.00
36	1	2870	C	C6-N1-C1'	9.28	131.94	120.80
36	1	716	A	C8-N9-C4	9.28	109.51	105.80
36	5	2601	A	N1-C6-N6	-9.27	113.04	118.60
36	5	1452	A	N9-C4-C5	-9.26	102.09	105.80
36	1	282	G	O5'-P-OP1	-9.26	97.37	105.70
36	1	1303	A	C8-N9-C4	9.25	109.50	105.80
1	2	577	G	C4-C5-N7	9.25	114.50	110.80
36	1	435	C	C6-N1-C2	9.24	124.00	120.30
36	1	3181	C	N3-C2-O2	-9.24	115.43	121.90
36	5	2830	G	C4-C5-N7	-9.23	107.11	110.80
36	5	57	A	C8-N9-C4	9.23	109.49	105.80
36	5	1390	A	N1-C6-N6	-9.22	113.07	118.60
36	1	1492	G	C5-N7-C8	9.21	108.91	104.30
36	1	2996	U	C6-N1-C1'	-9.21	108.31	121.20
38	4	103	G	N3-C4-C5	-9.20	124.00	128.60
1	6	163	G	N3-C2-N2	-9.19	113.47	119.90
36	5	1187	C	C6-N1-C2	9.18	123.97	120.30
36	5	2875	U	N1-C2-N3	9.18	120.41	114.90
36	5	3188	G	N1-C6-O6	-9.17	114.40	119.90
36	1	1165	A	C8-N9-C4	9.15	109.46	105.80
36	1	2402	A	O5'-P-OP2	-9.15	97.46	105.70
36	5	1483	G	O4'-C1'-N9	9.15	115.52	108.20
36	5	1513	G	C8-N9-C4	-9.14	102.74	106.40
38	4	113	U	N1-C2-N3	9.13	120.38	114.90
36	1	2714	G	C2-N3-C4	-9.12	107.34	111.90
1	2	73	U	O4'-C1'-N1	9.12	115.49	108.20
36	5	2764	C	N3-C4-C5	9.11	125.54	121.90
36	5	189	G	N1-C6-O6	-9.10	114.44	119.90
36	5	1911	A	O5'-P-OP2	-9.09	97.52	105.70
36	5	2189	U	O5'-P-OP1	-9.09	97.52	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	439	C	C2-N1-C1'	9.09	128.79	118.80
36	5	3100	U	O5'-P-OP1	-9.08	97.53	105.70
36	5	923	C	C6-N1-C2	9.07	123.93	120.30
1	2	542	A	O4'-C1'-N9	9.07	115.46	108.20
36	1	2617	U	N3-C4-O4	-9.06	113.06	119.40
36	5	776	U	C4-C5-C6	9.06	125.14	119.70
36	5	2372	A	C8-N9-C4	-9.03	102.19	105.80
36	1	672	A	N1-C6-N6	9.03	124.02	118.60
36	5	907	G	O5'-P-OP1	-9.03	97.58	105.70
36	5	3060	C	N1-C2-O2	-9.01	113.50	118.90
36	1	972	A	C8-N9-C4	9.00	109.40	105.80
36	5	515	C	O5'-P-OP2	-8.99	97.61	105.70
36	5	3043	C	C6-N1-C2	8.99	123.89	120.30
36	5	672	A	N1-C6-N6	8.98	123.99	118.60
1	6	139	C	N3-C2-O2	-8.97	115.62	121.90
36	5	1130	A	C2-N3-C4	8.97	115.08	110.60
1	6	782	U	N3-C2-O2	-8.97	115.92	122.20
36	5	2404	A	N1-C6-N6	8.97	123.98	118.60
36	5	2281	A	O5'-P-OP2	-8.96	97.63	105.70
36	1	681	U	C5-C4-O4	-8.95	120.53	125.90
36	1	1556	C	C6-N1-C2	-8.95	116.72	120.30
36	5	2393	G	C5-C6-O6	-8.95	123.23	128.60
36	1	421	G	N9-C4-C5	-8.94	101.82	105.40
36	1	2409	G	N3-C4-C5	-8.94	124.13	128.60
36	1	2865	U	C5-C4-O4	-8.93	120.54	125.90
36	5	2980	U	N3-C2-O2	-8.93	115.95	122.20
1	2	558	U	N3-C2-O2	-8.93	115.95	122.20
36	5	1148	G	C5-C6-O6	-8.92	123.25	128.60
36	5	1370	G	N3-C2-N2	8.92	126.14	119.90
1	6	163	G	C2-N3-C4	-8.90	107.45	111.90
1	2	1560	U	N3-C2-O2	-8.90	115.97	122.20
36	1	2836	C	C4-C5-C6	8.88	121.84	117.40
1	2	553	G	C6-C5-N7	-8.87	125.08	130.40
36	1	2726	C	N3-C4-N4	-8.87	111.79	118.00
36	1	636	C	C2-N3-C4	-8.86	115.47	119.90
36	1	922	U	N1-C2-O2	8.86	129.00	122.80
36	5	404	G	O5'-P-OP2	-8.86	97.73	105.70
36	1	1148	G	C8-N9-C4	8.85	109.94	106.40
36	5	2954	U	O4'-C1'-N1	8.84	115.27	108.20
1	2	453	U	N3-C2-O2	-8.84	116.01	122.20
36	1	885	U	C5-C6-N1	-8.84	118.28	122.70
36	1	2768	U	O5'-P-OP2	-8.84	97.75	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3122	A	O5'-P-OP1	-8.82	97.76	105.70
36	1	979	U	P-O3'-C3'	8.81	130.28	119.70
36	1	339	C	N3-C2-O2	-8.80	115.74	121.90
36	1	2856	G	C8-N9-C4	8.81	109.92	106.40
37	3	88	G	N1-C6-O6	-8.80	114.62	119.90
36	5	63	A	N1-C6-N6	8.80	123.88	118.60
36	5	2893	C	N3-C4-C5	-8.80	118.38	121.90
1	6	337	G	C6-C5-N7	-8.79	125.13	130.40
1	6	1657	U	O5'-P-OP2	-8.79	97.79	105.70
36	5	2954	U	C6-N1-C1'	-8.79	108.90	121.20
36	1	1795	U	C5-C4-O4	-8.78	120.63	125.90
36	5	838	G	C5-C6-O6	8.77	133.86	128.60
36	1	2693	C	C6-N1-C2	8.77	123.81	120.30
36	1	716	A	N1-C6-N6	8.76	123.86	118.60
36	1	2279	A	C8-N9-C4	8.76	109.30	105.80
36	5	2315	G	O5'-P-OP1	-8.76	97.82	105.70
36	5	2353	G	C5-C6-O6	-8.76	123.35	128.60
36	1	639	G	O5'-P-OP1	8.75	121.20	110.70
36	5	3214	U	N3-C2-O2	-8.75	116.08	122.20
36	1	2867	C	N3-C4-C5	8.75	125.40	121.90
1	6	795	U	N3-C2-O2	-8.74	116.08	122.20
36	1	1556	C	C2-N1-C1'	8.74	128.41	118.80
1	6	1596	C	N3-C2-O2	-8.74	115.78	121.90
36	5	874	U	O5'-P-OP1	-8.74	97.83	105.70
36	5	2904	U	C5-C6-N1	-8.74	118.33	122.70
36	1	350	C	C6-N1-C2	-8.72	116.81	120.30
36	1	681	U	N3-C4-O4	8.72	125.51	119.40
36	5	2815	G	N7-C8-N9	-8.72	108.74	113.10
36	1	648	C	C6-N1-C2	-8.72	116.81	120.30
36	5	1897	G	C5-C6-O6	-8.71	123.37	128.60
36	1	3178	A	N1-C6-N6	8.70	123.82	118.60
36	1	2935	U	O5'-P-OP2	-8.68	97.89	105.70
36	5	1152	G	C4-C5-N7	8.68	114.27	110.80
36	5	2272	G	O4'-C1'-N9	8.68	115.14	108.20
36	5	640	U	N1-C2-O2	-8.67	116.73	122.80
36	5	2816	G	N1-C6-O6	8.65	125.09	119.90
36	5	3185	U	O5'-P-OP2	-8.65	97.91	105.70
36	1	1838	G	C5-C6-O6	-8.64	123.42	128.60
36	1	2130	G	N1-C6-O6	-8.64	114.72	119.90
36	5	1320	C	O5'-P-OP2	-8.63	97.93	105.70
1	6	17	C	N1-C2-O2	8.62	124.07	118.90
36	1	1116	G	C8-N9-C4	-8.62	102.95	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2257	C	C6-N1-C2	-8.61	116.86	120.30
36	1	2621	G	N1-C6-O6	8.61	125.07	119.90
36	5	636	C	N3-C4-C5	8.61	125.34	121.90
36	5	2199	G	N1-C6-O6	8.60	125.06	119.90
36	5	3042	U	N3-C4-O4	-8.59	113.39	119.40
36	5	222	A	O5'-P-OP2	-8.59	97.97	105.70
36	5	2524	A	O4'-C1'-N9	8.58	115.06	108.20
36	5	941	G	N1-C6-O6	-8.58	114.75	119.90
36	5	1047	A	C5-C6-N6	-8.56	116.85	123.70
36	5	1856	C	C6-N1-C2	-8.56	116.88	120.30
1	6	314	C	C6-N1-C2	-8.55	116.88	120.30
1	6	1473	U	N3-C2-O2	-8.55	116.22	122.20
36	1	2846	U	C5-C4-O4	8.53	131.02	125.90
36	5	424	G	C5-C6-O6	-8.53	123.48	128.60
36	1	2874	G	C5-C6-N1	-8.52	107.24	111.50
36	5	719	U	N1-C2-O2	8.52	128.76	122.80
1	6	453	U	N1-C2-O2	8.52	128.76	122.80
36	5	2213	A	O5'-P-OP2	-8.51	98.04	105.70
36	1	2827	U	C2-N1-C1'	-8.50	107.50	117.70
37	3	86	U	C2-N3-C4	-8.50	121.90	127.00
36	1	1556	C	N3-C2-O2	-8.50	115.95	121.90
1	6	609	U	C5-C4-O4	8.49	131.00	125.90
36	1	439	C	C6-N1-C1'	-8.49	110.62	120.80
1	6	1745	G	C5-C6-O6	-8.48	123.51	128.60
36	1	2314	U	C2-N1-C1'	8.48	127.87	117.70
36	5	1108	U	O5'-P-OP2	-8.47	98.07	105.70
36	5	3308	C	N1-C2-O2	-8.47	113.82	118.90
36	5	398	A	O5'-P-OP2	-8.47	98.08	105.70
36	1	3362	A	O4'-C1'-N9	8.46	114.97	108.20
36	5	1929	G	N3-C2-N2	-8.46	113.98	119.90
37	3	86	U	C5-C4-O4	-8.44	120.83	125.90
36	5	966	U	N3-C2-O2	-8.44	116.29	122.20
36	1	2643	A	C8-N9-C4	8.44	109.17	105.80
36	1	2400	G	N3-C2-N2	-8.43	114.00	119.90
36	5	2314	U	C5-C4-O4	-8.43	120.84	125.90
36	5	1848	G	C5-C6-O6	-8.43	123.54	128.60
1	2	553	G	C5-C6-O6	-8.43	123.55	128.60
36	5	1161	G	C5-C6-N1	8.42	115.71	111.50
36	5	2278	C	C4-C5-C6	-8.42	113.19	117.40
36	1	646	A	C8-N9-C4	-8.42	102.43	105.80
52	m6	78	ARG	NE-CZ-NH2	-8.42	116.09	120.30
36	1	2622	C	N3-C4-C5	-8.41	118.53	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1700	C	N1-C2-O2	8.41	123.95	118.90
36	5	952	A	O5'-P-OP2	-8.40	98.14	105.70
36	1	1847	A	O5'-P-OP1	-8.40	98.14	105.70
36	1	421	G	O5'-P-OP1	-8.39	98.14	105.70
36	1	1433	A	N1-C6-N6	8.39	123.63	118.60
36	5	2634	U	C2-N3-C4	-8.39	121.97	127.00
36	1	645	A	C6-N1-C2	-8.39	113.57	118.60
36	1	1414	G	N1-C6-O6	8.39	124.93	119.90
36	5	3218	A	C4-C5-N7	8.39	114.89	110.70
36	1	2314	U	C6-N1-C1'	-8.38	109.47	121.20
36	1	979	U	N1-C2-N3	8.37	119.92	114.90
36	1	650	C	N1-C2-O2	-8.37	113.88	118.90
36	5	1336	U	O5'-P-OP2	-8.37	98.17	105.70
36	5	2667	A	O5'-P-OP1	-8.37	98.17	105.70
36	1	3143	C	O5'-P-OP2	-8.37	98.17	105.70
1	6	17	C	C6-N1-C2	-8.37	116.95	120.30
36	5	2824	G	O5'-P-OP2	-8.36	98.17	105.70
36	1	939	U	N1-C2-O2	-8.36	116.95	122.80
36	1	2572	C	N1-C2-O2	8.36	123.92	118.90
36	5	1592	G	C8-N9-C4	-8.36	103.06	106.40
36	1	2396	G	C4-C5-N7	-8.36	107.46	110.80
1	2	577	G	C5-C6-O6	-8.35	123.59	128.60
36	1	776	U	C5-C6-N1	-8.35	118.52	122.70
36	1	2374	C	C2-N1-C1'	-8.35	109.62	118.80
36	1	2572	C	C2-N1-C1'	8.35	127.98	118.80
36	5	1390	A	C8-N9-C4	-8.35	102.46	105.80
36	1	1445	U	N1-C2-O2	-8.35	116.96	122.80
37	3	82	G	N1-C2-N2	-8.34	108.69	116.20
36	5	2857	C	N3-C4-C5	8.34	125.24	121.90
36	1	655	C	C6-N1-C2	-8.32	116.97	120.30
36	5	3362	A	C2-N3-C4	-8.31	106.44	110.60
36	1	1429	G	N3-C2-N2	8.31	125.72	119.90
36	1	578	A	O5'-P-OP1	-8.31	98.22	105.70
36	1	895	A	C4-C5-N7	8.30	114.85	110.70
36	1	1377	G	C4-C5-N7	8.30	114.12	110.80
36	1	2393	G	C5-C6-O6	-8.30	123.62	128.60
1	6	941	A	N1-C6-N6	-8.30	113.62	118.60
36	1	2870	C	C4-C5-C6	-8.29	113.25	117.40
36	1	2409	G	N1-C6-O6	-8.29	114.93	119.90
36	1	770	G	O4'-C1'-N9	8.29	114.83	108.20
36	5	3127	A	N1-C6-N6	-8.29	113.63	118.60
36	1	922	U	C5-C4-O4	8.28	130.87	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1405	U	C5-C4-O4	-8.28	120.93	125.90
36	1	922	U	N3-C4-O4	-8.28	113.61	119.40
36	5	2980	U	C6-N1-C2	-8.27	116.04	121.00
36	1	1365	G	C8-N9-C4	-8.27	103.09	106.40
36	1	776	U	N1-C2-N3	8.26	119.86	114.90
1	6	1700	C	C2-N1-C1'	8.26	127.89	118.80
36	5	860	G	O5'-P-OP2	-8.26	98.26	105.70
36	1	2811	A	N1-C6-N6	-8.26	113.65	118.60
36	5	960	U	C2-N3-C4	-8.24	122.06	127.00
36	1	933	A	C4-C5-C6	8.23	121.12	117.00
36	1	1118	C	C6-N1-C2	-8.23	117.01	120.30
1	6	65	A	C2-N3-C4	-8.23	106.48	110.60
1	2	75	U	N1-C2-O2	8.23	128.56	122.80
36	1	922	U	N3-C2-O2	-8.23	116.44	122.20
1	6	139	C	C6-N1-C2	-8.21	117.01	120.30
36	1	1380	G	C2-N3-C4	-8.21	107.79	111.90
1	6	957	G	N1-C6-O6	8.21	124.83	119.90
36	1	1495	U	C2-N3-C4	-8.21	122.08	127.00
36	5	1148	G	N9-C4-C5	-8.21	102.12	105.40
36	1	963	G	O5'-P-OP1	8.20	120.54	110.70
36	5	2142	A	C5-C6-N1	8.20	121.80	117.70
48	m1	112	LEU	CA-CB-CG	8.20	134.15	115.30
1	6	416	A	N1-C6-N6	8.19	123.52	118.60
36	5	922	U	C2-N3-C4	-8.19	122.09	127.00
36	1	3265	C	C6-N1-C2	8.18	123.57	120.30
36	1	3269	U	C5-C4-O4	8.18	130.81	125.90
36	5	2945	G	C5-C6-O6	-8.18	123.69	128.60
1	2	75	U	N3-C2-O2	-8.18	116.48	122.20
36	1	1176	C	N3-C4-C5	8.16	125.17	121.90
36	1	2808	A	N9-C4-C5	-8.16	102.53	105.80
36	5	2794	G	C5-C6-O6	-8.16	123.70	128.60
36	5	923	C	N3-C4-C5	8.16	125.16	121.90
36	5	38	U	O5'-P-OP2	-8.15	98.36	105.70
36	1	3278	C	C5-C4-N4	8.15	125.90	120.20
36	1	963	G	O5'-P-OP2	-8.15	98.37	105.70
36	1	1094	U	C5-C6-N1	8.15	126.77	122.70
36	5	2796	G	O5'-P-OP2	-8.15	98.37	105.70
36	5	3362	A	N1-C2-N3	8.14	133.37	129.30
36	1	610	G	O5'-P-OP2	-8.14	98.38	105.70
36	1	2404	A	C6-C5-N7	-8.14	126.60	132.30
1	6	1773	C	N1-C2-O2	-8.13	114.02	118.90
36	5	419	G	N3-C4-N9	8.13	130.88	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2899	C	N3-C2-O2	-8.13	116.21	121.90
36	1	961	C	C6-N1-C2	8.12	123.55	120.30
36	1	2816	G	C8-N9-C4	8.12	109.65	106.40
36	1	2983	C	C5-C4-N4	8.12	125.88	120.20
36	5	658	G	C5-C6-O6	-8.12	123.73	128.60
36	5	960	U	N3-C4-C5	8.11	119.47	114.60
38	4	94	C	N3-C4-C5	8.10	125.14	121.90
70	O4	51	LEU	CA-CB-CG	8.10	133.94	115.30
36	1	421	G	C4-C5-N7	8.10	114.04	110.80
36	1	1414	G	C5-C6-O6	-8.10	123.74	128.60
1	6	543	C	C5-C6-N1	8.10	125.05	121.00
36	5	1879	A	N1-C6-N6	8.09	123.45	118.60
36	1	611	A	O5'-P-OP2	-8.08	98.42	105.70
36	1	3055	U	C5-C4-O4	-8.07	121.06	125.90
36	5	189	G	C5-C6-O6	8.06	133.44	128.60
36	1	1510	G	N3-C4-N9	8.06	130.84	126.00
36	5	2293	C	C2-N1-C1'	8.06	127.66	118.80
36	1	2345	A	N1-C6-N6	8.05	123.43	118.60
36	1	2756	C	C6-N1-C2	-8.05	117.08	120.30
36	1	2917	G	C5-C6-O6	-8.05	123.77	128.60
38	4	47	C	N3-C2-O2	-8.04	116.27	121.90
36	5	1130	A	N1-C2-N3	-8.02	125.29	129.30
36	1	2138	A	C8-N9-C4	-8.02	102.59	105.80
36	1	2374	C	N1-C2-O2	-8.02	114.09	118.90
36	5	2323	G	O5'-P-OP2	8.02	120.32	110.70
36	5	2404	A	N9-C4-C5	-8.02	102.59	105.80
1	6	25	C	N1-C2-O2	-8.01	114.09	118.90
36	1	1168	U	O5'-P-OP1	8.01	120.31	110.70
36	1	2808	A	C6-C5-N7	-8.01	126.70	132.30
36	1	893	C	C6-N1-C2	-8.00	117.10	120.30
36	1	2419	A	OP1-P-OP2	-8.00	107.60	119.60
36	1	1419	A	O5'-P-OP1	8.00	120.30	110.70
1	2	577	G	C5-N7-C8	-7.99	100.31	104.30
36	5	1452	A	N1-C6-N6	7.99	123.39	118.60
36	5	945	C	C6-N1-C2	7.98	123.49	120.30
36	1	3217	C	C2-N1-C1'	7.98	127.58	118.80
25	d3	33	LEU	CA-CB-CG	-7.98	96.94	115.30
36	5	519	A	N1-C6-N6	7.98	123.39	118.60
36	1	2817	A	C5-C6-N1	7.97	121.69	117.70
36	5	646	A	C8-N9-C4	-7.97	102.61	105.80
36	5	578	A	O5'-P-OP2	7.96	120.25	110.70
36	5	1450	G	N3-C2-N2	-7.96	114.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	N1-C2-N2	7.96	123.36	116.20
36	1	1168	U	N3-C2-O2	-7.96	116.63	122.20
36	1	1163	A	O5'-P-OP2	-7.95	98.54	105.70
1	6	1581	C	C6-N1-C2	7.95	123.48	120.30
36	1	2959	C	N1-C2-O2	-7.95	114.13	118.90
1	2	453	U	C2-N1-C1'	7.94	127.23	117.70
36	1	2812	C	C6-N1-C2	7.94	123.48	120.30
36	5	2234	G	C5-C6-O6	-7.94	123.83	128.60
36	5	2825	C	C6-N1-C2	7.94	123.48	120.30
36	5	1118	C	O5'-P-OP1	-7.94	98.56	105.70
38	4	140	G	C8-N9-C4	-7.94	103.22	106.40
1	6	1773	C	N3-C4-N4	7.94	123.56	118.00
1	6	1560	U	N3-C2-O2	-7.93	116.65	122.20
36	1	1389	G	C4-C5-N7	7.92	113.97	110.80
36	5	2667	A	C8-N9-C4	-7.92	102.63	105.80
1	6	901	G	N9-C4-C5	-7.92	102.23	105.40
36	1	2385	G	N3-C4-C5	7.92	132.56	128.60
36	1	2279	A	N1-C6-N6	7.92	123.35	118.60
36	5	2572	C	N3-C2-O2	-7.92	116.36	121.90
36	1	645	A	N3-C4-C5	-7.91	121.26	126.80
36	5	941	G	C5-C6-N1	7.91	115.45	111.50
36	5	960	U	N3-C2-O2	-7.91	116.66	122.20
37	7	110	G	O5'-P-OP2	-7.91	98.58	105.70
36	5	1149	G	O5'-P-OP2	-7.91	98.58	105.70
38	4	15	G	C5-C6-O6	-7.90	123.86	128.60
38	4	25	G	C5-C6-O6	7.90	133.34	128.60
38	4	113	U	C5-C4-O4	7.90	130.64	125.90
36	1	2247	G	C5-C6-O6	-7.89	123.86	128.60
36	5	1456	A	N1-C6-N6	7.89	123.33	118.60
36	5	437	G	N7-C8-N9	7.89	117.04	113.10
36	1	29	C	C5-C4-N4	-7.88	114.68	120.20
36	1	1116	G	N3-C4-C5	-7.88	124.66	128.60
36	5	2754	G	C5-C6-O6	7.88	133.33	128.60
1	2	1432	U	C6-N1-C2	7.87	125.72	121.00
36	5	2872	A	O5'-P-OP2	-7.87	98.62	105.70
36	1	1130	A	C2-N3-C4	7.86	114.53	110.60
36	1	660	A	O5'-P-OP2	-7.85	98.63	105.70
36	5	824	C	C6-N1-C2	-7.85	117.16	120.30
36	5	2572	C	C2-N1-C1'	7.85	127.43	118.80
36	5	1419	A	O5'-P-OP2	-7.84	98.64	105.70
1	2	577	G	N1-C6-O6	7.84	124.61	119.90
36	5	2950	G	O4'-C1'-N9	7.84	114.47	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2790	A	O5'-P-OP2	-7.83	98.65	105.70
36	1	3344	A	N7-C8-N9	7.83	117.72	113.80
1	6	44	U	N1-C2-O2	-7.83	117.32	122.80
1	6	57	G	O5'-P-OP2	-7.83	98.66	105.70
36	1	2850	G	C5-C6-O6	-7.82	123.91	128.60
1	6	103	A	C8-N9-C4	-7.82	102.67	105.80
36	1	1351	U	N1-C2-O2	7.82	128.27	122.80
36	5	56	G	N1-C6-O6	-7.82	115.21	119.90
36	5	1208	U	N3-C2-O2	-7.82	116.72	122.20
36	5	2758	A	C2-N3-C4	7.82	114.51	110.60
1	6	973	A	O5'-P-OP2	-7.81	98.67	105.70
36	1	936	A	N1-C6-N6	7.81	123.28	118.60
36	1	1525	G	O5'-P-OP2	-7.81	98.67	105.70
52	m6	78	ARG	NE-CZ-NH1	7.81	124.20	120.30
36	5	881	C	C5-C6-N1	7.79	124.90	121.00
1	2	830	U	N3-C2-O2	-7.79	116.75	122.20
36	1	1177	G	N3-C2-N2	-7.79	114.45	119.90
36	1	1149	G	N1-C6-O6	7.78	124.57	119.90
36	1	1949	G	O5'-P-OP1	-7.78	98.70	105.70
36	5	1452	A	C5-C6-N6	-7.78	117.48	123.70
36	1	2827	U	C6-N1-C1'	7.78	132.09	121.20
1	6	119	A	C2-N3-C4	-7.77	106.71	110.60
1	6	453	U	C2-N1-C1'	7.77	127.03	117.70
37	7	120	C	C6-N1-C2	7.76	123.41	120.30
36	1	421	G	C5-C6-O6	-7.76	123.94	128.60
36	1	2875	U	C2-N1-C1'	7.76	127.01	117.70
37	7	35	C	C6-N1-C2	7.75	123.40	120.30
42	l5	152	ARG	NE-CZ-NH1	7.75	124.17	120.30
36	1	96	G	C2-N3-C4	-7.75	108.03	111.90
36	5	1004	U	N1-C2-O2	7.75	128.22	122.80
36	5	2889	C	N3-C4-C5	7.74	125.00	121.90
36	5	1054	A	C8-N9-C4	7.74	108.89	105.80
36	5	2871	G	N1-C6-O6	-7.74	115.26	119.90
36	1	1157	G	C4-C5-N7	-7.73	107.71	110.80
36	1	2827	U	C5-C4-O4	7.73	130.54	125.90
36	5	2372	A	P-O3'-C3'	7.73	128.97	119.70
36	5	3005	A	C8-N9-C4	-7.73	102.71	105.80
36	1	2404	A	N9-C4-C5	-7.72	102.71	105.80
36	1	2875	U	C5-C4-O4	-7.72	121.27	125.90
44	l7	229	PHE	CB-CG-CD1	7.72	126.20	120.80
36	5	3041	U	N3-C2-O2	7.72	127.60	122.20
36	5	2852	C	O5'-P-OP1	7.71	119.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	144	U	N3-C2-O2	-7.71	116.80	122.20
36	5	908	G	C5-C6-O6	-7.71	123.97	128.60
36	5	835	G	O4'-C1'-N9	7.71	114.36	108.20
36	5	2308	C	N1-C2-O2	-7.71	114.28	118.90
36	5	881	C	N1-C2-O2	7.70	123.52	118.90
36	5	1897	G	N1-C6-O6	7.70	124.52	119.90
36	1	1306	G	C8-N9-C4	7.70	109.48	106.40
36	1	640	U	C5-C4-O4	-7.69	121.28	125.90
36	5	1049	C	C4-C5-C6	-7.69	113.55	117.40
36	5	2927	C	OP2-P-O3'	7.68	122.11	105.20
36	5	1176	C	C2-N3-C4	-7.68	116.06	119.90
36	5	1450	G	N1-C2-N2	7.68	123.11	116.20
1	2	1600	A	C2-N3-C4	-7.68	106.76	110.60
1	6	17	C	N3-C2-O2	-7.67	116.53	121.90
1	2	1039	A	O4'-C1'-N9	7.67	114.33	108.20
36	5	3154	C	C2-N1-C1'	7.67	127.23	118.80
36	5	2944	U	N1-C2-O2	7.67	128.17	122.80
36	5	1154	A	C2-N3-C4	7.66	114.43	110.60
36	5	1886	A	O5'-P-OP2	-7.66	98.80	105.70
36	5	2754	G	N1-C6-O6	-7.66	115.30	119.90
1	6	1473	U	C5-C4-O4	7.66	130.50	125.90
36	5	947	G	O5'-P-OP2	-7.66	98.81	105.70
36	1	1140	G	C4-C5-N7	7.66	113.86	110.80
36	5	2345	A	N1-C6-N6	7.66	123.19	118.60
36	1	2884	C	N3-C4-C5	7.65	124.96	121.90
36	5	1049	C	C5-C6-N1	7.65	124.83	121.00
36	5	2726	C	N3-C2-O2	-7.65	116.55	121.90
36	5	3245	A	C4-C5-N7	7.65	114.52	110.70
36	5	215	G	C8-N9-C4	-7.64	103.34	106.40
36	1	2693	C	N3-C4-C5	7.64	124.96	121.90
36	5	2211	U	C4-C5-C6	7.64	124.29	119.70
36	5	3188	G	N9-C4-C5	7.64	108.46	105.40
38	8	113	U	C2-N1-C1'	7.64	126.87	117.70
36	5	2861	U	O5'-P-OP1	-7.64	98.82	105.70
36	1	1366	A	N1-C2-N3	-7.64	125.48	129.30
1	6	630	A	N1-C6-N6	7.64	123.18	118.60
1	2	1761	U	C6-N1-C2	-7.63	116.42	121.00
38	4	27	U	OP1-P-OP2	-7.63	108.15	119.60
36	5	999	G	N1-C6-O6	-7.63	115.32	119.90
36	5	1464	G	C8-N9-C4	7.62	109.45	106.40
38	4	40	A	N1-C6-N6	7.62	123.17	118.60
36	1	2355	G	N1-C6-O6	7.62	124.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3034	C	C6-N1-C2	7.61	123.34	120.30
1	6	321	C	N3-C2-O2	-7.61	116.57	121.90
36	5	1449	A	N1-C6-N6	7.61	123.16	118.60
36	5	877	C	C4-C5-C6	-7.61	113.60	117.40
36	1	648	C	N3-C4-N4	7.60	123.32	118.00
36	5	1192	C	C5-C4-N4	-7.59	114.88	120.20
1	2	1291	G	N3-C4-N9	-7.59	121.44	126.00
36	1	895	A	C5-N7-C8	-7.59	100.11	103.90
12	C0	88	PRO	N-CA-CB	7.58	112.40	103.30
36	5	2199	G	C5-C6-O6	-7.58	124.05	128.60
36	1	3172	A	N7-C8-N9	-7.58	110.01	113.80
36	1	1838	G	C4-C5-N7	7.58	113.83	110.80
36	5	2831	G	C5-C6-O6	-7.58	124.05	128.60
36	1	1161	G	O5'-P-OP2	-7.57	98.88	105.70
36	1	2943	G	O5'-P-OP2	-7.57	98.89	105.70
1	6	1354	G	C8-N9-C4	-7.57	103.37	106.40
36	5	2377	G	O5'-P-OP2	-7.57	98.89	105.70
36	1	3362	A	N7-C8-N9	7.56	117.58	113.80
36	1	671	U	O5'-P-OP1	-7.55	98.90	105.70
36	5	3078	U	N3-C2-O2	-7.55	116.92	122.20
36	5	1392	G	C8-N9-C4	7.54	109.42	106.40
36	5	2865	U	N1-C2-O2	7.54	128.08	122.80
36	1	2302	G	C5-C6-O6	7.54	133.12	128.60
36	1	2983	C	N3-C4-N4	-7.54	112.72	118.00
36	1	2816	G	N1-C6-O6	7.53	124.42	119.90
36	5	2858	U	N3-C2-O2	-7.53	116.93	122.20
36	5	1838	G	C5-C6-O6	-7.52	124.09	128.60
36	5	2117	A	N1-C6-N6	-7.52	114.09	118.60
36	1	3306	U	C5-C4-O4	7.52	130.41	125.90
36	1	1198	C	N1-C2-O2	-7.51	114.39	118.90
36	5	914	A	O5'-P-OP1	-7.51	98.94	105.70
36	1	2831	G	C6-C5-N7	-7.51	125.90	130.40
36	1	661	G	C8-N9-C4	-7.50	103.40	106.40
36	5	645	A	C6-N1-C2	-7.50	114.10	118.60
36	1	2878	G	O5'-P-OP2	-7.49	98.96	105.70
36	1	810	A	N1-C6-N6	-7.49	114.11	118.60
36	5	1006	A	O5'-P-OP2	-7.49	98.96	105.70
49	m3	21	ARG	NE-CZ-NH1	-7.49	116.56	120.30
36	5	2857	C	C6-N1-C2	7.49	123.29	120.30
36	1	2633	U	OP1-P-O3'	7.48	121.67	105.20
36	1	2283	G	N1-C6-O6	7.48	124.39	119.90
36	1	2816	G	O4'-C1'-N9	7.48	114.18	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	805	G	C8-N9-C4	7.48	109.39	106.40
1	6	1777	G	O5'-P-OP1	-7.48	98.97	105.70
36	5	679	U	C5-C4-O4	7.48	130.39	125.90
36	5	1838	G	N1-C6-O6	7.47	124.38	119.90
36	1	2833	A	O5'-P-OP2	-7.47	98.98	105.70
36	5	963	G	O5'-P-OP2	-7.46	98.98	105.70
36	1	1329	U	O4'-C1'-N1	7.46	114.17	108.20
36	1	54	C	N3-C4-C5	7.46	124.89	121.90
36	5	3140	G	C5-C6-O6	-7.46	124.12	128.60
36	1	954	U	C6-N1-C2	-7.45	116.53	121.00
36	1	2726	C	N3-C2-O2	-7.45	116.69	121.90
36	5	1152	G	C5-C6-N1	-7.44	107.78	111.50
36	5	2343	C	C5-C6-N1	-7.44	117.28	121.00
1	6	542	A	C6-C5-N7	-7.44	127.09	132.30
36	5	2726	C	N1-C2-N3	7.44	124.41	119.20
36	5	585	A	O5'-P-OP2	-7.44	99.00	105.70
36	1	1495	U	N3-C2-O2	-7.43	117.00	122.20
37	3	82	G	N3-C2-N2	7.43	125.10	119.90
36	5	3095	U	N3-C2-O2	-7.43	117.00	122.20
36	5	1154	A	N1-C2-N3	-7.43	125.58	129.30
41	l4	339	LEU	CA-CB-CG	7.43	132.38	115.30
36	5	871	U	C5-C4-O4	7.42	130.35	125.90
36	1	98	G	C2-N3-C4	-7.42	108.19	111.90
36	1	2400	G	C5-C6-O6	-7.42	124.15	128.60
36	1	714	G	N9-C4-C5	-7.42	102.43	105.40
36	5	660	A	C8-N9-C4	7.42	108.77	105.80
36	5	2343	C	C6-N1-C2	7.42	123.27	120.30
36	5	2875	U	N3-C4-O4	-7.42	114.21	119.40
37	7	89	G	N3-C2-N2	7.42	125.09	119.90
1	2	933	A	C8-N9-C4	-7.41	102.83	105.80
36	5	1399	A	N1-C6-N6	7.41	123.05	118.60
36	5	2293	C	C5-C4-N4	-7.41	115.01	120.20
36	5	2843	U	N3-C2-O2	-7.41	117.01	122.20
36	1	304	G	N1-C2-N2	7.41	122.87	116.20
36	5	2870	C	C2-N1-C1'	-7.41	110.66	118.80
36	5	1406	A	N1-C6-N6	7.40	123.04	118.60
36	5	2889	C	C2-N3-C4	-7.40	116.20	119.90
36	1	1886	A	O5'-P-OP2	-7.40	99.04	105.70
36	5	1875	G	N1-C6-O6	-7.40	115.46	119.90
36	5	2295	A	C5-C6-N1	7.40	121.40	117.70
36	5	2942	C	C6-N1-C1'	-7.40	111.92	120.80
36	1	2942	C	C6-N1-C2	7.40	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1157	G	N9-C4-C5	7.39	108.36	105.40
1	6	782	U	N1-C2-O2	7.39	127.98	122.80
36	1	2329	C	O5'-P-OP2	-7.39	99.05	105.70
52	m6	94	ARG	NE-CZ-NH1	-7.39	116.60	120.30
36	5	838	G	N1-C6-O6	-7.39	115.47	119.90
36	5	3059	G	O5'-P-OP1	-7.39	99.05	105.70
36	5	2135	U	N3-C4-C5	7.38	119.03	114.60
36	5	2693	C	N3-C4-C5	7.38	124.85	121.90
36	1	2827	U	O4'-C1'-N1	7.38	114.10	108.20
36	5	3351	U	N3-C2-O2	-7.38	117.03	122.20
36	5	2834	G	O5'-P-OP1	-7.38	99.06	105.70
36	1	1331	U	C5-C4-O4	-7.38	121.47	125.90
1	2	1745	G	N3-C4-N9	7.37	130.42	126.00
36	5	3127	A	O5'-P-OP2	-7.37	99.06	105.70
36	1	876	A	N1-C6-N6	7.37	123.02	118.60
1	6	609	U	C5-C6-N1	-7.37	119.02	122.70
36	5	2753	G	N3-C2-N2	-7.37	114.74	119.90
36	5	719	U	N3-C2-O2	-7.37	117.04	122.20
36	5	2402	A	C8-N9-C4	-7.37	102.85	105.80
36	1	964	G	N1-C6-O6	-7.36	115.48	119.90
1	6	1	U	C2-N1-C1'	7.36	126.53	117.70
36	5	1375	G	C2-N3-C4	7.36	115.58	111.90
36	1	920	A	N1-C2-N3	7.36	132.98	129.30
36	1	2772	C	P-O3'-C3'	7.36	128.53	119.70
36	5	1331	U	N3-C4-C5	7.36	119.01	114.60
36	1	304	G	N3-C2-N2	-7.35	114.75	119.90
36	1	636	C	C5-C4-N4	-7.35	115.05	120.20
38	4	115	C	O5'-P-OP2	-7.35	99.09	105.70
36	5	39	A	N1-C6-N6	7.35	123.01	118.60
36	5	3200	G	N1-C6-O6	7.35	124.31	119.90
36	5	1879	A	C6-C5-N7	-7.34	127.16	132.30
36	5	2875	U	N1-C2-O2	-7.34	117.66	122.80
36	1	1148	G	N9-C4-C5	-7.34	102.46	105.40
1	2	1118	G	N1-C6-O6	7.34	124.30	119.90
38	4	109	A	N1-C6-N6	7.34	123.00	118.60
36	5	1925	U	O5'-P-OP2	-7.34	99.09	105.70
36	5	908	G	N1-C6-O6	7.34	124.30	119.90
1	6	308	C	C5-C6-N1	-7.33	117.33	121.00
36	1	2827	U	N1-C2-N3	7.32	119.29	114.90
1	6	421	A	C8-N9-C4	7.32	108.73	105.80
36	1	2343	C	N3-C4-C5	7.32	124.83	121.90
36	1	52	A	O5'-P-OP2	-7.31	99.12	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2726	C	C5-C4-N4	7.31	125.32	120.20
1	2	453	U	N1-C2-O2	7.31	127.92	122.80
1	6	557	G	N1-C6-O6	-7.31	115.51	119.90
36	5	882	A	N1-C2-N3	7.31	132.95	129.30
36	1	1906	G	C5-C6-O6	-7.30	124.22	128.60
36	1	2374	C	C6-N1-C1'	7.30	129.57	120.80
1	6	1514	U	N3-C4-O4	-7.30	114.29	119.40
36	5	2996	U	O5'-P-OP1	7.30	119.47	110.70
36	1	1896	A	O5'-P-OP1	-7.30	99.13	105.70
36	1	421	G	N3-C4-N9	7.30	130.38	126.00
36	1	697	A	C8-N9-C4	7.30	108.72	105.80
36	1	1599	G	O5'-P-OP2	-7.30	99.13	105.70
1	6	1600	A	C2-N3-C4	-7.30	106.95	110.60
36	1	650	C	C2-N3-C4	-7.30	116.25	119.90
36	5	655	C	C6-N1-C2	-7.30	117.38	120.30
36	1	1166	G	N1-C6-O6	7.29	124.28	119.90
37	7	7	G	O5'-P-OP1	7.29	119.45	110.70
36	5	1412	G	N9-C4-C5	7.29	108.31	105.40
36	1	2621	G	N1-C2-N2	7.29	122.76	116.20
36	5	3374	U	C5-C6-N1	-7.28	119.06	122.70
36	5	2351	U	N3-C2-O2	-7.28	117.10	122.20
36	5	2806	U	C5-C6-N1	-7.28	119.06	122.70
1	6	542	A	O4'-C1'-N9	7.28	114.02	108.20
36	1	2366	C	C5-C6-N1	7.28	124.64	121.00
36	1	3214	U	N3-C2-O2	-7.27	117.11	122.20
36	1	1923	C	C6-N1-C2	7.27	123.21	120.30
36	1	2642	A	C5-C6-N1	-7.26	114.07	117.70
1	6	901	G	C6-C5-N7	-7.26	126.04	130.40
38	4	9	A	O5'-P-OP2	-7.26	99.17	105.70
36	5	3046	A	N1-C6-N6	-7.26	114.25	118.60
36	5	2764	C	C6-N1-C2	7.26	123.20	120.30
36	5	3218	A	N9-C4-C5	-7.25	102.90	105.80
36	1	802	C	O5'-P-OP2	7.25	119.40	110.70
36	1	697	A	N9-C4-C5	-7.25	102.90	105.80
36	5	2953	U	C4-C5-C6	7.25	124.05	119.70
36	5	3103	A	C5-C6-N1	7.25	121.32	117.70
36	1	2169	G	C4-C5-N7	-7.25	107.90	110.80
36	1	2699	G	N1-C6-O6	7.25	124.25	119.90
36	5	3377	G	C4-C5-N7	7.25	113.70	110.80
36	1	2176	U	N3-C2-O2	-7.24	117.13	122.20
1	6	194	U	C2-N1-C1'	7.24	126.39	117.70
36	5	339	C	N3-C4-N4	-7.23	112.94	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	88	A	N1-C6-N6	7.23	122.94	118.60
36	1	645	A	N3-C4-N9	7.23	133.18	127.40
36	1	936	A	O5'-P-OP2	-7.23	99.19	105.70
24	d2	93	LEU	CA-CB-CG	7.23	131.92	115.30
36	5	2181	C	O5'-P-OP1	-7.22	99.20	105.70
36	1	1351	U	N3-C2-O2	-7.22	117.15	122.20
36	1	2550	U	N3-C2-O2	-7.22	117.15	122.20
36	5	2821	C	C5-C4-N4	-7.22	115.15	120.20
36	1	2808	A	O4'-C1'-N9	-7.22	102.43	108.20
36	5	3339	A	N1-C6-N6	7.22	122.93	118.60
36	1	2953	U	N1-C2-N3	7.21	119.22	114.90
36	1	802	C	O5'-P-OP1	-7.21	99.21	105.70
36	1	2173	U	N1-C2-O2	-7.21	117.76	122.80
36	5	1112	A	C5-C6-N6	-7.21	117.94	123.70
36	1	2255	A	C8-N9-C4	7.20	108.68	105.80
36	1	960	U	C2-N3-C4	-7.20	122.68	127.00
36	1	1405	U	C6-N1-C2	7.20	125.32	121.00
36	5	1311	G	O5'-P-OP2	-7.19	99.22	105.70
36	1	1389	G	C5-C6-O6	-7.19	124.28	128.60
36	1	1846	C	N1-C2-O2	-7.19	114.58	118.90
36	5	341	G	C5-C6-O6	-7.19	124.29	128.60
36	1	793	C	C5-C4-N4	-7.19	115.17	120.20
36	1	407	A	C5-C6-N6	-7.18	117.95	123.70
36	1	2936	A	O5'-P-OP1	-7.18	99.23	105.70
36	5	3218	A	C5-N7-C8	-7.18	100.31	103.90
36	5	3218	A	C6-C5-N7	-7.18	127.27	132.30
36	1	1165	A	N7-C8-N9	-7.18	110.21	113.80
36	5	1380	G	C8-N9-C4	7.18	109.27	106.40
36	5	1607	U	N3-C2-O2	-7.18	117.17	122.20
36	5	750	G	O5'-P-OP2	-7.18	99.24	105.70
36	1	1547	G	N7-C8-N9	-7.18	109.51	113.10
38	4	79	A	C8-N9-C4	-7.18	102.93	105.80
36	5	2796	G	N9-C4-C5	-7.18	102.53	105.40
36	5	804	C	N3-C4-C5	-7.18	119.03	121.90
36	5	2621	G	C5-C6-O6	-7.18	124.30	128.60
36	5	3188	G	C4-C5-N7	-7.18	107.93	110.80
36	1	2827	U	N3-C4-O4	-7.17	114.38	119.40
36	1	2406	C	C6-N1-C2	7.17	123.17	120.30
36	5	923	C	C5-C4-N4	-7.17	115.18	120.20
36	1	1205	A	O5'-P-OP2	-7.17	99.25	105.70
36	5	1607	U	P-O3'-C3'	7.17	128.30	119.70
36	1	1382	G	C8-N9-C4	7.17	109.27	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	861	C	C6-N1-C2	7.17	123.17	120.30
37	7	100	C	C6-N1-C2	7.17	123.17	120.30
36	5	200	C	N3-C4-N4	7.16	123.01	118.00
36	5	2928	C	C6-N1-C2	-7.16	117.44	120.30
36	1	699	A	C2-N3-C4	-7.16	107.02	110.60
36	1	2773	C	O5'-P-OP2	-7.16	99.25	105.70
36	1	1307	G	P-O3'-C3'	7.16	128.29	119.70
36	5	2362	C	N1-C2-O2	7.16	123.20	118.90
36	5	2765	C	C5-C6-N1	7.16	124.58	121.00
36	1	651	G	N3-C4-N9	7.16	130.29	126.00
1	6	1634	C	C2-N1-C1'	7.16	126.67	118.80
36	5	1859	A	O5'-P-OP2	-7.16	99.26	105.70
36	1	417	A	N1-C6-N6	7.15	122.89	118.60
36	1	895	A	C6-C5-N7	-7.15	127.29	132.30
38	4	140	G	N9-C4-C5	7.15	108.26	105.40
1	2	36	C	C6-N1-C2	7.15	123.16	120.30
1	6	139	C	P-O3'-C3'	7.15	128.28	119.70
36	1	2420	C	C6-N1-C2	-7.15	117.44	120.30
36	5	2813	A	C8-N9-C4	-7.15	102.94	105.80
36	1	2816	G	C5-C6-O6	-7.14	124.31	128.60
53	M7	23	ARG	NE-CZ-NH1	-7.14	116.73	120.30
36	5	1208	U	C5-C4-O4	7.14	130.18	125.90
36	5	2366	C	C5-C6-N1	7.14	124.57	121.00
36	1	668	G	N1-C6-O6	-7.13	115.62	119.90
36	1	422	A	N9-C4-C5	7.13	108.65	105.80
1	6	542	A	N1-C6-N6	7.13	122.88	118.60
36	5	911	C	C2-N3-C4	-7.13	116.33	119.90
36	5	2392	C	C2-N3-C4	-7.13	116.33	119.90
36	5	2824	G	C5-C6-O6	-7.13	124.32	128.60
36	1	701	G	OP2-P-O3'	7.13	120.89	105.20
50	M4	135	LEU	CA-CB-CG	7.13	131.70	115.30
36	5	1449	A	C2-N3-C4	-7.13	107.03	110.60
36	5	922	U	N3-C4-O4	-7.12	114.41	119.40
36	1	802	C	N3-C2-O2	-7.12	116.91	121.90
36	1	1405	U	N1-C2-O2	-7.12	117.81	122.80
36	5	1208	U	N3-C4-O4	-7.12	114.41	119.40
36	5	911	C	N1-C2-O2	-7.12	114.63	118.90
36	5	2631	U	OP1-P-O3'	7.12	120.87	105.20
36	1	369	A	C8-N9-C4	-7.12	102.95	105.80
36	1	922	U	C5-C6-N1	7.12	126.26	122.70
36	1	2639	G	C5-C6-O6	-7.12	124.33	128.60
1	2	942	G	N1-C6-O6	-7.12	115.63	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	419	G	N1-C2-N2	-7.12	109.79	116.20
36	1	3265	C	N3-C4-C5	7.12	124.75	121.90
36	5	2822	U	C6-N1-C2	7.12	125.27	121.00
36	5	1452	A	C8-N9-C4	7.12	108.65	105.80
1	2	1280	C	N3-C4-C5	-7.12	119.05	121.90
36	5	216	G	N1-C6-O6	7.12	124.17	119.90
36	1	827	A	C8-N9-C4	7.11	108.65	105.80
36	1	968	G	C5-C6-O6	-7.11	124.33	128.60
37	3	88	G	C5-C6-O6	7.11	132.87	128.60
36	5	2870	C	C4-C5-C6	-7.11	113.84	117.40
36	1	641	C	C2-N3-C4	-7.11	116.35	119.90
36	5	914	A	C2-N3-C4	-7.10	107.05	110.60
36	1	1216	C	C6-N1-C2	-7.10	117.46	120.30
36	1	2954	U	C6-N1-C2	7.10	125.26	121.00
1	2	74	U	O5'-P-OP1	-7.10	99.31	105.70
36	1	2836	C	C6-N1-C2	-7.10	117.46	120.30
36	1	639	G	C5-C6-O6	-7.10	124.34	128.60
36	1	644	G	C6-C5-N7	-7.10	126.14	130.40
36	1	1342	C	N3-C4-C5	7.10	124.74	121.90
36	1	2314	U	N1-C2-N3	-7.10	110.64	114.90
36	1	3109	G	O5'-P-OP2	7.10	119.22	110.70
36	5	2186	U	N3-C2-O2	-7.10	117.23	122.20
36	5	1190	A	C8-N9-C4	-7.09	102.96	105.80
1	2	1082	C	N1-C2-O2	7.09	123.16	118.90
36	1	960	U	C6-N1-C2	7.09	125.25	121.00
36	5	53	G	C8-N9-C4	7.09	109.24	106.40
1	2	1280	C	C6-N1-C2	-7.09	117.46	120.30
36	1	2169	G	C5-C6-O6	7.09	132.85	128.60
36	5	349	A	O5'-P-OP2	-7.09	99.32	105.70
36	5	869	G	C5-C6-N1	7.09	115.05	111.50
36	5	3039	C	O5'-P-OP2	-7.09	99.32	105.70
36	1	671	U	N1-C2-O2	-7.09	117.84	122.80
1	6	1535	U	N3-C2-O2	-7.09	117.24	122.20
36	1	196	G	C5-C6-O6	-7.08	124.35	128.60
1	2	1432	U	C5-C6-N1	-7.08	119.16	122.70
36	1	608	A	C5-C6-N6	-7.08	118.03	123.70
1	2	1200	G	C5-C6-N1	-7.08	107.96	111.50
1	2	1745	G	C5-C6-O6	-7.08	124.35	128.60
36	1	662	U	C5-C4-O4	7.08	130.15	125.90
36	5	1157	G	OP2-P-O3'	7.08	120.77	105.20
38	4	94	C	C6-N1-C2	7.08	123.13	120.30
36	5	1116	G	C4-C5-N7	-7.07	107.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1314	C	N3-C4-C5	7.07	124.73	121.90
36	1	908	G	O4'-C1'-N9	-7.07	102.54	108.20
36	1	1279	C	C6-N1-C2	-7.07	117.47	120.30
36	1	2144	A	C5-C6-N6	-7.07	118.04	123.70
36	1	2194	G	C6-C5-N7	-7.07	126.16	130.40
36	5	974	G	N3-C4-C5	-7.07	125.06	128.60
37	7	11	A	N1-C6-N6	7.07	122.84	118.60
36	1	2874	G	N1-C2-N3	7.07	128.14	123.90
36	1	111	C	C6-N1-C2	7.07	123.13	120.30
36	5	3136	G	C2-N3-C4	-7.06	108.37	111.90
36	5	1307	G	O5'-P-OP1	-7.06	99.34	105.70
36	5	1371	G	N1-C6-O6	-7.06	115.66	119.90
36	5	3195	U	P-O3'-C3'	7.06	128.17	119.70
36	5	1184	A	N1-C6-N6	-7.05	114.37	118.60
18	C6	40	GLU	C-N-CD	-7.05	105.09	120.60
36	5	1131	G	O5'-P-OP2	-7.05	99.35	105.70
36	1	1920	U	N3-C2-O2	-7.05	117.27	122.20
1	2	1773	C	C6-N1-C2	-7.05	117.48	120.30
36	5	1192	C	C2-N3-C4	-7.05	116.38	119.90
1	6	163	G	C8-N9-C1'	7.04	136.16	127.00
36	1	1365	G	N3-C4-C5	-7.04	125.08	128.60
36	5	646	A	N7-C8-N9	7.04	117.32	113.80
36	5	864	G	C5-C6-O6	-7.04	124.38	128.60
36	5	2937	G	N1-C6-O6	7.04	124.12	119.90
36	5	872	U	C5-C4-O4	-7.04	121.68	125.90
36	5	993	G	O5'-P-OP2	-7.04	99.37	105.70
36	5	936	A	C8-N9-C4	-7.03	102.99	105.80
36	5	2371	G	N3-C2-N2	7.03	124.82	119.90
36	5	2797	C	N3-C4-C5	-7.03	119.09	121.90
1	6	1614	A	N1-C6-N6	7.03	122.82	118.60
36	5	424	G	C4-C5-N7	7.03	113.61	110.80
36	1	34	A	OP2-P-O3'	7.03	120.65	105.20
1	6	1537	C	N1-C2-O2	-7.03	114.68	118.90
36	5	869	G	N1-C6-O6	-7.03	115.69	119.90
36	1	2243	A	O5'-P-OP2	-7.02	99.38	105.70
36	5	1321	G	C6-C5-N7	-7.02	126.19	130.40
62	N6	126	LEU	CA-CB-CG	7.01	131.43	115.30
36	1	2874	G	N9-C4-C5	7.01	108.20	105.40
36	1	2659	G	N1-C6-O6	7.00	124.10	119.90
38	4	82	U	C5-C6-N1	7.00	126.20	122.70
36	5	911	C	C5-C6-N1	-7.00	117.50	121.00
36	1	1429	G	N1-C2-N2	-7.00	109.90	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	999	G	OP2-P-O3'	7.00	120.59	105.20
36	5	3188	G	C5-C6-O6	7.00	132.80	128.60
1	2	75	U	C2-N1-C1'	7.00	126.09	117.70
36	1	2409	G	N3-C2-N2	6.99	124.80	119.90
36	1	1316	C	O5'-P-OP2	-6.99	99.41	105.70
36	1	2283	G	C5-C6-O6	-6.99	124.41	128.60
36	5	641	C	C2-N3-C4	-6.99	116.41	119.90
36	5	1111	U	C5-C4-O4	-6.99	121.71	125.90
36	5	3093	C	N1-C2-O2	-6.99	114.71	118.90
38	8	100	U	C2-N1-C1'	6.99	126.09	117.70
36	1	874	U	OP1-P-O3'	6.99	120.57	105.20
1	6	385	A	N1-C6-N6	-6.99	114.41	118.60
36	5	3333	G	O5'-P-OP2	-6.99	99.41	105.70
36	5	1496	C	N3-C4-C5	6.98	124.69	121.90
36	5	2419	A	C8-N9-C4	-6.98	103.01	105.80
36	1	817	A	C4-C5-C6	6.98	120.49	117.00
1	6	771	A	N1-C6-N6	6.97	122.78	118.60
36	1	92	G	C5-C6-O6	-6.97	124.42	128.60
36	1	675	C	N1-C2-O2	-6.97	114.72	118.90
1	6	1003	A	C8-N9-C4	6.97	108.59	105.80
36	5	3041	U	C4-C5-C6	-6.97	115.52	119.70
1	2	934	C	C2-N1-C1'	6.97	126.47	118.80
36	5	353	G	C4-N9-C1'	-6.97	117.44	126.50
36	5	1170	A	N1-C6-N6	6.97	122.78	118.60
36	5	1520	G	C5-C6-O6	-6.97	124.42	128.60
36	1	2373	A	OP1-P-O3'	6.97	120.53	105.20
36	5	2211	U	N3-C2-O2	-6.97	117.32	122.20
36	1	909	G	C8-N9-C4	6.97	109.19	106.40
36	5	2117	A	N9-C4-C5	6.97	108.59	105.80
1	6	352	A	O5'-P-OP2	-6.96	99.43	105.70
1	2	1118	G	C5-C6-O6	-6.96	124.42	128.60
36	5	3060	C	N3-C2-O2	6.96	126.77	121.90
37	7	73	C	C6-N1-C2	-6.96	117.52	120.30
36	1	2732	G	N3-C2-N2	6.96	124.77	119.90
36	1	2879	C	C6-N1-C2	6.96	123.08	120.30
36	1	1116	G	OP2-P-O3'	6.95	120.49	105.20
36	1	2879	C	N3-C2-O2	6.95	126.77	121.90
39	L2	96	LEU	CA-CB-CG	6.95	131.28	115.30
36	5	2138	A	C8-N9-C4	-6.95	103.02	105.80
36	5	2815	G	C5-N7-C8	6.95	107.77	104.30
36	5	1298	C	C6-N1-C2	-6.95	117.52	120.30
36	5	2343	C	N3-C4-C5	6.95	124.68	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	m0	167	LEU	CA-CB-CG	6.95	131.27	115.30
36	1	714	G	C6-C5-N7	-6.94	126.23	130.40
36	5	1370	G	N1-C6-O6	-6.94	115.73	119.90
36	1	1139	G	O5'-P-OP1	-6.94	99.45	105.70
36	5	1110	U	N1-C2-O2	6.94	127.66	122.80
36	5	2278	C	N3-C4-C5	6.94	124.68	121.90
36	5	2283	G	O5'-P-OP2	-6.94	99.45	105.70
36	1	2986	U	N1-C2-N3	6.94	119.06	114.90
36	1	2878	G	O5'-P-OP1	6.94	119.02	110.70
38	8	56	G	N1-C6-O6	6.94	124.06	119.90
36	5	1496	C	O5'-P-OP2	-6.93	99.46	105.70
36	1	880	G	N1-C6-O6	-6.93	115.74	119.90
38	4	98	U	C5-C4-O4	-6.93	121.74	125.90
36	5	1010	G	O5'-P-OP2	-6.93	99.47	105.70
36	1	984	G	C8-N9-C4	-6.93	103.63	106.40
36	5	907	G	N9-C4-C5	-6.93	102.63	105.40
36	5	950	G	C5-C6-O6	-6.93	124.44	128.60
36	5	3093	C	C6-N1-C2	6.93	123.07	120.30
1	2	581	U	C2-N1-C1'	6.92	126.01	117.70
36	1	1429	G	N3-C4-C5	-6.92	125.14	128.60
36	1	2640	A	C6-N1-C2	-6.92	114.44	118.60
36	1	3344	A	C5-N7-C8	-6.92	100.44	103.90
1	6	163	G	C5-N7-C8	-6.92	100.84	104.30
15	C3	22	ALA	C-N-CD	-6.92	105.38	120.60
36	1	28	C	N3-C4-C5	6.92	124.67	121.90
36	1	1429	G	N3-C4-N9	6.92	130.15	126.00
36	1	2372	A	C2-N3-C4	6.92	114.06	110.60
36	5	946	U	O5'-P-OP2	-6.92	99.47	105.70
36	5	1101	G	N3-C2-N2	6.92	124.74	119.90
36	1	639	G	N3-C2-N2	-6.91	115.06	119.90
36	1	809	G	N9-C4-C5	-6.91	102.64	105.40
36	5	633	C	N1-C2-O2	-6.91	114.75	118.90
36	1	640	U	N3-C4-O4	6.91	124.23	119.40
36	1	1307	G	OP1-P-O3'	6.91	120.39	105.20
36	5	672	A	C5-C6-N6	-6.90	118.18	123.70
36	1	1137	C	C5-C4-N4	-6.90	115.37	120.20
36	5	3043	C	N3-C4-C5	6.90	124.66	121.90
36	1	3344	A	O4'-C1'-N9	6.90	113.72	108.20
36	1	2867	C	N3-C4-N4	-6.89	113.17	118.00
36	5	3343	G	N3-C4-N9	6.89	130.14	126.00
1	2	359	A	C8-N9-C4	6.89	108.56	105.80
36	1	1140	G	N9-C4-C5	-6.89	102.64	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	426	G	N7-C8-N9	-6.89	109.65	113.10
36	5	3190	C	C6-N1-C2	-6.89	117.54	120.30
1	2	378	A	N1-C6-N6	6.89	122.73	118.60
1	2	830	U	N1-C2-O2	6.89	127.62	122.80
36	1	2983	C	C5-C6-N1	-6.89	117.56	121.00
36	5	425	G	C5-C6-O6	-6.89	124.47	128.60
36	1	1838	G	C6-C5-N7	-6.89	126.27	130.40
38	4	40	A	C5-C6-N6	-6.89	118.19	123.70
36	5	1181	U	O5'-P-OP1	-6.89	99.50	105.70
36	1	970	A	C8-N9-C4	-6.88	103.05	105.80
36	1	942	U	OP1-P-OP2	-6.88	109.28	119.60
37	3	93	C	N3-C4-N4	-6.88	113.18	118.00
36	1	918	C	C6-N1-C2	-6.88	117.55	120.30
1	6	1780	G	N3-C2-N2	6.88	124.71	119.90
36	5	509	U	N1-C2-O2	-6.88	117.99	122.80
36	5	2364	G	N1-C6-O6	-6.88	115.77	119.90
36	1	2140	U	O5'-P-OP2	-6.87	99.51	105.70
36	1	2944	U	O5'-P-OP1	-6.87	99.51	105.70
36	1	3178	A	C2-N3-C4	-6.87	107.16	110.60
36	5	2822	U	C5-C6-N1	-6.87	119.26	122.70
37	7	33	U	N3-C2-O2	-6.87	117.39	122.20
36	1	3092	C	O5'-P-OP1	-6.87	99.52	105.70
37	7	36	C	O5'-P-OP2	6.87	118.94	110.70
36	1	1300	G	C5-C6-O6	-6.87	124.48	128.60
36	1	2760	C	N3-C4-C5	-6.87	119.15	121.90
36	1	3212	C	C6-N1-C2	6.87	123.05	120.30
1	2	323	A	C8-N9-C4	-6.87	103.05	105.80
36	1	1177	G	O5'-P-OP2	-6.87	99.52	105.70
36	1	1307	G	N1-C6-O6	-6.86	115.78	119.90
36	5	2404	A	C8-N9-C4	6.86	108.55	105.80
36	5	2407	C	O5'-P-OP2	-6.86	99.52	105.70
36	1	1712	G	C6-C5-N7	-6.86	126.28	130.40
36	5	1452	A	C4-C5-N7	6.86	114.13	110.70
36	5	2754	G	N3-C2-N2	6.86	124.70	119.90
36	1	1412	G	O5'-P-OP1	-6.86	99.53	105.70
36	1	2308	C	N1-C2-O2	-6.85	114.79	118.90
36	5	75	G	C5-C6-O6	-6.85	124.49	128.60
36	1	2315	G	C5-C6-O6	6.85	132.71	128.60
36	5	2278	C	C5-C6-N1	6.85	124.43	121.00
36	1	3079	U	C5-C6-N1	-6.85	119.28	122.70
36	1	1144	U	C5-C6-N1	-6.85	119.28	122.70
36	1	3362	A	C2-N3-C4	-6.85	107.18	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	SM	167	PRO	N-CA-CB	6.84	111.51	103.30
36	1	1420	C	C5-C4-N4	6.84	124.99	120.20
36	5	1060	U	N3-C4-O4	-6.84	114.61	119.40
36	1	1197	A	C5-C6-N6	-6.84	118.23	123.70
36	5	776	U	N1-C2-N3	6.84	119.00	114.90
36	5	1882	G	O5'-P-OP1	-6.84	99.55	105.70
36	5	3269	U	P-O3'-C3'	6.84	127.91	119.70
36	1	2836	C	N3-C4-C5	-6.83	119.17	121.90
37	3	96	U	C5-C6-N1	-6.83	119.28	122.70
1	6	1600	A	C5-N7-C8	-6.83	100.48	103.90
36	5	1112	A	N1-C6-N6	6.83	122.70	118.60
36	5	2942	C	C5-C4-N4	-6.83	115.42	120.20
38	8	26	U	O5'-P-OP2	-6.83	99.55	105.70
36	1	96	G	C4-C5-N7	6.83	113.53	110.80
36	1	1306	G	N1-C6-O6	6.83	124.00	119.90
38	4	103	G	N9-C4-C5	6.83	108.13	105.40
36	5	1395	G	OP2-P-O3'	6.83	120.22	105.20
36	5	2806	U	C2-N3-C4	-6.83	122.90	127.00
36	5	3374	U	C6-N1-C2	6.83	125.10	121.00
36	1	2177	G	N3-C4-N9	6.82	130.09	126.00
1	6	1600	A	N9-C1'-C2'	6.82	122.87	114.00
36	5	644	G	N9-C4-C5	6.82	108.13	105.40
36	5	2875	U	C6-N1-C1'	6.82	130.75	121.20
38	4	89	A	C8-N9-C4	6.82	108.53	105.80
36	5	612	U	O5'-P-OP1	-6.82	99.56	105.70
36	5	2821	C	N3-C4-C5	6.82	124.63	121.90
1	2	287	G	O4'-C1'-N9	6.82	113.65	108.20
36	1	805	G	N7-C8-N9	-6.82	109.69	113.10
36	1	2942	C	N3-C4-C5	6.82	124.63	121.90
36	1	220	G	N1-C6-O6	6.82	123.99	119.90
36	1	1303	A	N9-C4-C5	-6.82	103.07	105.80
36	1	2808	A	C4-C5-N7	6.82	114.11	110.70
1	6	609	U	N3-C2-O2	-6.82	117.43	122.20
36	5	1513	G	N7-C8-N9	6.82	116.51	113.10
36	5	2763	U	C5-C4-O4	-6.82	121.81	125.90
73	O7	65	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	2	728	U	C2-N1-C1'	6.81	125.88	117.70
36	1	1132	C	C5-C6-N1	-6.81	117.59	121.00
36	1	1902	G	N1-C6-O6	-6.81	115.81	119.90
36	5	648	C	O5'-P-OP2	-6.81	99.57	105.70
36	5	1456	A	N9-C4-C5	-6.81	103.08	105.80
36	5	1657	C	N1-C2-O2	6.81	122.99	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1462	G	C5-C6-O6	-6.81	124.52	128.60
36	5	2234	G	C8-N9-C4	6.81	109.12	106.40
36	1	639	G	N9-C1'-C2'	-6.80	104.52	112.00
1	6	308	C	C2-N1-C1'	-6.80	111.31	118.80
1	6	942	G	N1-C6-O6	-6.80	115.82	119.90
36	5	644	G	C4-C5-N7	-6.80	108.08	110.80
36	5	3123	A	C8-N9-C4	6.80	108.52	105.80
1	2	90	C	C6-N1-C2	-6.80	117.58	120.30
1	6	965	U	N1-C2-O2	6.80	127.56	122.80
36	1	1661	G	N3-C4-N9	6.80	130.08	126.00
38	4	47	C	N1-C2-O2	6.80	122.98	118.90
36	5	61	A	C2-N3-C4	-6.80	107.20	110.60
36	5	2389	C	C2-N3-C4	-6.80	116.50	119.90
36	5	2754	G	N1-C2-N2	-6.80	110.08	116.20
36	1	1308	A	C5-N7-C8	-6.79	100.50	103.90
36	1	1604	G	C4-N9-C1'	6.79	135.33	126.50
36	5	1838	G	N3-C2-N2	-6.79	115.14	119.90
36	1	339	C	N3-C4-N4	-6.79	113.25	118.00
36	1	2862	U	C5-C6-N1	-6.79	119.31	122.70
36	5	419	G	N9-C4-C5	-6.79	102.68	105.40
36	5	1116	G	N3-C4-C5	-6.79	125.20	128.60
36	1	821	U	C5-C4-O4	6.79	129.97	125.90
36	5	1148	G	C4-C5-N7	6.79	113.52	110.80
1	6	1632	C	N1-C2-O2	6.79	122.97	118.90
36	1	666	A	N1-C6-N6	-6.79	114.53	118.60
36	5	3362	A	O4'-C1'-N9	6.79	113.63	108.20
1	2	507	U	N1-C2-O2	6.78	127.55	122.80
1	2	1112	G	N1-C6-O6	6.78	123.97	119.90
36	1	1060	U	C5-C6-N1	-6.78	119.31	122.70
36	5	2694	A	C2-N3-C4	6.77	113.99	110.60
36	5	361	A	N1-C6-N6	-6.77	114.54	118.60
36	5	1301	A	C5-C6-N6	-6.77	118.28	123.70
1	6	453	U	C6-N1-C2	-6.77	116.94	121.00
1	6	1537	C	C6-N1-C2	-6.77	117.59	120.30
1	2	647	G	N3-C4-N9	-6.76	121.94	126.00
36	5	2816	G	O4'-C1'-N9	6.76	113.61	108.20
36	1	3110	C	C6-N1-C2	-6.76	117.60	120.30
36	1	386	A	N1-C6-N6	6.76	122.66	118.60
1	6	1614	A	C4-C5-N7	6.76	114.08	110.70
36	5	216	G	C5-C6-O6	-6.76	124.54	128.60
36	1	1168	U	N1-C2-O2	6.76	127.53	122.80
36	1	206	G	C2-N3-C4	6.76	115.28	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2388	U	N1-C2-O2	-6.75	118.07	122.80
36	5	1205	A	O5'-P-OP2	-6.75	99.62	105.70
36	1	24	G	N3-C2-N2	-6.75	115.17	119.90
36	1	3048	A	O5'-P-OP2	-6.75	99.62	105.70
36	1	970	A	C5-N7-C8	-6.75	100.53	103.90
36	1	2130	G	C5-C6-O6	6.75	132.65	128.60
36	5	953	G	C4-C5-N7	6.75	113.50	110.80
36	1	1377	G	N9-C4-C5	-6.75	102.70	105.40
36	5	32	U	C6-N1-C2	-6.74	116.95	121.00
36	1	894	G	C5-C6-O6	-6.74	124.56	128.60
1	6	371	G	N3-C4-N9	6.74	130.04	126.00
36	1	1616	U	O5'-P-OP1	-6.74	99.63	105.70
38	4	113	U	C5-C6-N1	-6.74	119.33	122.70
36	5	1115	G	C8-N9-C4	-6.74	103.70	106.40
36	1	2314	U	N3-C4-O4	6.74	124.12	119.40
36	1	1396	C	C6-N1-C2	6.74	123.00	120.30
36	1	1396	C	N3-C4-C5	6.74	124.59	121.90
36	1	2983	C	C4-C5-C6	6.74	120.77	117.40
36	1	876	A	C5-C6-N6	-6.73	118.31	123.70
36	1	2115	G	C5-C6-O6	-6.73	124.56	128.60
36	5	926	A	N1-C6-N6	6.73	122.64	118.60
36	1	2870	C	N3-C4-N4	-6.73	113.29	118.00
36	1	632	G	OP2-P-O3'	6.73	120.00	105.20
36	1	1133	A	C8-N9-C4	6.72	108.49	105.80
1	6	163	G	N9-C4-C5	6.72	108.09	105.40
36	5	1858	A	C8-N9-C4	-6.72	103.11	105.80
36	5	1456	A	C8-N9-C4	6.72	108.49	105.80
36	5	3218	A	P-O3'-C3'	6.72	127.77	119.70
36	1	2249	G	N3-C4-N9	6.71	130.03	126.00
36	1	3305	A	N1-C6-N6	-6.71	114.57	118.60
36	5	389	A	C8-N9-C4	-6.71	103.11	105.80
36	1	718	G	C4-C5-N7	6.71	113.48	110.80
36	1	817	A	C8-N9-C4	-6.71	103.11	105.80
36	5	573	C	C6-N1-C2	-6.71	117.61	120.30
36	5	1513	G	N3-C4-C5	-6.71	125.25	128.60
1	2	579	A	N1-C2-N3	6.71	132.65	129.30
1	6	459	G	N1-C6-O6	6.71	123.92	119.90
1	6	609	U	N3-C4-O4	-6.71	114.70	119.40
36	5	413	U	N1-C2-O2	-6.71	118.10	122.80
36	5	751	A	O5'-P-OP2	-6.71	99.66	105.70
36	1	3368	U	C2-N1-C1'	-6.71	109.65	117.70
36	5	1113	G	C2-N3-C4	-6.71	108.55	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1461	A	C8-N9-C4	6.70	108.48	105.80
36	5	1902	G	C5-C6-N1	6.70	114.85	111.50
36	5	2902	A	N1-C6-N6	6.70	122.62	118.60
36	5	1101	G	C8-N9-C4	6.70	109.08	106.40
36	5	2391	G	N1-C6-O6	-6.70	115.88	119.90
36	1	974	G	N3-C4-C5	-6.70	125.25	128.60
1	2	1761	U	P-O3'-C3'	6.70	127.74	119.70
36	1	1405	U	N3-C2-O2	6.70	126.89	122.20
36	1	1515	A	N1-C6-N6	6.70	122.62	118.60
36	1	2144	A	C2-N3-C4	6.70	113.95	110.60
36	5	433	A	C2-N3-C4	-6.70	107.25	110.60
1	2	1654	G	C5-C6-O6	-6.70	124.58	128.60
36	1	2115	G	N1-C6-O6	6.70	123.92	119.90
36	1	1144	U	C2-N3-C4	-6.69	122.98	127.00
36	1	1433	A	C5-C6-N1	6.69	121.05	117.70
36	5	1085	A	C2-N3-C4	-6.69	107.25	110.60
36	5	2900	A	OP2-P-O3'	6.69	119.92	105.20
36	1	1489	A	C8-N9-C4	6.69	108.48	105.80
1	6	1773	C	C4-C5-C6	6.69	120.75	117.40
36	1	2356	A	N1-C6-N6	6.69	122.61	118.60
36	1	644	G	C8-N9-C4	-6.69	103.72	106.40
36	1	1191	U	N1-C2-O2	-6.69	118.12	122.80
36	1	3278	C	N3-C4-N4	-6.69	113.32	118.00
36	5	1170	A	N9-C4-C5	-6.69	103.12	105.80
36	5	2278	C	N1-C2-O2	6.68	122.91	118.90
36	5	2634	U	C5-C4-O4	-6.68	121.89	125.90
36	1	640	U	N1-C2-O2	-6.68	118.12	122.80
1	6	977	A	N1-C6-N6	6.68	122.61	118.60
36	1	1496	C	C5-C6-N1	6.68	124.34	121.00
38	4	16	G	C8-N9-C4	6.68	109.07	106.40
36	1	1867	A	C8-N9-C4	6.67	108.47	105.80
1	6	1794	A	O5'-P-OP1	-6.67	99.69	105.70
36	5	218	G	O5'-P-OP2	-6.67	99.69	105.70
77	q1	9	ARG	NE-CZ-NH1	6.67	123.64	120.30
38	4	13	A	N7-C8-N9	6.67	117.14	113.80
36	5	1487	G	N9-C4-C5	6.67	108.07	105.40
36	5	2953	U	N1-C2-O2	-6.67	118.13	122.80
36	1	2936	A	O5'-P-OP2	6.67	118.70	110.70
36	1	196	G	N9-C4-C5	-6.67	102.73	105.40
36	1	2865	U	N3-C4-C5	6.66	118.60	114.60
36	5	2818	U	O5'-P-OP1	-6.66	99.70	105.70
36	5	2942	C	C2-N1-C1'	6.66	126.13	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3154	C	N3-C2-O2	-6.66	117.23	121.90
1	6	1489	U	C2-N1-C1'	6.66	125.69	117.70
1	2	507	U	N3-C2-O2	-6.66	117.54	122.20
36	1	2899	C	C2-N1-C1'	6.66	126.13	118.80
36	1	3036	G	N3-C4-C5	-6.66	125.27	128.60
36	5	2728	G	C2-N3-C4	6.66	115.23	111.90
36	1	2996	U	N1-C2-O2	6.66	127.46	122.80
36	5	892	U	N3-C4-O4	-6.66	114.74	119.40
36	5	2417	U	N3-C4-O4	6.66	124.06	119.40
36	1	2414	G	N3-C2-N2	-6.66	115.24	119.90
1	2	864	U	N3-C2-O2	-6.66	117.54	122.20
36	5	213	A	O5'-P-OP1	6.66	118.69	110.70
36	5	931	C	C5-C6-N1	-6.66	117.67	121.00
36	5	994	G	N3-C4-N9	6.66	129.99	126.00
36	5	2333	C	N3-C4-C5	6.66	124.56	121.90
36	1	895	A	C8-N9-C4	-6.65	103.14	105.80
36	5	2796	G	C4-C5-N7	6.65	113.46	110.80
36	1	1589	A	O4'-C1'-N9	-6.65	102.88	108.20
1	6	18	C	N3-C4-C5	-6.65	119.24	121.90
1	6	639	U	N3-C2-O2	-6.65	117.55	122.20
36	1	419	G	N3-C2-N2	6.65	124.55	119.90
36	5	2851	A	N1-C2-N3	6.65	132.62	129.30
36	5	1371	G	C4-C5-N7	-6.65	108.14	110.80
36	1	648	C	O5'-P-OP1	-6.64	99.72	105.70
1	6	453	U	C5-C4-O4	6.64	129.89	125.90
36	5	3362	A	C5-N7-C8	-6.64	100.58	103.90
1	6	1100	G	N3-C4-C5	-6.64	125.28	128.60
36	1	695	C	N3-C4-C5	6.64	124.55	121.90
36	1	2869	U	OP2-P-O3'	6.64	119.80	105.20
36	5	3154	C	C5-C6-N1	6.64	124.32	121.00
36	1	397	A	C5-C6-N1	6.63	121.02	117.70
1	6	858	G	O4'-C1'-N9	6.63	113.51	108.20
1	6	543	C	C6-N1-C2	-6.63	117.65	120.30
36	1	2836	C	C5-C4-N4	6.63	124.84	120.20
36	1	608	A	C6-C5-N7	-6.63	127.66	132.30
36	5	931	C	C2-N3-C4	-6.62	116.59	119.90
36	5	2331	C	N3-C4-C5	-6.62	119.25	121.90
36	5	2368	A	N1-C6-N6	-6.62	114.63	118.60
1	6	1043	A	N1-C6-N6	6.62	122.57	118.60
36	5	1370	G	N3-C4-N9	6.62	129.97	126.00
36	1	933	A	N1-C2-N3	6.62	132.61	129.30
36	1	2281	A	C8-N9-C4	6.62	108.45	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2418	G	OP2-P-O3'	6.62	119.76	105.20
1	6	1773	C	C6-N1-C2	-6.62	117.65	120.30
36	5	1825	G	O5'-P-OP2	-6.62	99.74	105.70
36	1	2615	G	C5-C6-O6	-6.62	124.63	128.60
36	5	2634	U	N1-C2-O2	-6.62	118.17	122.80
36	1	1119	C	N3-C4-N4	-6.61	113.37	118.00
1	6	402	C	O5'-P-OP2	-6.61	99.75	105.70
1	6	794	U	N1-C2-O2	6.61	127.43	122.80
36	5	1307	G	C2'-C3'-O3'	6.61	124.28	113.70
36	1	1181	U	N3-C2-O2	-6.61	117.57	122.20
36	5	326	U	OP2-P-O3'	6.61	119.74	105.20
36	1	2661	G	C5-C6-O6	-6.61	124.64	128.60
36	5	681	U	N3-C4-O4	6.61	124.03	119.40
38	4	26	U	OP1-P-O3'	6.61	119.73	105.20
36	1	3181	C	C6-N1-C2	-6.60	117.66	120.30
1	6	103	A	N7-C8-N9	6.60	117.10	113.80
36	5	3285	C	C2-N1-C1'	6.60	126.06	118.80
36	1	2618	G	N1-C2-N2	-6.60	110.26	116.20
1	6	1106	U	O5'-P-OP1	-6.60	99.76	105.70
36	5	2234	G	N1-C6-O6	6.60	123.86	119.90
1	6	543	C	N1-C2-O2	6.60	122.86	118.90
36	5	2870	C	C6-N1-C1'	6.60	128.72	120.80
36	1	1324	U	O5'-P-OP1	6.59	118.61	110.70
41	L4	327	LEU	CA-CB-CG	6.59	130.47	115.30
36	5	86	G	O5'-P-OP2	-6.59	99.77	105.70
36	5	673	U	C5-C6-N1	-6.59	119.40	122.70
1	2	1486	G	C8-N9-C4	-6.59	103.76	106.40
36	5	2953	U	N3-C4-C5	-6.59	110.65	114.60
36	1	1310	G	C5-C6-O6	6.59	132.55	128.60
36	1	1351	U	C2-N1-C1'	6.59	125.61	117.70
36	1	1405	U	C5-C6-N1	-6.59	119.41	122.70
36	5	343	U	O5'-P-OP1	-6.59	99.77	105.70
36	5	2954	U	C5-C4-O4	-6.59	121.95	125.90
37	7	85	G	O5'-P-OP2	6.59	118.61	110.70
36	1	52	A	OP1-P-OP2	6.59	129.48	119.60
36	1	54	C	C2-N1-C1'	-6.59	111.56	118.80
36	1	1346	G	C5-C6-N1	-6.59	108.21	111.50
38	4	113	U	N3-C2-O2	-6.59	117.59	122.20
36	1	2392	C	N3-C4-C5	6.58	124.53	121.90
36	5	415	G	N1-C6-O6	-6.58	115.95	119.90
36	5	2411	U	N3-C4-O4	-6.58	114.79	119.40
1	6	914	G	N9-C4-C5	-6.58	102.77	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	662	U	N3-C4-O4	-6.58	114.80	119.40
36	1	212	G	O4'-C1'-N9	6.58	113.46	108.20
36	5	2289	U	N1-C2-O2	6.58	127.40	122.80
36	5	1016	C	O5'-P-OP1	-6.57	99.79	105.70
36	5	1317	A	C2-N3-C4	6.57	113.89	110.60
36	1	716	A	C4-C5-N7	6.57	113.98	110.70
36	1	2349	U	N3-C4-C5	6.57	118.54	114.60
1	6	18	C	C6-N1-C2	-6.57	117.67	120.30
36	1	1820	U	P-O3'-C3'	6.57	127.58	119.70
36	1	2874	G	C8-N9-C4	-6.57	103.77	106.40
36	1	3344	A	C6-C5-N7	-6.57	127.70	132.30
38	4	109	A	C5-C6-N6	-6.57	118.45	123.70
36	5	3026	G	C5-C6-O6	-6.57	124.66	128.60
36	5	2889	C	N3-C2-O2	-6.57	117.30	121.90
36	1	655	C	N3-C4-C5	-6.56	119.28	121.90
36	1	2816	G	N9-C4-C5	-6.56	102.78	105.40
36	1	2621	G	C5-C6-O6	-6.56	124.66	128.60
1	6	272	U	N3-C2-O2	-6.56	117.61	122.20
1	6	1097	U	P-O3'-C3'	6.56	127.57	119.70
36	5	2741	C	N1-C2-O2	-6.56	114.97	118.90
1	6	914	G	C5-C6-O6	-6.56	124.67	128.60
36	5	984	G	C4-C5-C6	6.56	122.73	118.80
36	5	1135	A	N1-C6-N6	-6.56	114.67	118.60
1	2	1765	A	O5'-P-OP1	-6.55	99.80	105.70
36	1	3235	C	O5'-P-OP1	-6.55	99.80	105.70
36	5	2830	G	N1-C2-N3	6.55	127.83	123.90
36	5	2858	U	N1-C2-O2	6.55	127.39	122.80
37	7	13	A	N1-C6-N6	6.55	122.53	118.60
36	1	1849	C	N1-C2-O2	-6.55	114.97	118.90
36	1	1906	G	N1-C6-O6	6.55	123.83	119.90
37	3	38	U	O5'-P-OP2	-6.55	99.81	105.70
36	5	2379	U	C5-C6-N1	-6.55	119.43	122.70
36	1	2309	A	O5'-P-OP1	-6.54	99.81	105.70
36	5	810	A	N1-C2-N3	-6.54	126.03	129.30
36	5	1148	G	N1-C6-O6	6.54	123.83	119.90
1	2	532	U	O5'-P-OP1	-6.54	99.81	105.70
36	5	3266	G	C5-C6-O6	6.54	132.53	128.60
41	L4	139	GLY	N-CA-C	-6.54	96.75	113.10
36	5	2703	A	N9-C4-C5	6.54	108.42	105.80
36	1	3362	A	C5-N7-C8	-6.54	100.63	103.90
38	4	120	C	N1-C2-O2	-6.54	114.98	118.90
1	6	337	G	C4-N9-C1'	6.54	135.00	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3042	U	N3-C4-C5	6.54	118.52	114.60
1	6	163	G	C8-N9-C4	-6.53	103.79	106.40
36	5	3306	U	N3-C4-C5	6.53	118.52	114.60
36	5	2400	G	N1-C6-O6	6.53	123.82	119.90
36	5	2130	G	C5-C6-O6	6.53	132.52	128.60
36	5	2364	G	C5-C6-O6	6.53	132.52	128.60
36	5	3187	A	N1-C6-N6	-6.53	114.68	118.60
36	1	2376	G	C5-N7-C8	-6.53	101.03	104.30
36	1	1140	G	C6-C5-N7	-6.53	126.48	130.40
36	1	2886	U	C5-C4-O4	-6.53	121.98	125.90
36	1	1100	U	C5-C6-N1	-6.53	119.44	122.70
36	1	1890	U	C2-N3-C4	-6.53	123.08	127.00
38	4	6	U	C5-C4-O4	-6.53	121.98	125.90
1	6	610	G	C8-N9-C1'	-6.53	118.52	127.00
1	6	1644	C	O5'-P-OP2	-6.53	99.83	105.70
1	6	308	C	C2-N3-C4	-6.52	116.64	119.90
1	2	1200	G	N3-C2-N2	-6.52	115.33	119.90
36	1	282	G	N9-C4-C5	6.52	108.01	105.40
36	5	2249	G	C8-N9-C4	-6.52	103.79	106.40
36	1	1510	G	N3-C2-N2	6.52	124.47	119.90
36	5	2650	U	N3-C4-O4	-6.52	114.83	119.40
1	6	1340	U	N3-C2-O2	-6.52	117.64	122.20
36	5	34	A	OP2-P-O3'	6.52	119.54	105.20
36	5	2965	U	N1-C2-O2	-6.52	118.24	122.80
36	1	2417	U	C2-N3-C4	-6.52	123.09	127.00
36	1	859	G	C6-C5-N7	-6.51	126.49	130.40
36	1	960	U	N3-C4-C5	6.51	118.51	114.60
36	1	3217	C	N1-C2-O2	6.51	122.81	118.90
36	5	2700	G	O5'-P-OP2	-6.51	99.84	105.70
36	1	407	A	N1-C6-N6	6.51	122.51	118.60
36	5	3195	U	OP1-P-O3'	6.51	119.53	105.20
36	1	1382	G	N7-C8-N9	-6.51	109.84	113.10
36	1	2937	G	C8-N9-C4	6.51	109.00	106.40
36	5	2667	A	N7-C8-N9	6.51	117.05	113.80
1	2	49	C	C6-N1-C2	-6.50	117.70	120.30
36	5	912	G	C2-N3-C4	6.50	115.15	111.90
1	2	158	U	N3-C2-O2	-6.50	117.65	122.20
36	1	362	U	OP1-P-O3'	6.50	119.51	105.20
36	1	2978	U	O4'-C1'-N1	6.50	113.40	108.20
1	6	794	U	N3-C2-O2	-6.50	117.65	122.20
36	5	2190	U	C6-N1-C2	-6.50	117.10	121.00
1	6	1596	C	N3-C4-N4	-6.50	113.45	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2726	C	N3-C4-N4	-6.50	113.45	118.00
36	5	1212	A	O5'-P-OP2	-6.50	99.85	105.70
36	5	2132	C	C6-N1-C2	-6.50	117.70	120.30
1	6	158	U	P-O3'-C3'	6.50	127.50	119.70
36	5	210	U	C5-C6-N1	-6.50	119.45	122.70
36	1	1114	U	N1-C2-O2	6.50	127.35	122.80
36	5	1112	A	N9-C4-C5	-6.50	103.20	105.80
36	5	2393	G	N1-C6-O6	6.50	123.80	119.90
36	5	2824	G	C6-C5-N7	-6.50	126.50	130.40
36	1	2169	G	C6-C5-N7	6.49	134.30	130.40
36	5	2199	G	C4-C5-N7	6.49	113.40	110.80
36	5	2602	G	O5'-P-OP2	-6.49	99.86	105.70
36	1	709	A	C8-N9-C4	6.49	108.40	105.80
36	5	908	G	C6-C5-N7	-6.49	126.51	130.40
36	5	313	A	C8-N9-C4	-6.49	103.20	105.80
36	1	1547	G	C5-N7-C8	6.49	107.54	104.30
1	2	1431	C	C6-N1-C2	6.49	122.89	120.30
1	6	543	C	C4-C5-C6	-6.49	114.16	117.40
36	5	1169	A	N1-C2-N3	6.49	132.54	129.30
36	5	1198	C	N1-C2-O2	6.49	122.79	118.90
36	1	1790	G	N1-C6-O6	6.48	123.79	119.90
36	5	971	G	C4-C5-N7	-6.48	108.21	110.80
36	5	1464	G	N9-C4-C5	-6.48	102.81	105.40
36	1	65	A	P-O3'-C3'	6.48	127.48	119.70
36	5	907	G	N3-C4-N9	6.48	129.89	126.00
36	5	994	G	N3-C2-N2	6.48	124.44	119.90
36	1	673	U	N3-C4-O4	-6.48	114.86	119.40
36	1	2660	G	C8-N9-C4	6.48	108.99	106.40
36	5	2372	A	N9-C4-C5	6.48	108.39	105.80
1	2	1777	G	N1-C6-O6	6.48	123.79	119.90
36	5	1496	C	O5'-P-OP1	6.48	118.47	110.70
36	5	3049	A	C8-N9-C4	6.48	108.39	105.80
36	1	2653	C	N3-C2-O2	-6.47	117.37	121.90
1	6	1614	A	C5-N7-C8	-6.47	100.66	103.90
36	5	3245	A	C6-C5-N7	-6.47	127.77	132.30
1	6	1756	A	N1-C6-N6	-6.47	114.72	118.60
36	5	1430	U	C6-N1-C2	6.47	124.88	121.00
36	5	2531	C	C2-N1-C1'	6.47	125.92	118.80
36	5	2818	U	C5-C4-O4	-6.47	122.02	125.90
36	1	2279	A	C5-C6-N6	-6.47	118.53	123.70
36	1	421	G	C8-N9-C4	6.47	108.99	106.40
36	1	2376	G	O5'-P-OP1	-6.47	99.88	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3375	A	C8-N9-C4	-6.47	103.21	105.80
38	8	98	U	C5-C4-O4	-6.46	122.02	125.90
36	1	1313	G	C4-C5-N7	6.46	113.38	110.80
36	1	2142	A	C6-N1-C2	-6.46	114.72	118.60
36	1	965	A	OP1-P-OP2	-6.46	109.91	119.60
36	1	2624	G	O5'-P-OP1	-6.46	99.89	105.70
36	5	1152	G	N1-C2-N3	6.46	127.77	123.90
36	1	887	G	C5-C6-O6	6.46	132.47	128.60
36	5	53	G	N9-C4-C5	-6.46	102.82	105.40
36	1	1197	A	C6-C5-N7	-6.45	127.78	132.30
36	1	1420	C	N3-C2-O2	-6.45	117.38	121.90
36	1	1585	C	C6-N1-C2	6.45	122.88	120.30
36	5	1319	G	N9-C4-C5	6.45	107.98	105.40
36	1	1294	A	O4'-C1'-N9	6.45	113.36	108.20
36	5	950	G	C5-C6-N1	6.45	114.73	111.50
36	1	2393	G	N1-C6-O6	6.45	123.77	119.90
36	5	975	C	N1-C2-O2	-6.45	115.03	118.90
36	1	1848	G	C5-C6-O6	-6.45	124.73	128.60
1	6	328	A	O5'-P-OP2	-6.45	99.90	105.70
36	1	3368	U	C6-N1-C1'	6.45	130.22	121.20
36	1	54	C	N3-C4-N4	-6.45	113.49	118.00
36	1	655	C	C5-C4-N4	6.45	124.71	120.20
36	1	961	C	C5-C6-N1	-6.45	117.78	121.00
36	1	1556	C	N1-C2-O2	6.45	122.77	118.90
36	5	2834	G	OP1-P-OP2	6.45	129.27	119.60
36	1	645	A	C5-C6-N1	6.44	120.92	117.70
36	1	972	A	N7-C8-N9	-6.44	110.58	113.80
36	5	2305	G	C6-C5-N7	-6.44	126.53	130.40
36	1	190	U	O4'-C1'-N1	6.44	113.35	108.20
36	1	1392	G	C5-C6-O6	-6.44	124.73	128.60
36	1	2867	C	O5'-P-OP2	-6.44	99.90	105.70
36	1	2637	A	O5'-P-OP1	-6.44	99.91	105.70
36	5	369	A	C8-N9-C4	-6.44	103.22	105.80
1	2	1762	A	C8-N9-C4	6.43	108.37	105.80
1	2	1674	C	C6-N1-C2	-6.43	117.73	120.30
36	5	926	A	C5-C6-N6	-6.43	118.56	123.70
36	5	2187	G	N9-C4-C5	-6.43	102.83	105.40
1	2	158	U	N1-C2-O2	6.43	127.30	122.80
1	6	358	U	O5'-P-OP1	-6.43	99.91	105.70
1	6	794	U	C2-N1-C1'	6.43	125.41	117.70
36	1	895	A	N1-C6-N6	6.43	122.45	118.60
36	1	2389	C	C6-N1-C2	6.43	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2374	C	N3-C2-O2	6.42	126.39	121.90
36	1	2861	U	O5'-P-OP1	-6.42	99.92	105.70
38	4	114	G	C8-N9-C4	6.42	108.97	106.40
36	5	1239	C	C5-C6-N1	6.42	124.21	121.00
36	5	1891	A	O5'-P-OP2	-6.42	99.92	105.70
36	5	2746	A	C8-N9-C4	6.42	108.37	105.80
36	5	2871	G	O5'-P-OP2	-6.42	99.92	105.70
36	5	1321	G	N1-C6-O6	6.42	123.75	119.90
36	5	1436	U	OP1-P-O3'	6.42	119.32	105.20
1	2	704	C	N1-C2-O2	6.42	122.75	118.90
36	1	663	C	N1-C2-O2	-6.42	115.05	118.90
36	5	831	G	C5-C6-O6	-6.42	124.75	128.60
36	1	1468	A	C2-N3-C4	-6.41	107.39	110.60
37	3	86	U	N1-C2-O2	-6.41	118.31	122.80
36	1	895	A	N7-C8-N9	6.41	117.01	113.80
36	1	2808	A	C2-N3-C4	-6.41	107.39	110.60
36	5	2293	C	C6-N1-C1'	-6.41	113.11	120.80
36	1	1300	G	N3-C4-N9	6.41	129.84	126.00
36	1	2367	A	C4-C5-C6	6.41	120.20	117.00
36	5	86	G	N1-C6-O6	-6.41	116.06	119.90
36	5	804	C	C4-C5-C6	6.41	120.61	117.40
36	5	1912	U	N3-C2-O2	6.41	126.69	122.20
1	6	1354	G	N7-C8-N9	6.41	116.30	113.10
36	1	797	U	OP1-P-OP2	-6.41	109.99	119.60
36	1	2603	G	N3-C2-N2	6.41	124.38	119.90
1	6	1783	C	N1-C2-O2	6.41	122.74	118.90
36	1	1175	C	C2-N3-C4	-6.40	116.70	119.90
36	1	3114	A	O5'-P-OP2	-6.40	99.94	105.70
1	6	106	U	OP2-P-O3'	6.40	119.29	105.20
36	5	2373	A	OP1-P-OP2	-6.40	110.00	119.60
36	1	3209	A	N1-C6-N6	6.40	122.44	118.60
37	7	89	G	C8-N9-C4	6.40	108.96	106.40
36	5	2375	G	O4'-C1'-N9	6.40	113.32	108.20
1	6	390	G	O5'-P-OP2	-6.40	99.94	105.70
1	6	805	U	C6-N1-C2	-6.40	117.16	121.00
36	5	3330	A	N1-C6-N6	-6.40	114.76	118.60
36	5	2176	U	N3-C2-O2	-6.40	117.72	122.20
36	1	1329	U	C6-N1-C2	-6.39	117.16	121.00
1	6	351	C	C2-N1-C1'	6.39	125.83	118.80
1	6	362	G	O5'-P-OP2	-6.39	99.94	105.70
36	5	790	U	C5-C4-O4	6.39	129.74	125.90
36	1	2372	A	O5'-P-OP2	-6.39	99.95	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	637	C	N3-C4-N4	-6.39	113.53	118.00
36	5	776	U	C2-N3-C4	-6.39	123.17	127.00
36	5	1481	A	C8-N9-C4	-6.39	103.24	105.80
36	1	1419	A	O5'-P-OP2	-6.39	99.95	105.70
36	5	407	A	N1-C6-N6	6.39	122.44	118.60
36	5	339	C	C6-N1-C2	-6.39	117.74	120.30
36	5	809	G	N9-C4-C5	-6.39	102.84	105.40
36	1	92	G	C8-N9-C4	6.39	108.95	106.40
36	5	1115	G	C4-N9-C1'	6.38	134.80	126.50
36	5	2385	G	C5-C6-O6	-6.38	124.77	128.60
38	4	53	A	C2-N3-C4	6.38	113.79	110.60
36	5	1187	C	N3-C4-C5	6.38	124.45	121.90
1	2	1339	C	P-O3'-C3'	6.38	127.35	119.70
36	1	662	U	N3-C2-O2	-6.38	117.73	122.20
36	5	2728	G	N9-C4-C5	6.38	107.95	105.40
76	q0	103	LEU	CB-CG-CD2	-6.38	100.16	111.00
1	6	542	A	N7-C8-N9	6.38	116.99	113.80
36	5	805	G	N9-C4-C5	-6.38	102.85	105.40
36	5	1419	A	N1-C6-N6	-6.38	114.78	118.60
36	5	2405	C	C2-N3-C4	-6.38	116.71	119.90
36	1	49	A	O5'-P-OP1	-6.38	99.96	105.70
36	1	893	C	C5-C6-N1	6.38	124.19	121.00
36	1	2359	C	O5'-P-OP2	-6.38	99.96	105.70
36	5	2944	U	N3-C2-O2	-6.38	117.74	122.20
1	2	1116	A	C8-N9-C4	6.37	108.35	105.80
36	5	3197	G	N3-C2-N2	-6.37	115.44	119.90
36	1	116	A	O4'-C1'-N9	6.37	113.30	108.20
36	1	220	G	C6-C5-N7	-6.37	126.58	130.40
36	5	2364	G	C8-N9-C4	-6.37	103.85	106.40
36	1	930	U	O5'-P-OP1	-6.37	99.97	105.70
36	1	1433	A	N3-C4-N9	6.37	132.50	127.40
38	8	84	C	C6-N1-C2	-6.37	117.75	120.30
36	1	2777	G	C5-C6-O6	6.37	132.42	128.60
36	1	3306	U	N3-C2-O2	-6.37	117.74	122.20
36	5	1521	G	N3-C2-N2	6.37	124.36	119.90
36	1	2712	U	C5-C4-O4	6.37	129.72	125.90
36	5	872	U	N3-C4-C5	6.37	118.42	114.60
36	5	1331	U	N3-C2-O2	6.37	126.66	122.20
36	5	1440	G	N9-C4-C5	6.37	107.95	105.40
36	5	2417	U	C4-C5-C6	6.37	123.52	119.70
36	1	655	C	OP2-P-O3'	6.36	119.20	105.20
36	1	680	G	O5'-P-OP1	-6.36	99.97	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	44	U	N1-C2-O2	-6.36	118.35	122.80
36	5	1395	G	N1-C6-O6	6.36	123.72	119.90
36	5	923	C	N3-C2-O2	6.36	126.35	121.90
36	5	1495	U	C6-N1-C2	-6.36	117.18	121.00
36	1	1858	A	N1-C2-N3	-6.36	126.12	129.30
36	5	1198	C	N3-C2-O2	-6.36	117.45	121.90
36	5	3260	G	C5-C6-O6	6.36	132.41	128.60
36	5	341	G	N1-C6-O6	6.35	123.71	119.90
1	2	314	C	O5'-P-OP1	-6.35	99.98	105.70
36	1	979	U	N1-C2-O2	6.35	127.25	122.80
1	2	507	U	C2-N1-C1'	6.35	125.32	117.70
36	1	2850	G	C4-C5-N7	6.35	113.34	110.80
47	M0	24	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	6	385	A	C5-C6-N6	6.35	128.78	123.70
36	5	1319	G	C8-N9-C4	-6.35	103.86	106.40
40	l3	3	HIS	N-CA-C	-6.35	93.86	111.00
1	2	320	U	C5-C4-O4	-6.35	122.09	125.90
81	sM	167	PRO	N-CA-CB	6.35	110.92	103.30
36	5	1155	C	N3-C4-C5	6.35	124.44	121.90
36	1	718	G	C5-N7-C8	-6.34	101.13	104.30
36	1	959	C	C6-N1-C2	6.34	122.84	120.30
1	6	1783	C	O5'-P-OP2	-6.34	99.99	105.70
36	1	895	A	C5-C6-N1	-6.34	114.53	117.70
36	5	2820	A	C8-N9-C4	-6.34	103.26	105.80
36	1	2411	U	N3-C4-O4	-6.34	114.96	119.40
36	1	2679	A	O4'-C1'-N9	6.34	113.27	108.20
36	5	2531	C	N1-C2-O2	6.34	122.70	118.90
10	s8	29	LEU	CA-CB-CG	6.34	129.87	115.30
36	5	1391	C	N3-C2-O2	6.34	126.34	121.90
36	5	641	C	N1-C2-N3	6.33	123.63	119.20
36	5	2825	C	C5-C4-N4	-6.33	115.77	120.20
36	5	958	C	N1-C2-O2	6.33	122.70	118.90
36	5	2191	U	N3-C4-O4	-6.33	114.97	119.40
36	5	660	A	N7-C8-N9	-6.32	110.64	113.80
1	6	394	C	N1-C2-O2	-6.32	115.11	118.90
37	7	101	G	C6-C5-N7	-6.32	126.61	130.40
36	1	1663	C	O5'-P-OP1	-6.32	100.01	105.70
38	4	82	U	N1-C2-O2	-6.32	118.38	122.80
36	5	960	U	N1-C2-O2	6.32	127.22	122.80
36	5	2302	G	N1-C6-O6	-6.32	116.11	119.90
36	5	2976	A	OP2-P-O3'	6.32	119.10	105.20
36	5	3225	C	C2-N1-C1'	6.32	125.75	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	633	C	N1-C2-O2	-6.32	115.11	118.90
36	1	2215	A	C4-C5-C6	-6.32	113.84	117.00
1	6	1361	U	C2-N1-C1'	6.32	125.28	117.70
36	5	714	G	C8-N9-C4	6.32	108.93	106.40
36	5	922	U	C5-C6-N1	-6.32	119.54	122.70
36	1	645	A	C2-N3-C4	6.31	113.76	110.60
36	1	2900	A	C8-N9-C4	6.31	108.33	105.80
36	1	651	G	N3-C4-C5	-6.31	125.44	128.60
1	6	767	U	N3-C2-O2	-6.31	117.78	122.20
1	6	795	U	N1-C2-O2	6.31	127.22	122.80
36	5	1516	C	N3-C4-C5	6.31	124.42	121.90
36	5	1372	C	C6-N1-C2	6.31	122.82	120.30
36	1	1216	C	C5-C6-N1	6.31	124.16	121.00
38	4	109	A	N9-C4-C5	-6.31	103.28	105.80
1	6	1776	A	O5'-P-OP2	-6.31	100.02	105.70
1	2	1568	C	P-O3'-C3'	6.31	127.27	119.70
36	1	498	A	N1-C6-N6	-6.31	114.82	118.60
36	1	1429	G	N1-C6-O6	-6.31	116.12	119.90
36	1	2572	C	N3-C2-O2	-6.31	117.48	121.90
36	1	3302	U	C6-N1-C2	6.31	124.78	121.00
1	6	337	G	C4-C5-N7	6.31	113.32	110.80
1	6	1655	A	C8-N9-C4	6.31	108.32	105.80
36	5	3245	A	N1-C2-N3	6.31	132.45	129.30
36	1	1127	G	C4-C5-N7	6.31	113.32	110.80
1	6	558	U	C2-N1-C1'	6.30	125.26	117.70
38	4	98	U	N3-C4-O4	6.30	123.81	119.40
36	5	1879	A	C4-C5-N7	6.30	113.85	110.70
1	6	337	G	N3-C4-N9	6.30	129.78	126.00
36	1	1201	C	N3-C4-N4	6.30	122.41	118.00
36	5	2711	C	C6-N1-C2	-6.30	117.78	120.30
36	1	1510	G	C6-C5-N7	-6.30	126.62	130.40
36	1	3362	A	C6-C5-N7	-6.30	127.89	132.30
36	1	876	A	C8-N9-C4	6.29	108.32	105.80
36	1	3344	A	C8-N9-C4	-6.29	103.28	105.80
1	6	864	U	O4'-C1'-N1	6.29	113.24	108.20
36	5	930	U	OP1-P-O3'	6.29	119.04	105.20
36	1	2202	C	O5'-P-OP2	6.29	118.25	110.70
1	6	914	G	N1-C6-O6	6.29	123.67	119.90
36	5	2772	C	P-O3'-C3'	6.29	127.25	119.70
1	6	1560	U	N1-C2-O2	6.29	127.20	122.80
36	5	2928	C	C2-N1-C1'	6.29	125.72	118.80
1	2	1657	U	O4'-C1'-N1	6.29	113.23	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3362	A	N1-C2-N3	6.29	132.44	129.30
36	5	308	A	O5'-P-OP1	6.29	118.25	110.70
1	6	1597	A	C8-N9-C4	6.29	108.31	105.80
36	1	407	A	O5'-P-OP2	-6.29	100.04	105.70
36	1	1356	U	O5'-P-OP1	-6.29	100.04	105.70
36	5	3004	C	N3-C4-N4	6.29	122.40	118.00
36	1	350	C	N3-C2-O2	-6.28	117.50	121.90
36	5	1792	C	O5'-P-OP2	-6.28	100.05	105.70
36	5	2150	G	C8-N9-C4	-6.28	103.89	106.40
36	5	2199	G	C6-C5-N7	-6.28	126.63	130.40
36	1	1179	A	O5'-P-OP1	-6.28	100.05	105.70
36	1	2126	A	C8-N9-C4	6.28	108.31	105.80
36	5	647	A	C2-N3-C4	-6.28	107.46	110.60
36	1	1551	C	N1-C2-O2	6.28	122.67	118.90
36	1	2314	U	N1-C2-O2	6.28	127.19	122.80
45	L8	189	LEU	CA-CB-CG	6.28	129.74	115.30
36	1	2355	G	N3-C2-N2	-6.28	115.51	119.90
36	1	2361	A	OP2-P-O3'	6.28	119.01	105.20
36	5	3099	C	N1-C2-O2	-6.28	115.14	118.90
36	5	3272	C	N1-C2-O2	-6.28	115.14	118.90
36	1	960	U	N3-C4-O4	6.27	123.79	119.40
36	1	2283	G	N3-C2-N2	-6.27	115.51	119.90
36	5	1116	G	N9-C4-C5	6.27	107.91	105.40
36	1	2812	C	C5-C6-N1	-6.27	117.86	121.00
36	5	3377	G	N9-C4-C5	-6.27	102.89	105.40
1	2	1198	G	C8-N9-C4	-6.27	103.89	106.40
36	1	639	G	OP1-P-OP2	-6.27	110.19	119.60
36	1	2642	A	C6-N1-C2	6.27	122.36	118.60
36	1	709	A	O5'-P-OP2	6.27	118.22	110.70
36	1	2383	C	C6-N1-C2	6.27	122.81	120.30
36	1	908	G	C8-N9-C1'	-6.27	118.85	127.00
36	1	2356	A	C5-N7-C8	-6.27	100.77	103.90
36	1	2411	U	N1-C2-N3	6.27	118.66	114.90
1	6	1766	A	N1-C6-N6	6.27	122.36	118.60
36	5	1799	A	N1-C6-N6	6.27	122.36	118.60
38	8	151	C	C6-N1-C2	6.27	122.81	120.30
36	1	1157	G	C5-C6-O6	6.27	132.36	128.60
36	1	895	A	O5'-P-OP1	-6.26	100.06	105.70
36	5	3245	A	C8-N9-C4	-6.26	103.29	105.80
36	5	890	C	C4-C5-C6	6.26	120.53	117.40
37	7	89	G	N9-C4-C5	-6.26	102.90	105.40
36	1	797	U	OP2-P-O3'	6.26	118.97	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2879	C	N3-C4-N4	6.26	122.38	118.00
36	5	1127	G	C6-N1-C2	-6.26	121.34	125.10
36	5	2327	U	C5-C6-N1	-6.26	119.57	122.70
36	5	2912	G	N1-C2-N2	6.26	121.83	116.20
36	5	1605	A	O4'-C1'-N9	6.26	113.20	108.20
1	2	1092	A	N1-C6-N6	6.25	122.35	118.60
36	5	1592	G	N9-C4-C5	6.25	107.90	105.40
36	1	304	G	C6-C5-N7	6.25	134.15	130.40
36	1	372	A	N9-C4-C5	-6.25	103.30	105.80
36	1	651	G	C8-N9-C1'	-6.25	118.88	127.00
36	5	2334	U	O5'-P-OP1	6.25	118.20	110.70
36	5	3214	U	C5-C4-O4	6.25	129.65	125.90
1	2	1200	G	C6-C5-N7	-6.25	126.65	130.40
36	1	714	G	C4-C5-N7	6.25	113.30	110.80
36	5	587	U	C6-N1-C2	6.25	124.75	121.00
36	1	2418	G	C2-N3-C4	6.25	115.02	111.90
36	5	1481	A	N7-C8-N9	6.25	116.92	113.80
36	5	2281	A	C8-N9-C4	6.25	108.30	105.80
36	1	813	G	C2-N3-C4	6.24	115.02	111.90
1	6	914	G	C4-C5-N7	6.24	113.30	110.80
36	5	2813	A	C4-C5-C6	6.24	120.12	117.00
36	1	1409	G	N1-C6-O6	-6.24	116.16	119.90
1	6	1503	A	C2-N3-C4	-6.24	107.48	110.60
36	5	2362	C	N3-C2-O2	-6.24	117.53	121.90
36	1	220	G	C5-C6-O6	-6.24	124.86	128.60
1	6	609	U	N1-C2-N3	6.24	118.64	114.90
1	2	1291	G	N3-C4-C5	6.24	131.72	128.60
36	1	724	U	C6-N1-C2	6.24	124.74	121.00
36	5	931	C	N3-C4-C5	6.24	124.39	121.90
36	5	2421	U	N1-C2-O2	-6.24	118.44	122.80
36	5	2914	G	O5'-P-OP2	-6.24	100.09	105.70
36	1	2323	G	N3-C4-C5	-6.23	125.48	128.60
