Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 02:06 am GMT

PDB ID	:	4U4Y
Title	:	Crystal structure of Pactamycin bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-24
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

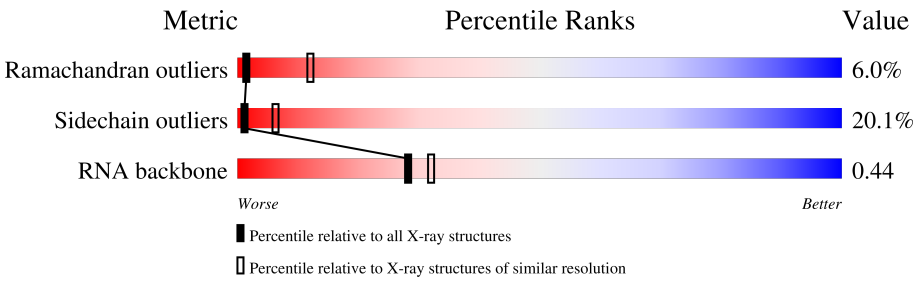
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et 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 3.20 Å.

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



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

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	62% 30% 5% •
1	6	1800	60% 33% 6%
2	S0	251	61% 20% • 18%
2	s0	251	62% 18% • 18%
3	S1	254	57% 24% • 16%
3	s1	254	63% 21% • 15%
4	S2	253	67% 18% • 14%
4	s2	253	62% 22% • 14%

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Mol	Chain	Length	Quality of chain
5	S3	239	74% 17% • 7%
5	s3	239	72% 19% • 7%
6	S4	260	73% 24% •
6	s4	260	77% 21% •
7	S5	224	70% 20% • 8%
7	s5	224	69% 22% • 8%
8	S6	236	76% 19% • •
8	s6	236	74% 17% • 8%
9	S7	189	72% 21% • •
9	s7	189	77% 20% • •
10	S8	200	76% 16% • 6%
10	s8	200	76% 17% • 6%
11	S9	196	71% 22% • 6%
11	s9	196	71% 22% • 6%
12	C0	105	69% 20% • 9%
12	c0	105	70% 17% • 9%
13	C1	155	79% 19% •
13	c1	155	74% 19% • 6%
14	C2	142	58% 27% • 13%
14	c2	142	60% 24% • • 13%
15	C3	150	79% 20% •
15	c3	150	79% 18% •
16	C4	136	71% 18% • 7%
16	c4	136	69% 22% • 6%
17	C5	141	67% 16% • 12%

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Mol	Chain	Length	Quality of chain
17	c5	141	68% 24%
18	C6	142	77% 21%
18	c6	142	81% 19%
19	C7	136	68% 16% 12%
19	c7	136	63% 21% 14%
20	C8	145	74% 22%
20	c8	145	77% 20%
21	C9	143	79% 20%
21	c9	143	82% 17%
22	D0	120	67% 22% 11%
22	d0	120	60% 30% 8%
23	D1	87	78% 18%
23	d1	87	77% 23%
24	D2	129	77% 22%
24	d2	129	85% 13%
25	D3	144	77% 22%
25	d3	144	82% 17%
26	D4	134	79% 20%
26	d4	134	80% 19%
27	D5	107	40% 24% 35%
27	d5	107	52% 11% 36%
28	D6	97	68% 26% 5%
28	d6	97	77% 22%
29	D7	81	88% 12%
29	d7	81	84% 15%

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Mol	Chain	Length	Quality of chain
30	D8	66	70% 24% 5%
30	d8	66	67% 26% 5%
31	D9	55	82% 13%
31	d9	55	69% 25%
32	E0	60	82% 15%
33	E1	76	49% 39% 5% 7%
33	e1	76	55% 41%
34	SR	318	82% 17%
34	sR	318	87% 12%
35	SM	273	45% 12% 42%
35	sM	273	27% 10% 62%
36	1	3396	47% 38% 8% 7%
36	5	3396	45% 40% 7% 7%
37	3	121	70% 27%
37	7	121	59% 32% 9%
38	4	158	49% 44% 7%
38	8	158	57% 35% 8%
39	L2	253	81% 18%
39	l2	253	83% 15%
40	L3	386	77% 22%
40	l3	386	81% 18%
41	L4	361	79% 19%
41	l4	361	80% 19%
42	L5	296	80% 19%
42	l5	296	79% 19%

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Mol	Chain	Length	Quality of chain
43	L6	175	77% 12% • 11%
43	l6	175	75% 14% • 10%
44	L7	243	75% 14% • 9%
44	l7	243	79% 11% • 8%
45	L8	255	74% 17% 9%
45	l8	255	69% 21% • 9%
46	L9	191	81% 18% •
46	l9	191	77% 21% •
47	M0	220	77% 18% • •
47	m0	220	73% 22% • •
48	M1	173	72% 22% • •
48	m1	173	71% 24% • •
49	M3	198	80% 15% • •
49	m3	198	75% 22% • •
50	M4	137	81% 18% • •
50	m4	137	80% 18% •
51	M5	203	82% 17%
51	m5	203	82% 16% •
52	M6	198	85% 13% • • •
52	m6	198	76% 21% • • •
53	M7	183	80% 19% •
53	m7	183	70% 15% 15%
54	M8	185	83% 16% •
54	m8	185	78% 21% •
55	M9	188	82% 18% •

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Mol	Chain	Length	Quality of chain
55	m9	188	80% 19% •
56	N0	172	80% 18% •
56	n0	172	75% 24% •
57	N1	159	77% 21% •
57	n1	159	82% 16% •
58	N2	120	65% 17% • 17%
58	n2	120	67% 13% • 18%
59	N3	136	83% 17%
59	n3	136	85% 15%
60	N4	155	55% 8% • 37%
60	n4	155	74% 13% • 13%
61	N5	141	65% 18% • 14%
61	n5	141	66% 18% • 15%
62	N6	126	77% 21% •
62	n6	126	78% 21% •
63	N7	135	79% 21% •
63	n7	135	77% 22% •
64	N8	148	84% 14% •
64	n8	148	79% 20% •
65	N9	58	78% 22%
65	n9	58	76% 17% 5% •
66	O0	104	76% 16% • 7%
66	o0	104	74% 22% •
67	O1	112	71% 24% • •
67	o1	112	72% 23% •• •

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Mol	Chain	Length	Quality of chain
68	O2	129	82% 15%
68	o2	129	73% 24%
69	O3	106	85% 15%
69	o3	106	84% 15%
70	O4	120	78% 13% 7%
70	o4	120	73% 18% 7%
71	O5	119	78% 20%
71	o5	119	76% 24%
72	O6	99	77% 19%
72	o6	99	70% 26%
73	O7	87	75% 23%
73	o7	87	78% 21%
74	O8	77	73% 26%
74	o8	77	81% 19%
75	O9	50	78% 22%
75	o9	50	82% 18%
76	Q0	52	81% 17%
76	q0	52	71% 29%
77	Q1	25	56% 44%
77	q1	25	72% 28%
78	Q2	105	73% 26%
78	q2	105	80% 19%
79	Q3	91	80% 19%
79	q3	91	81% 19%
80	e0	62	71% 26%

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Mol	Chain	Length	Quality of chain
81	m2	160	93% 6%
82	p0	311	39% 6% 54%
83	p1	47	100%
84	p2	46	100%

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 411223 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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C5	137	SER	ARG	conflict	UNP Q01855
c5	137	SER	ARG	conflict	UNP Q01855

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
35	SM	159	1104	652	221	231	0	0	0
35	sM	104	679	402	140	137	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	121	LYS	-	expression tag	UNP P87262
o4	121	LYS	-	expression tag	UNP P87262

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 84 is a protein called unknown protein chain p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	2	124	124	124	0	0
85	S2	2	2	2	0	0
85	S8	1	1	1	0	0
85	D0	1	1	1	0	0
85	D3	1	1	1	0	0
85	SM	1	1	1	0	0
85	1	471	471	471	0	0
85	3	14	14	14	0	0
85	4	21	21	21	0	0
85	L2	1	1	1	0	0
85	L3	2	2	2	0	0
85	L4	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	L5	1	1	1	0	0
85	L7	3	3	3	0	0
85	L8	1	1	1	0	0
85	M0	2	2	2	0	0
85	M1	1	1	1	0	0
85	M3	3	3	3	0	0
85	M5	2	2	2	0	0
85	M6	2	2	2	0	0
85	M7	4	4	4	0	0
85	M9	3	3	3	0	0
85	N0	1	1	1	0	0
85	N3	2	2	2	0	0
85	N5	1	1	1	0	0
85	N6	1	1	1	0	0
85	N8	4	4	4	0	0
85	N9	1	1	1	0	0
85	O2	1	1	1	0	0
85	O3	1	1	1	0	0
85	O7	2	2	2	0	0
85	Q2	1	1	1	0	0
85	6	147	147	147	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	s1	1	1	1	0	0
85	s2	1	1	1	0	0
85	s8	2	2	2	0	0
85	c1	1	1	1	0	0
85	c7	1	1	1	0	0
85	c8	2	2	2	0	0
85	d3	2	2	2	0	0
85	d6	1	1	1	0	0
85	sM	2	2	2	0	0
85	5	504	504	504	0	0
85	7	14	14	14	0	0
85	8	16	16	16	0	0
85	l2	1	1	1	0	0
85	l3	2	2	2	0	0
85	l4	1	1	1	0	0
85	l5	2	2	2	0	0
85	l7	2	2	2	0	0
85	l8	1	1	1	0	0
85	m1	2	2	2	0	0
85	m5	4	4	4	0	0
85	m6	2	2	2	0	0

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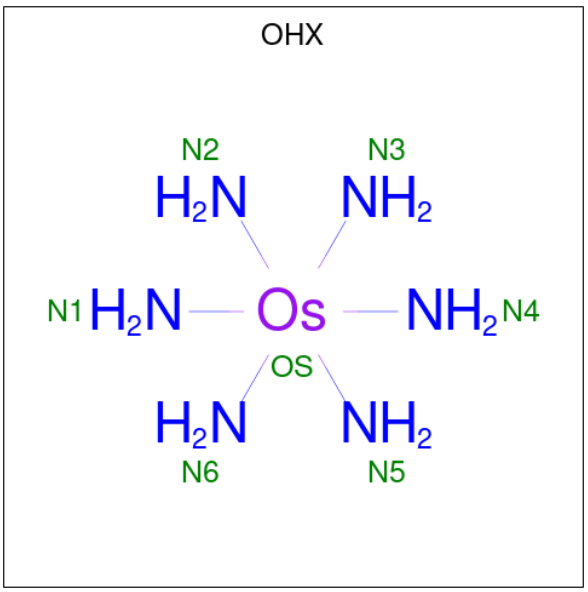
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	m7	5	Total Mg 5 5	0	0
85	n0	2	Total Mg 2 2	0	0
85	n3	2	Total Mg 2 2	0	0
85	n6	1	Total Mg 1 1	0	0
85	n8	4	Total Mg 4 4	0	0
85	o1	1	Total Mg 1 1	0	0
85	o3	1	Total Mg 1 1	0	0
85	o4	1	Total Mg 1 1	0	0
85	q0	1	Total Mg 1 1	0	0
85	q1	1	Total Mg 1 1	0	0
85	q3	2	Total Mg 2 2	0	0

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



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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	L3	1	7	6	1	0	0
			Total	N	Os		
86	L3	1	7	6	1	0	0
			Total	N	Os		
86	L3	1	7	6	1	0	0
			Total	N	Os		
86	L4	1	7	6	1	0	0
			Total	N	Os		
86	M0	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	M5	1	7	6	1	0	0
86	M7	1	7	6	1	0	0
86	M7	1	7	6	1	0	0
86	M9	1	7	6	1	0	0
86	N1	1	7	6	1	0	0
86	N9	1	7	6	1	0	0
86	O3	1	7	6	1	0	0
86	O7	1	7	6	1	0	0
86	Q2	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
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86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	s1	1	7	6	1	0	0
86	s4	1	7	6	1	0	0
86	s8	1	7	6	1	0	0
86	s9	1	7	6	1	0	0
86	c3	1	7	6	1	0	0
86	c5	1	7	6	1	0	0
86	c8	1	7	6	1	0	0
86	d4	1	7	6	1	0	0
86	d9	1	7	6	1	0	0
86	sR	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
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86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	7	6	1	0	0
			Total	N	Os		
86	5	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
86	5	1	7	6	1	0	0
			Total	N	Os		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	l3	1	7	6	1	0	0
			Total	N	Os		
86	l4	1	7	6	1	0	0
			Total	N	Os		
86	l4	1	7	6	1	0	0
			Total	N	Os		
86	l5	1	7	6	1	0	0
			Total	N	Os		
86	l5	1	7	6	1	0	0
			Total	N	Os		
86	l5	1	7	6	1	0	0
			Total	N	Os		
86	l9	1	7	6	1	0	0
			Total	N	Os		
86	m0	1	7	6	1	0	0

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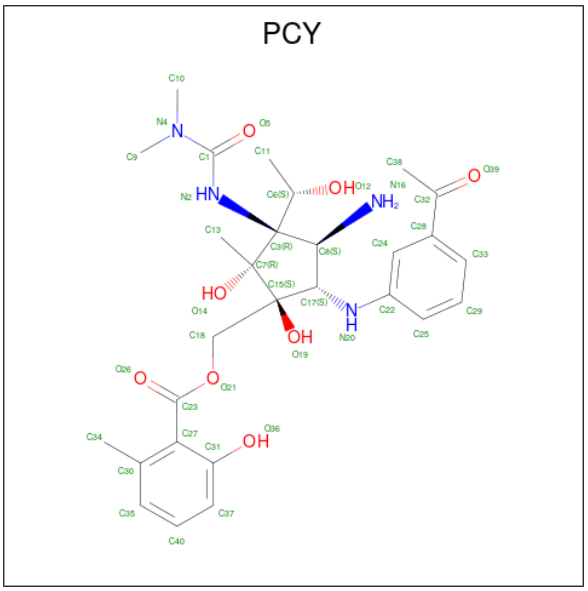
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	m0	1	7	6	1	0	0
86	m1	1	7	6	1	0	0
86	m4	1	7	6	1	0	0
86	m5	1	7	6	1	0	0
86	m6	1	7	6	1	0	0
86	m7	1	7	6	1	0	0
86	m8	1	7	6	1	0	0
86	n3	1	7	6	1	0	0
86	n9	1	7	6	1	0	0
86	n9	1	7	6	1	0	0
86	o2	1	7	6	1	0	0
86	o3	1	7	6	1	0	0
86	o7	1	7	6	1	0	0
86	o7	1	7	6	1	0	0
86	q1	1	7	6	1	0	0
86	q2	1	7	6	1	0	0

- Molecule 87 is Pactamycin (three-letter code: PCY) (formula: $C_{28}H_{38}N_4O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
87	2	1	40	28	4	8	0	0
			Total	C	N	O		
87	6	1	40	28	4	8	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
			Total	Zn		
88	D7	1	1	1	0	0
			Total	Zn		
88	D9	1	1	1	0	0
			Total	Zn		
88	E1	1	1	1	0	0
			Total	Zn		
88	O7	1	1	1	0	0
			Total	Zn		
88	Q0	1	1	1	0	0
			Total	Zn		
88	Q2	1	1	1	0	0
			Total	Zn		
88	Q3	1	1	1	0	0
			Total	Zn		
88	d6	1	1	1	0	0
			Total	Zn		
88	d7	1	1	1	0	0