36	1	2381	G	C2-N3-C4	6.23	115.02	111.90
36	5	1521	G	C5-C6-O6	6.23	132.34	128.60
1	6	44	U	N3-C2-O2	6.23	126.56	122.20
36	1	2222	A	C8-N9-C4	-6.23	103.31	105.80
36	1	2811	A	N9-C4-C5	6.23	108.29	105.80
1	6	1472	C	C2-N1-C1'	-6.23	111.95	118.80
36	5	895	A	C8-N9-C4	6.23	108.29	105.80
36	5	1331	U	C6-N1-C2	6.23	124.74	121.00
36	5	1906	G	N9-C4-C5	-6.23	102.91	105.40
36	5	1910	A	OP2-P-O3'	6.23	118.90	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1149	G	C5-C6-O6	-6.22	124.87	128.60
36	5	2338	C	N1-C2-O2	-6.22	115.17	118.90
36	5	57	A	N9-C4-C5	-6.22	103.31	105.80
36	5	639	G	O5'-P-OP1	6.22	118.16	110.70
36	1	220	G	C4-C5-N7	6.22	113.29	110.80
36	1	231	G	N1-C6-O6	-6.22	116.17	119.90
36	5	141	C	N1-C2-O2	-6.22	115.17	118.90
36	5	1116	G	OP2-P-O3'	6.22	118.88	105.20
36	5	2341	A	N7-C8-N9	-6.22	110.69	113.80
36	1	958	C	N3-C4-N4	-6.21	113.65	118.00
36	5	282	G	O5'-P-OP1	-6.21	100.11	105.70
36	1	1807	G	C8-N9-C4	-6.21	103.92	106.40
36	5	65	A	O5'-P-OP2	-6.21	100.11	105.70
36	5	1175	C	N3-C4-C5	6.21	124.38	121.90
36	5	2234	G	N9-C4-C5	-6.21	102.92	105.40
36	5	2790	A	O5'-P-OP2	-6.21	100.11	105.70
36	1	59	G	N1-C6-O6	6.21	123.62	119.90
36	1	644	G	C4-C5-C6	6.21	122.53	118.80
36	5	699	A	C2-N3-C4	-6.21	107.50	110.60
36	5	1847	A	N3-C4-C5	6.21	131.15	126.80
36	5	3017	A	C5-C6-N6	-6.21	118.73	123.70
36	1	57	A	C2-N3-C4	-6.21	107.50	110.60
36	5	954	U	C5-C6-N1	6.21	125.80	122.70
36	1	2773	C	OP1-P-OP2	6.21	128.91	119.60
1	6	308	C	C6-N1-C1'	6.21	128.25	120.80
1	6	431	C	N1-C2-O2	6.20	122.62	118.90
10	S8	29	LEU	CA-CB-CG	6.20	129.56	115.30
12	c0	83	PRO	N-CA-CB	6.20	110.74	103.30
36	5	3174	A	C5-N7-C8	-6.20	100.80	103.90
36	5	714	G	N9-C4-C5	-6.20	102.92	105.40
36	1	3181	C	N1-C2-N3	6.20	123.54	119.20
36	5	36	C	C5-C6-N1	6.20	124.10	121.00
36	1	2356	A	C4-C5-N7	6.19	113.80	110.70
36	1	3094	A	O5'-P-OP1	-6.19	100.13	105.70
36	5	32	U	N1-C2-N3	6.19	118.62	114.90
36	1	2901	G	N1-C6-O6	6.19	123.61	119.90
36	5	2874	G	C5-C6-O6	6.19	132.31	128.60
36	1	674	G	N9-C4-C5	6.19	107.88	105.40
36	1	2142	A	O5'-P-OP2	6.19	118.12	110.70
36	1	2357	A	N1-C6-N6	6.19	122.31	118.60
36	5	3144	G	C8-N9-C4	-6.19	103.92	106.40
36	1	2874	G	C2-N3-C4	-6.18	108.81	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	321	C	N1-C2-O2	6.18	122.61	118.90
1	6	337	G	C8-N9-C1'	-6.18	118.96	127.00
36	5	2524	A	N9-C1'-C2'	6.18	122.04	114.00
36	5	133	U	N1-C2-O2	6.18	127.13	122.80
36	5	3110	C	C2-N3-C4	-6.18	116.81	119.90
36	1	2901	G	N3-C2-N2	-6.18	115.57	119.90
38	8	43	A	C8-N9-C4	-6.18	103.33	105.80
43	l6	173	MET	CB-CG-SD	-6.18	93.86	112.40
36	5	1879	A	C5-N7-C8	-6.18	100.81	103.90
36	1	2381	G	N3-C4-C5	-6.18	125.51	128.60
36	5	1733	G	C5-C6-O6	-6.18	124.89	128.60
36	1	363	G	N1-C6-O6	6.17	123.61	119.90
36	1	671	U	N3-C2-O2	6.17	126.52	122.20
36	1	963	G	C5-C6-O6	-6.17	124.89	128.60
36	1	1156	C	N3-C4-N4	-6.17	113.68	118.00
36	1	1492	G	C4-C5-C6	6.17	122.50	118.80
36	1	3269	U	N3-C2-O2	-6.17	117.88	122.20
36	5	209	A	C8-N9-C4	-6.17	103.33	105.80
1	2	1560	U	C5-C4-O4	6.17	129.60	125.90
36	1	660	A	N1-C2-N3	-6.17	126.22	129.30
36	1	663	C	C5-C4-N4	-6.17	115.88	120.20
36	1	859	G	N3-C4-N9	6.17	129.70	126.00
36	1	2983	C	N1-C2-N3	6.17	123.52	119.20
36	5	283	G	C5-N7-C8	-6.17	101.22	104.30
36	5	1296	C	O5'-P-OP1	-6.17	100.15	105.70
36	5	1524	A	C8-N9-C4	6.17	108.27	105.80
36	5	3104	U	N3-C4-C5	6.17	118.30	114.60
36	1	2850	G	C6-C5-N7	-6.17	126.70	130.40
36	5	640	U	N1-C2-N3	6.17	118.60	114.90
36	5	3009	G	N1-C6-O6	-6.17	116.20	119.90
36	5	1112	A	N3-C4-N9	6.16	132.33	127.40
36	5	2330	C	O5'-P-OP2	-6.16	100.15	105.70
1	2	1654	G	O5'-P-OP2	-6.16	100.16	105.70
36	1	585	A	O5'-P-OP2	-6.16	100.16	105.70
36	1	810	A	C8-N9-C4	-6.16	103.34	105.80
12	c0	97	PRO	N-CA-CB	6.16	110.69	103.30
36	5	2634	U	N1-C2-N3	6.16	118.60	114.90
36	5	423	A	N7-C8-N9	-6.16	110.72	113.80
36	5	1493	G	O4'-C1'-N9	6.16	113.13	108.20
36	5	2364	G	O4'-C1'-N9	6.16	113.13	108.20
36	5	2916	U	N3-C4-O4	6.16	123.71	119.40
38	4	40	A	C6-C5-N7	-6.15	127.99	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2295	A	C5-C6-N6	-6.15	118.78	123.70
36	5	3315	G	N1-C6-O6	-6.15	116.21	119.90
36	5	1878	G	C4-N9-C1'	6.15	134.50	126.50
36	5	297	G	O4'-C1'-N9	6.15	113.12	108.20
36	5	1331	U	C5-C4-O4	-6.15	122.21	125.90
36	5	2187	G	C8-N9-C4	6.15	108.86	106.40
36	5	2283	G	C5-C6-O6	-6.15	124.91	128.60
36	5	2838	A	N1-C6-N6	6.15	122.29	118.60
36	1	816	A	OP2-P-O3'	6.15	118.72	105.20
36	5	2709	C	N3-C4-C5	6.15	124.36	121.90
36	5	3204	C	N3-C4-C5	6.15	124.36	121.90
36	1	3090	U	N3-C2-O2	6.15	126.50	122.20
36	5	3041	U	N3-C4-C5	6.15	118.29	114.60
1	6	542	A	C4-C5-C6	6.14	120.07	117.00
36	5	416	A	C4-C5-C6	6.14	120.07	117.00
36	1	98	G	N3-C4-C5	6.14	131.67	128.60
36	1	1330	A	N1-C6-N6	6.14	122.28	118.60
36	5	937	G	O4'-C1'-N9	6.14	113.11	108.20
1	2	337	G	C5-C6-O6	-6.14	124.92	128.60
36	1	2815	G	N1-C2-N2	-6.14	110.67	116.20
36	5	2244	A	O5'-P-OP1	6.14	118.07	110.70
36	5	993	G	O4'-C1'-N9	6.14	113.11	108.20
36	5	2404	A	C4-C5-N7	6.14	113.77	110.70
36	1	111	C	N3-C4-C5	6.14	124.36	121.90
36	1	1890	U	C5-C6-N1	-6.14	119.63	122.70
36	5	516	A	C8-N9-C4	6.14	108.25	105.80
36	5	3217	C	C2-N1-C1'	-6.14	112.05	118.80
1	6	1537	C	N3-C4-C5	-6.13	119.45	121.90
36	5	916	G	N3-C4-C5	6.13	131.67	128.60
36	5	2650	U	N1-C2-N3	6.13	118.58	114.90
36	5	2824	G	N9-C4-C5	-6.13	102.95	105.40
36	5	2933	A	OP2-P-O3'	6.13	118.69	105.20
36	1	63	A	C8-N9-C4	-6.13	103.35	105.80
36	5	3060	C	C5-C4-N4	-6.13	115.91	120.20
1	2	1096	C	N1-C2-O2	6.13	122.58	118.90
36	1	326	U	O5'-P-OP2	-6.13	100.18	105.70
36	1	1434	G	N7-C8-N9	6.13	116.17	113.10
36	1	2295	A	N1-C6-N6	6.13	122.28	118.60
36	5	419	G	C6-C5-N7	-6.13	126.72	130.40
36	5	809	G	N3-C4-N9	6.13	129.68	126.00
36	1	1802	C	C6-N1-C2	-6.13	117.85	120.30
36	5	674	G	C8-N9-C4	-6.13	103.95	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	767	U	N3-C2-O2	-6.13	117.91	122.20
36	1	811	U	C4-C5-C6	6.13	123.38	119.70
36	5	1317	A	OP2-P-O3'	6.13	118.68	105.20
36	5	1791	C	C6-N1-C2	-6.13	117.85	120.30
36	5	3174	A	N7-C8-N9	6.12	116.86	113.80
1	2	110	U	N3-C2-O2	-6.12	117.91	122.20
1	2	448	C	C6-N1-C2	-6.12	117.85	120.30
36	1	2349	U	N3-C2-O2	-6.12	117.91	122.20
1	6	1700	C	C6-N1-C1'	-6.12	113.45	120.80
36	5	3362	A	N7-C8-N9	6.12	116.86	113.80
36	1	1183	C	N3-C4-C5	6.12	124.35	121.90
1	6	944	A	O5'-P-OP1	-6.12	100.19	105.70
1	6	1514	U	C5-C4-O4	6.12	129.57	125.90
1	6	1614	A	C2-N3-C4	-6.12	107.54	110.60
36	5	2371	G	N9-C4-C5	-6.12	102.95	105.40
36	1	1452	A	C8-N9-C4	6.12	108.25	105.80
1	2	1462	G	C4-C5-N7	6.12	113.25	110.80
36	1	1189	C	C4-C5-C6	6.12	120.46	117.40
36	5	1239	C	C2-N1-C1'	6.12	125.53	118.80
36	1	1305	U	N1-C2-O2	6.12	127.08	122.80
36	1	1374	G	N3-C2-N2	6.12	124.18	119.90
36	1	2662	G	N1-C6-O6	6.12	123.57	119.90
36	1	120	G	C8-N9-C4	6.12	108.85	106.40
36	1	815	G	C8-N9-C4	-6.12	103.95	106.40
36	1	1139	G	C5-C6-O6	6.11	132.27	128.60
36	1	1176	C	C6-N1-C2	6.11	122.75	120.30
36	5	609	G	N1-C6-O6	6.11	123.57	119.90
36	5	908	G	C4-C5-N7	6.11	113.25	110.80
36	1	3298	C	C6-N1-C2	6.11	122.75	120.30
36	5	1448	U	C6-N1-C2	6.11	124.67	121.00
37	7	11	A	C4-C5-N7	6.11	113.76	110.70
36	1	938	C	C5-C4-N4	-6.11	115.92	120.20
36	1	72	C	C2-N1-C1'	-6.11	112.08	118.80
1	6	542	A	O5'-P-OP1	-6.11	100.20	105.70
36	5	2985	C	C5-C6-N1	6.11	124.05	121.00
36	1	1141	C	N3-C4-C5	-6.11	119.46	121.90
36	1	1367	G	C6-C5-N7	-6.11	126.74	130.40
36	1	2298	U	C5-C6-N1	-6.11	119.65	122.70
36	1	3135	U	C5-C6-N1	-6.10	119.65	122.70
36	1	3217	C	C6-N1-C1'	-6.10	113.47	120.80
36	5	326	U	N3-C2-O2	6.10	126.47	122.20
36	5	680	G	O5'-P-OP2	-6.10	100.21	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2848	G	C6-C5-N7	-6.10	126.74	130.40
1	6	1119	G	C6-C5-N7	-6.10	126.74	130.40
36	5	2660	G	O5'-P-OP2	-6.10	100.21	105.70
36	5	3050	U	C5-C4-O4	6.10	129.56	125.90
36	5	2396	G	N9-C4-C5	6.10	107.84	105.40
36	1	340	C	C2-N3-C4	-6.10	116.85	119.90
36	1	2944	U	OP1-P-O3'	6.10	118.62	105.20
36	5	2352	A	C4-C5-C6	6.10	120.05	117.00
36	5	2729	U	N1-C2-O2	6.10	127.07	122.80
36	1	2409	G	C8-N9-C4	-6.10	103.96	106.40
36	5	2824	G	C4-C5-N7	6.10	113.24	110.80
36	1	1879	A	O4'-C1'-N9	6.09	113.08	108.20
36	5	641	C	O4'-C1'-N1	6.09	113.08	108.20
36	5	911	C	C6-N1-C2	6.09	122.74	120.30
36	1	1199	C	C6-N1-C2	6.09	122.74	120.30
36	1	1433	A	C2-N3-C4	6.09	113.65	110.60
36	5	1468	A	N1-C6-N6	6.09	122.26	118.60
1	2	1733	C	N3-C4-N4	6.09	122.26	118.00
36	1	369	A	N9-C4-C5	6.09	108.24	105.80
1	2	402	C	O5'-P-OP1	-6.09	100.22	105.70
1	6	756	A	N7-C8-N9	6.09	116.84	113.80
36	5	652	G	O5'-P-OP2	-6.09	100.22	105.70
36	5	1151	U	N1-C2-O2	-6.09	118.54	122.80
36	5	1131	G	OP1-P-OP2	6.09	128.73	119.60
36	1	1380	G	O5'-P-OP1	6.09	118.00	110.70
1	6	57	G	N3-C4-N9	6.09	129.65	126.00
1	6	408	C	N3-C4-C5	-6.09	119.47	121.90
36	1	910	G	C5-C6-N1	-6.08	108.46	111.50
36	1	2812	C	O5'-P-OP2	6.08	118.00	110.70
1	6	338	C	C5-C4-N4	-6.08	115.94	120.20
36	5	416	A	C6-C5-N7	-6.08	128.04	132.30
36	5	668	G	N3-C2-N2	6.08	124.16	119.90
36	5	884	A	C4-C5-C6	-6.08	113.96	117.00
36	1	805	G	N9-C4-C5	-6.08	102.97	105.40
36	5	369	A	N7-C8-N9	6.08	116.84	113.80
36	1	199	A	O4'-C1'-N9	6.08	113.06	108.20
36	1	611	A	O5'-P-OP1	6.08	117.99	110.70
36	5	1476	G	N3-C4-C5	6.08	131.64	128.60
36	5	1150	A	O5'-P-OP2	-6.08	100.23	105.70
36	5	922	U	N1-C2-O2	6.08	127.05	122.80
36	1	1149	G	N3-C2-N2	-6.07	115.65	119.90
1	6	1596	C	C5-C4-N4	6.07	124.45	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	514	G	N1-C6-O6	6.07	123.54	119.90
36	5	3140	G	N1-C6-O6	6.07	123.54	119.90
36	1	283	G	O4'-C1'-N9	-6.07	103.34	108.20
36	1	2107	A	O5'-P-OP1	-6.07	100.24	105.70
36	5	1085	A	N1-C6-N6	6.07	122.24	118.60
36	1	2388	U	N3-C2-O2	6.07	126.45	122.20
1	6	416	A	C4-C5-N7	6.07	113.73	110.70
36	5	3060	C	N3-C4-N4	6.07	122.25	118.00
36	1	580	C	N1-C2-O2	-6.07	115.26	118.90
36	1	2382	G	C5-C6-O6	6.07	132.24	128.60
36	1	2728	G	C5-C6-N1	6.07	114.53	111.50
38	4	40	A	N9-C4-C5	-6.07	103.37	105.80
36	1	695	C	N3-C4-N4	-6.06	113.75	118.00
36	5	2656	A	C8-N9-C4	-6.06	103.38	105.80
36	1	405	U	N3-C2-O2	6.06	126.44	122.20
36	1	1151	U	C5-C6-N1	6.06	125.73	122.70
36	1	2892	A	N1-C6-N6	-6.06	114.96	118.60
36	1	835	G	O4'-C1'-N9	6.06	113.05	108.20
36	1	1904	C	C6-N1-C2	-6.06	117.88	120.30
36	5	1481	A	P-O3'-C3'	6.06	126.97	119.70
36	5	2416	U	C6-N1-C2	-6.06	117.36	121.00
36	5	2601	A	N9-C4-C5	6.06	108.22	105.80
36	5	2765	C	C6-N1-C2	-6.06	117.88	120.30
36	1	911	C	O5'-P-OP1	-6.06	100.25	105.70
36	1	1298	C	O5'-P-OP1	-6.06	100.25	105.70
36	5	101	G	O4'-C1'-N9	6.06	113.05	108.20
36	5	3154	C	C6-N1-C2	-6.06	117.88	120.30
36	1	1683	A	N1-C6-N6	6.06	122.23	118.60
36	5	2824	G	N1-C6-O6	6.06	123.53	119.90
1	6	1700	C	N3-C2-O2	-6.05	117.66	121.90
36	5	2865	U	C4-C5-C6	-6.05	116.07	119.70
36	1	936	A	C5-C6-N6	-6.05	118.86	123.70
36	1	2632	G	N1-C6-O6	-6.05	116.27	119.90
1	6	337	G	C5-C6-O6	-6.05	124.97	128.60
36	5	966	U	O5'-P-OP2	-6.05	100.25	105.70
36	5	1858	A	O4'-C1'-N9	6.05	113.04	108.20
36	5	2360	C	N1-C2-O2	-6.05	115.27	118.90
36	1	2397	A	N1-C6-N6	6.05	122.23	118.60
37	3	96	U	C2-N3-C4	-6.05	123.37	127.00
1	6	1796	C	N3-C4-N4	-6.05	113.77	118.00
36	5	939	U	O5'-P-OP1	6.05	117.96	110.70
36	5	1582	C	C6-N1-C2	-6.05	117.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2618	G	C5-C6-N1	6.05	114.53	111.50
36	5	2878	G	C5-C6-O6	-6.05	124.97	128.60
36	5	2831	G	C5-C6-N1	6.05	114.52	111.50
36	5	2945	G	N1-C6-O6	6.05	123.53	119.90
36	5	61	A	N1-C2-N3	6.04	132.32	129.30
1	2	831	U	C5-C6-N1	6.04	125.72	122.70
36	1	969	C	N3-C4-C5	6.04	124.32	121.90
36	1	2891	U	C5-C4-O4	-6.04	122.28	125.90
36	5	2124	G	N1-C6-O6	6.04	123.52	119.90
36	5	2142	A	C6-N1-C2	-6.04	114.98	118.60
36	5	2383	C	N3-C4-N4	6.04	122.23	118.00
36	5	2653	C	C6-N1-C2	-6.04	117.88	120.30
36	1	94	G	O4'-C1'-N9	6.04	113.03	108.20
36	1	284	A	O4'-C1'-N9	6.04	113.03	108.20
36	1	1376	C	C4-C5-C6	6.04	120.42	117.40
1	6	1094	G	N1-C6-O6	-6.04	116.28	119.90
36	1	674	G	C8-N9-C4	-6.04	103.98	106.40
36	1	3053	G	N1-C6-O6	-6.03	116.28	119.90
1	6	1472	C	C6-N1-C1'	6.03	128.04	120.80
36	5	1008	U	C2-N1-C1'	-6.03	110.46	117.70
36	5	1790	G	O5'-P-OP1	-6.03	100.27	105.70
36	5	2822	U	O5'-P-OP1	-6.03	100.27	105.70
36	1	2719	U	N1-C2-N3	6.03	118.52	114.90
36	5	880	G	C4-N9-C1'	-6.03	118.66	126.50
36	5	1304	A	N1-C2-N3	-6.03	126.28	129.30
36	1	2856	G	N7-C8-N9	-6.03	110.08	113.10
36	5	1897	G	C4-C5-N7	6.03	113.21	110.80
36	1	422	A	C5-C6-N6	6.03	128.52	123.70
36	1	1459	C	N3-C4-C5	6.03	124.31	121.90
36	5	2830	G	C5-C6-O6	6.03	132.22	128.60
36	5	2130	G	N1-C6-O6	-6.03	116.28	119.90
36	5	3374	U	N3-C4-C5	6.03	118.22	114.60
36	1	206	G	C5-C6-N1	6.02	114.51	111.50
36	1	2404	A	C5-C6-N6	-6.02	118.88	123.70
36	5	2293	C	N1-C2-O2	6.02	122.51	118.90
36	1	765	C	N3-C2-O2	-6.02	117.69	121.90
1	2	765	G	O4'-C1'-N9	-6.02	103.39	108.20
36	1	101	G	O4'-C1'-N9	6.02	113.02	108.20
36	1	2356	A	C5-C6-N6	-6.02	118.89	123.70
1	2	402	C	C6-N1-C2	6.02	122.71	120.30
1	2	1777	G	C6-C5-N7	-6.02	126.79	130.40
36	1	1420	C	C6-N1-C2	-6.02	117.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	959	C	O4'-C1'-N1	6.02	113.01	108.20
36	5	1170	A	C8-N9-C4	6.02	108.21	105.80
36	5	2138	A	C4-C5-C6	6.02	120.01	117.00
36	1	1445	U	C2-N3-C4	-6.01	123.39	127.00
1	6	1768	G	C5-C6-O6	6.01	132.21	128.60
36	5	1907	C	N1-C2-O2	-6.01	115.29	118.90
36	1	2821	C	OP1-P-OP2	-6.01	110.58	119.60
36	5	659	G	OP2-P-O3'	6.01	118.42	105.20
36	5	2914	G	C8-N9-C1'	-6.01	119.18	127.00
38	8	37	A	N1-C6-N6	-6.01	114.99	118.60
36	1	795	G	C2-N3-C4	6.01	114.91	111.90
36	1	2366	C	C6-N1-C2	-6.01	117.90	120.30
1	6	1141	G	O5'-P-OP1	-6.01	100.29	105.70
36	5	2699	G	C5-C6-O6	-6.01	125.00	128.60
36	5	2892	A	N9-C4-C5	6.01	108.20	105.80
36	5	3092	C	O4'-C1'-N1	6.01	113.01	108.20
36	1	814	U	O5'-P-OP2	6.01	117.91	110.70
36	5	639	G	N3-C2-N2	-6.01	115.69	119.90
36	5	966	U	C2-N1-C1'	6.01	124.91	117.70
36	5	1399	A	C5-C6-N6	-6.01	118.89	123.70
36	5	3078	U	N1-C2-O2	6.01	127.00	122.80
36	1	2806	U	O5'-P-OP2	-6.00	100.30	105.70
36	5	2984	C	OP1-P-O3'	6.00	118.41	105.20
52	M6	101	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	6	804	A	N1-C6-N6	6.00	122.20	118.60
36	5	631	U	N3-C2-O2	-6.00	118.00	122.20
36	5	2920	U	N1-C2-O2	-6.00	118.60	122.80
36	1	2130	G	N1-C2-N2	-6.00	110.80	116.20
36	5	925	A	N1-C6-N6	6.00	122.20	118.60
36	1	3361	G	N3-C4-N9	6.00	129.60	126.00
37	7	93	C	N3-C2-O2	-6.00	117.70	121.90
36	1	1269	U	C2-N1-C1'	6.00	124.90	117.70
36	1	1484	U	N3-C2-O2	-6.00	118.00	122.20
1	6	113	U	N1-C2-O2	-6.00	118.60	122.80
1	6	1537	C	C6-N1-C1'	6.00	128.00	120.80
36	5	2964	G	N1-C6-O6	-6.00	116.30	119.90
36	5	3245	A	N1-C6-N6	6.00	122.20	118.60
36	1	352	A	O4'-C1'-N9	6.00	113.00	108.20
36	1	1437	C	N1-C2-O2	-6.00	115.30	118.90
36	1	1858	A	C8-N9-C4	-6.00	103.40	105.80
36	1	2216	G	N9-C4-C5	6.00	107.80	105.40
36	1	579	G	OP2-P-O3'	6.00	118.39	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2142	A	C2-N3-C4	6.00	113.60	110.60
1	6	630	A	C2-N3-C4	-5.99	107.60	110.60
36	5	2364	G	N9-C4-C5	5.99	107.80	105.40
36	5	2757	U	N1-C2-N3	5.99	118.50	114.90
36	5	2865	U	N1-C2-N3	-5.99	111.30	114.90
38	4	113	U	C4-C5-C6	5.99	123.30	119.70
36	5	622	A	N1-C6-N6	5.99	122.19	118.60
36	5	2871	G	C5-C6-O6	5.99	132.19	128.60
1	6	31	C	C5-C4-N4	5.99	124.39	120.20
1	6	107	C	C6-N1-C2	5.99	122.69	120.30
36	5	2248	C	C6-N1-C2	5.99	122.70	120.30
36	5	283	G	O4'-C1'-N9	-5.99	103.41	108.20
36	5	1450	G	C6-C5-N7	5.99	133.99	130.40
36	1	641	C	C2-N1-C1'	-5.99	112.22	118.80
36	5	1306	G	C5-C6-O6	-5.99	125.01	128.60
36	5	2341	A	C8-N9-C4	5.99	108.19	105.80
36	5	2993	G	C4-C5-N7	5.99	113.19	110.80
36	1	346	C	C5-C6-N1	-5.98	118.01	121.00
36	1	3318	G	C8-N9-C4	-5.98	104.01	106.40
36	1	206	G	N7-C8-N9	-5.98	110.11	113.10
36	1	2169	G	N9-C4-C5	5.98	107.79	105.40
37	3	57	G	N1-C6-O6	-5.98	116.31	119.90
36	5	2401	A	C2-N3-C4	-5.98	107.61	110.60
36	1	2879	C	C5-C4-N4	-5.98	116.01	120.20
1	6	1776	A	OP2-P-O3'	5.98	118.36	105.20
36	5	2957	G	O5'-P-OP1	-5.98	100.32	105.70
36	1	91	G	N3-C4-C5	5.98	131.59	128.60
36	1	1116	G	N9-C4-C5	5.98	107.79	105.40
36	1	2585	G	N3-C4-C5	-5.98	125.61	128.60
36	5	1161	G	C2-N3-C4	5.98	114.89	111.90
36	5	2996	U	O4'-C1'-N1	-5.98	103.42	108.20
36	5	1338	C	N1-C2-O2	-5.98	115.31	118.90
36	1	1112	A	O5'-P-OP2	-5.97	100.32	105.70
36	1	1314	C	C6-N1-C2	-5.97	117.91	120.30
36	1	2614	G	C5-N7-C8	5.97	107.29	104.30
36	1	3103	A	O5'-P-OP2	-5.97	100.32	105.70
38	4	25	G	C4-C5-N7	-5.97	108.41	110.80
38	4	52	A	O5'-P-OP1	-5.97	100.32	105.70
1	6	1082	C	C6-N1-C2	-5.97	117.91	120.30
36	5	2411	U	N3-C4-C5	5.97	118.19	114.60
37	3	42	A	C8-N9-C4	5.97	108.19	105.80
1	6	444	C	C6-N1-C2	5.97	122.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	871	U	N3-C4-O4	-5.97	115.22	119.40
36	1	1421	G	N7-C8-N9	-5.97	110.11	113.10
36	5	1226	G	N3-C4-N9	5.97	129.58	126.00
36	1	2412	G	C8-N9-C4	-5.97	104.01	106.40
48	M1	112	LEU	CA-CB-CG	5.97	129.02	115.30
1	6	542	A	C4-N9-C1'	5.97	137.04	126.30
36	5	2345	A	C5-C6-N6	-5.97	118.93	123.70
1	2	1324	G	N3-C2-N2	-5.96	115.72	119.90
36	1	331	G	C2-N3-C4	5.96	114.88	111.90
36	5	881	C	C2-N3-C4	5.96	122.88	119.90
38	4	13	A	C8-N9-C4	-5.96	103.42	105.80
1	6	619	A	OP2-P-O3'	5.96	118.32	105.20
38	8	7	U	C5-C4-O4	-5.96	122.32	125.90
36	1	1349	G	C2-N3-C4	5.96	114.88	111.90
36	1	1890	U	C5-C4-O4	-5.96	122.32	125.90
36	1	2572	C	C6-N1-C1'	-5.96	113.65	120.80
36	1	1902	G	C8-N9-C4	-5.96	104.02	106.40
36	5	681	U	C5-C4-O4	-5.96	122.33	125.90
39	l2	190	ARG	NE-CZ-NH1	-5.96	117.32	120.30
36	1	1846	C	N3-C4-C5	-5.96	119.52	121.90
36	1	3275	U	OP1-P-O3'	5.96	118.31	105.20
36	1	398	A	C5-C6-N6	-5.96	118.94	123.70
69	O3	67	MET	CG-SD-CE	-5.96	90.67	100.20
1	2	1560	U	N1-C2-N3	5.95	118.47	114.90
36	1	92	G	N9-C4-C5	-5.95	103.02	105.40
36	1	2245	C	C6-N1-C2	-5.95	117.92	120.30
36	1	2747	A	N1-C6-N6	-5.95	115.03	118.60
36	5	3107	U	OP2-P-O3'	5.95	118.30	105.20
1	2	158	U	P-O3'-C3'	5.95	126.84	119.70
36	1	709	A	N7-C8-N9	-5.95	110.83	113.80
36	1	2339	C	C6-N1-C2	-5.95	117.92	120.30
36	5	659	G	C5-C6-O6	-5.95	125.03	128.60
36	5	1303	A	N1-C2-N3	-5.95	126.33	129.30
36	1	2846	U	N1-C2-O2	5.95	126.96	122.80
36	5	980	A	N1-C6-N6	-5.95	115.03	118.60
1	2	1560	U	C6-N1-C2	-5.95	117.43	121.00
1	2	323	A	N7-C8-N9	5.95	116.77	113.80
36	5	204	A	C5-C6-N1	5.95	120.67	117.70
36	5	659	G	P-O3'-C3'	5.95	126.83	119.70
36	1	646	A	N1-C2-N3	5.94	132.27	129.30
36	5	3377	G	C6-C5-N7	-5.94	126.83	130.40
36	1	1140	G	N3-C2-N2	5.94	124.06	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1312	C	N1-C2-O2	-5.94	115.33	118.90
36	1	2406	C	C5-C6-N1	-5.94	118.03	121.00
36	1	1409	G	C6-C5-N7	5.94	133.96	130.40
36	1	2354	C	O5'-P-OP1	-5.94	100.35	105.70
36	1	2978	U	P-O3'-C3'	5.94	126.83	119.70
36	5	1406	A	C5-N7-C8	-5.94	100.93	103.90
36	1	964	G	C5-C6-N1	5.94	114.47	111.50
36	5	3382	U	C2-N1-C1'	5.94	124.83	117.70
1	2	1657	U	C4-C5-C6	5.94	123.26	119.70
36	5	1880	U	O5'-P-OP2	5.94	117.83	110.70
1	2	158	U	C2-N1-C1'	5.94	124.82	117.70
36	1	2811	A	C5-C6-N1	5.94	120.67	117.70
36	5	2880	U	C6-N1-C2	-5.94	117.44	121.00
36	1	200	C	N1-C2-O2	5.93	122.46	118.90
36	5	283	G	C5-C6-O6	-5.93	125.04	128.60
36	5	974	G	C2-N3-C4	5.93	114.87	111.90
36	5	2434	U	C5-C4-O4	5.93	129.46	125.90
1	2	1652	C	C5-C6-N1	5.93	123.97	121.00
36	1	785	G	C2-N3-C4	5.93	114.87	111.90
36	1	1589	A	OP2-P-O3'	5.93	118.25	105.20
38	4	73	U	N1-C2-O2	5.93	126.95	122.80
1	6	57	G	N3-C4-C5	-5.93	125.63	128.60
36	5	1733	G	N1-C6-O6	5.93	123.46	119.90
36	1	673	U	N3-C4-C5	5.93	118.16	114.60
36	5	283	G	C8-N9-C4	-5.93	104.03	106.40
38	8	45	C	C6-N1-C2	-5.93	117.93	120.30
36	5	2404	A	C5-C6-N6	-5.93	118.96	123.70
36	5	2408	U	C2-N3-C4	-5.93	123.44	127.00
1	6	804	A	N9-C4-C5	-5.93	103.43	105.80
36	5	1226	G	N9-C4-C5	-5.93	103.03	105.40
36	5	3214	U	N3-C4-O4	-5.93	115.25	119.40
37	3	15	C	C6-N1-C2	5.93	122.67	120.30
36	5	335	G	O5'-P-OP2	5.93	117.81	110.70
36	1	1792	C	C4-C5-C6	5.92	120.36	117.40
36	1	2861	U	N3-C2-O2	-5.92	118.05	122.20
37	3	81	U	C2-N3-C4	-5.92	123.44	127.00
36	5	933	A	C6-N1-C2	-5.92	115.05	118.60
38	8	56	G	C6-C5-N7	-5.92	126.84	130.40
36	1	2712	U	N3-C2-O2	-5.92	118.05	122.20
1	2	879	G	O5'-P-OP2	-5.92	100.37	105.70
36	5	631	U	N1-C2-O2	5.92	126.94	122.80
36	5	1213	G	C4-C5-N7	5.92	113.17	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3188	G	C8-N9-C4	-5.92	104.03	106.40
36	1	1169	A	OP2-P-O3'	5.92	118.22	105.20
36	5	859	G	O5'-P-OP1	-5.92	100.37	105.70
36	5	913	A	O5'-P-OP1	-5.92	100.37	105.70
36	1	1176	C	C5-C4-N4	-5.92	116.06	120.20
36	1	2947	G	C5-C6-O6	-5.92	125.05	128.60
36	1	793	C	N3-C4-N4	5.92	122.14	118.00
1	6	1111	G	N3-C4-N9	5.92	129.55	126.00
36	5	3218	A	C5-C6-N6	-5.92	118.97	123.70
37	7	102	A	C5-C6-N1	-5.92	114.74	117.70
36	1	109	A	N1-C6-N6	-5.91	115.05	118.60
36	1	1294	A	C2-N3-C4	5.91	113.56	110.60
36	1	2298	U	O4'-C1'-N1	5.91	112.93	108.20
1	6	977	A	C8-N9-C4	5.91	108.17	105.80
36	5	2400	G	C5-C6-O6	-5.91	125.05	128.60
36	5	3306	U	C6-N1-C2	5.91	124.55	121.00
1	2	1174	C	N1-C2-O2	5.91	122.45	118.90
36	5	940	G	C2-N3-C4	5.91	114.86	111.90
36	5	960	U	OP2-P-O3'	5.91	118.21	105.20
36	5	2650	U	C2-N3-C4	-5.91	123.45	127.00
36	1	2619	G	OP1-P-OP2	5.91	128.47	119.60
1	6	1012	U	C5-C4-O4	-5.91	122.35	125.90
36	5	2421	U	N1-C2-N3	5.91	118.45	114.90
36	1	333	G	C5-C6-O6	5.91	132.15	128.60
36	1	2859	U	C4-C5-C6	5.91	123.25	119.70
36	5	776	U	N3-C2-O2	-5.91	118.06	122.20
1	2	553	G	C4-C5-C6	5.91	122.34	118.80
36	1	361	A	N1-C6-N6	-5.91	115.06	118.60
1	6	957	G	N3-C2-N2	-5.91	115.77	119.90
1	2	1258	U	N3-C2-O2	-5.91	118.07	122.20
36	1	29	C	C6-N1-C2	5.91	122.66	120.30
36	1	200	C	C6-N1-C1'	-5.91	113.71	120.80
36	1	1843	C	N1-C2-O2	-5.91	115.36	118.90
1	6	1745	G	N1-C6-O6	5.91	123.44	119.90
20	c8	116	LEU	CA-CB-CG	5.91	128.88	115.30
37	7	37	G	N3-C4-C5	-5.91	125.65	128.60
36	1	940	G	O5'-P-OP1	-5.90	100.39	105.70
36	5	1476	G	C8-N9-C4	5.90	108.76	106.40
36	5	2337	C	N3-C4-C5	5.90	124.26	121.90
36	5	3076	C	N3-C4-C5	5.90	124.26	121.90
36	1	934	G	C8-N9-C1'	-5.90	119.33	127.00
36	5	264	G	N9-C4-C5	-5.90	103.04	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1307	G	C2-N3-C4	5.90	114.85	111.90
36	5	2890	A	C5-C6-N1	-5.90	114.75	117.70
36	5	3174	A	C8-N9-C4	-5.90	103.44	105.80
36	1	1394	A	OP2-P-O3'	5.90	118.18	105.20
36	1	2846	U	N1-C2-N3	5.90	118.44	114.90
1	6	542	A	C8-N9-C4	-5.90	103.44	105.80
36	5	1473	G	C8-N9-C4	5.90	108.76	106.40
1	6	639	U	C2-N1-C1'	5.90	124.78	117.70
36	5	56	G	C6-C5-N7	5.90	133.94	130.40
36	5	92	G	C5-C6-N1	5.90	114.45	111.50
36	5	892	U	C5-C6-N1	-5.90	119.75	122.70
36	5	2899	C	N3-C2-O2	-5.90	117.77	121.90
38	8	56	G	C5-C6-O6	-5.90	125.06	128.60
36	5	1881	A	O5'-P-OP2	-5.90	100.39	105.70
36	1	1184	A	OP2-P-O3'	5.89	118.17	105.20
36	1	2898	G	O4'-C1'-N9	-5.89	103.48	108.20
38	4	30	C	O5'-P-OP1	-5.89	100.39	105.70
36	5	982	C	OP2-P-O3'	5.89	118.17	105.20
36	5	3120	C	C2-N3-C4	5.89	122.85	119.90
36	1	3055	U	N3-C4-C5	5.89	118.14	114.60
1	6	272	U	P-O3'-C3'	5.89	126.77	119.70
36	5	795	G	N1-C2-N3	-5.89	120.36	123.90
36	5	1147	G	C4-C5-N7	-5.89	108.44	110.80
36	1	66	A	O5'-P-OP1	-5.89	100.40	105.70
36	1	517	G	C8-N9-C4	-5.89	104.05	106.40
36	1	970	A	N7-C8-N9	5.89	116.75	113.80
36	1	1294	A	N1-C6-N6	-5.89	115.07	118.60
36	1	2305	G	N1-C6-O6	5.89	123.43	119.90
36	1	2958	A	C5-C6-N1	5.89	120.64	117.70
1	6	114	C	N1-C2-O2	5.89	122.43	118.90
36	5	2902	A	C5-C6-N6	-5.89	118.99	123.70
36	1	2726	C	N1-C2-N3	5.89	123.32	119.20
36	1	2917	G	C2-N3-C4	5.89	114.84	111.90
1	6	965	U	N3-C4-C5	5.89	118.13	114.60
36	1	1362	G	C8-N9-C4	5.89	108.75	106.40
1	6	402	C	O4'-C1'-N1	5.89	112.91	108.20
36	5	648	C	C2-N1-C1'	5.89	125.28	118.80
36	5	869	G	N3-C4-C5	-5.89	125.66	128.60
36	5	2870	C	N3-C4-C5	5.89	124.25	121.90
36	1	1891	A	C2-N3-C4	-5.88	107.66	110.60
1	6	426	G	C4-N9-C1'	5.88	134.15	126.50
1	6	1120	U	N3-C2-O2	-5.88	118.08	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1655	A	N1-C6-N6	5.88	122.13	118.60
36	5	788	C	OP2-P-O3'	5.88	118.14	105.20
36	5	795	G	C2-N3-C4	5.88	114.84	111.90
36	5	953	G	N1-C6-O6	5.88	123.43	119.90
36	5	1833	G	N1-C6-O6	-5.88	116.37	119.90
36	1	714	G	C8-N9-C1'	-5.88	119.35	127.00
1	6	687	G	N3-C4-N9	-5.88	122.47	126.00
37	3	95	A	N1-C6-N6	5.88	122.13	118.60
1	6	558	U	N1-C2-O2	5.88	126.92	122.80
36	5	1406	A	C5-C6-N6	-5.88	119.00	123.70
36	5	212	G	OP1-P-O3'	5.88	118.14	105.20
36	1	1007	U	C5-C4-O4	-5.88	122.37	125.90
36	1	2662	G	C6-C5-N7	-5.88	126.87	130.40
36	5	2257	C	C5-C6-N1	5.88	123.94	121.00
36	1	102	C	N1-C2-O2	-5.88	115.37	118.90
36	1	2434	U	C5-C4-O4	5.88	129.43	125.90
36	1	2634	U	C2-N3-C4	-5.88	123.47	127.00
36	1	2953	U	N3-C4-O4	5.88	123.51	119.40
36	5	1398	U	OP2-P-O3'	5.88	118.13	105.20
36	5	2142	A	O5'-P-OP1	5.88	117.75	110.70
1	6	1354	G	C4-N9-C1'	5.88	134.14	126.50
36	5	883	A	C8-N9-C4	5.88	108.15	105.80
36	1	645	A	C5-C6-N6	-5.87	119.00	123.70
36	1	810	A	N9-C4-C5	5.87	108.15	105.80
36	1	2831	G	C4-C5-N7	5.87	113.15	110.80
1	6	1582	U	C5-C6-N1	-5.87	119.76	122.70
36	5	966	U	N1-C2-O2	5.87	126.91	122.80
37	7	13	A	C5-C6-N6	-5.87	119.00	123.70
1	2	1273	G	O4'-C1'-N9	5.87	112.90	108.20
36	1	198	A	C8-N9-C4	-5.87	103.45	105.80
36	1	2286	U	N3-C2-O2	-5.87	118.09	122.20
47	M0	152	LEU	CA-CB-CG	-5.87	101.80	115.30
36	5	1017	C	N1-C2-O2	5.87	122.42	118.90
36	5	1592	G	OP2-P-O3'	5.87	118.12	105.20
36	5	2691	A	C8-N9-C4	-5.87	103.45	105.80
36	5	3183	A	OP1-P-OP2	-5.87	110.79	119.60
36	5	1878	G	C8-N9-C4	-5.87	104.05	106.40
36	1	2653	C	N1-C2-O2	5.87	122.42	118.90
52	M6	37	ARG	NE-CZ-NH1	-5.87	117.37	120.30
36	5	982	C	N1-C2-O2	5.87	122.42	118.90
36	5	2866	U	OP1-P-O3'	5.87	118.11	105.20
1	2	1012	U	C2-N3-C4	5.87	130.52	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	282	G	N1-C6-O6	-5.87	116.38	119.90
36	1	1712	G	C4-C5-N7	5.87	113.15	110.80
36	5	2360	C	N3-C4-N4	5.87	122.11	118.00
1	2	380	U	N1-C2-O2	5.86	126.90	122.80
36	1	2830	G	N3-C2-N2	-5.86	115.80	119.90
36	5	1148	G	C8-N9-C4	5.86	108.75	106.40
36	5	3322	A	O5'-P-OP2	-5.86	100.42	105.70
36	5	3351	U	N1-C2-O2	5.86	126.90	122.80
36	1	2585	G	C2-N3-C4	5.86	114.83	111.90
36	1	3178	A	N9-C4-C5	-5.86	103.45	105.80
36	1	196	G	C4-C5-N7	5.86	113.14	110.80
36	1	2362	C	N1-C2-O2	5.86	122.42	118.90
1	6	426	G	N3-C4-C5	-5.86	125.67	128.60
36	1	217	U	OP1-P-O3'	5.86	118.09	105.20
36	1	398	A	N1-C6-N6	5.86	122.11	118.60
36	1	1335	C	N3-C4-N4	-5.86	113.90	118.00
36	1	2121	G	C5-C6-O6	5.86	132.12	128.60
36	1	282	G	C2'-C3'-O3'	5.86	123.07	113.70
36	5	846	A	O5'-P-OP2	-5.86	100.43	105.70
36	5	881	C	C2-N1-C1'	5.86	125.24	118.80
36	5	948	C	C5-C4-N4	-5.86	116.10	120.20
36	5	1513	G	N1-C6-O6	-5.86	116.39	119.90
36	1	660	A	C2-N3-C4	5.86	113.53	110.60
36	5	809	G	C5-C6-O6	-5.86	125.09	128.60
36	5	1449	A	C6-C5-N7	-5.86	128.20	132.30
36	5	3186	A	O5'-P-OP2	-5.86	100.43	105.70
36	5	339	C	C5-C4-N4	5.85	124.30	120.20
36	5	2685	C	C2-N3-C4	-5.85	116.97	119.90
36	1	1292	C	C6-N1-C2	5.85	122.64	120.30
36	5	2643	A	N1-C2-N3	-5.85	126.37	129.30
56	n0	137	ARG	NE-CZ-NH1	5.85	123.23	120.30
36	1	1530	U	C6-N1-C2	5.85	124.51	121.00
36	1	2345	A	C5-C6-N6	-5.85	119.02	123.70
36	5	2382	G	N9-C4-C5	5.85	107.74	105.40
36	1	1300	G	N1-C6-O6	5.85	123.41	119.90
36	1	2142	A	N3-C4-C5	-5.85	122.71	126.80
36	1	2526	C	C2-N1-C1'	5.85	125.23	118.80
36	1	2656	A	C2-N3-C4	5.85	113.52	110.60
37	7	99	G	N1-C6-O6	-5.85	116.39	119.90
36	5	1132	C	N3-C4-C5	5.84	124.24	121.90
36	5	2131	A	N1-C6-N6	5.84	122.11	118.60
36	5	2395	G	C4-C5-N7	5.84	113.14	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3140	G	C6-C5-N7	-5.84	126.89	130.40
36	1	2944	U	N3-C4-C5	5.84	118.11	114.60
36	5	63	A	C6-C5-N7	-5.84	128.21	132.30
36	5	210	U	C2-N1-C1'	-5.84	110.69	117.70
1	2	1503	A	N1-C6-N6	5.84	122.11	118.60
36	1	155	G	N3-C4-N9	5.84	129.50	126.00
36	1	870	G	C5-C6-O6	-5.84	125.09	128.60
1	6	1503	A	C5-N7-C8	-5.84	100.98	103.90
36	5	1517	G	O5'-P-OP2	-5.84	100.44	105.70
36	1	58	G	C5-C6-O6	-5.84	125.10	128.60
36	1	2878	G	C8-N9-C4	5.84	108.73	106.40
36	5	2985	C	C6-N1-C2	-5.84	117.97	120.30
36	1	1842	A	N1-C6-N6	-5.84	115.10	118.60
36	1	2292	U	C2-N1-C1'	5.84	124.70	117.70
36	1	2808	A	C5-C6-N6	-5.84	119.03	123.70
37	3	5	G	C2-N3-C4	-5.84	108.98	111.90
1	6	1596	C	N1-C2-O2	5.84	122.40	118.90
36	5	1301	A	C6-C5-N7	-5.84	128.21	132.30
36	5	2377	G	C5-C6-O6	5.83	132.10	128.60
36	5	3239	G	N1-C6-O6	5.83	123.40	119.90
1	2	1798	U	C2-N1-C1'	5.83	124.70	117.70
36	1	1201	C	C5-C4-N4	-5.83	116.12	120.20
36	1	1380	G	N3-C4-C5	5.83	131.52	128.60
36	5	2817	A	OP1-P-OP2	-5.83	110.85	119.60
36	1	300	G	O5'-P-OP1	-5.83	100.45	105.70
36	1	426	G	N3-C4-N9	5.83	129.50	126.00
1	6	914	G	C8-N9-C4	5.83	108.73	106.40
1	6	1037	C	C6-N1-C2	5.83	122.63	120.30
36	5	1190	A	N7-C8-N9	5.83	116.72	113.80
36	5	2117	A	O5'-P-OP2	-5.83	100.45	105.70
36	1	2300	G	OP2-P-O3'	5.83	118.03	105.20
36	5	2618	G	C5-C6-O6	-5.83	125.10	128.60
36	1	2142	A	OP1-P-OP2	-5.83	110.86	119.60
1	6	75	U	O4'-C1'-N1	5.83	112.86	108.20
57	n1	106	LEU	CA-CB-CG	-5.83	101.90	115.30
36	5	1848	G	N1-C6-O6	5.83	123.40	119.90
36	1	965	A	OP1-P-O3'	5.83	118.02	105.20
36	1	1125	U	OP2-P-O3'	5.83	118.02	105.20
36	5	609	G	N3-C2-N2	-5.83	115.82	119.90
36	5	1047	A	C4-C5-N7	5.83	113.61	110.70
36	1	395	A	O5'-P-OP2	-5.82	100.46	105.70
36	5	2190	U	N1-C2-N3	5.82	118.39	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1114	G	C8-N9-C4	5.82	108.73	106.40
36	1	2815	G	N3-C2-N2	5.82	123.98	119.90
36	5	1301	A	C4-C5-N7	5.82	113.61	110.70
1	2	704	C	O4'-C1'-N1	5.82	112.86	108.20
36	1	1858	A	N3-C4-C5	-5.82	122.73	126.80
36	5	2305	G	C4-C5-N7	5.82	113.13	110.80
1	2	973	A	O5'-P-OP2	-5.82	100.46	105.70
36	1	730	C	C6-N1-C2	5.82	122.63	120.30
36	1	1103	A	N9-C4-C5	-5.82	103.47	105.80
36	1	1333	C	O5'-P-OP1	5.82	117.68	110.70
36	5	2211	U	C5-C6-N1	-5.82	119.79	122.70
36	1	788	C	C2-N1-C1'	-5.82	112.40	118.80
36	1	1507	G	O4'-C1'-N9	-5.82	103.55	108.20
36	5	709	A	O5'-P-OP1	-5.82	100.47	105.70
36	5	838	G	C4-C5-N7	-5.82	108.47	110.80
36	5	2399	A	OP1-P-OP2	-5.82	110.88	119.60
1	6	139	C	N1-C2-O2	5.81	122.39	118.90
36	5	636	C	C5-C6-N1	-5.81	118.09	121.00
36	1	206	G	C8-N9-C4	5.81	108.72	106.40
36	5	2290	C	C5-C4-N4	-5.81	116.13	120.20
36	1	21	G	N1-C6-O6	-5.81	116.41	119.90
1	6	771	A	N9-C4-C5	-5.81	103.48	105.80
36	5	3050	U	N3-C2-O2	-5.81	118.13	122.20
36	1	793	C	N1-C2-O2	-5.81	115.42	118.90
36	1	2247	G	C6-C5-N7	-5.81	126.92	130.40
1	6	901	G	C5-N7-C8	-5.81	101.40	104.30
36	1	2405	C	C4-C5-C6	5.81	120.30	117.40
36	1	3078	U	N3-C2-O2	-5.81	118.14	122.20
1	6	647	G	N3-C4-N9	-5.81	122.52	126.00
36	1	2714	G	C5-N7-C8	-5.81	101.40	104.30
36	5	2391	G	OP1-P-OP2	-5.81	110.89	119.60
36	5	3214	U	N1-C2-N3	5.81	118.38	114.90
36	1	44	U	C2-N1-C1'	-5.80	110.73	117.70
36	1	2376	G	N7-C8-N9	5.80	116.00	113.10
45	l8	69	LEU	CA-CB-CG	5.80	128.65	115.30
1	2	337	G	C6-C5-N7	-5.80	126.92	130.40
1	2	190	C	O4'-C1'-N1	5.80	112.84	108.20
1	2	1462	G	N9-C4-C5	-5.80	103.08	105.40
36	1	325	A	C5-C6-N1	5.80	120.60	117.70
36	5	2621	G	N1-C6-O6	5.80	123.38	119.90
36	5	3197	G	C8-N9-C4	-5.80	104.08	106.40
1	6	1649	G	N3-C2-N2	5.80	123.96	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1151	U	N3-C2-O2	5.80	126.26	122.20
37	7	19	C	O5'-P-OP2	-5.80	100.48	105.70
36	5	1506	A	N9-C4-C5	5.80	108.12	105.80
36	5	1884	A	N1-C6-N6	5.80	122.08	118.60
36	5	2874	G	C5-C6-N1	-5.80	108.60	111.50
1	2	145	A	C8-N9-C4	-5.80	103.48	105.80
36	1	821	U	N3-C4-O4	-5.80	115.34	119.40
36	1	1604	G	C8-N9-C1'	-5.79	119.47	127.00
36	1	2870	C	O4'-C1'-N1	5.79	112.84	108.20
36	1	2875	U	N3-C2-O2	-5.79	118.14	122.20
1	2	186	C	C2-N1-C1'	5.79	125.17	118.80
36	1	515	C	N3-C4-N4	5.79	122.06	118.00
36	1	666	A	C6-C5-N7	5.79	136.35	132.30
36	1	1141	C	C6-N1-C2	-5.79	117.98	120.30
36	1	2993	G	N9-C4-C5	-5.79	103.08	105.40
36	5	1369	A	N1-C2-N3	-5.79	126.40	129.30
36	5	514	G	C4-C5-N7	5.79	113.12	110.80
36	5	1825	G	O5'-P-OP1	5.79	117.65	110.70
36	5	780	A	N1-C6-N6	5.79	122.07	118.60
36	5	2882	U	O5'-P-OP2	-5.79	100.49	105.70
36	5	3105	U	OP2-P-O3'	5.79	117.94	105.20
36	1	1507	G	N3-C2-N2	-5.79	115.85	119.90
1	6	1194	A	N1-C6-N6	5.79	122.07	118.60
6	s4	38	LEU	CA-CB-CG	5.79	128.62	115.30
36	5	1506	A	C8-N9-C4	-5.79	103.48	105.80
36	1	2404	A	C4-C5-C6	5.79	119.89	117.00
36	5	417	A	N7-C8-N9	-5.79	110.91	113.80
36	5	1181	U	OP1-P-OP2	5.79	128.28	119.60
36	5	2334	U	N3-C2-O2	-5.79	118.15	122.20
36	1	1657	C	C6-N1-C2	5.79	122.61	120.30
1	6	957	G	C8-N9-C4	5.79	108.71	106.40
36	5	74	G	O5'-P-OP1	-5.79	100.49	105.70
1	2	271	A	O5'-P-OP2	-5.78	100.49	105.70
36	1	827	A	N7-C8-N9	-5.78	110.91	113.80
36	1	2816	G	O5'-P-OP2	-5.78	100.49	105.70
36	5	43	A	O5'-P-OP2	-5.78	100.50	105.70
36	5	2873	U	O5'-P-OP2	-5.78	100.50	105.70
36	1	347	G	C5-N7-C8	-5.78	101.41	104.30
36	1	2130	G	N3-C2-N2	5.78	123.95	119.90
36	1	2850	G	N1-C6-O6	5.78	123.37	119.90
36	5	2857	C	C2-N3-C4	-5.78	117.01	119.90
1	6	400	A	OP2-P-O3'	5.78	117.91	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1400	G	O5'-P-OP2	-5.78	100.50	105.70
36	1	1510	G	N9-C4-C5	-5.78	103.09	105.40
1	6	90	C	N3-C2-O2	-5.78	117.86	121.90
36	5	410	U	OP2-P-O3'	5.78	117.91	105.20
36	5	2135	U	C6-N1-C2	5.78	124.47	121.00
36	5	2818	U	N3-C4-C5	5.78	118.07	114.60
36	5	3175	U	O5'-P-OP2	-5.78	100.50	105.70
36	1	885	U	C4-C5-C6	5.78	123.17	119.70
36	5	50	U	C5-C6-N1	5.78	125.59	122.70
36	5	1104	G	C8-N9-C4	-5.78	104.09	106.40
36	5	2140	U	N1-C2-O2	-5.78	118.76	122.80
36	5	2753	G	C8-N9-C4	-5.78	104.09	106.40
1	2	1200	G	C5-C6-O6	-5.77	125.14	128.60
36	1	1371	G	C8-N9-C4	5.77	108.71	106.40
36	5	2186	U	C5-C4-O4	5.77	129.36	125.90
36	1	934	G	C4-N9-C1'	5.77	134.00	126.50
36	1	2869	U	C2-N1-C1'	5.77	124.62	117.70
1	6	1151	A	C8-N9-C4	-5.77	103.49	105.80
1	2	2	A	O4'-C1'-N9	-5.77	103.59	108.20
1	2	1291	G	C2-N3-C4	-5.77	109.02	111.90
37	3	40	C	C6-N1-C2	-5.77	117.99	120.30
36	5	213	A	O5'-P-OP2	-5.77	100.51	105.70
36	5	3178	A	O5'-P-OP1	-5.77	100.51	105.70
36	1	1492	G	C4-C5-N7	-5.76	108.49	110.80
44	L7	215	GLY	N-CA-C	-5.76	98.69	113.10
36	5	770	G	O4'-C1'-N9	5.76	112.81	108.20
36	5	1884	A	C5-N7-C8	-5.76	101.02	103.90
36	5	2186	U	O5'-P-OP2	-5.76	100.51	105.70
1	2	1573	A	P-O3'-C3'	5.76	126.61	119.70
1	2	1773	C	N3-C4-N4	5.76	122.03	118.00
36	1	860	G	C5-C6-O6	-5.76	125.14	128.60
36	1	894	G	N1-C6-O6	5.76	123.36	119.90
36	1	976	U	C5-C4-O4	-5.76	122.44	125.90
36	1	2314	U	P-O3'-C3'	-5.76	112.79	119.70
36	5	584	G	N9-C4-C5	5.76	107.70	105.40
36	1	1320	C	O5'-P-OP2	-5.76	100.52	105.70
36	5	908	G	O4'-C1'-N9	-5.76	103.59	108.20
36	1	656	A	N9-C4-C5	5.76	108.10	105.80
36	5	668	G	C5-C6-N1	5.76	114.38	111.50
36	5	1487	G	C8-N9-C4	-5.76	104.10	106.40
36	5	2820	A	N7-C8-N9	5.76	116.68	113.80
36	1	919	U	O5'-P-OP2	-5.75	100.52	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1434	G	C8-N9-C4	-5.75	104.10	106.40
1	6	310	C	N3-C4-C5	-5.75	119.60	121.90
1	6	361	C	OP1-P-OP2	-5.75	110.97	119.60
36	5	625	G	N9-C4-C5	5.75	107.70	105.40
36	5	2699	G	N1-C6-O6	5.75	123.35	119.90
68	O2	16	LYS	CD-CE-NZ	5.75	124.93	111.70
1	6	1031	U	C6-N1-C2	5.75	124.45	121.00
1	6	1697	G	N3-C4-C5	-5.75	125.72	128.60
36	5	519	A	O5'-P-OP2	-5.75	100.52	105.70
36	5	2872	A	O5'-P-OP1	5.75	117.61	110.70
36	1	1510	G	C4-C5-N7	5.75	113.10	110.80
36	1	3305	A	O5'-P-OP2	-5.75	100.52	105.70
36	5	1561	G	O4'-C1'-N9	5.75	112.80	108.20
1	2	1241	G	O4'-C1'-N9	5.75	112.80	108.20
36	1	2728	G	C5-C6-O6	-5.75	125.15	128.60
1	6	1600	A	N7-C8-N9	5.75	116.67	113.80
36	5	426	G	N9-C4-C5	-5.75	103.10	105.40
36	5	1926	C	C2-N1-C1'	-5.75	112.48	118.80
36	1	3143	C	N1-C2-O2	-5.75	115.45	118.90
36	5	1529	A	C8-N9-C4	5.75	108.10	105.80
36	5	2541	U	C2-N1-C1'	5.75	124.60	117.70
36	5	2704	A	C5'-C4'-O4'	-5.75	102.20	109.10
36	1	200	C	C2-N1-C1'	5.74	125.12	118.80
21	c9	57	ARG	NE-CZ-NH2	-5.74	117.43	120.30
36	5	3014	U	C5-C4-O4	-5.74	122.45	125.90
37	7	35	C	C5-C6-N1	-5.74	118.13	121.00
36	1	2979	U	N1-C2-N3	5.74	118.34	114.90
36	5	670	C	C6-N1-C2	-5.74	118.00	120.30
36	5	2333	C	C6-N1-C2	5.74	122.60	120.30
36	5	2350	C	C2-N3-C4	-5.74	117.03	119.90
1	2	408	C	O5'-P-OP2	-5.74	100.53	105.70
1	2	447	U	C6-N1-C2	-5.74	117.56	121.00
36	1	2181	C	N3-C4-C5	5.74	124.20	121.90
38	4	84	C	C6-N1-C2	5.74	122.60	120.30
36	5	679	U	N3-C4-O4	-5.74	115.38	119.40
36	5	793	C	N3-C4-N4	5.74	122.02	118.00
36	5	969	C	C6-N1-C2	5.74	122.60	120.30
37	7	92	A	N1-C6-N6	5.74	122.04	118.60
36	1	347	G	C5-C6-O6	-5.74	125.16	128.60
36	1	646	A	N9-C4-C5	5.74	108.09	105.80
1	6	1119	G	N3-C4-C5	-5.74	125.73	128.60
36	5	353	G	C8-N9-C1'	5.74	134.46	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1168	U	C5-C6-N1	5.74	125.57	122.70
36	1	1197	A	N9-C4-C5	-5.74	103.50	105.80
36	1	1516	C	N1-C2-O2	-5.74	115.46	118.90
36	5	1365	G	N1-C2-N2	-5.74	111.04	116.20
37	7	85	G	OP2-P-O3'	5.74	117.82	105.20
36	1	35	A	N1-C6-N6	5.74	122.04	118.60
36	5	2345	A	C6-C5-N7	-5.73	128.29	132.30
36	1	944	C	OP2-P-O3'	5.73	117.81	105.20
38	4	93	U	C5-C4-O4	-5.73	122.46	125.90
1	6	53	G	O5'-P-OP2	-5.73	100.54	105.70
36	5	672	A	C6-C5-N7	-5.73	128.29	132.30
36	5	3101	G	O5'-P-OP1	-5.73	100.54	105.70
44	l7	163	LEU	CB-CG-CD1	-5.73	101.25	111.00
36	1	601	U	N1-C2-O2	5.73	126.81	122.80
1	6	1663	G	C8-N9-C4	-5.73	104.11	106.40
36	5	1363	A	N1-C6-N6	-5.73	115.16	118.60
36	5	2354	C	N3-C2-O2	5.73	125.91	121.90
36	5	2366	C	C6-N1-C2	-5.73	118.01	120.30
36	1	221	A	O5'-P-OP2	-5.73	100.54	105.70
36	1	304	G	C2-N3-C4	5.73	114.76	111.90
36	5	883	A	N7-C8-N9	-5.73	110.94	113.80
36	1	907	G	N3-C2-N2	5.73	123.91	119.90
36	1	3043	C	OP2-P-O3'	5.73	117.80	105.20
1	6	542	A	P-O3'-C3'	5.73	126.57	119.70
1	6	1747	G	C8-N9-C4	5.73	108.69	106.40
1	2	1486	G	N7-C8-N9	5.73	115.96	113.10
36	1	648	C	C2-N1-C1'	5.73	125.10	118.80
36	1	2139	A	N1-C6-N6	-5.73	115.17	118.60
36	1	1119	C	N3-C4-C5	5.72	124.19	121.90
36	1	1133	A	N1-C2-N3	-5.72	126.44	129.30
36	1	1878	G	O5'-P-OP1	-5.72	100.55	105.70
36	5	1331	U	N1-C2-N3	-5.72	111.47	114.90
36	5	2385	G	N1-C6-O6	5.72	123.33	119.90
36	5	2916	U	N1-C2-O2	-5.72	118.79	122.80
36	1	1367	G	N9-C4-C5	-5.72	103.11	105.40
36	1	2357	A	C6-C5-N7	-5.72	128.29	132.30
36	1	2947	G	N1-C6-O6	5.72	123.33	119.90
36	1	3344	A	N1-C6-N6	5.72	122.03	118.60
36	5	966	U	C6-N1-C2	-5.72	117.57	121.00
36	5	1359	C	N3-C4-N4	5.72	122.01	118.00
36	1	2176	U	N1-C2-O2	5.72	126.81	122.80
36	1	3277	U	N3-C2-O2	-5.72	118.19	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	4	37	A	C8-N9-C4	-5.72	103.51	105.80
1	2	1363	U	N3-C2-O2	-5.72	118.20	122.20
36	1	1367	G	C4-C5-N7	5.72	113.09	110.80
36	5	1878	G	N3-C4-C5	-5.72	125.74	128.60
36	5	2737	C	O5'-P-OP2	-5.72	100.55	105.70
36	5	2849	C	C5-C6-N1	5.72	123.86	121.00
36	5	3129	A	OP1-P-OP2	5.72	128.18	119.60
36	1	2129	U	C6-N1-C2	-5.72	117.57	121.00
1	6	795	U	C6-N1-C2	-5.72	117.57	121.00
36	5	1302	A	C8-N9-C4	-5.72	103.51	105.80
36	5	2341	A	C2-N3-C4	5.72	113.46	110.60
1	2	1777	G	C4-C5-N7	5.72	113.09	110.80
36	5	1906	G	N3-C4-N9	5.72	129.43	126.00
37	3	85	G	C5-C6-O6	-5.71	125.17	128.60
37	7	98	C	O5'-P-OP2	-5.71	100.56	105.70
36	1	2152	A	N1-C6-N6	-5.71	115.17	118.60
36	1	1495	U	C5-C4-O4	5.71	129.33	125.90
36	1	1506	A	N1-C6-N6	-5.71	115.17	118.60
36	1	2982	A	C8-N9-C4	5.71	108.08	105.80
36	5	2147	A	N1-C6-N6	5.71	122.03	118.60
36	5	3092	C	N3-C2-O2	-5.71	117.90	121.90
36	1	2980	U	N3-C2-O2	-5.71	118.20	122.20
1	6	687	G	N3-C2-N2	-5.71	115.90	119.90
36	5	407	A	N3-C4-N9	5.71	131.97	127.40
36	5	3093	C	C5-C6-N1	-5.71	118.14	121.00
36	1	1294	A	N9-C4-C5	5.71	108.08	105.80
36	1	3201	C	N3-C4-C5	-5.71	119.62	121.90
1	6	1141	G	C8-N9-C4	5.71	108.68	106.40
36	5	1866	C	O4'-C1'-N1	-5.71	103.63	108.20
36	1	1172	G	N9-C4-C5	-5.71	103.12	105.40
36	1	2884	C	C6-N1-C2	5.71	122.58	120.30
36	5	909	G	C5-C6-O6	5.71	132.02	128.60
36	5	1604	G	C4-N9-C1'	5.71	133.92	126.50
36	5	1884	A	C2-N3-C4	-5.71	107.75	110.60
36	5	2637	A	N9-C4-C5	-5.71	103.52	105.80
36	1	3244	A	C8-N9-C4	5.71	108.08	105.80
36	1	974	G	N3-C4-N9	5.70	129.42	126.00
36	1	1195	A	O5'-P-OP2	5.70	117.54	110.70
36	1	2624	G	N7-C8-N9	5.70	115.95	113.10
1	6	416	A	C6-C5-N7	-5.70	128.31	132.30
36	5	2174	G	N1-C6-O6	5.70	123.32	119.90
36	5	2191	U	N3-C4-C5	5.70	118.02	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2985	C	N3-C4-C5	-5.70	119.62	121.90
36	1	828	A	N1-C6-N6	5.70	122.02	118.60
37	3	88	G	N3-C2-N2	5.70	123.89	119.90
68	O2	19	ARG	NE-CZ-NH2	5.70	123.15	120.30
36	5	393	U	O5'-P-OP1	-5.70	100.57	105.70
36	5	2729	U	N3-C2-O2	-5.70	118.21	122.20
36	1	1002	A	O5'-P-OP1	5.70	117.54	110.70
36	1	3090	U	C5-C4-O4	-5.70	122.48	125.90
36	1	422	A	C6-C5-N7	5.70	136.29	132.30
36	1	2398	A	C5-N7-C8	5.70	106.75	103.90
36	5	648	C	OP1-P-OP2	5.70	128.15	119.60
36	5	833	G	C5-C6-O6	-5.70	125.18	128.60
1	2	969	C	C5-C4-N4	-5.70	116.21	120.20
36	1	734	C	C2-N1-C1'	5.70	125.07	118.80
36	1	1129	A	N1-C6-N6	5.70	122.02	118.60
36	1	1189	C	C2-N3-C4	-5.70	117.05	119.90
36	5	2754	G	N3-C4-C5	-5.70	125.75	128.60
1	2	73	U	OP1-P-O3'	5.69	117.73	105.20
1	2	736	C	C2-N1-C1'	5.69	125.06	118.80
36	1	1344	G	C8-N9-C4	5.69	108.68	106.40
36	1	1419	A	C5'-C4'-O4'	5.69	115.93	109.10
36	1	1926	C	N3-C4-C5	5.69	124.18	121.90
36	1	2682	C	O5'-P-OP2	-5.69	100.58	105.70
36	5	53	G	O5'-P-OP2	-5.69	100.58	105.70
1	6	337	G	N1-C6-O6	5.69	123.31	119.90
36	5	2904	U	C2-N3-C4	-5.69	123.59	127.00
36	5	3096	C	N1-C2-O2	-5.69	115.49	118.90
1	2	728	U	N1-C2-O2	5.69	126.78	122.80
1	2	1096	C	C2-N1-C1'	5.69	125.06	118.80
36	1	1189	C	C5-C6-N1	-5.69	118.16	121.00
36	1	1802	C	C5-C6-N1	5.69	123.84	121.00
36	1	2385	G	N3-C4-N9	-5.69	122.59	126.00
36	5	869	G	C6-N1-C2	-5.69	121.69	125.10
36	5	1096	U	N1-C2-O2	-5.69	118.82	122.80
49	m3	85	LEU	CA-CB-CG	5.69	128.38	115.30
1	2	794	U	P-O3'-C3'	5.69	126.53	119.70
1	2	1363	U	C2-N1-C1'	5.69	124.53	117.70
36	1	1168	U	OP1-P-OP2	-5.69	111.07	119.60
36	1	1923	C	N3-C4-C5	5.69	124.17	121.90
1	6	297	U	N3-C4-O4	5.69	123.38	119.40
36	1	955	U	N1-C2-O2	-5.69	118.82	122.80
36	1	2800	G	C5-C6-O6	-5.69	125.19	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	610	G	C4-N9-C1'	5.69	133.89	126.50
36	5	922	U	N1-C2-N3	5.68	118.31	114.90
36	5	1304	A	C5-C6-N6	-5.68	119.15	123.70
36	1	308	A	OP2-P-O3'	5.68	117.70	105.20
36	1	829	U	N3-C2-O2	-5.68	118.22	122.20
36	1	2661	G	C4-C5-N7	5.68	113.07	110.80
36	5	1192	C	N3-C4-N4	5.68	121.98	118.00
41	l4	194	TYR	CA-CB-CG	5.68	124.20	113.40
36	1	1153	A	C4-C5-C6	5.68	119.84	117.00
38	4	16	G	O4'-C1'-N9	5.68	112.75	108.20
1	6	1333	C	N3-C4-C5	5.68	124.17	121.90
36	1	334	A	C8-N9-C4	-5.68	103.53	105.80
36	1	2631	U	OP1-P-O3'	5.68	117.69	105.20
36	5	86	G	N3-C2-N2	5.68	123.87	119.90
36	5	278	U	N1-C2-O2	-5.68	118.83	122.80
36	1	2323	G	N3-C4-N9	5.68	129.41	126.00
1	2	1324	G	N3-C4-N9	-5.67	122.59	126.00
36	1	1837	U	N3-C2-O2	5.67	126.17	122.20
37	3	81	U	C5-C6-N1	-5.67	119.86	122.70
1	6	39	A	O4'-C1'-N9	5.67	112.74	108.20
36	5	1390	A	C5-C6-N6	5.67	128.24	123.70
36	1	2623	G	N1-C2-N2	-5.67	111.09	116.20
37	3	86	U	N3-C4-C5	5.67	118.00	114.60
1	6	29	U	C5-C4-O4	5.67	129.30	125.90
36	1	945	C	N3-C4-C5	5.67	124.17	121.90
36	1	1657	C	N3-C2-O2	5.67	125.87	121.90
36	5	3362	A	C6-C5-N7	-5.67	128.33	132.30
36	1	655	C	N1-C2-N3	5.67	123.17	119.20
70	O4	58	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	6	1749	A	C2-N3-C4	-5.67	107.77	110.60
36	1	2836	C	N1-C2-N3	5.67	123.17	119.20
36	5	428	A	OP2-P-O3'	5.67	117.67	105.20
36	5	2382	G	C4-C5-N7	-5.67	108.53	110.80
36	1	2640	A	N1-C6-N6	-5.67	115.20	118.60
36	1	2824	G	N3-C4-N9	-5.67	122.60	126.00
1	6	869	A	O5'-P-OP1	-5.67	100.60	105.70
36	5	1192	C	C4-C5-C6	5.67	120.23	117.40
36	1	1589	A	C5-C6-N6	-5.67	119.17	123.70
1	6	1736	G	N3-C2-N2	-5.67	115.93	119.90
36	5	1847	A	N3-C4-N9	-5.67	122.87	127.40
36	5	2361	A	C4-C5-C6	5.67	119.83	117.00
36	1	803	C	O5'-P-OP1	5.66	117.50	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	631	U	C4-C5-C6	-5.66	116.30	119.70
1	2	1389	C	N1-C2-O2	5.66	122.30	118.90
36	1	1468	A	N1-C2-N3	5.66	132.13	129.30
36	1	1685	C	N1-C2-O2	5.66	122.30	118.90
36	1	2945	G	N1-C6-O6	5.66	123.30	119.90
36	5	283	G	N7-C8-N9	5.66	115.93	113.10
36	5	3105	U	N1-C2-O2	-5.66	118.84	122.80
48	m1	30	LEU	CA-CB-CG	5.66	128.32	115.30
1	2	720	G	P-O3'-C3'	5.66	126.49	119.70
1	6	1535	U	O5'-P-OP1	5.66	117.49	110.70
36	5	2389	C	C6-N1-C2	5.66	122.56	120.30
1	2	1780	G	N1-C6-O6	5.66	123.30	119.90
36	1	2627	C	C6-N1-C2	5.66	122.56	120.30
1	6	1117	U	C6-N1-C2	-5.66	117.61	121.00
1	6	1796	C	C5-C6-N1	-5.66	118.17	121.00
36	5	2601	A	C5-C6-N6	5.66	128.23	123.70
37	3	95	A	C6-C5-N7	-5.66	128.34	132.30
36	5	1419	A	O5'-P-OP1	5.66	117.49	110.70
36	1	651	G	OP2-P-O3'	5.66	117.64	105.20
36	1	964	G	OP2-P-O3'	5.66	117.64	105.20
1	6	1145	U	N3-C4-O4	5.66	123.36	119.40
36	5	57	A	N7-C8-N9	-5.66	110.97	113.80
36	1	1174	G	C4-N9-C1'	5.65	133.85	126.50
36	1	2304	C	N3-C2-O2	-5.65	117.94	121.90
36	1	1136	A	C8-N9-C4	-5.65	103.54	105.80
1	2	794	U	N1-C2-O2	5.65	126.75	122.80
36	1	3090	U	N1-C2-O2	-5.65	118.84	122.80
36	5	1375	G	N1-C2-N3	-5.65	120.51	123.90
36	5	2608	G	OP1-P-OP2	-5.65	111.12	119.60
36	1	2730	G	N3-C4-N9	-5.65	122.61	126.00
36	1	3201	C	C6-N1-C2	-5.65	118.04	120.30
36	5	936	A	N9-C4-C5	5.65	108.06	105.80
37	7	26	C	OP1-P-O3'	5.65	117.63	105.20
36	1	1310	G	N1-C2-N3	5.65	127.29	123.90
36	1	1374	G	OP2-P-O3'	5.65	117.62	105.20
1	6	1026	A	O5'-P-OP1	-5.65	100.62	105.70
1	2	435	C	C5-C4-N4	5.64	124.15	120.20
1	2	1241	G	C4-N9-C1'	5.64	133.84	126.50
1	2	1596	C	N3-C2-O2	-5.64	117.95	121.90
36	5	326	U	N1-C2-O2	-5.64	118.85	122.80
36	5	1881	A	N1-C6-N6	5.64	121.99	118.60
36	5	2767	U	O5'-P-OP2	-5.64	100.62	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	720	G	OP1-P-O3'	5.64	117.61	105.20
36	1	1156	C	N3-C4-C5	5.64	124.16	121.90
36	1	3326	G	C8-N9-C4	5.64	108.66	106.40
36	5	349	A	OP2-P-O3'	5.64	117.61	105.20
36	5	1937	U	C5-C6-N1	-5.64	119.88	122.70
36	5	2928	C	N3-C2-O2	-5.64	117.95	121.90
36	5	3004	C	C5-C4-N4	-5.64	116.25	120.20
36	5	3214	U	C5-C6-N1	-5.64	119.88	122.70
38	8	39	G	N3-C4-C5	-5.64	125.78	128.60
1	2	734	A	P-O3'-C3'	5.64	126.47	119.70
36	1	1909	A	C8-N9-C4	5.64	108.06	105.80
36	1	2190	U	C5-C4-O4	-5.64	122.52	125.90
1	6	352	A	OP2-P-O3'	5.64	117.61	105.20
36	5	1049	C	N3-C4-C5	5.64	124.16	121.90
36	1	776	U	C2-N3-C4	-5.64	123.62	127.00
36	1	1129	A	C5-C6-N6	-5.64	119.19	123.70
36	1	1926	C	N1-C2-O2	-5.64	115.52	118.90
36	1	2238	G	C5-C6-O6	-5.64	125.22	128.60
36	1	1148	G	C5-C6-O6	-5.63	125.22	128.60
1	6	401	A	O5'-P-OP2	-5.63	100.63	105.70
36	5	925	A	N9-C4-C5	-5.63	103.55	105.80
36	5	2121	G	C5-C6-O6	-5.63	125.22	128.60
36	1	1168	U	C5-C4-O4	5.63	129.28	125.90
36	5	50	U	O5'-P-OP1	-5.63	100.63	105.70
36	5	1461	A	N7-C8-N9	-5.63	110.98	113.80
36	5	2704	A	OP1-P-OP2	5.63	128.05	119.60
36	5	1592	G	C5-C6-N1	-5.63	108.68	111.50
36	5	2632	G	N1-C6-O6	-5.63	116.52	119.90
1	2	1761	U	C5-C4-O4	5.63	129.28	125.90
1	2	380	U	N3-C2-O2	-5.63	118.26	122.20
40	L3	17	LEU	CA-CB-CG	5.63	128.25	115.30
36	5	348	A	O5'-P-OP1	-5.63	100.64	105.70
36	5	658	G	N1-C6-O6	5.63	123.28	119.90
1	2	992	A	N3-C4-C5	5.63	130.74	126.80
36	1	86	G	O5'-P-OP1	5.63	117.45	110.70
36	5	506	U	C5-C6-N1	-5.63	119.89	122.70
36	5	2353	G	N1-C6-O6	5.63	123.28	119.90
36	5	2996	U	N1-C2-O2	5.63	126.74	122.80
36	5	776	U	C5-C4-O4	5.62	129.28	125.90
36	5	1297	C	O5'-P-OP1	-5.62	100.64	105.70
36	1	1837	U	N1-C2-O2	-5.62	118.86	122.80
54	M8	170	ARG	NE-CZ-NH1	-5.62	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	459	G	C6-C5-N7	-5.62	127.03	130.40
36	5	2810	C	O5'-P-OP2	-5.62	100.64	105.70
1	6	971	A	OP1-P-OP2	-5.62	111.17	119.60
36	5	2165	G	C5-C6-O6	-5.62	125.23	128.60
36	1	372	A	O5'-P-OP2	-5.62	100.64	105.70
36	1	979	U	C5-C4-O4	5.62	129.27	125.90
64	N8	57	GLY	N-CA-C	5.62	127.15	113.10
1	6	1748	G	C8-N9-C4	5.62	108.65	106.40
36	5	2687	G	O5'-P-OP2	-5.62	100.64	105.70
36	5	2915	U	C2-N3-C4	-5.62	123.63	127.00
36	5	3271	G	O5'-P-OP2	-5.62	100.64	105.70
36	1	651	G	C4-N9-C1'	5.62	133.80	126.50
36	1	1349	G	N3-C4-C5	-5.62	125.79	128.60
36	1	3344	A	C4-C5-N7	5.62	113.51	110.70
36	1	283	G	C5-C6-O6	-5.62	125.23	128.60
36	1	3217	C	N3-C2-O2	-5.62	117.97	121.90
38	4	40	A	N3-C4-N9	5.61	131.89	127.40
1	6	365	G	N3-C4-N9	5.61	129.37	126.00
36	5	1307	G	OP2-P-O3'	5.61	117.55	105.20
37	7	11	A	C6-C5-N7	-5.61	128.37	132.30
1	2	1650	U	C6-N1-C2	5.61	124.37	121.00
36	1	641	C	N3-C4-C5	5.61	124.14	121.90
36	1	1795	U	N1-C2-O2	-5.61	118.87	122.80
36	5	964	G	C8-N9-C4	-5.61	104.16	106.40
36	5	1127	G	C5-C6-O6	-5.61	125.23	128.60
36	5	2621	G	N3-C2-N2	-5.61	115.97	119.90
36	5	2948	C	O5'-P-OP1	5.61	117.43	110.70
1	2	110	U	C6-N1-C2	-5.61	117.64	121.00
1	2	1082	C	N3-C2-O2	-5.61	117.97	121.90
36	1	1741	A	C2-N3-C4	-5.61	107.80	110.60
36	1	2860	U	N3-C4-O4	5.61	123.33	119.40
70	O4	8	ARG	NE-CZ-NH2	-5.61	117.50	120.30
36	5	974	G	C8-N9-C4	-5.61	104.16	106.40
1	2	1652	C	C6-N1-C2	-5.61	118.06	120.30
1	2	1657	U	N3-C4-O4	5.61	123.32	119.40
36	1	2938	G	OP1-P-OP2	5.61	128.01	119.60
1	6	65	A	N1-C6-N6	5.61	121.96	118.60
36	5	1406	A	C4-C5-N7	5.61	113.50	110.70
37	3	72	A	C8-N9-C4	-5.60	103.56	105.80
38	8	54	A	C2-N3-C4	-5.60	107.80	110.60
38	4	69	U	C6-N1-C2	5.60	124.36	121.00
36	5	1592	G	N7-C8-N9	5.60	115.90	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1496	C	C6-N1-C2	-5.60	118.06	120.30
36	5	1841	A	N1-C6-N6	5.60	121.96	118.60
36	1	412	G	O5'-P-OP2	-5.60	100.66	105.70
36	1	1098	A	C8-N9-C4	-5.60	103.56	105.80
36	1	2404	A	C4-C5-N7	5.60	113.50	110.70
1	6	1	U	C6-N1-C1'	-5.60	113.36	121.20
36	5	1096	U	N3-C2-O2	5.60	126.12	122.20
36	5	1449	A	C4-C5-C6	5.60	119.80	117.00
36	1	427	C	N1-C2-O2	-5.60	115.54	118.90
36	1	876	A	C4-C5-N7	5.60	113.50	110.70
36	1	921	A	O4'-C1'-N9	-5.60	103.72	108.20
36	1	2315	G	N1-C6-O6	-5.60	116.54	119.90
36	1	3055	U	C6-N1-C1'	-5.60	113.36	121.20
36	5	712	G	O5'-P-OP2	-5.60	100.66	105.70
36	5	2360	C	OP1-P-OP2	-5.60	111.20	119.60
36	1	1391	C	N3-C4-C5	-5.59	119.66	121.90
36	1	2378	C	C6-N1-C2	5.59	122.54	120.30
36	1	2973	G	N1-C6-O6	5.59	123.26	119.90
1	6	1292	G	N1-C6-O6	5.59	123.26	119.90
36	5	219	A	N1-C6-N6	5.59	121.96	118.60
36	5	230	U	N1-C2-N3	5.59	118.26	114.90
36	1	3344	A	C2-N3-C4	-5.59	107.80	110.60
36	5	1846	C	C2-N3-C4	-5.59	117.10	119.90
36	1	227	G	C5-C6-O6	-5.59	125.25	128.60
36	1	1472	U	C6-N1-C2	5.59	124.36	121.00
36	1	2412	G	OP1-P-O3'	5.59	117.50	105.20
36	5	2385	G	N3-C4-C5	5.59	131.40	128.60
36	5	2841	G	OP1-P-OP2	5.59	127.99	119.60
36	5	2917	G	C5-C6-O6	-5.59	125.25	128.60
36	1	2399	A	OP1-P-OP2	-5.59	111.22	119.60
36	1	2640	A	C5-C6-N1	5.59	120.50	117.70
36	1	2688	U	N1-C2-N3	-5.59	111.55	114.90
36	1	3266	G	N9-C4-C5	5.59	107.64	105.40
36	5	1115	G	P-O3'-C3'	5.59	126.41	119.70
36	1	1353	U	N3-C2-O2	-5.59	118.29	122.20
49	m3	46	ILE	CG1-CB-CG2	-5.59	99.11	111.40
36	1	2804	A	OP2-P-O3'	5.59	117.49	105.20
36	1	3209	A	N9-C4-C5	-5.59	103.56	105.80
36	5	1075	A	C8-N9-C4	5.59	108.03	105.80
36	5	1126	G	C5-C6-N1	-5.59	108.71	111.50
36	5	1340	G	C8-N9-C4	5.59	108.64	106.40
36	5	1722	U	N3-C2-O2	5.59	126.11	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2395	G	C5-C6-O6	-5.59	125.25	128.60
36	1	942	U	C5-C4-O4	-5.58	122.55	125.90
36	1	1300	G	C6-C5-N7	-5.58	127.05	130.40
36	1	1838	G	OP1-P-O3'	5.58	117.48	105.20
36	1	2874	G	C5-C6-O6	5.58	131.95	128.60
1	6	443	C	C6-N1-C2	5.58	122.53	120.30
12	c0	88	PRO	N-CA-CB	5.58	110.00	103.30
36	5	423	A	OP2-P-O3'	5.58	117.48	105.20
36	5	654	C	O5'-P-OP1	-5.58	100.67	105.70
36	5	2111	G	C8-N9-C4	5.58	108.63	106.40
36	1	2651	G	N7-C8-N9	-5.58	110.31	113.10
38	4	25	G	C5-N7-C8	5.58	107.09	104.30
1	6	1269	U	N3-C2-O2	-5.58	118.29	122.20
36	5	47	C	C6-N1-C2	5.58	122.53	120.30
36	5	767	U	O4'-C1'-N1	5.58	112.67	108.20
36	5	950	G	C4-C5-N7	5.58	113.03	110.80
36	1	2138	A	N9-C4-C5	5.58	108.03	105.80
41	L4	84	ARG	NE-CZ-NH1	-5.58	117.51	120.30
36	5	2416	U	OP1-P-OP2	-5.58	111.23	119.60
36	1	363	G	C5-C6-O6	-5.58	125.25	128.60
36	1	369	A	O5'-P-OP1	5.58	117.39	110.70
36	1	1183	C	C6-N1-C2	5.58	122.53	120.30
36	1	2754	G	C8-N9-C4	5.58	108.63	106.40
36	5	1509	A	N9-C4-C5	-5.58	103.57	105.80
36	5	2866	U	N3-C2-O2	-5.58	118.30	122.20
36	5	3052	G	N3-C4-N9	-5.58	122.65	126.00
36	1	2624	G	N1-C6-O6	5.58	123.25	119.90
36	5	437	G	N9-C4-C5	5.58	107.63	105.40
36	5	2836	C	C2-N3-C4	-5.58	117.11	119.90
36	5	2984	C	C6-N1-C2	-5.58	118.07	120.30
36	1	641	C	N1-C2-O2	-5.58	115.56	118.90
36	5	3298	C	O5'-P-OP2	-5.58	100.68	105.70
1	2	1175	U	OP1-P-O3'	5.57	117.46	105.20
36	1	63	A	N9-C4-C5	5.57	108.03	105.80
36	1	1893	A	N1-C2-N3	5.57	132.09	129.30
36	1	2688	U	C6-N1-C1'	-5.57	113.40	121.20
36	5	1380	G	N9-C4-C5	-5.57	103.17	105.40
36	5	2372	A	O5'-P-OP2	5.57	117.39	110.70
36	5	2402	A	C5-C6-N6	5.57	128.16	123.70
36	1	349	A	OP2-P-O3'	5.57	117.46	105.20
36	1	776	U	N1-C2-O2	-5.57	118.90	122.80
36	5	2142	A	C2-N3-C4	5.57	113.39	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2661	G	OP1-P-O3'	5.57	117.46	105.20
36	5	2848	G	C4-N9-C1'	5.57	133.74	126.50
36	1	1130	A	N1-C2-N3	-5.57	126.51	129.30
36	1	1417	G	N3-C4-N9	-5.57	122.66	126.00
36	5	1204	A	N1-C6-N6	-5.57	115.26	118.60
36	5	2139	A	C5-C6-N6	5.57	128.16	123.70
36	5	3141	A	O5'-P-OP1	-5.57	100.69	105.70
36	1	2293	C	C5-C4-N4	-5.57	116.30	120.20
1	2	17	C	C6-N1-C2	-5.57	118.07	120.30
36	1	2714	G	C4-C5-C6	-5.57	115.46	118.80
36	1	2802	A	N9-C4-C5	5.57	108.03	105.80
1	6	100	A	C5-C6-N1	-5.57	114.92	117.70
1	6	454	U	O5'-P-OP2	-5.57	100.69	105.70
36	5	887	G	N3-C2-N2	5.57	123.80	119.90
36	5	3041	U	N1-C2-N3	-5.57	111.56	114.90
36	5	3315	G	N9-C4-C5	5.57	107.63	105.40
36	1	344	A	C4-C5-C6	-5.57	114.22	117.00
36	1	3361	G	C4-N9-C1'	5.57	133.74	126.50
36	5	215	G	N7-C8-N9	5.57	115.88	113.10
36	5	501	A	O5'-P-OP2	-5.57	100.69	105.70
36	5	717	C	OP2-P-O3'	5.57	117.44	105.20
37	7	48	U	N1-C2-O2	-5.57	118.90	122.80
37	7	105	C	C6-N1-C2	-5.57	118.07	120.30
36	1	1304	A	OP1-P-OP2	5.56	127.95	119.60
36	5	1371	G	C5-N7-C8	5.56	107.08	104.30
36	5	961	C	C2-N1-C1'	5.56	124.92	118.80
36	5	2299	A	O5'-P-OP2	-5.56	100.69	105.70
36	5	2960	C	N3-C4-N4	-5.56	114.11	118.00
37	3	85	G	OP2-P-O3'	5.56	117.44	105.20
1	6	1584	G	O5'-P-OP1	-5.56	100.69	105.70
36	5	3181	C	C6-N1-C2	-5.56	118.08	120.30
36	1	2396	G	N9-C4-C5	5.56	107.62	105.40
39	L2	191	LEU	CA-CB-CG	-5.56	102.51	115.30
1	6	610	G	N3-C4-N9	5.56	129.34	126.00
1	6	623	A	N1-C6-N6	5.56	121.94	118.60
36	5	617	G	C4-C5-N7	5.56	113.02	110.80
36	1	1377	G	C5-C6-O6	-5.56	125.27	128.60
36	1	1445	U	N3-C2-O2	5.56	126.09	122.20
41	L4	182	LEU	CA-CB-CG	5.56	128.08	115.30
36	5	1487	G	C4-C5-N7	-5.56	108.58	110.80
38	4	28	C	N1-C2-O2	5.56	122.23	118.90
36	5	2864	A	OP2-P-O3'	5.56	117.42	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	226	C	N3-C4-C5	-5.55	119.68	121.90
36	1	1137	C	N3-C4-N4	5.55	121.89	118.00
36	1	1712	G	N1-C6-O6	5.55	123.23	119.90
36	5	1604	G	C8-N9-C1'	-5.55	119.78	127.00
36	5	622	A	N9-C4-C5	-5.55	103.58	105.80
36	5	2623	G	N9-C4-C5	-5.55	103.18	105.40
36	1	808	A	C8-N9-C4	5.55	108.02	105.80
36	1	1607	U	C5-C4-O4	5.55	129.23	125.90
36	1	2345	A	N9-C4-C5	-5.55	103.58	105.80
1	6	630	A	N9-C4-C5	-5.55	103.58	105.80
36	5	63	A	C5-C6-N6	-5.55	119.26	123.70
36	5	2360	C	N3-C4-C5	-5.55	119.68	121.90
36	1	805	G	C5-N7-C8	5.55	107.07	104.30
1	6	996	U	C2-N1-C1'	5.55	124.36	117.70
36	5	102	C	N3-C4-N4	5.55	121.88	118.00
36	5	1127	G	N3-C4-N9	5.55	129.33	126.00
36	5	1449	A	N1-C2-N3	5.55	132.07	129.30
36	5	2840	C	O5'-P-OP1	-5.55	100.70	105.70
36	5	407	A	C6-C5-N7	-5.55	128.42	132.30
36	5	2300	G	C5-C6-N1	5.55	114.27	111.50
36	5	2704	A	C8-N9-C4	5.55	108.02	105.80
36	1	2238	G	C4-C5-N7	5.55	113.02	110.80
1	6	1039	A	O4'-C1'-N9	5.55	112.64	108.20
36	5	2622	C	C4-C5-C6	5.55	120.17	117.40
36	1	1480	G	N1-C6-O6	5.54	123.23	119.90
36	1	1547	G	C6-C5-N7	5.54	133.73	130.40
36	1	2550	U	C5-C4-O4	5.54	129.23	125.90
36	5	1554	U	OP1-P-O3'	5.54	117.40	105.20
36	5	2382	G	N1-C6-O6	-5.54	116.57	119.90
36	1	671	U	N3-C4-O4	5.54	123.28	119.40
36	1	1313	G	C5-C6-O6	-5.54	125.27	128.60
36	5	639	G	N1-C6-O6	5.54	123.23	119.90
36	5	3200	G	N3-C2-N2	-5.54	116.02	119.90
1	2	966	A	N1-C6-N6	5.54	121.92	118.60
36	1	672	A	C6-C5-N7	-5.54	128.42	132.30
36	1	2984	C	C6-N1-C2	-5.54	118.08	120.30
36	5	1101	G	N9-C4-C5	-5.54	103.18	105.40
36	5	1152	G	N7-C8-N9	5.54	115.87	113.10
36	5	201	A	OP1-P-OP2	-5.54	111.29	119.60
36	5	2175	U	C2-N3-C4	-5.54	123.68	127.00
36	1	92	G	C5-C6-N1	5.54	114.27	111.50
36	1	3092	C	C6-N1-C2	5.54	122.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	389	A	N9-C4-C5	5.54	108.02	105.80
36	5	884	A	C2-N3-C4	-5.54	107.83	110.60
36	1	1661	G	C8-N9-C1'	-5.54	119.80	127.00
36	5	423	A	C8-N9-C4	5.54	108.02	105.80
36	5	2117	A	C4-C5-N7	-5.54	107.93	110.70
36	1	325	A	C2-N3-C4	5.54	113.37	110.60
36	1	1050	U	N1-C2-O2	5.54	126.67	122.80
36	1	2859	U	N1-C2-N3	5.54	118.22	114.90
1	6	350	U	N1-C2-N3	5.54	118.22	114.90
36	5	622	A	C5-C6-N6	-5.54	119.27	123.70
36	5	861	C	C5-C4-N4	-5.54	116.33	120.20
36	5	964	G	N7-C8-N9	5.54	115.87	113.10
36	1	2354	C	C4-C5-C6	5.53	120.17	117.40
36	5	1014	U	C2-N1-C1'	5.53	124.34	117.70
36	5	1373	A	OP2-P-O3'	5.53	117.37	105.20
36	5	3188	G	N3-C4-C5	-5.53	125.83	128.60
36	1	200	C	C5-C4-N4	-5.53	116.33	120.20
36	1	960	U	C2-N1-C1'	-5.53	111.06	117.70
36	1	1926	C	N3-C2-O2	5.53	125.77	121.90
38	4	103	G	N1-C6-O6	-5.53	116.58	119.90
37	7	8	G	N3-C2-N2	5.53	123.77	119.90
36	1	350	C	C2-N1-C1'	5.53	124.88	118.80
36	1	920	A	C2-N3-C4	-5.53	107.83	110.60
9	s7	118	LEU	CA-CB-CG	5.53	128.02	115.30
36	5	864	G	N1-C6-O6	5.53	123.22	119.90
38	8	96	A	C8-N9-C4	5.53	108.01	105.80
41	L4	313	LEU	CA-CB-CG	5.53	128.02	115.30
1	6	536	C	C2-N1-C1'	5.53	124.88	118.80
36	1	895	A	N3-C4-C5	5.53	130.67	126.80
36	1	2772	C	O4'-C1'-N1	5.53	112.62	108.20
36	5	1376	C	OP1-P-OP2	5.53	127.89	119.60
36	5	2836	C	O4'-C1'-N1	5.53	112.62	108.20
77	q1	9	ARG	NE-CZ-NH2	-5.53	117.54	120.30
36	1	1340	G	N3-C4-N9	5.53	129.31	126.00
1	6	558	U	N3-C2-O2	-5.53	118.33	122.20
36	5	41	G	N1-C6-O6	5.53	123.22	119.90
36	5	1846	C	N1-C2-O2	-5.53	115.58	118.90
36	5	3049	A	N1-C6-N6	5.53	121.92	118.60
1	2	458	G	C5-C6-N1	-5.52	108.74	111.50
1	2	1514	U	O5'-P-OP1	-5.52	100.73	105.70
1	6	536	C	C6-N1-C2	-5.52	118.09	120.30
1	2	1761	U	N3-C2-O2	-5.52	118.33	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1796	G	C8-N9-C4	-5.52	104.19	106.40
36	1	2700	G	C6-C5-N7	-5.52	127.09	130.40
36	5	907	G	N3-C2-N2	5.52	123.77	119.90
36	5	2281	A	O4'-C1'-N9	5.52	112.62	108.20
36	5	2572	C	C6-N1-C2	-5.52	118.09	120.30
36	1	907	G	N3-C4-N9	5.52	129.31	126.00
36	1	2622	C	C5-C6-N1	5.52	123.76	121.00
1	6	1746	A	O5'-P-OP1	-5.52	100.73	105.70
36	1	284	A	C8-N9-C4	-5.52	103.59	105.80
36	1	1842	A	OP1-P-O3'	5.52	117.34	105.20
36	5	1929	G	C2-N3-C4	-5.52	109.14	111.90
36	1	1115	G	OP1-P-O3'	5.52	117.34	105.20
36	1	1116	G	C4-C5-C6	5.52	122.11	118.80
36	1	2408	U	O5'-P-OP1	-5.52	100.73	105.70
38	4	32	C	C6-N1-C1'	5.52	127.42	120.80
1	6	1697	G	N3-C4-N9	5.52	129.31	126.00
36	5	948	C	C6-N1-C2	5.52	122.51	120.30
1	2	734	A	OP1-P-O3'	5.52	117.33	105.20
36	5	1751	G	C8-N9-C4	5.52	108.61	106.40
36	1	635	G	C5-C6-O6	-5.51	125.29	128.60
36	1	1402	C	C2-N3-C4	-5.51	117.14	119.90
36	1	2631	U	C5-C6-N1	-5.51	119.94	122.70
36	1	2850	G	N3-C4-N9	5.51	129.31	126.00
36	1	2852	C	C6-N1-C2	5.51	122.51	120.30
1	6	678	A	P-O3'-C3'	5.51	126.32	119.70
36	5	2124	G	C6-C5-N7	-5.51	127.09	130.40
36	5	2158	A	C5-C6-N1	5.51	120.46	117.70
36	5	2855	U	N3-C4-C5	5.51	117.91	114.60
36	5	661	G	C4-C5-N7	5.51	113.00	110.80
36	1	2599	U	C5-C6-N1	5.51	125.46	122.70
36	5	2285	C	C6-N1-C2	-5.51	118.09	120.30
1	2	704	C	C2-N1-C1'	5.51	124.86	118.80
36	1	197	G	N1-C6-O6	5.51	123.21	119.90
36	1	1206	G	O5'-P-OP2	-5.51	100.74	105.70
36	1	2661	G	N1-C6-O6	5.51	123.21	119.90
1	6	1058	U	OP1-P-O3'	5.51	117.32	105.20
1	6	1481	C	C6-N1-C2	-5.51	118.10	120.30
1	6	1774	G	C5-C6-O6	5.51	131.91	128.60
36	5	2141	U	OP2-P-O3'	5.51	117.32	105.20
36	5	2859	U	N1-C2-O2	-5.51	118.94	122.80
1	2	1600	A	C5-C6-N1	-5.51	114.95	117.70
36	1	609	G	C2-N3-C4	5.51	114.65	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	403	G	C2-N3-C4	-5.51	109.15	111.90
1	6	1280	C	N3-C4-C5	-5.51	119.70	121.90
36	5	300	G	O5'-P-OP1	-5.50	100.75	105.70
36	5	933	A	N1-C2-N3	5.50	132.05	129.30
36	5	1151	U	C5-C6-N1	5.50	125.45	122.70
36	5	2636	A	O5'-P-OP2	5.50	117.31	110.70
1	2	985	G	C5-C6-O6	-5.50	125.30	128.60
36	1	2237	C	C6-N1-C2	5.50	122.50	120.30
1	6	308	C	N1-C2-N3	5.50	123.05	119.20
36	5	2601	A	OP2-P-O3'	5.50	117.31	105.20
36	5	3092	C	N1-C2-O2	5.50	122.20	118.90
36	1	407	A	C4-C5-N7	5.50	113.45	110.70
36	1	984	G	C5-C6-O6	5.50	131.90	128.60
36	5	2245	C	N3-C4-C5	-5.50	119.70	121.90
36	5	2978	U	C5-C6-N1	-5.50	119.95	122.70
37	7	44	C	N1-C2-O2	-5.50	115.60	118.90
36	1	2933	A	N1-C2-N3	-5.50	126.55	129.30
36	1	1157	G	OP2-P-O3'	5.50	117.30	105.20
36	1	1417	G	N3-C4-C5	5.50	131.35	128.60
36	1	2836	C	N3-C2-O2	-5.50	118.05	121.90
36	1	3057	U	N3-C4-O4	-5.50	115.55	119.40
36	5	159	A	C8-N9-C4	5.50	108.00	105.80
36	5	1392	G	N7-C8-N9	-5.50	110.35	113.10
36	5	1907	C	N3-C4-N4	5.50	121.85	118.00
36	1	668	G	C5-C6-O6	5.50	131.90	128.60
36	1	1379	G	OP2-P-O3'	5.50	117.29	105.20
36	5	2234	G	C4-C5-N7	5.50	113.00	110.80
36	5	2333	C	C2-N3-C4	-5.50	117.15	119.90
36	5	2914	G	C4-N9-C1'	5.50	133.65	126.50
36	1	1157	G	N1-C2-N3	5.50	127.20	123.90
36	1	3036	G	N3-C4-N9	5.50	129.30	126.00
1	6	1457	C	O4'-C1'-N1	5.50	112.60	108.20
36	5	2996	U	N1-C2-N3	-5.50	111.60	114.90
5	S3	202	LEU	CA-CB-CG	5.49	127.93	115.30
36	1	1148	G	N7-C8-N9	-5.49	110.35	113.10
38	4	22	U	C5-C6-N1	-5.49	119.95	122.70
36	1	2278	C	C5-C6-N1	5.49	123.75	121.00
36	1	2945	G	OP1-P-OP2	-5.49	111.36	119.60
1	2	992	A	N3-C4-N9	-5.49	123.01	127.40
36	5	625	G	C4-C5-N7	-5.49	108.60	110.80
1	2	402	C	O5'-P-OP2	5.49	117.29	110.70
36	1	61	A	N1-C6-N6	5.49	121.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	320	G	O5'-P-OP2	-5.49	100.76	105.70
36	1	2911	A	C8-N9-C4	5.49	108.00	105.80
1	6	434	G	O5'-P-OP2	-5.49	100.76	105.70
36	5	39	A	O5'-P-OP2	-5.49	100.76	105.70
36	5	214	G	C8-N9-C4	5.49	108.59	106.40
36	5	907	G	N1-C2-N2	-5.49	111.26	116.20
36	1	54	C	C6-N1-C2	5.49	122.50	120.30
1	6	337	G	N9-C4-C5	-5.49	103.20	105.40
42	L5	163	LEU	CA-CB-CG	5.49	127.92	115.30
25	d3	16	ARG	NE-CZ-NH2	-5.49	117.56	120.30
36	5	2949	U	C5-C6-N1	5.49	125.44	122.70
36	5	2984	C	N3-C2-O2	-5.49	118.06	121.90
36	5	3206	C	N1-C2-O2	5.49	122.19	118.90
36	5	1212	A	N1-C6-N6	5.48	121.89	118.60
1	2	577	G	C6-C5-N7	-5.48	127.11	130.40
36	1	2314	U	C5-C6-N1	5.48	125.44	122.70
36	5	192	C	C4-C5-C6	5.48	120.14	117.40
1	6	421	A	N9-C4-C5	-5.48	103.61	105.80
36	5	1314	C	C2-N1-C1'	5.48	124.83	118.80
1	2	73	U	P-O3'-C3'	5.48	126.28	119.70
36	1	979	U	C2-N1-C1'	5.48	124.28	117.70
36	1	2372	A	N3-C4-C5	-5.48	122.97	126.80
36	1	2381	G	N9-C4-C5	5.48	107.59	105.40
36	5	2993	G	C5-C6-O6	-5.48	125.31	128.60
37	7	93	C	O5'-P-OP2	-5.48	100.77	105.70
36	5	200	C	OP2-P-O3'	5.48	117.25	105.20
36	5	936	A	P-O3'-C3'	5.48	126.27	119.70
38	8	63	G	N1-C6-O6	-5.48	116.61	119.90
36	5	3309	G	N3-C4-C5	-5.47	125.86	128.60
38	4	40	A	C4-C5-N7	5.47	113.44	110.70
38	4	56	G	N1-C6-O6	-5.47	116.62	119.90
1	6	431	C	N3-C2-O2	-5.47	118.07	121.90
36	5	1882	G	O5'-P-OP2	5.47	117.27	110.70
36	5	1906	G	N1-C2-N2	-5.47	111.28	116.20
36	5	2930	A	O4'-C1'-N9	5.47	112.58	108.20
38	8	77	A	N1-C6-N6	5.47	121.88	118.60
1	6	400	A	N1-C6-N6	5.47	121.88	118.60
1	6	1058	U	P-O3'-C3'	5.47	126.27	119.70
38	8	22	U	O5'-P-OP1	-5.47	100.78	105.70
1	2	95	G	C4-C5-N7	-5.47	108.61	110.80
36	5	424	G	N1-C6-O6	5.47	123.18	119.90
36	5	2611	U	C4-C5-C6	5.47	122.98	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2613	U	N3-C4-C5	-5.47	111.32	114.60
1	2	435	C	N3-C4-N4	-5.47	114.17	118.00
36	1	1075	A	C8-N9-C4	5.47	107.99	105.80
36	1	2240	G	OP2-P-O3'	5.47	117.23	105.20
36	1	2424	A	O5'-P-OP2	-5.47	100.78	105.70
36	1	3034	C	N1-C2-O2	5.47	122.18	118.90
36	5	2383	C	C4-C5-C6	5.47	120.13	117.40
36	1	2616	C	O5'-P-OP1	-5.47	100.78	105.70
36	5	2212	C	OP2-P-O3'	5.47	117.23	105.20
38	8	37	A	N9-C4-C5	5.47	107.99	105.80
1	2	829	A	P-O3'-C3'	5.46	126.26	119.70
36	1	981	U	O5'-P-OP2	-5.46	100.78	105.70
36	5	3343	G	N3-C2-N2	5.46	123.72	119.90
56	N0	155	ARG	NE-CZ-NH2	5.46	123.03	120.30
36	5	590	G	O5'-P-OP1	-5.46	100.78	105.70
37	7	76	A	C8-N9-C4	5.46	107.98	105.80
1	2	139	C	P-O3'-C3'	5.46	126.25	119.70
1	2	1747	G	C5-C6-N1	-5.46	108.77	111.50
36	1	1168	U	N3-C4-O4	-5.46	115.58	119.40
36	1	1906	G	C6-C5-N7	-5.46	127.12	130.40
36	1	2278	C	O5'-P-OP1	-5.46	100.78	105.70
36	1	3017	A	N1-C6-N6	5.46	121.88	118.60
36	5	2390	A	OP2-P-O3'	5.46	117.22	105.20
36	5	2978	U	O4'-C1'-N1	5.46	112.57	108.20
36	1	2700	G	C8-N9-C4	-5.46	104.22	106.40
61	N5	34	LEU	CA-CB-CG	5.46	127.86	115.30
36	1	192	C	O5'-P-OP1	-5.46	100.79	105.70
36	1	374	A	P-O3'-C3'	5.46	126.25	119.70
36	1	1870	C	C6-N1-C2	5.46	122.48	120.30
36	1	2980	U	OP1-P-O3'	5.46	117.21	105.20
36	5	889	U	N3-C4-C5	5.46	117.88	114.60
36	1	924	G	O5'-P-OP1	-5.46	100.79	105.70
36	1	2165	G	C6-C5-N7	-5.46	127.13	130.40
36	1	2366	C	C2-N1-C1'	5.46	124.80	118.80
1	6	1192	C	N1-C2-O2	5.46	122.17	118.90
1	6	1361	U	C6-N1-C1'	-5.46	113.56	121.20
36	5	826	G	C4-C5-N7	5.46	112.98	110.80
36	5	931	C	N3-C4-N4	-5.46	114.18	118.00
36	5	960	U	C2-N1-C1'	5.46	124.25	117.70
36	5	2310	U	O5'-P-OP2	-5.46	100.79	105.70
36	5	2412	G	N3-C4-C5	-5.46	125.87	128.60
36	1	701	G	OP1-P-O3'	-5.46	93.20	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	N8	116	GLY	N-CA-C	5.46	126.74	113.10
1	6	62	A	N1-C6-N6	5.46	121.87	118.60
1	6	579	A	P-O3'-C3'	5.46	126.25	119.70
36	5	526	C	C5-C4-N4	-5.46	116.38	120.20
36	1	1492	G	N7-C8-N9	-5.45	110.37	113.10
36	1	2349	U	C2-N3-C4	-5.45	123.73	127.00
36	5	297	G	N1-C6-O6	-5.45	116.63	119.90
36	5	654	C	OP1-P-OP2	5.45	127.78	119.60
36	5	2147	A	C5-C6-N6	-5.45	119.34	123.70
36	5	2748	A	OP2-P-O3'	5.45	117.20	105.20
36	5	2991	A	OP2-P-O3'	5.45	117.20	105.20
38	8	7	U	N3-C2-O2	5.45	126.02	122.20
36	1	3133	C	C5-C6-N1	5.45	123.73	121.00
1	6	1634	C	N1-C2-O2	5.45	122.17	118.90
36	1	1414	G	C4-C5-N7	5.45	112.98	110.80
36	1	2209	U	C5-C6-N1	5.45	125.42	122.70
36	5	419	G	C8-N9-C1'	-5.45	119.92	127.00
36	5	2830	G	N3-C2-N2	-5.45	116.08	119.90
36	1	72	C	N1-C2-O2	-5.45	115.63	118.90
36	1	883	A	N1-C6-N6	-5.45	115.33	118.60
36	1	1152	G	O4'-C1'-N9	5.45	112.56	108.20
36	1	1373	A	OP2-P-O3'	5.45	117.19	105.20
36	1	1389	G	OP1-P-OP2	5.45	127.77	119.60
36	1	2601	A	N1-C2-N3	-5.45	126.58	129.30
54	M8	164	ARG	NE-CZ-NH1	5.45	123.02	120.30
36	5	961	C	N3-C2-O2	-5.45	118.09	121.90
36	5	2632	G	O5'-P-OP1	-5.45	100.80	105.70
36	5	3176	G	N3-C2-N2	-5.45	116.09	119.90
36	1	1406	A	N1-C6-N6	5.45	121.87	118.60
36	1	2859	U	N3-C4-C5	-5.45	111.33	114.60
37	3	84	A	N1-C6-N6	5.45	121.87	118.60
38	4	116	G	C8-N9-C4	5.45	108.58	106.40
36	5	2708	C	C5-C4-N4	-5.45	116.39	120.20
36	1	99	A	O4'-C1'-N9	5.44	112.56	108.20
36	1	1845	G	OP2-P-O3'	5.44	117.18	105.20
36	1	2305	G	C5-C6-O6	-5.44	125.33	128.60
36	5	1879	A	N7-C8-N9	5.44	116.52	113.80
36	1	950	G	C4-C5-N7	5.44	112.98	110.80
36	1	2192	C	C5-C6-N1	-5.44	118.28	121.00
36	1	2610	G	O4'-C1'-N9	5.44	112.55	108.20
36	5	632	G	OP2-P-O3'	5.44	117.17	105.20
36	5	1400	G	O5'-P-OP1	-5.44	100.80	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	282	G	P-O3'-C3'	5.44	126.23	119.70
36	1	1846	C	C6-N1-C2	-5.44	118.12	120.30
36	1	2802	A	OP2-P-O3'	5.44	117.17	105.20
1	6	1653	C	O5'-P-OP2	-5.44	100.81	105.70
36	5	2758	A	O4'-C1'-N9	5.44	112.55	108.20
1	2	1129	U	N3-C4-C5	5.44	117.86	114.60
36	1	2953	U	N3-C2-O2	5.43	126.00	122.20
36	5	631	U	N3-C4-O4	-5.43	115.60	119.40
36	5	2861	U	O5'-P-OP2	5.43	117.22	110.70
1	2	1196	A	OP1-P-O3'	5.43	117.15	105.20
36	1	2249	G	C3'-C2'-C1'	-5.43	97.15	101.50
36	1	3272	C	O5'-P-OP1	-5.43	100.81	105.70
1	6	801	G	N1-C6-O6	-5.43	116.64	119.90
36	5	424	G	O5'-P-OP2	-5.43	100.81	105.70
36	5	514	G	C6-C5-N7	-5.43	127.14	130.40
36	5	1884	A	C4-C5-N7	5.43	113.42	110.70
36	5	3174	A	O4'-C1'-N9	5.43	112.55	108.20
36	1	1116	G	C5'-C4'-O4'	5.43	115.62	109.10
36	1	1159	A	N1-C6-N6	-5.43	115.34	118.60
38	8	29	U	C2-N1-C1'	5.43	124.22	117.70
1	6	1297	G	O5'-P-OP2	-5.43	100.81	105.70
36	5	362	U	C5-C6-N1	5.43	125.42	122.70
36	5	439	C	C4-C5-C6	5.43	120.11	117.40
36	5	661	G	P-O3'-C3'	5.43	126.22	119.70
36	5	2728	G	C5-C6-N1	5.43	114.21	111.50
36	1	1329	U	N3-C2-O2	-5.43	118.40	122.20
36	1	2296	A	C2-N3-C4	-5.43	107.89	110.60
36	5	2333	C	OP2-P-O3'	5.43	117.14	105.20
1	2	934	C	C6-N1-C1'	-5.43	114.29	120.80
36	1	650	C	OP2-P-O3'	5.43	117.14	105.20
36	1	1421	G	C8-N9-C4	5.43	108.57	106.40
36	1	1795	U	N3-C2-O2	5.43	126.00	122.20
36	5	1128	U	C5-C6-N1	-5.43	119.99	122.70
36	5	3206	C	OP1-P-OP2	5.43	127.74	119.60
36	1	878	G	C5-C6-N1	-5.42	108.79	111.50
36	1	3198	U	N3-C2-O2	5.42	126.00	122.20
1	6	767	U	N1-C2-N3	5.42	118.15	114.90
36	5	866	A	C8-N9-C4	5.42	107.97	105.80
36	1	155	G	N3-C4-C5	-5.42	125.89	128.60
36	1	1340	G	N9-C4-C5	-5.42	103.23	105.40
36	1	1528	G	C8-N9-C4	-5.42	104.23	106.40
1	6	1607	G	C4-C5-N7	-5.42	108.63	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c9	57	ARG	NE-CZ-NH1	5.42	123.01	120.30
36	5	879	U	C2-N1-C1'	5.42	124.20	117.70
36	1	2249	G	N9-C1'-C2'	-5.42	106.04	112.00
36	1	2916	U	O5'-P-OP1	5.42	117.20	110.70
36	1	3269	U	N1-C2-N3	5.42	118.15	114.90
36	5	63	A	N9-C4-C5	-5.42	103.63	105.80
36	5	1830	G	OP1-P-O3'	5.42	117.12	105.20
36	5	2818	U	C4-C5-C6	-5.42	116.45	119.70
36	1	1126	G	N1-C6-O6	5.42	123.15	119.90
36	1	3314	A	C8-N9-C4	-5.42	103.63	105.80
38	4	38	U	N1-C2-N3	5.42	118.15	114.90
1	6	1547	A	N1-C6-N6	-5.42	115.35	118.60
4	s2	58	LEU	CA-CB-CG	5.42	127.76	115.30
36	1	2805	G	N3-C2-N2	5.42	123.69	119.90
36	1	918	C	N1-C2-O2	-5.41	115.65	118.90
1	6	323	A	C8-N9-C4	-5.41	103.64	105.80
36	1	2952	G	C5-C6-N1	-5.41	108.79	111.50
1	2	624	G	N1-C6-O6	-5.41	116.65	119.90
36	1	2114	C	OP1-P-OP2	5.41	127.72	119.60
36	1	2413	A	O5'-P-OP1	-5.41	100.83	105.70
36	1	2700	G	N7-C8-N9	5.41	115.81	113.10
36	1	2800	G	C6-N1-C2	-5.41	121.85	125.10
36	1	2846	U	N3-C4-O4	-5.41	115.61	119.40
36	1	2916	U	OP1-P-O3'	5.41	117.10	105.20
1	6	639	U	N1-C2-O2	5.41	126.59	122.80
36	5	504	A	C8-N9-C4	5.41	107.96	105.80
36	5	1385	C	C4-C5-C6	-5.41	114.69	117.40
36	5	2770	G	C8-N9-C4	-5.41	104.24	106.40
1	2	1363	U	N1-C2-O2	5.41	126.59	122.80
1	6	454	U	C6-N1-C2	5.41	124.25	121.00
36	5	1335	C	OP2-P-O3'	5.41	117.10	105.20
52	m6	94	ARG	NE-CZ-NH2	5.41	123.00	120.30
36	1	2689	A	N1-C6-N6	-5.41	115.36	118.60
36	5	2524	A	C4-N9-C1'	5.41	136.03	126.30
36	1	49	A	C5-C6-N1	-5.41	115.00	117.70
36	1	1343	A	N1-C6-N6	5.41	121.84	118.60
36	1	1815	U	P-O3'-C3'	5.41	126.19	119.70
1	6	1111	G	N3-C4-C5	-5.41	125.90	128.60
36	5	415	G	OP1-P-OP2	-5.41	111.49	119.60
36	5	1304	A	C2-N3-C4	5.41	113.30	110.60
36	5	3309	G	C4-N9-C1'	5.41	133.53	126.50
36	1	1362	G	N7-C8-N9	-5.40	110.40	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2728	G	C2-N3-C4	5.40	114.60	111.90
36	1	2973	G	OP1-P-O3'	5.40	117.09	105.20
36	1	3207	U	OP2-P-O3'	5.40	117.09	105.20
36	5	999	G	C6-C5-N7	5.40	133.64	130.40
36	1	614	C	C6-N1-C2	5.40	122.46	120.30
36	1	919	U	N1-C2-O2	5.40	126.58	122.80
36	1	1329	U	C5-C6-N1	5.40	125.40	122.70
36	1	1604	G	N3-C4-C5	-5.40	125.90	128.60
36	1	2854	U	OP2-P-O3'	5.40	117.08	105.20
38	4	80	A	C8-N9-C4	5.40	107.96	105.80
36	5	2353	G	C6-N1-C2	-5.40	121.86	125.10
1	2	1268	G	O5'-P-OP2	-5.40	100.84	105.70
36	1	343	U	C2-N3-C4	5.40	130.24	127.00
36	5	1837	U	OP2-P-O3'	5.40	117.08	105.20
36	5	2231	C	O4'-C1'-N1	5.40	112.52	108.20
1	2	109	G	N1-C6-O6	5.40	123.14	119.90
1	2	1324	G	C6-C5-N7	5.40	133.64	130.40
36	1	1428	A	N1-C6-N6	5.40	121.84	118.60
36	1	2257	C	C2-N1-C1'	5.40	124.74	118.80
56	N0	155	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	6	1119	G	C8-N9-C4	-5.40	104.24	106.40
36	5	969	C	N3-C4-C5	5.40	124.06	121.90
36	5	1607	U	N1-C2-N3	5.40	118.14	114.90
40	l3	102	LEU	CA-CB-CG	5.40	127.72	115.30
1	6	383	G	C8-N9-C4	-5.40	104.24	106.40
36	5	1098	A	N7-C8-N9	5.40	116.50	113.80
36	5	2870	C	O4'-C1'-N1	5.40	112.52	108.20
36	5	3285	C	N1-C2-O2	5.40	122.14	118.90
68	o2	33	ARG	NE-CZ-NH2	-5.40	117.60	120.30
36	1	2693	C	C4-C5-C6	-5.40	114.70	117.40
36	1	1194	G	OP1-P-O3'	5.39	117.07	105.20
36	1	2241	U	O5'-P-OP1	-5.39	100.84	105.70
36	1	2662	G	C4-C5-N7	5.39	112.96	110.80
1	6	826	U	C5-C6-N1	5.39	125.40	122.70
1	2	121	U	N3-C2-O2	-5.39	118.43	122.20
1	2	378	A	C5-C6-N6	-5.39	119.39	123.70
36	1	920	A	OP1-P-O3'	5.39	117.06	105.20
36	1	1136	A	C6-N1-C2	-5.39	115.36	118.60
36	1	1496	C	C2-N1-C1'	5.39	124.73	118.80
36	5	192	C	C2-N1-C1'	5.39	124.73	118.80
36	5	407	A	C5-C6-N6	-5.39	119.39	123.70
36	5	635	G	N3-C4-C5	5.39	131.30	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1049	C	N1-C2-O2	5.39	122.14	118.90
36	1	228	U	N3-C2-O2	-5.39	118.43	122.20
36	1	662	U	N1-C2-O2	5.39	126.57	122.80
36	1	1329	U	N1-C1'-C2'	-5.39	106.07	112.00
1	6	1481	C	N3-C2-O2	-5.39	118.13	121.90
36	5	39	A	C5-C6-N6	-5.39	119.39	123.70
36	1	109	A	C5-C6-N6	5.39	128.01	123.70
36	1	631	U	C5-C4-O4	-5.39	122.67	125.90
36	5	2724	U	C6-N1-C2	-5.39	117.77	121.00
36	1	1409	G	C4-N9-C1'	-5.39	119.50	126.50
36	5	75	G	N1-C6-O6	5.39	123.13	119.90
36	5	1770	G	C4-N9-C1'	5.39	133.50	126.50
68	o2	4	LEU	C-N-CA	-5.39	99.38	122.00
36	1	517	G	C4-N9-C1'	5.38	133.50	126.50
36	1	3368	U	N1-C2-O2	-5.38	119.03	122.80
36	5	1194	G	C2-N3-C4	5.38	114.59	111.90
36	5	2849	C	N1-C2-O2	-5.38	115.67	118.90
36	1	307	A	O5'-P-OP2	-5.38	100.86	105.70
36	1	1433	A	O5'-P-OP1	-5.38	100.86	105.70
36	1	2797	C	N1-C2-O2	-5.38	115.67	118.90
1	6	711	U	C2-N1-C1'	5.38	124.16	117.70
36	5	1440	G	N3-C4-N9	-5.38	122.77	126.00
1	2	61	A	N7-C8-N9	5.38	116.49	113.80
36	5	1407	A	C2-N3-C4	-5.38	107.91	110.60
1	6	767	U	C5-C4-O4	5.38	129.13	125.90
1	6	1745	G	C4-C5-N7	5.38	112.95	110.80
36	1	439	C	C4-C5-C6	-5.38	114.71	117.40
36	1	2664	C	N3-C4-C5	5.38	124.05	121.90
38	4	8	C	OP2-P-O3'	5.38	117.03	105.20
38	4	52	A	C8-N9-C4	-5.38	103.65	105.80
36	5	1670	C	C6-N1-C2	5.38	122.45	120.30
36	5	2860	U	OP1-P-O3'	5.38	117.03	105.20
36	5	2983	C	C4-C5-C6	5.38	120.09	117.40
52	m6	27	LEU	CB-CG-CD1	-5.38	101.86	111.00
36	1	1420	C	N1-C2-N3	5.38	122.96	119.20
36	1	1481	A	O4'-C1'-N9	5.38	112.50	108.20
36	1	2937	G	N7-C8-N9	-5.38	110.41	113.10
38	4	9	A	N1-C6-N6	-5.38	115.37	118.60
1	6	1643	U	C2-N3-C4	-5.38	123.77	127.00
36	5	352	A	O4'-C1'-N9	5.38	112.50	108.20
36	5	648	C	OP1-P-O3'	5.38	117.03	105.20
36	5	2836	C	N3-C4-N4	-5.38	114.24	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2993	G	P-O3'-C3'	5.38	126.15	119.70
1	2	831	U	C6-N1-C2	-5.38	117.78	121.00
36	1	2134	G	OP1-P-OP2	-5.38	111.54	119.60
1	2	558	U	C2-N1-C1'	5.37	124.15	117.70
36	5	83	U	OP1-P-OP2	5.37	127.66	119.60
36	5	2645	G	C2-N3-C4	5.37	114.59	111.90
36	1	580	C	N3-C2-O2	5.37	125.66	121.90
36	5	416	A	N1-C6-N6	5.37	121.82	118.60
36	5	811	U	C5-C4-O4	-5.37	122.68	125.90
36	5	1308	A	N1-C6-N6	-5.37	115.38	118.60
36	5	2643	A	C8-N9-C4	5.37	107.95	105.80
36	5	3294	A	C8-N9-C4	-5.37	103.65	105.80
36	1	3050	U	N1-C2-O2	5.37	126.56	122.80
38	4	15	G	C5-C6-N1	5.37	114.18	111.50
1	6	2	A	O5'-P-OP2	-5.37	100.87	105.70
36	5	422	A	C8-N9-C4	-5.37	103.65	105.80
36	5	2208	A	O4'-C1'-N9	5.37	112.49	108.20
36	5	2286	U	N3-C2-O2	-5.37	118.44	122.20
36	5	2343	C	O5'-P-OP2	-5.37	100.87	105.70
36	5	2593	A	P-O3'-C3'	5.37	126.14	119.70
1	6	1539	G	O4'-C1'-N9	-5.37	103.91	108.20
36	5	1180	A	O4'-C1'-N9	-5.37	103.91	108.20
39	l2	212	GLY	N-CA-C	5.37	126.52	113.10
1	2	969	C	N3-C2-O2	5.37	125.66	121.90
1	2	1202	A	C2-N3-C4	5.37	113.28	110.60
36	1	1926	C	C5-C4-N4	-5.37	116.44	120.20
36	5	414	U	C5-C6-N1	-5.37	120.02	122.70
36	5	1014	U	C6-N1-C1'	-5.37	113.69	121.20
36	5	2175	U	N1-C2-O2	-5.37	119.04	122.80
36	5	2336	U	C5-C4-O4	-5.37	122.68	125.90
36	5	3206	C	N3-C2-O2	-5.37	118.14	121.90
1	2	736	C	C5-C6-N1	5.36	123.68	121.00
36	1	639	G	N1-C2-N2	5.36	121.03	116.20
36	1	2163	C	C5-C6-N1	-5.36	118.32	121.00
36	1	2257	C	O4'-C1'-N1	5.36	112.49	108.20
1	6	194	U	N1-C2-O2	5.36	126.55	122.80
1	6	755	A	C8-N9-C4	-5.36	103.65	105.80
36	5	708	G	C8-N9-C4	-5.36	104.25	106.40
36	1	1156	C	N3-C2-O2	-5.36	118.15	121.90
1	6	1535	U	N1-C2-O2	5.36	126.55	122.80
36	1	1607	U	N3-C2-O2	-5.36	118.45	122.20
36	1	2993	G	N3-C4-N9	5.36	129.22	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1303	A	C8-N9-C4	5.36	107.94	105.80
36	5	2857	C	C5-C4-N4	-5.36	116.45	120.20
36	5	2912	G	C5-C6-O6	-5.36	125.38	128.60
36	1	339	C	C5-C4-N4	5.36	123.95	120.20
36	1	2620	G	C8-N9-C4	5.36	108.54	106.40
36	1	2173	U	N1-C2-N3	5.36	118.11	114.90
1	6	366	A	C2-N3-C4	-5.36	107.92	110.60
36	5	932	U	C6-N1-C2	5.36	124.21	121.00
36	5	2848	G	N1-C6-O6	5.36	123.11	119.90
36	1	388	G	C8-N9-C4	-5.36	104.26	106.40
36	1	896	A	C8-N9-C4	-5.36	103.66	105.80
36	1	906	A	C5-C6-N6	-5.36	119.42	123.70
36	1	2281	A	C2-N3-C4	-5.36	107.92	110.60
36	5	1112	A	C8-N9-C1'	-5.36	118.06	127.70
36	5	1208	U	N1-C2-O2	5.36	126.55	122.80
36	5	2892	A	C8-N9-C4	-5.36	103.66	105.80
36	5	3082	C	C6-N1-C2	-5.36	118.16	120.30
1	6	1660	A	N1-C6-N6	-5.35	115.39	118.60
36	5	2293	C	N3-C4-N4	5.35	121.75	118.00
36	5	2339	C	OP1-P-O3'	5.35	116.98	105.20
36	1	979	U	C5-C6-N1	5.35	125.38	122.70
36	1	1396	C	OP2-P-O3'	5.35	116.98	105.20
36	1	1655	G	N3-C4-N9	5.35	129.21	126.00
1	6	407	A	N1-C6-N6	5.35	121.81	118.60
37	7	37	G	N3-C4-N9	5.35	129.21	126.00
36	1	1330	A	N9-C4-C5	-5.35	103.66	105.80
36	1	1407	A	C8-N9-C4	5.35	107.94	105.80
36	5	2572	C	C6-N1-C1'	-5.35	114.38	120.80
36	5	2726	C	C4-C5-C6	5.35	120.08	117.40
36	1	333	G	N9-C4-C5	5.35	107.54	105.40
36	1	645	A	C4-C5-C6	5.35	119.67	117.00
36	1	909	G	N7-C8-N9	-5.35	110.43	113.10
36	1	2286	U	N3-C4-O4	-5.35	115.66	119.40
36	1	2301	U	N3-C2-O2	-5.35	118.45	122.20
38	4	98	U	N3-C2-O2	5.35	125.94	122.20
1	6	25	C	P-O3'-C3'	5.35	126.12	119.70
1	6	287	G	C5-C6-O6	-5.35	125.39	128.60
36	5	423	A	C5-N7-C8	5.35	106.58	103.90
36	5	2419	A	O5'-P-OP2	5.35	117.12	110.70
36	5	2726	C	N3-C4-C5	-5.35	119.76	121.90
1	2	1781	A	C5-C6-N1	-5.35	115.03	117.70
36	1	2362	C	C2-N3-C4	5.35	122.57	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2403	G	N9-C4-C5	-5.35	103.26	105.40
36	1	2901	G	C5-C6-O6	-5.35	125.39	128.60
1	6	1751	C	C6-N1-C2	5.35	122.44	120.30
36	5	359	U	OP2-P-O3'	5.35	116.96	105.20
36	5	683	U	O5'-P-OP2	-5.35	100.89	105.70
36	5	1884	A	OP2-P-O3'	5.35	116.96	105.20
36	1	1389	G	N9-C4-C5	-5.35	103.26	105.40
36	5	662	U	N3-C4-O4	-5.34	115.66	119.40
36	5	2908	G	C8-N9-C4	-5.34	104.26	106.40
36	5	3105	U	C2-N3-C4	-5.34	123.79	127.00
36	5	359	U	N1-C2-O2	-5.34	119.06	122.80
1	2	1780	G	C4-C5-N7	5.34	112.94	110.80
36	1	575	G	C8-N9-C4	5.34	108.54	106.40
36	1	1891	A	C8-N9-C4	5.34	107.94	105.80
38	4	115	C	C6-N1-C2	5.34	122.44	120.30
1	6	165	G	C8-N9-C4	-5.34	104.26	106.40
1	6	813	U	N1-C2-O2	5.34	126.54	122.80
1	6	1200	G	N1-C6-O6	5.34	123.11	119.90
36	5	1906	G	OP1-P-O3'	5.34	116.95	105.20
36	5	2136	C	C2-N3-C4	-5.34	117.23	119.90
36	1	805	G	N1-C6-O6	-5.34	116.70	119.90
36	1	1133	A	N7-C8-N9	-5.34	111.13	113.80
36	1	2633	U	N3-C2-O2	-5.34	118.46	122.20
36	1	2798	C	C5-C6-N1	5.34	123.67	121.00
1	6	858	G	C4-N9-C1'	5.34	133.44	126.50
1	6	1600	A	N1-C2-N3	5.34	131.97	129.30
1	6	1767	G	C8-N9-C4	5.34	108.53	106.40
36	5	2654	C	N1-C2-O2	-5.34	115.70	118.90
36	5	2799	A	N1-C6-N6	-5.34	115.40	118.60
24	D2	65	LEU	CA-CB-CG	5.34	127.58	115.30
36	1	716	A	O4'-C1'-N9	-5.34	103.93	108.20
36	1	796	U	OP2-P-O3'	5.34	116.94	105.20
1	6	1473	U	N1-C2-O2	5.34	126.54	122.80
36	1	1113	G	N3-C2-N2	-5.34	116.17	119.90
36	1	1329	U	OP1-P-OP2	5.34	127.61	119.60
36	1	2754	G	C5-C6-O6	5.34	131.80	128.60
36	1	2865	U	C6-N1-C2	5.34	124.20	121.00
36	1	2917	G	N3-C4-N9	5.34	129.20	126.00
36	5	2807	U	OP1-P-O3'	5.34	116.94	105.20
36	5	3127	A	N9-C4-C5	5.34	107.93	105.80
1	2	1745	G	C6-C5-N7	-5.33	127.20	130.40
36	1	75	G	C4-N9-C1'	5.33	133.44	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	308	C	N1-C2-O2	-5.33	115.70	118.90
1	2	553	G	N3-C2-N2	-5.33	116.17	119.90
1	2	1773	C	N3-C4-C5	-5.33	119.77	121.90
36	1	636	C	C5-C6-N1	-5.33	118.33	121.00
36	1	636	C	OP1-P-OP2	5.33	127.60	119.60
36	5	1716	U	P-O3'-C3'	5.33	126.10	119.70
36	5	2980	U	C5-C4-O4	5.33	129.10	125.90
36	5	3245	A	N3-C4-C5	5.33	130.53	126.80
36	1	341	G	C5-C6-O6	-5.33	125.40	128.60
36	1	1100	U	C2-N3-C4	-5.33	123.80	127.00
36	1	1547	G	N1-C2-N2	5.33	121.00	116.20
36	1	2409	G	N9-C4-C5	5.33	107.53	105.40
36	1	2633	U	N1-C2-O2	5.33	126.53	122.80
36	5	504	A	N1-C2-N3	-5.33	126.63	129.30
36	5	1338	C	C4-C5-C6	5.33	120.07	117.40
38	8	36	G	O5'-P-OP1	-5.33	100.90	105.70
36	1	1345	G	OP2-P-O3'	5.33	116.93	105.20
37	7	72	A	OP2-P-O3'	5.33	116.92	105.20
36	1	656	A	O5'-P-OP2	-5.33	100.90	105.70
1	6	7	G	N3-C2-N2	5.33	123.63	119.90
36	5	941	G	C2-N3-C4	5.33	114.56	111.90
1	2	704	C	N3-C2-O2	-5.33	118.17	121.90
36	1	2308	C	C2-N3-C4	-5.33	117.24	119.90
36	1	2403	G	C8-N9-C4	5.33	108.53	106.40
1	6	52	U	N1-C2-N3	5.33	118.09	114.90
1	2	1081	A	O4'-C1'-N9	5.32	112.46	108.20
36	1	407	A	C6-C5-N7	-5.32	128.57	132.30
36	1	658	G	C4-N9-C1'	5.32	133.42	126.50
36	1	765	C	N1-C2-O2	5.32	122.09	118.90
36	1	1297	C	C6-N1-C2	5.32	122.43	120.30
36	1	1392	G	C2-N3-C4	5.32	114.56	111.90
36	1	2993	G	C5-C6-O6	-5.32	125.41	128.60
1	6	392	G	C8-N9-C4	-5.32	104.27	106.40
1	6	448	C	C6-N1-C2	-5.32	118.17	120.30
36	1	439	C	C5-C6-N1	5.32	123.66	121.00
36	1	1487	G	N9-C4-C5	5.32	107.53	105.40
20	c8	15	LEU	CA-CB-CG	5.32	127.54	115.30
36	1	1296	C	N3-C4-C5	-5.32	119.77	121.90
36	1	1474	A	O5'-P-OP2	5.32	117.08	110.70
38	4	113	U	C6-N1-C1'	5.32	128.65	121.20
36	5	1399	A	C6-C5-N7	-5.32	128.58	132.30
36	5	1547	G	N1-C6-O6	5.32	123.09	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1929	G	N1-C2-N3	5.32	127.09	123.90
38	8	45	C	N3-C4-C5	-5.32	119.77	121.90
36	1	3302	U	C5-C6-N1	-5.32	120.04	122.70
36	5	934	G	C4-N9-C1'	5.32	133.41	126.50
36	5	2134	G	N3-C4-N9	5.32	129.19	126.00
36	5	2285	C	N1-C2-O2	-5.32	115.71	118.90
36	1	28	C	C6-N1-C2	5.32	122.43	120.30
36	1	1592	G	N3-C4-C5	-5.32	125.94	128.60
36	5	2342	U	N3-C2-O2	-5.32	118.48	122.20
36	1	2177	G	N3-C4-C5	-5.32	125.94	128.60
36	1	2212	C	OP2-P-O3'	5.32	116.89	105.20
36	1	3310	A	N9-C4-C5	-5.32	103.67	105.80
36	5	1480	G	O4'-C1'-N9	5.32	112.45	108.20
36	1	824	C	N3-C4-N4	-5.31	114.28	118.00
36	1	984	G	N1-C6-O6	-5.31	116.71	119.90
36	1	1794	G	O4'-C1'-N9	-5.31	103.95	108.20
36	1	2623	G	N3-C2-N2	5.31	123.62	119.90
11	s9	99	LEU	CA-CB-CG	5.31	127.52	115.30
1	2	1483	A	C8-N9-C4	-5.31	103.67	105.80
37	3	88	G	O5'-P-OP1	-5.31	100.92	105.70
36	5	1907	C	N3-C2-O2	5.31	125.62	121.90
36	5	2158	A	C6-N1-C2	-5.31	115.41	118.60
36	5	3140	G	C4-C5-N7	5.31	112.92	110.80
37	7	11	A	C5-C6-N6	-5.31	119.45	123.70
36	1	40	A	N9-C4-C5	-5.31	103.68	105.80
36	1	2169	G	OP2-P-O3'	5.31	116.88	105.20
36	5	2753	G	N1-C6-O6	5.31	123.09	119.90
36	1	394	G	N3-C4-N9	-5.31	122.81	126.00
36	1	800	G	C5-C6-O6	5.31	131.79	128.60
36	1	1151	U	C6-N1-C2	-5.31	117.81	121.00
36	1	1192	C	C6-N1-C1'	-5.31	114.43	120.80
36	1	2861	U	O5'-P-OP2	5.31	117.07	110.70
36	1	2920	U	C2-N3-C4	-5.31	123.81	127.00
36	1	3138	U	OP2-P-O3'	5.31	116.88	105.20
36	5	30	G	OP1-P-O3'	5.31	116.88	105.20
36	5	313	A	N7-C8-N9	5.31	116.45	113.80
36	1	341	G	N3-C4-N9	5.31	129.19	126.00
36	1	805	G	C5-C6-N1	5.31	114.15	111.50
38	4	115	C	N3-C4-C5	5.31	124.02	121.90
36	5	100	A	N1-C6-N6	5.31	121.78	118.60
36	5	2300	G	N1-C6-O6	-5.31	116.72	119.90
1	2	1600	A	N1-C6-N6	5.31	121.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	423	A	N9-C4-C5	5.31	107.92	105.80
36	1	1017	C	C5-C6-N1	5.31	123.65	121.00
36	1	694	C	N1-C2-O2	-5.30	115.72	118.90
36	1	1838	G	N9-C4-C5	-5.30	103.28	105.40
52	M6	78	ARG	NE-CZ-NH2	-5.30	117.65	120.30
36	5	363	G	OP1-P-O3'	5.30	116.87	105.20
36	5	908	G	C8-N9-C1'	-5.30	120.10	127.00
36	5	1301	A	C5-N7-C8	-5.30	101.25	103.90
1	6	333	A	C8-N9-C4	5.30	107.92	105.80
36	5	1047	A	N9-C4-C5	-5.30	103.68	105.80
36	5	1048	A	OP1-P-O3'	5.30	116.87	105.20
36	1	973	A	N1-C2-N3	5.30	131.95	129.30
36	1	1179	A	OP2-P-O3'	5.30	116.86	105.20
36	1	1586	G	N3-C4-N9	5.30	129.18	126.00
38	4	1	A	C4-C5-C6	-5.30	114.35	117.00
38	4	55	U	C5-C6-N1	-5.30	120.05	122.70
36	5	500	C	C6-N1-C2	5.30	122.42	120.30
36	5	2153	U	C5-C4-O4	-5.30	122.72	125.90
36	5	2310	U	O5'-P-OP1	5.30	117.06	110.70
1	2	337	G	N1-C6-O6	5.30	123.08	119.90
36	1	131	C	C6-N1-C2	-5.30	118.18	120.30
36	1	1501	U	C5-C6-N1	5.30	125.35	122.70
36	1	2115	G	C4-C5-N7	5.30	112.92	110.80
36	1	2763	U	N1-C2-O2	-5.30	119.09	122.80
36	1	2988	C	C2-N1-C1'	-5.30	112.97	118.80
36	1	3178	A	C6-C5-N7	-5.30	128.59	132.30
1	6	366	A	C8-N9-C4	5.30	107.92	105.80
1	6	756	A	C8-N9-C4	-5.30	103.68	105.80
36	5	205	C	N3-C4-C5	5.30	124.02	121.90
36	5	338	A	OP2-P-O3'	5.30	116.86	105.20
36	5	3164	C	O4'-C1'-N1	5.30	112.44	108.20
36	5	3225	C	N3-C4-N4	5.30	121.71	118.00
36	1	406	G	O5'-P-OP2	-5.30	100.93	105.70
36	5	78	U	O5'-P-OP1	-5.30	100.93	105.70
36	5	2875	U	C6-N1-C2	5.30	124.18	121.00
36	5	3055	U	C5-C4-O4	-5.30	122.72	125.90
36	5	38	U	C5-C4-O4	-5.30	122.72	125.90
36	1	1670	C	N1-C2-O2	-5.29	115.72	118.90
41	l4	187	LEU	CA-CB-CG	5.29	127.48	115.30
36	1	229	G	N3-C2-N2	-5.29	116.19	119.90
36	1	1136	A	C5-C6-N6	-5.29	119.47	123.70
1	6	338	C	N3-C4-N4	5.29	121.70	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1509	C	N3-C2-O2	-5.29	118.19	121.90
1	6	1766	A	OP1-P-O3'	5.29	116.84	105.20
36	5	704	U	C2-N1-C1'	-5.29	111.35	117.70
36	5	2877	G	C5-C6-O6	5.29	131.78	128.60
1	2	1189	A	C8-N9-C4	5.29	107.92	105.80
36	1	1398	U	OP2-P-O3'	5.29	116.84	105.20
36	1	3355	U	C2-N1-C1'	5.29	124.05	117.70
36	5	2923	U	N1-C2-O2	-5.29	119.09	122.80
36	1	1174	G	C8-N9-C1'	-5.29	120.12	127.00
36	1	2550	U	N1-C2-N3	5.29	118.07	114.90
36	1	2830	G	C4-C5-N7	-5.29	108.68	110.80
36	5	864	G	OP2-P-O3'	5.29	116.84	105.20
38	8	126	A	OP1-P-O3'	5.29	116.84	105.20
36	1	329	U	N1-C2-N3	5.29	118.07	114.90
36	1	2984	C	C5-C4-N4	5.29	123.90	120.20
1	6	17	C	N3-C4-N4	-5.29	114.30	118.00
36	5	2913	C	N1-C2-N3	5.29	122.90	119.20
36	5	3181	C	N3-C4-C5	-5.29	119.78	121.90
1	2	1773	C	C5-C6-N1	5.29	123.64	121.00
36	1	2133	U	O4'-C1'-N1	5.29	112.43	108.20
36	1	2206	G	C5-C6-O6	-5.29	125.43	128.60
36	5	1879	A	P-O3'-C3'	5.29	126.04	119.70
36	5	2409	G	O5'-P-OP2	-5.29	100.94	105.70
36	5	2971	A	N9-C4-C5	-5.29	103.69	105.80
36	5	3138	U	OP2-P-O3'	5.29	116.83	105.20
36	1	225	C	N3-C4-N4	5.29	121.70	118.00
38	4	79	A	N7-C8-N9	5.29	116.44	113.80
70	O4	8	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	6	457	G	N1-C6-O6	5.29	123.07	119.90
36	5	2174	G	OP1-P-O3'	5.29	116.83	105.20
1	2	1747	G	N1-C6-O6	5.28	123.07	119.90
36	5	907	G	C8-N9-C4	5.28	108.51	106.40
36	5	3154	C	C2-N3-C4	5.28	122.54	119.90
36	1	2176	U	C5-C4-O4	5.28	129.07	125.90
36	5	3382	U	N1-C2-O2	5.28	126.50	122.80
1	6	114	C	C2-N1-C1'	5.28	124.61	118.80
1	6	351	C	N3-C2-O2	-5.28	118.20	121.90
36	5	293	C	C6-N1-C2	5.28	122.41	120.30
36	5	2942	C	N3-C4-N4	5.28	121.70	118.00
36	1	2791	G	C8-N9-C4	-5.28	104.29	106.40
36	1	917	A	C5-C6-N6	5.28	127.92	123.70
36	1	1359	C	N3-C2-O2	5.28	125.59	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2688	U	C2-N1-C1'	5.28	124.03	117.70
1	6	539	G	C8-N9-C4	-5.28	104.29	106.40
36	5	1047	A	C6-C5-N7	-5.28	128.61	132.30
36	5	1416	C	C2-N1-C1'	5.28	124.61	118.80
36	5	2704	A	C4-C5-N7	5.28	113.34	110.70
1	2	15	U	C6-N1-C2	-5.28	117.83	121.00
36	1	1158	A	C5-C6-N6	-5.28	119.48	123.70
36	1	2159	U	C6-N1-C2	5.28	124.17	121.00
36	1	2939	G	OP1-P-O3'	-5.28	93.59	105.20
47	M0	167	LEU	CA-CB-CG	5.28	127.44	115.30
36	5	658	G	N3-C2-N2	-5.28	116.21	119.90
38	4	7	U	N1-C2-N3	5.27	118.06	114.90
36	5	643	U	C2-N3-C4	-5.27	123.84	127.00
36	5	1446	A	OP1-P-O3'	5.27	116.80	105.20
36	5	1450	G	C2-N3-C4	5.27	114.54	111.90
36	5	2153	U	N3-C4-O4	5.27	123.09	119.40
38	8	137	C	N3-C4-N4	5.27	121.69	118.00
36	1	718	G	C2-N3-C4	-5.27	109.26	111.90
36	1	1297	C	O5'-P-OP1	-5.27	100.95	105.70
1	6	1620	C	C6-N1-C2	-5.27	118.19	120.30
36	5	2891	U	C5-C6-N1	-5.27	120.06	122.70
1	6	1698	G	P-O3'-C3'	5.27	126.03	119.70
36	5	2893	C	C4-C5-C6	5.27	120.04	117.40
36	5	3288	G	C5-C6-N1	5.27	114.14	111.50
36	5	694	C	N3-C2-O2	-5.27	118.21	121.90
3	S1	96	LEU	CA-CB-CG	5.27	127.42	115.30
36	1	2619	G	O5'-P-OP1	-5.27	100.96	105.70
38	4	6	U	N3-C4-C5	5.27	117.76	114.60
1	6	87	C	C6-N1-C2	-5.27	118.19	120.30
36	5	1295	G	OP2-P-O3'	5.27	116.79	105.20
36	1	1379	G	N3-C2-N2	-5.27	116.21	119.90
36	1	1406	A	C5-C6-N6	-5.27	119.49	123.70
36	1	1500	G	OP2-P-O3'	5.27	116.78	105.20
1	6	539	G	N7-C8-N9	5.27	115.73	113.10
36	5	99	A	C8-N9-C4	5.27	107.91	105.80
36	5	822	G	O5'-P-OP1	-5.27	100.96	105.70
36	5	3309	G	C8-N9-C4	-5.27	104.29	106.40
36	1	730	C	N3-C4-C5	5.26	124.00	121.90
38	4	82	U	N3-C2-O2	5.26	125.89	122.20
77	Q1	9	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	6	431	C	O5'-P-OP1	-5.26	100.96	105.70
1	6	1491	U	P-O3'-C3'	5.26	126.02	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	637	C	N3-C4-C5	5.26	124.01	121.90
36	5	1321	G	N9-C4-C5	-5.26	103.29	105.40
36	5	1489	A	N1-C6-N6	5.26	121.76	118.60
36	5	2531	C	N3-C2-O2	-5.26	118.21	121.90
36	5	2601	A	C6-C5-N7	5.26	135.99	132.30
36	5	2733	A	O5'-P-OP2	-5.26	100.96	105.70
36	1	2930	A	N1-C6-N6	-5.26	115.44	118.60
36	5	1199	C	C4-C5-C6	5.26	120.03	117.40
36	5	1338	C	N3-C4-N4	5.26	121.68	118.00
36	5	2354	C	N3-C4-N4	5.26	121.68	118.00
36	5	2602	G	C8-N9-C4	-5.26	104.30	106.40
37	7	53	U	O5'-P-OP2	-5.26	100.96	105.70
38	8	22	U	O5'-P-OP2	5.26	117.02	110.70
36	1	343	U	N3-C4-C5	-5.26	111.44	114.60
36	1	2551	U	N3-C2-O2	-5.26	118.52	122.20
36	1	3269	U	N3-C4-O4	-5.26	115.72	119.40
1	6	1129	U	N3-C4-O4	-5.26	115.72	119.40
36	5	2137	U	N3-C4-C5	5.26	117.76	114.60
36	5	2352	A	N3-C4-C5	-5.26	123.12	126.80
36	5	2398	A	N1-C6-N6	-5.26	115.44	118.60
38	8	39	G	N3-C4-N9	5.26	129.16	126.00
1	2	453	U	C6-N1-C1'	-5.26	113.84	121.20
36	1	3362	A	C8-N9-C4	-5.26	103.70	105.80
36	5	584	G	C4-C5-N7	-5.26	108.70	110.80
36	5	809	G	C8-N9-C4	5.26	108.50	106.40
36	5	994	G	N3-C4-C5	-5.26	125.97	128.60
36	5	2354	C	N1-C2-O2	-5.26	115.74	118.90
36	5	2830	G	C5-N7-C8	5.26	106.93	104.30
36	5	2851	A	C6-N1-C2	-5.26	115.44	118.60
25	D3	111	GLY	N-CA-C	-5.26	99.95	113.10
1	6	417	A	C4-C5-C6	5.26	119.63	117.00
1	6	426	G	O5'-P-OP2	-5.26	100.97	105.70
1	2	186	C	C5-C6-N1	5.26	123.63	121.00
1	2	1324	G	N9-C4-C5	5.26	107.50	105.40
36	1	425	G	OP1-P-OP2	-5.26	111.72	119.60
36	1	2637	A	C8-N9-C4	-5.26	103.70	105.80
36	1	2660	G	N9-C4-C5	-5.26	103.30	105.40
36	1	3053	G	N3-C2-N2	5.26	123.58	119.90
1	6	1137	A	N7-C8-N9	-5.26	111.17	113.80
36	5	915	A	C8-N9-C4	-5.26	103.70	105.80
36	5	942	U	C6-N1-C2	-5.26	117.85	121.00
36	5	1047	A	C5-N7-C8	-5.26	101.27	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1314	C	C5-C4-N4	-5.26	116.52	120.20
36	5	1391	C	N1-C2-O2	-5.26	115.75	118.90
36	5	2343	C	C2-N3-C4	-5.26	117.27	119.90
36	5	2632	G	N3-C2-N2	5.26	123.58	119.90
36	1	2148	U	N1-C2-O2	-5.25	119.12	122.80
37	7	93	C	C6-N1-C2	-5.25	118.20	120.30
1	2	1494	C	C6-N1-C2	-5.25	118.20	120.30
36	5	633	C	OP2-P-O3'	5.25	116.76	105.20
36	5	3386	G	O5'-P-OP2	-5.25	100.97	105.70
36	1	592	A	N9-C4-C5	-5.25	103.70	105.80
36	1	1140	G	C8-N9-C1'	-5.25	120.17	127.00
1	6	365	G	N1-C2-N2	-5.25	111.47	116.20
1	6	1340	U	N1-C2-O2	5.25	126.48	122.80
36	5	1456	A	C5-C6-N6	-5.25	119.50	123.70
36	5	2165	G	N3-C4-N9	5.25	129.15	126.00
36	5	2637	A	N1-C6-N6	5.25	121.75	118.60
36	1	1177	G	N1-C2-N2	5.25	120.92	116.20
36	1	1890	U	N3-C4-C5	5.25	117.75	114.60
36	1	2732	G	N1-C2-N2	-5.25	111.47	116.20
36	5	2397	A	N1-C6-N6	-5.25	115.45	118.60
36	5	2927	C	C5-C6-N1	5.25	123.62	121.00
1	2	610	G	C4-N9-C1'	5.25	133.32	126.50
56	N0	115	ARG	NE-CZ-NH1	5.25	122.92	120.30
36	5	721	G	C5-C6-N1	5.25	114.12	111.50
36	5	2283	G	N1-C6-O6	5.25	123.05	119.90
36	5	3324	C	N3-C2-O2	5.25	125.57	121.90
36	1	545	U	N1-C2-O2	5.25	126.47	122.80
36	1	3361	G	N3-C4-C5	-5.25	125.98	128.60
36	5	2675	C	N1-C2-O2	-5.25	115.75	118.90
37	7	28	C	N3-C4-C5	-5.25	119.80	121.90
36	1	88	A	N9-C4-C5	-5.24	103.70	105.80
36	1	2853	A	C2-N3-C4	5.24	113.22	110.60
1	6	194	U	C5-C6-N1	5.24	125.32	122.70
1	6	408	C	C6-N1-C2	-5.24	118.20	120.30
36	5	437	G	N1-C2-N3	5.24	127.05	123.90
36	5	3306	U	C5-C4-O4	-5.24	122.75	125.90
1	6	1463	C	C6-N1-C2	5.24	122.40	120.30
36	5	519	A	C6-C5-N7	-5.24	128.63	132.30
36	1	2288	G	C5-C6-O6	5.24	131.74	128.60
36	1	2541	U	P-O3'-C3'	5.24	125.99	119.70
36	5	873	C	P-O3'-C3'	5.24	125.99	119.70
36	5	1317	A	N1-C2-N3	-5.24	126.68	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3186	A	N1-C6-N6	-5.24	115.46	118.60
1	2	380	U	C2-N1-C1'	5.24	123.99	117.70
1	2	1241	G	C6-C5-N7	-5.24	127.26	130.40
36	1	282	G	C5-C6-O6	5.24	131.74	128.60
36	1	706	A	C8-N9-C4	5.24	107.89	105.80
36	1	2343	C	C5-C4-N4	-5.24	116.53	120.20
37	3	82	G	C8-N9-C1'	-5.24	120.19	127.00
36	5	3315	G	C5-C6-O6	5.24	131.74	128.60
1	6	782	U	C2-N1-C1'	5.24	123.98	117.70
36	5	2187	G	O5'-P-OP2	5.24	116.98	110.70
36	5	2830	G	N3-C4-N9	-5.24	122.86	126.00
36	5	3225	C	O5'-P-OP1	-5.24	100.99	105.70
1	2	553	G	C5-C6-N1	-5.24	108.88	111.50
36	1	99	A	C5'-C4'-O4'	5.24	115.38	109.10
36	1	1848	G	N1-C6-O6	5.24	123.04	119.90
1	6	194	U	N3-C2-O2	-5.24	118.54	122.20
36	5	514	G	C5-C6-O6	-5.24	125.46	128.60
36	5	867	G	C8-N9-C4	5.24	108.49	106.40
36	5	901	G	N3-C2-N2	5.24	123.56	119.90
36	5	1138	U	C2-N3-C4	-5.24	123.86	127.00
36	5	3209	A	N1-C2-N3	5.24	131.92	129.30
36	1	1114	U	N3-C4-O4	-5.23	115.74	119.40
36	5	1129	A	O5'-P-OP2	-5.23	100.99	105.70
36	5	2367	A	C8-N9-C4	-5.23	103.71	105.80
36	5	2746	A	N7-C8-N9	-5.23	111.18	113.80
1	2	447	U	C5-C6-N1	5.23	125.32	122.70
36	1	96	G	N3-C4-C5	5.23	131.22	128.60
36	1	339	C	N1-C2-O2	5.23	122.04	118.90
73	o7	65	ARG	NE-CZ-NH1	5.23	122.92	120.30
36	1	1484	U	N1-C2-O2	5.23	126.46	122.80
36	1	1515	A	N9-C4-C5	-5.23	103.71	105.80
36	1	2200	U	N1-C2-O2	-5.23	119.14	122.80
1	6	1003	A	N9-C4-C5	-5.23	103.71	105.80
36	5	162	G	N1-C6-O6	-5.23	116.76	119.90
36	5	1323	G	C8-N9-C4	-5.23	104.31	106.40
46	L9	166	ARG	NE-CZ-NH2	5.23	122.92	120.30
36	5	431	U	C5-C4-O4	-5.23	122.76	125.90
36	5	636	C	C2-N3-C4	-5.23	117.28	119.90
36	5	776	U	P-O3'-C3'	5.23	125.97	119.70
36	5	1193	A	C4-C5-C6	5.23	119.61	117.00
36	1	355	A	C2-N3-C4	-5.23	107.99	110.60
36	1	2961	G	O5'-P-OP2	-5.23	101.00	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	765	G	O4'-C1'-N9	-5.23	104.02	108.20
36	5	362	U	C5-C4-O4	-5.23	122.76	125.90
36	5	1794	G	N1-C2-N2	-5.23	111.49	116.20
36	5	2800	G	N9-C4-C5	5.23	107.49	105.40
38	8	116	G	N1-C6-O6	5.23	123.04	119.90
1	2	1745	G	N3-C4-C5	-5.22	125.99	128.60
1	2	1777	G	C5-C6-O6	-5.22	125.47	128.60
36	1	96	G	C5-N7-C8	-5.22	101.69	104.30
36	1	716	A	C2-N3-C4	-5.22	107.99	110.60
36	1	1297	C	C5-C6-N1	-5.22	118.39	121.00
36	1	2623	G	C8-N9-C4	5.22	108.49	106.40
1	6	792	U	C6-N1-C2	-5.22	117.86	121.00
36	5	866	A	OP1-P-OP2	-5.22	111.76	119.60
54	m8	176	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	2	381	C	N1-C2-O2	5.22	122.03	118.90
15	C3	22	ALA	C-N-CA	5.22	143.94	122.00
36	1	1389	G	N1-C6-O6	5.22	123.03	119.90
1	6	578	U	C5-C6-N1	-5.22	120.09	122.70
36	5	864	G	C6-N1-C2	-5.22	121.97	125.10
36	5	1133	A	C2-N3-C4	5.22	113.21	110.60
36	5	1914	G	N1-C6-O6	-5.22	116.77	119.90
36	5	2627	C	OP2-P-O3'	5.22	116.69	105.20
36	5	2816	G	C8-N9-C4	5.22	108.49	106.40
36	1	376	G	C5-C6-N1	-5.22	108.89	111.50
11	s9	3	ARG	NE-CZ-NH2	5.22	122.91	120.30
36	5	960	U	C6-N1-C1'	-5.22	113.89	121.20
36	5	1589	A	C2-N3-C4	5.22	113.21	110.60
36	5	2745	G	O4'-C1'-N9	5.22	112.38	108.20
36	1	332	C	N1-C2-O2	5.22	122.03	118.90
36	1	410	U	OP1-P-OP2	-5.22	111.77	119.60
1	6	1629	G	OP2-P-O3'	5.22	116.68	105.20
36	5	513	G	N9-C4-C5	-5.22	103.31	105.40
36	5	1047	A	OP2-P-O3'	5.22	116.68	105.20
36	5	663	C	O5'-P-OP1	5.22	116.96	110.70
36	5	2601	A	C4-C5-N7	-5.22	108.09	110.70
36	1	197	G	O5'-P-OP2	5.22	116.96	110.70
36	1	2114	C	O5'-P-OP2	-5.22	101.00	105.70
36	1	2163	C	C4-C5-C6	5.22	120.01	117.40
36	5	1162	U	O5'-P-OP2	-5.22	101.00	105.70
36	5	1300	G	N1-C6-O6	5.22	123.03	119.90
36	5	2249	G	N3-C4-C5	-5.22	125.99	128.60
36	5	3142	A	O5'-P-OP1	-5.22	101.00	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3339	A	C5-C6-N6	-5.22	119.53	123.70
37	7	50	U	C5-C6-N1	5.22	125.31	122.70
1	2	1269	U	C2-N1-C1'	5.21	123.96	117.70
36	1	639	G	C8-N9-C4	5.21	108.49	106.40
36	1	893	C	C2-N3-C4	5.21	122.51	119.90
36	1	1097	G	P-O3'-C3'	5.21	125.96	119.70
1	6	1629	G	N3-C4-C5	-5.21	125.99	128.60
1	6	1634	C	C6-N1-C2	-5.21	118.21	120.30
36	5	1316	C	N1-C2-O2	-5.21	115.77	118.90
54	m8	151	ARG	NE-CZ-NH1	-5.21	117.69	120.30
36	1	2411	U	C2-N3-C4	-5.21	123.87	127.00
36	5	1060	U	N3-C4-C5	5.21	117.73	114.60
36	5	2285	C	O5'-P-OP1	-5.21	101.01	105.70
36	1	594	U	C5-C6-N1	-5.21	120.09	122.70
36	1	2954	U	OP1-P-O3'	5.21	116.67	105.20
37	3	57	G	OP2-P-O3'	5.21	116.67	105.20
65	N9	14	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	6	1745	G	N9-C4-C5	-5.21	103.31	105.40
36	5	714	G	C5-C6-O6	-5.21	125.47	128.60
36	1	109	A	OP1-P-O3'	5.21	116.66	105.20
36	1	2626	A	N1-C2-N3	5.21	131.91	129.30
36	5	3032	A	N9-C4-C5	-5.21	103.72	105.80
1	2	1006	C	C6-N1-C2	-5.21	118.22	120.30
36	1	315	C	O5'-P-OP1	-5.21	101.01	105.70
36	1	593	C	N1-C2-O2	-5.21	115.78	118.90
36	5	630	A	C2-N3-C4	-5.21	108.00	110.60
36	5	2108	C	N1-C2-O2	-5.21	115.78	118.90
36	5	2138	A	N9-C4-C5	5.21	107.88	105.80
38	8	80	A	C4-C5-C6	5.21	119.61	117.00
36	1	697	A	C5-C6-N6	-5.21	119.53	123.70
36	1	2292	U	C5-C4-O4	-5.21	122.78	125.90
36	1	3102	G	C5-C6-O6	5.21	131.72	128.60
1	6	1031	U	C2-N1-C1'	-5.21	111.45	117.70
36	5	2279	A	N1-C6-N6	5.21	121.72	118.60
36	5	2350	C	OP1-P-OP2	-5.21	111.79	119.60
36	5	3272	C	C6-N1-C2	5.21	122.38	120.30
36	1	156	G	N3-C2-N2	5.21	123.54	119.90
36	1	2627	C	N3-C4-N4	-5.21	114.36	118.00
1	2	360	A	C8-N9-C4	5.20	107.88	105.80
36	1	1416	C	N3-C4-N4	-5.20	114.36	118.00
36	1	1904	C	C5-C6-N1	5.20	123.60	121.00
36	1	2408	U	N3-C2-O2	-5.20	118.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	421	A	N1-C6-N6	5.20	121.72	118.60
36	5	965	A	C5-C6-N6	-5.20	119.54	123.70
36	5	1695	U	N3-C2-O2	-5.20	118.56	122.20
36	5	1794	G	O4'-C1'-N9	-5.20	104.04	108.20
52	m6	27	LEU	CB-CG-CD2	-5.20	102.16	111.00
36	1	2800	G	O5'-P-OP1	5.20	116.94	110.70
36	5	419	G	C4-C5-N7	5.20	112.88	110.80
36	5	1124	U	C4-C5-C6	-5.20	116.58	119.70
36	5	2367	A	N7-C8-N9	5.20	116.40	113.80
36	5	2865	U	N3-C4-C5	5.20	117.72	114.60
1	2	1314	U	N3-C2-O2	-5.20	118.56	122.20
36	1	2623	G	OP1-P-OP2	-5.20	111.80	119.60
36	1	2960	C	N3-C4-C5	5.20	123.98	121.90
36	5	799	G	C5-C6-N1	5.20	114.10	111.50
36	5	2144	A	O5'-P-OP2	-5.20	101.02	105.70
41	l4	188	ARG	NE-CZ-NH2	-5.20	117.70	120.30
36	1	2286	U	C5-C4-O4	5.20	129.02	125.90
1	6	622	A	C4-C5-N7	-5.20	108.10	110.70
1	6	1781	A	C8-N9-C4	-5.20	103.72	105.80
36	5	666	A	O5'-P-OP1	-5.20	101.02	105.70
36	5	893	C	C2-N3-C4	5.20	122.50	119.90
36	5	1298	C	N1-C2-O2	-5.20	115.78	118.90
36	5	2759	U	C5-C6-N1	-5.20	120.10	122.70
37	3	98	C	N3-C4-C5	-5.20	119.82	121.90
1	6	1541	G	N3-C4-C5	-5.20	126.00	128.60
36	5	2784	G	N3-C4-C5	-5.20	126.00	128.60
1	2	240	U	OP2-P-O3'	5.20	116.63	105.20
36	1	716	A	N3-C4-C5	5.20	130.44	126.80
36	1	2826	U	OP2-P-O3'	5.20	116.63	105.20
36	5	215	G	N9-C4-C5	5.20	107.48	105.40
36	5	2312	A	C5-C6-N1	5.20	120.30	117.70
36	1	1053	A	C8-N9-C4	5.19	107.88	105.80
36	1	2255	A	N7-C8-N9	-5.19	111.20	113.80
36	5	1317	A	P-O3'-C3'	5.19	125.93	119.70
36	5	3020	U	C6-N1-C2	-5.19	117.88	121.00
1	2	1121	C	C2-N1-C1'	-5.19	113.09	118.80
1	2	1455	G	C8-N9-C4	-5.19	104.32	106.40
36	1	954	U	N1-C2-N3	5.19	118.02	114.90
1	6	1196	A	O4'-C1'-N9	5.19	112.35	108.20
1	6	1509	C	N1-C2-O2	5.19	122.02	118.90
36	5	209	A	N7-C8-N9	5.19	116.40	113.80
36	5	3093	C	C2-N3-C4	-5.19	117.30	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2389	C	N1-C2-O2	5.19	122.01	118.90
1	6	543	C	N3-C2-O2	-5.19	118.27	121.90
36	5	1170	A	C5-C6-N6	-5.19	119.55	123.70
37	7	32	U	C5-C6-N1	-5.19	120.11	122.70
1	2	1600	A	N9-C4-C5	-5.19	103.72	105.80
36	1	281	G	N1-C2-N3	5.19	127.01	123.90
36	1	590	G	C5-C6-O6	-5.19	125.49	128.60
36	1	1546	A	N1-C2-N3	-5.19	126.70	129.30
36	1	2365	C	N1-C2-O2	5.19	122.01	118.90
1	6	31	C	N3-C4-N4	-5.19	114.37	118.00
1	2	1426	C	N3-C2-O2	5.19	125.53	121.90
36	1	1331	U	C6-N1-C1'	-5.19	113.94	121.20
36	1	1429	G	C5-N7-C8	5.19	106.89	104.30
36	1	2121	G	N1-C6-O6	-5.19	116.79	119.90
36	1	2795	U	O5'-P-OP1	-5.19	101.03	105.70
36	1	3150	A	C8-N9-C4	5.19	107.88	105.80
61	N5	38	LEU	CA-CB-CG	5.19	127.23	115.30
36	1	95	A	C5-C6-N1	-5.19	115.11	117.70
36	5	3027	A	N1-C6-N6	5.19	121.71	118.60
36	1	1192	C	C2-N1-C1'	5.18	124.50	118.80
36	1	2983	C	C2-N3-C4	-5.18	117.31	119.90
36	1	3323	A	N1-C6-N6	5.18	121.71	118.60
36	5	47	C	C5-C6-N1	-5.18	118.41	121.00
36	5	1302	A	N9-C4-C5	5.18	107.87	105.80
38	8	39	G	C4-N9-C1'	5.18	133.24	126.50
41	l4	359	LEU	CA-CB-CG	5.18	127.22	115.30
35	SM	134	ASP	CB-CG-OD2	5.18	122.97	118.30
36	1	648	C	C5-C4-N4	-5.18	116.57	120.20
36	5	528	U	N3-C2-O2	-5.18	118.57	122.20
36	5	2796	G	N3-C4-N9	5.18	129.11	126.00
36	5	2887	A	O5'-P-OP1	-5.18	101.03	105.70
36	1	29	C	N3-C4-N4	5.18	121.63	118.00
36	1	98	G	N3-C4-N9	-5.18	122.89	126.00
36	1	427	C	C6-N1-C2	-5.18	118.23	120.30
36	1	2520	A	OP2-P-O3'	5.18	116.60	105.20
1	6	965	U	C2-N1-C1'	5.18	123.92	117.70
1	2	779	U	O4'-C1'-N1	5.18	112.34	108.20
36	1	96	G	C6-C5-N7	-5.18	127.29	130.40
36	1	517	G	N7-C8-N9	5.18	115.69	113.10
36	1	797	U	C5-C6-N1	-5.18	120.11	122.70
36	1	1116	G	O5'-P-OP1	-5.18	101.04	105.70
36	1	1441	G	N3-C4-C5	-5.18	126.01	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	417	A	N1-C6-N6	-5.18	115.49	118.60
36	5	934	G	C8-N9-C1'	-5.18	120.27	127.00
36	5	1794	G	N9-C4-C5	-5.18	103.33	105.40
36	5	2366	C	C2-N3-C4	5.18	122.49	119.90
36	5	2584	G	OP2-P-O3'	5.18	116.59	105.20
1	2	795	U	C4-C5-C6	5.18	122.81	119.70
1	6	1779	U	N1-C2-O2	5.18	126.42	122.80
36	5	939	U	C2-N3-C4	-5.18	123.89	127.00
36	1	184	U	N3-C2-O2	-5.18	118.58	122.20
36	1	889	U	N3-C2-O2	-5.18	118.58	122.20
36	1	1330	A	C4-C5-N7	5.18	113.29	110.70
36	1	2618	G	N3-C2-N2	5.18	123.52	119.90
36	1	2939	G	OP2-P-O3'	5.18	116.59	105.20
36	5	884	A	N3-C4-C5	5.18	130.42	126.80
36	5	1130	A	N1-C6-N6	-5.18	115.49	118.60
36	5	1434	G	C2-N3-C4	5.18	114.49	111.90
37	7	102	A	N1-C6-N6	5.18	121.70	118.60
1	2	602	U	O5'-P-OP1	-5.17	101.04	105.70
1	2	782	U	P-O3'-C3'	5.17	125.91	119.70
1	2	1014	G	N9-C4-C5	5.17	107.47	105.40
1	2	1462	G	N1-C6-O6	5.17	123.00	119.90
36	1	201	A	O5'-P-OP1	5.17	116.91	110.70
36	1	958	C	C5-C6-N1	-5.17	118.41	121.00
36	1	964	G	C2-N3-C4	5.17	114.49	111.90
36	1	2400	G	C6-N1-C2	-5.17	122.00	125.10
36	1	2412	G	N3-C4-C5	-5.17	126.01	128.60
1	6	455	C	N1-C2-O2	-5.17	115.80	118.90
1	6	1737	G	N1-C6-O6	5.17	123.00	119.90
36	5	58	G	O5'-P-OP1	5.17	116.91	110.70
36	5	2725	U	OP1-P-OP2	-5.17	111.84	119.60
4	s2	113	LEU	CA-CB-CG	5.17	127.20	115.30
36	5	3298	C	C4-C5-C6	5.17	119.99	117.40
38	8	113	U	C2-N3-C4	5.17	130.10	127.00
36	1	2216	G	O5'-P-OP2	5.17	116.91	110.70
36	1	2874	G	N3-C4-N9	-5.17	122.90	126.00
1	6	280	U	C2-N1-C1'	5.17	123.91	117.70
36	5	1476	G	N7-C8-N9	-5.17	110.51	113.10
36	5	2994	A	C4-C5-C6	5.17	119.59	117.00
36	1	1520	G	C5-N7-C8	5.17	106.89	104.30
1	6	416	A	C5-N7-C8	-5.17	101.31	103.90
36	5	345	G	C5-C6-O6	-5.17	125.50	128.60
36	5	1115	G	N7-C8-N9	5.17	115.69	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2145	A	C6-N1-C2	-5.17	115.50	118.60
36	1	635	G	C5-C6-N1	5.17	114.08	111.50
36	1	2860	U	N3-C2-O2	5.17	125.82	122.20
36	5	99	A	N1-C6-N6	5.17	121.70	118.60
36	5	2340	U	C4-C5-C6	-5.17	116.60	119.70
36	1	582	G	N3-C4-N9	-5.17	122.90	126.00
36	1	765	C	C6-N1-C2	-5.17	118.23	120.30
36	1	2606	G	OP2-P-O3'	5.17	116.57	105.20
36	5	2113	A	O4'-C1'-N9	-5.17	104.07	108.20
1	2	1164	G	C5-C6-O6	-5.17	125.50	128.60
36	1	2385	G	C8-N9-C4	5.17	108.47	106.40
36	1	2614	G	N7-C8-N9	-5.17	110.52	113.10
36	5	3098	G	OP2-P-O3'	5.17	116.56	105.20
44	l7	221	LYS	N-CA-C	-5.17	97.05	111.00
1	2	187	G	P-O3'-C3'	5.16	125.90	119.70
36	1	405	U	C6-N1-C2	5.16	124.10	121.00
36	1	896	A	O4'-C1'-N9	5.16	112.33	108.20
36	1	2761	G	C5-C6-N1	-5.16	108.92	111.50
36	1	3013	U	O5'-P-OP2	-5.16	101.05	105.70
36	5	1879	A	O5'-P-OP2	-5.16	101.05	105.70
36	5	3319	U	O4'-C1'-N1	5.16	112.33	108.20
1	2	1092	A	N9-C4-C5	-5.16	103.73	105.80
36	5	714	G	N1-C6-O6	5.16	123.00	119.90
36	1	197	G	C5-C6-O6	-5.16	125.50	128.60
36	1	980	A	C8-N9-C4	-5.16	103.73	105.80
1	6	144	U	O4'-C1'-N1	5.16	112.33	108.20
36	5	775	A	C8-N9-C4	-5.16	103.74	105.80
36	5	1362	G	OP2-P-O3'	5.16	116.55	105.20
38	8	116	G	C6-C5-N7	-5.16	127.30	130.40
41	l4	134	LEU	CA-CB-CG	5.16	127.17	115.30
36	1	124	U	N3-C2-O2	-5.16	118.59	122.20
36	1	1142	G	C5-C6-N1	5.16	114.08	111.50
1	6	358	U	OP1-P-OP2	5.16	127.34	119.60
36	5	1591	G	C8-N9-C4	-5.16	104.34	106.40
1	6	1656	U	O5'-P-OP1	5.16	116.89	110.70
36	5	393	U	C6-N1-C2	-5.16	117.91	121.00
36	5	2186	U	N1-C2-O2	5.16	126.41	122.80
36	5	2351	U	C6-N1-C2	-5.16	117.91	121.00
1	2	301	A	OP2-P-O3'	5.16	116.54	105.20
36	1	2302	G	N1-C6-O6	-5.16	116.81	119.90
36	1	2974	U	O5'-P-OP1	-5.16	101.06	105.70
36	1	3214	U	C5-C4-O4	5.16	128.99	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	17	C	C5-C6-N1	5.16	123.58	121.00
36	5	289	A	C5-C6-N6	-5.16	119.58	123.70
36	5	895	A	N7-C8-N9	-5.16	111.22	113.80
36	5	1410	U	O5'-P-OP2	-5.16	101.06	105.70
37	7	41	G	C5-C6-O6	-5.16	125.51	128.60
1	2	499	U	C3'-C2'-C1'	5.15	105.62	101.50
36	1	1054	A	N1-C2-N3	-5.15	126.72	129.30
36	5	2848	G	C8-N9-C1'	-5.15	120.30	127.00
1	2	969	C	C6-N1-C2	5.15	122.36	120.30
18	C6	40	GLU	C-N-CA	5.15	143.64	122.00
36	1	158	G	N3-C2-N2	-5.15	116.29	119.90
36	1	714	G	N1-C6-O6	5.15	122.99	119.90
36	1	817	A	N9-C1'-C2'	5.15	120.70	114.00
36	1	932	U	N1-C2-O2	-5.15	119.19	122.80
36	1	1056	U	C5-C6-N1	5.15	125.28	122.70
36	1	2335	G	C5-C6-N1	5.15	114.08	111.50
36	1	2789	U	C6-N1-C2	-5.15	117.91	121.00
36	1	2983	C	N3-C2-O2	-5.15	118.29	121.90
36	1	3022	G	O4'-C1'-N9	5.15	112.32	108.20
36	5	399	A	N1-C2-N3	-5.15	126.72	129.30
36	5	3078	U	N1-C1'-C2'	-5.15	106.33	112.00
36	1	1359	C	C5-C4-N4	-5.15	116.59	120.20
36	1	1359	C	N1-C2-O2	-5.15	115.81	118.90
36	1	2144	A	C5-C6-N1	5.15	120.28	117.70
1	6	965	U	C6-N1-C1'	-5.15	113.99	121.20
1	6	1584	G	OP1-P-O3'	5.15	116.53	105.20
36	5	389	A	N1-C6-N6	-5.15	115.51	118.60
36	5	1875	G	C5-C6-O6	5.15	131.69	128.60
37	7	26	C	C4-C5-C6	5.15	119.97	117.40
1	2	499	U	P-O3'-C3'	5.15	125.88	119.70
36	1	95	A	N1-C2-N3	5.15	131.88	129.30
36	1	1177	G	C5-C6-O6	-5.15	125.51	128.60
38	4	93	U	C2-N1-C1'	5.15	123.88	117.70
1	6	1472	C	N1-C2-O2	-5.15	115.81	118.90
36	5	267	G	O4'-C1'-N9	-5.15	104.08	108.20
36	5	407	A	N9-C4-C5	-5.15	103.74	105.80
36	1	426	G	C8-N9-C1'	-5.15	120.31	127.00
36	1	1445	U	C2-N1-C1'	-5.15	111.52	117.70
36	5	516	A	O5'-P-OP2	-5.15	101.07	105.70
36	5	581	U	C6-N1-C2	-5.15	117.91	121.00
36	5	590	G	C2-N3-C4	5.15	114.47	111.90
36	5	2997	G	N3-C4-C5	5.15	131.17	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1505	C	N3-C4-C5	-5.15	119.84	121.90
37	7	57	G	C5-C6-O6	5.15	131.69	128.60
36	1	756	U	OP2-P-O3'	5.14	116.52	105.20
36	1	1183	C	N3-C2-O2	5.14	125.50	121.90
36	1	2596	U	C5-C4-O4	-5.14	122.81	125.90
36	1	2899	C	C4-C5-C6	5.14	119.97	117.40
36	5	1158	A	N1-C6-N6	5.14	121.69	118.60
36	5	2699	G	C2-N3-C4	5.14	114.47	111.90
36	5	3037	U	N1-C2-N3	5.14	117.99	114.90
1	2	1339	C	C3'-C2'-C1'	5.14	105.61	101.50
36	1	217	U	OP1-P-OP2	5.14	127.31	119.60
36	1	1269	U	N1-C2-O2	5.14	126.40	122.80
36	1	1466	G	N3-C2-N2	5.14	123.50	119.90
36	1	2293	C	N3-C4-N4	5.14	121.60	118.00
1	6	1607	G	C5-C6-O6	5.14	131.69	128.60
36	5	1352	A	P-O3'-C3'	5.14	125.87	119.70
36	5	2112	U	P-O3'-C3'	5.14	125.87	119.70
36	5	2277	C	O5'-P-OP2	-5.14	101.07	105.70
36	1	3107	U	O5'-P-OP2	-5.14	101.07	105.70
36	5	1200	A	N1-C6-N6	5.14	121.69	118.60
36	1	805	G	N3-C4-N9	5.14	129.08	126.00
37	3	58	C	C6-N1-C2	-5.14	118.25	120.30
1	6	457	G	C4-C5-N7	5.14	112.86	110.80
36	5	893	C	N3-C4-C5	-5.14	119.84	121.90
36	5	2796	G	C8-N9-C1'	-5.14	120.32	127.00
36	5	3387	U	N3-C2-O2	-5.14	118.60	122.20
1	2	1200	G	C4-C5-C6	5.14	121.88	118.80
36	1	628	A	N1-C6-N6	5.14	121.68	118.60
36	1	807	A	N1-C6-N6	5.14	121.68	118.60
36	1	1421	G	C5-C6-N1	5.14	114.07	111.50
1	6	1145	U	N1-C2-O2	-5.14	119.20	122.80
36	5	644	G	C5-N7-C8	5.14	106.87	104.30
36	5	2174	G	C6-C5-N7	-5.14	127.32	130.40
47	m0	57	LEU	CA-CB-CG	5.14	127.12	115.30
36	1	608	A	N9-C4-C5	-5.14	103.75	105.80
36	1	878	G	C5-C6-O6	5.14	131.68	128.60
36	1	1661	G	N9-C4-C5	-5.14	103.35	105.40
36	1	2350	C	N1-C2-N3	5.14	122.80	119.20
36	1	2408	U	C2-N1-C1'	5.14	123.86	117.70
1	6	418	G	C6-C5-N7	-5.14	127.32	130.40
36	5	2117	A	C5-C6-N6	5.14	127.81	123.70
36	5	2401	A	O5'-P-OP1	-5.14	101.08	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	694	U	C2-N1-C1'	5.13	123.86	117.70
36	1	1197	A	C4-C5-C6	5.13	119.57	117.00
39	L2	123	ARG	NE-CZ-NH1	-5.13	117.73	120.30
53	M7	19	GLY	N-CA-C	-5.13	100.26	113.10
36	5	960	U	OP1-P-O3'	-5.13	93.90	105.20
36	5	1926	C	C6-N1-C2	5.13	122.35	120.30
36	5	2377	G	N3-C2-N2	5.13	123.49	119.90
36	1	1556	C	C6-N1-C1'	-5.13	114.64	120.80
36	1	2144	A	N1-C6-N6	5.13	121.68	118.60
36	1	2400	G	N1-C6-O6	5.13	122.98	119.90
36	1	2726	C	C2-N3-C4	-5.13	117.33	119.90
36	1	3306	U	O5'-P-OP2	-5.13	101.08	105.70
37	3	82	G	N3-C4-N9	5.13	129.08	126.00
1	6	380	U	N3-C2-O2	-5.13	118.61	122.20
1	6	1624	C	O5'-P-OP1	-5.13	101.08	105.70
36	5	1099	A	N1-C6-N6	5.13	121.68	118.60
36	5	2654	C	N3-C2-O2	5.13	125.49	121.90
37	7	49	G	O4'-C1'-N9	5.13	112.31	108.20
36	1	215	G	N3-C4-C5	-5.13	126.03	128.60
1	6	970	A	P-O3'-C3'	5.13	125.86	119.70
36	1	2192	C	C4-C5-C6	5.13	119.96	117.40
36	1	3267	A	N1-C6-N6	-5.13	115.52	118.60
36	5	280	U	C5-C4-O4	-5.13	122.82	125.90
36	5	1541	G	N9-C4-C5	-5.13	103.35	105.40
37	7	8	G	N3-C4-C5	-5.13	126.04	128.60
38	8	104	A	N9-C4-C5	-5.13	103.75	105.80
36	1	351	A	C8-N9-C4	5.13	107.85	105.80
36	1	356	C	C6-N1-C2	5.13	122.35	120.30
36	1	545	U	C2-N1-C1'	5.13	123.85	117.70
36	1	1000	C	O4'-C1'-N1	5.13	112.30	108.20
36	1	2572	C	C6-N1-C2	-5.13	118.25	120.30
36	1	2772	C	O3'-P-O5'	5.13	113.74	104.00
1	6	1043	A	O5'-P-OP2	-5.13	101.09	105.70
1	2	1479	A	N1-C6-N6	5.12	121.67	118.60
36	1	425	G	C8-N9-C4	-5.12	104.35	106.40
1	6	664	U	C2-N1-C1'	5.12	123.85	117.70
1	2	1314	U	N1-C2-N3	5.12	117.97	114.90
36	1	1122	U	N3-C4-C5	5.12	117.67	114.60
36	1	2402	A	N9-C4-C5	5.12	107.85	105.80
1	6	265	A	N1-C6-N6	5.12	121.67	118.60
1	6	794	U	OP2-P-O3'	5.12	116.47	105.20
36	5	2857	C	C5-C6-N1	-5.12	118.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	58	G	N1-C6-O6	5.12	122.97	119.90
36	5	358	G	N1-C6-O6	5.12	122.97	119.90
36	5	1166	G	C5-C6-O6	5.12	131.67	128.60
36	5	1364	C	OP2-P-O3'	5.12	116.47	105.20
36	5	2712	U	C5-C4-O4	5.12	128.97	125.90
36	5	2838	A	C5-C6-N6	-5.12	119.60	123.70
36	1	663	C	N3-C4-N4	5.12	121.58	118.00
36	1	1659	U	C6-N1-C2	-5.12	117.93	121.00
36	1	1414	G	OP1-P-O3'	5.12	116.46	105.20
36	1	2396	G	C5-N7-C8	5.12	106.86	104.30
38	4	73	U	C4-C5-C6	-5.12	116.63	119.70
1	6	339	C	OP2-P-O3'	5.12	116.46	105.20
1	6	1137	A	C8-N9-C4	5.12	107.85	105.80
36	5	1338	C	N3-C2-O2	5.12	125.48	121.90
36	5	1390	A	C4-C5-N7	-5.12	108.14	110.70
36	5	1487	G	C5-C6-O6	5.12	131.67	128.60
36	5	2849	C	N3-C4-C5	-5.12	119.85	121.90
37	7	39	C	C6-N1-C2	-5.12	118.25	120.30
1	2	144	U	N3-C2-O2	-5.12	118.62	122.20
1	2	937	C	C6-N1-C2	-5.12	118.25	120.30
36	1	2714	G	C4-N9-C1'	-5.12	119.85	126.50
37	3	88	G	N3-C4-N9	5.12	129.07	126.00
36	1	3006	A	O5'-P-OP1	-5.12	101.09	105.70
36	5	1110	U	N3-C2-O2	-5.12	118.62	122.20
1	2	305	C	C6-N1-C2	-5.11	118.25	120.30
1	2	1096	C	C6-N1-C1'	-5.11	114.66	120.80
24	D2	93	LEU	CA-CB-CG	5.11	127.06	115.30
36	1	2409	G	C5-C6-O6	5.11	131.67	128.60
1	6	1000	C	N3-C2-O2	-5.11	118.32	121.90
36	5	645	A	N1-C2-N3	5.11	131.86	129.30
36	5	897	U	N1-C2-N3	5.11	117.97	114.90
36	5	1422	G	N7-C8-N9	5.11	115.66	113.10
36	5	2113	A	C8-N9-C4	5.11	107.84	105.80
36	5	2978	U	OP2-P-O3'	5.11	116.45	105.20
36	1	371	G	O5'-P-OP2	-5.11	101.10	105.70
36	1	1480	G	O5'-P-OP2	-5.11	101.10	105.70
37	3	39	C	OP1-P-OP2	5.11	127.27	119.60
36	5	1307	G	OP1-P-OP2	5.11	127.27	119.60
36	5	1321	G	C5-C6-N1	-5.11	108.94	111.50
36	5	2817	A	C2-N3-C4	5.11	113.16	110.60
36	5	2956	A	N7-C8-N9	5.11	116.36	113.80
36	5	3127	A	C5-C6-N1	5.11	120.26	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1650	U	C5-C6-N1	-5.11	120.14	122.70
36	1	97	U	OP2-P-O3'	5.11	116.44	105.20
36	1	158	G	N1-C6-O6	5.11	122.97	119.90
36	1	1586	G	O5'-P-OP2	-5.11	101.10	105.70
36	5	672	A	N9-C4-C5	-5.11	103.76	105.80
36	5	1202	A	O5'-P-OP1	-5.11	101.10	105.70
36	5	2619	G	C5-C6-O6	-5.11	125.53	128.60
36	1	933	A	N3-C4-C5	-5.11	123.22	126.80
41	L4	186	LYS	CD-CE-NZ	5.11	123.45	111.70
36	1	767	U	O4'-C1'-N1	5.11	112.29	108.20
36	1	799	G	OP1-P-O3'	5.11	116.44	105.20
44	L7	216	VAL	N-CA-C	5.11	124.79	111.00
36	5	1678	G	N1-C6-O6	-5.11	116.83	119.90
36	1	652	G	O5'-P-OP2	-5.11	101.11	105.70
36	1	1378	U	C2-N1-C1'	5.11	123.83	117.70
36	1	2383	C	O5'-P-OP1	-5.11	101.11	105.70
36	5	205	C	N3-C4-N4	-5.11	114.43	118.00
36	5	1476	G	C4-N9-C1'	-5.11	119.86	126.50
36	5	1868	G	N9-C4-C5	-5.11	103.36	105.40
36	5	2941	A	C8-N9-C4	5.11	107.84	105.80
36	5	2971	A	C4-C5-N7	5.11	113.25	110.70
36	5	2978	U	P-O3'-C3'	5.11	125.83	119.70
36	5	3051	U	N3-C2-O2	-5.11	118.63	122.20
36	5	3374	U	N3-C4-O4	-5.11	115.83	119.40
36	1	341	G	C5-C6-N1	5.10	114.05	111.50
36	5	1476	G	N3-C4-N9	-5.10	122.94	126.00
38	8	80	A	N3-C4-C5	-5.10	123.23	126.80
36	1	340	C	N3-C4-C5	5.10	123.94	121.90
36	1	2957	G	N9-C4-C5	5.10	107.44	105.40
1	6	2	A	O5'-P-OP1	5.10	116.82	110.70
36	5	1119	C	N3-C4-C5	5.10	123.94	121.90
36	5	2130	G	O5'-P-OP2	-5.10	101.11	105.70
36	1	608	A	N3-C4-N9	5.10	131.48	127.40
41	L4	194	TYR	CA-CB-CG	5.10	123.09	113.40
36	5	642	U	C5-C6-N1	-5.10	120.15	122.70
36	5	999	G	C5-C6-O6	5.10	131.66	128.60
36	5	2389	C	C5-C6-N1	-5.10	118.45	121.00
1	2	590	C	C2-N1-C1'	5.10	124.41	118.80
36	1	1127	G	C6-C5-N7	-5.10	127.34	130.40
36	1	1332	A	OP2-P-O3'	5.10	116.41	105.20
36	1	1436	U	OP1-P-OP2	-5.10	111.95	119.60
36	1	2984	C	N3-C4-N4	-5.10	114.43	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1300	G	C5-C6-O6	-5.10	125.54	128.60
37	7	67	G	N3-C2-N2	-5.10	116.33	119.90
36	1	675	C	N3-C2-O2	5.10	125.47	121.90
36	1	1389	G	C5-N7-C8	-5.10	101.75	104.30
36	5	3153	U	N1-C2-O2	5.10	126.37	122.80
36	1	828	A	C4-C5-C6	5.09	119.55	117.00
36	1	1317	A	N1-C2-N3	-5.09	126.75	129.30
36	1	2875	U	C6-N1-C1'	-5.09	114.07	121.20
36	1	3154	C	C2-N1-C1'	5.09	124.40	118.80
1	6	1136	U	C5-C6-N1	5.09	125.25	122.70
1	6	1588	G	N1-C6-O6	-5.09	116.84	119.90
36	5	810	A	C2-N3-C4	5.09	113.15	110.60
36	5	1387	G	OP1-P-OP2	5.09	127.24	119.60
36	1	943	U	N3-C2-O2	-5.09	118.64	122.20
36	1	999	G	C5-C6-N1	5.09	114.05	111.50
36	1	1153	A	N1-C6-N6	5.09	121.66	118.60
36	1	2679	A	C2-N3-C4	-5.09	108.05	110.60
36	5	1434	G	C5-N7-C8	-5.09	101.75	104.30
36	5	2215	A	C2-N3-C4	-5.09	108.05	110.60
36	5	2353	G	N3-C2-N2	-5.09	116.33	119.90
36	1	363	G	C6-C5-N7	-5.09	127.34	130.40
36	1	633	C	C4-C5-C6	5.09	119.94	117.40
36	1	930	U	N3-C4-O4	-5.09	115.83	119.40
36	1	2867	C	C6-N1-C2	5.09	122.34	120.30
1	6	1615	C	C3'-C2'-C1'	5.09	105.57	101.50
36	5	641	C	OP1-P-OP2	5.09	127.24	119.60
36	5	1455	U	OP1-P-O3'	5.09	116.40	105.20
36	5	1607	U	C6-N1-C2	-5.09	117.95	121.00
36	5	2116	G	C6-C5-N7	-5.09	127.34	130.40
36	5	2633	U	OP1-P-O3'	5.09	116.40	105.20
1	2	335	U	N1-C2-O2	-5.09	119.24	122.80
24	D2	104	LEU	CA-CB-CG	5.09	127.01	115.30
36	1	2238	G	O5'-P-OP2	5.09	116.81	110.70
36	1	2885	C	C6-N1-C2	5.09	122.33	120.30
1	6	418	G	N1-C6-O6	5.09	122.95	119.90
36	5	424	G	N9-C4-C5	-5.09	103.36	105.40
36	5	909	G	N1-C6-O6	-5.09	116.85	119.90
36	5	1445	U	N1-C2-O2	-5.09	119.24	122.80
36	5	2645	G	N1-C6-O6	-5.09	116.85	119.90
36	5	2783	U	O5'-P-OP1	5.09	116.81	110.70
36	1	2373	A	O5'-P-OP1	-5.09	101.12	105.70
36	5	1004	U	N3-C2-O2	-5.09	118.64	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1305	U	C5-C4-O4	5.09	128.95	125.90
1	2	1781	A	C5-C6-N6	5.09	127.77	123.70
36	5	2606	G	C5-C6-O6	5.09	131.65	128.60
36	5	3272	C	C5-C6-N1	-5.09	118.46	121.00
37	7	48	U	C5-C4-O4	-5.09	122.85	125.90
36	1	92	G	C4-C5-N7	5.08	112.83	110.80
36	1	948	C	O5'-P-OP1	5.08	116.80	110.70
36	1	2699	G	C5-C6-O6	-5.08	125.55	128.60
38	4	4	C	C6-N1-C1'	-5.08	114.70	120.80
36	5	2215	A	C8-N9-C4	5.08	107.83	105.80
37	7	120	C	C5-C6-N1	-5.08	118.46	121.00
36	1	1834	U	N3-C4-C5	-5.08	111.55	114.60
36	5	2531	C	C6-N1-C2	-5.08	118.27	120.30
36	5	2817	A	OP2-P-O3'	5.08	116.39	105.20
36	5	3113	A	C5-N7-C8	5.08	106.44	103.90
36	1	810	A	OP1-P-OP2	-5.08	111.98	119.60
36	1	1103	A	N3-C4-N9	5.08	131.47	127.40
36	1	1822	C	C6-N1-C2	-5.08	118.27	120.30
36	1	2424	A	N1-C2-N3	-5.08	126.76	129.30
36	1	2828	G	N3-C4-N9	5.08	129.05	126.00
36	5	264	G	C4-C5-N7	5.08	112.83	110.80
36	5	2372	A	N7-C8-N9	5.08	116.34	113.80
37	7	99	G	N3-C2-N2	5.08	123.46	119.90
36	1	1144	U	N1-C2-N3	5.08	117.95	114.90
36	5	2608	G	N3-C2-N2	5.08	123.46	119.90
36	5	2796	G	C6-C5-N7	-5.08	127.35	130.40
36	1	1307	G	C5'-C4'-O4'	-5.08	103.01	109.10
36	1	2314	U	O5'-P-OP2	-5.08	101.13	105.70
36	1	3055	U	C6-N1-C2	5.08	124.05	121.00
38	4	93	U	N3-C4-O4	5.08	122.95	119.40
36	5	945	C	N1-C2-O2	5.08	121.95	118.90
36	5	412	G	C8-N9-C4	-5.08	104.37	106.40
36	5	948	C	N3-C4-N4	5.08	121.55	118.00
36	1	42	C	C6-N1-C2	-5.08	118.27	120.30
36	1	2632	G	N3-C2-N2	5.08	123.45	119.90
36	1	2923	U	C6-N1-C2	5.08	124.05	121.00
38	4	4	C	C2-N1-C1'	5.08	124.38	118.80
56	N0	14	LEU	CB-CG-CD1	-5.08	102.37	111.00
71	O5	36	LEU	CA-CB-CG	5.08	126.97	115.30
36	5	840	C	O5'-P-OP2	-5.08	101.13	105.70
36	1	1195	A	O5'-P-OP1	-5.07	101.13	105.70
36	1	2865	U	N3-C2-O2	5.07	125.75	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2944	U	C5-C6-N1	5.07	125.24	122.70
36	1	2964	G	O5'-P-OP2	-5.07	101.13	105.70
36	5	192	C	N3-C4-C5	-5.07	119.87	121.90
36	5	880	G	C8-N9-C1'	5.07	133.59	127.00
36	5	1667	A	N1-C6-N6	5.07	121.64	118.60
36	5	1846	C	C5-C6-N1	-5.07	118.46	121.00
36	5	2656	A	C5-C6-N6	5.07	127.76	123.70
37	7	83	U	N3-C4-C5	5.07	117.64	114.60
1	2	70	C	C6-N1-C2	5.07	122.33	120.30
36	1	969	C	C2-N3-C4	-5.07	117.36	119.90
36	1	1336	U	OP1-P-OP2	-5.07	111.99	119.60
36	1	1893	A	C8-N9-C4	-5.07	103.77	105.80
36	5	530	G	O4'-C1'-N9	5.07	112.26	108.20
36	5	824	C	N3-C2-O2	-5.07	118.35	121.90
1	2	1596	C	N1-C2-O2	5.07	121.94	118.90
36	1	1332	A	N7-C8-N9	5.07	116.34	113.80
36	1	1344	G	N9-C4-C5	-5.07	103.37	105.40
36	1	1371	G	OP2-P-O3'	5.07	116.36	105.20
1	6	1615	C	N1-C1'-C2'	-5.07	106.42	112.00
36	5	1041	U	O5'-P-OP2	-5.07	101.14	105.70
36	5	1838	G	OP1-P-O3'	5.07	116.36	105.20
36	5	1894	U	C2-N1-C1'	-5.07	111.61	117.70
36	5	3128	G	N3-C4-N9	5.07	129.04	126.00
36	1	2643	A	N9-C4-C5	-5.07	103.77	105.80
1	6	1667	A	OP1-P-OP2	-5.07	112.00	119.60
36	5	1314	C	C6-N1-C1'	-5.07	114.72	120.80
36	5	2145	A	C8-N9-C4	-5.07	103.77	105.80
36	5	2951	G	OP1-P-O3'	5.07	116.35	105.20
36	1	28	C	C4-C5-C6	-5.07	114.87	117.40
36	1	782	U	N3-C4-C5	5.07	117.64	114.60
36	1	816	A	O5'-P-OP2	-5.07	101.14	105.70
36	1	1683	A	C5-C6-N6	-5.07	119.65	123.70
36	1	2400	G	N1-C2-N2	5.07	120.76	116.20
36	1	2611	U	N3-C4-C5	5.07	117.64	114.60
1	6	911	U	C6-N1-C2	-5.07	117.96	121.00
1	6	1117	U	N3-C4-C5	-5.07	111.56	114.60
36	5	2376	G	N7-C8-N9	5.07	115.63	113.10
36	5	2856	G	OP1-P-O3'	5.07	116.35	105.20
1	2	187	G	OP1-P-O3'	5.07	116.35	105.20
36	1	69	C	N3-C4-C5	-5.07	119.87	121.90
36	1	666	A	C4-C5-C6	-5.07	114.47	117.00
36	1	1515	A	C6-C5-N7	-5.07	128.75	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	96	G	OP2-P-O3'	5.07	116.34	105.20
36	5	1436	U	C5-C4-O4	-5.07	122.86	125.90
36	5	2926	A	C8-N9-C4	-5.07	103.77	105.80
36	1	2408	U	N1-C2-O2	5.06	126.34	122.80
36	1	3316	A	C2-N3-C4	-5.06	108.07	110.60
1	6	418	G	C4-C5-N7	5.06	112.83	110.80
36	5	406	G	C5-C6-N1	5.06	114.03	111.50
36	5	803	C	N3-C4-N4	5.06	121.55	118.00
36	5	2135	U	N1-C2-N3	-5.06	111.86	114.90
36	5	2620	G	N9-C4-C5	5.06	107.43	105.40
36	5	1430	U	N1-C2-N3	-5.06	111.86	114.90
36	5	2310	U	N3-C2-O2	-5.06	118.66	122.20
36	1	718	G	N7-C8-N9	5.06	115.63	113.10
36	1	3382	U	N3-C2-O2	-5.06	118.66	122.20
36	5	2794	G	N1-C6-O6	5.06	122.94	119.90
1	2	404	G	C8-N9-C4	5.06	108.42	106.40
36	1	2126	A	N9-C4-C5	-5.06	103.78	105.80
36	1	2964	G	OP1-P-O3'	5.06	116.33	105.20
37	3	73	C	N1-C2-O2	5.06	121.94	118.90
36	5	648	C	O5'-P-OP1	-5.06	101.15	105.70
36	5	2394	G	OP1-P-O3'	5.06	116.33	105.20
36	1	907	G	O4'-C1'-N9	5.06	112.25	108.20
36	1	1304	A	N1-C6-N6	-5.06	115.57	118.60
36	1	1510	G	N3-C4-C5	-5.06	126.07	128.60
36	1	2120	A	O5'-P-OP2	-5.06	101.15	105.70
37	3	103	A	OP2-P-O3'	5.06	116.33	105.20
36	5	359	U	OP1-P-OP2	-5.06	112.01	119.60
36	5	884	A	C4-N9-C1'	-5.06	117.20	126.30
37	7	86	U	C2-N3-C4	-5.06	123.97	127.00
1	6	1600	A	C4-C5-N7	5.06	113.23	110.70
36	5	2433	U	N3-C4-C5	5.06	117.63	114.60
36	5	2725	U	N3-C4-C5	5.06	117.63	114.60
36	1	863	C	OP2-P-O3'	5.05	116.32	105.20
36	1	1135	A	O5'-P-OP2	-5.05	101.15	105.70
36	1	1496	C	N1-C2-O2	5.05	121.93	118.90
1	6	1549	C	C6-N1-C2	-5.05	118.28	120.30
36	5	35	A	N1-C6-N6	5.05	121.63	118.60
36	5	3245	A	C5-C6-N1	-5.05	115.17	117.70
36	1	2525	G	C4-C5-N7	5.05	112.82	110.80
36	1	3311	C	C6-N1-C2	5.05	122.32	120.30
36	5	2281	A	N1-C6-N6	5.05	121.63	118.60
36	5	2402	A	N3-C4-N9	-5.05	123.36	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2729	U	C5-C4-O4	5.05	128.93	125.90
1	2	1120	U	N3-C2-O2	-5.05	118.66	122.20
36	1	1901	A	N1-C6-N6	-5.05	115.57	118.60
36	1	2244	A	P-O3'-C3'	5.05	125.76	119.70
1	6	514	G	N3-C2-N2	5.05	123.44	119.90
36	5	217	U	C5-C6-N1	-5.05	120.17	122.70
36	5	431	U	N3-C4-C5	5.05	117.63	114.60
36	5	1072	G	OP1-P-O3'	5.05	116.31	105.20
36	5	1159	A	O5'-P-OP2	5.05	116.76	110.70
36	5	1416	C	N3-C2-O2	-5.05	118.36	121.90
36	5	2176	U	C2-N1-C1'	5.05	123.76	117.70
36	5	2860	U	C6-N1-C2	5.05	124.03	121.00
36	1	936	A	C5-N7-C8	-5.05	101.38	103.90
36	1	946	U	N1-C2-N3	5.05	117.93	114.90
36	1	2899	C	C6-N1-C1'	-5.05	114.74	120.80
36	5	835	G	C5-C6-N1	5.05	114.03	111.50
36	5	1919	G	N1-C6-O6	5.05	122.93	119.90
36	5	2796	G	C5-C6-O6	-5.05	125.57	128.60
36	5	2980	U	N3-C4-O4	-5.05	115.86	119.40
44	l7	229	PHE	CB-CG-CD2	-5.05	117.27	120.80
36	1	933	A	C6-N1-C2	-5.05	115.57	118.60
36	1	1607	U	C6-N1-C2	-5.05	117.97	121.00
36	1	3172	A	N9-C4-C5	-5.05	103.78	105.80
36	5	1514	G	C5-C6-O6	-5.05	125.57	128.60
36	5	2719	U	N1-C2-N3	5.05	117.93	114.90
36	5	3048	A	O5'-P-OP2	-5.05	101.16	105.70
31	D9	36	LEU	CA-CB-CG	5.05	126.91	115.30
36	1	59	G	C6-C5-N7	-5.05	127.37	130.40
36	1	2123	G	N7-C8-N9	-5.05	110.58	113.10
36	1	3209	A	C5-N7-C8	-5.05	101.38	103.90
38	4	40	A	C4-N9-C1'	5.05	135.38	126.30
38	4	103	G	N7-C8-N9	5.05	115.62	113.10
1	6	600	U	O5'-P-OP2	-5.05	101.16	105.70
36	5	413	U	N3-C2-O2	5.05	125.73	122.20
36	5	419	G	N3-C2-N2	5.05	123.43	119.90
36	5	788	C	N1-C2-O2	-5.05	115.87	118.90
36	5	2350	C	O5'-P-OP1	5.05	116.75	110.70
36	5	3150	A	N1-C6-N6	5.05	121.63	118.60
36	5	2607	G	OP2-P-O3'	5.04	116.30	105.20
36	5	2917	G	N1-C6-O6	5.04	122.93	119.90
36	1	1508	C	C5-C6-N1	5.04	123.52	121.00
36	1	2215	A	C8-N9-C4	5.04	107.82	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2772	C	C3'-C2'-C1'	-5.04	97.47	101.50
1	6	977	A	N9-C4-C5	-5.04	103.78	105.80
1	6	1082	C	OP1-P-OP2	5.04	127.16	119.60
1	2	412	A	N1-C6-N6	5.04	121.62	118.60
36	1	1064	A	O4'-C1'-N9	-5.04	104.17	108.20
36	1	1081	U	C2-N1-C1'	5.04	123.75	117.70
37	3	86	U	OP1-P-O3'	5.04	116.29	105.20
36	5	1199	C	N3-C4-C5	-5.04	119.88	121.90
36	5	1304	A	N1-C6-N6	5.04	121.62	118.60
1	2	337	G	C4-C5-N7	5.04	112.82	110.80
38	4	116	G	C8-N9-C1'	-5.04	120.45	127.00
54	M8	138	LEU	CA-CB-CG	5.04	126.89	115.30
36	5	1898	G	O4'-C1'-N9	5.04	112.23	108.20
36	5	2618	G	N3-C4-N9	5.04	129.02	126.00
36	5	3144	G	C5-C6-O6	5.04	131.62	128.60
36	1	705	A	OP1-P-O3'	5.04	116.29	105.20
36	1	1315	U	N3-C2-O2	-5.04	118.67	122.20
36	1	1685	C	N3-C2-O2	-5.04	118.37	121.90
36	1	2351	U	O5'-P-OP2	5.04	116.75	110.70
65	N9	20	GLY	N-CA-C	5.04	125.70	113.10
36	5	425	G	N1-C6-O6	5.04	122.92	119.90
36	5	1336	U	OP2-P-O3'	5.04	116.28	105.20
36	5	1733	G	C6-C5-N7	-5.04	127.38	130.40
36	5	2400	G	O5'-P-OP2	-5.04	101.17	105.70
36	5	2992	U	N1-C2-O2	5.04	126.33	122.80
36	5	1082	U	N1-C2-O2	-5.04	119.27	122.80
1	2	501	U	P-O3'-C3'	5.04	125.74	119.70
36	1	873	C	C6-N1-C2	-5.04	118.29	120.30
36	1	1002	A	C4-C5-C6	-5.04	114.48	117.00
36	1	1115	G	P-O3'-C3'	5.04	125.74	119.70
36	1	2249	G	C5-C6-N1	5.04	114.02	111.50
36	1	2857	C	C5-C4-N4	-5.04	116.67	120.20
38	4	112	U	C2-N1-C1'	-5.04	111.66	117.70
38	4	125	U	C2-N1-C1'	5.04	123.74	117.70
1	6	472	U	N1-C2-N3	5.04	117.92	114.90
36	5	200	C	C5-C4-N4	-5.04	116.68	120.20
36	5	530	G	N9-C4-C5	5.04	107.41	105.40
36	5	1060	U	C6-N1-C2	5.04	124.02	121.00
36	5	1434	G	C5-C6-O6	-5.04	125.58	128.60
36	5	1912	U	N1-C2-O2	-5.04	119.28	122.80
36	5	2687	G	N3-C4-C5	-5.04	126.08	128.60
36	1	304	G	C5-C6-N1	5.03	114.02	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	304	G	N9-C4-C5	5.03	107.41	105.40
36	1	417	A	C5-C6-N6	-5.03	119.67	123.70
36	1	828	A	C6-C5-N7	-5.03	128.78	132.30
36	1	1213	G	C5'-C4'-O4'	-5.03	103.06	109.10
36	1	1392	G	N1-C2-N3	-5.03	120.88	123.90
38	4	111	A	N1-C6-N6	5.03	121.62	118.60
36	5	884	A	N3-C4-N9	-5.03	123.37	127.40
36	5	1586	G	C6-C5-N7	-5.03	127.38	130.40
36	5	3276	G	OP1-P-OP2	-5.03	112.05	119.60
36	1	1380	G	O5'-P-OP2	-5.03	101.17	105.70
36	1	665	A	N1-C6-N6	-5.03	115.58	118.60
36	5	1085	A	O5'-P-OP1	-5.03	101.17	105.70
36	5	1171	G	C6-N1-C2	-5.03	122.08	125.10
36	5	1183	C	N3-C4-C5	5.03	123.91	121.90
36	5	2204	C	N3-C4-N4	-5.03	114.48	118.00
36	5	3115	C	C6-N1-C2	-5.03	118.29	120.30
38	8	109	A	O5'-P-OP2	-5.03	101.17	105.70
36	5	2374	C	N3-C2-O2	5.03	125.42	121.90
1	2	53	G	N1-C6-O6	-5.03	116.88	119.90
1	2	305	C	N3-C2-O2	-5.03	118.38	121.90
36	1	681	U	C2-N3-C4	-5.03	123.98	127.00
36	1	1177	G	N1-C6-O6	5.03	122.92	119.90
36	1	1352	A	P-O3'-C3'	5.03	125.73	119.70
36	1	2176	U	N3-C4-O4	-5.03	115.88	119.40
36	5	673	U	C2-N3-C4	-5.03	123.98	127.00
36	5	749	C	N1-C2-O2	-5.03	115.88	118.90
36	5	779	G	OP2-P-O3'	5.03	116.26	105.20
36	5	981	U	C5-C6-N1	5.03	125.21	122.70
36	5	3314	A	OP2-P-O3'	5.03	116.26	105.20
1	2	794	U	N3-C2-O2	-5.03	118.68	122.20
1	2	1747	G	C2-N3-C4	-5.03	109.39	111.90
36	1	659	G	C5-C6-O6	-5.03	125.58	128.60
36	1	2123	G	C8-N9-C4	5.03	108.41	106.40
36	1	2311	G	C5-N7-C8	-5.03	101.79	104.30
1	6	1124	A	N9-C4-C5	-5.03	103.79	105.80
25	d3	104	LEU	CB-CG-CD1	-5.03	102.45	111.00
36	5	410	U	O5'-P-OP1	-5.03	101.18	105.70
36	5	1521	G	N1-C2-N2	-5.03	111.68	116.20
36	5	2319	U	OP1-P-O3'	5.03	116.26	105.20
36	5	2383	C	N3-C2-O2	5.03	125.42	121.90
38	8	109	A	C5-C6-N1	5.03	120.21	117.70
36	1	78	U	N1-C2-O2	-5.02	119.28	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	419	G	N3-C4-N9	5.02	129.01	126.00
36	1	1300	G	C8-N9-C1'	-5.02	120.47	127.00
36	1	1389	G	O5'-P-OP1	-5.02	101.18	105.70
36	1	2122	G	O5'-P-OP2	-5.02	101.18	105.70
1	6	622	A	N1-C6-N6	-5.02	115.58	118.60
36	5	361	A	C5-C6-N6	5.02	127.72	123.70
36	5	892	U	N3-C4-C5	5.02	117.61	114.60
36	5	1412	G	N3-C4-N9	-5.02	122.99	126.00
38	8	104	A	C8-N9-C4	5.02	107.81	105.80
52	m6	28	LEU	CA-CB-CG	-5.02	103.74	115.30
36	1	2621	G	OP1-P-OP2	-5.02	112.07	119.60
36	1	2714	G	C4-C5-N7	5.02	112.81	110.80
36	1	3316	A	N3-C4-C5	5.02	130.32	126.80
36	5	86	G	O5'-P-OP1	5.02	116.73	110.70
36	5	1830	G	O5'-P-OP2	-5.02	101.18	105.70
36	5	2279	A	C5-C6-N6	-5.02	119.68	123.70
1	2	1212	G	C4-C5-N7	5.02	112.81	110.80
36	1	2912	G	C5-C6-N1	5.02	114.01	111.50
1	6	1581	C	N3-C4-C5	5.02	123.91	121.90
36	5	133	U	N3-C2-O2	-5.02	118.69	122.20
36	5	2271	A	N1-C2-N3	-5.02	126.79	129.30
1	2	1324	G	C8-N9-C1'	5.02	133.53	127.00
36	1	922	U	C4-C5-C6	-5.02	116.69	119.70
36	1	1141	C	C4-C5-C6	5.02	119.91	117.40
1	6	297	U	C5-C4-O4	-5.02	122.89	125.90
36	5	497	C	OP2-P-O3'	5.02	116.24	105.20
1	2	310	C	C6-N1-C2	-5.02	118.29	120.30
36	1	1330	A	C8-N9-C4	5.02	107.81	105.80
36	1	2986	U	N1-C2-O2	-5.02	119.29	122.80
36	5	925	A	C8-N9-C4	5.02	107.81	105.80
36	5	3200	G	C5-C6-O6	-5.02	125.59	128.60
36	5	3368	U	C2-N1-C1'	-5.02	111.68	117.70
36	1	73	C	C6-N1-C2	5.02	122.31	120.30
36	1	636	C	O5'-P-OP2	5.02	116.72	110.70
36	5	617	G	N9-C4-C5	-5.02	103.39	105.40
36	5	1126	G	C8-N9-C4	-5.02	104.39	106.40
36	5	2913	C	N1-C2-O2	-5.02	115.89	118.90
36	5	3027	A	C5-C6-N6	-5.02	119.69	123.70
1	2	581	U	C5-C6-N1	5.01	125.21	122.70
36	1	1169	A	OP1-P-OP2	-5.01	112.08	119.60
36	1	2322	C	C2-N1-C1'	-5.01	113.28	118.80
36	1	3318	G	N3-C4-C5	-5.01	126.09	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	408	C	O5'-P-OP2	-5.01	101.19	105.70
36	5	674	G	N9-C4-C5	5.01	107.41	105.40
36	5	927	C	O5'-P-OP1	-5.01	101.19	105.70
36	5	1044	U	OP1-P-OP2	-5.01	112.08	119.60
36	5	2413	A	C2-N3-C4	-5.01	108.09	110.60
36	5	2875	U	C4-C5-C6	5.01	122.71	119.70
36	1	988	U	C6-N1-C2	5.01	124.01	121.00
36	1	1154	A	C8-N9-C4	-5.01	103.80	105.80
36	1	1880	U	N3-C2-O2	5.01	125.71	122.20
36	1	3055	U	C2-N3-C4	-5.01	123.99	127.00
36	5	1132	C	N3-C4-N4	-5.01	114.49	118.00
6	S4	38	LEU	CA-CB-CG	5.01	126.83	115.30
36	1	1446	A	N1-C6-N6	5.01	121.61	118.60
36	1	2373	A	C5'-C4'-O4'	-5.01	103.09	109.10
36	5	2805	G	C5-C6-O6	-5.01	125.59	128.60
36	5	2939	G	N1-C2-N2	5.01	120.71	116.20
36	1	295	A	N7-C8-N9	5.01	116.31	113.80
36	1	859	G	C8-N9-C1'	-5.01	120.49	127.00
36	5	180	C	N3-C2-O2	-5.01	118.39	121.90
36	5	909	G	C4-C5-N7	-5.01	108.80	110.80
36	5	2155	G	N1-C2-N3	-5.01	120.89	123.90
36	5	2724	U	C5-C4-O4	5.01	128.91	125.90
36	5	2974	U	OP1-P-O3'	5.01	116.22	105.20
36	5	3131	U	O5'-P-OP1	-5.01	101.19	105.70
36	1	1476	G	N1-C6-O6	-5.01	116.89	119.90
36	1	1870	C	N3-C4-C5	5.01	123.90	121.90
37	3	89	G	C5-N7-C8	5.01	106.80	104.30
36	5	216	G	C6-C5-N7	-5.01	127.39	130.40
36	5	2728	G	O4'-C1'-N9	5.01	112.21	108.20
36	1	608	A	C4-C5-C6	5.01	119.50	117.00
36	1	2714	G	C8-N9-C1'	5.01	133.51	127.00
78	Q2	71	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	6	163	G	C4-N9-C1'	-5.01	119.99	126.50
1	6	804	A	C8-N9-C4	5.01	107.80	105.80
36	5	170	G	C4-N9-C1'	5.01	133.01	126.50
36	5	867	G	N9-C4-C5	-5.01	103.40	105.40
36	5	1393	A	C5-N7-C8	-5.01	101.40	103.90
36	5	1492	G	C4-C5-N7	5.01	112.80	110.80
36	5	1683	A	N1-C6-N6	5.01	121.60	118.60
36	5	3082	C	O5'-P-OP2	-5.01	101.19	105.70
36	5	3084	C	N3-C4-C5	5.01	123.90	121.90
36	1	333	G	N3-C4-N9	-5.00	123.00	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2177	G	C5-C6-N1	5.00	114.00	111.50
36	5	1130	A	C5-N7-C8	5.00	106.40	103.90
36	5	1816	A	P-O3'-C3'	5.00	125.71	119.70
36	5	2181	C	OP2-P-O3'	5.00	116.21	105.20
36	5	2973	G	C8-N9-C4	-5.00	104.40	106.40
56	n0	155	ARG	NE-CZ-NH2	5.00	122.80	120.30
1	2	427	C	N3-C2-O2	-5.00	118.40	121.90
36	1	2362	C	O5'-P-OP2	-5.00	101.20	105.70
36	1	2869	U	O5'-P-OP1	-5.00	101.20	105.70
36	1	2949	U	O5'-P-OP2	-5.00	101.20	105.70
37	3	33	U	N1-C2-O2	5.00	126.30	122.80
36	5	3094	A	C8-N9-C4	5.00	107.80	105.80
38	8	139	U	C5-C4-O4	5.00	128.90	125.90
1	2	872	G	N3-C4-N9	-5.00	123.00	126.00
36	1	1121	U	O5'-P-OP2	-5.00	101.20	105.70
36	1	3130	A	O5'-P-OP2	-5.00	101.20	105.70
1	6	1138	A	C2-N3-C4	-5.00	108.10	110.60
1	6	1459	C	O5'-P-OP2	-5.00	101.20	105.70
36	5	1919	G	C6-C5-N7	-5.00	127.40	130.40