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

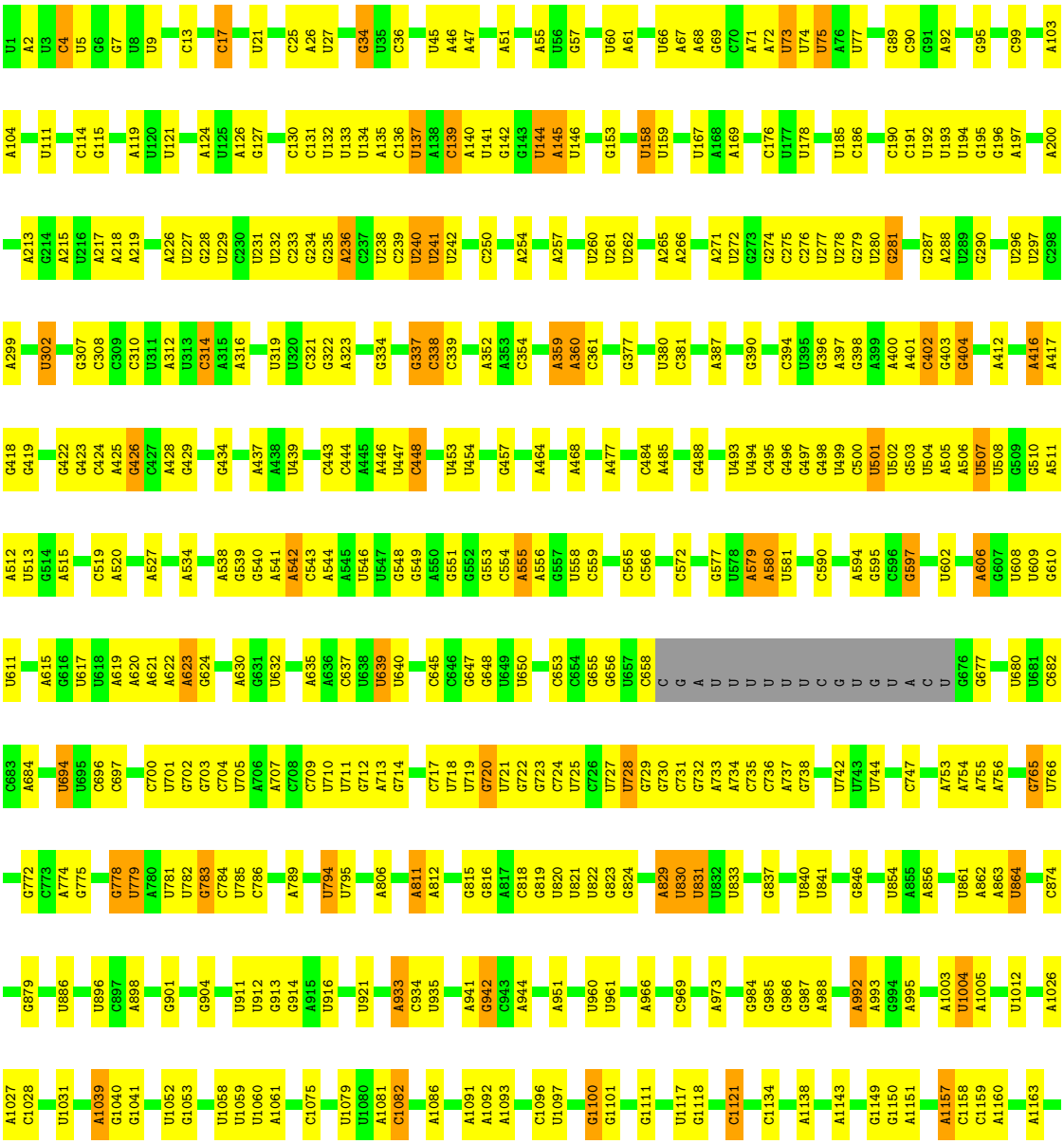
3 Residue-property plots (i)

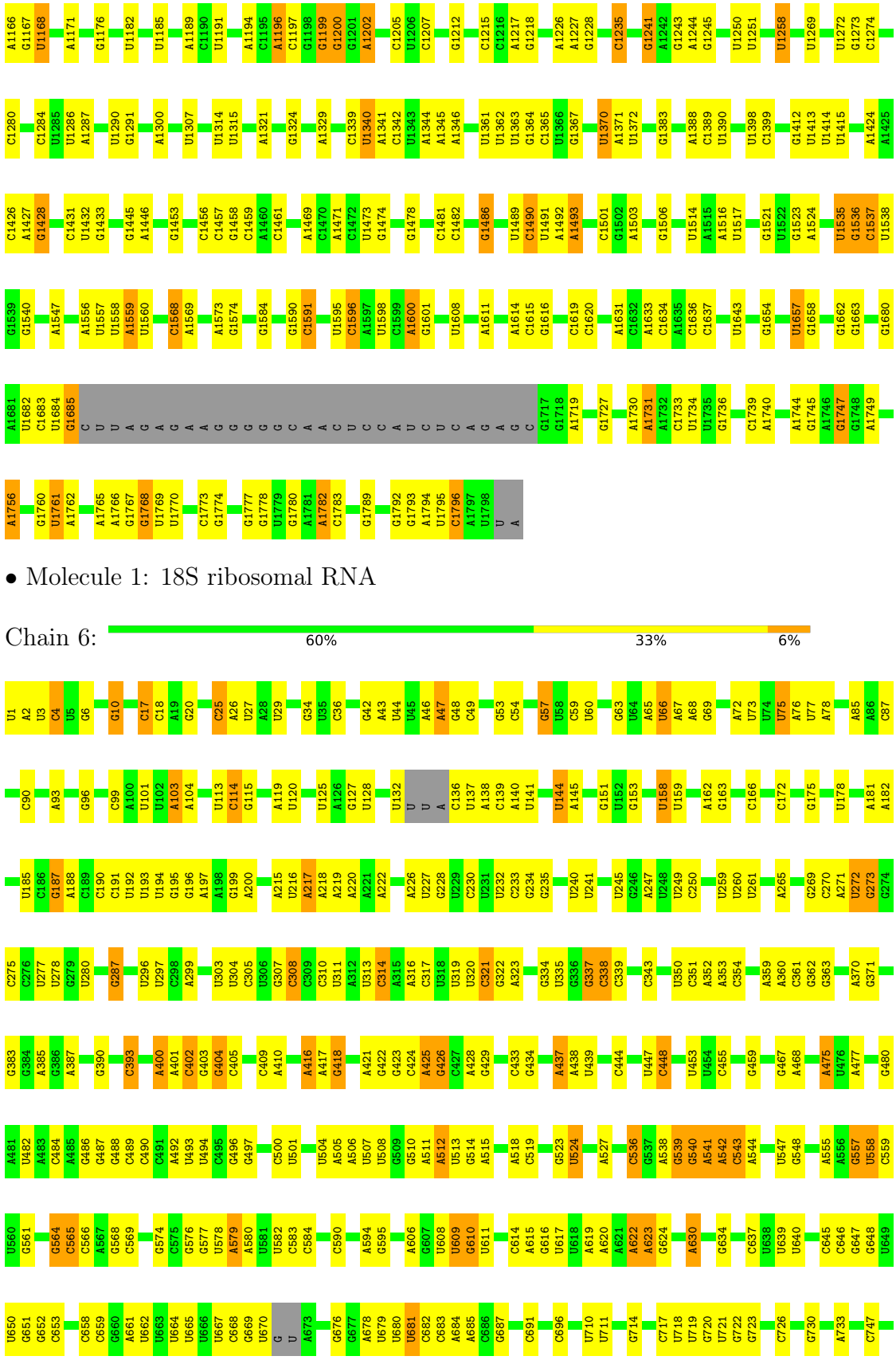
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

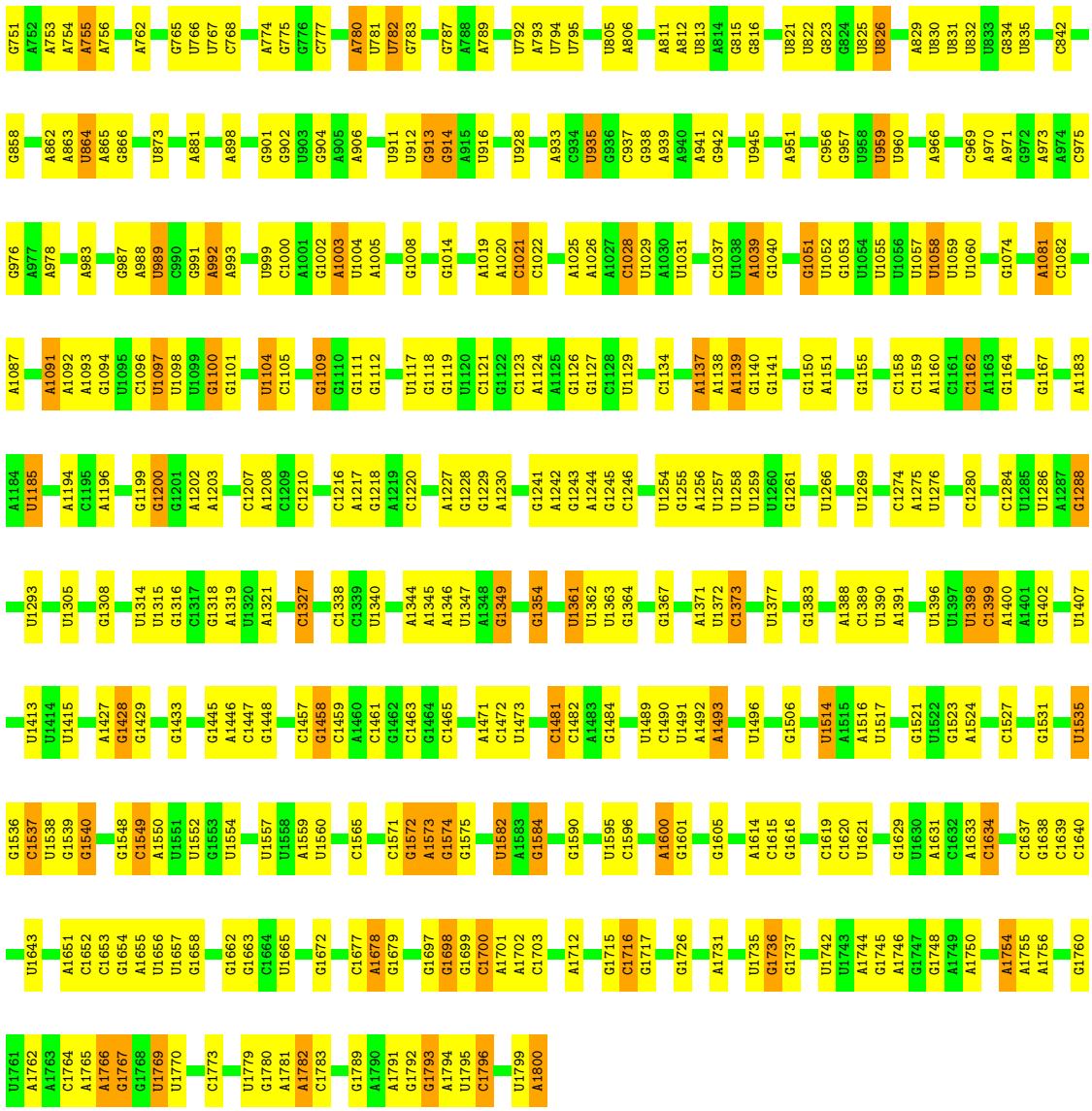
Chain 2: 62% 30% 5% •





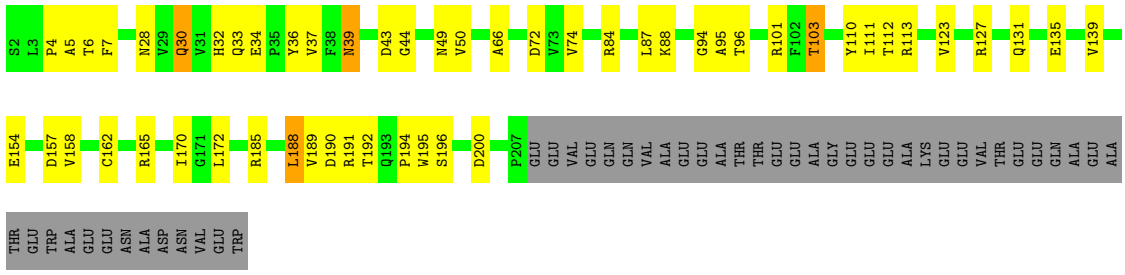
• Molecule 1: 18S ribosomal RNA

Chain 6: 60% 33% 6%



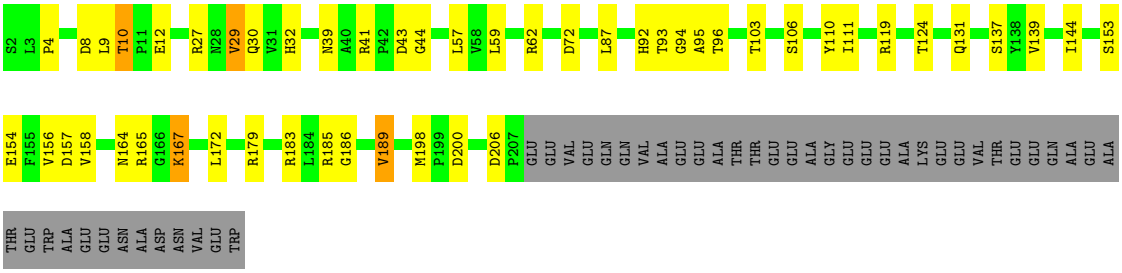
- Molecule 2: 40S ribosomal protein S0-A

Chain S0:



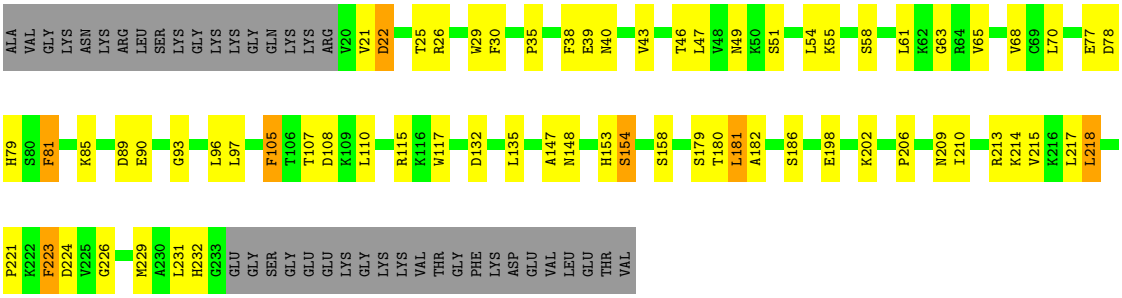
- Molecule 2: 40S ribosomal protein S0-A

Chain s0:



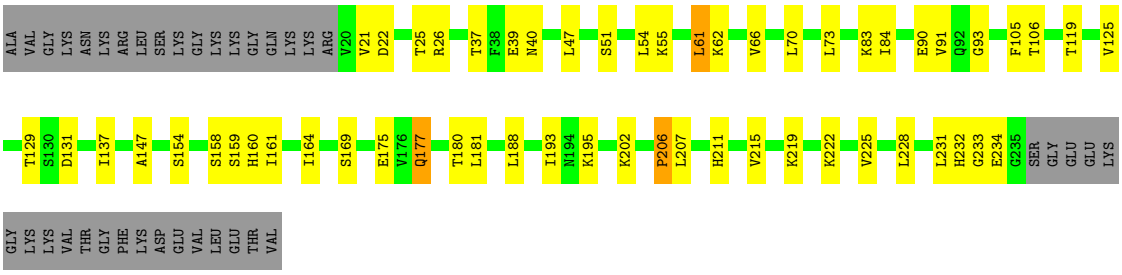
- Molecule 3: 40S ribosomal protein S1-A

Chain S1:



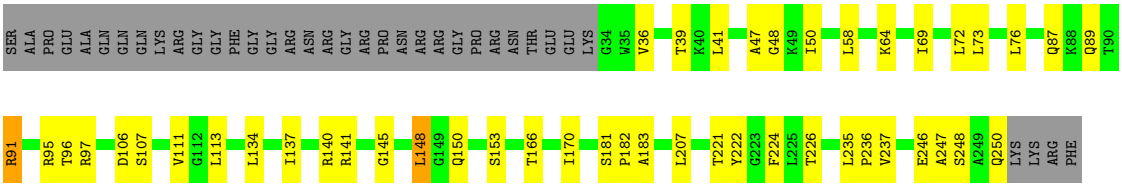
- Molecule 3: 40S ribosomal protein S1-A

Chain s1:



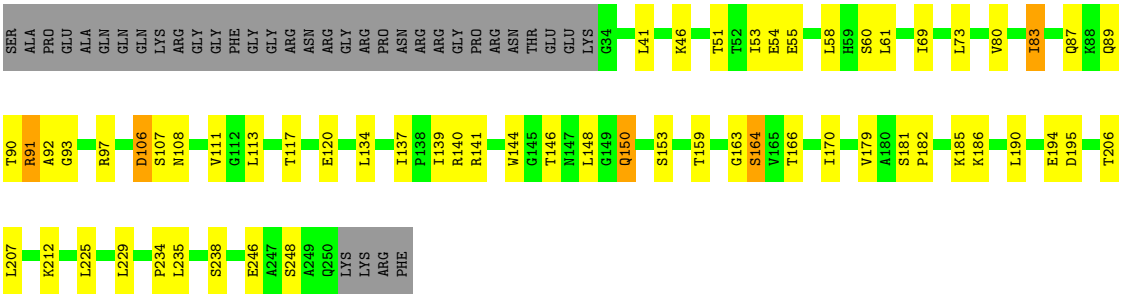
- Molecule 4: 40S ribosomal protein S2

Chain S2:



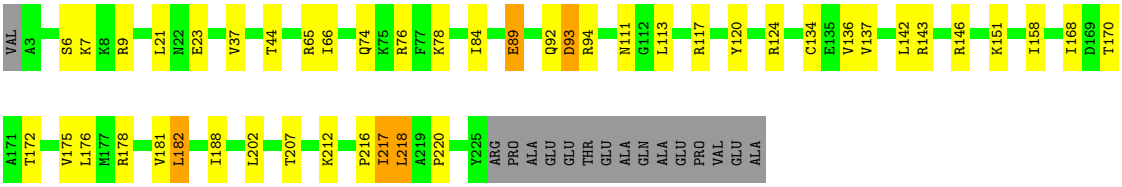
- Molecule 4: 40S ribosomal protein S2

Chain s2:



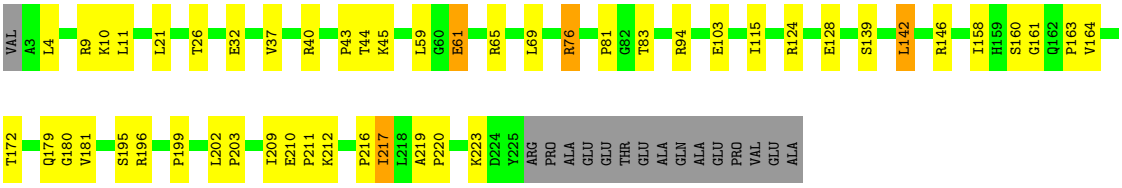
• Molecule 5: 40S ribosomal protein S3

Chain S3:



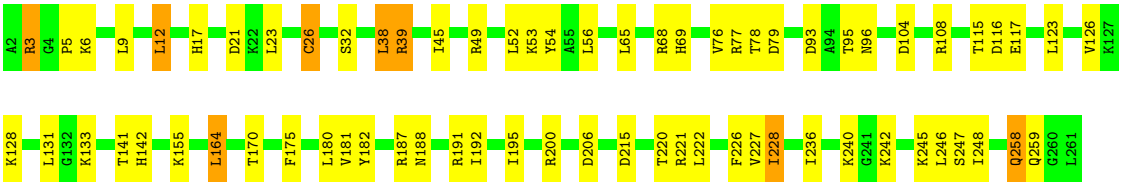
• Molecule 5: 40S ribosomal protein S3

Chain s3:



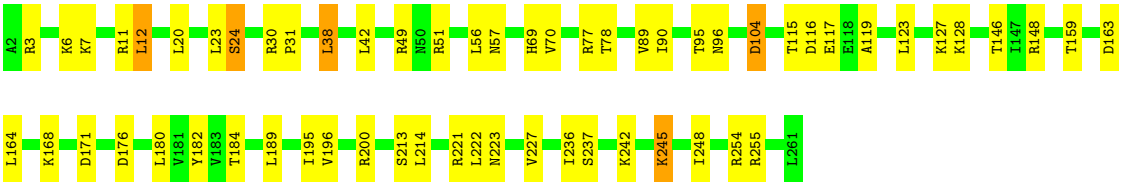
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



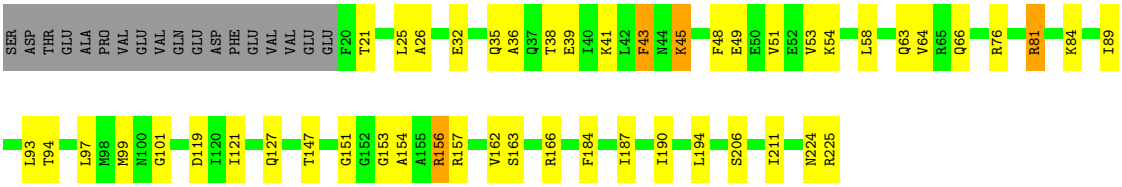
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



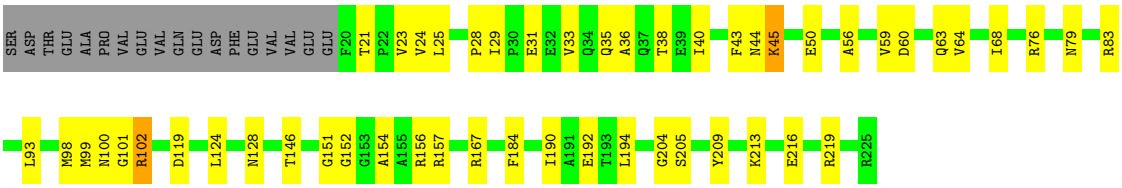
- Molecule 7: 40S ribosomal protein S5

Chain S5:



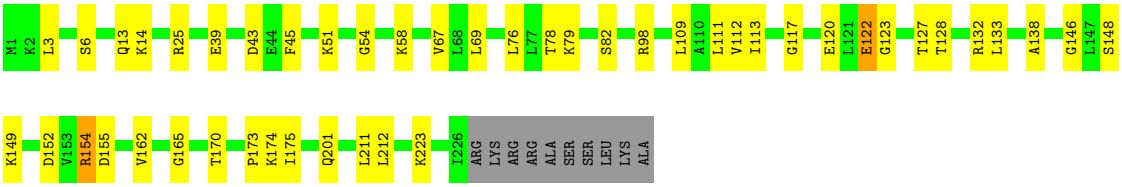
- Molecule 7: 40S ribosomal protein S5

Chain s5:



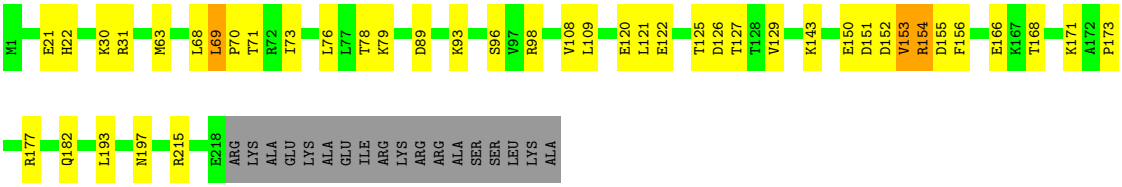
- Molecule 8: 40S ribosomal protein S6-A

Chain S6:



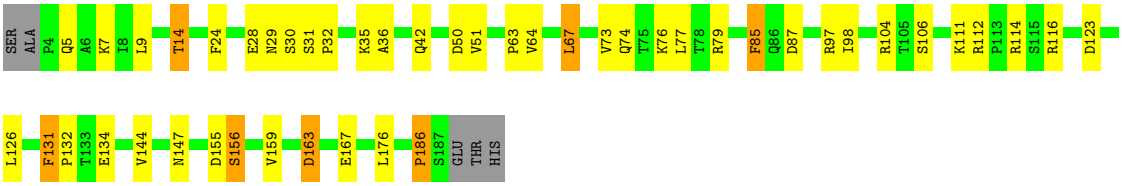
- Molecule 8: 40S ribosomal protein S6-A

Chain s6:



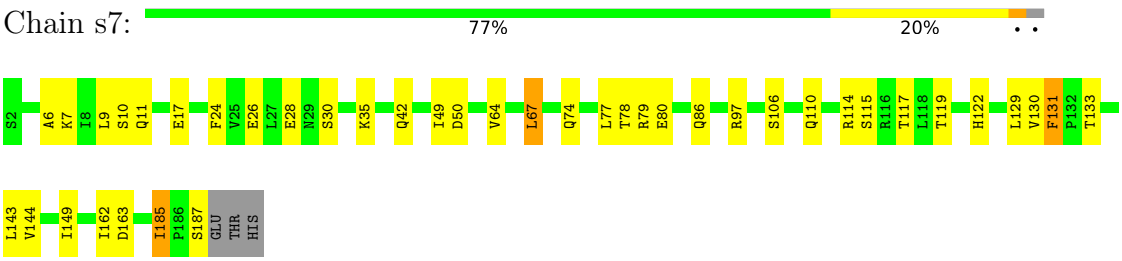
- Molecule 9: 40S ribosomal protein S7-A

Chain S7:



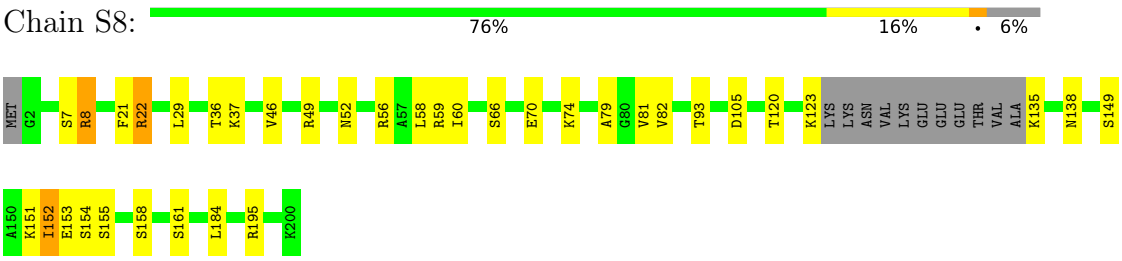
• Molecule 9: 40S ribosomal protein S7-A

Chain s7:



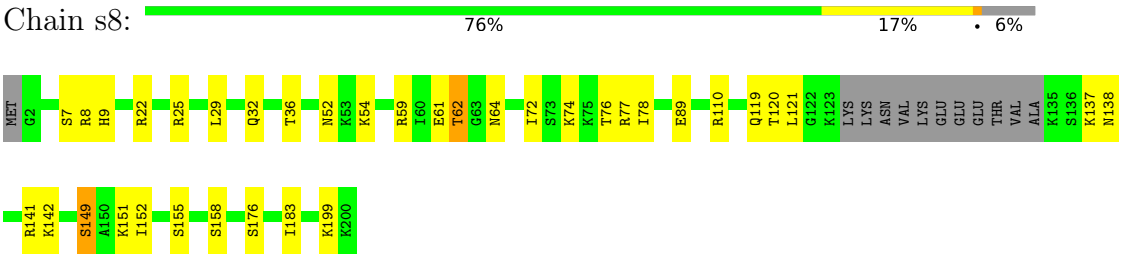
• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



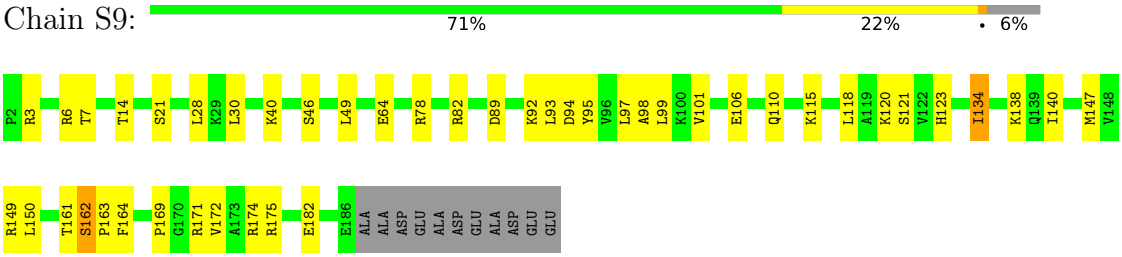
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



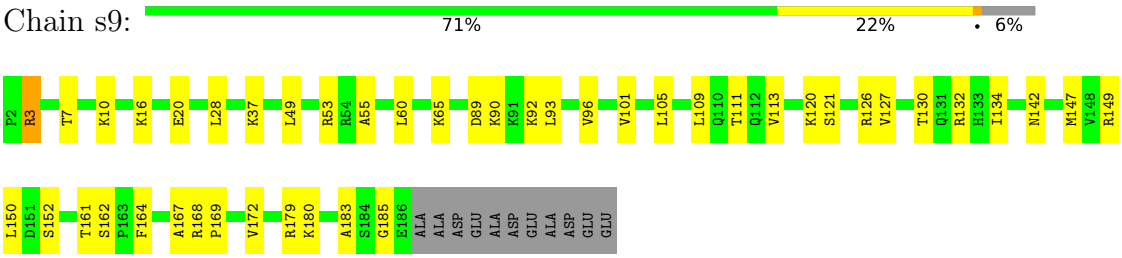
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



• Molecule 12: 40S ribosomal protein S10-A

Chain C0: 69% 20% • 9%

M1 K5 E6 Q13 F27 N28 E34 L40 L46 L49 V55 K56 S60 L76 R77 E78 Y79 L80 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% 17% • 9%

M1 L2 M3 P4 K5 V20 V21 V22 A23 K24 K25 A30 K31 H32 I35 L40 V55 K56 T57 V73 L76 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% 19% •

S2 T3 E4 V7 N21 V25 K29 R30 T31 L40 K43 T44 D55 L63 V64 R67 G68 K69 I70 L71 T72 G73 T74 N80 L91 P95 K96 V107 P113 Q127 I131 N138 V139 V140 K141 A145 A146 A154 K155 F156