There are no chirality outliers.

All (43) 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
19	C7	85	VAL	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
28	D6	97	PRO	Peptide
33	E1	105	TYR	Peptide
43	L6	51	ARG	Peptide
45	L8	30	THR	Peptide
48	M1	64	LYS	Peptide
48	M1	8	PRO	Peptide
51	M5	182	ASN	Peptide
52	M6	110	PRO	Peptide
53	M7	8	SER	Peptide
56	N0	1	MET	Peptide
56	N0	22	PRO	Peptide
57	N1	16	GLN	Peptide

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Mol	Chain	Res	Type	Group
64	N8	15	VAL	Peptide
65	N9	19	ASN	Peptide
67	O1	5	LYS	Peptide
9	S7	131	PHE	Peptide
10	S8	147	ALA	Peptide
17	c5	52	LYS	Peptide
18	c6	41	PRO	Peptide
22	d0	70	THR	Peptide
39	l2	143	GLU	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
55	m9	56	THR	Peptide
56	n0	133	ALA	Peptide
56	n0	87	THR	Peptide
62	n6	111	LEU	Peptide
64	n8	26	ARG	Peptide
64	n8	66	ALA	Peptide
67	o1	64	VAL	Peptide
67	o1	90	PHE	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%)	152 (74%)	31 (15%)	21 (10%)	0	2
2	s0	204/251 (81%)	153 (75%)	26 (13%)	25 (12%)	0	1
3	S1	212/254 (84%)	146 (69%)	39 (18%)	27 (13%)	0	1
3	s1	214/254 (84%)	177 (83%)	26 (12%)	11 (5%)	2	12
4	S2	215/253 (85%)	187 (87%)	17 (8%)	11 (5%)	2	12
4	s2	215/253 (85%)	186 (86%)	16 (7%)	13 (6%)	1	9
5	S3	221/239 (92%)	179 (81%)	29 (13%)	13 (6%)	1	9
5	s3	221/239 (92%)	183 (83%)	19 (9%)	19 (9%)	1	3
6	S4	258/260 (99%)	206 (80%)	41 (16%)	11 (4%)	2	15
6	s4	258/260 (99%)	216 (84%)	24 (9%)	18 (7%)	1	6
7	S5	204/224 (91%)	158 (78%)	32 (16%)	14 (7%)	1	6
7	s5	204/224 (91%)	164 (80%)	25 (12%)	15 (7%)	1	5
8	S6	224/236 (95%)	194 (87%)	17 (8%)	13 (6%)	1	10
8	s6	216/236 (92%)	189 (88%)	15 (7%)	12 (6%)	2	10
9	S7	182/189 (96%)	137 (75%)	25 (14%)	20 (11%)	0	2
9	s7	184/189 (97%)	148 (80%)	21 (11%)	15 (8%)	1	4
10	S8	184/200 (92%)	154 (84%)	21 (11%)	9 (5%)	2	13
10	s8	184/200 (92%)	163 (89%)	16 (9%)	5 (3%)	5	26
11	S9	183/196 (93%)	151 (82%)	23 (13%)	9 (5%)	2	13
11	s9	183/196 (93%)	140 (76%)	34 (19%)	9 (5%)	2	13
12	C0	94/105 (90%)	68 (72%)	15 (16%)	11 (12%)	0	1
12	c0	92/105 (88%)	64 (70%)	14 (15%)	14 (15%)	0	1
13	C1	153/155 (99%)	126 (82%)	16 (10%)	11 (7%)	1	5
13	c1	144/155 (93%)	118 (82%)	17 (12%)	9 (6%)	1	7
14	C2	122/142 (86%)	70 (57%)	25 (20%)	27 (22%)	0	0
14	c2	122/142 (86%)	68 (56%)	32 (26%)	22 (18%)	0	0
15	C3	148/150 (99%)	123 (83%)	18 (12%)	7 (5%)	2	14
15	c3	148/150 (99%)	120 (81%)	17 (12%)	11 (7%)	1	5
16	C4	125/136 (92%)	94 (75%)	15 (12%)	16 (13%)	0	1
16	c4	126/136 (93%)	101 (80%)	16 (13%)	9 (7%)	1	5
17	C5	122/141 (86%)	88 (72%)	23 (19%)	11 (9%)	1	3
17	c5	133/141 (94%)	92 (69%)	22 (16%)	19 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	116 (84%)	16 (12%)	7 (5%)	2	12
18	c6	140/142 (99%)	116 (83%)	16 (11%)	8 (6%)	1	10
19	C7	116/136 (85%)	91 (78%)	13 (11%)	12 (10%)	0	2
19	c7	113/136 (83%)	87 (77%)	18 (16%)	8 (7%)	1	5
20	C8	143/145 (99%)	115 (80%)	16 (11%)	12 (8%)	1	4
20	c8	143/145 (99%)	114 (80%)	20 (14%)	9 (6%)	1	7
21	C9	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	5	25
21	c9	141/143 (99%)	119 (84%)	16 (11%)	6 (4%)	2	15
22	D0	105/120 (88%)	88 (84%)	13 (12%)	4 (4%)	3	18
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	0	3
23	D1	85/87 (98%)	61 (72%)	16 (19%)	8 (9%)	0	3
23	d1	85/87 (98%)	72 (85%)	8 (9%)	5 (6%)	1	9
24	D2	127/129 (98%)	106 (84%)	19 (15%)	2 (2%)	9	40
24	d2	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	19	57
25	D3	142/144 (99%)	113 (80%)	19 (13%)	10 (7%)	1	6
25	d3	142/144 (99%)	123 (87%)	16 (11%)	3 (2%)	7	33
26	D4	132/134 (98%)	103 (78%)	20 (15%)	9 (7%)	1	6
26	d4	132/134 (98%)	103 (78%)	21 (16%)	8 (6%)	1	8
27	D5	68/107 (64%)	47 (69%)	9 (13%)	12 (18%)	0	0
27	d5	67/107 (63%)	52 (78%)	9 (13%)	6 (9%)	1	3
28	D6	95/97 (98%)	59 (62%)	18 (19%)	18 (19%)	0	0
28	d6	95/97 (98%)	74 (78%)	12 (13%)	9 (10%)	0	3
29	D7	79/81 (98%)	66 (84%)	8 (10%)	5 (6%)	1	7
29	d7	79/81 (98%)	60 (76%)	12 (15%)	7 (9%)	1	3
30	D8	61/66 (92%)	51 (84%)	6 (10%)	4 (7%)	1	6
30	d8	61/66 (92%)	42 (69%)	15 (25%)	4 (7%)	1	6
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3	17
31	d9	51/55 (93%)	41 (80%)	6 (12%)	4 (8%)	1	4
32	E0	58/60 (97%)	44 (76%)	12 (21%)	2 (3%)	3	20
33	E1	69/76 (91%)	36 (52%)	17 (25%)	16 (23%)	0	0
33	e1	74/76 (97%)	36 (49%)	17 (23%)	21 (28%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	271 (86%)	35 (11%)	10 (3%)	4	22
34	sR	316/318 (99%)	270 (85%)	36 (11%)	10 (3%)	4	22
35	SM	155/273 (57%)	113 (73%)	23 (15%)	19 (12%)	0	1
39	L2	250/253 (99%)	223 (89%)	21 (8%)	6 (2%)	6	29
39	l2	250/253 (99%)	210 (84%)	30 (12%)	10 (4%)	3	17
40	L3	384/386 (100%)	326 (85%)	45 (12%)	13 (3%)	3	20
40	l3	384/386 (100%)	340 (88%)	32 (8%)	12 (3%)	4	23
41	L4	359/361 (99%)	299 (83%)	43 (12%)	17 (5%)	2	14
41	l4	359/361 (99%)	300 (84%)	39 (11%)	20 (6%)	2	10
42	L5	294/296 (99%)	242 (82%)	31 (10%)	21 (7%)	1	5
42	l5	292/296 (99%)	255 (87%)	30 (10%)	7 (2%)	6	29
43	L6	152/175 (87%)	132 (87%)	16 (10%)	4 (3%)	5	27
43	l6	153/175 (87%)	129 (84%)	20 (13%)	4 (3%)	5	27
44	L7	220/243 (90%)	198 (90%)	12 (6%)	10 (4%)	2	14
44	l7	221/243 (91%)	195 (88%)	20 (9%)	6 (3%)	5	26
45	L8	231/255 (91%)	188 (81%)	35 (15%)	8 (4%)	3	20
45	l8	229/255 (90%)	188 (82%)	21 (9%)	20 (9%)	1	3
46	L9	189/191 (99%)	167 (88%)	15 (8%)	7 (4%)	3	19
46	l9	189/191 (99%)	171 (90%)	15 (8%)	3 (2%)	9	40
47	M0	207/220 (94%)	178 (86%)	18 (9%)	11 (5%)	2	11
47	m0	209/220 (95%)	167 (80%)	27 (13%)	15 (7%)	1	5
48	M1	167/173 (96%)	131 (78%)	21 (13%)	15 (9%)	1	3
48	m1	167/173 (96%)	139 (83%)	16 (10%)	12 (7%)	1	5
49	M3	191/198 (96%)	164 (86%)	16 (8%)	11 (6%)	1	10
49	m3	192/198 (97%)	159 (83%)	17 (9%)	16 (8%)	1	4
50	M4	134/137 (98%)	117 (87%)	12 (9%)	5 (4%)	3	19
50	m4	135/137 (98%)	122 (90%)	10 (7%)	3 (2%)	6	31
51	M5	201/203 (99%)	181 (90%)	12 (6%)	8 (4%)	3	17
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	4	24
52	M6	195/198 (98%)	181 (93%)	11 (6%)	3 (2%)	10	42
52	m6	195/198 (98%)	179 (92%)	8 (4%)	8 (4%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	M7	181/183 (99%)	152 (84%)	22 (12%)	7 (4%)	3	17
53	m7	153/183 (84%)	138 (90%)	13 (8%)	2 (1%)	12	45
54	M8	183/185 (99%)	165 (90%)	14 (8%)	4 (2%)	6	31
54	m8	183/185 (99%)	155 (85%)	22 (12%)	6 (3%)	4	21
55	M9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	68
55	m9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	68
56	N0	170/172 (99%)	150 (88%)	15 (9%)	5 (3%)	4	24
56	n0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	25	64
57	N1	157/159 (99%)	133 (85%)	18 (12%)	6 (4%)	3	18
57	n1	157/159 (99%)	141 (90%)	12 (8%)	4 (2%)	5	28
58	N2	98/120 (82%)	76 (78%)	17 (17%)	5 (5%)	2	12
58	n2	96/120 (80%)	77 (80%)	13 (14%)	6 (6%)	1	7
59	N3	134/136 (98%)	124 (92%)	9 (7%)	1 (1%)	22	60
59	n3	134/136 (98%)	121 (90%)	11 (8%)	2 (2%)	10	42
60	N4	96/155 (62%)	74 (77%)	13 (14%)	9 (9%)	0	3
60	n4	133/155 (86%)	107 (80%)	17 (13%)	9 (7%)	1	6
61	N5	119/141 (84%)	106 (89%)	12 (10%)	1 (1%)	19	57
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	1	5
62	N6	124/126 (98%)	110 (89%)	8 (6%)	6 (5%)	2	13
62	n6	124/126 (98%)	113 (91%)	7 (6%)	4 (3%)	4	22
63	N7	133/135 (98%)	109 (82%)	18 (14%)	6 (4%)	2	14
63	n7	133/135 (98%)	104 (78%)	18 (14%)	11 (8%)	1	4
64	N8	146/148 (99%)	121 (83%)	15 (10%)	10 (7%)	1	6
64	n8	146/148 (99%)	119 (82%)	22 (15%)	5 (3%)	3	20
65	N9	56/58 (97%)	48 (86%)	6 (11%)	2 (4%)	3	19
65	n9	56/58 (97%)	40 (71%)	12 (21%)	4 (7%)	1	5
66	O0	95/104 (91%)	89 (94%)	4 (4%)	2 (2%)	7	33
66	o0	98/104 (94%)	88 (90%)	6 (6%)	4 (4%)	3	16
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	2	14
67	o1	107/112 (96%)	90 (84%)	12 (11%)	5 (5%)	2	14
68	O2	125/129 (97%)	112 (90%)	10 (8%)	3 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	o2	125/129 (97%)	106 (85%)	13 (10%)	6 (5%)	2	13
69	O3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	4	24
69	o3	104/106 (98%)	92 (88%)	8 (8%)	4 (4%)	3	18
70	O4	110/119 (92%)	97 (88%)	12 (11%)	1 (1%)	17	55
70	o4	110/119 (92%)	93 (84%)	11 (10%)	6 (6%)	2	10
71	O5	117/119 (98%)	104 (89%)	12 (10%)	1 (1%)	17	55
71	o5	117/119 (98%)	102 (87%)	13 (11%)	2 (2%)	9	39
72	O6	97/99 (98%)	77 (79%)	15 (16%)	5 (5%)	2	12
72	o6	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	5
73	O7	85/87 (98%)	74 (87%)	8 (9%)	3 (4%)	3	20
73	o7	85/87 (98%)	75 (88%)	8 (9%)	2 (2%)	6	29
74	O8	75/77 (97%)	62 (83%)	11 (15%)	2 (3%)	5	26
74	o8	75/77 (97%)	60 (80%)	11 (15%)	4 (5%)	2	11
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	7	33
75	o9	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	33
76	Q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	17
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	7	34
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	15
78	Q2	103/105 (98%)	84 (82%)	13 (13%)	6 (6%)	1	10
78	q2	103/105 (98%)	92 (89%)	10 (10%)	1 (1%)	15	53
79	Q3	89/91 (98%)	77 (86%)	8 (9%)	4 (4%)	2	14
79	q3	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	14	50
80	e0	60/62 (97%)	43 (72%)	11 (18%)	6 (10%)	0	2
81	sM	98/273 (36%)	62 (63%)	22 (22%)	14 (14%)	0	1
83	p0	139/311 (45%)	120 (86%)	15 (11%)	4 (3%)	4	24
All	All	22333/24141 (92%)	18562 (83%)	2524 (11%)	1247 (6%)	2	10

All (1247) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN

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Mol	Chain	Res	Type
2	S0	66	ALA
2	S0	158	VAL
2	S0	191	ARG
3	S1	49	ASN
3	S1	58	SER
3	S1	60	ALA
3	S1	63	GLY
3	S1	177	GLN
3	S1	179	SER
3	S1	206	PRO
3	S1	213	ARG
4	S2	107	SER
5	S3	62	ASN
5	S3	65	ARG
5	S3	93	ASP
5	S3	220	PRO
6	S4	3	ARG
6	S4	104	ASP
6	S4	142	HIS
7	S5	26	ALA
7	S5	35	GLN
7	S5	39	GLU
7	S5	51	VAL
7	S5	63	GLN
7	S5	101	GLY
8	S6	122	GLU
8	S6	154	ARG
8	S6	173	PRO
8	S6	174	LYS
9	S7	31	SER
9	S7	32	PRO
9	S7	64	VAL
9	S7	85	PHE
9	S7	111	LYS
9	S7	112	ARG
9	S7	116	ARG
9	S7	131	PHE
9	S7	133	THR
9	S7	134	GLU
10	S8	40	ALA
10	S8	52	ASN
10	S8	153	GLU

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Mol	Chain	Res	Type
11	S9	98	ALA
11	S9	121	SER
11	S9	134	ILE
11	S9	164	PHE
11	S9	168	ARG
12	C0	54	TYR
12	C0	60	SER
12	C0	81	ASN
12	C0	88	PRO
12	C0	94	GLU
13	C1	7	VAL
13	C1	29	LYS
14	C2	69	ALA
14	C2	83	GLU
14	C2	89	ILE
14	C2	90	LYS
14	C2	91	VAL
14	C2	93	ASP
14	C2	127	GLY
15	C3	138	ASN
16	C4	39	ILE
16	C4	124	ASP
16	C4	125	SER
17	C5	54	ALA
17	C5	125	PRO
17	C5	126	VAL
18	C6	40	GLU
18	C6	41	PRO
18	C6	59	LYS
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	124	VAL
20	C8	14	ILE
20	C8	60	GLU
20	C8	82	PRO
20	C8	91	ASP
20	C8	92	ILE
20	C8	144	ARG
21	C9	31	PRO
21	C9	50	ALA
21	C9	53	TRP

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Mol	Chain	Res	Type
23	D1	21	ASN
24	D2	57	ARG
24	D2	83	ILE
25	D3	3	LYS
25	D3	114	LYS
25	D3	138	GLU
26	D4	36	SER
27	D5	39	ALA
27	D5	44	GLN
27	D5	71	ILE
27	D5	97	LYS
28	D6	45	VAL
28	D6	65	PRO
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
29	D7	38	PRO
29	D7	62	ILE
32	E0	47	VAL
33	E1	84	VAL
33	E1	102	VAL
33	E1	103	LEU
33	E1	106	TYR
33	E1	128	ALA
33	E1	138	ARG
34	SR	318	ALA
35	SM	47	ALA
35	SM	52	PRO
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
40	L3	4	ARG
40	L3	5	LYS
40	L3	140	ASP
40	L3	174	LYS
41	L4	291	ASN
41	L4	338	LYS
42	L5	215	ASP
42	L5	233	ALA
42	L5	234	ASP
43	L6	98	VAL

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Mol	Chain	Res	Type
44	L7	24	GLU
44	L7	26	VAL
44	L7	216	VAL
45	L8	25	PRO
45	L8	31	PRO
45	L8	36	ILE
45	L8	37	GLY
46	L9	50	ASN
46	L9	109	ALA
47	M0	189	GLU
47	M0	211	ARG
48	M1	8	PRO
48	M1	9	MET
48	M1	11	ASP
48	M1	74	PRO
48	M1	94	ARG
48	M1	115	LYS
48	M1	165	GLN
49	M3	47	ALA
49	M3	129	ASN
50	M4	8	LYS
50	M4	9	ALA
50	M4	10	SER
51	M5	74	PRO
51	M5	75	VAL
52	M6	111	PRO
53	M7	157	VAL
54	M8	41	ASP
54	M8	99	THR
56	N0	2	ALA
56	N0	13	ARG
57	N1	159	PHE
60	N4	64	THR
60	N4	81	PRO
61	N5	44	PRO
62	N6	52	ARG
62	N6	53	ASP
62	N6	83	ASP
63	N7	125	GLY
64	N8	57	GLY
64	N8	66	ALA
64	N8	76	ASP

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Mol	Chain	Res	Type
67	O1	6	ASP
67	O1	84	ASP
71	O5	119	LYS
72	O6	33	ALA
75	O9	50	ASN
76	Q0	78	ILE
78	Q2	15	LYS
78	Q2	30	ALA
78	Q2	60	LYS
79	Q3	58	SER
2	s0	4	PRO
2	s0	8	ASP
2	s0	111	ILE
2	s0	158	VAL
2	s0	164	ASN
2	s0	186	GLY
2	s0	189	VAL
2	s0	203	PHE
2	s0	206	ASP
3	s1	147	ALA
3	s1	179	SER
3	s1	206	PRO
3	s1	223	PHE
4	s2	91	ARG
4	s2	92	ALA
4	s2	107	SER
5	s3	61	GLU
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	104	ASP
6	s4	163	ASP
6	s4	164	LEU
6	s4	195	ILE
6	s4	196	VAL
7	s5	28	PRO
7	s5	39	GLU
7	s5	184	PHE
7	s5	204	GLY
8	s6	153	VAL
8	s6	154	ARG

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Mol	Chain	Res	Type
8	s6	156	PHE
8	s6	173	PRO
8	s6	174	LYS
9	s7	10	SER
9	s7	64	VAL
9	s7	66	SER
9	s7	67	LEU
9	s7	74	GLN
9	s7	131	PHE
9	s7	185	ILE
10	s8	136	SER
11	s9	121	SER
11	s9	134	ILE
12	c0	32	HIS
12	c0	82	LEU
12	c0	83	PRO
12	c0	88	PRO
12	c0	92	ILE
12	c0	94	GLU
12	c0	97	PRO
13	c1	133	LYS
13	c1	146	ALA
14	c2	89	ILE
15	c3	19	SER
15	c3	43	LYS
15	c3	66	ILE
15	c3	137	PRO
15	c3	140	LYS
16	c4	126	THR
16	c4	132	ARG
17	c5	11	VAL
17	c5	50	THR
17	c5	51	SER
17	c5	52	LYS
17	c5	125	PRO
17	c5	126	VAL
17	c5	132	GLY
18	c6	42	GLU
18	c6	116	LEU
19	c7	88	VAL
19	c7	99	VAL
19	c7	104	ASN

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Mol	Chain	Res	Type
19	c7	116	LYS
20	c8	91	ASP
20	c8	92	ILE
20	c8	135	GLY
21	c9	29	GLU
21	c9	33	TYR
21	c9	34	VAL
22	d0	15	GLN
22	d0	49	ASN
22	d0	51	VAL
22	d0	52	LYS
22	d0	96	PRO
22	d0	97	VAL
22	d0	118	VAL
23	d1	44	ARG
24	d2	68	ARG
26	d4	33	ALA
26	d4	35	VAL
26	d4	132	ARG
27	d5	85	LYS
27	d5	104	ALA
28	d6	34	LYS
28	d6	35	ALA
28	d6	47	ALA
29	d7	38	PRO
29	d7	60	SER
30	d8	57	MET
30	d8	61	ARG
31	d9	6	VAL
31	d9	7	TRP
80	e0	60	PRO
33	e1	79	LYS
33	e1	84	VAL
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	103	LEU
33	e1	106	TYR
34	sR	4	ASN
34	sR	163	ASP
34	sR	165	ASP
34	sR	318	ALA

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Mol	Chain	Res	Type
81	sM	50	ASN
81	sM	63	ASP
81	sM	66	ALA
39	l2	56	ALA
39	l2	96	LEU
39	l2	212	GLY
40	l3	3	HIS
40	l3	129	ALA
40	l3	140	ASP
40	l3	142	ALA
40	l3	235	THR
40	l3	347	SER
41	l4	14	GLU
41	l4	15	ALA
41	l4	232	SER
41	l4	272	VAL
41	l4	302	ALA
41	l4	329	PRO
42	l5	260	PHE
43	l6	98	VAL
44	l7	159	GLN
45	l8	25	PRO
45	l8	34	PHE
45	l8	112	GLU
45	l8	121	SER
45	l8	122	LYS
45	l8	133	LYS
45	l8	240	ASN
47	m0	82	ARG
47	m0	170	LYS
47	m0	175	ASN
47	m0	179	PRO
47	m0	207	GLU
48	m1	8	PRO
48	m1	9	MET
48	m1	10	ARG
48	m1	108	GLU
49	m3	13	HIS
49	m3	47	ALA
49	m3	101	ARG
49	m3	134	GLU
49	m3	150	PRO

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Mol	Chain	Res	Type
50	m4	136	ALA
51	m5	76	PRO
52	m6	16	VAL
52	m6	110	PRO
52	m6	180	SER
54	m8	41	ASP
54	m8	99	THR
56	n0	2	ALA
57	n1	122	GLN
57	n1	135	PRO
58	n2	91	ASP
59	n3	42	SER
60	n4	25	ASP
60	n4	63	ILE
60	n4	71	ARG
60	n4	76	VAL
60	n4	77	LYS
61	n5	24	LEU
61	n5	25	LYS
61	n5	44	PRO
62	n6	83	ASP
62	n6	84	LYS
62	n6	126	LEU
63	n7	17	ARG
63	n7	125	GLY
63	n7	129	TRP
64	n8	76	ASP
65	n9	21	ILE
65	n9	25	LYS
65	n9	39	PHE
66	o0	100	ILE
67	o1	7	VAL
67	o1	45	GLY
68	o2	4	LEU
68	o2	5	PRO
68	o2	27	ARG
70	o4	79	SER
72	o6	33	ALA
72	o6	63	ASN
72	o6	64	SER
72	o6	98	ARG
83	p0	93	LEU

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Mol	Chain	Res	Type
2	S0	5	ALA
2	S0	49	ASN
2	S0	94	GLY
2	S0	95	ALA
2	S0	139	VAL
2	S0	187	ALA
2	S0	190	ASP
2	S0	203	PHE
3	S1	116	LYS
3	S1	147	ALA
3	S1	148	ASN
3	S1	176	VAL
3	S1	221	PRO
4	S2	148	LEU
4	S2	236	PRO
5	S3	216	PRO
6	S4	26	CYS
6	S4	77	ARG
6	S4	195	ILE
7	S5	43	PHE
7	S5	58	LEU
7	S5	150	GLY
7	S5	153	GLY
8	S6	25	ARG
8	S6	149	LYS
9	S7	98	ILE
9	S7	186	PRO
10	S8	22	ARG
10	S8	105	ASP
10	S8	149	SER
10	S8	152	ILE
11	S9	150	LEU
11	S9	163	PRO
12	C0	64	TYR
13	C1	30	ARG
13	C1	55	ASP
13	C1	146	ALA
13	C1	154	ALA
14	C2	101	ALA
14	C2	126	TRP
14	C2	131	ASP
15	C3	19	SER

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Mol	Chain	Res	Type
15	C3	22	ALA
15	C3	27	LYS
15	C3	68	GLY
16	C4	42	VAL
16	C4	50	ALA
16	C4	123	SER
16	C4	126	THR
17	C5	101	ALA
18	C6	113	ASP
18	C6	138	PHE
19	C7	6	THR
19	C7	23	LYS
19	C7	72	LYS
19	C7	87	GLU
19	C7	113	LEU
19	C7	115	LEU
19	C7	123	ASN
20	C8	61	LEU
20	C8	83	ALA
20	C8	142	GLY
23	D1	12	TYR
23	D1	44	ARG
25	D3	40	SER
25	D3	70	LYS
25	D3	112	LYS
25	D3	144	ARG
26	D4	5	VAL
26	D4	34	ASN
27	D5	43	ASP
27	D5	56	THR
28	D6	15	ARG
28	D6	18	VAL
28	D6	36	ILE
28	D6	63	ALA
29	D7	51	GLN
29	D7	63	LEU
30	D8	36	THR
33	E1	98	VAL
33	E1	111	GLU
33	E1	127	GLY
34	SR	51	ASP
34	SR	136	ILE

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Mol	Chain	Res	Type
34	SR	160	GLU
34	SR	161	LYS
34	SR	295	SER
35	SM	87	THR
35	SM	89	ARG
35	SM	102	THR
35	SM	139	GLU
39	L2	47	GLN
39	L2	143	GLU
39	L2	250	GLN
40	L3	347	SER
40	L3	351	LEU
40	L3	385	LYS
40	L3	386	ASP
41	L4	15	ALA
41	L4	190	GLY
41	L4	232	SER
41	L4	268	ALA
41	L4	294	GLU
41	L4	311	HIS
42	L5	57	ASN
42	L5	58	LYS
42	L5	137	ASP
42	L5	253	PHE
42	L5	260	PHE
42	L5	276	LYS
44	L7	164	SER
45	L8	39	ALA
45	L8	156	ASP
45	L8	254	ASP
47	M0	117	GLY
47	M0	194	GLY
48	M1	65	ILE
48	M1	95	ASN
48	M1	167	TYR
49	M3	13	HIS
49	M3	164	GLU
51	M5	184	LYS
52	M6	16	VAL
53	M7	162	GLU
55	M9	53	LYS
56	N0	142	GLN

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Mol	Chain	Res	Type
57	N1	124	VAL
58	N2	31	ALA
58	N2	51	GLY
60	N4	97	LYS
62	N6	84	LYS
62	N6	92	GLY
64	N8	24	LYS
64	N8	96	LYS
67	O1	82	GLU
68	O2	123	LYS
68	O2	127	ALA
70	O4	77	GLY
72	O6	34	SER
73	O7	86	ALA
78	Q2	94	GLY
2	s0	29	VAL
2	s0	44	GLY
2	s0	66	ALA
2	s0	95	ALA
2	s0	185	ARG
2	s0	191	ARG
3	s1	26	ARG
3	s1	39	GLU
3	s1	82	ARG
3	s1	93	GLY
3	s1	232	HIS
4	s2	93	GLY
4	s2	163	GLY
4	s2	182	PRO
5	s3	90	ARG
5	s3	179	GLN
6	s4	12	LEU
6	s4	24	SER
7	s5	36	ALA
7	s5	43	PHE
8	s6	25	ARG
8	s6	68	LEU
8	s6	70	PRO
9	s7	155	ASP
10	s8	62	THR
11	s9	150	LEU
11	s9	164	PHE

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Mol	Chain	Res	Type
12	c0	31	LYS
12	c0	35	ILE
13	c1	61	THR
13	c1	121	ASP
13	c1	144	ALA
14	c2	22	VAL
14	c2	58	LEU
14	c2	66	VAL
14	c2	82	PRO
14	c2	101	ALA
14	c2	119	SER
14	c2	131	ASP
15	c3	60	VAL
15	c3	87	ASP
17	c5	68	PRO
17	c5	117	GLY
18	c6	113	ASP
20	c8	102	ALA
22	d0	17	GLN
23	d1	21	ASN
25	d3	131	SER
27	d5	87	GLY
28	d6	13	LYS
28	d6	62	TYR
29	d7	20	LYS
29	d7	62	ILE
31	d9	16	LYS
80	e0	38	LEU
80	e0	47	VAL
80	e0	51	ASN
33	e1	100	LEU
33	e1	102	VAL
33	e1	127	GLY
33	e1	145	HIS
34	sR	75	ALA
34	sR	160	GLU
81	sM	42	ALA
81	sM	48	ARG
81	sM	65	THR
81	sM	67	GLY
39	l2	13	GLY
39	l2	24	GLN

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Mol	Chain	Res	Type
39	l2	127	ALA
39	l2	194	ASN
39	l2	249	SER
40	l3	141	GLY
40	l3	155	ALA
40	l3	187	SER
41	l4	146	PRO
41	l4	154	THR
41	l4	301	PRO
41	l4	311	HIS
42	l5	279	LYS
45	l8	39	ALA
45	l8	117	ALA
45	l8	120	LYS
45	l8	150	LEU
45	l8	203	VAL
46	l9	2	LYS
46	l9	144	ILE
47	m0	101	LYS
47	m0	204	GLY
48	m1	7	ASN
48	m1	15	GLU
48	m1	94	ARG
48	m1	115	LYS
48	m1	167	TYR
49	m3	93	ILE
49	m3	129	ASN
49	m3	135	ALA
49	m3	141	ALA
49	m3	162	ASN
51	m5	81	TYR
51	m5	184	LYS
52	m6	12	LYS
54	m8	98	LYS
55	m9	36	ASN
58	n2	50	LEU
61	n5	40	LEU
63	n7	16	GLY
63	n7	56	LYS
67	o1	5	LYS
67	o1	83	GLU
67	o1	99	ALA

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Mol	Chain	Res	Type
71	o5	82	ALA
71	o5	119	LYS
76	q0	78	ILE
77	q1	23	ARG
83	p0	198	PRO
2	S0	27	ARG
2	S0	103	THR
2	S0	163	ASN
2	S0	189	VAL
3	S1	35	PRO
3	S1	37	THR
3	S1	51	SER
3	S1	54	LEU
3	S1	158	SER
4	S2	91	ARG
5	S3	44	THR
5	S3	59	LEU
5	S3	211	PRO
5	S3	218	LEU
6	S4	12	LEU
6	S4	153	ASN
6	S4	240	LYS
6	S4	245	LYS
7	S5	76	ARG
7	S5	127	GLN
8	S6	123	GLY
8	S6	148	SER
9	S7	29	ASN
9	S7	30	SER
9	S7	84	LYS
10	S8	120	THR
13	C1	6	THR
13	C1	145	ALA
14	C2	21	GLU
14	C2	66	VAL
14	C2	87	PRO
14	C2	107	ASP
14	C2	112	ALA
14	C2	119	SER
14	C2	130	THR
15	C3	137	PRO
16	C4	38	THR

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Mol	Chain	Res	Type
16	C4	40	ALA
16	C4	51	ASP
16	C4	109	GLY
17	C5	22	LEU
17	C5	48	GLY
18	C6	33	GLY
19	C7	83	GLN
20	C8	25	ASN
22	D0	17	GLN
23	D1	2	GLU
23	D1	7	GLN
23	D1	8	LEU
23	D1	10	GLU
23	D1	15	ARG
25	D3	41	SER
26	D4	4	ALA
26	D4	11	LYS
27	D5	55	PRO
27	D5	57	TYR
28	D6	11	ASN
28	D6	61	GLU
28	D6	62	TYR
30	D8	20	GLY
32	E0	33	ARG
33	E1	87	THR
33	E1	118	ARG
33	E1	137	ASP
34	SR	50	ASP
35	SM	17	VAL
35	SM	88	ARG
35	SM	153	ASP
39	L2	13	GLY
39	L2	127	ALA
41	L4	130	ALA
41	L4	146	PRO
41	L4	339	LEU
41	L4	352	ALA
42	L5	188	GLU
42	L5	228	ALA
42	L5	252	ALA
42	L5	258	LYS
46	L9	190	ASP