• Molecule 13: 40S ribosomal protein S11-A

Chain c1: 74% 19% • 6%

S2 L5 T6 V7 E10 N21 K24 T27 R30 T31 K32 L40 T44 D55 K56 F60 R67 G68 K69 T74 S77 M80 H81 R82 R87 V107 P113 V119 G120 D121 C128 R129 N138 V139 V140 S143 A144 A145 A146

A147 LYS ALA ASN LYS GLN PHE ALA LYS PHE

• Molecule 14: 40S ribosomal protein S12

Chain C2: 58% 27% • 13%

SER ASP VAL GLU GLU VAL VAL GLU VAL GLN GLU GLU THR VAL VAL GLU GLN THR A20 E21 V22 E25 R33 V37 R43 G44 L45 R46 T49 K50 A51 L52 T53 R54 L59 L62 V66 I71 L74 E83 V86 P87 L88 I89 K90 V91 A92

A101 G102 L103 I106 D107 R108 A112 V115 S119 N125 W126 G127 A128 E129 T130 D131 E132 M135 H139 F140 Q143

• Molecule 14: 40S ribosomal protein S12

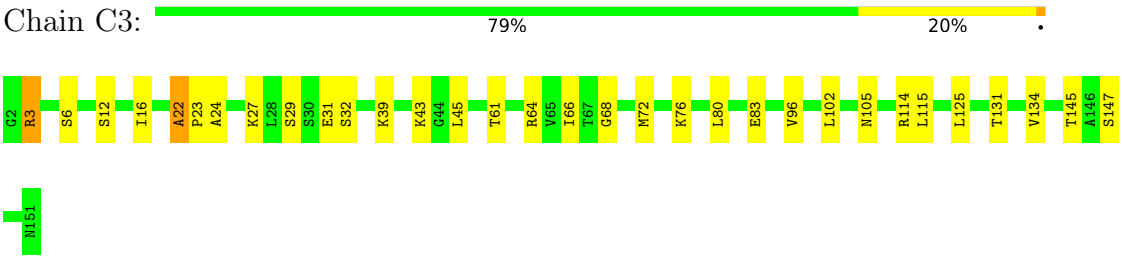
Chain c2: 60% 24% • • 13%

SER ASP VAL GLU GLU VAL VAL GLU VAL GLN GLU GLU THR VAL VAL GLU GLN THR A20 E21 V22 D26 A27 L28 K29 V30 L36 V37 H38 D39 G40 L45 L52 L53 V61 T67 I71 L74 P82 E83 N84 K85 V86 P87 L88 I89 K90 D93

L97 L103 I106 D107 R108 V115 A118 S119 V120 V121 E129 T130 D131 E132 I136 F140 S141 Q142 Q143

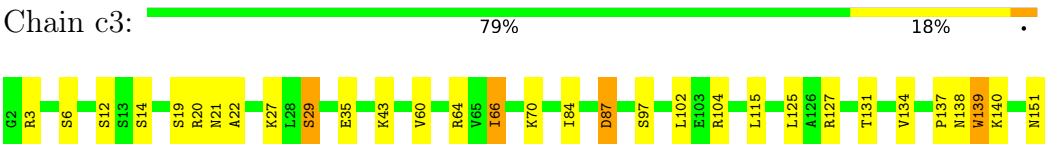
• Molecule 15: 40S ribosomal protein S13

Chain C3:



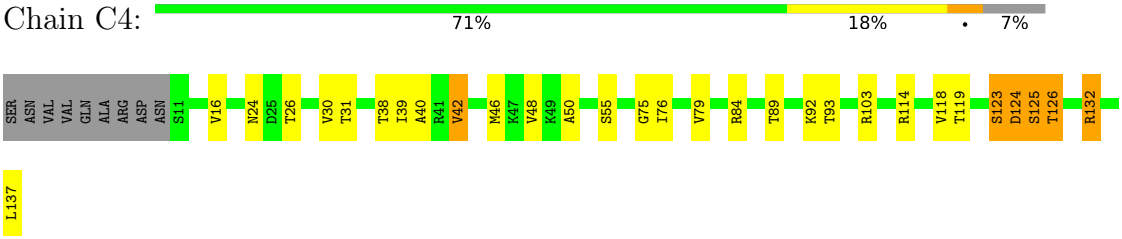
• Molecule 15: 40S ribosomal protein S13

Chain c3:



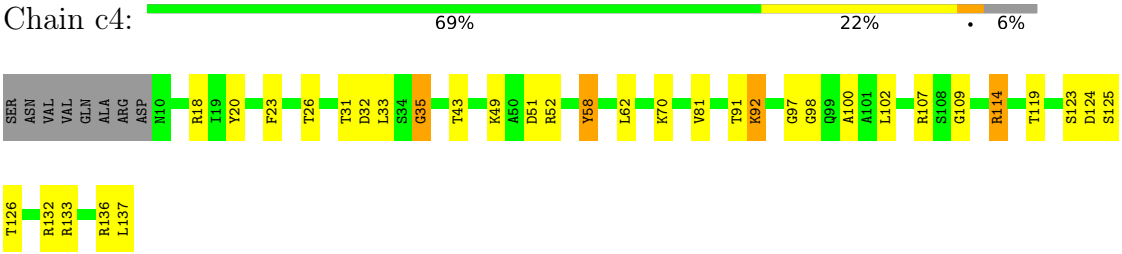
• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



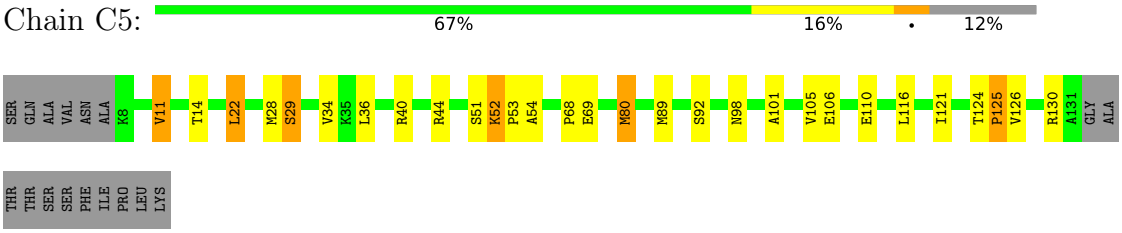
• Molecule 16: 40S ribosomal protein S14-A

Chain c4:



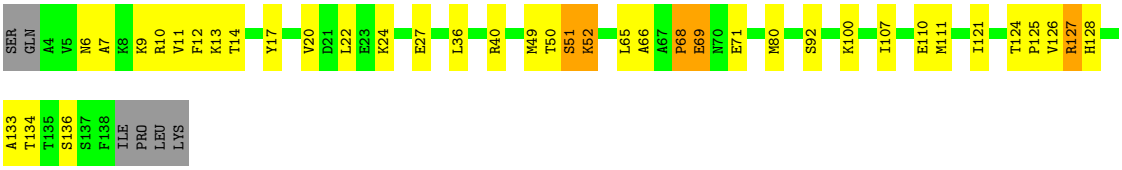
• Molecule 17: 40S ribosomal protein S15

Chain C5:



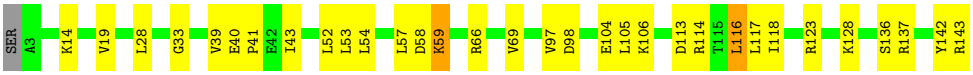
• Molecule 17: 40S ribosomal protein S15

Chain c5:



• Molecule 18: 40S ribosomal protein S16-A

Chain C6:

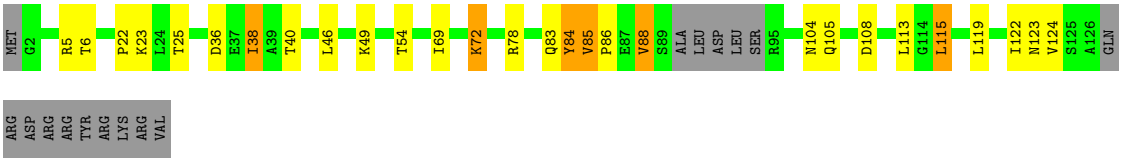


• Molecule 18: 40S ribosomal protein S16-A

Chain c6:

• Molecule 19: 40S ribosomal protein S17-A

Chain C7:

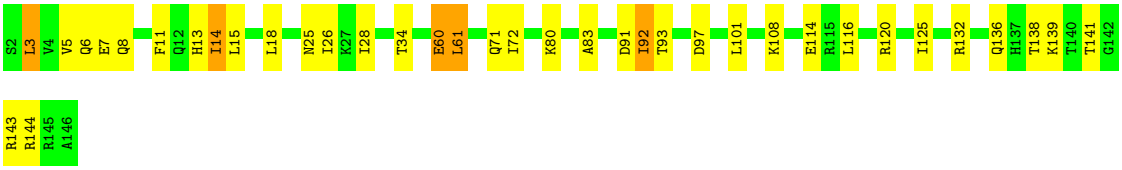


• Molecule 19: 40S ribosomal protein S17-A

Chain c7:

• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



• Molecule 20: 40S ribosomal protein S18-A

Chain c8: 77% 20%

S2 L3 V4 V5 Q6 E7 Q8 G9 Q12 H13 I14 T20 N25 I28 V29 T33 T34 R40 V46 R57 E60 L61 T62 Q63 L66 K80 D91 I92 T93 D94 V105 L116 I119 G135 R143 R144 R145 A146

- Molecule 21: 40S ribosomal protein S19-A

Chain C9: 79% 20%

P2 G3 V4 S5 V6 D13 Y18 L22 K27 L28 E29 V30 P31 G32 Y33 V34 D35 I36 V37 K38 T39 W53 R57 M67 R68 K69 Q70 V71 I94 I111 R122 R123 I124 S125 E126 R130 D131 L132 T139 E144

- Molecule 21: 40S ribosomal protein S19-A

Chain c9: 82% 17%

P2 G3 V6 L28 E29 Y33 V34 V37 S41 E51 R57 R68 K69 Q70 V71 R86 Y91 R102 I116 S117 P118 K119 R123 E126 D131 L132 D133 T139 L140 E141 E142 D143 E144

- Molecule 22: 40S ribosomal protein S20

Chain D0: 67% 22% 11%

SER ASP PHE GLN LYS GLU LYS VAL GLU GLU GLN GLU GLN Q15 Q16 Q17 Q18 I19 I20 R23 T27 V31 L34 S39 N40 I41 N49 L50 V51 R57 L58 K61 R68 E74 G75 S76 T81 R89 I99 I103 I106 N121

- Molecule 22: 40S ribosomal protein S20

Chain d0: 60% 30% 8%

SER ASP PHE GLN LYS GLU LYS VAL GLU GLU Q12 E13 Q14 Q15 Q16 Q17 Q18 I19 R23 I24 T25 L26 T27 K30 V31 L34 N44 A45 N49 L50 V51 K52 R57 T60 K61 V62 L63 T70 P71 N72 G73 E74 K77 T81 K88 R89 P96 V97

Q98 I99 R102 I103 T104 Q105 I106 T107 D113 V114 E115 V118 N121

- Molecule 23: 40S ribosomal protein S21-A

Chain D1: 78% 18%

M1 E2 N3 D4 Q7 L8 V9 E10 L11 Y12 S18 D27 V36 E41 E42 G43 T52 S68 L69 L78 V82 R87

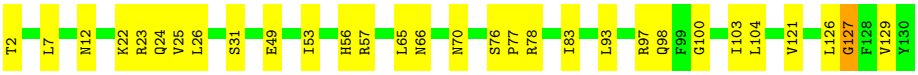
- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 77% 23%

M1 E2 N3 D4 K5 G6 E10 L11 Y12 K25 V32 K38 G43 R44 Y50 V51 T52 S68 L69 N75 L78 N81 R87

• Molecule 24: 40S ribosomal protein S22-A

Chain D2:

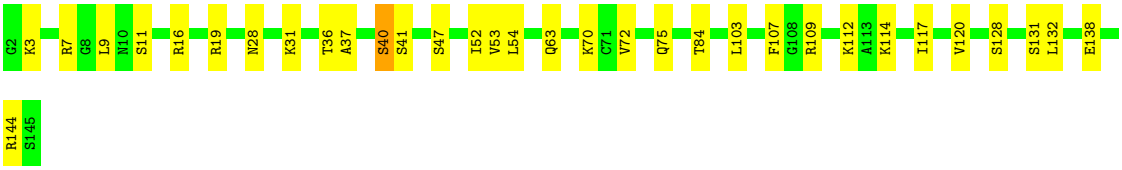


• Molecule 24: 40S ribosomal protein S22-A

Chain d2:

• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



• Molecule 25: 40S ribosomal protein S23-A

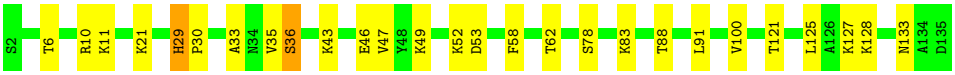
Chain d3:

• Molecule 26: 40S ribosomal protein S24-A

Chain D4:

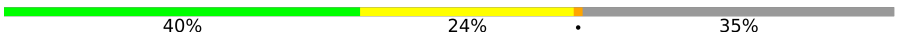
• Molecule 26: 40S ribosomal protein S24-A

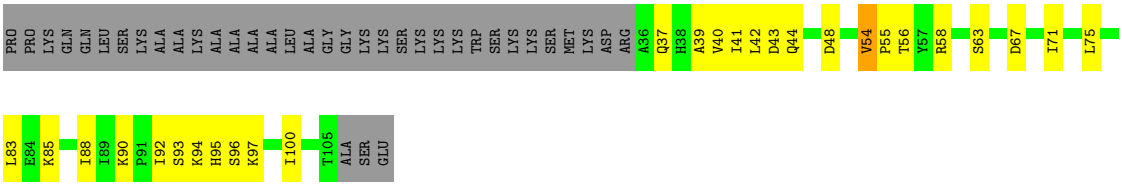
Chain d4:



• Molecule 27: 40S ribosomal protein S25-A

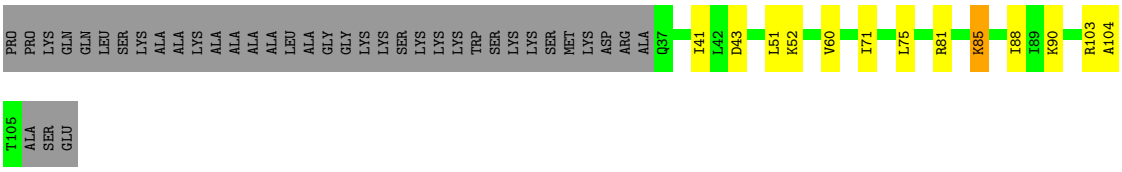
Chain D5:





• Molecule 27: 40S ribosomal protein S25-A

Chain d5:



• Molecule 28: 40S ribosomal protein S26-B

Chain D6:

• Molecule 28: 40S ribosomal protein S26-B

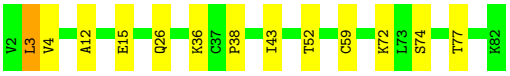
Chain d6:

• Molecule 29: 40S ribosomal protein S27-A

Chain D7:

• Molecule 29: 40S ribosomal protein S27-A

Chain d7:

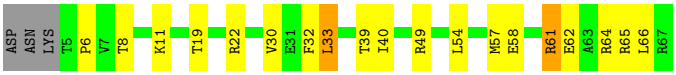


• Molecule 30: 40S ribosomal protein S28-A

Chain D8:

• Molecule 30: 40S ribosomal protein S28-A

Chain d8:

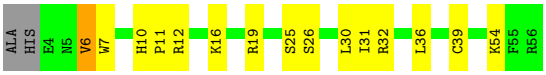


• Molecule 31: 40S ribosomal protein S29-A

Chain D9:

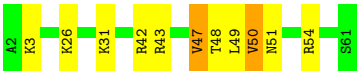
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



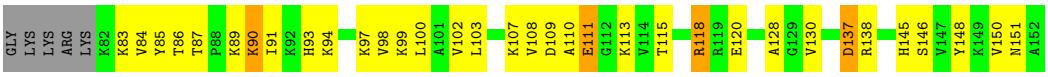
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:

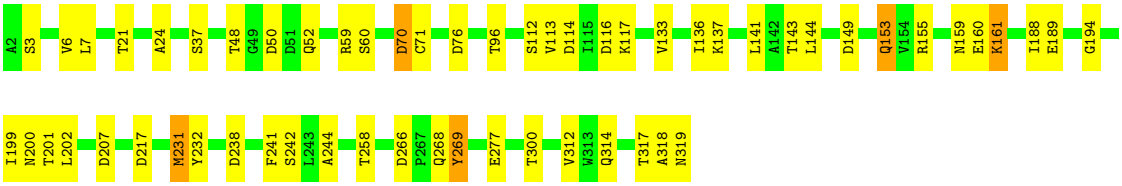


• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:

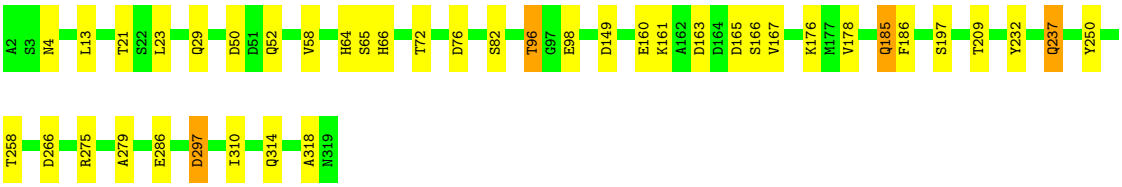
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



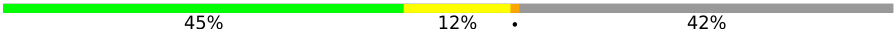
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

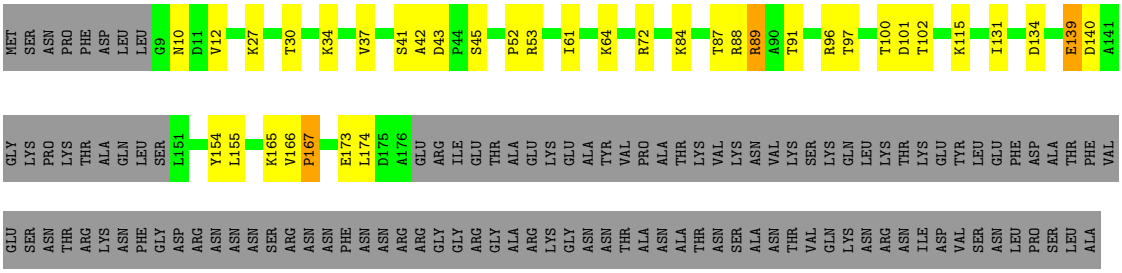
Chain sR:



• Molecule 35: Suppressor protein STM1

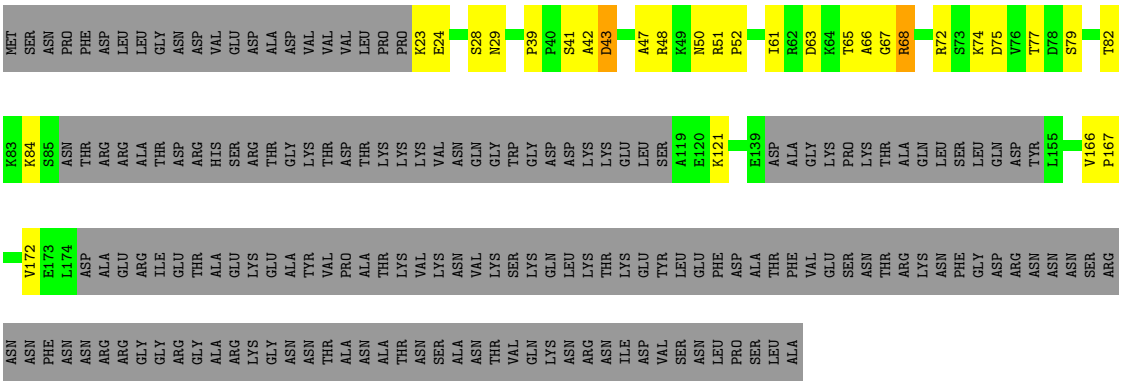
Chain SM:





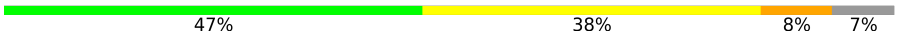
• Molecule 35: Suppressor protein STM1

Chain sM:

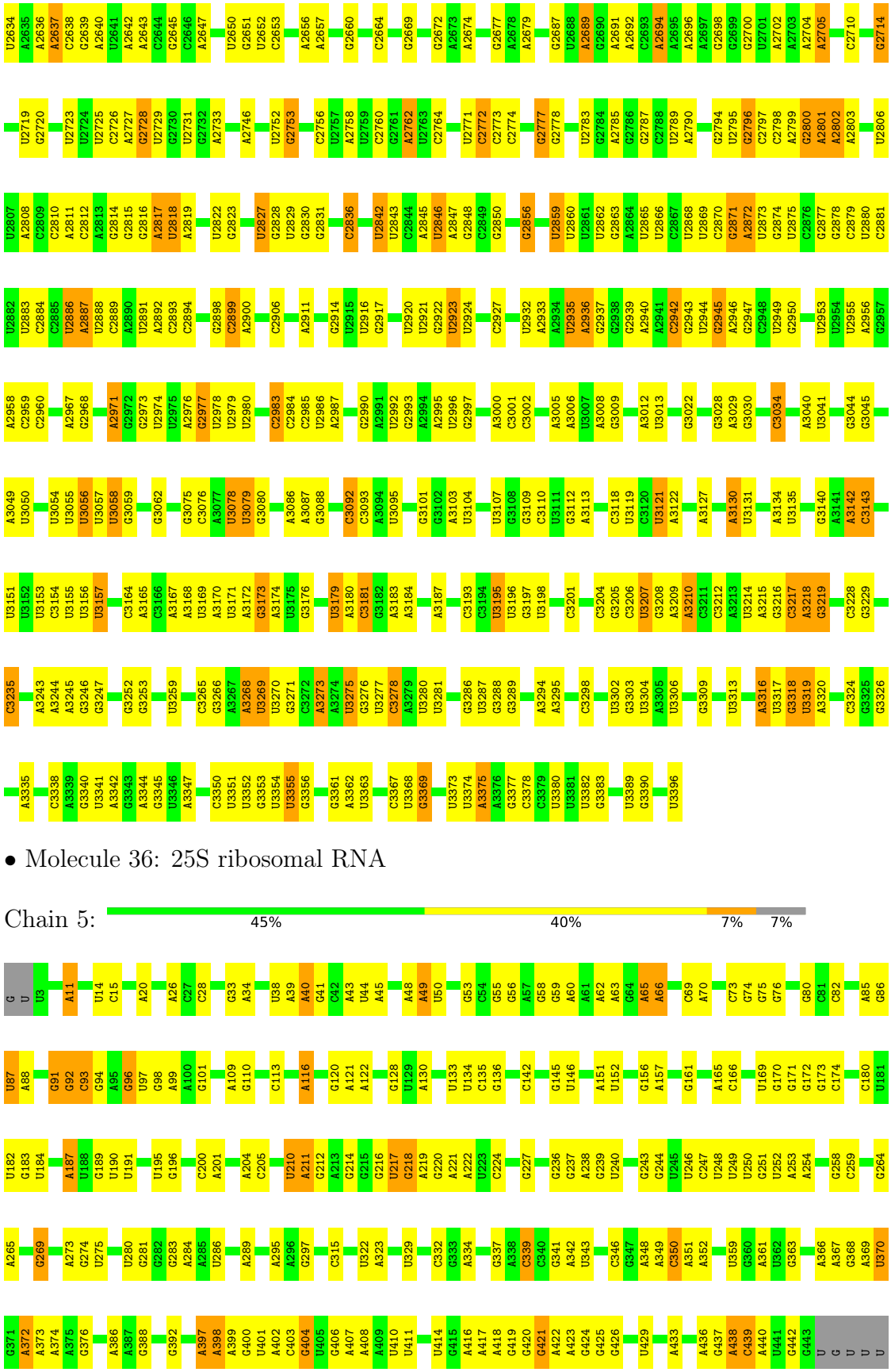


• Molecule 36: 25S ribosomal RNA

Chain 1:

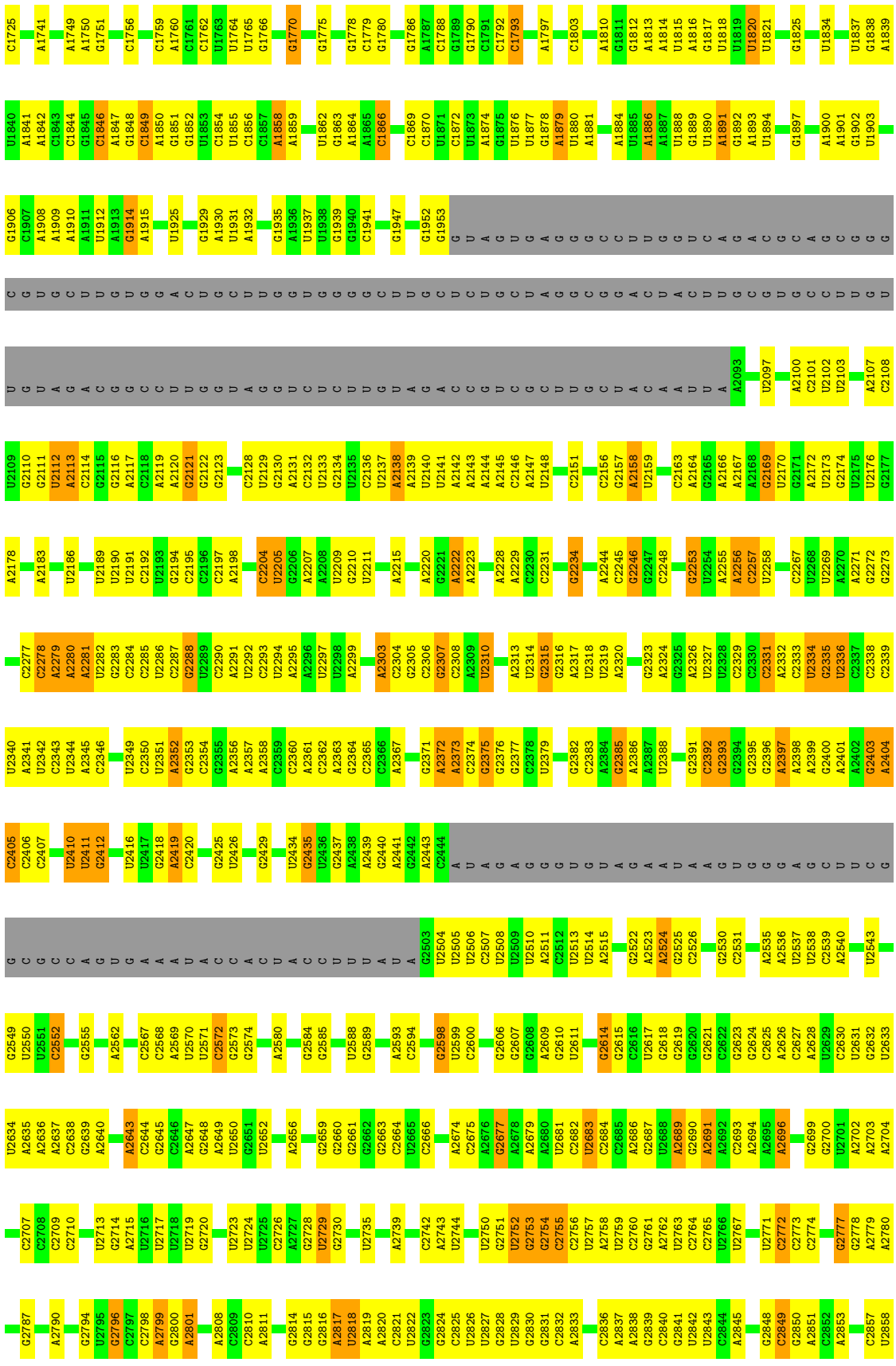


G U U3 A13 U14 C15 A16 G22 U25 A26 C27 C28 C29 G30 C31 U32 G33 A34 A35 C36 U37 U38 A39 A40 G41 C42 A43 U44 A45 U46 C47 A48 A49 U50 A51 A52 G53 C54 G55 G56 G59 A60 A61 G64 A65 A66 A67 C68 C69 A70 A71 C72 C73 G74 G75
G76 A77 U78 U79 G80 C81 C82 U83 U84 A85 G86 A89 C90 G91 G92 C93 G94 A95 G96 U97 G98 A99 A100 G101 G104 C105 A106 A107 A108 A109 G110 C111 U112 C113 A114 A115 A116 U117 A121 A122 A123 U124 G127 C131 C132 U133 U134 C135 G136 C142 G143 A144 G145 U146
U147 G148 U153 U154 G155 G156 A157 G158 A165 C166 U169 G170 G171 G176 A187 U188 G189 U190 U191 C192 G196 G197 A198 A199 C200 C205 G206 U207 U210 A211 G212 A213 G216 U217 G218 A219 G220 A221 A222 U223 C224 C225 U228 G229 G232 C233 G237 A238
G239 U240 G241 C242 G243 G244 U245 U246 C247 U248 U249 U250 U251 U252 G264 A265 G269 U270 U278 G282 G283 A284 A285 U286 G287 G290 C291 U292 A295 A296 G297 U298 G304 U305 C311 C315 U316 A317 A318 A319 G320 A323 A324 A325 U326 U329 G330 G331 C332
A336 G337 A338 C339 C340 U343 A344 G345 C346 A349 C350 C356 A357 G358 U359 G360 A361 U362 G363 G368 A369 U370 G371 A372 A373 G376 G388 G392 U393 G394 A395 A396 A397 A398 U401 A402 C403 G404 U405 G406 A407 A408 A409 U410 U411 G412 U413 A416 A417
G420 G421 A422 A423 G424 G425 G426 C427 A428 U429 C435 A438 C439 A440 U G G U U U U U G U G C C C C U U C C U C C U U G U G G G U A G G G G G C G C
A U U U C A C U G G494 G495 A498 G499 C500 A501 A504 G505 U506 U507 G511 A519 U520 A521 G535 U541 C544 U545 C546 C547 G548 U549 A550 A551 G552 U555 U556 A557 U558 A559 G560 C573 C577 A578 G579 C580 U581 G584 A585 C586
U587 G588 A589 G590 G591 A592 C593 U594 G600 U601 G604 A607 A608 G609 G610 A611 C614 A619 U620 A621 G624 U627 A628 U629 A630 U631 G632 C633 C634 G635 C636 C637 C638 G639 U640 C641 U642 U643 G644 A645 A646 A647 C648 A649 C650 G651 G652 A653 C654 C655 A656 A657 G658
G659 A660 G661 U662 C663 U664 A665 A666 C667 G668 U669 C670 U671 A672 U673 G674 C675 G676 A677 G678 U679 G680 U681 U682 U683 G684 G685 G686 U687 G688 A691 A692 A693 C694 C695 C696 A697 U698 A699 C700 G701 C702 A705 A706 U707 G708 A709 G712 A715 A716 C717 G718 U719 A720 G721
G725 G726 C730 C743 C758 G763 U764 C765 U766 U767 G770 U776 U777 U778 G779 A780 G781 G785 A786 G787 C788 A789 U790 A791 G792 C793 U794 G795 U796 U797 G798 G799 G800 A801 C802 C803 C804 G805 A806 A807 A808 G809 A810 U811 G815 A816 A817 A820 U821 G826
A830 G835 A836 A837 A843 C849 G857 A858 G859 C860 C861 U862 C863 G864 U865 G870 U871 U872 C873 U874 C877 G878 U879 G880 C881 A882 A883 A884 U885 C886 G887 A888 U889 C890 G894 A895 A896 G901 G902 A906 G907 G908 G909 G910 C911 G912 A913 A914 A915 G916
A917 C918 U919 A920 A921 U922 C923 G924 A925 C928 A929 U930 C931 U932 A933 G934 G937 C938 U939 G940 G941 U942 U943 C944 C945 U946 G947 C948 G949 A952 G953 U954 U955 U956 C957 C958 C959 U960 C961 G964 A965 U966 A967 G968 C969 A970 A973 U979 A980 U981 C982 A983 G984
G993 G994 A997 A998 G999 C1000 G1001 A1002 A1003 A1006 U1007 U1008 A1009 G1010 A1011 G1012 G1013 U1014 U1015 C1016 C1017 G1018 G1019 U1020 G1021 G1024 A1025 G1029 A1036 C1037 U1041 U1042 C1045 A1046 A1047 A1048 C1049 U1050 A1053 A1054 A1055 U1056 U1060 A1064 A1065 C1068 C1069 G1072
U1081 U1082 G1083 G1087 A1093 U1094 U1095 U1096 G1097 A1098 A1099 U1100 G1101 A1102 A1103 G1104 C1107 U1111 A1112 G1113 U1114 G1115 G1116 G1117 C1118 C1119 A1120 U1124 G1127 U1128 A1129 A1130 G1131 C1132 A1133 C1137 U1138 G1139 G1140 C1141 G1142 A1143 U1144 G1149 A1150 U1151 G1152 A1153 A1154 C1155 C1156
G1157 A1158 A1159 C1160 A1163 G1164 A1165 G1166 A1169 A1170 G1171 G1174 C1175 C1176 G1177 G1178 A1179 A1180 U1181 A1182 C1183 A1184 C1187 U1188 C1189 A1190 U1191 C1192 C1196 A1197 C1198 C1201 G1209 G1213 C1216 A1217 U1218 G1222 A1225 G1226 C1227 C1232 G1233 G1234 U1235 G1236 G1237
U1241 G1242 G1243 A1244 A1245 G1246 U1247 C1248 G1249 U1253 U1258 A1259 G1262 A1263 G1264 U1265 G1266 U1267 G1268 A1269 A1270 A1271 C1272 A1273 A1274 A1278 C1279 C1280 G1285 A1286 A1287 A1294 G1295 C1296 C1297 C1298 U1299 G1300 A1304 U1305 G1306 G1307 A1308 U1309 G1310 G1313 C1314 U1315 C1316 A1317 C1320



• Molecule 36: 25S ribosomal RNA

Chain 5: 45% 40% 7% 7%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A2790 C2708 A2635 U2550 C G 2110 C2277 A2341 C2406 G1907 G U A1741 A1841
G2794 C2709 A2636 U2551 C G 2111 C2278 U2342 C2407 A1908 U G A1842
U2795 C2710 A2637 C2552 C C U2112 A2279 C2343 U2410 A1909 G A C1843
G2796 U2713 C2638 G2555 A C 2113 A2280 U2344 U2411 A1910 C G C1844
C2797 G2714 G2639 A G U 2114 A2281 A2345 G2412 A1911 U A C1845
C2798 A2715 A2640 A2562 G U 2115 U2282 C2346 A1912 U C C1846
A2799 U2716 A2643 U G 2116 G2283 U2349 U2416 A1913 G G A1847
G2800 U2717 C2644 C2567 A 2117 C2284 C2350 U2417 G1914 G G G1848
A2801 U2718 C2645 C2568 A 2118 C2285 U2351 G2418 A1915 U C C1849
A2808 U2719 C2646 A2569 A 2119 U2286 A2352 A2419 U1925 C U A1850
C2809 G2720 A2647 U2570 U 2120 C2287 G2353 C2420 U U G1851
C2810 U2723 G2648 U2571 A 2121 G2288 C2354 G2425 G G1925 G G1852
A2811 U2724 A2649 C2572 C 2122 U2289 C2355 U2426 G U G U1853
G2814 U2725 U2650 G2573 C 2123 C2290 A2356 G1929 U G C1854
G2815 C2726 G2651 G2574 A 2128 A2291 A2357 G2429 G1930 U C U1855
G2816 A2727 U2652 C U 2129 C2292 A2358 U2434 U1931 U U C1856
A2817 G2728 A2656 A 2130 C2293 C2359 G2435 A1932 U U C1857
U2818 U2729 G2659 C 2131 U2294 G2360 U2436 G1935 G G A1858
A2819 G2730 G2660 C 2132 G2295 A2361 G2437 A1936 G U A1859
A2820 U2735 U2588 U 2133 A2296 C2362 A2438 U1937 U G U1862
C2821 G2589 U 2134 U2297 A2363 A2439 U1938 G G G1863
U2822 A2739 G2663 U 2135 U2298 G2364 G2440 G1939 G G A1864
G2823 C2742 A2593 G2664 A 2136 U2209 C2365 A2441 G1940 G C A1865
G2824 A2743 C2594 U2665 2137 G2299 C2366 G2442 C1941 U C C1866
C2825 U2744 G2666 G2503 2138 A2303 A2367 A2443 G1947 U U C1869
U2826 U2750 G2598 U2504 2139 C2304 G2371 C2444 G1952 G U C1870
U2827 G2751 U2599 U2505 2140 G2305 A2372 A G1953 U G U1871
G2828 U2752 G2600 U2506 2141 C2306 A2373 U G U U1872
U2829 G2753 G2606 C2507 2142 G2307 C2374 A G U U1873
G2830 G2754 G2607 U2508 2143 C2308 G2375 G G U U1874
G2831 C2755 G2678 U2509 2144 A2309 G2376 G G U U1875
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A2833 U2757 G2680 A2511 2146 A2313 C2378 G U U1877
C2836 A2758 U2681 G2609 2147 U2314 U2379 C U G1878
A2837 U2759 C2682 C2610 2148 G2315 A U A1879
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C2839 G2761 C2684 G2614 C2151 U2513 A2317 G U A1881
C2840 A2762 C2685 G2615 U2514 U2318 G U
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U2842 C2764 G2687 U2617 G2522 U2319 G2157 C A2164 C U U1885
U2843 C2765 U2688 G2618 A2523 A2320 A2158 U G2165 U U A1886
C2844 U2766 A2689 G2619 A2524 G2323 U2159 A A2166 A U A1887
A2845 U2767 G2690 G2620 G2525 A2324 C A2167 C U U1888
G2848 U2771 A2691 G2621 A2526 G2525 C U A2168 G U G1889
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C2852 G2777 A2695 C2625 A2536 A2256 A2166 A2172 A G1893
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A2702 C2630 U2543 U2268 G2171 C
A2703 U2631 U2269 A2172 A
A2704 G2632 A2270 U2173 G
U2633 A2271 G2174 C A1900
G2272 U2175 U A1901
G2273 U2176 G A1902
G2177 G A1903
A2093 U1819 C1725 A1741 A1749 A1750 G1751 C1756 C1759 A1760 C1761 C1762 U1763 U1764 U1765 G1766 G1770 G1775 G1778 C1779 G1780 G1786 A1787 C1788 G1789 G1790 C1791 C1792 C1793 A1797 C1803 A1810 G1811 G1812 A1813 A1814 U1815 A1816 G1817 U1818 U1820 U1821 G1825 U1834 U1837 G1838 A1839
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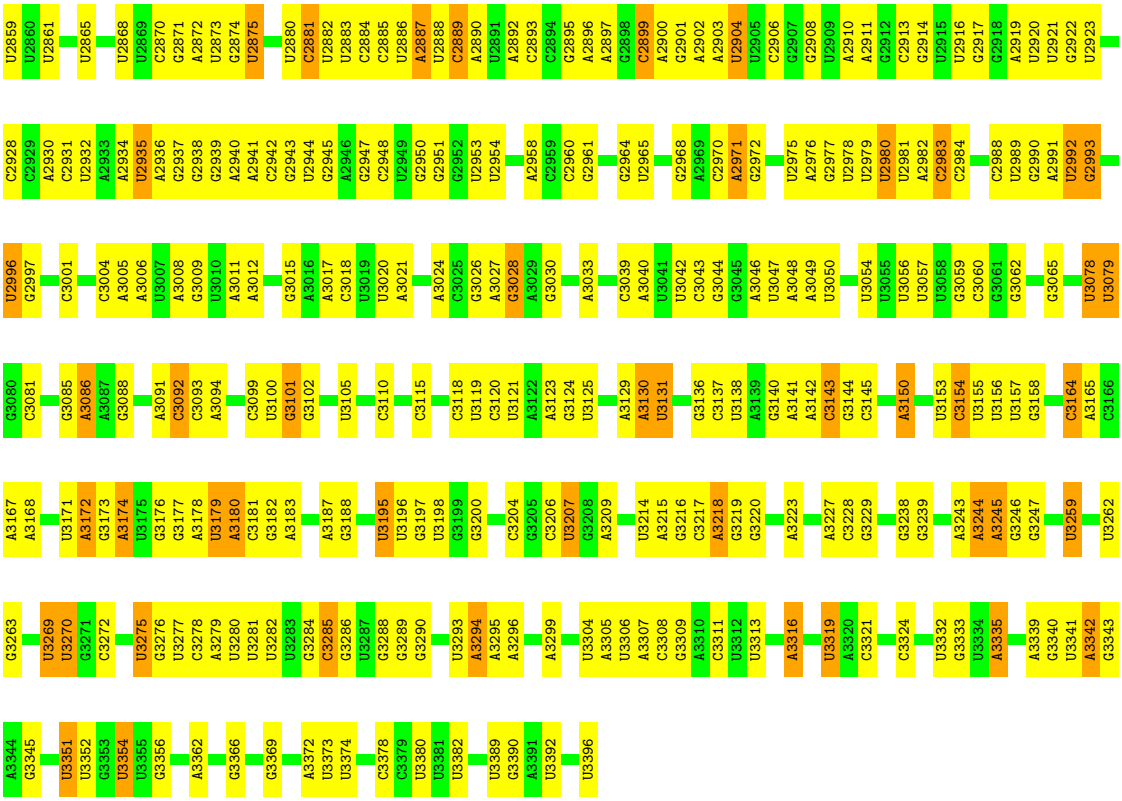
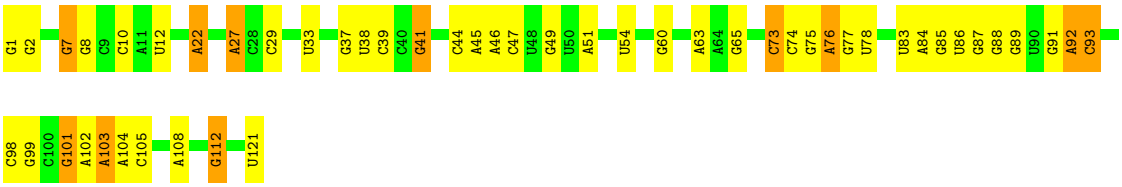


- Molecule 37: 5S ribosomal RNA

Chain 3:

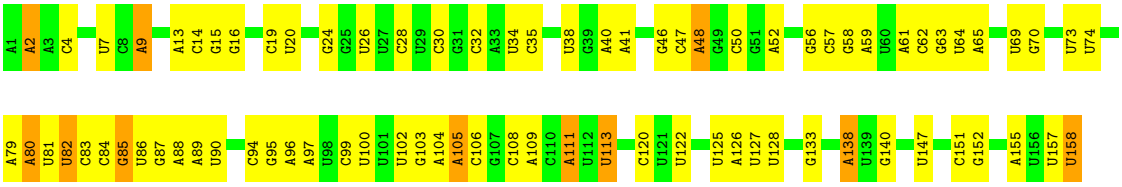
- Molecule 37: 5S ribosomal RNA

Chain 7:



- Molecule 38: 5.8S ribosomal RNA

Chain 4:



• Molecule 38: 5.8S ribosomal RNA

Chain 8: 57% 35% 8%

A1 A2 A3 C4 U7 C8 A9 A10 C11 A12 G16 A17 U18 C19 U20 C21 G25 U29 C32 A33 U34 C35 G36 A37 U38 G39 A40 A41 G42 A43 C47 A48 G49 C50 G51 A52 A53 A54 U55 G56 A59 C62 G63 G68 U74 A79 A80 U81 U82

C83 C84 G85 U86 G87 U93 C94 G95 A96 A97 U98 C99 A104 A105 C106 G107 C108 A109 C110 A111 U112 U113 U125 A126 G140 G152 A155 U156 U157 U158

• Molecule 39: 60S ribosomal protein L2-A

Chain L2: 81% 18%

G2 G13 S18 H19 G25 K28 L32 E36 R37 I44 V45 K46 Q47 I48 V62 R70 L71 R72 E73 S95 L96 N97 V101 L104 S114 N115 V116 A127 I137 G138 H139 E143 N144 R149 V157 R163 G164 V165 I169

K177 P178 L179 L180 K181 L191 K192 R193 V202 V207 R227 V230 R241 L246 Q250 K251 T252 Q253 ASP

• Molecule 39: 60S ribosomal protein L2-A

Chain l2: 83% 15% •

G2 I15 Q24 L32 I41 I44 V45 I48 A56 V61 V62 K68 E80 G81 V82 V101 L102 P103 L104 E109 S114 N115 V116 R123 L126 S130 I137 P141 D142 E143 V157 K177 P178 L179 L191 K192 R193 N194

M204 M205 P206 N215 R227 V230 I238 R241 R242 L245 L246 S249 Q253 ASP

• Molecule 40: 60S ribosomal protein L3

Chain L3: 77% 22% •

S2 H3 R4 K5 Y6 E7 R10 L17 P18 R19 K20 R21 S24 I25 K30 R37 L47 I56 K66 R70 V73 V79 D80 T81 V84 V85 V86 V87 R100 S101 L102 T103 V114 K115 R116 K126 K127 K128 S134 A138 Q139 D140 G141