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Mol	Chain	Res	Type
47	M0	24	ARG
47	M0	91	VAL
47	M0	207	GLU
47	M0	218	ALA
47	M0	220	GLN
49	M3	130	GLY
49	M3	136	GLU
49	M3	165	SER
49	M3	166	ALA
50	M4	29	ALA
51	M5	144	ARG
53	M7	160	ALA
53	M7	164	LYS
56	N0	167	ARG
57	N1	101	CYS
58	N2	11	ILE
58	N2	32	SER
58	N2	44	GLU
59	N3	82	ALA
63	N7	35	SER
63	N7	78	ASN
63	N7	102	GLU
64	N8	117	ARG
72	O6	3	VAL
73	O7	65	ARG
74	O8	33	LYS
2	s0	5	ALA
2	s0	10	THR
2	s0	30	GLN
2	s0	92	HIS
2	s0	94	GLY
2	s0	183	ARG
4	s2	106	ASP
5	s3	93	ASP
5	s3	142	LEU
5	s3	144	ALA
5	s3	180	GLY
5	s3	221	SER
6	s4	171	ASP
6	s4	245	LYS
7	s5	56	ALA
7	s5	57	SER

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Mol	Chain	Res	Type
7	s5	58	LEU
7	s5	60	ASP
8	s6	152	ASP
9	s7	111	LYS
12	c0	23	ALA
12	c0	30	ALA
13	c1	114	ALA
14	c2	45	LEU
14	c2	106	ILE
14	c2	108	ARG
15	c3	20	ARG
15	c3	22	ALA
15	c3	139	TRP
16	c4	92	LYS
17	c5	7	ALA
17	c5	14	THR
17	c5	17	TYR
17	c5	69	GLU
17	c5	127	ARG
17	c5	135	THR
17	c5	136	SER
18	c6	40	GLU
19	c7	113	LEU
19	c7	120	SER
20	c8	14	ILE
20	c8	61	LEU
21	c9	25	GLN
25	d3	70	LYS
26	d4	48	TYR
26	d4	50	ALA
26	d4	58	PHE
26	d4	77	ASN
29	d7	3	LEU
29	d7	59	CYS
33	e1	83	LYS
33	e1	85	TYR
33	e1	128	ALA
33	e1	146	SER
34	sR	161	LYS
81	sM	30	THR
81	sM	43	ASP
81	sM	47	ALA

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Mol	Chain	Res	Type
81	sM	64	LYS
39	l2	80	GLU
40	l3	4	ARG
40	l3	302	LYS
41	l4	120	TYR
41	l4	145	ILE
41	l4	305	ALA
41	l4	330	TYR
42	l5	215	ASP
43	l6	10	TYR
44	l7	157	ASN
45	l8	81	THR
45	l8	118	GLU
45	l8	196	ALA
45	l8	237	ILE
47	m0	3	ARG
47	m0	25	ALA
47	m0	176	LEU
47	m0	187	ALA
47	m0	219	ALA
50	m4	135	LEU
51	m5	183	THR
52	m6	184	THR
53	m7	66	SER
54	m8	91	ALA
54	m8	112	ALA
58	n2	52	ASN
60	n4	26	SER
60	n4	74	LYS
60	n4	132	GLY
61	n5	38	LEU
62	n6	125	LYS
63	n7	34	LYS
63	n7	102	GLU
63	n7	121	ARG
64	n8	47	LYS
66	o0	10	ILE
68	o2	122	PRO
70	o4	47	CYS
70	o4	77	GLY
70	o4	78	GLY
70	o4	82	ALA

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Mol	Chain	Res	Type
72	o6	34	SER
72	o6	67	LYS
73	o7	87	SER
74	o8	17	ARG
75	o9	4	GLN
2	S0	164	ASN
2	S0	195	TRP
3	S1	62	LYS
3	S1	132	ASP
4	S2	145	GLY
4	S2	150	GLN
4	S2	225	LEU
4	S2	248	SER
5	S3	92	GLN
5	S3	178	ARG
5	S3	217	ILE
7	S5	64	VAL
8	S6	70	PRO
8	S6	152	ASP
9	S7	73	VAL
9	S7	155	ASP
12	C0	25	LYS
12	C0	34	GLU
13	C1	4	GLU
13	C1	147	ALA
14	C2	25	GLU
14	C2	106	ILE
14	C2	125	ASN
16	C4	18	ARG
16	C4	127	ARG
17	C5	29	SER
17	C5	52	LYS
17	C5	66	ALA
17	C5	127	ARG
18	C6	39	VAL
25	D3	5	LYS
26	D4	6	THR
26	D4	58	PHE
27	D5	54	VAL
28	D6	46	GLU
28	D6	47	ALA
28	D6	64	LEU

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Mol	Chain	Res	Type
28	D6	97	PRO
30	D8	61	ARG
33	E1	100	LEU
34	SR	98	GLU
34	SR	194	GLY
35	SM	53	ARG
35	SM	86	ASN
35	SM	172	VAL
35	SM	173	GLU
35	SM	174	LEU
39	L2	246	LEU
40	L3	155	ALA
41	L4	5	GLN
41	L4	14	GLU
41	L4	270	SER
42	L5	115	LEU
42	L5	125	VAL
42	L5	151	GLN
42	L5	295	GLY
43	L6	100	LYS
44	L7	100	ARG
45	L8	157	VAL
46	L9	96	HIS
46	L9	120	ASP
47	M0	41	ALA
47	M0	142	ASP
48	M1	114	ILE
49	M3	5	LYS
49	M3	44	ALA
51	M5	34	ASN
51	M5	81	TYR
52	M6	182	ASN
53	M7	75	GLU
53	M7	163	LYS
54	M8	162	ALA
57	N1	16	GLN
60	N4	86	SER
62	N6	42	GLN
63	N7	103	GLN
64	N8	47	LYS
65	N9	25	LYS
67	O1	7	VAL

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Mol	Chain	Res	Type
72	O6	21	THR
73	O7	68	LYS
74	O8	18	ALA
79	Q3	7	LYS
2	s0	103	THR
4	s2	85	PRO
4	s2	235	LEU
4	s2	238	SER
5	s3	43	PRO
5	s3	45	LYS
6	s4	57	ASN
6	s4	90	ILE
6	s4	95	THR
7	s5	29	ILE
7	s5	59	VAL
7	s5	100	ASN
8	s6	165	GLY
9	s7	30	SER
9	s7	133	THR
11	s9	22	SER
12	c0	3	MET
12	c0	24	LYS
13	c1	129	ARG
14	c2	87	PRO
14	c2	103	LEU
14	c2	118	ALA
16	c4	11	SER
16	c4	12	GLN
17	c5	71	GLU
17	c5	130	ARG
18	c6	39	VAL
18	c6	97	VAL
18	c6	142	TYR
20	c8	139	LYS
23	d1	42	GLU
26	d4	4	ALA
28	d6	63	ALA
31	d9	11	PRO
80	e0	54	ARG
80	e0	61	SER
33	e1	81	LYS
33	e1	131	PHE

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Mol	Chain	Res	Type
33	e1	136	LYS
34	sR	146	GLY
41	l4	5	GLN
41	l4	233	LEU
44	l7	191	VAL
45	l8	26	LEU
45	l8	69	LEU
45	l8	188	THR
48	m1	95	ASN
48	m1	114	ILE
49	m3	76	THR
49	m3	121	SER
49	m3	152	THR
50	m4	10	SER
51	m5	181	ASN
52	m6	13	GLY
52	m6	122	GLN
57	n1	136	ARG
58	n2	49	ASN
58	n2	90	ARG
61	n5	47	ALA
61	n5	57	LEU
63	n7	127	ASN
63	n7	134	LEU
66	o0	103	THR
68	o2	6	HIS
69	o3	41	ALA
70	o4	46	ASP
73	o7	86	ALA
78	q2	78	LYS
79	q3	4	ARG
2	S0	36	TYR
3	S1	26	ARG
3	S1	82	ARG
3	S1	130	SER
3	S1	210	ILE
4	S2	36	VAL
4	S2	39	THR
4	S2	235	LEU
5	S3	70	THR
6	S4	260	GLY
8	S6	69	LEU

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Mol	Chain	Res	Type
9	S7	74	GLN
10	S8	10	LYS
11	S9	162	SER
12	C0	87	VAL
14	C2	22	VAL
14	C2	81	ASP
14	C2	113	ARG
15	C3	3	ARG
16	C4	92	LYS
16	C4	114	ARG
17	C5	51	SER
21	C9	69	LYS
22	D0	59	PRO
25	D3	96	VAL
26	D4	60	PHE
28	D6	35	ALA
30	D8	34	GLU
31	D9	8	PHE
33	E1	85	TYR
33	E1	86	THR
34	SR	105	GLY
40	L3	3	HIS
40	L3	139	GLN
40	L3	317	ILE
41	L4	4	PRO
42	L5	6	ASP
42	L5	221	GLU
42	L5	259	LYS
43	L6	6	ALA
46	L9	2	LYS
46	L9	66	ALA
48	M1	64	LYS
48	M1	108	GLU
48	M1	117	ASP
49	M3	193	ALA
50	M4	6	ILE
51	M5	94	TYR
54	M8	4	ASP
60	N4	69	LYS
60	N4	80	ARG
60	N4	89	LEU
63	N7	36	HIS

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Mol	Chain	Res	Type
64	N8	70	LYS
65	N9	21	ILE
66	O0	100	ILE
69	O3	14	LEU
69	O3	94	PHE
72	O6	27	SER
78	Q2	17	CYS
79	Q3	51	ALA
79	Q3	60	CYS
2	s0	49	ASN
3	s1	22	ASP
3	s1	207	LEU
4	s2	150	GLN
4	s2	151	PRO
5	s3	163	PRO
5	s3	196	ARG
6	s4	105	VAL
6	s4	168	LYS
7	s5	54	LYS
8	s6	131	LYS
9	s7	13	PRO
9	s7	106	SER
10	s8	78	ILE
10	s8	94	ASN
11	s9	110	GLN
11	s9	162	SER
11	s9	167	ALA
11	s9	183	ALA
12	c0	95	ARG
13	c1	7	VAL
14	c2	107	ASP
16	c4	51	ASP
20	c8	18	LEU
20	c8	60	GLU
22	d0	16	GLN
22	d0	119	ALA
23	d1	10	GLU
25	d3	27	ASN
27	d5	38	HIS
28	d6	59	TYR
29	d7	58	SER
30	d8	33	LEU

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Mol	Chain	Res	Type
33	e1	112	GLY
33	e1	148	TYR
34	sR	186	PHE
81	sM	167	PRO
39	l2	238	ILE
41	l4	190	GLY
41	l4	328	ASN
42	l5	125	VAL
42	l5	178	ASN
42	l5	258	LYS
43	l6	97	ASN
44	l7	32	ALA
46	l9	167	VAL
47	m0	100	ASN
47	m0	220	GLN
48	m1	118	PRO
49	m3	140	SER
51	m5	68	ARG
54	m8	113	LYS
58	n2	23	THR
60	n4	83	THR
61	n5	45	LYS
63	n7	103	GLN
64	n8	28	HIS
64	n8	129	PHE
66	o0	96	GLY
68	o2	124	GLY
69	o3	91	ALA
72	o6	9	ILE
74	o8	18	ALA
83	p0	33	VAL
83	p0	68	SER
3	S1	61	LEU
3	S1	81	PHE
3	S1	209	ASN
8	S6	9	VAL
9	S7	13	PRO
11	S9	160	PRO
13	C1	113	PRO
14	C2	39	ASP
14	C2	82	PRO
20	C8	139	LYS

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Mol	Chain	Res	Type
22	D0	21	LYS
26	D4	47	VAL
27	D5	38	HIS
29	D7	75	GLU
33	E1	148	TYR
35	SM	12	VAL
42	L5	178	ASN
44	L7	91	GLY
44	L7	178	ILE
48	M1	151	SER
51	M5	145	ASP
57	N1	18	ASP
60	N4	82	ILE
76	Q0	79	GLU
78	Q2	100	LYS
5	s3	44	THR
5	s3	115	ILE
5	s3	219	ALA
6	s4	30	ARG
6	s4	32	SER
6	s4	157	ASN
9	s7	11	GLN
10	s8	101	ILE
14	c2	90	LYS
14	c2	110	ALA
16	c4	37	GLU
16	c4	124	ASP
17	c5	65	LEU
18	c6	4	VAL
27	d5	44	GLN
28	d6	8	ASN
34	sR	281	TYR
81	sM	51	ARG
42	l5	168	ASP
43	l6	151	LYS
44	l7	59	GLU
44	l7	178	ILE
49	m3	60	ALA
52	m6	183	ALA
53	m7	75	GLU
57	n1	16	GLN
61	n5	48	SER

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Mol	Chain	Res	Type
64	n8	87	ARG
7	S5	21	THR
9	S7	132	PRO
12	C0	92	ILE
14	C2	115	VAL
16	C4	75	GLY
31	D9	11	PRO
44	L7	212	GLY
60	N4	76	VAL
69	O3	59	VAL
14	c2	40	GLY
14	c2	115	VAL
16	c4	131	GLY
19	c7	98	GLY
23	d1	77	GLY
41	l4	277	PRO
45	l8	239	GLY
2	S0	194	PRO
20	C8	125	ILE
22	D0	106	ILE
2	s0	194	PRO
8	s6	69	LEU
14	c2	91	VAL
15	c3	82	PRO
41	l4	142	VAL
69	o3	59	VAL
14	C2	55	GLY
27	D5	41	ILE
27	D5	88	ILE
35	SM	39	PRO
44	L7	188	ILE
44	L7	191	VAL
56	N0	129	ILE
57	N1	123	GLY
68	O2	68	PRO
4	s2	234	PRO
6	s4	150	PRO
13	c1	139	VAL
14	c2	63	VAL
19	c7	50	ILE
21	c9	26	GLY
21	c9	100	ILE

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Mol	Chain	Res	Type
30	d8	6	PRO
33	e1	124	PRO
81	sM	172	VAL
49	m3	50	PRO
65	n9	24	PRO
74	o8	37	PRO
12	C0	86	ILE
41	L4	23	PRO
64	N8	148	ILE
66	O0	96	GLY
67	O1	33	VAL
2	s0	139	VAL
9	s7	159	VAL
14	c2	127	GLY
47	m0	194	GLY
59	n3	41	GLY
69	o3	61	GLY
8	S6	146	GLY
43	L6	149	ILE
53	M7	51	VAL
64	N8	116	GLY
7	s5	21	THR
27	d5	55	PRO
28	d6	58	VAL
40	l3	239	PRO
74	o8	35	GLY
40	L3	257	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	S0	164/209 (78%)	133 (81%)	31 (19%)	1 8
2	s0	165/209 (79%)	131 (79%)	34 (21%)	1 6
3	S1	191/223 (86%)	155 (81%)	36 (19%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	s1	192/223 (86%)	163 (85%)	29 (15%)	3	14
4	S2	176/204 (86%)	142 (81%)	34 (19%)	1	8
4	s2	176/204 (86%)	133 (76%)	43 (24%)	0	3
5	S3	182/194 (94%)	145 (80%)	37 (20%)	1	6
5	s3	182/194 (94%)	151 (83%)	31 (17%)	2	10
6	S4	221/221 (100%)	183 (83%)	38 (17%)	2	10
6	s4	221/221 (100%)	183 (83%)	38 (17%)	2	10
7	S5	173/190 (91%)	142 (82%)	31 (18%)	2	9
7	s5	173/190 (91%)	133 (77%)	40 (23%)	1	4
8	S6	188/201 (94%)	148 (79%)	40 (21%)	1	5
8	s6	187/201 (93%)	151 (81%)	36 (19%)	1	8
9	S7	165/169 (98%)	140 (85%)	25 (15%)	3	14
9	s7	165/169 (98%)	138 (84%)	27 (16%)	2	11
10	S8	150/161 (93%)	130 (87%)	20 (13%)	4	17
10	s8	150/161 (93%)	128 (85%)	22 (15%)	3	15
11	S9	158/165 (96%)	123 (78%)	35 (22%)	1	4
11	s9	158/165 (96%)	128 (81%)	30 (19%)	1	8
12	C0	77/98 (79%)	67 (87%)	10 (13%)	4	19
12	c0	73/98 (74%)	63 (86%)	10 (14%)	3	17
13	C1	129/136 (95%)	107 (83%)	22 (17%)	2	10
13	c1	129/136 (95%)	106 (82%)	23 (18%)	2	9
14	C2	88/118 (75%)	66 (75%)	22 (25%)	0	3
14	c2	88/118 (75%)	66 (75%)	22 (25%)	0	3
15	C3	127/127 (100%)	100 (79%)	27 (21%)	1	5
15	c3	127/127 (100%)	103 (81%)	24 (19%)	1	8
16	C4	81/104 (78%)	60 (74%)	21 (26%)	0	2
16	c4	97/104 (93%)	76 (78%)	21 (22%)	1	5
17	C5	101/117 (86%)	85 (84%)	16 (16%)	2	12
17	c5	103/117 (88%)	84 (82%)	19 (18%)	1	9
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1	7
18	c6	118/118 (100%)	93 (79%)	25 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	C7	94/124 (76%)	72 (77%)	22 (23%)	1	4
19	c7	92/124 (74%)	78 (85%)	14 (15%)	3	14
20	C8	128/128 (100%)	95 (74%)	33 (26%)	0	2
20	c8	128/128 (100%)	103 (80%)	25 (20%)	1	7
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	7
21	c9	115/115 (100%)	93 (81%)	22 (19%)	1	8
22	D0	100/113 (88%)	78 (78%)	22 (22%)	1	4
22	d0	103/113 (91%)	78 (76%)	25 (24%)	0	3
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	10
23	d1	74/74 (100%)	56 (76%)	18 (24%)	0	3
24	D2	110/110 (100%)	94 (86%)	16 (14%)	3	15
24	d2	110/110 (100%)	93 (84%)	17 (16%)	2	13
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2	10
25	d3	119/119 (100%)	104 (87%)	15 (13%)	4	20
26	D4	112/112 (100%)	93 (83%)	19 (17%)	2	10
26	d4	112/112 (100%)	94 (84%)	18 (16%)	2	12
27	D5	61/88 (69%)	46 (75%)	15 (25%)	0	3
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	11
28	D6	83/83 (100%)	67 (81%)	16 (19%)	1	8
28	d6	83/83 (100%)	73 (88%)	10 (12%)	5	22
29	D7	70/70 (100%)	64 (91%)	6 (9%)	10	37
29	d7	70/70 (100%)	60 (86%)	10 (14%)	3	15
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1	5
30	d8	56/59 (95%)	44 (79%)	12 (21%)	1	5
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	10
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	5
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1	7
33	E1	62/66 (94%)	46 (74%)	16 (26%)	0	2
33	e1	66/66 (100%)	51 (77%)	15 (23%)	1	4
34	SR	260/261 (100%)	222 (85%)	38 (15%)	3	15
34	sR	260/261 (100%)	233 (90%)	27 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	SM	97/228 (42%)	76 (78%)	21 (22%)	1	5
39	L2	193/195 (99%)	150 (78%)	43 (22%)	1	4
39	l2	192/195 (98%)	152 (79%)	40 (21%)	1	5
40	L3	321/322 (100%)	257 (80%)	64 (20%)	1	7
40	l3	320/322 (99%)	251 (78%)	69 (22%)	1	5
41	L4	288/288 (100%)	228 (79%)	60 (21%)	1	5
41	l4	288/288 (100%)	229 (80%)	59 (20%)	1	6
42	L5	244/244 (100%)	197 (81%)	47 (19%)	1	8
42	l5	243/244 (100%)	196 (81%)	47 (19%)	1	8
43	L6	134/152 (88%)	112 (84%)	22 (16%)	2	11
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	10
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4	19
44	l7	187/204 (92%)	160 (86%)	27 (14%)	3	15
45	L8	187/207 (90%)	152 (81%)	35 (19%)	1	8
45	l8	177/207 (86%)	147 (83%)	30 (17%)	2	11
46	L9	171/171 (100%)	134 (78%)	37 (22%)	1	5
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1	7
47	M0	177/186 (95%)	143 (81%)	34 (19%)	1	8
47	m0	179/186 (96%)	142 (79%)	37 (21%)	1	6
48	M1	147/150 (98%)	115 (78%)	32 (22%)	1	5
48	m1	147/150 (98%)	122 (83%)	25 (17%)	2	10
49	M3	154/158 (98%)	128 (83%)	26 (17%)	2	11
49	m3	154/158 (98%)	130 (84%)	24 (16%)	2	13
50	M4	107/108 (99%)	84 (78%)	23 (22%)	1	5
50	m4	108/108 (100%)	88 (82%)	20 (18%)	1	8
51	M5	175/175 (100%)	138 (79%)	37 (21%)	1	5
51	m5	175/175 (100%)	149 (85%)	26 (15%)	3	14
52	M6	160/161 (99%)	133 (83%)	27 (17%)	2	11
52	m6	160/161 (99%)	132 (82%)	28 (18%)	2	10
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	4
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	M8	150/150 (100%)	128 (85%)	22 (15%)	3	15
54	m8	150/150 (100%)	118 (79%)	32 (21%)	1	5
55	M9	153/153 (100%)	132 (86%)	21 (14%)	3	17
55	m9	153/153 (100%)	120 (78%)	33 (22%)	1	5
56	N0	156/156 (100%)	121 (78%)	35 (22%)	1	4
56	n0	156/156 (100%)	124 (80%)	32 (20%)	1	6
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1	6
57	n1	136/136 (100%)	108 (79%)	28 (21%)	1	6
58	N2	87/106 (82%)	74 (85%)	13 (15%)	3	14
58	n2	85/106 (80%)	72 (85%)	13 (15%)	2	13
59	N3	104/104 (100%)	86 (83%)	18 (17%)	2	10
59	n3	104/104 (100%)	94 (90%)	10 (10%)	8	32
60	N4	57/129 (44%)	50 (88%)	7 (12%)	4	21
60	n4	100/129 (78%)	82 (82%)	18 (18%)	1	9
61	N5	104/117 (89%)	84 (81%)	20 (19%)	1	8
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	6
62	N6	109/109 (100%)	83 (76%)	26 (24%)	0	3
62	n6	109/109 (100%)	82 (75%)	27 (25%)	0	3
63	N7	115/115 (100%)	94 (82%)	21 (18%)	1	9
63	n7	115/115 (100%)	93 (81%)	22 (19%)	1	8
64	N8	118/118 (100%)	96 (81%)	22 (19%)	1	8
64	n8	118/118 (100%)	93 (79%)	25 (21%)	1	5
65	N9	46/46 (100%)	35 (76%)	11 (24%)	0	3
65	n9	46/46 (100%)	37 (80%)	9 (20%)	1	7
66	O0	81/87 (93%)	68 (84%)	13 (16%)	2	12
66	o0	84/87 (97%)	70 (83%)	14 (17%)	2	11
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	4
67	o1	94/96 (98%)	74 (79%)	20 (21%)	1	5
68	O2	109/110 (99%)	87 (80%)	22 (20%)	1	6
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	4
69	O3	90/90 (100%)	81 (90%)	9 (10%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	o3	90/90 (100%)	77 (86%)	13 (14%)	3	15
70	O4	95/101 (94%)	74 (78%)	21 (22%)	1	4
70	o4	95/101 (94%)	75 (79%)	20 (21%)	1	5
71	O5	104/104 (100%)	80 (77%)	24 (23%)	1	4
71	o5	103/104 (99%)	80 (78%)	23 (22%)	1	4
72	O6	81/81 (100%)	65 (80%)	16 (20%)	1	7
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	10
73	o7	70/70 (100%)	58 (83%)	12 (17%)	2	10
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	3
74	o8	67/68 (98%)	53 (79%)	14 (21%)	1	5
75	O9	45/45 (100%)	40 (89%)	5 (11%)	6	25
75	o9	45/45 (100%)	36 (80%)	9 (20%)	1	7
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	0	3
76	q0	47/47 (100%)	35 (74%)	12 (26%)	0	3
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	67 (74%)	23 (26%)	0	3
78	q2	90/90 (100%)	73 (81%)	17 (19%)	1	8
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1	5
79	q3	71/71 (100%)	63 (89%)	8 (11%)	6	24
80	e0	53/53 (100%)	42 (79%)	11 (21%)	1	5
81	sM	54/228 (24%)	40 (74%)	14 (26%)	0	2
83	p0	105/253 (42%)	80 (76%)	25 (24%)	0	3
All	All	18729/20239 (92%)	15175 (81%)	3554 (19%)	1	8

All (3554) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	7	PHE
2	S0	27	ARG
2	S0	30	GLN
2	S0	32	HIS
2	S0	33	GLN

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Mol	Chain	Res	Type
2	S0	37	VAL
2	S0	49	ASN
2	S0	50	VAL
2	S0	57	LEU
2	S0	59	LEU
2	S0	62	ARG
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	101	ARG
2	S0	111	ILE
2	S0	119	ARG
2	S0	123	VAL
2	S0	140	ASN
2	S0	146	LEU
2	S0	154	GLU
2	S0	156	VAL
2	S0	157	ASP
2	S0	170	ILE
2	S0	172	LEU
2	S0	177	LEU
2	S0	184	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	196	SER
3	S1	21	VAL
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	46	THR
3	S1	51	SER
3	S1	61	LEU
3	S1	70	LEU
3	S1	73	LEU
3	S1	77	GLU
3	S1	78	ASP
3	S1	81	PHE
3	S1	89	ASP
3	S1	91	VAL
3	S1	96	LEU
3	S1	97	LEU

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Mol	Chain	Res	Type
3	S1	105	PHE
3	S1	110	LEU
3	S1	111	ARG
3	S1	112	SER
3	S1	117	TRP
3	S1	131	ASP
3	S1	154	SER
3	S1	177	GLN
3	S1	180	THR
3	S1	181	LEU
3	S1	184	LEU
3	S1	193	ILE
3	S1	198	GLU
3	S1	202	LYS
3	S1	214	LYS
3	S1	218	LEU
3	S1	219	LYS
3	S1	220	GLN
3	S1	223	PHE
3	S1	229	MET
4	S2	41	LEU
4	S2	53	ILE
4	S2	54	GLU
4	S2	55	GLU
4	S2	58	LEU
4	S2	68	ILE
4	S2	77	GLN
4	S2	89	GLN
4	S2	90	THR
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	106	ASP
4	S2	111	VAL
4	S2	117	THR
4	S2	119	LYS
4	S2	130	ILE
4	S2	134	LEU
4	S2	140	ARG
4	S2	141	ARG
4	S2	148	LEU
4	S2	166	THR

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Mol	Chain	Res	Type
4	S2	181	SER
4	S2	187	LEU
4	S2	222	TYR
4	S2	224	PHE
4	S2	226	THR
4	S2	229	LEU
4	S2	235	LEU
4	S2	237	VAL
4	S2	240	LEU
4	S2	245	ASP
4	S2	246	GLU
4	S2	250	GLN
5	S3	4	LEU
5	S3	5	ILE
5	S3	9	ARG
5	S3	21	LEU
5	S3	23	GLU
5	S3	37	VAL
5	S3	41	VAL
5	S3	65	ARG
5	S3	66	ILE
5	S3	67	ASN
5	S3	76	ARG
5	S3	84	ILE
5	S3	89	GLU
5	S3	92	GLN
5	S3	93	ASP
5	S3	94	ARG
5	S3	105	MET
5	S3	111	ASN
5	S3	113	LEU
5	S3	117	ARG
5	S3	122	VAL
5	S3	127	MET
5	S3	134	CYS
5	S3	135	GLU
5	S3	137	VAL
5	S3	142	LEU
5	S3	143	ARG
5	S3	151	LYS
5	S3	158	ILE
5	S3	172	THR

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Mol	Chain	Res	Type
5	S3	175	VAL
5	S3	176	LEU
5	S3	177	MET
5	S3	178	ARG
5	S3	181	VAL
5	S3	190	ARG
5	S3	195	SER
6	S4	6	LYS
6	S4	7	LYS
6	S4	9	LEU
6	S4	23	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	48	LEU
6	S4	70	VAL
6	S4	77	ARG
6	S4	92	LEU
6	S4	95	THR
6	S4	102	VAL
6	S4	115	THR
6	S4	116	ASP
6	S4	117	GLU
6	S4	123	LEU
6	S4	131	LEU
6	S4	133	LYS
6	S4	155	LYS
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	191	ARG
6	S4	197	HIS
6	S4	198	LYS
6	S4	206	ASP
6	S4	215	ASP
6	S4	221	ARG
6	S4	223	ASN
6	S4	226	PHE
6	S4	227	VAL
6	S4	237	SER
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU

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Mol	Chain	Res	Type
6	S4	247	SER
6	S4	258	GLN
6	S4	259	GLN
7	S5	25	LEU
7	S5	27	THR
7	S5	38	THR
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS
7	S5	63	GLN
7	S5	65	ARG
7	S5	76	ARG
7	S5	79	ASN
7	S5	86	GLN
7	S5	89	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	104	ASN
7	S5	109	LYS
7	S5	119	ASP
7	S5	139	ASN
7	S5	146	THR
7	S5	147	THR
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	162	VAL
7	S5	163	SER
7	S5	166	ARG
7	S5	194	LEU
7	S5	203	LYS
7	S5	206	SER
7	S5	216	GLU
7	S5	225	ARG
8	S6	13	GLN
8	S6	14	LYS
8	S6	25	ARG
8	S6	32	ILE
8	S6	45	PHE
8	S6	51	LYS
8	S6	58	LYS
8	S6	65	GLN

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Mol	Chain	Res	Type
8	S6	67	VAL
8	S6	68	LEU
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	81	VAL
8	S6	82	SER
8	S6	93	LYS
8	S6	98	ARG
8	S6	109	LEU
8	S6	120	GLU
8	S6	124	LEU
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	129	VAL
8	S6	132	ARG
8	S6	133	LEU
8	S6	143	LYS
8	S6	150	GLU
8	S6	154	ARG
8	S6	155	ASP
8	S6	169	TYR
8	S6	170	THR
8	S6	175	ILE
8	S6	176	GLN
8	S6	177	ARG
8	S6	183	ARG
8	S6	211	LEU
8	S6	216	LEU
8	S6	217	SER
8	S6	223	LYS
9	S7	9	LEU
9	S7	38	LEU
9	S7	46	ILE
9	S7	50	ASP
9	S7	51	VAL
9	S7	70	PHE
9	S7	75	THR
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG

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Mol	Chain	Res	Type
9	S7	105	THR
9	S7	107	ARG
9	S7	114	ARG
9	S7	116	ARG
9	S7	123	ASP
9	S7	126	LEU
9	S7	130	VAL
9	S7	134	GLU
9	S7	136	VAL
9	S7	147	ASN
9	S7	158	ASP
9	S7	163	ASP
9	S7	167	GLU
9	S7	174	ASN
9	S7	185	ILE
10	S8	7	SER
10	S8	8	ARG
10	S8	14	THR
10	S8	21	PHE
10	S8	26	LYS
10	S8	29	LEU
10	S8	36	THR
10	S8	46	VAL
10	S8	49	ARG
10	S8	58	LEU
10	S8	69	SER
10	S8	82	VAL
10	S8	138	ASN
10	S8	151	LYS
10	S8	152	ILE
10	S8	154	SER
10	S8	158	SER
10	S8	161	SER
10	S8	187	GLU
10	S8	196	LEU
11	S9	3	ARG
11	S9	7	THR
11	S9	14	THR
11	S9	16	LYS
11	S9	28	LEU
11	S9	40	LYS
11	S9	46	SER

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Mol	Chain	Res	Type
11	S9	49	LEU
11	S9	54	ARG
11	S9	60	LEU
11	S9	63	ASP
11	S9	78	ARG
11	S9	79	ARG
11	S9	82	ARG
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	97	LEU
11	S9	99	LEU
11	S9	105	LEU
11	S9	109	LEU
11	S9	110	GLN
11	S9	113	VAL
11	S9	118	LEU
11	S9	134	ILE
11	S9	138	LYS
11	S9	145	SER
11	S9	149	ARG
11	S9	151	ASP
11	S9	157	ASP
11	S9	161	THR
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	182	GLU
12	C0	1	MET
12	C0	8	ARG
12	C0	27	PHE
12	C0	29	GLN
12	C0	32	HIS
12	C0	55	VAL
12	C0	56	LYS
12	C0	71	GLU
12	C0	76	LEU
12	C0	82	LEU
13	C1	8	GLN
13	C1	21	ASN
13	C1	27	THR
13	C1	29	LYS

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Mol	Chain	Res	Type
13	C1	37	ASN
13	C1	40	LEU
13	C1	44	THR
13	C1	63	LEU
13	C1	67	ARG
13	C1	69	LYS
13	C1	72	THR
13	C1	74	THR
13	C1	79	LYS
13	C1	83	THR
13	C1	109	VAL
13	C1	112	SER
13	C1	118	GLN
13	C1	123	VAL
13	C1	127	GLN
13	C1	131	ILE
13	C1	140	VAL
13	C1	143	SER
14	C2	28	LEU
14	C2	33	ARG
14	C2	37	VAL
14	C2	43	ARG
14	C2	46	ARG
14	C2	50	LYS
14	C2	52	LEU
14	C2	54	ARG
14	C2	58	LEU
14	C2	61	VAL
14	C2	66	VAL
14	C2	71	ILE
14	C2	74	LEU
14	C2	86	VAL
14	C2	89	ILE
14	C2	103	LEU
14	C2	121	VAL
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	139	HIS
14	C2	140	PHE
15	C3	3	ARG
15	C3	9	LYS

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Mol	Chain	Res	Type
15	C3	11	ILE
15	C3	13	SER
15	C3	16	ILE
15	C3	27	LYS
15	C3	32	SER
15	C3	39	LYS
15	C3	42	ARG
15	C3	45	LEU
15	C3	50	ILE
15	C3	56	ASP
15	C3	58	HIS
15	C3	64	ARG
15	C3	66	ILE
15	C3	76	LYS
15	C3	83	GLU
15	C3	88	LEU
15	C3	102	LEU
15	C3	110	ASP
15	C3	114	ARG
15	C3	115	LEU
15	C3	125	LEU
15	C3	134	VAL
15	C3	142	GLU
15	C3	145	THR
15	C3	151	ASN
16	C4	13	VAL
16	C4	14	PHE
16	C4	16	VAL
16	C4	24	ASN
16	C4	29	HIS
16	C4	30	VAL
16	C4	31	THR
16	C4	39	ILE
16	C4	42	VAL
16	C4	48	VAL
16	C4	51	ASP
16	C4	92	LYS
16	C4	102	LEU
16	C4	103	ARG
16	C4	118	VAL
16	C4	123	SER
16	C4	126	THR

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Mol	Chain	Res	Type
16	C4	132	ARG
16	C4	133	ARG
16	C4	136	ARG
16	C4	137	LEU
17	C5	22	LEU
17	C5	26	LEU
17	C5	34	VAL
17	C5	35	LYS
17	C5	36	LEU
17	C5	40	ARG
17	C5	44	ARG
17	C5	47	ARG
17	C5	52	LYS
17	C5	60	LEU
17	C5	89	MET
17	C5	100	LYS
17	C5	110	GLU
17	C5	116	LEU
17	C5	121	ILE
17	C5	124	THR
18	C6	4	VAL
18	C6	13	LYS
18	C6	14	LYS
18	C6	17	THR
18	C6	26	LYS
18	C6	28	LEU
18	C6	44	LEU
18	C6	58	ASP
18	C6	66	ARG
18	C6	68	ARG
18	C6	69	VAL
18	C6	98	ASP
18	C6	106	LYS
18	C6	114	ARG
18	C6	118	ILE
18	C6	121	SER
18	C6	123	ARG
18	C6	127	LYS
18	C6	128	LYS
18	C6	136	SER
18	C6	137	ARG
18	C6	141	SER

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Mol	Chain	Res	Type
18	C6	143	ARG
19	C7	5	ARG
19	C7	25	THR
19	C7	29	GLN
19	C7	30	THR
19	C7	34	LEU
19	C7	38	ILE
19	C7	46	LEU
19	C7	49	LYS
19	C7	54	THR
19	C7	69	ILE
19	C7	71	PHE
19	C7	72	LYS
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	87	GLU
19	C7	104	ASN
19	C7	105	GLN
19	C7	107	SER
19	C7	113	LEU
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	6	GLN
20	C8	8	GLN
20	C8	11	PHE
20	C8	12	GLN
20	C8	13	HIS
20	C8	14	ILE
20	C8	17	LEU
20	C8	18	LEU
20	C8	20	THR
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	32	LEU
20	C8	40	ARG
20	C8	53	ASP
20	C8	54	LEU
20	C8	60	GLU

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Mol	Chain	Res	Type
20	C8	61	LEU
20	C8	71	GLN
20	C8	80	LYS
20	C8	89	GLN
20	C8	92	ILE
20	C8	97	ASP
20	C8	108	LYS
20	C8	115	ARG
20	C8	116	LEU
20	C8	120	ARG
20	C8	132	ARG
20	C8	136	GLN
20	C8	140	THR
20	C8	143	ARG
21	C9	4	VAL
21	C9	6	VAL
21	C9	18	TYR
21	C9	22	LEU
21	C9	28	LEU
21	C9	30	VAL
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	57	ARG
21	C9	67	MET
21	C9	70	GLN
21	C9	84	LYS
21	C9	94	ILE
21	C9	111	ILE
21	C9	116	ILE
21	C9	117	SER
21	C9	130	ARG
21	C9	131	ASP
21	C9	134	ARG
21	C9	140	LEU
21	C9	144	GLU
22	D0	15	GLN
22	D0	22	ILE
22	D0	23	ARG
22	D0	27	THR
22	D0	30	LYS

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Mol	Chain	Res	Type
22	D0	47	GLN
22	D0	48	HIS
22	D0	51	VAL
22	D0	57	ARG
22	D0	61	LYS
22	D0	66	SER
22	D0	72	ASN
22	D0	74	GLU
22	D0	76	SER
22	D0	81	THR
22	D0	88	LYS
22	D0	89	ARG
22	D0	99	ILE
22	D0	103	ILE
22	D0	105	GLN
22	D0	108	ILE
22	D0	121	ASN
23	D1	5	LYS
23	D1	11	LEU
23	D1	18	SER
23	D1	25	LYS
23	D1	41	GLU
23	D1	49	GLU
23	D1	52	THR
23	D1	61	SER
23	D1	68	SER
23	D1	69	LEU
23	D1	78	LEU
23	D1	80	LYS
23	D1	84	SER
24	D2	7	LEU
24	D2	24	GLN
24	D2	25	VAL
24	D2	29	PRO
24	D2	53	ILE
24	D2	65	LEU
24	D2	81	VAL
24	D2	93	LEU
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR

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Mol	Chain	Res	Type
24	D2	119	LYS
24	D2	121	VAL
24	D2	122	SER
24	D2	129	VAL
25	D3	7	ARG
25	D3	9	LEU
25	D3	18	HIS
25	D3	19	ARG
25	D3	28	ASN
25	D3	41	SER
25	D3	73	ARG
25	D3	84	THR
25	D3	97	ASP
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	127	VAL
25	D3	131	SER
25	D3	136	TRP
25	D3	138	GLU
25	D3	140	LYS
25	D3	144	ARG
26	D4	10	ARG
26	D4	17	LEU
26	D4	21	LYS
26	D4	29	HIS
26	D4	32	ARG
26	D4	34	ASN
26	D4	47	VAL
26	D4	51	GLU
26	D4	52	LYS
26	D4	57	VAL
26	D4	61	ARG
26	D4	62	THR
26	D4	74	LEU
26	D4	96	LEU
26	D4	99	LYS
26	D4	102	LYS
26	D4	121	THR

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Mol	Chain	Res	Type
26	D4	127	LYS
26	D4	128	LYS
27	D5	42	LEU
27	D5	48	ASP
27	D5	50	ILE
27	D5	58	ARG
27	D5	59	TYR
27	D5	60	VAL
27	D5	63	SER
27	D5	67	ASP
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	85	LYS
27	D5	92	ILE
27	D5	95	HIS
27	D5	100	ILE
28	D6	36	ILE
28	D6	38	ARG
28	D6	44	ILE
28	D6	45	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	67	THR
28	D6	68	TYR
28	D6	69	ASN
28	D6	70	LYS
28	D6	82	ARG
28	D6	83	ILE
28	D6	85	ARG
28	D6	86	VAL
28	D6	90	GLU
28	D6	91	ASP
29	D7	3	LEU
29	D7	20	LYS
29	D7	26	GLN
29	D7	33	LEU
29	D7	55	THR
29	D7	67	THR
30	D8	13	ILE
30	D8	15	VAL
30	D8	19	THR

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Mol	Chain	Res	Type
30	D8	32	PHE
30	D8	33	LEU
30	D8	35	ASP
30	D8	36	THR
30	D8	44	VAL
30	D8	49	ARG
30	D8	57	MET
30	D8	58	GLU
30	D8	64	ARG
31	D9	6	VAL
31	D9	7	TRP
31	D9	22	ARG
31	D9	25	SER
31	D9	30	LEU
31	D9	32	ARG
31	D9	36	LEU
31	D9	38	ILE
32	E0	3	LYS
32	E0	20	LYS
32	E0	21	VAL
32	E0	22	GLU
32	E0	28	LYS
32	E0	29	LYS
32	E0	39	LEU
32	E0	42	ARG
32	E0	47	VAL
32	E0	56	MET
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
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	137	ASP
33	E1	140	TYR
33	E1	146	SER
33	E1	147	VAL
33	E1	149	LYS

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Mol	Chain	Res	Type
33	E1	151	ASN
34	SR	3	SER
34	SR	6	VAL
34	SR	7	LEU
34	SR	10	ARG
34	SR	12	THR
34	SR	16	HIS
34	SR	29	GLN
34	SR	46	LYS
34	SR	48	THR
34	SR	52	GLN
34	SR	59	ARG
34	SR	66	HIS
34	SR	76	ASP
34	SR	94	VAL
34	SR	96	THR
34	SR	106	HIS
34	SR	108	SER
34	SR	112	SER
34	SR	117	LYS
34	SR	118	LYS
34	SR	136	ILE
34	SR	137	LYS
34	SR	141	LEU
34	SR	165	ASP
34	SR	166	SER
34	SR	191	ASP
34	SR	199	ILE
34	SR	202	LEU
34	SR	222	LEU
34	SR	238	ASP
34	SR	266	ASP
34	SR	268	GLN
34	SR	277	GLU
34	SR	300	THR
34	SR	308	ASN
34	SR	314	GLN
34	SR	316	MET
34	SR	317	THR
35	SM	34	LYS
35	SM	46	LYS
35	SM	51	ARG

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Mol	Chain	Res	Type
35	SM	55	SER
35	SM	61	ILE
35	SM	64	LYS
35	SM	68	ARG
35	SM	78	ASP
35	SM	79	SER
35	SM	84	LYS
35	SM	89	ARG
35	SM	91	THR
35	SM	96	ARG
35	SM	97	THR
35	SM	100	THR
35	SM	103	LYS
35	SM	105	LYS
35	SM	116	GLU
35	SM	130	GLU
35	SM	131	ILE
35	SM	139	GLU
39	L2	8	GLN
39	L2	10	LYS
39	L2	20	THR
39	L2	23	ARG
39	L2	30	ARG
39	L2	31	THR
39	L2	32	LEU
39	L2	37	ARG
39	L2	44	ILE
39	L2	45	VAL
39	L2	46	LYS
39	L2	62	VAL
39	L2	70	ARG
39	L2	74	GLU
39	L2	82	VAL
39	L2	88	ILE
39	L2	95	SER
39	L2	96	LEU
39	L2	97	ASN
39	L2	101	VAL
39	L2	104	LEU
39	L2	109	GLU
39	L2	116	VAL
39	L2	134	VAL

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Mol	Chain	Res	Type
39	L2	141	PRO
39	L2	142	ASP
39	L2	143	GLU
39	L2	158	ILE
39	L2	165	VAL
39	L2	169	ILE
39	L2	177	LYS
39	L2	179	LEU
39	L2	180	LEU
39	L2	181	LYS
39	L2	190	ARG
39	L2	191	LEU
39	L2	193	ARG
39	L2	202	VAL
39	L2	204	MET
39	L2	207	VAL
39	L2	226	SER
39	L2	230	VAL
39	L2	247	ARG
40	L3	2	SER
40	L3	7	GLU
40	L3	17	LEU
40	L3	19	ARG
40	L3	25	ILE
40	L3	30	LYS
40	L3	37	ARG
40	L3	47	LEU
40	L3	50	LYS
40	L3	56	ILE
40	L3	73	VAL
40	L3	84	VAL
40	L3	85	VAL
40	L3	102	LEU
40	L3	103	THR
40	L3	114	VAL
40	L3	116	ARG
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	169	THR
40	L3	173	GLN
40	L3	188	ILE
40	L3	192	VAL
40	L3	196	ARG
40	L3	200	GLU
40	L3	201	LYS
40	L3	202	THR
40	L3	205	VAL
40	L3	207	SER
40	L3	212	ASN
40	L3	218	ILE
40	L3	229	VAL
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	238	LEU
40	L3	241	LYS
40	L3	244	ARG
40	L3	252	ILE
40	L3	284	ARG
40	L3	300	ARG
40	L3	304	THR
40	L3	305	ILE
40	L3	308	MET
40	L3	316	GLU
40	L3	319	ASN
40	L3	320	ASP
40	L3	324	VAL
40	L3	328	ILE
40	L3	332	ARG
40	L3	337	THR
40	L3	338	LEU
40	L3	341	SER
40	L3	343	TYR
40	L3	347	SER
40	L3	355	SER
40	L3	361	THR
40	L3	364	LYS
40	L3	380	MET
40	L3	385	LYS
41	L4	4	PRO

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Mol	Chain	Res	Type
41	L4	18	ASN
41	L4	22	LEU
41	L4	25	VAL
41	L4	37	THR
41	L4	40	THR
41	L4	54	GLU
41	L4	60	THR
41	L4	71	VAL
41	L4	74	ILE
41	L4	85	SER
41	L4	93	MET
41	L4	99	MET
41	L4	133	SER
41	L4	135	VAL
41	L4	136	LEU
41	L4	138	ARG
41	L4	145	ILE
41	L4	150	LEU
41	L4	152	VAL
41	L4	153	SER
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	187	LEU
41	L4	191	LYS
41	L4	193	LYS
41	L4	194	TYR
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	230	VAL
41	L4	246	ARG
41	L4	256	THR
41	L4	258	LEU
41	L4	267	VAL
41	L4	270	SER

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Mol	Chain	Res	Type
41	L4	275	THR
41	L4	287	THR
41	L4	292	SER
41	L4	293	SER
41	L4	306	THR
41	L4	307	GLN
41	L4	308	LYS
41	L4	313	LEU
41	L4	314	LYS
41	L4	321	LYS
41	L4	323	VAL
41	L4	332	LYS
41	L4	339	LEU
41	L4	343	LYS
41	L4	346	LYS
41	L4	350	LYS
41	L4	354	VAL
42	L5	5	LYS
42	L5	23	ARG
42	L5	34	LYS
42	L5	35	ARG
42	L5	41	LYS
42	L5	66	SER
42	L5	69	ILE
42	L5	80	SER
42	L5	85	ARG
42	L5	89	THR
42	L5	92	LEU
42	L5	93	THR
42	L5	95	TRP
42	L5	105	ILE
42	L5	109	THR
42	L5	112	LYS
42	L5	115	LEU
42	L5	118	THR
42	L5	122	VAL
42	L5	123	GLU
42	L5	131	LEU
42	L5	132	THR
42	L5	137	ASP
42	L5	140	ARG
42	L5	144	VAL

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Mol	Chain	Res	Type
42	L5	146	LEU
42	L5	148	ILE
42	L5	152	ARG
42	L5	155	THR
42	L5	158	ARG
42	L5	159	VAL
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE
42	L5	196	ARG
42	L5	216	GLU
42	L5	222	LEU
42	L5	232	ASP
42	L5	242	SER
42	L5	254	LYS
42	L5	258	LYS
42	L5	259	LYS
42	L5	261	THR
42	L5	263	GLU
42	L5	273	ARG
42	L5	277	LEU
42	L5	293	LEU
43	L6	2	SER
43	L6	5	LYS
43	L6	15	VAL
43	L6	21	THR
43	L6	31	ARG
43	L6	35	VAL
43	L6	46	ARG
43	L6	48	ARG
43	L6	52	VAL
43	L6	56	LYS
43	L6	65	ILE
43	L6	79	VAL
43	L6	84	VAL
43	L6	89	THR
43	L6	90	LYS
43	L6	93	VAL
43	L6	94	GLU
43	L6	98	VAL
43	L6	129	GLU
43	L6	134	ARG

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Mol	Chain	Res	Type
43	L6	152	THR
43	L6	155	LEU
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	40	LYS
44	L7	60	ARG
44	L7	77	VAL
44	L7	82	LYS
44	L7	88	ARG
44	L7	93	ASN
44	L7	100	ARG
44	L7	101	LYS
44	L7	110	ARG
44	L7	121	LYS
44	L7	124	LEU
44	L7	143	THR
44	L7	157	ASN
44	L7	158	LYS
44	L7	164	SER
44	L7	178	ILE
44	L7	179	LEU
44	L7	184	LEU
44	L7	228	SER
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	27	THR
45	L8	41	GLN
45	L8	47	SER
45	L8	63	LYS
45	L8	74	THR
45	L8	79	GLN
45	L8	81	THR
45	L8	84	ARG
45	L8	89	GLU
45	L8	92	LYS
45	L8	95	ASN
45	L8	101	THR
45	L8	106	LYS
45	L8	110	THR
45	L8	132	VAL

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Mol	Chain	Res	Type
45	L8	136	LEU
45	L8	145	ASN
45	L8	149	LYS
45	L8	150	LEU
45	L8	156	ASP
45	L8	160	ILE
45	L8	169	LEU
45	L8	172	LYS
45	L8	185	ARG
45	L8	190	VAL
45	L8	194	THR
45	L8	203	VAL
45	L8	206	GLU
45	L8	208	GLU
45	L8	214	LEU
45	L8	238	LEU
45	L8	241	LYS
45	L8	246	MET
45	L8	248	LYS
46	L9	4	ILE
46	L9	5	GLN
46	L9	6	THR
46	L9	12	VAL
46	L9	16	VAL
46	L9	18	VAL
46	L9	19	SER
46	L9	24	ILE
46	L9	33	THR
46	L9	34	LEU
46	L9	41	ILE
46	L9	48	VAL
46	L9	49	ASN
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	107	ASP
46	L9	123	ILE
46	L9	124	ARG

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Mol	Chain	Res	Type
46	L9	133	THR
46	L9	135	GLU
46	L9	138	THR
46	L9	139	ASN
46	L9	151	VAL
46	L9	152	GLU
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	164	ILE
46	L9	172	ILE
46	L9	189	GLU
46	L9	190	ASP
46	L9	191	LEU
47	M0	3	ARG
47	M0	21	ARG
47	M0	24	ARG
47	M0	30	LYS
47	M0	32	ARG
47	M0	33	ILE
47	M0	36	LEU
47	M0	39	LYS
47	M0	40	LYS
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	57	LEU
47	M0	63	GLU
47	M0	87	LEU
47	M0	91	VAL
47	M0	99	ILE
47	M0	129	VAL
47	M0	139	ARG
47	M0	140	THR
47	M0	162	GLN
47	M0	163	GLN
47	M0	165	ILE
47	M0	167	LEU
47	M0	169	LYS
47	M0	174	THR
47	M0	175	ASN
47	M0	176	LEU

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Mol	Chain	Res	Type
47	M0	177	ASP
47	M0	184	LYS
47	M0	185	ARG
47	M0	200	LEU
47	M0	203	LYS
47	M0	207	GLU
48	M1	6	GLN
48	M1	7	ASN
48	M1	9	MET
48	M1	10	ARG
48	M1	11	ASP
48	M1	12	LEU
48	M1	13	LYS
48	M1	22	SER
48	M1	28	ASP
48	M1	34	SER
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	82	ARG
48	M1	94	ARG
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	115	LYS
48	M1	119	SER
48	M1	130	VAL
48	M1	138	VAL
48	M1	140	ARG
48	M1	142	LYS
48	M1	143	ARG
48	M1	148	VAL
48	M1	158	ASP
48	M1	166	LYS
48	M1	173	ASP
49	M3	23	LYS
49	M3	35	ARG
49	M3	46	ILE
49	M3	54	LEU

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Mol	Chain	Res	Type
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	70	ARG
49	M3	85	LEU
49	M3	100	ARG
49	M3	115	ARG
49	M3	120	GLN
49	M3	122	LYS
49	M3	124	ILE
49	M3	128	ARG
49	M3	131	LYS
49	M3	136	GLU
49	M3	164	GLU
49	M3	168	ARG
49	M3	171	ARG
49	M3	175	SER
49	M3	182	ILE
49	M3	190	LYS
50	M4	5	SER
50	M4	8	LYS
50	M4	20	VAL
50	M4	25	LYS
50	M4	27	GLN
50	M4	38	ILE
50	M4	50	LYS
50	M4	53	VAL
50	M4	55	ARG
50	M4	58	ILE
50	M4	63	VAL
50	M4	64	VAL
50	M4	69	THR
50	M4	72	LEU
50	M4	83	LYS
50	M4	90	VAL
50	M4	92	GLU
50	M4	93	LYS
50	M4	102	LYS
50	M4	125	LYS

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Mol	Chain	Res	Type
50	M4	126	GLN
50	M4	130	THR
50	M4	135	LEU
51	M5	10	LEU
51	M5	11	GLN
51	M5	15	GLN
51	M5	20	ARG
51	M5	22	LEU
51	M5	46	ASP
51	M5	50	ARG
51	M5	68	ARG
51	M5	77	LYS
51	M5	80	THR
51	M5	83	LYS
51	M5	85	THR
51	M5	91	GLU
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	117	ASN
51	M5	133	ILE
51	M5	138	GLN
51	M5	144	ARG
51	M5	151	ILE
51	M5	153	ASP
51	M5	155	VAL
51	M5	159	ARG
51	M5	167	THR
51	M5	170	LYS
51	M5	183	THR
51	M5	187	ARG
51	M5	190	THR
51	M5	194	GLN
51	M5	196	THR
51	M5	204	LYS
52	M6	25	LYS
52	M6	33	ILE

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Mol	Chain	Res	Type
52	M6	34	VAL
52	M6	46	GLU
52	M6	58	LEU
52	M6	68	ARG
52	M6	74	ARG
52	M6	78	ARG
52	M6	79	ILE
52	M6	84	LEU
52	M6	85	ARG
52	M6	94	ARG
52	M6	106	GLU
52	M6	111	PRO
52	M6	116	LYS
52	M6	117	ARG
52	M6	122	GLN
52	M6	124	LEU
52	M6	126	VAL
52	M6	128	ARG
52	M6	143	THR
52	M6	144	SER
52	M6	155	LYS
52	M6	160	ARG
52	M6	180	SER
52	M6	182	ASN
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	34	GLN
53	M7	36	ILE
53	M7	41	LEU
53	M7	52	LEU
53	M7	53	ASP
53	M7	65	SER
53	M7	67	ILE
53	M7	69	ARG
53	M7	78	VAL
53	M7	79	THR
53	M7	107	LEU
53	M7	112	LEU

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Mol	Chain	Res	Type
53	M7	118	GLN
53	M7	119	VAL
53	M7	123	PRO
53	M7	126	ARG
53	M7	127	ARG
53	M7	136	ILE
53	M7	138	LYS
53	M7	142	SER
53	M7	144	SER
53	M7	157	VAL
53	M7	168	LEU
53	M7	171	ARG
53	M7	180	LYS
53	M7	181	ARG
54	M8	3	ILE
54	M8	17	THR
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	34	THR
54	M8	46	LYS
54	M8	49	LEU
54	M8	57	ILE
54	M8	64	VAL
54	M8	73	GLN
54	M8	95	GLU
54	M8	111	ARG
54	M8	113	LYS
54	M8	120	GLU
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	150	VAL
54	M8	170	ARG
54	M8	178	ARG
54	M8	180	ARG
55	M9	29	THR
55	M9	44	LEU
55	M9	46	LYS
55	M9	51	VAL
55	M9	55	VAL
55	M9	71	ARG

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Mol	Chain	Res	Type
55	M9	74	ARG
55	M9	91	SER
55	M9	98	ARG
55	M9	99	LEU
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	115	ILE
55	M9	116	ASP
55	M9	135	LYS
55	M9	138	LEU
55	M9	146	LYS
55	M9	164	LEU
55	M9	173	ARG
55	M9	182	ASP
56	N0	1	MET
56	N0	8	GLN
56	N0	12	ARG
56	N0	21	GLU
56	N0	45	LEU
56	N0	51	VAL
56	N0	57	GLU
56	N0	61	ILE
56	N0	71	LYS
56	N0	80	ARG
56	N0	85	SER
56	N0	87	THR
56	N0	92	LYS
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	122	HIS
56	N0	125	LYS
56	N0	130	GLU
56	N0	131	LYS
56	N0	132	THR
56	N0	136	LYS
56	N0	137	ARG
56	N0	138	GLN

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Mol	Chain	Res	Type
56	N0	142	GLN
56	N0	145	THR
56	N0	155	ARG
56	N0	156	VAL
56	N0	158	LYS
56	N0	161	LYS
56	N0	167	ARG
56	N0	169	SER
57	N1	9	SER
57	N1	12	ARG
57	N1	18	ASP
57	N1	25	VAL
57	N1	26	HIS
57	N1	27	LEU
57	N1	55	LYS
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	80	VAL
57	N1	83	ARG
57	N1	88	ARG
57	N1	96	ILE
57	N1	104	GLU
57	N1	106	LEU
57	N1	110	LYS
57	N1	118	GLU
57	N1	124	VAL
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	136	ARG
57	N1	139	ARG
57	N1	143	THR
57	N1	149	GLN
57	N1	158	THR
57	N1	159	PHE
58	N2	10	LYS
58	N2	14	THR
58	N2	16	THR
58	N2	29	ASP
58	N2	32	SER
58	N2	43	VAL

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Mol	Chain	Res	Type
58	N2	52	ASN
58	N2	66	VAL
58	N2	75	TYR
58	N2	88	GLN
58	N2	93	ILE
58	N2	100	THR
58	N2	105	LEU
59	N3	13	ILE
59	N3	32	ARG
59	N3	48	ARG
59	N3	63	LYS
59	N3	69	LEU
59	N3	71	LYS
59	N3	72	LYS
59	N3	73	VAL
59	N3	74	MET
59	N3	79	VAL
59	N3	83	LYS
59	N3	102	ILE
59	N3	109	MET
59	N3	110	LYS
59	N3	115	THR
59	N3	120	LYS
59	N3	125	LEU
59	N3	135	VAL
60	N4	4	GLU
60	N4	5	ILE
60	N4	17	ARG
60	N4	39	LEU
60	N4	47	ARG
60	N4	54	LEU
60	N4	64	THR
61	N5	27	ARG
61	N5	37	THR
61	N5	38	LEU
61	N5	39	LYS
61	N5	40	LEU
61	N5	63	ILE
61	N5	71	THR
61	N5	86	VAL
61	N5	92	LYS
61	N5	108	LEU

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Mol	Chain	Res	Type
61	N5	115	ARG
61	N5	120	LYS
61	N5	125	ARG
61	N5	127	THR
61	N5	129	ASP
61	N5	133	LEU
61	N5	135	ILE
61	N5	138	ARG
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	5	SER
62	N6	13	ARG
62	N6	17	LYS
62	N6	36	SER
62	N6	37	LYS
62	N6	39	LEU
62	N6	42	GLN
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	60	ARG
62	N6	64	LYS
62	N6	70	ILE
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	88	GLU
62	N6	89	LYS
62	N6	94	SER
62	N6	105	VAL
62	N6	115	ARG
62	N6	125	LYS
63	N7	14	VAL
63	N7	17	ARG
63	N7	21	LYS
63	N7	24	VAL
63	N7	30	ASP
63	N7	34	LYS

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Mol	Chain	Res	Type
63	N7	46	ILE
63	N7	54	THR
63	N7	60	LYS
63	N7	64	LYS
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	90	GLU
63	N7	97	SER
63	N7	102	GLU
63	N7	108	GLU
63	N7	109	GLU
63	N7	120	GLU
63	N7	121	ARG
63	N7	134	LEU
64	N8	4	ARG
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	19	LYS
64	N8	32	ARG
64	N8	34	MET
64	N8	42	ARG
64	N8	46	ASP
64	N8	47	LYS
64	N8	60	TYR
64	N8	76	ASP
64	N8	78	LEU
64	N8	85	ASP
64	N8	91	LEU
64	N8	92	LYS
64	N8	115	LYS
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
64	N8	135	GLU
64	N8	139	ARG
65	N9	14	ARG
65	N9	18	ARG
65	N9	21	ILE
65	N9	22	LYS
65	N9	23	LYS

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Mol	Chain	Res	Type
65	N9	25	LYS
65	N9	28	LYS
65	N9	38	LYS
65	N9	40	ARG
65	N9	50	THR
65	N9	59	LYS
66	O0	16	LEU
66	O0	22	LYS
66	O0	34	LEU
66	O0	40	LYS
66	O0	54	SER
66	O0	61	MET
66	O0	79	THR
66	O0	83	LYS
66	O0	93	LEU
66	O0	99	ASP
66	O0	100	ILE
66	O0	101	LEU
66	O0	104	LEU
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	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	86	LYS
67	O1	89	LEU
67	O1	94	GLU
67	O1	96	VAL
67	O1	106	THR
67	O1	107	VAL
67	O1	110	GLU
68	O2	15	LYS
68	O2	16	LYS

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Mol	Chain	Res	Type
68	O2	18	LYS
68	O2	19	ARG
68	O2	33	ARG
68	O2	41	VAL
68	O2	51	SER
68	O2	59	SER
68	O2	61	LYS
68	O2	62	LYS
68	O2	67	SER
68	O2	73	THR
68	O2	75	LEU
68	O2	76	VAL
68	O2	82	LEU
68	O2	84	THR
68	O2	89	THR
68	O2	91	THR
68	O2	106	VAL
68	O2	109	LEU
68	O2	111	ARG
68	O2	128	LEU
69	O3	4	SER
69	O3	15	SER
69	O3	49	ILE
69	O3	59	VAL
69	O3	70	LYS
69	O3	78	SER
69	O3	80	VAL
69	O3	93	THR
69	O3	106	ASN
70	O4	3	GLN
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	33	GLN
70	O4	51	LEU
70	O4	58	ARG
70	O4	65	VAL
70	O4	66	SER

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Mol	Chain	Res	Type
70	O4	71	THR
70	O4	74	ARG
70	O4	81	CYS
70	O4	86	LYS
70	O4	87	GLU
70	O4	90	ILE
70	O4	104	VAL
70	O4	107	GLU
71	O5	5	LYS
71	O5	21	LEU
71	O5	27	GLU
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	85	THR
71	O5	89	ARG
71	O5	90	ARG
71	O5	94	LYS
71	O5	99	GLN
71	O5	100	VAL
71	O5	101	THR
71	O5	102	GLU
71	O5	107	LYS
71	O5	115	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	34	SER
72	O6	36	ARG
72	O6	45	ARG
72	O6	57	LEU
72	O6	58	ILE

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Mol	Chain	Res	Type
72	O6	60	LEU
72	O6	68	ARG
72	O6	76	ARG
72	O6	81	THR
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	37	CYS
73	O7	44	THR
73	O7	55	ARG
73	O7	58	THR
73	O7	59	THR
73	O7	65	ARG
73	O7	67	LEU
74	O8	5	ILE
74	O8	12	LEU
74	O8	22	THR
74	O8	24	THR
74	O8	32	ASN
74	O8	41	THR
74	O8	45	VAL
74	O8	50	SER
74	O8	53	THR
74	O8	54	LEU
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	72	THR
74	O8	77	ARG
74	O8	78	LEU
75	O9	5	LYS
75	O9	11	GLN
75	O9	21	ARG
75	O9	45	ARG
75	O9	51	ILE
76	Q0	77	ILE
76	Q0	78	ILE
76	Q0	83	LYS

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Mol	Chain	Res	Type
76	Q0	85	LEU
76	Q0	97	ARG
76	Q0	106	ARG
76	Q0	108	THR
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	127	LEU
76	Q0	128	LYS
77	Q1	2	ARG
77	Q1	4	LYS
77	Q1	6	ARG
77	Q1	9	ARG
77	Q1	11	ARG
77	Q1	16	LYS
77	Q1	19	LYS
77	Q1	21	ARG
78	Q2	2	VAL
78	Q2	3	ASN
78	Q2	8	ARG
78	Q2	16	THR
78	Q2	26	THR
78	Q2	35	LEU
78	Q2	47	GLN
78	Q2	48	SER
78	Q2	54	THR
78	Q2	60	LYS
78	Q2	66	LYS
78	Q2	72	LEU
78	Q2	76	LYS
78	Q2	78	LYS
78	Q2	79	THR
78	Q2	80	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	93	LEU
78	Q2	100	LYS
78	Q2	104	LEU
78	Q2	105	GLN
79	Q3	7	LYS
79	Q3	11	THR

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Mol	Chain	Res	Type
79	Q3	25	GLN
79	Q3	45	LYS
79	Q3	46	THR
79	Q3	49	ARG
79	Q3	56	THR
79	Q3	59	CYS
79	Q3	60	CYS
79	Q3	64	VAL
79	Q3	73	THR
79	Q3	78	THR
79	Q3	82	THR
79	Q3	84	ARG
79	Q3	90	VAL
2	s0	9	LEU
2	s0	10	THR
2	s0	12	GLU
2	s0	24	LEU
2	s0	29	VAL
2	s0	30	GLN
2	s0	39	ASN
2	s0	41	ARG
2	s0	45	VAL
2	s0	55	GLU
2	s0	59	LEU
2	s0	62	ARG
2	s0	72	ASP
2	s0	87	LEU
2	s0	88	LYS
2	s0	93	THR
2	s0	96	THR
2	s0	101	ARG
2	s0	106	SER
2	s0	110	TYR
2	s0	111	ILE
2	s0	112	THR
2	s0	119	ARG
2	s0	124	THR
2	s0	144	ILE
2	s0	151	SER
2	s0	153	SER
2	s0	154	GLU
2	s0	157	ASP

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Mol	Chain	Res	Type
2	s0	172	LEU
2	s0	183	ARG
2	s0	184	LEU
2	s0	185	ARG
2	s0	189	VAL
3	s1	21	VAL
3	s1	25	THR
3	s1	37	THR
3	s1	47	LEU
3	s1	51	SER
3	s1	55	LYS
3	s1	62	LYS
3	s1	70	LEU
3	s1	83	LYS
3	s1	85	LYS
3	s1	105	PHE
3	s1	126	THR
3	s1	129	THR
3	s1	137	ILE
3	s1	154	SER
3	s1	173	THR
3	s1	177	GLN
3	s1	180	THR
3	s1	181	LEU
3	s1	184	LEU
3	s1	202	LYS
3	s1	203	ASP
3	s1	204	ILE
3	s1	212	VAL
3	s1	215	VAL
3	s1	217	LEU
3	s1	219	LYS
3	s1	222	LYS
3	s1	223	PHE
4	s2	39	THR
4	s2	41	LEU
4	s2	53	ILE
4	s2	55	GLU
4	s2	58	LEU
4	s2	60	SER
4	s2	61	LEU
4	s2	69	ILE

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Mol	Chain	Res	Type
4	s2	72	LEU
4	s2	73	LEU
4	s2	76	LEU
4	s2	81	MET
4	s2	83	ILE
4	s2	84	LYS
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	117	THR
4	s2	139	ILE
4	s2	140	ARG
4	s2	141	ARG
4	s2	153	SER
4	s2	159	THR
4	s2	164	SER
4	s2	165	VAL
4	s2	166	THR
4	s2	170	ILE
4	s2	185	LYS
4	s2	194	GLU
4	s2	195	ASP
4	s2	206	THR
4	s2	218	ILE
4	s2	222	TYR
4	s2	225	LEU
4	s2	229	LEU
4	s2	233	GLN
4	s2	237	VAL
4	s2	244	SER
4	s2	248	SER
5	s3	4	LEU
5	s3	10	LYS
5	s3	21	LEU
5	s3	32	GLU
5	s3	39	VAL
5	s3	44	THR
5	s3	59	LEU

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Mol	Chain	Res	Type
5	s3	61	GLU
5	s3	69	LEU
5	s3	70	THR
5	s3	83	THR
5	s3	84	ILE
5	s3	89	GLU
5	s3	90	ARG
5	s3	93	ASP
5	s3	111	ASN
5	s3	115	ILE
5	s3	142	LEU
5	s3	143	ARG
5	s3	146	ARG
5	s3	148	LYS
5	s3	158	ILE
5	s3	162	GLN
5	s3	168	ILE
5	s3	172	THR
5	s3	202	LEU
5	s3	204	ASP
5	s3	208	ILE
5	s3	212	LYS
5	s3	213	GLU
5	s3	225	TYR
6	s4	7	LYS
6	s4	12	LEU
6	s4	23	LEU
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	69	HIS
6	s4	70	VAL
6	s4	77	ARG
6	s4	78	THR
6	s4	81	THR
6	s4	102	VAL
6	s4	105	VAL
6	s4	108	ARG
6	s4	113	ARG

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Mol	Chain	Res	Type
6	s4	116	ASP
6	s4	123	LEU
6	s4	126	VAL
6	s4	131	LEU
6	s4	143	ASP
6	s4	146	THR
6	s4	147	ILE
6	s4	148	ARG
6	s4	159	THR
6	s4	180	LEU
6	s4	182	TYR
6	s4	187	ARG
6	s4	191	ARG
6	s4	219	VAL
6	s4	221	ARG
6	s4	222	LEU
6	s4	227	VAL
6	s4	237	SER
6	s4	245	LYS
6	s4	248	ILE
7	s5	23	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU
7	s5	32	GLU
7	s5	38	THR
7	s5	41	LYS
7	s5	43	PHE
7	s5	44	ASN
7	s5	45	LYS
7	s5	58	LEU
7	s5	59	VAL
7	s5	63	GLN
7	s5	64	VAL
7	s5	68	ILE
7	s5	76	ARG
7	s5	83	ARG
7	s5	89	ILE
7	s5	93	LEU
7	s5	94	THR
7	s5	102	ARG
7	s5	109	LYS

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Mol	Chain	Res	Type
7	s5	119	ASP
7	s5	122	ASN
7	s5	125	THR
7	s5	128	ASN
7	s5	140	THR
7	s5	147	THR
7	s5	148	ARG
7	s5	157	ARG
7	s5	163	SER
7	s5	167	ARG
7	s5	170	GLN
7	s5	186	ASN
7	s5	194	LEU
7	s5	203	LYS
7	s5	208	SER
7	s5	213	LYS
7	s5	216	GLU
7	s5	225	ARG
8	s6	17	GLU
8	s6	21	GLU
8	s6	25	ARG
8	s6	30	LYS
8	s6	34	GLN
8	s6	43	ASP
8	s6	65	GLN
8	s6	68	LEU
8	s6	71	THR
8	s6	76	LEU
8	s6	78	THR
8	s6	79	LYS
8	s6	81	VAL
8	s6	93	LYS
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU
8	s6	111	LEU
8	s6	115	LYS
8	s6	120	GLU
8	s6	121	LEU
8	s6	126	ASP
8	s6	127	THR
8	s6	128	THR

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Mol	Chain	Res	Type
8	s6	129	VAL
8	s6	143	LYS
8	s6	150	GLU
8	s6	151	ASP
8	s6	153	VAL
8	s6	155	ASP
8	s6	156	PHE
8	s6	170	THR
8	s6	193	LEU
8	s6	203	GLU
8	s6	212	LEU
8	s6	215	ARG
9	s7	11	GLN
9	s7	28	GLU
9	s7	33	GLU
9	s7	42	GLN
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	87	ASP
9	s7	97	ARG
9	s7	103	SER
9	s7	105	THR
9	s7	108	GLN
9	s7	114	ARG
9	s7	115	SER
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	126	LEU
9	s7	136	VAL
9	s7	139	ARG
9	s7	143	LEU
9	s7	159	VAL
9	s7	185	ILE
9	s7	187	SER
10	s8	20	GLN
10	s8	25	ARG
10	s8	26	LYS

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Mol	Chain	Res	Type
10	s8	29	LEU
10	s8	32	GLN
10	s8	36	THR
10	s8	46	VAL
10	s8	58	LEU
10	s8	59	ARG
10	s8	74	LYS
10	s8	76	THR
10	s8	89	GLU
10	s8	111	GLN
10	s8	120	THR
10	s8	121	LEU
10	s8	151	LYS
10	s8	152	ILE
10	s8	155	SER
10	s8	158	SER
10	s8	161	SER
10	s8	176	SER
10	s8	183	ILE
11	s9	3	ARG
11	s9	7	THR
11	s9	22	SER
11	s9	28	LEU
11	s9	33	GLU
11	s9	39	LYS
11	s9	49	LEU
11	s9	54	ARG
11	s9	78	ARG
11	s9	82	ARG
11	s9	90	LYS
11	s9	93	LEU
11	s9	101	VAL
11	s9	109	LEU
11	s9	110	GLN
11	s9	111	THR
11	s9	115	LYS
11	s9	126	ARG
11	s9	127	VAL
11	s9	130	THR
11	s9	133	HIS
11	s9	134	ILE
11	s9	142	ASN

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Mol	Chain	Res	Type
11	s9	149	ARG
11	s9	161	THR
11	s9	162	SER
11	s9	168	ARG
11	s9	172	VAL
11	s9	180	LYS
11	s9	182	GLU
12	c0	2	LEU
12	c0	3	MET
12	c0	5	LYS
12	c0	8	ARG
12	c0	12	HIS
12	c0	15	LEU
12	c0	20	VAL
12	c0	55	VAL
12	c0	57	THR
12	c0	71	GLU
13	c1	3	THR
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	31	THR
13	c1	32	LYS
13	c1	33	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	60	PHE
13	c1	67	ARG
13	c1	74	THR
13	c1	76	VAL
13	c1	80	MET
13	c1	83	THR
13	c1	86	ILE
13	c1	122	ILE
13	c1	123	VAL
13	c1	129	ARG
13	c1	140	VAL
14	c2	28	LEU
14	c2	36	LEU

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Mol	Chain	Res	Type
14	c2	39	ASP
14	c2	43	ARG
14	c2	52	LEU
14	c2	58	LEU
14	c2	59	LEU
14	c2	62	LEU
14	c2	71	ILE
14	c2	74	LEU
14	c2	82	PRO
14	c2	83	GLU
14	c2	85	LYS
14	c2	89	ILE
14	c2	97	LEU
14	c2	103	LEU
14	c2	116	VAL
14	c2	121	VAL
14	c2	129	GLU
14	c2	132	GLU
14	c2	136	ILE
14	c2	140	PHE
15	c3	12	SER
15	c3	14	SER
15	c3	16	ILE
15	c3	35	GLU
15	c3	39	LYS
15	c3	49	GLN
15	c3	64	ARG
15	c3	66	ILE
15	c3	70	LYS
15	c3	80	LEU
15	c3	83	GLU
15	c3	84	ILE
15	c3	87	ASP
15	c3	88	LEU
15	c3	97	SER
15	c3	102	LEU
15	c3	106	ARG
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	134	VAL
15	c3	138	ASN

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Mol	Chain	Res	Type
15	c3	147	SER
15	c3	150	VAL
16	c4	16	VAL
16	c4	18	ARG
16	c4	20	TYR
16	c4	26	THR
16	c4	33	LEU
16	c4	51	ASP
16	c4	52	ARG
16	c4	66	ASP
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	123	SER
16	c4	127	ARG
16	c4	132	ARG
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
17	c5	12	PHE
17	c5	27	GLU
17	c5	28	MET
17	c5	36	LEU
17	c5	40	ARG
17	c5	51	SER
17	c5	52	LYS
17	c5	69	GLU
17	c5	72	LYS
17	c5	77	ARG
17	c5	92	SER
17	c5	107	ILE
17	c5	110	GLU
17	c5	121	ILE
17	c5	122	THR
17	c5	124	THR
17	c5	125	PRO
17	c5	127	ARG
17	c5	128	HIS

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Mol	Chain	Res	Type
18	c6	17	THR
18	c6	23	LYS
18	c6	28	LEU
18	c6	37	THR
18	c6	39	VAL
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	66	ARG
18	c6	68	ARG
18	c6	69	VAL
18	c6	70	THR
18	c6	81	ILE
18	c6	94	GLN
18	c6	98	ASP
18	c6	106	LYS
18	c6	110	THR
18	c6	114	ARG
18	c6	115	THR
18	c6	123	ARG
18	c6	137	ARG
18	c6	143	ARG
19	c7	3	ARG
19	c7	8	THR
19	c7	29	GLN
19	c7	34	LEU
19	c7	46	LEU
19	c7	49	LYS
19	c7	60	ARG
19	c7	62	GLN
19	c7	63	LYS
19	c7	69	ILE
19	c7	85	VAL
19	c7	88	VAL
19	c7	110	VAL
19	c7	113	LEU
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL

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Mol	Chain	Res	Type
20	c8	6	GLN
20	c8	10	SER
20	c8	13	HIS
20	c8	15	LEU
20	c8	25	ASN
20	c8	26	ILE
20	c8	28	ILE
20	c8	33	THR
20	c8	38	VAL
20	c8	40	ARG
20	c8	61	LEU
20	c8	63	GLN
20	c8	66	LEU
20	c8	68	ARG
20	c8	116	LEU
20	c8	119	ILE
20	c8	120	ARG
20	c8	133	VAL
20	c8	138	THR
20	c8	143	ARG
20	c8	144	ARG
20	c8	145	ARG
21	c9	6	VAL
21	c9	20	SER
21	c9	27	LYS
21	c9	28	LEU
21	c9	34	VAL
21	c9	36	ILE
21	c9	37	VAL
21	c9	57	ARG
21	c9	70	GLN
21	c9	71	VAL
21	c9	75	LYS
21	c9	84	LYS
21	c9	86	ARG
21	c9	88	VAL
21	c9	111	ILE
21	c9	123	ARG
21	c9	132	LEU
21	c9	133	ASP
21	c9	139	THR
21	c9	140	LEU

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Mol	Chain	Res	Type
21	c9	142	GLU
21	c9	143	ASP
22	d0	23	ARG
22	d0	27	THR
22	d0	30	LYS
22	d0	31	VAL
22	d0	34	LEU
22	d0	44	ASN
22	d0	47	GLN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	61	LYS
22	d0	63	LEU
22	d0	70	THR
22	d0	74	GLU
22	d0	77	LYS
22	d0	81	THR
22	d0	88	LYS
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	105	GLN
22	d0	108	ILE
22	d0	113	ASP
22	d0	115	GLU
22	d0	116	VAL
23	d1	2	GLU
23	d1	5	LYS
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	15	ARG
23	d1	18	SER
23	d1	32	VAL
23	d1	34	ILE
23	d1	38	LYS
23	d1	49	GLU
23	d1	52	THR
23	d1	68	SER
23	d1	69	LEU
23	d1	78	LEU

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Mol	Chain	Res	Type
23	d1	81	ASN
23	d1	86	SER
23	d1	87	ARG
24	d2	6	VAL
24	d2	7	LEU
24	d2	15	ASN
24	d2	20	THR
24	d2	23	ARG
24	d2	25	VAL
24	d2	31	SER
24	d2	65	LEU
24	d2	74	VAL
24	d2	81	VAL
24	d2	88	LYS
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	105	THR
24	d2	119	LYS
24	d2	129	VAL
25	d3	9	LEU
25	d3	14	LYS
25	d3	19	ARG
25	d3	23	ARG
25	d3	40	SER
25	d3	72	VAL
25	d3	73	ARG
25	d3	83	VAL
25	d3	84	THR
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	109	ARG
25	d3	121	ARG
25	d3	131	SER
26	d4	10	ARG
26	d4	13	ILE
26	d4	21	LYS
26	d4	26	ASP
26	d4	34	ASN
26	d4	36	SER
26	d4	43	LYS

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Mol	Chain	Res	Type
26	d4	44	LEU
26	d4	47	VAL
26	d4	49	LYS
26	d4	55	VAL
26	d4	62	THR
26	d4	77	ASN
26	d4	78	SER
26	d4	83	LYS
26	d4	88	THR
26	d4	105	ARG
26	d4	128	LYS
27	d5	42	LEU
27	d5	43	ASP
27	d5	46	LYS
27	d5	51	LEU
27	d5	53	GLU
27	d5	57	TYR
27	d5	60	VAL
27	d5	81	ARG
27	d5	88	ILE
27	d5	93	SER
28	d6	10	ARG
28	d6	11	ASN
28	d6	24	VAL
28	d6	44	ILE
28	d6	46	GLU
28	d6	53	LEU
28	d6	67	THR
28	d6	82	ARG
28	d6	85	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	8	LEU
29	d7	17	ARG
29	d7	41	LEU
29	d7	43	ILE
29	d7	44	THR
29	d7	52	THR
29	d7	61	THR
29	d7	72	LYS
29	d7	81	ARG
30	d8	5	THR

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Mol	Chain	Res	Type
30	d8	7	VAL
30	d8	16	LEU
30	d8	22	ARG
30	d8	32	PHE
30	d8	33	LEU
30	d8	40	ILE
30	d8	42	ARG
30	d8	52	ASP
30	d8	54	LEU
30	d8	58	GLU
30	d8	62	GLU
31	d9	4	GLU
31	d9	10	HIS
31	d9	19	ARG
31	d9	21	CYS
31	d9	26	SER
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	38	ILE
31	d9	54	LYS
80	e0	13	LYS
80	e0	22	GLU
80	e0	23	LYS
80	e0	26	LYS
80	e0	29	LYS
80	e0	41	THR
80	e0	42	ARG
80	e0	44	PHE
80	e0	47	VAL
80	e0	49	LEU
80	e0	55	ARG
33	e1	80	ARG
33	e1	84	VAL
33	e1	87	THR
33	e1	90	LYS
33	e1	96	LYS
33	e1	97	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	107	LYS

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Mol	Chain	Res	Type
33	e1	113	LYS
33	e1	120	GLU
33	e1	140	TYR
33	e1	144	CYS
33	e1	151	ASN
34	sR	23	LEU
34	sR	25	THR
34	sR	29	GLN
34	sR	52	GLN
34	sR	58	VAL
34	sR	59	ARG
34	sR	65	SER
34	sR	76	ASP
34	sR	96	THR
34	sR	98	GLU
34	sR	102	ARG
34	sR	106	HIS
34	sR	108	SER
34	sR	145	LEU
34	sR	168	THR
34	sR	176	LYS
34	sR	199	ILE
34	sR	203	THR
34	sR	228	LYS
34	sR	232	TYR
34	sR	275	ARG
34	sR	277	GLU
34	sR	286	GLU
34	sR	297	ASP
34	sR	309	VAL
34	sR	310	ILE
34	sR	312	VAL
81	sM	23	LYS
81	sM	33	LYS
81	sM	43	ASP
81	sM	45	SER
81	sM	51	ARG
81	sM	53	ARG
81	sM	55	SER
81	sM	61	ILE
81	sM	68	ARG
81	sM	74	LYS

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Mol	Chain	Res	Type
81	sM	75	ASP
81	sM	77	THR
81	sM	78	ASP
81	sM	82	THR
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	48	ILE
39	l2	49	VAL
39	l2	52	SER
39	l2	61	VAL
39	l2	62	VAL
39	l2	64	ARG
39	l2	71	LEU
39	l2	74	GLU
39	l2	82	VAL
39	l2	84	THR
39	l2	101	VAL
39	l2	116	VAL
39	l2	128	ARG
39	l2	134	VAL
39	l2	137	ILE
39	l2	142	ASP
39	l2	147	ARG
39	l2	152	SER
39	l2	155	LYS
39	l2	157	VAL
39	l2	158	ILE
39	l2	165	VAL
39	l2	169	ILE
39	l2	179	LEU
39	l2	181	LYS
39	l2	188	LYS
39	l2	190	ARG
39	l2	193	ARG
39	l2	200	ARG
39	l2	202	VAL
39	l2	227	ARG
39	l2	230	VAL

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Mol	Chain	Res	Type
39	l2	243	THR
39	l2	246	LEU
40	l3	3	HIS
40	l3	10	ARG
40	l3	17	LEU
40	l3	20	LYS
40	l3	24	SER
40	l3	30	LYS
40	l3	34	LYS
40	l3	37	ARG
40	l3	43	LEU
40	l3	44	THR
40	l3	47	LEU
40	l3	50	LYS
40	l3	55	THR
40	l3	56	ILE
40	l3	69	LYS
40	l3	73	VAL
40	l3	77	THR
40	l3	79	VAL
40	l3	84	VAL
40	l3	85	VAL
40	l3	103	THR
40	l3	114	VAL
40	l3	116	ARG
40	l3	134	SER
40	l3	139	GLN
40	l3	145	GLU
40	l3	146	ARG
40	l3	148	LEU
40	l3	150	ARG
40	l3	169	THR
40	l3	178	LEU
40	l3	183	LEU
40	l3	184	ASN
40	l3	188	ILE
40	l3	192	VAL
40	l3	196	ARG
40	l3	201	LYS
40	l3	202	THR
40	l3	205	VAL
40	l3	211	GLN

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Mol	Chain	Res	Type
40	l3	221	THR
40	l3	222	LYS
40	l3	229	VAL
40	l3	232	ARG
40	l3	235	THR
40	l3	238	LEU
40	l3	242	THR
40	l3	249	VAL
40	l3	252	ILE
40	l3	264	VAL
40	l3	266	ARG
40	l3	274	SER
40	l3	284	ARG
40	l3	287	LYS
40	l3	296	THR
40	l3	304	THR
40	l3	308	MET
40	l3	319	ASN
40	l3	322	ILE
40	l3	324	VAL
40	l3	328	ILE
40	l3	332	ARG
40	l3	338	LEU
40	l3	340	LYS
40	l3	341	SER
40	l3	346	THR
40	l3	347	SER
40	l3	348	ARG
40	l3	361	THR
41	l4	2	SER
41	l4	3	ARG
41	l4	11	LEU
41	l4	18	ASN
41	l4	22	LEU
41	l4	25	VAL
41	l4	47	ARG
41	l4	48	GLN
41	l4	60	THR
41	l4	71	VAL
41	l4	82	THR
41	l4	93	MET
41	l4	99	MET

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Mol	Chain	Res	Type
41	l4	112	LYS
41	l4	120	TYR
41	l4	136	LEU
41	l4	144	LYS
41	l4	145	ILE
41	l4	148	ILE
41	l4	150	LEU
41	l4	156	LEU
41	l4	158	SER
41	l4	170	LYS
41	l4	172	VAL
41	l4	177	ASP
41	l4	179	LEU
41	l4	182	LEU
41	l4	185	LYS
41	l4	186	LYS
41	l4	187	LEU
41	l4	191	LYS
41	l4	194	TYR
41	l4	203	ARG
41	l4	206	LEU
41	l4	211	GLU
41	l4	215	ILE
41	l4	217	LYS
41	l4	220	ARG
41	l4	222	VAL
41	l4	230	VAL
41	l4	246	ARG
41	l4	252	GLU
41	l4	265	GLU
41	l4	266	THR
41	l4	297	SER
41	l4	301	PRO
41	l4	306	THR
41	l4	307	GLN
41	l4	313	LEU
41	l4	319	LYS
41	l4	327	LEU
41	l4	338	LYS
41	l4	339	LEU
41	l4	342	LYS
41	l4	345	GLU

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Mol	Chain	Res	Type
41	l4	347	THR
41	l4	356	THR
41	l4	358	THR
41	l4	359	LEU
42	l5	4	GLN
42	l5	5	LYS
42	l5	15	ARG
42	l5	34	LYS
42	l5	35	ARG
42	l5	41	LYS
42	l5	51	LEU
42	l5	68	THR
42	l5	70	THR
42	l5	73	VAL
42	l5	75	LEU
42	l5	89	THR
42	l5	93	THR
42	l5	110	LEU
42	l5	112	LYS
42	l5	115	LEU
42	l5	118	THR
42	l5	120	LYS
42	l5	124	GLU
42	l5	128	GLU
42	l5	133	GLU
42	l5	140	ARG
42	l5	144	VAL
42	l5	146	LEU
42	l5	152	ARG
42	l5	155	THR
42	l5	158	ARG
42	l5	177	GLU
42	l5	185	PHE
42	l5	187	THR
42	l5	194	LEU
42	l5	205	SER
42	l5	211	LEU
42	l5	218	ARG
42	l5	227	LEU
42	l5	236	LEU
42	l5	242	SER
42	l5	254	LYS

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Mol	Chain	Res	Type
42	l5	258	LYS
42	l5	259	LYS
42	l5	260	PHE
42	l5	268	GLU
42	l5	269	SER
42	l5	273	ARG
42	l5	276	LYS
42	l5	279	LYS
42	l5	282	ARG
43	l6	5	LYS
43	l6	8	LYS
43	l6	15	VAL
43	l6	20	LYS
43	l6	21	THR
43	l6	50	LYS
43	l6	64	LEU
43	l6	65	ILE
43	l6	78	ARG
43	l6	79	VAL
43	l6	89	THR
43	l6	98	VAL
43	l6	99	GLU
43	l6	108	LYS
43	l6	109	GLU
43	l6	130	ILE
43	l6	131	LYS
43	l6	133	GLU
43	l6	152	THR
43	l6	155	LEU
43	l6	160	SER
43	l6	162	SER
43	l6	171	PRO
44	l7	22	THR
44	l7	26	VAL
44	l7	39	GLU
44	l7	40	LYS
44	l7	45	LEU
44	l7	54	GLU
44	l7	60	ARG
44	l7	82	LYS
44	l7	83	LEU
44	l7	88	ARG

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Mol	Chain	Res	Type
44	l7	100	ARG
44	l7	121	LYS
44	l7	124	LEU
44	l7	130	ILE
44	l7	157	ASN
44	l7	158	LYS
44	l7	159	GLN
44	l7	173	LEU
44	l7	175	LYS
44	l7	179	LEU
44	l7	181	ILE
44	l7	184	LEU
44	l7	196	LYS
44	l7	219	LYS
44	l7	229	PHE
44	l7	234	GLU
44	l7	239	LEU
45	l8	26	LEU
45	l8	41	GLN
45	l8	65	LEU
45	l8	68	ARG
45	l8	71	VAL
45	l8	74	THR
45	l8	79	GLN
45	l8	81	THR
45	l8	90	THR
45	l8	95	ASN
45	l8	98	ARG
45	l8	109	LEU
45	l8	136	LEU
45	l8	149	LYS
45	l8	150	LEU
45	l8	153	ILE
45	l8	160	ILE
45	l8	164	VAL
45	l8	169	LEU
45	l8	183	LYS
45	l8	185	ARG
45	l8	191	ASN
45	l8	208	GLU
45	l8	213	LYS
45	l8	214	LEU

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Mol	Chain	Res	Type
45	l8	217	THR
45	l8	230	LYS
45	l8	241	LYS
45	l8	245	LYS
45	l8	248	LYS
46	l9	5	GLN
46	l9	6	THR
46	l9	18	VAL
46	l9	22	SER
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	82	VAL
46	l9	91	ARG
46	l9	92	TYR
46	l9	105	GLU
46	l9	106	LYS
46	l9	107	ASP
46	l9	129	ARG
46	l9	132	VAL
46	l9	133	THR
46	l9	138	THR
46	l9	143	GLU
46	l9	144	ILE
46	l9	151	VAL
46	l9	157	ASN
46	l9	161	LEU
46	l9	162	GLN
46	l9	166	ARG
46	l9	176	LEU
46	l9	179	ILE
46	l9	191	LEU
47	m0	3	ARG
47	m0	24	ARG
47	m0	26	VAL

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Mol	Chain	Res	Type
47	m0	35	ASP
47	m0	36	LEU
47	m0	42	THR
47	m0	44	ASP
47	m0	52	LEU
47	m0	58	GLU
47	m0	60	LEU
47	m0	63	GLU
47	m0	71	CYS
47	m0	74	LYS
47	m0	76	MET
47	m0	77	THR
47	m0	87	LEU
47	m0	91	VAL
47	m0	99	ILE
47	m0	129	VAL
47	m0	139	ARG
47	m0	143	SER
47	m0	144	ASN
47	m0	162	GLN
47	m0	163	GLN
47	m0	167	LEU
47	m0	169	LYS
47	m0	176	LEU
47	m0	177	ASP
47	m0	178	ARG
47	m0	197	VAL
47	m0	200	LEU
47	m0	205	SER
47	m0	206	LEU
47	m0	208	ASN
47	m0	211	ARG
47	m0	212	GLU
47	m0	217	PHE
48	m1	10	ARG
48	m1	13	LYS
48	m1	23	VAL
48	m1	31	THR
48	m1	35	LYS
48	m1	37	LEU
48	m1	44	THR
48	m1	46	VAL

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Mol	Chain	Res	Type
48	m1	56	THR
48	m1	61	ARG
48	m1	71	VAL
48	m1	80	LEU
48	m1	94	ARG
48	m1	101	ASN
48	m1	106	ILE
48	m1	107	ASP
48	m1	112	LEU
48	m1	115	LYS
48	m1	129	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	153	LYS
48	m1	158	ASP
48	m1	159	THR
48	m1	161	SER
49	m3	58	VAL
49	m3	59	ARG
49	m3	63	VAL
49	m3	67	ARG
49	m3	69	VAL
49	m3	73	ARG
49	m3	76	THR
49	m3	85	LEU
49	m3	100	ARG
49	m3	103	ASN
49	m3	107	GLU
49	m3	114	GLN
49	m3	118	GLU
49	m3	121	SER
49	m3	123	ILE
49	m3	124	ILE
49	m3	131	LYS
49	m3	149	GLN
49	m3	152	THR
49	m3	157	ARG
49	m3	164	GLU
49	m3	165	SER
49	m3	168	ARG
49	m3	194	GLU
50	m4	2	SER

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Mol	Chain	Res	Type
50	m4	3	THR
50	m4	4	ASP
50	m4	15	VAL
50	m4	20	VAL
50	m4	24	LYS
50	m4	53	VAL
50	m4	55	ARG
50	m4	62	GLN
50	m4	64	VAL
50	m4	66	THR
50	m4	72	LEU
50	m4	80	THR
50	m4	82	SER
50	m4	107	GLU
50	m4	113	THR
50	m4	123	LEU
50	m4	124	ARG
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	8	GLU
51	m5	10	LEU
51	m5	15	GLN
51	m5	22	LEU
51	m5	24	ARG
51	m5	50	ARG
51	m5	66	VAL
51	m5	67	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	97	SER
51	m5	98	LEU
51	m5	105	ARG
51	m5	106	VAL
51	m5	114	ARG
51	m5	138	GLN
51	m5	153	ASP
51	m5	155	VAL

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Mol	Chain	Res	Type
51	m5	171	SER
51	m5	176	LYS
51	m5	188	ARG
52	m6	25	LYS
52	m6	41	LEU
52	m6	59	ARG
52	m6	60	LYS
52	m6	66	LYS
52	m6	67	THR
52	m6	68	ARG
52	m6	74	ARG
52	m6	78	ARG
52	m6	79	ILE
52	m6	84	LEU
52	m6	85	ARG
52	m6	106	GLU
52	m6	108	ILE
52	m6	110	PRO
52	m6	117	ARG
52	m6	124	LEU
52	m6	126	VAL
52	m6	128	ARG
52	m6	152	VAL
52	m6	160	ARG
52	m6	166	GLU
52	m6	170	LYS
52	m6	171	LYS
52	m6	175	THR
52	m6	182	ASN
52	m6	190	VAL
52	m6	197	LEU
53	m7	9	THR
53	m7	24	VAL
53	m7	29	THR
53	m7	32	THR
53	m7	41	LEU
53	m7	52	LEU
53	m7	56	ARG
53	m7	79	THR
53	m7	80	LYS
53	m7	86	LYS
53	m7	94	LEU

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Mol	Chain	Res	Type
53	m7	107	LEU
53	m7	114	VAL
53	m7	118	GLN
53	m7	119	VAL
53	m7	120	ASN
53	m7	126	ARG
53	m7	127	ARG
53	m7	136	ILE
53	m7	138	LYS
53	m7	144	SER
53	m7	155	GLU
54	m8	3	ILE
54	m8	7	SER
54	m8	12	ARG
54	m8	17	THR
54	m8	20	LYS
54	m8	26	LEU
54	m8	31	LYS
54	m8	32	LEU
54	m8	34	THR
54	m8	41	ASP
54	m8	49	LEU
54	m8	57	ILE
54	m8	63	SER
54	m8	64	VAL
54	m8	66	ARG
54	m8	69	ARG
54	m8	80	THR
54	m8	86	THR
54	m8	93	ILE
54	m8	100	THR
54	m8	113	LYS
54	m8	127	LEU
54	m8	135	GLN
54	m8	138	LEU
54	m8	147	ARG
54	m8	150	VAL
54	m8	159	LYS
54	m8	161	LYS
54	m8	165	ILE
54	m8	170	ARG
54	m8	178	ARG

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Mol	Chain	Res	Type
54	m8	180	ARG
55	m9	7	GLN
55	m9	8	LYS
55	m9	9	ARG
55	m9	10	LEU
55	m9	17	VAL
55	m9	20	ARG
55	m9	29	THR
55	m9	30	SER
55	m9	36	ASN
55	m9	43	LYS
55	m9	49	THR
55	m9	52	LYS
55	m9	55	VAL
55	m9	56	THR
55	m9	63	THR
55	m9	71	ARG
55	m9	74	ARG
55	m9	76	SER
55	m9	88	ARG
55	m9	91	SER
55	m9	99	LEU
55	m9	116	ASP
55	m9	117	LYS
55	m9	126	GLU
55	m9	138	LEU
55	m9	152	GLU
55	m9	153	LYS
55	m9	162	ARG
55	m9	164	LEU
55	m9	167	ARG
55	m9	170	ARG
55	m9	173	ARG
55	m9	180	LYS
56	n0	1	MET
56	n0	13	ARG
56	n0	17	GLU
56	n0	23	LYS
56	n0	32	SER
56	n0	50	LYS
56	n0	51	VAL
56	n0	52	LYS

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Mol	Chain	Res	Type
56	n0	53	LYS
56	n0	58	ILE
56	n0	62	ASN
56	n0	70	THR
56	n0	71	LYS
56	n0	73	LYS
56	n0	87	THR
56	n0	92	LYS
56	n0	97	VAL
56	n0	100	VAL
56	n0	104	GLU
56	n0	105	THR
56	n0	117	ARG
56	n0	130	GLU
56	n0	132	THR
56	n0	136	LYS
56	n0	137	ARG
56	n0	142	GLN
56	n0	148	LEU
56	n0	157	GLN
56	n0	160	THR
56	n0	162	THR
56	n0	167	ARG
56	n0	172	TYR
57	n1	12	ARG
57	n1	17	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	35	LYS
57	n1	36	VAL
57	n1	55	LYS
57	n1	68	THR
57	n1	72	VAL
57	n1	80	VAL
57	n1	83	ARG
57	n1	86	GLU
57	n1	88	ARG
57	n1	89	LEU
57	n1	96	ILE
57	n1	97	LYS
57	n1	102	ARG

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Mol	Chain	Res	Type
57	n1	122	GLN
57	n1	126	VAL
57	n1	127	GLN
57	n1	130	ARG
57	n1	135	PRO
57	n1	139	ARG
57	n1	143	THR
57	n1	149	GLN
57	n1	150	THR
57	n1	160	ILE
58	n2	16	THR
58	n2	27	VAL
58	n2	37	LEU
58	n2	43	VAL
58	n2	50	LEU
58	n2	54	VAL
58	n2	55	THR
58	n2	63	VAL
58	n2	68	THR
58	n2	75	TYR
58	n2	90	ARG
58	n2	96	VAL
58	n2	100	THR
59	n3	7	GLN
59	n3	13	ILE
59	n3	14	SER
59	n3	17	LEU
59	n3	42	SER
59	n3	70	ARG
59	n3	73	VAL
59	n3	88	ARG
59	n3	115	THR
59	n3	135	VAL
60	n4	1	MET
60	n4	5	ILE
60	n4	19	THR
60	n4	26	SER
60	n4	39	LEU
60	n4	43	ARG
60	n4	54	LEU
60	n4	57	LYS
60	n4	63	ILE

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Mol	Chain	Res	Type
60	n4	89	LEU
60	n4	96	LEU
60	n4	97	LYS
60	n4	105	ARG
60	n4	107	GLU
60	n4	126	GLU
60	n4	127	LYS
60	n4	134	GLN
60	n4	135	SER
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	39	LYS
61	n5	40	LEU
61	n5	45	LYS
61	n5	56	ARG
61	n5	63	ILE
61	n5	71	THR
61	n5	74	LYS
61	n5	86	VAL
61	n5	105	VAL
61	n5	108	LEU
61	n5	109	LYS
61	n5	115	ARG
61	n5	125	ARG
61	n5	127	THR
61	n5	135	ILE
61	n5	137	ASN
61	n5	142	ILE
62	n6	9	SER
62	n6	11	ASP
62	n6	12	ARG
62	n6	13	ARG
62	n6	14	LYS
62	n6	17	LYS
62	n6	37	LYS
62	n6	39	LEU
62	n6	40	ARG
62	n6	45	ILE
62	n6	50	ILE
62	n6	51	ARG

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Mol	Chain	Res	Type
62	n6	57	LEU
62	n6	62	SER
62	n6	66	GLN
62	n6	70	ILE
62	n6	74	TYR
62	n6	76	LEU
62	n6	80	VAL
62	n6	83	ASP
62	n6	89	LYS
62	n6	94	SER
62	n6	95	VAL
62	n6	105	VAL
62	n6	108	LYS
62	n6	120	GLN
62	n6	127	GLU
63	n7	5	LEU
63	n7	14	VAL
63	n7	15	ARG
63	n7	17	ARG
63	n7	24	VAL
63	n7	34	LYS
63	n7	46	ILE
63	n7	52	LYS
63	n7	65	ARG
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	98	THR
63	n7	100	THR
63	n7	103	GLN
63	n7	121	ARG
63	n7	127	ASN
63	n7	134	LEU
63	n7	135	ARG
64	n8	3	SER
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	10	LYS

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Mol	Chain	Res	Type
64	n8	24	LYS
64	n8	26	ARG
64	n8	42	ARG
64	n8	46	ASP
64	n8	47	LYS
64	n8	56	VAL
64	n8	60	TYR
64	n8	78	LEU
64	n8	82	ILE
64	n8	85	ASP
64	n8	87	ARG
64	n8	91	LEU
64	n8	97	GLU
64	n8	98	THR
64	n8	115	LYS
64	n8	123	VAL
64	n8	128	ARG
64	n8	132	LYS
64	n8	133	LEU
64	n8	139	ARG
65	n9	14	ARG
65	n9	21	ILE
65	n9	22	LYS
65	n9	23	LYS
65	n9	26	THR
65	n9	33	LYS
65	n9	38	LYS
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	9	SER
66	o0	10	ILE
66	o0	18	ILE
66	o0	19	LYS
66	o0	32	LYS
66	o0	34	LEU
66	o0	40	LYS
66	o0	41	LEU
66	o0	61	MET
66	o0	68	TYR
66	o0	86	ARG
66	o0	99	ASP

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Mol	Chain	Res	Type
66	o0	103	THR
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	28	ARG
67	o1	31	ARG
67	o1	34	LYS
67	o1	36	ILE
67	o1	44	MET
67	o1	46	THR
67	o1	64	VAL
67	o1	76	SER
67	o1	84	ASP
67	o1	98	VAL
67	o1	100	SER
67	o1	102	LYS
67	o1	104	LEU
67	o1	106	THR
67	o1	107	VAL
67	o1	110	GLU
68	o2	3	SER
68	o2	4	LEU
68	o2	6	HIS
68	o2	16	LYS
68	o2	18	LYS
68	o2	19	ARG
68	o2	24	ARG
68	o2	27	ARG
68	o2	33	ARG
68	o2	34	LYS
68	o2	41	VAL
68	o2	51	SER
68	o2	54	LYS
68	o2	71	HIS
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	86	THR
68	o2	89	THR
68	o2	95	GLU
68	o2	101	SER

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Mol	Chain	Res	Type
68	o2	109	LEU
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	10	LYS
69	o3	20	LYS
69	o3	28	SER
69	o3	31	LYS
69	o3	33	GLU
69	o3	49	ILE
69	o3	70	LYS
69	o3	74	THR
69	o3	84	THR
69	o3	98	VAL
69	o3	105	SER
69	o3	107	ILE
70	o4	5	VAL
70	o4	20	ILE
70	o4	24	LYS
70	o4	25	THR
70	o4	29	ILE
70	o4	30	LEU
70	o4	49	SER
70	o4	58	ARG
70	o4	64	THR
70	o4	65	VAL
70	o4	66	SER
70	o4	68	THR
70	o4	71	THR
70	o4	79	SER
70	o4	86	LYS
70	o4	87	GLU
70	o4	88	ARG
70	o4	98	GLN
70	o4	104	VAL
70	o4	105	VAL
71	o5	11	THR
71	o5	15	GLU
71	o5	20	GLN
71	o5	27	GLU
71	o5	28	LEU
71	o5	37	SER

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Mol	Chain	Res	Type
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	80	LEU
71	o5	84	LYS
71	o5	85	THR
71	o5	86	ARG
71	o5	89	ARG
71	o5	90	ARG
71	o5	100	VAL
71	o5	101	THR
71	o5	107	LYS
71	o5	119	LYS
72	o6	3	VAL
72	o6	7	ILE
72	o6	9	ILE
72	o6	12	ASN
72	o6	21	THR
72	o6	26	ILE
72	o6	29	LYS
72	o6	34	SER
72	o6	36	ARG
72	o6	37	THR
72	o6	42	SER
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	59	ASP
72	o6	60	LEU
72	o6	68	ARG
72	o6	75	LYS
72	o6	76	ARG
72	o6	79	SER
72	o6	88	GLU
72	o6	94	ILE
72	o6	98	ARG
73	o7	3	LYS

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Mol	Chain	Res	Type
73	o7	17	THR
73	o7	25	ARG
73	o7	33	THR
73	o7	36	SER
73	o7	44	THR
73	o7	58	THR
73	o7	59	THR
73	o7	65	ARG
73	o7	67	LEU
73	o7	71	SER
73	o7	80	THR
74	o8	5	ILE
74	o8	12	LEU
74	o8	16	ARG
74	o8	17	ARG
74	o8	24	THR
74	o8	41	THR
74	o8	46	ARG
74	o8	50	SER
74	o8	53	THR
74	o8	61	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	72	THR
74	o8	78	LEU
75	o9	4	GLN
75	o9	11	GLN
75	o9	15	LYS
75	o9	17	LYS
75	o9	21	ARG
75	o9	23	LEU
75	o9	29	LEU
75	o9	48	LYS
75	o9	51	ILE
76	q0	78	ILE
76	q0	79	GLU
76	q0	80	PRO
76	q0	83	LYS
76	q0	85	LEU
76	q0	91	CYS
76	q0	97	ARG
76	q0	106	ARG

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Mol	Chain	Res	Type
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	13	LEU
77	q1	14	LYS
77	q1	16	LYS
77	q1	19	LYS
77	q1	21	ARG
77	q1	23	ARG
77	q1	24	SER
78	q2	3	ASN
78	q2	7	THR
78	q2	8	ARG
78	q2	16	THR
78	q2	35	LEU
78	q2	61	LYS
78	q2	66	LYS
78	q2	71	ARG
78	q2	78	LYS
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	89	LYS
78	q2	91	PHE
78	q2	93	LEU
78	q2	97	LYS
78	q2	105	GLN
79	q3	20	SER
79	q3	24	ARG
79	q3	40	SER
79	q3	42	CYS
79	q3	54	ILE
79	q3	56	THR
79	q3	70	THR
79	q3	72	SER
83	p0	4	ILE
83	p0	5	ARG
83	p0	7	LYS
83	p0	10	GLU

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Mol	Chain	Res	Type
83	p0	14	LYS
83	p0	15	LEU
83	p0	25	LEU
83	p0	39	HIS
83	p0	42	ARG
83	p0	43	LYS
83	p0	44	GLU
83	p0	48	ARG
83	p0	51	VAL
83	p0	52	LEU
83	p0	55	LYS
83	p0	67	LEU
83	p0	70	LEU
83	p0	74	GLU
83	p0	76	LEU
83	p0	80	VAL
83	p0	81	LYS
83	p0	84	VAL
83	p0	93	LEU
83	p0	97	LYS
83	p0	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
3	S1	79	HIS
4	S2	201	ASN
5	S3	165	ASN
6	S4	142	HIS
6	S4	231	GLN
7	S5	128	ASN
7	S5	224	ASN
9	S7	74	GLN
9	S7	89	HIS
12	C0	58	GLN
12	C0	62	GLN
13	C1	37	ASN
18	C6	83	GLN
20	C8	75	ASN
20	C8	78	HIS
23	D1	74	GLN
27	D5	95	HIS

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Mol	Chain	Res	Type
34	SR	159	ASN
39	L2	8	GLN
39	L2	83	HIS
39	L2	209	HIS
39	L2	218	HIS
40	L3	256	HIS
42	L5	40	HIS
42	L5	90	HIS
42	L5	264	GLN
48	M1	109	HIS
69	O3	106	ASN
74	O8	32	ASN
78	Q2	23	HIS
3	s1	209	ASN
6	s4	36	HIS
9	s7	71	HIS
11	s9	110	GLN
11	s9	124	HIS
11	s9	142	ASN
12	c0	32	HIS
20	c8	8	GLN
21	c9	64	HIS
22	d0	98	GLN
26	d4	22	GLN
27	d5	37	GLN
39	l2	83	HIS
42	l5	264	GLN
44	l7	80	GLN
49	m3	162	ASN
56	n0	138	GLN
59	n3	33	ASN
63	n7	57	HIS
64	n8	25	HIS
64	n8	44	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	451 (25%)	62 (3%)
1	6	1793/1800 (99%)	468 (26%)	56 (3%)
36	1	3145/3396 (92%)	662 (21%)	85 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
36	5	3145/3396 (92%)	673 (21%)	84 (2%)
37	3	120/121 (99%)	16 (13%)	3 (2%)
37	7	120/121 (99%)	21 (17%)	0
38	4	157/158 (99%)	39 (24%)	3 (1%)
38	8	157/158 (99%)	36 (22%)	3 (1%)
All	All	10384/10950 (94%)	2366 (22%)	296 (2%)

All (2366) 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	47	A
1	2	50	C
1	2	57	G
1	2	60	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	104	A
1	2	114	C
1	2	127	G
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U

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Mol	Chain	Res	Type
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	166	C
1	2	167	U
1	2	169	A
1	2	170	U
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	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	233	C
1	2	234	G
1	2	235	G
1	2	236	A
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U

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Mol	Chain	Res	Type
1	2	250	C
1	2	260	U
1	2	261	U
1	2	265	A
1	2	266	A
1	2	267	U
1	2	271	A
1	2	272	U
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	284	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	308	C
1	2	314	C
1	2	316	A
1	2	321	C
1	2	322	G
1	2	325	G
1	2	337	G
1	2	338	C
1	2	341	A
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	418	G
1	2	419	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A

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Mol	Chain	Res	Type
1	2	434	G
1	2	439	U
1	2	444	C
1	2	445	A
1	2	448	C
1	2	454	U
1	2	468	A
1	2	484	C
1	2	485	A
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	511	A
1	2	512	A
1	2	513	U
1	2	515	A
1	2	516	G
1	2	527	A
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
1	2	543	C
1	2	544	A
1	2	546	U

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Mol	Chain	Res	Type
1	2	548	G
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	579	A
1	2	580	A
1	2	582	U
1	2	585	A
1	2	594	A
1	2	595	G
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	650	U
1	2	653	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A

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Mol	Chain	Res	Type
1	2	709	C
1	2	710	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	743	U
1	2	745	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	779	U
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	789	A
1	2	793	A

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Mol	Chain	Res	Type
1	2	794	U
1	2	795	U
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G
1	2	824	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	848	C
1	2	854	U
1	2	856	A
1	2	862	A
1	2	863	A
1	2	864	U
1	2	886	U
1	2	896	U
1	2	898	A
1	2	912	U
1	2	913	G
1	2	914	G
1	2	916	U
1	2	921	U
1	2	933	A
1	2	935	U
1	2	942	G
1	2	944	A
1	2	951	A
1	2	960	U
1	2	966	A
1	2	971	A
1	2	992	A

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Mol	Chain	Res	Type
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	1026	A
1	2	1028	C
1	2	1029	U
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1064	G
1	2	1074	G
1	2	1080	U
1	2	1082	C
1	2	1086	A
1	2	1087	A
1	2	1091	A
1	2	1092	A
1	2	1093	A
1	2	1096	C
1	2	1097	U
1	2	1098	U
1	2	1100	G
1	2	1109	G
1	2	1111	G
1	2	1138	A
1	2	1150	G
1	2	1151	A
1	2	1152	A
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1167	G
1	2	1185	U
1	2	1191	U

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Mol	Chain	Res	Type
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G
1	2	1226	A
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1257	U
1	2	1258	U
1	2	1286	U
1	2	1292	G
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
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1349	G
1	2	1354	G
1	2	1355	C
1	2	1361	U
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1370	U

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Mol	Chain	Res	Type
1	2	1371	A
1	2	1379	C
1	2	1383	G
1	2	1388	A
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1412	G
1	2	1413	U
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1435	G
1	2	1446	A
1	2	1447	C
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	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	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1535	U
1	2	1536	G
1	2	1537	C

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Mol	Chain	Res	Type
1	2	1538	U
1	2	1548	G
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1573	A
1	2	1574	G
1	2	1583	A
1	2	1584	G
1	2	1591	C
1	2	1600	A
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1626	U
1	2	1627	U
1	2	1631	A
1	2	1635	A
1	2	1638	G
1	2	1652	C
1	2	1657	U
1	2	1658	G
1	2	1683	C
1	2	1684	U
1	2	1719	A
1	2	1729	C
1	2	1756	A
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1768	G
1	2	1769	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	14	U

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Mol	Chain	Res	Type
36	1	16	A
36	1	26	A
36	1	40	A
36	1	43	A
36	1	49	A
36	1	57	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	68	C
36	1	73	C
36	1	74	G
36	1	75	G
36	1	76	G
36	1	83	U
36	1	85	A
36	1	92	G
36	1	93	C
36	1	94	G
36	1	99	A
36	1	109	A
36	1	110	G
36	1	111	C
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	147	U
36	1	156	G
36	1	157	A
36	1	166	C
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	235	A

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Mol	Chain	Res	Type
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	265	A
36	1	269	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	315	C
36	1	323	A
36	1	329	U
36	1	343	U
36	1	349	A
36	1	350	C
36	1	375	A
36	1	376	G
36	1	395	A
36	1	398	A
36	1	399	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	410	U
36	1	417	A
36	1	421	G
36	1	422	A
36	1	440	A
36	1	495	G
36	1	520	U
36	1	521	A
36	1	535	G
36	1	537	A
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G

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Mol	Chain	Res	Type
36	1	551	A
36	1	552	G
36	1	553	U
36	1	555	U
36	1	556	U
36	1	557	A
36	1	559	A
36	1	560	G
36	1	573	C
36	1	578	A
36	1	579	G
36	1	592	A
36	1	604	G
36	1	608	A
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	639	G
36	1	647	A
36	1	649	A
36	1	656	A
36	1	658	G
36	1	660	A
36	1	661	G
36	1	677	A
36	1	681	U
36	1	691	A
36	1	705	A
36	1	712	G
36	1	715	A
36	1	716	A
36	1	719	U
36	1	764	U
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	780	A
36	1	781	G

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Mol	Chain	Res	Type
36	1	785	G
36	1	786	A
36	1	804	C
36	1	806	A
36	1	817	A
36	1	830	A
36	1	849	C
36	1	861	C
36	1	874	U
36	1	875	G
36	1	879	U
36	1	890	C
36	1	895	A
36	1	896	A
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	923	C
36	1	924	G
36	1	937	G
36	1	938	C
36	1	943	U
36	1	944	C
36	1	959	C
36	1	960	U
36	1	974	G
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	991	G
36	1	993	G
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

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Mol	Chain	Res	Type
36	1	1020	G
36	1	1021	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1037	C
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1063	G
36	1	1064	A
36	1	1065	A
36	1	1071	U
36	1	1072	G
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1087	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1128	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	1190	A
36	1	1191	U
36	1	1192	C
36	1	1196	C
36	1	1197	A
36	1	1201	C
36	1	1209	G

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Mol	Chain	Res	Type
36	1	1213	G
36	1	1216	C
36	1	1218	U
36	1	1222	G
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1235	U
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1242	G
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1267	U
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1272	C
36	1	1274	A
36	1	1277	C
36	1	1278	A
36	1	1279	C
36	1	1285	G
36	1	1287	A
36	1	1306	G
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1329	U
36	1	1330	A
36	1	1331	U
36	1	1333	C

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Mol	Chain	Res	Type
36	1	1345	G
36	1	1348	U
36	1	1349	G
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1354	G
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1368	U
36	1	1386	A
36	1	1399	A
36	1	1400	G
36	1	1418	A
36	1	1419	A
36	1	1429	G
36	1	1434	G
36	1	1437	C
36	1	1440	G
36	1	1446	A
36	1	1448	U
36	1	1450	G
36	1	1454	A
36	1	1455	U
36	1	1468	A
36	1	1481	A
36	1	1482	A
36	1	1503	A
36	1	1508	C
36	1	1526	U
36	1	1527	C
36	1	1528	G
36	1	1529	A
36	1	1533	U
36	1	1555	U
36	1	1556	C
36	1	1557	A
36	1	1560	G
36	1	1561	G
36	1	1562	C
36	1	1563	C

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Mol	Chain	Res	Type
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	1572	U
36	1	1575	A
36	1	1576	G
36	1	1580	A
36	1	1581	C
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1607	U
36	1	1620	U
36	1	1629	U
36	1	1639	C
36	1	1642	A
36	1	1643	A
36	1	1645	U
36	1	1657	C
36	1	1683	A
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1725	C
36	1	1735	G
36	1	1736	G
36	1	1741	A
36	1	1742	U
36	1	1745	C
36	1	1750	A
36	1	1751	G
36	1	1760	A
36	1	1761	C
36	1	1762	C
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1770	G

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Mol	Chain	Res	Type
36	1	1780	G
36	1	1781	C
36	1	1783	U
36	1	1797	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
36	1	1845	G
36	1	1846	C
36	1	1849	C
36	1	1866	C
36	1	1871	U
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1901	A
36	1	1906	G
36	1	1948	G
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	1954	G
36	1	2094	C
36	1	2101	C
36	1	2102	U
36	1	2106	A
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2116	G
36	1	2121	G
36	1	2122	G
36	1	2131	A

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Mol	Chain	Res	Type
36	1	2133	U
36	1	2140	U
36	1	2144	A
36	1	2158	A
36	1	2164	A
36	1	2169	G
36	1	2170	U
36	1	2187	G
36	1	2188	A
36	1	2192	C
36	1	2193	U
36	1	2194	G
36	1	2198	A
36	1	2201	G
36	1	2205	U
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2223	A
36	1	2228	A
36	1	2239	G
36	1	2244	A
36	1	2245	C
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	2281	A
36	1	2282	U
36	1	2284	C
36	1	2298	U
36	1	2301	U
36	1	2307	G
36	1	2309	A
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2319	U
36	1	2330	C

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Mol	Chain	Res	Type
36	1	2334	U
36	1	2336	U
36	1	2362	C
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2393	G
36	1	2394	G
36	1	2397	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2405	C
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2424	A
36	1	2435	G
36	1	2437	G
36	1	2443	A
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2504	U
36	1	2513	U
36	1	2514	U
36	1	2515	A
36	1	2522	G
36	1	2523	A
36	1	2525	G
36	1	2526	C
36	1	2532	U
36	1	2533	G
36	1	2534	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U

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Mol	Chain	Res	Type
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	2567	C
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	2576	G
36	1	2581	U
36	1	2582	C
36	1	2585	G
36	1	2586	G
36	1	2593	A
36	1	2594	C
36	1	2606	G
36	1	2607	G
36	1	2613	U
36	1	2614	G
36	1	2619	G
36	1	2626	A
36	1	2629	U
36	1	2630	C
36	1	2637	A
36	1	2652	U
36	1	2654	C
36	1	2656	A
36	1	2672	G
36	1	2674	A
36	1	2677	G
36	1	2689	A
36	1	2691	A
36	1	2694	A
36	1	2696	A
36	1	2705	A

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Mol	Chain	Res	Type
36	1	2714	G
36	1	2728	G
36	1	2752	U
36	1	2753	G
36	1	2755	C
36	1	2762	A
36	1	2771	U
36	1	2772	C
36	1	2773	C
36	1	2777	G
36	1	2778	G
36	1	2779	A
36	1	2787	G
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2810	C
36	1	2816	G
36	1	2817	A
36	1	2818	U
36	1	2822	U
36	1	2825	C
36	1	2829	U
36	1	2830	G
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2849	C
36	1	2853	A
36	1	2860	U
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2875	U
36	1	2876	C
36	1	2882	U
36	1	2887	A
36	1	2889	C
36	1	2898	G
36	1	2899	C
36	1	2923	U

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Mol	Chain	Res	Type
36	1	2927	C
36	1	2935	U
36	1	2936	A
36	1	2942	C
36	1	2945	G
36	1	2947	G
36	1	2955	U
36	1	2971	A
36	1	2979	U
36	1	2983	C
36	1	2990	G
36	1	2992	U
36	1	2996	U
36	1	2997	G
36	1	3012	A
36	1	3025	C
36	1	3030	G
36	1	3040	A
36	1	3055	U
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3079	U
36	1	3086	A
36	1	3087	A
36	1	3092	C
36	1	3113	A
36	1	3119	U
36	1	3122	A
36	1	3128	G
36	1	3130	A
36	1	3131	U
36	1	3136	G
36	1	3139	A
36	1	3141	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

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Mol	Chain	Res	Type
36	1	3157	U
36	1	3158	G
36	1	3164	C
36	1	3165	A
36	1	3168	A
36	1	3169	U
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3180	A
36	1	3181	C
36	1	3187	A
36	1	3196	U
36	1	3198	U
36	1	3207	U
36	1	3208	G
36	1	3210	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3228	C
36	1	3229	G
36	1	3235	C
36	1	3242	G
36	1	3243	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3270	U
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	3293	U

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Mol	Chain	Res	Type
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
36	1	3320	A
36	1	3330	A
36	1	3335	A
36	1	3336	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3350	C
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3369	G
36	1	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
36	1	3396	U
37	3	5	G
37	3	13	A
37	3	14	U
37	3	21	G
37	3	22	A
37	3	42	A
37	3	53	U
37	3	54	U
37	3	65	G
37	3	74	C
37	3	76	A

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Mol	Chain	Res	Type
37	3	91	G
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	21	C
38	4	22	U
38	4	26	U
38	4	34	U
38	4	35	C
38	4	43	A
38	4	48	A
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	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	97	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	148	G
38	4	152	G

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Mol	Chain	Res	Type
38	4	155	A
38	4	158	U
1	6	2	A
1	6	4	C
1	6	13	C
1	6	17	C
1	6	24	U
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	47	A
1	6	57	G
1	6	68	A
1	6	69	G
1	6	71	A
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	78	A
1	6	100	A
1	6	104	A
1	6	114	C
1	6	116	U
1	6	127	G
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	142	G
1	6	143	G
1	6	144	U
1	6	145	A
1	6	146	U
1	6	158	U
1	6	159	U
1	6	166	C
1	6	177	U
1	6	178	U
1	6	185	U

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Mol	Chain	Res	Type
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	198	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	222	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	229	U
1	6	230	C
1	6	232	U
1	6	233	C
1	6	235	G
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	261	U
1	6	265	A
1	6	271	A
1	6	272	U
1	6	273	G
1	6	276	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	287	G
1	6	299	A
1	6	301	A
1	6	308	C
1	6	314	C

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Mol	Chain	Res	Type
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	333	A
1	6	335	U
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	393	C
1	6	396	G
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	417	A
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	439	U
1	6	444	C
1	6	448	C
1	6	454	U
1	6	468	A
1	6	470	A
1	6	477	A
1	6	480	G
1	6	484	C
1	6	485	A
1	6	486	G
1	6	487	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A

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Mol	Chain	Res	Type
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	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	515	A
1	6	519	C
1	6	527	A
1	6	534	A
1	6	536	C
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	564	G
1	6	565	C
1	6	566	C
1	6	570	A
1	6	574	G
1	6	578	U
1	6	579	A
1	6	580	A
1	6	582	U

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Mol	Chain	Res	Type
1	6	585	A
1	6	594	A
1	6	595	G
1	6	609	U
1	6	610	G
1	6	617	U
1	6	619	A
1	6	620	A
1	6	621	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	637	C
1	6	639	U
1	6	640	U
1	6	645	C
1	6	648	G
1	6	651	G
1	6	652	G
1	6	653	C
1	6	654	C
1	6	658	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	669	G
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	691	C
1	6	696	C
1	6	698	U
1	6	710	U
1	6	711	U
1	6	714	G

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Mol	Chain	Res	Type
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	726	C
1	6	730	G
1	6	742	U
1	6	743	U
1	6	753	A
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	767	U
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G
1	6	789	A
1	6	790	U
1	6	792	U
1	6	793	A
1	6	794	U
1	6	795	U
1	6	806	A
1	6	811	A
1	6	812	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	823	G
1	6	825	U
1	6	826	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U

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Mol	Chain	Res	Type
1	6	834	G
1	6	835	U
1	6	847	A
1	6	856	A
1	6	863	A
1	6	864	U
1	6	876	G
1	6	898	A
1	6	906	A
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	944	A
1	6	959	U
1	6	960	U
1	6	966	A
1	6	970	A
1	6	971	A
1	6	983	A
1	6	989	U
1	6	991	G
1	6	992	A
1	6	993	A
1	6	997	G
1	6	998	A
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1020	A
1	6	1021	C
1	6	1025	A
1	6	1026	A
1	6	1028	C
1	6	1031	U
1	6	1039	A
1	6	1040	G
1	6	1052	U
1	6	1053	G
1	6	1056	U

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Mol	Chain	Res	Type
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1063	U
1	6	1066	C
1	6	1071	U
1	6	1074	G
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	1137	A
1	6	1138	A
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1162	C
1	6	1167	G
1	6	1185	U
1	6	1194	A
1	6	1196	A
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1207	C
1	6	1208	A
1	6	1217	A
1	6	1218	G
1	6	1219	A
1	6	1220	C
1	6	1221	A
1	6	1226	A
1	6	1228	G
1	6	1229	G

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Mol	Chain	Res	Type
1	6	1230	A
1	6	1239	U
1	6	1241	G
1	6	1242	A
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1259	U
1	6	1262	U
1	6	1286	U
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1327	C
1	6	1337	A
1	6	1338	C
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1371	A
1	6	1372	U
1	6	1373	C
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1412	G
1	6	1413	U

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Mol	Chain	Res	Type
1	6	1414	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1429	G
1	6	1431	C
1	6	1433	G
1	6	1445	G
1	6	1446	A
1	6	1448	G
1	6	1454	G
1	6	1457	C
1	6	1458	G
1	6	1459	C
1	6	1461	C
1	6	1469	A
1	6	1471	A
1	6	1481	C
1	6	1482	C
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1496	U
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1554	U
1	6	1555	A
1	6	1557	U
1	6	1559	A
1	6	1569	A

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Mol	Chain	Res	Type
1	6	1573	A
1	6	1574	G
1	6	1575	G
1	6	1576	A
1	6	1577	A
1	6	1584	G
1	6	1590	G
1	6	1601	G
1	6	1615	C
1	6	1616	G
1	6	1619	C
1	6	1621	U
1	6	1622	G
1	6	1634	C
1	6	1637	C
1	6	1657	U
1	6	1658	G
1	6	1696	G
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1710	U
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1727	G
1	6	1731	A
1	6	1736	G
1	6	1742	U
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A
1	6	1783	C

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Mol	Chain	Res	Type
1	6	1789	G
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	14	U
36	5	15	C
36	5	26	A
36	5	33	G
36	5	38	U
36	5	40	A
36	5	49	A
36	5	60	A
36	5	65	A
36	5	66	A
36	5	73	C
36	5	76	G
36	5	83	U
36	5	88	A
36	5	92	G
36	5	93	C
36	5	97	U
36	5	99	A
36	5	109	A
36	5	110	G
36	5	113	C
36	5	116	A
36	5	121	A
36	5	122	A
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	142	C
36	5	150	A
36	5	152	U
36	5	156	G
36	5	157	A
36	5	160	G

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Mol	Chain	Res	Type
36	5	165	A
36	5	166	C
36	5	170	G
36	5	171	G
36	5	172	G
36	5	173	G
36	5	174	C
36	5	178	U
36	5	180	C
36	5	182	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	200	C
36	5	210	U
36	5	218	G
36	5	219	A
36	5	221	A
36	5	224	C
36	5	231	G
36	5	234	G
36	5	235	A
36	5	236	G
36	5	237	G
36	5	239	G
36	5	240	U
36	5	244	G
36	5	246	U
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	259	C
36	5	269	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	323	A
36	5	329	U

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Mol	Chain	Res	Type
36	5	339	C
36	5	349	A
36	5	350	C
36	5	370	U
36	5	376	G
36	5	395	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	417	A
36	5	421	G
36	5	422	A
36	5	425	G
36	5	436	A
36	5	439	C
36	5	441	U
36	5	442	G
36	5	443	G
36	5	492	U
36	5	495	G
36	5	503	C
36	5	521	A
36	5	531	G
36	5	535	G
36	5	542	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	551	A
36	5	552	G
36	5	553	U
36	5	555	U
36	5	557	A
36	5	559	A
36	5	578	A
36	5	579	G
36	5	592	A
36	5	600	G
36	5	604	G
36	5	608	A

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Mol	Chain	Res	Type
36	5	609	G
36	5	610	G
36	5	611	A
36	5	619	A
36	5	620	U
36	5	621	A
36	5	636	C
36	5	649	A
36	5	660	A
36	5	677	A
36	5	681	U
36	5	683	U
36	5	689	U
36	5	705	A
36	5	712	G
36	5	715	A
36	5	716	A
36	5	725	G
36	5	727	G
36	5	735	A
36	5	736	A
36	5	758	C
36	5	765	C
36	5	766	U
36	5	767	U
36	5	768	C
36	5	776	U
36	5	777	U
36	5	778	U
36	5	780	A
36	5	781	G
36	5	785	G
36	5	786	A
36	5	796	U
36	5	806	A
36	5	816	A
36	5	817	A
36	5	830	A
36	5	851	C
36	5	861	C
36	5	874	U
36	5	879	U

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Mol	Chain	Res	Type
36	5	881	C
36	5	896	A
36	5	897	U
36	5	907	G
36	5	908	G
36	5	910	G
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	923	C
36	5	924	G
36	5	937	G
36	5	944	C
36	5	946	U
36	5	959	C
36	5	960	U
36	5	963	G
36	5	979	U
36	5	993	G
36	5	994	G
36	5	1001	G
36	5	1002	A
36	5	1003	A
36	5	1006	A
36	5	1010	G
36	5	1014	U
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1019	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1027	A
36	5	1028	U
36	5	1029	G
36	5	1035	G
36	5	1047	A
36	5	1049	C

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Mol	Chain	Res	Type
36	5	1052	U
36	5	1064	A
36	5	1065	A
36	5	1066	G
36	5	1072	G
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	1116	G
36	5	1117	G
36	5	1121	U
36	5	1129	A
36	5	1131	G
36	5	1153	A
36	5	1159	A
36	5	1160	C
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1190	A
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1197	A
36	5	1201	C
36	5	1209	G
36	5	1213	G
36	5	1222	G
36	5	1232	C
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1243	G

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Mol	Chain	Res	Type
36	5	1245	A
36	5	1246	G
36	5	1252	A
36	5	1254	C
36	5	1258	U
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1312	C
36	5	1313	G
36	5	1321	G
36	5	1330	A
36	5	1331	U
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1354	G
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1366	A
36	5	1380	G
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1419	A
36	5	1424	C
36	5	1431	G
36	5	1433	A
36	5	1434	G
36	5	1435	A
36	5	1437	C
36	5	1446	A
36	5	1450	G

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Mol	Chain	Res	Type
36	5	1460	A
36	5	1465	A
36	5	1481	A
36	5	1482	A
36	5	1490	A
36	5	1495	U
36	5	1500	G
36	5	1502	C
36	5	1503	A
36	5	1508	C
36	5	1519	G
36	5	1522	U
36	5	1528	G
36	5	1533	U
36	5	1536	G
36	5	1541	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
36	5	1580	A
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1589	A

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Mol	Chain	Res	Type
36	5	1593	A
36	5	1605	A
36	5	1607	U
36	5	1608	C
36	5	1620	U
36	5	1629	U
36	5	1639	C
36	5	1641	U
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1657	C
36	5	1658	G
36	5	1683	A
36	5	1685	C
36	5	1687	U
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1725	C
36	5	1736	G
36	5	1750	A
36	5	1751	G
36	5	1756	C
36	5	1760	A
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1769	G
36	5	1770	G
36	5	1780	G
36	5	1796	G
36	5	1797	A
36	5	1813	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1820	U
36	5	1821	U

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Mol	Chain	Res	Type
36	5	1839	A
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	1906	G
36	5	1918	C
36	5	1932	A
36	5	1935	G
36	5	1953	G
36	5	2101	C
36	5	2102	U
36	5	2111	G
36	5	2112	U
36	5	2113	A
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2139	A
36	5	2144	A
36	5	2158	A
36	5	2169	G
36	5	2170	U
36	5	2176	U
36	5	2186	U
36	5	2188	A
36	5	2192	C
36	5	2198	A
36	5	2201	G
36	5	2205	U
36	5	2206	G
36	5	2210	G
36	5	2213	A
36	5	2222	A
36	5	2223	A
36	5	2225	U

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Mol	Chain	Res	Type
36	5	2228	A
36	5	2229	A
36	5	2244	A
36	5	2250	G
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2258	U
36	5	2269	U
36	5	2270	A
36	5	2273	G
36	5	2279	A
36	5	2281	A
36	5	2288	G
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2334	U
36	5	2336	U
36	5	2361	A
36	5	2366	C
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2392	C
36	5	2393	G
36	5	2394	G
36	5	2397	A
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2411	U
36	5	2418	G
36	5	2437	G
36	5	2439	A
36	5	2440	G
36	5	2441	A
36	5	2443	A

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Mol	Chain	Res	Type
36	5	2504	U
36	5	2505	U
36	5	2506	U
36	5	2507	C
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2512	C
36	5	2514	U
36	5	2515	A
36	5	2522	G
36	5	2523	A
36	5	2526	C
36	5	2529	A
36	5	2530	G
36	5	2531	C
36	5	2532	U
36	5	2534	G
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2549	G
36	5	2552	C
36	5	2555	G
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2593	A
36	5	2594	C
36	5	2599	U
36	5	2606	G
36	5	2607	G
36	5	2610	G

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Mol	Chain	Res	Type
36	5	2614	G
36	5	2615	G
36	5	2618	G
36	5	2628	A
36	5	2639	G
36	5	2652	U
36	5	2656	A
36	5	2667	A
36	5	2674	A
36	5	2677	G
36	5	2681	U
36	5	2682	C
36	5	2683	U
36	5	2689	A
36	5	2690	G
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2700	G
36	5	2705	A
36	5	2714	G
36	5	2719	U
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	2781	U
36	5	2796	G
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2810	C
36	5	2814	G
36	5	2816	G
36	5	2817	A

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Mol	Chain	Res	Type
36	5	2818	U
36	5	2819	A
36	5	2821	C
36	5	2829	U
36	5	2837	A
36	5	2838	A
36	5	2843	U
36	5	2845	A
36	5	2853	A
36	5	2871	G
36	5	2872	A
36	5	2876	C
36	5	2887	A
36	5	2889	C
36	5	2899	C
36	5	2904	U
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2947	G
36	5	2954	U
36	5	2955	U
36	5	2957	G
36	5	2971	A
36	5	2972	G
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	3028	G
36	5	3049	A
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3069	G
36	5	3078	U
36	5	3079	U
36	5	3080	G
36	5	3081	C

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Mol	Chain	Res	Type
36	5	3086	A
36	5	3092	C
36	5	3102	G
36	5	3119	U
36	5	3123	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3150	A
36	5	3153	U
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3159	C
36	5	3164	C
36	5	3165	A
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3179	U
36	5	3180	A
36	5	3181	C
36	5	3184	A
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3198	U
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3224	G
36	5	3228	C
36	5	3229	G
36	5	3238	G
36	5	3239	G
36	5	3243	A

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Mol	Chain	Res	Type
36	5	3244	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3260	G
36	5	3263	G
36	5	3270	U
36	5	3273	A
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3279	A
36	5	3280	U
36	5	3281	U
36	5	3282	U
36	5	3285	C
36	5	3286	G
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3307	A
36	5	3313	U
36	5	3317	U
36	5	3319	U
36	5	3325	G
36	5	3330	A
36	5	3332	U
36	5	3333	G
36	5	3335	A
36	5	3336	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3356	G
36	5	3358	U

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Mol	Chain	Res	Type
36	5	3369	G
36	5	3378	C
36	5	3382	U
36	5	3383	G
36	5	3389	U
36	5	3390	G
36	5	3393	U
36	5	3394	U
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	27	A
37	7	33	U
37	7	38	U
37	7	42	A
37	7	54	U
37	7	55	A
37	7	60	G
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	84	A
37	7	91	G
37	7	93	C
37	7	101	G
37	7	102	A
37	7	103	A
37	7	110	G
37	7	112	G
38	8	21	C
38	8	34	U
38	8	35	C
38	8	48	A
38	8	49	G
38	8	52	A
38	8	53	A
38	8	59	A
38	8	62	C
38	8	63	G
38	8	79	A
38	8	80	A

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Mol	Chain	Res	Type
38	8	81	U
38	8	83	C
38	8	84	C
38	8	85	G
38	8	86	U
38	8	87	G
38	8	90	U
38	8	95	G
38	8	96	A
38	8	97	A
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	138	A
38	8	152	G
38	8	155	A
38	8	156	U
38	8	157	U
38	8	158	U

All (296) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	73	U
1	2	74	U
1	2	103	A
1	2	114	C
1	2	126	A
1	2	130	C
1	2	131	C
1	2	139	C
1	2	158	U
1	2	187	G
1	2	217	A

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Mol	Chain	Res	Type
1	2	218	A
1	2	232	U
1	2	240	U
1	2	260	U
1	2	278	U
1	2	280	U
1	2	313	U
1	2	400	A
1	2	417	A
1	2	468	A
1	2	484	C
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	558	U
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	734	A
1	2	755	A
1	2	781	U
1	2	782	U
1	2	794	U
1	2	811	A
1	2	829	A
1	2	913	G
1	2	1058	U
1	2	1081	A
1	2	1150	G
1	2	1157	A
1	2	1196	A
1	2	1207	C
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1339	C
1	2	1344	A
1	2	1370	U
1	2	1481	C

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Mol	Chain	Res	Type
1	2	1489	U
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1657	U
1	2	1761	U
36	1	43	A
36	1	65	A
36	1	99	A
36	1	109	A
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	619	A
36	1	647	A
36	1	715	A
36	1	763	G
36	1	816	A
36	1	873	C
36	1	896	A
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	1507	G

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Mol	Chain	Res	Type
36	1	1554	U
36	1	1562	C
36	1	1582	C
36	1	1716	U
36	1	1724	U
36	1	1751	G
36	1	1815	U
36	1	1816	A
36	1	1820	U
36	1	1842	A
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	2418	G
36	1	2513	U
36	1	2522	G
36	1	2525	G
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2656	A
36	1	2704	A
36	1	2728	G
36	1	2772	C
36	1	2801	A
36	1	2818	U
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3139	A
36	1	3157	U
36	1	3195	U
36	1	3217	C
36	1	3218	A
36	1	3228	C

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Mol	Chain	Res	Type
36	1	3269	U
36	1	3275	U
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
37	3	13	A
37	3	49	G
37	3	52	G
38	4	85	G
38	4	111	A
38	4	125	U
1	6	25	C
1	6	103	A
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	512	A
1	6	514	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	555	A
1	6	557	G
1	6	558	U
1	6	651	G
1	6	667	U
1	6	678	A
1	6	697	C
1	6	717	C

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Mol	Chain	Res	Type
1	6	755	A
1	6	829	A
1	6	834	G
1	6	1051	G
1	6	1058	U
1	6	1081	A
1	6	1097	U
1	6	1137	A
1	6	1207	C
1	6	1227	A
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1481	C
1	6	1489	U
1	6	1491	U
1	6	1535	U
1	6	1568	C
1	6	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
1	6	1700	C
36	5	43	A
36	5	65	A
36	5	93	C
36	5	151	A
36	5	223	U
36	5	238	A
36	5	397	A
36	5	588	G
36	5	647	A
36	5	715	A
36	5	735	A
36	5	765	C
36	5	896	A
36	5	916	G
36	5	993	G

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Mol	Chain	Res	Type
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1181	U
36	5	1236	G
36	5	1238	C
36	5	1241	U
36	5	1307	G
36	5	1329	U
36	5	1352	A
36	5	1355	A
36	5	1370	G
36	5	1392	G
36	5	1434	G
36	5	1481	A
36	5	1507	G
36	5	1514	G
36	5	1560	G
36	5	1574	C
36	5	1580	A
36	5	1607	U
36	5	1716	U
36	5	1751	G
36	5	1816	A
36	5	1819	U
36	5	1841	A
36	5	1846	C
36	5	1879	A
36	5	2101	C
36	5	2112	U
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2257	C
36	5	2281	A
36	5	2372	A
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2522	G