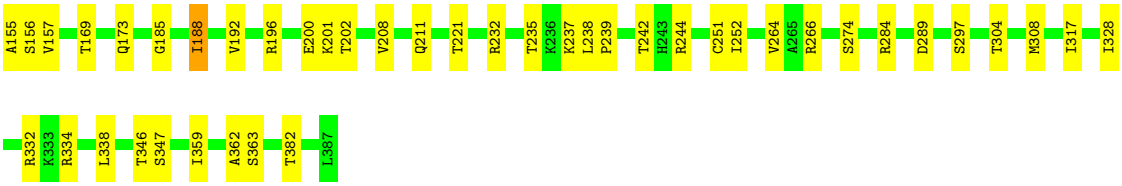
A142 R146 E147 L148 K153 Y154 A155 S156 V157 V160 Q165 I166 R167 K168 T169 G185 G186 S187 I188 S189 V192 R196 E200 K201 T202 V208 F209 E210 Q211 N212 R232 T235 K236 K237 L238 K241 I252 V264 A265 R266 S274 R284 R300

I305 M308 I317 D320 V324 I328 R332 L338 S341 L342 Y343 S347 R348 L351 E352 E353 V354 S355 K364 A378 T382 K385 D386 L387

• Molecule 40: 60S ribosomal protein L3

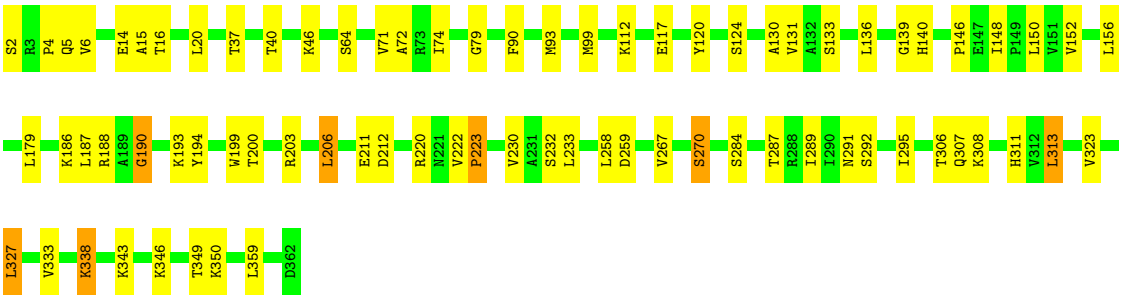
Chain l3: 81% 18% •

S2 H3 R4 R10 L17 P18 R19 K20 R21 A22 A23 S24 K30 S38 T44 I56 L60 K66 E74 T77 V78 V79 D80 T81 V85 V86 V87 T103 V114 K126 A129 K132 Q139 D140 G141 A142 R146 E147 L148 A149 R150



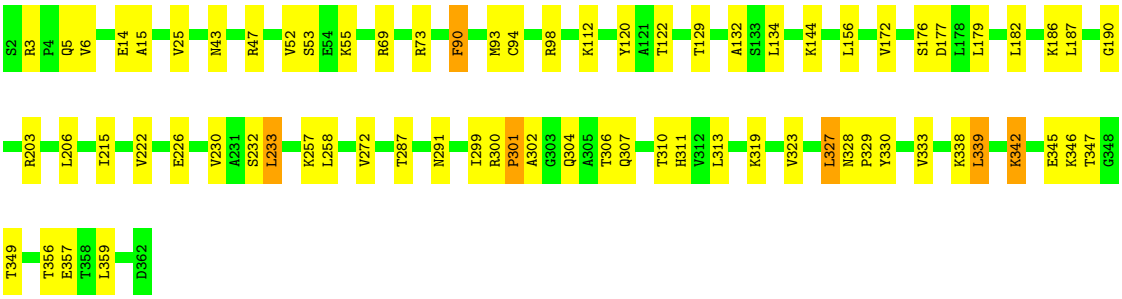
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



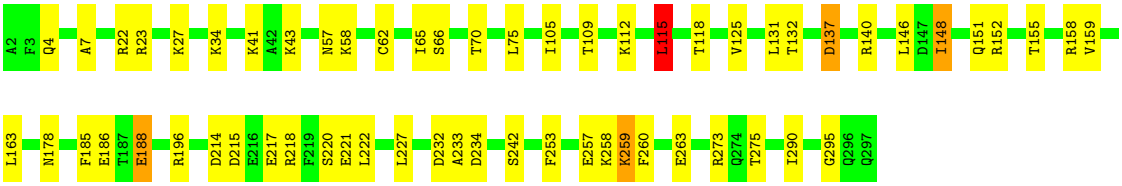
• Molecule 41: 60S ribosomal protein L4-A

Chain l4:



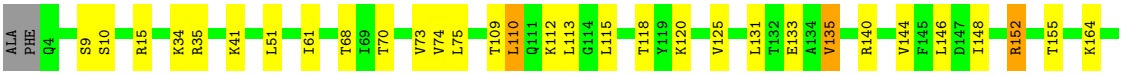
• Molecule 42: 60S ribosomal protein L5

Chain L5:



• Molecule 42: 60S ribosomal protein L5

Chain l5:



S176 E177 N178 W183 D184 F185 E186 T187 L194 L211 R218 L227 D230 L236 E237 D238 I239 K254 K258 K259 F260 T261 K262 Y265 A266 A267 E268 S269 K270 K271 T275 K276 L277 S278 K279 V286 L293 Q297

• Molecule 43: 60S ribosomal protein L6-A

Chain L6: 77% 12% • 11%

S2 K5 A6 P7 V15 L18 T21 R48 R51 V52 L64 I65 V79 V84 T89 K90 E94 V98 K108 E109 LYS LEU THR LYS LYS GLU LYS LYS GLU ALA ASN LEU PHE PRO GLU GLN GLN ASN LYS E129 R134 L155 S162

K166 F176

• Molecule 43: 60S ribosomal protein L6-A

Chain l6: 75% 14% • 10%

S2 K8 W9 Y10 D14 V15 K20 T21 L30 R31 R46 L64 I65 R78 R82 T89 K90 V91 N97 V98 E99 E109 LYS LEU THR LYS LYS GLU LYS LYS GLU ALA ASN LEU PHE PRO GLU GLN GLN ASN K128 K131 A132 E133 K150 K151 T152

L155 K170 M173 L174 K175 F176

• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 75% 14% • 9%

ALA ALA GLU LYS ILE LEU THR PRO GLU SER GLN LEU LYS LYS SER LYS ALA GLN GLN LYS THR A23 E24 Q25 V26 A32 R33 K38 E39 K40 E59 R60 V77 K82 I89 K90 G91 I92 N93 K98 R110 K118 V119 T120 L124 K128 L129 K158

Q159 R160 V161 P162 L163 S164 K175 I178 L179 D182 D183 L184 K206 L207 P217 I224 S228 L239 N244

• Molecule 44: 60S ribosomal protein L7-A

Chain l7: 79% 11% • 8%

ALA ALA GLU LYS ILE LEU THR PRO GLU SER GLN LEU LYS LYS SER LYS ALA GLN GLN LYS T22 A23 E24 R30 R41 L45 E54 R60 K82 L83 R88 K94 R100 K121 L124 L129 T130 I156 N157 K158 Q159 L173 T178 L179 S180

I181 L184 V191 G192 P193 K219 G226 F229 L239 S242 M243 N244

• Molecule 45: 60S ribosomal protein L8-A

Chain L8: 74% 17% 9%

ALA PRO GLY LYS LYS VAL ALA PRO ALA PRO PHE GLY ALA LYS SER THR LYS SER ASN LYS THR ARG N24 P25 L26 T27 I36 A39 V40 Q41 S47 V50 K63 V71 T74 Q79 Y80 T81 L82 D83 R84 N95 T101 K106 E118 K122

V132 G135 L136 N137 H138 K149 L150 D156 V157 V163 L169 K172 K181 R185 L189 V197 V203 E206 L211 D219 A220 N221 H232 L238 K241 M246 D247 K248 A256

• Molecule 45: 60S ribosomal protein L8-A

Chain l8: 69% 21% • 9%

ALA PRO GLY LYS LYS VAL ALA PRO ALA PRO PHE GLY ALA LYS SER THR LYS SER ASN LYS THR ARG N24 P25 S29 A39 V40 Q41 L46 L65 R68 L69 K70 V71 T74 I75 A76 Q79 Y80 T81 L82 D83 R84 N85 L93 F94 N95 L109 T110 K111

A117 K120 S121 K122 Q123 D124 K128 V132 K133 L136 K147 A148 K149 I153 I160 V163 V164 L169 K183 A196 L200 T201 E202 V203 E208 A209 A210 L211 A212 K213 L214 A223 D224 K231 I237 L238 G239 N240 K245 K248 D254

SER ALA

• Molecule 46: 60S ribosomal protein L9-A

Chain L9: 81% 18% •

M1 K2 Q5 T6 E14 V18 S19 I20 K21 S22 L34 T35 K36 I41 V48 L52 L68 R69 T70 V71 K72 M78 V82 P98 G108 R115 I123 R124 E135 T138 N139 S147 V151 E152 N157 L161 Q162 Q163 I164

R173 D177 E189 D190 L191

• Molecule 46: 60S ribosomal protein L9-A

Chain l9: 77% 21% •

M1 Q5 T6 V16 T17 V18 S19 R31 G32 T33 N37 V43 T44 Q51 L52 V55 R62 L68 R69 T70 T80 G81 V82 G85 Y92 A109 K110 R115 L118 K121 K122 I123 R129 V132 T133 T138 E143 I144 V151

N157 Q162 Q163 R166 V167 R173 I179 L191

• Molecule 47: 60S ribosomal protein L10

Chain M0: 77% 18% • •

A2 R3 R21 R24 A25 V26 K30 I31 R32 I33 K39 T42 L48 L52 L57 E63 L87 M102 LEU SER CYS ALA GLY ALA ASP ARG LEU Q112 G117 A127 R128 V129 D130 Q133 V138 R139 K145 D146 Q163 K164 I165 I166

T174 N175 L176 D177 R178 P179 E180 K184 E189 V190 K191 K203 G204 S205 L206 E207 N208 A219 Q220 A221

• Molecule 47: 60S ribosomal protein L10

Chain m0: 73% 22% • •

A2 R3 R4 R24 A25 D28 L36 T42 V43 D44 L48 C49 V50 H51 L52 L57 E58 E63 C71 T77 T78 R82 D83 L87 R88 V91 I99 N100 K101 M102 L103 SER CYS ALA GLY ALA ASP ARG L111 V129 I135 R139 S143

N144 K145 R156 S168 K169 K170 L176 D177 L182 R185 D193 G194 V197 L200 S201 K202 K203 G204 S205 L206 E207 I210 R211 E212 A219 Q220 A221

• Molecule 48: 60S ribosomal protein L11-B

Chain M1: 72% 22%

SER THR LYS ALA Q6 N7 P8 M9 R10 D11 L12 K13 S26 G27 D28 S34 E38 Q39 L40 T44 P45 V46 Y52 E63 K64 I65 V71 E77 L80 E81 R82 R94 N95 I106 D107 E108 L112 G113 I114 K115 Y116 D117 V130 R137 R140

R141 K142 K145 S151 T155 D158 S161 Q165 K166 Y167 V171 L172 D173 K174

• Molecule 48: 60S ribosomal protein L11-B

Chain m1: 71% 24%

SER THR LYS ALA Q6 N7 P8 M9 R10 D11 L12 K13 K16 V23 L37 E38 Q39 T44 P45 V46 K49 R60 I65 E78 I79 L80 K87 R94 T99 I106 D107 E108 L112 G113 I114 K115 Y116 D117 I122 V129 V130 R137 V138 T139

R140 R141 K142 T147 H152 K153 T154 D158 T159 Y167 V171 K174

• Molecule 49: 60S ribosomal protein L13-A

Chain M3: 80% 15%

A2 H13 K23 R35 A47 L54 R55 P56 V57 V58 R59 T62 R67 K68 V69 R70 T76 V80 L85 E107 Q114 K122 I123 I124 N129 G130 K131 E136 A141 T144 I147 G163 E164 S165 R168 T169 L170 R171 K190

A191 E192 A193 E194 ALA GLU LYS LYS LYS

• Molecule 49: 60S ribosomal protein L13-A

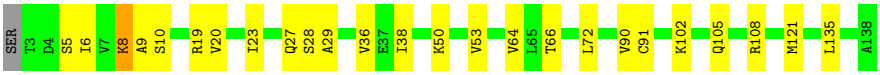
Chain m3: 75% 22%

A2 H13 R21 Q28 K31 R36 A44 K45 I46 A47 P50 L51 L54 R55 R59 A60 V63 R67 K68 V69 R73 T76 L85 I93 N103 R104 E107 I124 N129 G130 K131 E134 A135 S140 A141 Q149 P150 A151

T152 R157 N162 S165 R171 S175 E176 E184 A193 E194 A195 GLU LYS LYS LYS

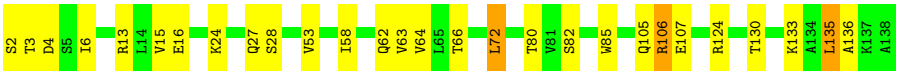
• Molecule 50: 60S ribosomal protein L14-A

Chain M4: 81% 18%



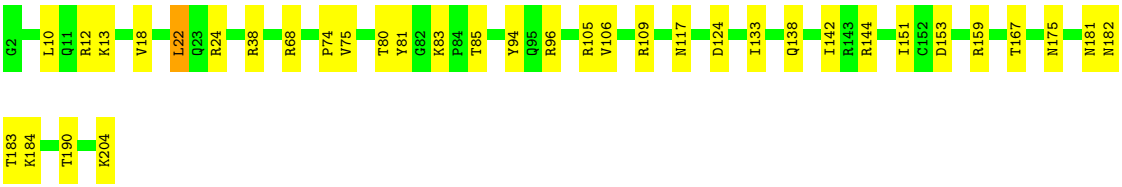
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



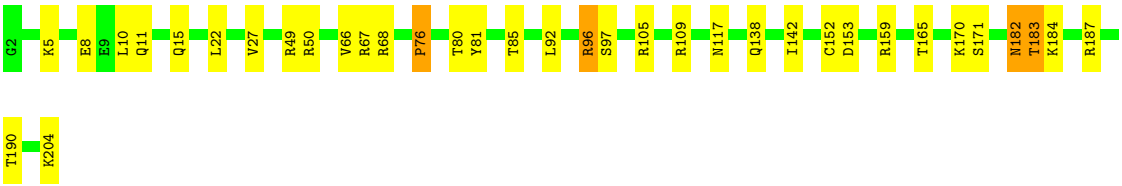
• Molecule 51: 60S ribosomal protein L15-A

Chain M5:



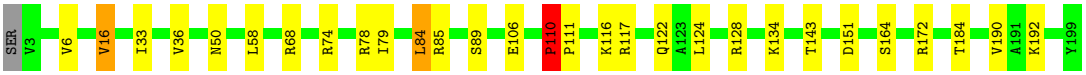
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



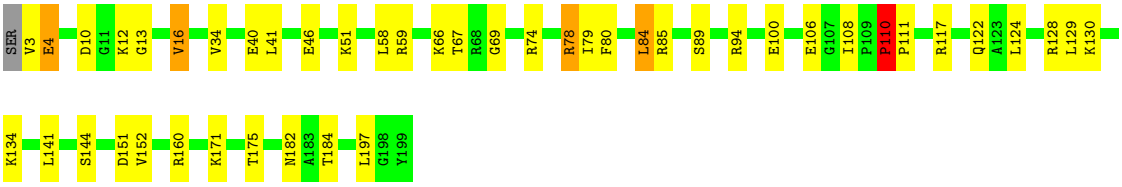
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