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Mol	Chain	Res	Type
36	5	2531	C
36	5	2539	C
36	5	2593	A
36	5	2682	C
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2818	U
36	5	2887	A
36	5	2971	A
36	5	3049	A
36	5	3056	U
36	5	3078	U
36	5	3154	C
36	5	3195	U
36	5	3207	U
36	5	3218	A
36	5	3228	C
36	5	3242	G
36	5	3259	U
36	5	3269	U
36	5	3275	U
36	5	3289	G
36	5	3303	G
36	5	3340	G
36	5	3341	U
36	5	3357	U
38	8	59	A
38	8	111	A
38	8	126	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2563 ligands modelled in this entry, 1428 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	$\#\|Z\| > 2$
87	OHX	2	2166	-	0,6,6	-	-	-		
87	OHX	2	2132	-	0,6,6	-	-	-		
87	OHX	1	4085	-	0,6,6	-	-	-		
87	OHX	2	2171	-	0,6,6	-	-	-		
87	OHX	1	4163	-	0,6,6	-	-	-		
87	OHX	5	4113	-	0,6,6	-	-	-		
87	OHX	1	3912	-	0,6,6	-	-	-		
87	OHX	5	4010	-	0,6,6	-	-	-		
87	OHX	1	4065	-	0,6,6	-	-	-		
87	OHX	5	4025	-	0,6,6	-	-	-		
87	OHX	1	3988	-	0,6,6	-	-	-		
87	OHX	5	3982	-	0,6,6	-	-	-		
87	OHX	2	2025	-	0,6,6	-	-	-		
87	OHX	1	4192	-	0,6,6	-	-	-		
87	OHX	1	3944	-	0,6,6	-	-	-		
87	OHX	1	4088	-	0,6,6	-	-	-		
87	OHX	6	2148	-	0,6,6	-	-	-		
87	OHX	5	4221	-	0,6,6	-	-	-		
87	OHX	4	231	-	0,6,6	-	-	-		
87	OHX	6	2076	-	0,6,6	-	-	-		
87	OHX	1	4152	-	0,6,6	-	-	-		
87	OHX	1	3933	-	0,6,6	-	-	-		
87	OHX	s9	201	-	0,6,6	-	-	-		
87	OHX	5	3963	-	0,6,6	-	-	-		
87	OHX	5	4074	-	0,6,6	-	-	-		
87	OHX	4	232	-	0,6,6	-	-	-		
87	OHX	5	4240	-	0,6,6	-	-	-		
87	OHX	6	2165	-	0,6,6	-	-	-		
87	OHX	5	4120	-	0,6,6	-	-	-		
87	OHX	1	4175	-	0,6,6	-	-	-		
87	OHX	5	4053	-	0,6,6	-	-	-		
87	OHX	1	4180	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	4171	-	0,6,6	-	-	-		
87	OHX	6	2158	-	0,6,6	-	-	-		
87	OHX	5	4032	-	0,6,6	-	-	-		
87	OHX	1	3891	-	0,6,6	-	-	-		
87	OHX	1	4104	-	0,6,6	-	-	-		
87	OHX	5	3972	-	0,6,6	-	-	-		
87	OHX	5	4003	-	0,6,6	-	-	-		
87	OHX	5	3974	-	0,6,6	-	-	-		
87	OHX	1	3872	-	0,6,6	-	-	-		
87	OHX	6	2171	-	0,6,6	-	-	-		
87	OHX	5	4157	-	0,6,6	-	-	-		
87	OHX	2	2172	-	0,6,6	-	-	-		
87	OHX	l3	404	-	0,6,6	-	-	-		
87	OHX	5	4173	-	0,6,6	-	-	-		
87	OHX	5	4017	-	0,6,6	-	-	-		
87	OHX	2	2110	-	0,6,6	-	-	-		
87	OHX	1	3960	-	0,6,6	-	-	-		
87	OHX	5	4135	-	0,6,6	-	-	-		
87	OHX	2	2068	-	0,6,6	-	-	-		
87	OHX	6	2099	-	0,6,6	-	-	-		
87	OHX	6	2107	-	0,6,6	-	-	-		
87	OHX	1	3982	-	0,6,6	-	-	-		
87	OHX	1	4179	-	0,6,6	-	-	-		
87	OHX	m7	206	-	0,6,6	-	-	-		
87	OHX	5	4045	-	0,6,6	-	-	-		
87	OHX	5	4047	-	0,6,6	-	-	-		
87	OHX	6	2108	-	0,6,6	-	-	-		
87	OHX	5	4196	-	0,6,6	-	-	-		
87	OHX	5	3983	-	0,6,6	-	-	-		
87	OHX	5	4022	-	0,6,6	-	-	-		
87	OHX	m9	201	-	0,6,6	-	-	-		
87	OHX	2	2038	-	0,6,6	-	-	-		
87	OHX	5	3904	-	0,6,6	-	-	-		
87	OHX	5	3993	-	0,6,6	-	-	-		
87	OHX	5	3999	-	0,6,6	-	-	-		
87	OHX	6	2085	-	0,6,6	-	-	-		
87	OHX	5	4180	-	0,6,6	-	-	-		
87	OHX	1	4129	-	0,6,6	-	-	-		
87	OHX	1	4121	-	0,6,6	-	-	-		
87	OHX	1	4055	-	0,6,6	-	-	-		
87	OHX	1	4190	-	0,6,6	-	-	-		
87	OHX	2	2153	-	0,6,6	-	-	-		
87	OHX	1	4114	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	4021	-	0,6,6	-	-	-		
87	OHX	8	227	-	0,6,6	-	-	-		
87	OHX	5	4178	-	0,6,6	-	-	-		
87	OHX	1	3991	-	0,6,6	-	-	-		
87	OHX	1	3917	-	0,6,6	-	-	-		
87	OHX	1	3896	-	0,6,6	-	-	-		
87	OHX	2	2120	-	0,6,6	-	-	-		
87	OHX	1	4134	-	0,6,6	-	-	-		
87	OHX	6	2191	-	0,6,6	-	-	-		
87	OHX	6	2086	-	0,6,6	-	-	-		
87	OHX	1	4156	-	0,6,6	-	-	-		
87	OHX	6	2065	-	0,6,6	-	-	-		
87	OHX	5	3910	-	0,6,6	-	-	-		
87	OHX	2	2026	-	0,6,6	-	-	-		
87	OHX	5	4169	-	0,6,6	-	-	-		
87	OHX	2	2090	-	0,6,6	-	-	-		
87	OHX	2	2107	-	0,6,6	-	-	-		
87	OHX	5	3976	-	0,6,6	-	-	-		
87	OHX	1	3964	-	0,6,6	-	-	-		
87	OHX	1	3970	-	0,6,6	-	-	-		
87	OHX	1	3877	-	0,6,6	-	-	-		
87	OHX	5	4202	-	0,6,6	-	-	-		
87	OHX	6	2195	-	0,6,6	-	-	-		
87	OHX	5	3961	-	0,6,6	-	-	-		
87	OHX	5	4161	-	0,6,6	-	-	-		
87	OHX	5	3909	-	0,6,6	-	-	-		
87	OHX	2	2030	-	0,6,6	-	-	-		
87	OHX	5	4041	-	0,6,6	-	-	-		
87	OHX	5	4241	-	0,6,6	-	-	-		
87	OHX	5	3911	-	0,6,6	-	-	-		
87	OHX	1	3998	-	0,6,6	-	-	-		
87	OHX	1	3929	-	0,6,6	-	-	-		
87	OHX	2	2168	-	0,6,6	-	-	-		
87	OHX	1	3873	-	0,6,6	-	-	-		
87	OHX	1	4146	-	0,6,6	-	-	-		
87	OHX	1	4133	-	0,6,6	-	-	-		
87	OHX	6	2152	-	0,6,6	-	-	-		
87	OHX	5	4182	-	0,6,6	-	-	-		
87	OHX	5	4198	-	0,6,6	-	-	-		
87	OHX	5	4215	-	0,6,6	-	-	-		
87	OHX	6	2178	-	0,6,6	-	-	-		
87	OHX	1	4144	-	0,6,6	-	-	-		
87	OHX	2	2118	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4070	-	0,6,6	-	-	-		
87	OHX	2	2159	-	0,6,6	-	-	-		
87	OHX	8	221	-	0,6,6	-	-	-		
87	OHX	5	3948	-	0,6,6	-	-	-		
87	OHX	1	3907	-	0,6,6	-	-	-		
87	OHX	1	3949	-	0,6,6	-	-	-		
87	OHX	6	2114	-	0,6,6	-	-	-		
87	OHX	5	4229	-	0,6,6	-	-	-		
87	OHX	5	3921	-	0,6,6	-	-	-		
87	OHX	1	4072	-	0,6,6	-	-	-		
87	OHX	1	3950	-	0,6,6	-	-	-		
87	OHX	4	233	-	0,6,6	-	-	-		
87	OHX	M9	202	-	0,6,6	-	-	-		
87	OHX	6	2140	-	0,6,6	-	-	-		
87	OHX	1	4199	-	0,6,6	-	-	-		
87	OHX	1	3981	-	0,6,6	-	-	-		
87	OHX	5	4149	-	0,6,6	-	-	-		
87	OHX	6	2194	-	0,6,6	-	-	-		
87	OHX	3	219	-	0,6,6	-	-	-		
87	OHX	1	3992	-	0,6,6	-	-	-		
87	OHX	6	2115	-	0,6,6	-	-	-		
87	OHX	5	4083	-	0,6,6	-	-	-		
87	OHX	5	4093	-	0,6,6	-	-	-		
87	OHX	1	3966	-	0,6,6	-	-	-		
87	OHX	2	2079	-	0,6,6	-	-	-		
87	OHX	1	4150	-	0,6,6	-	-	-		
87	OHX	5	4036	-	0,6,6	-	-	-		
87	OHX	1	4166	-	0,6,6	-	-	-		
87	OHX	1	4044	-	0,6,6	-	-	-		
87	OHX	6	2153	-	0,6,6	-	-	-		
87	OHX	2	2176	-	0,6,6	-	-	-		
87	OHX	3	221	-	0,6,6	-	-	-		
87	OHX	6	2117	-	0,6,6	-	-	-		
87	OHX	2	2145	-	0,6,6	-	-	-		
87	OHX	5	3995	-	0,6,6	-	-	-		
87	OHX	6	2192	-	0,6,6	-	-	-		
87	OHX	1	4023	-	0,6,6	-	-	-		
87	OHX	5	4094	-	0,6,6	-	-	-		
87	OHX	1	4029	-	0,6,6	-	-	-		
87	OHX	6	2101	-	0,6,6	-	-	-		
87	OHX	5	4082	-	0,6,6	-	-	-		
87	OHX	5	4243	-	0,6,6	-	-	-		
89	3KD	1	4218	-	24,25,25	0.80	0	30,39,39	1.10	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	8	228	-	0,6,6	-	-	-		
87	OHX	2	2103	-	0,6,6	-	-	-		
87	OHX	1	3875	-	0,6,6	-	-	-		
87	OHX	1	4008	-	0,6,6	-	-	-		
87	OHX	2	2128	-	0,6,6	-	-	-		
87	OHX	1	3884	-	0,6,6	-	-	-		
87	OHX	1	4168	-	0,6,6	-	-	-		
87	OHX	6	2066	-	0,6,6	-	-	-		
87	OHX	6	2162	-	0,6,6	-	-	-		
87	OHX	1	3926	-	0,6,6	-	-	-		
87	OHX	5	4037	-	0,6,6	-	-	-		
87	OHX	1	4153	-	0,6,6	-	-	-		
87	OHX	1	4174	-	0,6,6	-	-	-		
87	OHX	1	4099	-	0,6,6	-	-	-		
87	OHX	6	2111	-	0,6,6	-	-	-		
87	OHX	6	2200	-	0,6,6	-	-	-		
87	OHX	1	4024	-	0,6,6	-	-	-		
87	OHX	6	2182	-	0,6,6	-	-	-		
87	OHX	5	4181	-	0,6,6	-	-	-		
87	OHX	5	4191	-	0,6,6	-	-	-		
87	OHX	6	2146	-	0,6,6	-	-	-		
87	OHX	5	4183	-	0,6,6	-	-	-		
87	OHX	1	4108	-	0,6,6	-	-	-		
87	OHX	3	223	-	0,6,6	-	-	-		
87	OHX	2	2096	-	0,6,6	-	-	-		
87	OHX	2	2054	-	0,6,6	-	-	-		
87	OHX	1	3898	-	0,6,6	-	-	-		
87	OHX	1	3962	-	0,6,6	-	-	-		
87	OHX	5	4081	-	0,6,6	-	-	-		
87	OHX	1	4195	-	0,6,6	-	-	-		
87	OHX	6	2052	-	0,6,6	-	-	-		
87	OHX	1	4017	-	0,6,6	-	-	-		
87	OHX	5	4040	-	0,6,6	-	-	-		
87	OHX	5	4085	-	0,6,6	-	-	-		
87	OHX	1	4100	-	0,6,6	-	-	-		
87	OHX	2	2100	-	0,6,6	-	-	-		
87	OHX	1	3957	-	0,6,6	-	-	-		
87	OHX	6	2128	-	0,6,6	-	-	-		
87	OHX	1	4000	-	0,6,6	-	-	-		
87	OHX	5	3942	-	0,6,6	-	-	-		
87	OHX	1	4112	-	0,6,6	-	-	-		
87	OHX	2	2043	-	0,6,6	-	-	-		
87	OHX	1	3963	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	3998	-	0,6,6	-	-	-		
87	OHX	L3	404	-	0,6,6	-	-	-		
87	OHX	5	4133	-	0,6,6	-	-	-		
87	OHX	5	4023	-	0,6,6	-	-	-		
87	OHX	6	2119	-	0,6,6	-	-	-		
87	OHX	1	4038	-	0,6,6	-	-	-		
87	OHX	6	2087	-	0,6,6	-	-	-		
87	OHX	5	4190	-	0,6,6	-	-	-		
87	OHX	1	3990	-	0,6,6	-	-	-		
87	OHX	6	2142	-	0,6,6	-	-	-		
87	OHX	6	2188	-	0,6,6	-	-	-		
87	OHX	1	3888	-	0,6,6	-	-	-		
87	OHX	2	2137	-	0,6,6	-	-	-		
87	OHX	5	4142	-	0,6,6	-	-	-		
87	OHX	2	2065	-	0,6,6	-	-	-		
87	OHX	2	2126	-	0,6,6	-	-	-		
87	OHX	1	3972	-	0,6,6	-	-	-		
87	OHX	m5	304	-	0,6,6	-	-	-		
87	OHX	5	4247	-	0,6,6	-	-	-		
87	OHX	2	2124	-	0,6,6	-	-	-		
87	OHX	6	2123	-	0,6,6	-	-	-		
87	OHX	5	4130	-	0,6,6	-	-	-		
87	OHX	5	4197	-	0,6,6	-	-	-		
87	OHX	8	223	-	0,6,6	-	-	-		
87	OHX	5	4072	-	0,6,6	-	-	-		
87	OHX	7	227	-	0,6,6	-	-	-		
87	OHX	1	4096	-	0,6,6	-	-	-		
87	OHX	1	3986	-	0,6,6	-	-	-		
87	OHX	6	2109	-	0,6,6	-	-	-		
87	OHX	d9	102	-	0,6,6	-	-	-		
87	OHX	5	4131	-	0,6,6	-	-	-		
87	OHX	1	3883	-	0,6,6	-	-	-		
87	OHX	5	3992	-	0,6,6	-	-	-		
87	OHX	5	3920	-	0,6,6	-	-	-		
87	OHX	1	4058	-	0,6,6	-	-	-		
87	OHX	1	4071	-	0,6,6	-	-	-		
87	OHX	5	4107	-	0,6,6	-	-	-		
87	OHX	1	4013	-	0,6,6	-	-	-		
87	OHX	4	225	-	0,6,6	-	-	-		
87	OHX	5	4077	-	0,6,6	-	-	-		
87	OHX	2	2069	-	0,6,6	-	-	-		
87	OHX	5	4203	-	0,6,6	-	-	-		
87	OHX	2	2144	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	3989	-	0,6,6	-	-	-		
87	OHX	1	4006	-	0,6,6	-	-	-		
87	OHX	1	4212	-	0,6,6	-	-	-		
87	OHX	1	4002	-	0,6,6	-	-	-		
87	OHX	5	3981	-	0,6,6	-	-	-		
87	OHX	6	2127	-	0,6,6	-	-	-		
87	OHX	5	3937	-	0,6,6	-	-	-		
87	OHX	5	4224	-	0,6,6	-	-	-		
87	OHX	1	3939	-	0,6,6	-	-	-		
87	OHX	1	3971	-	0,6,6	-	-	-		
87	OHX	1	4207	-	0,6,6	-	-	-		
87	OHX	2	2160	-	0,6,6	-	-	-		
87	OHX	1	4007	-	0,6,6	-	-	-		
87	OHX	1	3975	-	0,6,6	-	-	-		
87	OHX	5	3918	-	0,6,6	-	-	-		
87	OHX	1	3928	-	0,6,6	-	-	-		
87	OHX	1	4043	-	0,6,6	-	-	-		
87	OHX	1	4057	-	0,6,6	-	-	-		
87	OHX	6	2163	-	0,6,6	-	-	-		
87	OHX	5	4199	-	0,6,6	-	-	-		
87	OHX	N1	201	-	0,6,6	-	-	-		
87	OHX	5	4008	-	0,6,6	-	-	-		
87	OHX	2	2063	-	0,6,6	-	-	-		
87	OHX	1	3895	-	0,6,6	-	-	-		
87	OHX	8	229	-	0,6,6	-	-	-		
87	OHX	2	2022	-	0,6,6	-	-	-		
87	OHX	1	4025	-	0,6,6	-	-	-		
87	OHX	2	2051	-	0,6,6	-	-	-		
87	OHX	C8	201	-	0,6,6	-	-	-		
87	OHX	1	3909	-	0,6,6	-	-	-		
87	OHX	1	3977	-	0,6,6	-	-	-		
87	OHX	2	2042	-	0,6,6	-	-	-		
87	OHX	5	4066	-	0,6,6	-	-	-		
87	OHX	5	4111	-	0,6,6	-	-	-		
87	OHX	5	4168	-	0,6,6	-	-	-		
87	OHX	6	2173	-	0,6,6	-	-	-		
87	OHX	5	4096	-	0,6,6	-	-	-		
87	OHX	5	4119	-	0,6,6	-	-	-		
87	OHX	1	4046	-	0,6,6	-	-	-		
87	OHX	1	3874	-	0,6,6	-	-	-		
87	OHX	5	4031	-	0,6,6	-	-	-		
87	OHX	2	2046	-	0,6,6	-	-	-		
87	OHX	2	2152	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	6	2106	-	0,6,6	-	-	-		
87	OHX	6	2190	-	0,6,6	-	-	-		
87	OHX	5	4251	-	0,6,6	-	-	-		
87	OHX	O7	103	-	0,6,6	-	-	-		
87	OHX	1	4032	-	0,6,6	-	-	-		
87	OHX	1	4035	-	0,6,6	-	-	-		
87	OHX	2	2154	-	0,6,6	-	-	-		
87	OHX	5	3978	-	0,6,6	-	-	-		
87	OHX	o3	203	-	0,6,6	-	-	-		
87	OHX	5	4216	-	0,6,6	-	-	-		
87	OHX	5	4026	-	0,6,6	-	-	-		
87	OHX	5	4228	-	0,6,6	-	-	-		
87	OHX	6	2135	-	0,6,6	-	-	-		
87	OHX	7	221	-	0,6,6	-	-	-		
87	OHX	5	4034	-	0,6,6	-	-	-		
87	OHX	1	4081	-	0,6,6	-	-	-		
87	OHX	6	2063	-	0,6,6	-	-	-		
87	OHX	5	3955	-	0,6,6	-	-	-		
87	OHX	5	4245	-	0,6,6	-	-	-		
87	OHX	1	3974	-	0,6,6	-	-	-		
87	OHX	5	4027	-	0,6,6	-	-	-		
87	OHX	5	3954	-	0,6,6	-	-	-		
87	OHX	2	2134	-	0,6,6	-	-	-		
87	OHX	6	2139	-	0,6,6	-	-	-		
87	OHX	8	222	-	0,6,6	-	-	-		
87	OHX	o7	503	-	0,6,6	-	-	-		
87	OHX	1	4142	-	0,6,6	-	-	-		
87	OHX	6	2121	-	0,6,6	-	-	-		
87	OHX	1	4193	-	0,6,6	-	-	-		
87	OHX	2	2099	-	0,6,6	-	-	-		
87	OHX	1	3901	-	0,6,6	-	-	-		
87	OHX	6	2133	-	0,6,6	-	-	-		
87	OHX	sR	401	-	0,6,6	-	-	-		
87	OHX	5	4009	-	0,6,6	-	-	-		
87	OHX	2	2086	-	0,6,6	-	-	-		
87	OHX	2	2083	-	0,6,6	-	-	-		
87	OHX	6	2179	-	0,6,6	-	-	-		
87	OHX	1	4155	-	0,6,6	-	-	-		
87	OHX	1	4170	-	0,6,6	-	-	-		
87	OHX	1	4067	-	0,6,6	-	-	-		
87	OHX	5	4156	-	0,6,6	-	-	-		
87	OHX	5	3979	-	0,6,6	-	-	-		
87	OHX	1	3996	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4150	-	0,6,6	-	-	-		
87	OHX	1	4084	-	0,6,6	-	-	-		
87	OHX	5	4116	-	0,6,6	-	-	-		
87	OHX	1	4136	-	0,6,6	-	-	-		
87	OHX	6	2079	-	0,6,6	-	-	-		
87	OHX	1	4083	-	0,6,6	-	-	-		
87	OHX	5	4105	-	0,6,6	-	-	-		
87	OHX	2	2034	-	0,6,6	-	-	-		
87	OHX	l5	305	-	0,6,6	-	-	-		
87	OHX	6	2150	-	0,6,6	-	-	-		
87	OHX	1	3923	-	0,6,6	-	-	-		
87	OHX	1	4068	-	0,6,6	-	-	-		
87	OHX	5	4038	-	0,6,6	-	-	-		
87	OHX	1	4145	-	0,6,6	-	-	-		
87	OHX	1	4191	-	0,6,6	-	-	-		
87	OHX	4	223	-	0,6,6	-	-	-		
87	OHX	5	3971	-	0,6,6	-	-	-		
87	OHX	1	4196	-	0,6,6	-	-	-		
87	OHX	1	4183	-	0,6,6	-	-	-		
87	OHX	1	4200	-	0,6,6	-	-	-		
87	OHX	5	3905	-	0,6,6	-	-	-		
87	OHX	2	2178	-	0,6,6	-	-	-		
87	OHX	5	3913	-	0,6,6	-	-	-		
87	OHX	5	3932	-	0,6,6	-	-	-		
87	OHX	5	4063	-	0,6,6	-	-	-		
87	OHX	5	4233	-	0,6,6	-	-	-		
87	OHX	1	4194	-	0,6,6	-	-	-		
87	OHX	5	4125	-	0,6,6	-	-	-		
87	OHX	2	2158	-	0,6,6	-	-	-		
87	OHX	5	3901	-	0,6,6	-	-	-		
87	OHX	1	4139	-	0,6,6	-	-	-		
87	OHX	5	3965	-	0,6,6	-	-	-		
87	OHX	5	4162	-	0,6,6	-	-	-		
87	OHX	5	4019	-	0,6,6	-	-	-		
87	OHX	5	4153	-	0,6,6	-	-	-		
87	OHX	1	4045	-	0,6,6	-	-	-		
87	OHX	6	2197	-	0,6,6	-	-	-		
87	OHX	3	225	-	0,6,6	-	-	-		
87	OHX	1	3945	-	0,6,6	-	-	-		
87	OHX	1	4138	-	0,6,6	-	-	-		
87	OHX	7	224	-	0,6,6	-	-	-		
87	OHX	5	4067	-	0,6,6	-	-	-		
87	OHX	5	4115	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4189	-	0,6,6	-	-	-		
87	OHX	1	3921	-	0,6,6	-	-	-		
87	OHX	2	2066	-	0,6,6	-	-	-		
87	OHX	5	3975	-	0,6,6	-	-	-		
87	OHX	5	3996	-	0,6,6	-	-	-		
87	OHX	5	4237	-	0,6,6	-	-	-		
87	OHX	6	2072	-	0,6,6	-	-	-		
87	OHX	5	3906	-	0,6,6	-	-	-		
87	OHX	M5	302	-	0,6,6	-	-	-		
87	OHX	5	3923	-	0,6,6	-	-	-		
87	OHX	2	2040	-	0,6,6	-	-	-		
87	OHX	1	3890	-	0,6,6	-	-	-		
87	OHX	6	2198	-	0,6,6	-	-	-		
87	OHX	5	4118	-	0,6,6	-	-	-		
87	OHX	5	4059	-	0,6,6	-	-	-		
87	OHX	1	4165	-	0,6,6	-	-	-		
87	OHX	1	3915	-	0,6,6	-	-	-		
87	OHX	1	4069	-	0,6,6	-	-	-		
87	OHX	d4	202	-	0,6,6	-	-	-		
87	OHX	5	4016	-	0,6,6	-	-	-		
87	OHX	5	3936	-	0,6,6	-	-	-		
87	OHX	1	4076	-	0,6,6	-	-	-		
87	OHX	1	4135	-	0,6,6	-	-	-		
87	OHX	s1	303	-	0,6,6	-	-	-		
87	OHX	2	2087	-	0,6,6	-	-	-		
87	OHX	6	2122	-	0,6,6	-	-	-		
87	OHX	1	4111	-	0,6,6	-	-	-		
87	OHX	1	4211	-	0,6,6	-	-	-		
87	OHX	5	4137	-	0,6,6	-	-	-		
87	OHX	2	2157	-	0,6,6	-	-	-		
87	OHX	1	4060	-	0,6,6	-	-	-		
87	OHX	1	3968	-	0,6,6	-	-	-		
87	OHX	5	4011	-	0,6,6	-	-	-		
87	OHX	1	4036	-	0,6,6	-	-	-		
87	OHX	3	220	-	0,6,6	-	-	-		
87	OHX	1	4208	-	0,6,6	-	-	-		
87	OHX	6	2102	-	0,6,6	-	-	-		
87	OHX	2	2131	-	0,6,6	-	-	-		
87	OHX	5	4246	-	0,6,6	-	-	-		
87	OHX	1	4092	-	0,6,6	-	-	-		
87	OHX	1	3983	-	0,6,6	-	-	-		
87	OHX	1	4107	-	0,6,6	-	-	-		
87	OHX	o7	502	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	2	2119	-	0,6,6	-	-	-		
87	OHX	2	2044	-	0,6,6	-	-	-		
87	OHX	1	4186	-	0,6,6	-	-	-		
87	OHX	1	4037	-	0,6,6	-	-	-		
87	OHX	5	3926	-	0,6,6	-	-	-		
87	OHX	6	2130	-	0,6,6	-	-	-		
87	OHX	6	2177	-	0,6,6	-	-	-		
87	OHX	3	224	-	0,6,6	-	-	-		
87	OHX	5	4101	-	0,6,6	-	-	-		
87	OHX	2	2072	-	0,6,6	-	-	-		
87	OHX	2	2055	-	0,6,6	-	-	-		
87	OHX	1	3946	-	0,6,6	-	-	-		
87	OHX	5	4167	-	0,6,6	-	-	-		
87	OHX	5	4201	-	0,6,6	-	-	-		
87	OHX	5	4065	-	0,6,6	-	-	-		
87	OHX	5	3997	-	0,6,6	-	-	-		
87	OHX	1	4169	-	0,6,6	-	-	-		
87	OHX	6	2180	-	0,6,6	-	-	-		
87	OHX	6	2187	-	0,6,6	-	-	-		
87	OHX	5	4152	-	0,6,6	-	-	-		
87	OHX	5	3933	-	0,6,6	-	-	-		
87	OHX	4	222	-	0,6,6	-	-	-		
87	OHX	5	4033	-	0,6,6	-	-	-		
87	OHX	2	2088	-	0,6,6	-	-	-		
87	OHX	1	4102	-	0,6,6	-	-	-		
87	OHX	5	4172	-	0,6,6	-	-	-		
87	OHX	6	2056	-	0,6,6	-	-	-		
87	OHX	5	4232	-	0,6,6	-	-	-		
87	OHX	2	2175	-	0,6,6	-	-	-		
87	OHX	s1	302	-	0,6,6	-	-	-		
87	OHX	5	4024	-	0,6,6	-	-	-		
87	OHX	4	228	-	0,6,6	-	-	-		
87	OHX	5	4164	-	0,6,6	-	-	-		
87	OHX	m6	202	-	0,6,6	-	-	-		
87	OHX	2	2130	-	0,6,6	-	-	-		
87	OHX	M7	207	-	0,6,6	-	-	-		
87	OHX	2	2115	-	0,6,6	-	-	-		
87	OHX	2	2052	-	0,6,6	-	-	-		
87	OHX	5	4112	-	0,6,6	-	-	-		
87	OHX	2	2102	-	0,6,6	-	-	-		
87	OHX	2	2125	-	0,6,6	-	-	-		
87	OHX	1	3870	-	0,6,6	-	-	-		
87	OHX	2	2021	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	4090	-	0,6,6	-	-	-		
87	OHX	1	4019	-	0,6,6	-	-	-		
87	OHX	1	4119	-	0,6,6	-	-	-		
87	OHX	L4	403	-	0,6,6	-	-	-		
87	OHX	1	3967	-	0,6,6	-	-	-		
87	OHX	1	3934	-	0,6,6	-	-	-		
87	OHX	1	4028	-	0,6,6	-	-	-		
87	OHX	5	4122	-	0,6,6	-	-	-		
87	OHX	5	4141	-	0,6,6	-	-	-		
87	OHX	6	2154	-	0,6,6	-	-	-		
87	OHX	6	2113	-	0,6,6	-	-	-		
87	OHX	5	3950	-	0,6,6	-	-	-		
87	OHX	1	3994	-	0,6,6	-	-	-		
87	OHX	2	2045	-	0,6,6	-	-	-		
87	OHX	6	2074	-	0,6,6	-	-	-		
87	OHX	1	3969	-	0,6,6	-	-	-		
87	OHX	6	2161	-	0,6,6	-	-	-		
87	OHX	8	226	-	0,6,6	-	-	-		
87	OHX	2	2143	-	0,6,6	-	-	-		
87	OHX	2	2141	-	0,6,6	-	-	-		
87	OHX	2	2150	-	0,6,6	-	-	-		
87	OHX	1	3905	-	0,6,6	-	-	-		
87	OHX	2	2039	-	0,6,6	-	-	-		
87	OHX	2	2167	-	0,6,6	-	-	-		
87	OHX	6	2175	-	0,6,6	-	-	-		
87	OHX	2	2036	-	0,6,6	-	-	-		
87	OHX	1	4015	-	0,6,6	-	-	-		
87	OHX	5	3945	-	0,6,6	-	-	-		
87	OHX	5	4075	-	0,6,6	-	-	-		
87	OHX	M7	208	-	0,6,6	-	-	-		
87	OHX	s8	303	-	0,6,6	-	-	-		
87	OHX	5	4014	-	0,6,6	-	-	-		
87	OHX	5	4176	-	0,6,6	-	-	-		
87	OHX	q2	502	-	0,6,6	-	-	-		
87	OHX	5	4055	-	0,6,6	-	-	-		
87	OHX	5	3938	-	0,6,6	-	-	-		
87	OHX	5	4138	-	0,6,6	-	-	-		
87	OHX	1	4079	-	0,6,6	-	-	-		
87	OHX	2	2098	-	0,6,6	-	-	-		
87	OHX	1	4009	-	0,6,6	-	-	-		
87	OHX	1	4082	-	0,6,6	-	-	-		
87	OHX	5	4060	-	0,6,6	-	-	-		
87	OHX	5	4160	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4163	-	0,6,6	-	-	-		
87	OHX	1	4056	-	0,6,6	-	-	-		
87	OHX	7	222	-	0,6,6	-	-	-		
87	OHX	6	2064	-	0,6,6	-	-	-		
87	OHX	2	2101	-	0,6,6	-	-	-		
87	OHX	1	4062	-	0,6,6	-	-	-		
87	OHX	5	4192	-	0,6,6	-	-	-		
87	OHX	5	3934	-	0,6,6	-	-	-		
87	OHX	1	4051	-	0,6,6	-	-	-		
87	OHX	5	4195	-	0,6,6	-	-	-		
87	OHX	1	4047	-	0,6,6	-	-	-		
87	OHX	n6	202	-	0,6,6	-	-	-		
87	OHX	5	4043	-	0,6,6	-	-	-		
87	OHX	1	3937	-	0,6,6	-	-	-		
87	OHX	6	2164	-	0,6,6	-	-	-		
87	OHX	5	4073	-	0,6,6	-	-	-		
87	OHX	2	2113	-	0,6,6	-	-	-		
87	OHX	1	4137	-	0,6,6	-	-	-		
87	OHX	6	2060	-	0,6,6	-	-	-		
87	OHX	5	4089	-	0,6,6	-	-	-		
87	OHX	2	2121	-	0,6,6	-	-	-		
87	OHX	6	2131	-	0,6,6	-	-	-		
87	OHX	C5	201	-	0,6,6	-	-	-		
87	OHX	2	2023	-	0,6,6	-	-	-		
87	OHX	1	4063	-	0,6,6	-	-	-		
87	OHX	2	2047	-	0,6,6	-	-	-		
87	OHX	5	3907	-	0,6,6	-	-	-		
87	OHX	5	3927	-	0,6,6	-	-	-		
87	OHX	5	3941	-	0,6,6	-	-	-		
87	OHX	6	2181	-	0,6,6	-	-	-		
87	OHX	5	4159	-	0,6,6	-	-	-		
87	OHX	1	3953	-	0,6,6	-	-	-		
87	OHX	1	4197	-	0,6,6	-	-	-		
87	OHX	5	4091	-	0,6,6	-	-	-		
87	OHX	6	2206	-	0,6,6	-	-	-		
87	OHX	5	4147	-	0,6,6	-	-	-		
87	OHX	2	2032	-	0,6,6	-	-	-		
87	OHX	8	220	-	0,6,6	-	-	-		
87	OHX	1	3978	-	0,6,6	-	-	-		
87	OHX	1	4101	-	0,6,6	-	-	-		
87	OHX	6	2082	-	0,6,6	-	-	-		
87	OHX	1	4061	-	0,6,6	-	-	-		
87	OHX	1	4185	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4248	-	0,6,6	-	-	-		
87	OHX	5	4231	-	0,6,6	-	-	-		
87	OHX	1	4167	-	0,6,6	-	-	-		
87	OHX	5	4044	-	0,6,6	-	-	-		
87	OHX	5	4175	-	0,6,6	-	-	-		
87	OHX	5	3917	-	0,6,6	-	-	-		
87	OHX	2	2106	-	0,6,6	-	-	-		
87	OHX	3	222	-	0,6,6	-	-	-		
87	OHX	1	4198	-	0,6,6	-	-	-		
87	OHX	8	217	-	0,6,6	-	-	-		
87	OHX	M0	303	-	0,6,6	-	-	-		
87	OHX	6	2169	-	0,6,6	-	-	-		
87	OHX	2	2077	-	0,6,6	-	-	-		
87	OHX	1	4026	-	0,6,6	-	-	-		
87	OHX	1	4033	-	0,6,6	-	-	-		
87	OHX	1	4054	-	0,6,6	-	-	-		
87	OHX	1	4130	-	0,6,6	-	-	-		
87	OHX	5	3988	-	0,6,6	-	-	-		
87	OHX	5	4029	-	0,6,6	-	-	-		
87	OHX	6	2059	-	0,6,6	-	-	-		
87	OHX	5	4188	-	0,6,6	-	-	-		
87	OHX	1	3900	-	0,6,6	-	-	-		
87	OHX	6	2144	-	0,6,6	-	-	-		
87	OHX	1	4078	-	0,6,6	-	-	-		
87	OHX	5	4211	-	0,6,6	-	-	-		
87	OHX	2	2122	-	0,6,6	-	-	-		
87	OHX	1	3954	-	0,6,6	-	-	-		
87	OHX	1	3931	-	0,6,6	-	-	-		
87	OHX	2	2105	-	0,6,6	-	-	-		
87	OHX	6	2183	-	0,6,6	-	-	-		
87	OHX	6	2207	-	0,6,6	-	-	-		
87	OHX	5	4123	-	0,6,6	-	-	-		
87	OHX	5	4092	-	0,6,6	-	-	-		
87	OHX	7	220	-	0,6,6	-	-	-		
87	OHX	1	4203	-	0,6,6	-	-	-		
87	OHX	6	2149	-	0,6,6	-	-	-		
87	OHX	5	3924	-	0,6,6	-	-	-		
87	OHX	1	4178	-	0,6,6	-	-	-		
87	OHX	m8	201	-	0,6,6	-	-	-		
87	OHX	1	3916	-	0,6,6	-	-	-		
87	OHX	2	2082	-	0,6,6	-	-	-		
87	OHX	6	2147	-	0,6,6	-	-	-		
87	OHX	N9	101	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	3878	-	0,6,6	-	-	-		
87	OHX	m0	301	-	0,6,6	-	-	-		
87	OHX	5	4039	-	0,6,6	-	-	-		
87	OHX	5	4015	-	0,6,6	-	-	-		
87	OHX	1	4080	-	0,6,6	-	-	-		
87	OHX	2	2177	-	0,6,6	-	-	-		
87	OHX	6	2051	-	0,6,6	-	-	-		
87	OHX	5	4100	-	0,6,6	-	-	-		
87	OHX	6	2145	-	0,6,6	-	-	-		
87	OHX	1	3913	-	0,6,6	-	-	-		
87	OHX	1	3918	-	0,6,6	-	-	-		
87	OHX	5	4187	-	0,6,6	-	-	-		
87	OHX	5	3951	-	0,6,6	-	-	-		
87	OHX	1	3961	-	0,6,6	-	-	-		
87	OHX	1	3997	-	0,6,6	-	-	-		
87	OHX	6	2129	-	0,6,6	-	-	-		
87	OHX	m4	201	-	0,6,6	-	-	-		
87	OHX	2	2057	-	0,6,6	-	-	-		
87	OHX	6	2088	-	0,6,6	-	-	-		
87	OHX	D9	102	-	0,6,6	-	-	-		
87	OHX	7	226	-	0,6,6	-	-	-		
87	OHX	6	2136	-	0,6,6	-	-	-		
87	OHX	M6	202	-	0,6,6	-	-	-		
87	OHX	1	4172	-	0,6,6	-	-	-		
87	OHX	1	3880	-	0,6,6	-	-	-		
87	OHX	2	2117	-	0,6,6	-	-	-		
87	OHX	1	3980	-	0,6,6	-	-	-		
87	OHX	5	3944	-	0,6,6	-	-	-		
87	OHX	1	4116	-	0,6,6	-	-	-		
87	OHX	7	217	-	0,6,6	-	-	-		
87	OHX	1	4066	-	0,6,6	-	-	-		
87	OHX	5	4184	-	0,6,6	-	-	-		
87	OHX	2	2112	-	0,6,6	-	-	-		
87	OHX	4	221	-	0,6,6	-	-	-		
87	OHX	5	4012	-	0,6,6	-	-	-		
87	OHX	2	2142	-	0,6,6	-	-	-		
87	OHX	6	2203	-	0,6,6	-	-	-		
87	OHX	1	4173	-	0,6,6	-	-	-		
87	OHX	6	2096	-	0,6,6	-	-	-		
87	OHX	6	2054	-	0,6,6	-	-	-		
87	OHX	5	4193	-	0,6,6	-	-	-		
87	OHX	1	3919	-	0,6,6	-	-	-		
87	OHX	1	4027	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	6	2092	-	0,6,6	-	-	-		
87	OHX	6	2143	-	0,6,6	-	-	-		
87	OHX	6	2071	-	0,6,6	-	-	-		
87	OHX	6	2053	-	0,6,6	-	-	-		
87	OHX	6	2155	-	0,6,6	-	-	-		
87	OHX	5	3986	-	0,6,6	-	-	-		
87	OHX	1	4118	-	0,6,6	-	-	-		
87	OHX	c3	201	-	0,6,6	-	-	-		
87	OHX	2	2094	-	0,6,6	-	-	-		
87	OHX	5	3947	-	0,6,6	-	-	-		
87	OHX	6	2055	-	0,6,6	-	-	-		
87	OHX	C3	201	-	0,6,6	-	-	-		
87	OHX	1	4034	-	0,6,6	-	-	-		
87	OHX	5	4005	-	0,6,6	-	-	-		
87	OHX	2	2041	-	0,6,6	-	-	-		
87	OHX	1	4113	-	0,6,6	-	-	-		
87	OHX	5	4128	-	0,6,6	-	-	-		
87	OHX	1	3927	-	0,6,6	-	-	-		
87	OHX	2	2129	-	0,6,6	-	-	-		
87	OHX	5	3930	-	0,6,6	-	-	-		
87	OHX	5	4220	-	0,6,6	-	-	-		
87	OHX	5	3959	-	0,6,6	-	-	-		
87	OHX	5	4250	-	0,6,6	-	-	-		
87	OHX	1	4031	-	0,6,6	-	-	-		
87	OHX	1	4094	-	0,6,6	-	-	-		
87	OHX	1	4181	-	0,6,6	-	-	-		
87	OHX	1	3911	-	0,6,6	-	-	-		
87	OHX	1	4074	-	0,6,6	-	-	-		
87	OHX	5	4108	-	0,6,6	-	-	-		
87	OHX	1	4049	-	0,6,6	-	-	-		
87	OHX	5	4165	-	0,6,6	-	-	-		
87	OHX	5	4143	-	0,6,6	-	-	-		
87	OHX	5	4207	-	0,6,6	-	-	-		
87	OHX	3	226	-	0,6,6	-	-	-		
87	OHX	5	4218	-	0,6,6	-	-	-		
87	OHX	8	216	-	0,6,6	-	-	-		
87	OHX	1	4188	-	0,6,6	-	-	-		
87	OHX	5	4095	-	0,6,6	-	-	-		
87	OHX	5	4057	-	0,6,6	-	-	-		
87	OHX	m1	202	-	0,6,6	-	-	-		
87	OHX	5	4121	-	0,6,6	-	-	-		
87	OHX	1	3897	-	0,6,6	-	-	-		
87	OHX	6	2170	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	3	217	-	0,6,6	-	-	-		
87	OHX	5	4021	-	0,6,6	-	-	-		
87	OHX	2	2161	-	0,6,6	-	-	-		
87	OHX	5	4114	-	0,6,6	-	-	-		
87	OHX	8	215	-	0,6,6	-	-	-		
87	OHX	5	3946	-	0,6,6	-	-	-		
87	OHX	5	4217	-	0,6,6	-	-	-		
87	OHX	1	3973	-	0,6,6	-	-	-		
87	OHX	1	3965	-	0,6,6	-	-	-		
87	OHX	5	4204	-	0,6,6	-	-	-		
87	OHX	5	3900	-	0,6,6	-	-	-		
87	OHX	1	4105	-	0,6,6	-	-	-		
87	OHX	5	3908	-	0,6,6	-	-	-		
87	OHX	5	4227	-	0,6,6	-	-	-		
87	OHX	l4	403	-	0,6,6	-	-	-		
87	OHX	1	4087	-	0,6,6	-	-	-		
87	OHX	5	4235	-	0,6,6	-	-	-		
87	OHX	1	3956	-	0,6,6	-	-	-		
87	OHX	4	229	-	0,6,6	-	-	-		
87	OHX	6	2069	-	0,6,6	-	-	-		
87	OHX	5	4225	-	0,6,6	-	-	-		
87	OHX	2	2027	-	0,6,6	-	-	-		
87	OHX	O7	104	-	0,6,6	-	-	-		
87	OHX	5	4209	-	0,6,6	-	-	-		
87	OHX	1	4187	-	0,6,6	-	-	-		
87	OHX	1	3894	-	0,6,6	-	-	-		
87	OHX	1	3903	-	0,6,6	-	-	-		
87	OHX	2	2147	-	0,6,6	-	-	-		
87	OHX	6	2201	-	0,6,6	-	-	-		
87	OHX	5	3922	-	0,6,6	-	-	-		
87	OHX	5	4004	-	0,6,6	-	-	-		
87	OHX	5	4124	-	0,6,6	-	-	-		
87	OHX	1	3904	-	0,6,6	-	-	-		
87	OHX	5	4205	-	0,6,6	-	-	-		
87	OHX	c5	201	-	0,6,6	-	-	-		
87	OHX	1	4042	-	0,6,6	-	-	-		
87	OHX	5	4242	-	0,6,6	-	-	-		
87	OHX	5	4013	-	0,6,6	-	-	-		
87	OHX	5	4144	-	0,6,6	-	-	-		
87	OHX	5	4179	-	0,6,6	-	-	-		
87	OHX	5	3915	-	0,6,6	-	-	-		
87	OHX	1	4189	-	0,6,6	-	-	-		
87	OHX	5	4002	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4086	-	0,6,6	-	-	-		
87	OHX	6	2083	-	0,6,6	-	-	-		
87	OHX	2	2031	-	0,6,6	-	-	-		
87	OHX	2	2085	-	0,6,6	-	-	-		
87	OHX	1	3871	-	0,6,6	-	-	-		
87	OHX	1	4064	-	0,6,6	-	-	-		
87	OHX	2	2070	-	0,6,6	-	-	-		
87	OHX	5	4253	-	0,6,6	-	-	-		
87	OHX	O9	101	-	0,6,6	-	-	-		
87	OHX	5	4087	-	0,6,6	-	-	-		
87	OHX	1	4059	-	0,6,6	-	-	-		
87	OHX	7	219	-	0,6,6	-	-	-		
87	OHX	2	2097	-	0,6,6	-	-	-		
87	OHX	1	3936	-	0,6,6	-	-	-		
87	OHX	6	2062	-	0,6,6	-	-	-		
87	OHX	6	2080	-	0,6,6	-	-	-		
87	OHX	1	4157	-	0,6,6	-	-	-		
87	OHX	2	2049	-	0,6,6	-	-	-		
87	OHX	1	4184	-	0,6,6	-	-	-		
87	OHX	2	2064	-	0,6,6	-	-	-		
87	OHX	5	4042	-	0,6,6	-	-	-		
87	OHX	1	4005	-	0,6,6	-	-	-		
87	OHX	1	4077	-	0,6,6	-	-	-		
87	OHX	5	4103	-	0,6,6	-	-	-		
87	OHX	7	223	-	0,6,6	-	-	-		
87	OHX	1	3902	-	0,6,6	-	-	-		
87	OHX	2	2174	-	0,6,6	-	-	-		
87	OHX	1	3892	-	0,6,6	-	-	-		
87	OHX	5	3952	-	0,6,6	-	-	-		
87	OHX	5	4127	-	0,6,6	-	-	-		
87	OHX	5	4158	-	0,6,6	-	-	-		
87	OHX	5	3956	-	0,6,6	-	-	-		
87	OHX	6	2132	-	0,6,6	-	-	-		
87	OHX	5	3931	-	0,6,6	-	-	-		
87	OHX	8	225	-	0,6,6	-	-	-		
87	OHX	6	2091	-	0,6,6	-	-	-		
87	OHX	2	2035	-	0,6,6	-	-	-		
87	OHX	3	216	-	0,6,6	-	-	-		
87	OHX	1	3924	-	0,6,6	-	-	-		
87	OHX	1	4148	-	0,6,6	-	-	-		
87	OHX	1	3999	-	0,6,6	-	-	-		
87	OHX	2	2092	-	0,6,6	-	-	-		
87	OHX	1	4206	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	2	2071	-	0,6,6	-	-	-		
87	OHX	5	4154	-	0,6,6	-	-	-		
87	OHX	2	2140	-	0,6,6	-	-	-		
87	OHX	5	3919	-	0,6,6	-	-	-		
87	OHX	1	4201	-	0,6,6	-	-	-		
87	OHX	1	3879	-	0,6,6	-	-	-		
87	OHX	5	4126	-	0,6,6	-	-	-		
87	OHX	2	2073	-	0,6,6	-	-	-		
87	OHX	1	3941	-	0,6,6	-	-	-		
87	OHX	5	3973	-	0,6,6	-	-	-		
87	OHX	2	2109	-	0,6,6	-	-	-		
87	OHX	1	3935	-	0,6,6	-	-	-		
87	OHX	1	3881	-	0,6,6	-	-	-		
87	OHX	5	4249	-	0,6,6	-	-	-		
87	OHX	1	4164	-	0,6,6	-	-	-		
87	OHX	2	2162	-	0,6,6	-	-	-		
87	OHX	4	227	-	0,6,6	-	-	-		
87	OHX	5	4050	-	0,6,6	-	-	-		
87	OHX	1	4205	-	0,6,6	-	-	-		
87	OHX	6	2084	-	0,6,6	-	-	-		
87	OHX	1	4091	-	0,6,6	-	-	-		
87	OHX	5	4170	-	0,6,6	-	-	-		
87	OHX	1	4160	-	0,6,6	-	-	-		
87	OHX	5	4206	-	0,6,6	-	-	-		
87	OHX	6	2151	-	0,6,6	-	-	-		
87	OHX	1	3987	-	0,6,6	-	-	-		
87	OHX	2	2059	-	0,6,6	-	-	-		
87	OHX	1	4141	-	0,6,6	-	-	-		
87	OHX	M8	202	-	0,6,6	-	-	-		
87	OHX	5	3916	-	0,6,6	-	-	-		
87	OHX	1	4122	-	0,6,6	-	-	-		
87	OHX	5	3960	-	0,6,6	-	-	-		
87	OHX	n3	203	-	0,6,6	-	-	-		
87	OHX	5	3943	-	0,6,6	-	-	-		
87	OHX	5	3968	-	0,6,6	-	-	-		
87	OHX	1	3955	-	0,6,6	-	-	-		
87	OHX	5	4068	-	0,6,6	-	-	-		
87	OHX	5	4145	-	0,6,6	-	-	-		
87	OHX	5	4051	-	0,6,6	-	-	-		
87	OHX	2	2146	-	0,6,6	-	-	-		
87	OHX	5	4236	-	0,6,6	-	-	-		
87	OHX	1	4147	-	0,6,6	-	-	-		
87	OHX	5	4177	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	S8	302	-	0,6,6	-	-	-		
87	OHX	1	3886	-	0,6,6	-	-	-		
87	OHX	2	2058	-	0,6,6	-	-	-		
87	OHX	1	3984	-	0,6,6	-	-	-		
87	OHX	1	4093	-	0,6,6	-	-	-		
87	OHX	5	4054	-	0,6,6	-	-	-		
87	OHX	2	2164	-	0,6,6	-	-	-		
87	OHX	1	4014	-	0,6,6	-	-	-		
87	OHX	1	4176	-	0,6,6	-	-	-		
87	OHX	6	2070	-	0,6,6	-	-	-		
87	OHX	5	4110	-	0,6,6	-	-	-		
87	OHX	5	4129	-	0,6,6	-	-	-		
87	OHX	1	4217	-	0,6,6	-	-	-		
87	OHX	6	2104	-	0,6,6	-	-	-		
87	OHX	5	3903	-	0,6,6	-	-	-		
87	OHX	1	4016	-	0,6,6	-	-	-		
87	OHX	4	226	-	0,6,6	-	-	-		
87	OHX	5	4064	-	0,6,6	-	-	-		
87	OHX	5	4106	-	0,6,6	-	-	-		
87	OHX	6	2050	-	0,6,6	-	-	-		
87	OHX	5	4194	-	0,6,6	-	-	-		
87	OHX	5	4223	-	0,6,6	-	-	-		
87	OHX	1	3995	-	0,6,6	-	-	-		
87	OHX	5	3991	-	0,6,6	-	-	-		
87	OHX	1	3914	-	0,6,6	-	-	-		
87	OHX	5	3925	-	0,6,6	-	-	-		
87	OHX	2	2053	-	0,6,6	-	-	-		
87	OHX	1	4140	-	0,6,6	-	-	-		
87	OHX	2	2084	-	0,6,6	-	-	-		
87	OHX	2	2076	-	0,6,6	-	-	-		
87	OHX	5	4102	-	0,6,6	-	-	-		
87	OHX	2	2170	-	0,6,6	-	-	-		
87	OHX	6	2184	-	0,6,6	-	-	-		
87	OHX	2	2135	-	0,6,6	-	-	-		
87	OHX	2	2111	-	0,6,6	-	-	-		
87	OHX	1	3925	-	0,6,6	-	-	-		
87	OHX	1	3882	-	0,6,6	-	-	-		
87	OHX	1	3940	-	0,6,6	-	-	-		
87	OHX	2	2037	-	0,6,6	-	-	-		
87	OHX	1	4073	-	0,6,6	-	-	-		
87	OHX	1	4125	-	0,6,6	-	-	-		
87	OHX	c8	201	-	0,6,6	-	-	-		
87	OHX	1	4089	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4069	-	0,6,6	-	-	-		
87	OHX	1	4020	-	0,6,6	-	-	-		
87	OHX	5	4088	-	0,6,6	-	-	-		
87	OHX	5	4076	-	0,6,6	-	-	-		
87	OHX	n9	101	-	0,6,6	-	-	-		
87	OHX	2	2050	-	0,6,6	-	-	-		
87	OHX	5	3929	-	0,6,6	-	-	-		
87	OHX	1	4162	-	0,6,6	-	-	-		
87	OHX	1	4010	-	0,6,6	-	-	-		
87	OHX	2	2123	-	0,6,6	-	-	-		
87	OHX	1	4052	-	0,6,6	-	-	-		
87	OHX	s4	302	-	0,6,6	-	-	-		
87	OHX	2	2075	-	0,6,6	-	-	-		
87	OHX	5	3990	-	0,6,6	-	-	-		
87	OHX	6	2186	-	0,6,6	-	-	-		
87	OHX	l5	304	-	0,6,6	-	-	-		
87	OHX	6	2077	-	0,6,6	-	-	-		
87	OHX	1	4095	-	0,6,6	-	-	-		
87	OHX	1	4159	-	0,6,6	-	-	-		
87	OHX	L3	403	-	0,6,6	-	-	-		
87	OHX	2	2169	-	0,6,6	-	-	-		
87	OHX	5	4208	-	0,6,6	-	-	-		
87	OHX	5	3914	-	0,6,6	-	-	-		
87	OHX	1	4040	-	0,6,6	-	-	-		
87	OHX	8	218	-	0,6,6	-	-	-		
87	OHX	6	2172	-	0,6,6	-	-	-		
87	OHX	5	4018	-	0,6,6	-	-	-		
87	OHX	2	2091	-	0,6,6	-	-	-		
87	OHX	6	2110	-	0,6,6	-	-	-		
87	OHX	6	2073	-	0,6,6	-	-	-		
87	OHX	5	3970	-	0,6,6	-	-	-		
87	OHX	5	4001	-	0,6,6	-	-	-		
87	OHX	5	4171	-	0,6,6	-	-	-		
87	OHX	8	224	-	0,6,6	-	-	-		
87	OHX	2	2078	-	0,6,6	-	-	-		
87	OHX	2	2029	-	0,6,6	-	-	-		
87	OHX	2	2114	-	0,6,6	-	-	-		
87	OHX	1	4151	-	0,6,6	-	-	-		
87	OHX	5	4035	-	0,6,6	-	-	-		
87	OHX	6	2157	-	0,6,6	-	-	-		
87	OHX	6	2168	-	0,6,6	-	-	-		
87	OHX	5	3966	-	0,6,6	-	-	-		
87	OHX	2	2127	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4214	-	0,6,6	-	-	-		
87	OHX	1	4075	-	0,6,6	-	-	-		
87	OHX	5	4166	-	0,6,6	-	-	-		
87	OHX	6	2067	-	0,6,6	-	-	-		
87	OHX	5	4238	-	0,6,6	-	-	-		
87	OHX	5	4134	-	0,6,6	-	-	-		
87	OHX	8	219	-	0,6,6	-	-	-		
87	OHX	6	2137	-	0,6,6	-	-	-		
87	OHX	2	2149	-	0,6,6	-	-	-		
87	OHX	2	2155	-	0,6,6	-	-	-		
87	OHX	m0	302	-	0,6,6	-	-	-		
87	OHX	2	2024	-	0,6,6	-	-	-		
87	OHX	1	3932	-	0,6,6	-	-	-		
87	OHX	6	2125	-	0,6,6	-	-	-		
87	OHX	1	3943	-	0,6,6	-	-	-		
87	OHX	2	2156	-	0,6,6	-	-	-		
87	OHX	2	2163	-	0,6,6	-	-	-		
87	OHX	6	2126	-	0,6,6	-	-	-		
87	OHX	5	3935	-	0,6,6	-	-	-		
87	OHX	5	4056	-	0,6,6	-	-	-		
87	OHX	1	3958	-	0,6,6	-	-	-		
87	OHX	l4	402	-	0,6,6	-	-	-		
87	OHX	6	2095	-	0,6,6	-	-	-		
87	OHX	1	4216	-	0,6,6	-	-	-		
87	OHX	6	2124	-	0,6,6	-	-	-		
87	OHX	1	4109	-	0,6,6	-	-	-		
87	OHX	3	218	-	0,6,6	-	-	-		
87	OHX	1	4022	-	0,6,6	-	-	-		
87	OHX	1	3930	-	0,6,6	-	-	-		
87	OHX	1	4103	-	0,6,6	-	-	-		
87	OHX	6	2078	-	0,6,6	-	-	-		
87	OHX	1	4131	-	0,6,6	-	-	-		
87	OHX	2	2139	-	0,6,6	-	-	-		
87	OHX	1	3920	-	0,6,6	-	-	-		
87	OHX	6	2061	-	0,6,6	-	-	-		
87	OHX	1	4123	-	0,6,6	-	-	-		
87	OHX	7	218	-	0,6,6	-	-	-		
87	OHX	2	2173	-	0,6,6	-	-	-		
87	OHX	1	3947	-	0,6,6	-	-	-		
87	OHX	5	3987	-	0,6,6	-	-	-		
87	OHX	8	230	-	0,6,6	-	-	-		
87	OHX	1	4050	-	0,6,6	-	-	-		
87	OHX	5	3964	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	2	2165	-	0,6,6	-	-	-		
87	OHX	5	4030	-	0,6,6	-	-	-		
87	OHX	1	4041	-	0,6,6	-	-	-		
87	OHX	1	4128	-	0,6,6	-	-	-		
87	OHX	5	4052	-	0,6,6	-	-	-		
87	OHX	6	2081	-	0,6,6	-	-	-		
87	OHX	1	3910	-	0,6,6	-	-	-		
87	OHX	5	3994	-	0,6,6	-	-	-		
87	OHX	5	4136	-	0,6,6	-	-	-		
87	OHX	6	2118	-	0,6,6	-	-	-		
87	OHX	5	3969	-	0,6,6	-	-	-		
87	OHX	5	3962	-	0,6,6	-	-	-		
87	OHX	5	4148	-	0,6,6	-	-	-		
87	OHX	6	2189	-	0,6,6	-	-	-		
87	OHX	2	2095	-	0,6,6	-	-	-		
87	OHX	1	4039	-	0,6,6	-	-	-		
87	OHX	6	2156	-	0,6,6	-	-	-		
87	OHX	6	2205	-	0,6,6	-	-	-		
87	OHX	5	3902	-	0,6,6	-	-	-		
87	OHX	5	3984	-	0,6,6	-	-	-		
87	OHX	1	4048	-	0,6,6	-	-	-		
87	OHX	1	4097	-	0,6,6	-	-	-		
87	OHX	1	3893	-	0,6,6	-	-	-		
87	OHX	1	3951	-	0,6,6	-	-	-		
87	OHX	6	2068	-	0,6,6	-	-	-		
87	OHX	1	4126	-	0,6,6	-	-	-		
87	OHX	5	3957	-	0,6,6	-	-	-		
87	OHX	2	2089	-	0,6,6	-	-	-		
87	OHX	1	4115	-	0,6,6	-	-	-		
87	OHX	6	2193	-	0,6,6	-	-	-		
87	OHX	6	2090	-	0,6,6	-	-	-		
87	OHX	5	4151	-	0,6,6	-	-	-		
87	OHX	5	4061	-	0,6,6	-	-	-		
87	OHX	1	4215	-	0,6,6	-	-	-		
87	OHX	5	4185	-	0,6,6	-	-	-		
87	OHX	2	2116	-	0,6,6	-	-	-		
87	OHX	1	4120	-	0,6,6	-	-	-		
87	OHX	5	4079	-	0,6,6	-	-	-		
87	OHX	1	4106	-	0,6,6	-	-	-		
87	OHX	1	4209	-	0,6,6	-	-	-		
87	OHX	6	2141	-	0,6,6	-	-	-		
87	OHX	5	4099	-	0,6,6	-	-	-		
87	OHX	2	2104	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4140	-	0,6,6	-	-	-		
87	OHX	1	3948	-	0,6,6	-	-	-		
87	OHX	1	4182	-	0,6,6	-	-	-		
87	OHX	7	225	-	0,6,6	-	-	-		
87	OHX	5	4244	-	0,6,6	-	-	-		
87	OHX	1	4012	-	0,6,6	-	-	-		
87	OHX	5	4109	-	0,6,6	-	-	-		
87	OHX	2	2062	-	0,6,6	-	-	-		
87	OHX	6	2199	-	0,6,6	-	-	-		
87	OHX	2	2061	-	0,6,6	-	-	-		
87	OHX	1	3942	-	0,6,6	-	-	-		
87	OHX	5	4020	-	0,6,6	-	-	-		
87	OHX	6	2159	-	0,6,6	-	-	-		
87	OHX	5	4062	-	0,6,6	-	-	-		
87	OHX	5	3967	-	0,6,6	-	-	-		
87	OHX	3	215	-	0,6,6	-	-	-		
87	OHX	5	4097	-	0,6,6	-	-	-		
87	OHX	5	4078	-	0,6,6	-	-	-		
87	OHX	6	2196	-	0,6,6	-	-	-		
87	OHX	1	4213	-	0,6,6	-	-	-		
87	OHX	6	2166	-	0,6,6	-	-	-		
87	OHX	5	4155	-	0,6,6	-	-	-		
87	OHX	o2	201	-	0,6,6	-	-	-		
87	OHX	6	2098	-	0,6,6	-	-	-		
87	OHX	1	4117	-	0,6,6	-	-	-		
87	OHX	5	4058	-	0,6,6	-	-	-		
87	OHX	2	2151	-	0,6,6	-	-	-		
87	OHX	2	2056	-	0,6,6	-	-	-		
87	OHX	5	3940	-	0,6,6	-	-	-		
87	OHX	5	4000	-	0,6,6	-	-	-		
87	OHX	1	3959	-	0,6,6	-	-	-		
87	OHX	6	2058	-	0,6,6	-	-	-		
87	OHX	6	2120	-	0,6,6	-	-	-		
87	OHX	D3	202	-	0,6,6	-	-	-		
87	OHX	1	4086	-	0,6,6	-	-	-		
87	OHX	1	4070	-	0,6,6	-	-	-		
87	OHX	1	4177	-	0,6,6	-	-	-		
87	OHX	5	3953	-	0,6,6	-	-	-		
87	OHX	5	4212	-	0,6,6	-	-	-		
87	OHX	6	2097	-	0,6,6	-	-	-		
87	OHX	6	2138	-	0,6,6	-	-	-		
87	OHX	5	4146	-	0,6,6	-	-	-		
87	OHX	1	4143	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	4132	-	0,6,6	-	-	-		
87	OHX	1	3906	-	0,6,6	-	-	-		
87	OHX	6	2176	-	0,6,6	-	-	-		
87	OHX	6	2204	-	0,6,6	-	-	-		
87	OHX	5	3958	-	0,6,6	-	-	-		
87	OHX	5	4139	-	0,6,6	-	-	-		
87	OHX	5	4186	-	0,6,6	-	-	-		
87	OHX	6	2174	-	0,6,6	-	-	-		
87	OHX	4	224	-	0,6,6	-	-	-		
87	OHX	Q2	503	-	0,6,6	-	-	-		
87	OHX	O3	201	-	0,6,6	-	-	-		
87	OHX	2	2074	-	0,6,6	-	-	-		
87	OHX	1	3899	-	0,6,6	-	-	-		
87	OHX	5	4213	-	0,6,6	-	-	-		
87	OHX	5	4234	-	0,6,6	-	-	-		
87	OHX	5	4006	-	0,6,6	-	-	-		
87	OHX	1	3922	-	0,6,6	-	-	-		
87	OHX	5	3912	-	0,6,6	-	-	-		
87	OHX	L3	405	-	0,6,6	-	-	-		
87	OHX	6	2167	-	0,6,6	-	-	-		
87	OHX	1	4204	-	0,6,6	-	-	-		
87	OHX	1	4161	-	0,6,6	-	-	-		
87	OHX	6	2202	-	0,6,6	-	-	-		
87	OHX	1	3908	-	0,6,6	-	-	-		
87	OHX	1	3985	-	0,6,6	-	-	-		
87	OHX	6	2075	-	0,6,6	-	-	-		
87	OHX	2	2028	-	0,6,6	-	-	-		
87	OHX	5	4252	-	0,6,6	-	-	-		
87	OHX	5	4222	-	0,6,6	-	-	-		
87	OHX	5	3977	-	0,6,6	-	-	-		
87	OHX	1	4210	-	0,6,6	-	-	-		
87	OHX	5	4239	-	0,6,6	-	-	-		
87	OHX	1	3889	-	0,6,6	-	-	-		
87	OHX	O2	201	-	0,6,6	-	-	-		
87	OHX	l5	303	-	0,6,6	-	-	-		
87	OHX	c1	202	-	0,6,6	-	-	-		
87	OHX	5	4226	-	0,6,6	-	-	-		
87	OHX	5	4048	-	0,6,6	-	-	-		
87	OHX	1	4003	-	0,6,6	-	-	-		
87	OHX	l9	202	-	0,6,6	-	-	-		
87	OHX	2	2048	-	0,6,6	-	-	-		
87	OHX	1	3938	-	0,6,6	-	-	-		
87	OHX	1	4004	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	4124	-	0,6,6	-	-	-		
87	OHX	5	3949	-	0,6,6	-	-	-		
87	OHX	5	4132	-	0,6,6	-	-	-		
87	OHX	1	4030	-	0,6,6	-	-	-		
87	OHX	SR	401	-	0,6,6	-	-	-		
87	OHX	2	2080	-	0,6,6	-	-	-		
87	OHX	2	2108	-	0,6,6	-	-	-		
87	OHX	4	230	-	0,6,6	-	-	-		
87	OHX	1	4018	-	0,6,6	-	-	-		
87	OHX	1	4149	-	0,6,6	-	-	-		
87	OHX	5	4028	-	0,6,6	-	-	-		
87	OHX	1	4001	-	0,6,6	-	-	-		
87	OHX	1	4098	-	0,6,6	-	-	-		
87	OHX	5	3989	-	0,6,6	-	-	-		
87	OHX	6	2089	-	0,6,6	-	-	-		
87	OHX	1	3887	-	0,6,6	-	-	-		
87	OHX	6	2103	-	0,6,6	-	-	-		
87	OHX	2	2081	-	0,6,6	-	-	-		
87	OHX	l3	403	-	0,6,6	-	-	-		
87	OHX	5	3985	-	0,6,6	-	-	-		
87	OHX	5	4080	-	0,6,6	-	-	-		
87	OHX	1	4214	-	0,6,6	-	-	-		
87	OHX	6	2116	-	0,6,6	-	-	-		
87	OHX	5	4049	-	0,6,6	-	-	-		
87	OHX	5	4071	-	0,6,6	-	-	-		
87	OHX	2	2093	-	0,6,6	-	-	-		
87	OHX	1	4053	-	0,6,6	-	-	-		
87	OHX	6	2105	-	0,6,6	-	-	-		
87	OHX	1	4158	-	0,6,6	-	-	-		
87	OHX	5	4090	-	0,6,6	-	-	-		
87	OHX	1	3993	-	0,6,6	-	-	-		
87	OHX	5	3928	-	0,6,6	-	-	-		
87	OHX	1	3976	-	0,6,6	-	-	-		
87	OHX	6	2112	-	0,6,6	-	-	-		
87	OHX	2	2033	-	0,6,6	-	-	-		
87	OHX	1	4110	-	0,6,6	-	-	-		
87	OHX	6	2057	-	0,6,6	-	-	-		
87	OHX	5	4098	-	0,6,6	-	-	-		
87	OHX	5	4117	-	0,6,6	-	-	-		
87	OHX	2	2060	-	0,6,6	-	-	-		
87	OHX	6	2100	-	0,6,6	-	-	-		
87	OHX	1	3876	-	0,6,6	-	-	-		
87	OHX	2	2067	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
89	3KD	5	4254	-	24,25,25	1.04	2 (8%)	30,39,39	1.06	1 (3%)
87	OHX	6	2160	-	0,6,6	-	-	-		
87	OHX	5	3980	-	0,6,6	-	-	-		
87	OHX	2	2148	-	0,6,6	-	-	-		
87	OHX	5	4084	-	0,6,6	-	-	-		
87	OHX	1	3952	-	0,6,6	-	-	-		
87	OHX	1	4127	-	0,6,6	-	-	-		
87	OHX	2	2133	-	0,6,6	-	-	-		
87	OHX	6	2094	-	0,6,6	-	-	-		
87	OHX	1	4011	-	0,6,6	-	-	-		
87	OHX	5	4174	-	0,6,6	-	-	-		
87	OHX	6	2134	-	0,6,6	-	-	-		
87	OHX	2	2136	-	0,6,6	-	-	-		
87	OHX	5	3939	-	0,6,6	-	-	-		
87	OHX	5	4210	-	0,6,6	-	-	-		
87	OHX	5	4219	-	0,6,6	-	-	-		
87	OHX	5	4046	-	0,6,6	-	-	-		
87	OHX	1	4202	-	0,6,6	-	-	-		
87	OHX	6	2185	-	0,6,6	-	-	-		
87	OHX	6	2093	-	0,6,6	-	-	-		
87	OHX	1	3885	-	0,6,6	-	-	-		
87	OHX	5	4200	-	0,6,6	-	-	-		
87	OHX	5	4104	-	0,6,6	-	-	-		
87	OHX	5	4230	-	0,6,6	-	-	-		
87	OHX	2	2138	-	0,6,6	-	-	-		
87	OHX	1	4154	-	0,6,6	-	-	-		
87	OHX	5	4007	-	0,6,6	-	-	-		
87	OHX	1	3979	-	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
89	3KD	1	4218	-	-	-	0/5/5/5
89	3KD	5	4254	-	-	-	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	5	4254	3KD	C13-C12	3.04	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	5	4254	3KD	C8-C9	-2.40	1.47	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
89	5	4254	3KD	O-C14-C9	-3.44	101.86	109.57
89	1	4218	3KD	O-C14-C9	-2.91	103.05	109.57

There are no chirality outliers.

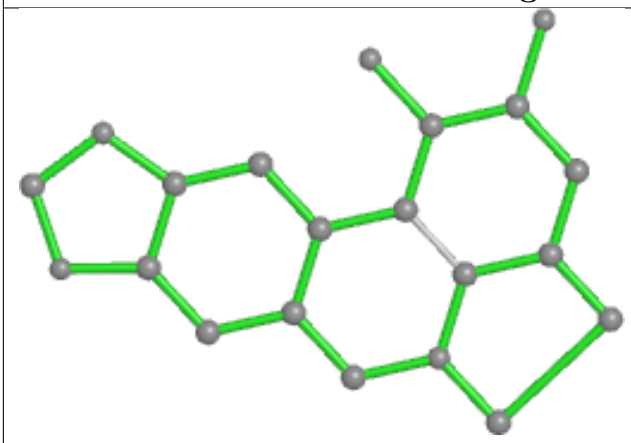
There are no torsion outliers.

There are no ring outliers.

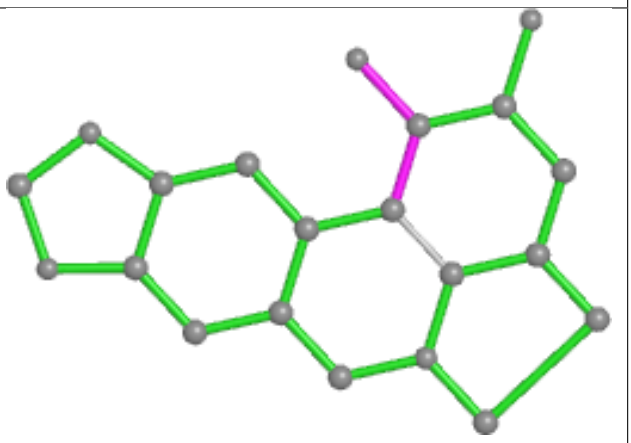
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

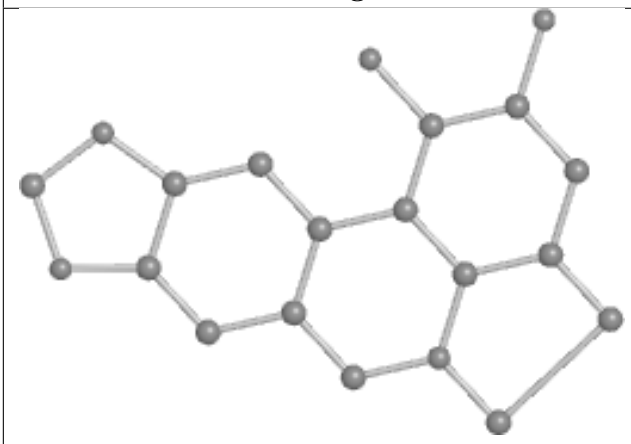
Ligand 3KD 1 4218



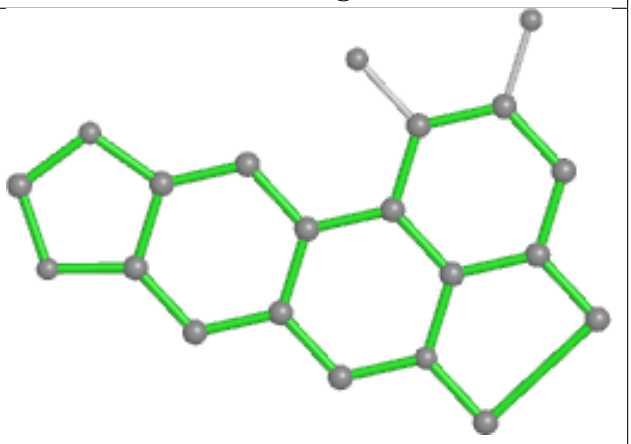
Bond lengths



Bond angles

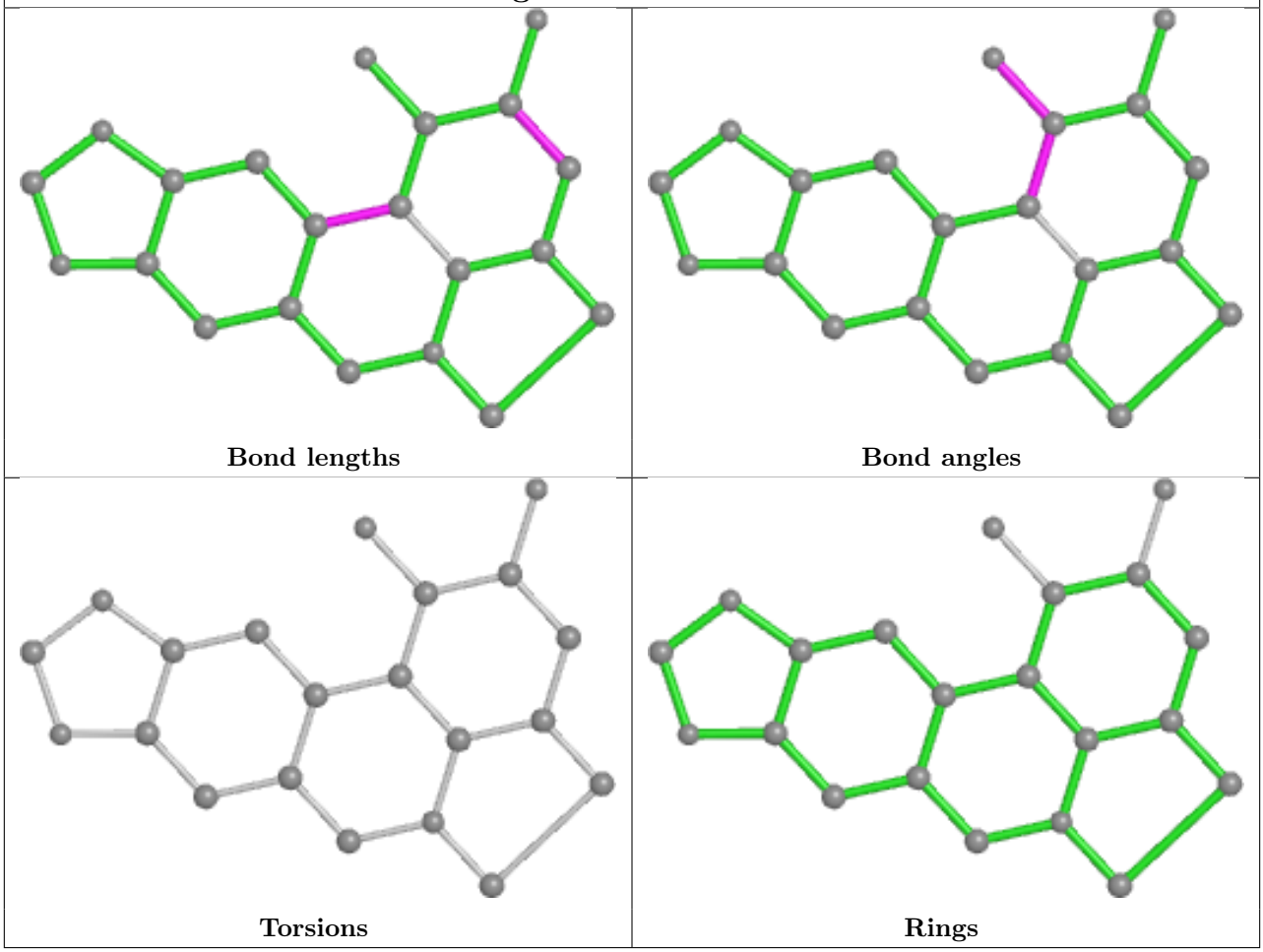


Torsions



Rings

Ligand 3KD 5 4254



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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