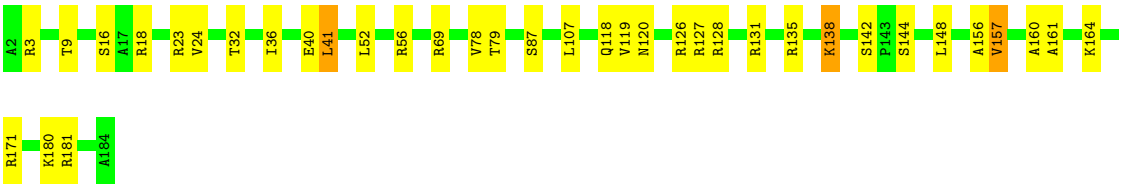
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



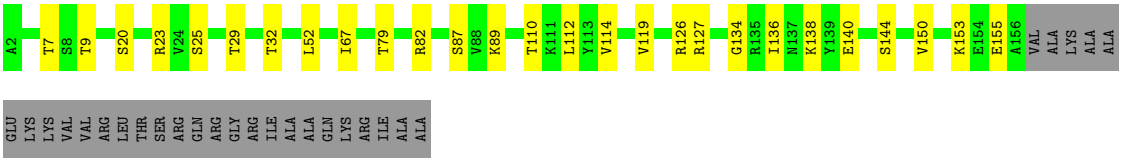
• Molecule 53: 60S ribosomal protein L17-A

Chain M7: 80% 19%



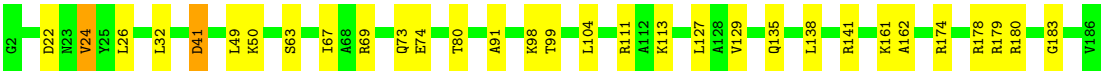
- Molecule 53: 60S ribosomal protein L17-A

Chain m7: 70% 15% 15%



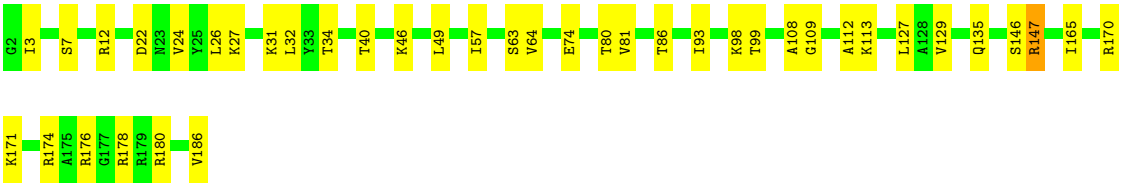
- Molecule 54: 60S ribosomal protein L18-A

Chain M8: 83% 16%



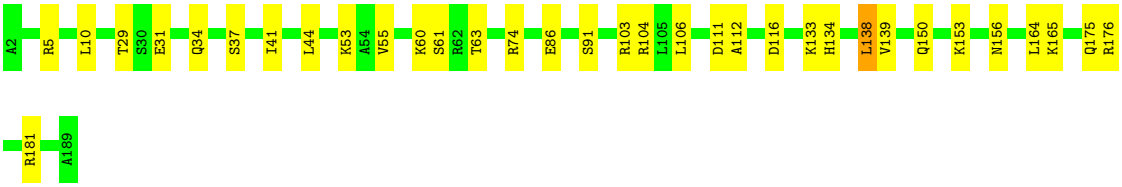
- Molecule 54: 60S ribosomal protein L18-A

Chain m8: 78% 21%



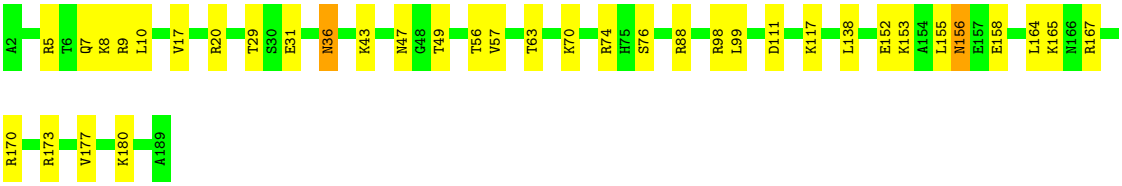
- Molecule 55: 60S ribosomal protein L19-A

Chain M9: 82% 18%



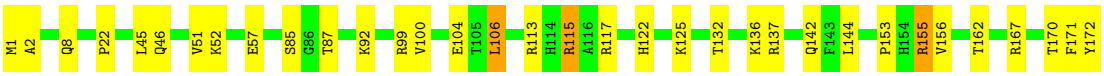
- Molecule 55: 60S ribosomal protein L19-A

Chain m9: 80% 19%



• Molecule 56: 60S ribosomal protein L20-A

Chain N0:

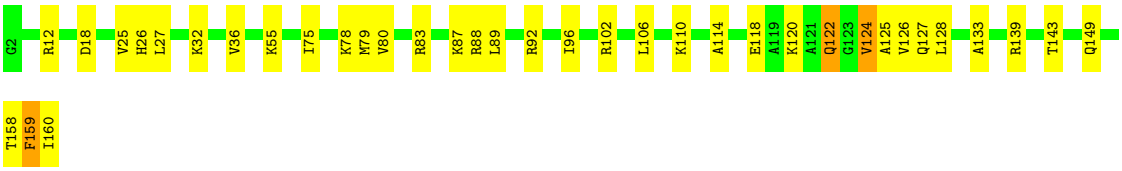


• Molecule 56: 60S ribosomal protein L20-A

Chain n0:

• Molecule 57: 60S ribosomal protein L21-A

Chain N1:

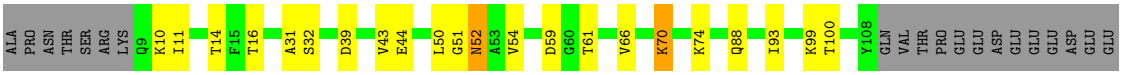


• Molecule 57: 60S ribosomal protein L21-A

Chain n1:

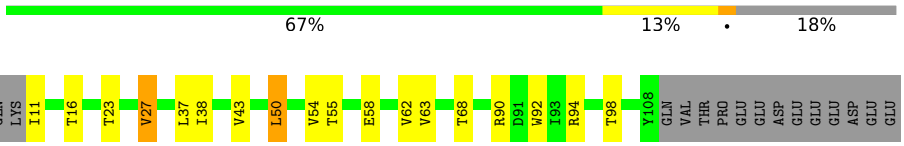
• Molecule 58: 60S ribosomal protein L22-A

Chain N2:



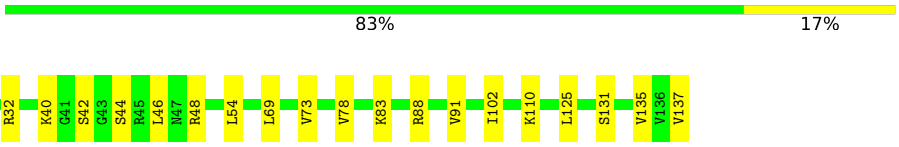
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



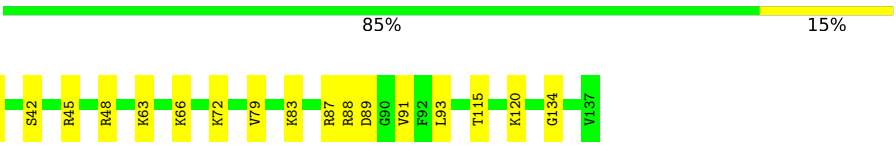
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



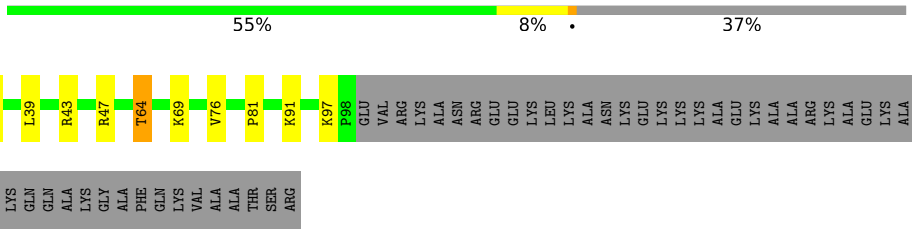
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



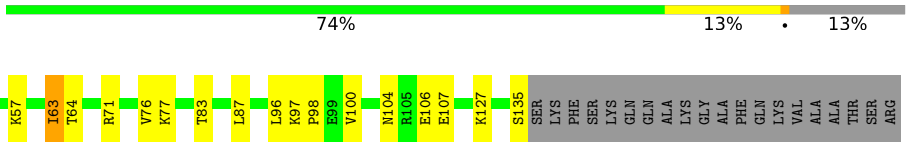
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



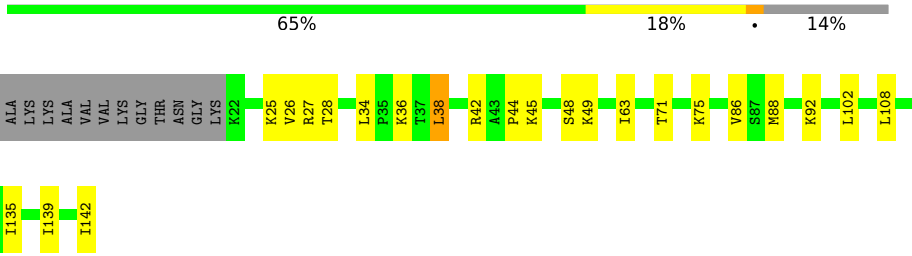
• Molecule 60: 60S ribosomal protein L24-A

Chain n4:



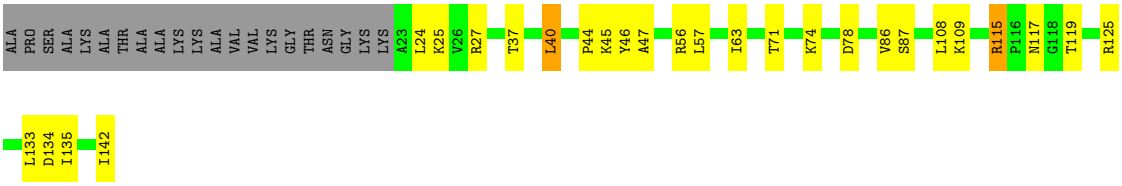
• Molecule 61: 60S ribosomal protein L25

Chain N5:



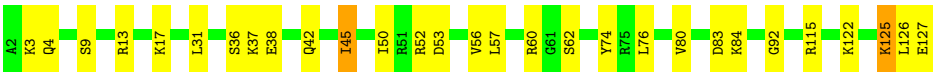
• Molecule 61: 60S ribosomal protein L25

Chain n5:



- Molecule 62: 60S ribosomal protein L26-A

Chain N6: 77% 21% •

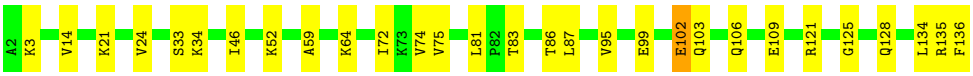


- Molecule 62: 60S ribosomal protein L26-A

Chain n6: 78% 21% •

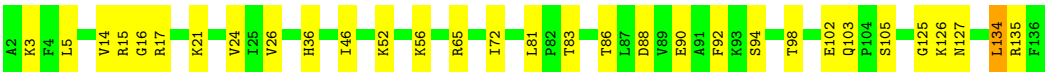
- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 79% 21% •



- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 77% 22% •

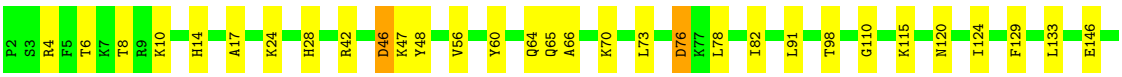


- Molecule 64: 60S ribosomal protein L28

Chain N8: 84% 14% •

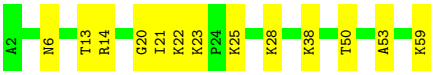
- Molecule 64: 60S ribosomal protein L28

Chain n8: 79% 20% •



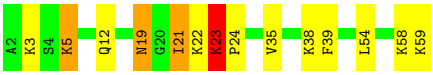
• Molecule 65: 60S ribosomal protein L29

Chain N9:



• Molecule 65: 60S ribosomal protein L29

Chain n9:



• Molecule 66: 60S ribosomal protein L30

Chain O0:

• Molecule 66: 60S ribosomal protein L30

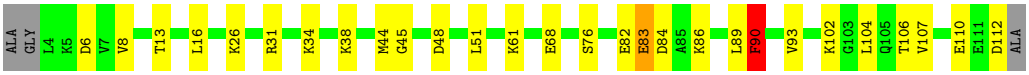
Chain o0:

• Molecule 67: 60S ribosomal protein L31-A

Chain O1:

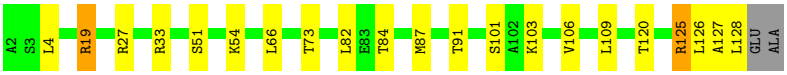
• Molecule 67: 60S ribosomal protein L31-A

Chain o1:



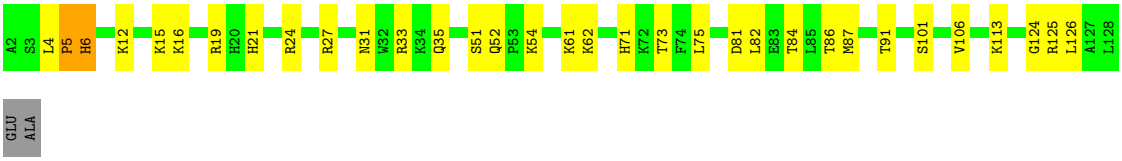
• Molecule 68: 60S ribosomal protein L32

Chain O2:



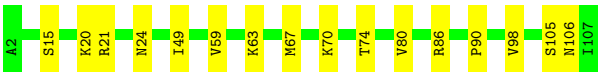
• Molecule 68: 60S ribosomal protein L32

Chain o2:



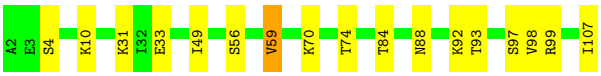
• Molecule 69: 60S ribosomal protein L33-A

Chain O3:



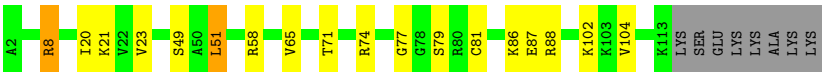
• Molecule 69: 60S ribosomal protein L33-A

Chain o3:



• Molecule 70: 60S ribosomal protein L34-A

Chain O4:

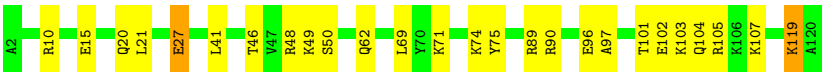


• Molecule 70: 60S ribosomal protein L34-A

Chain o4:

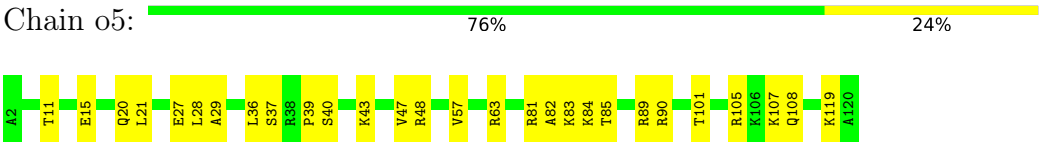
• Molecule 71: 60S ribosomal protein L35-A

Chain O5:



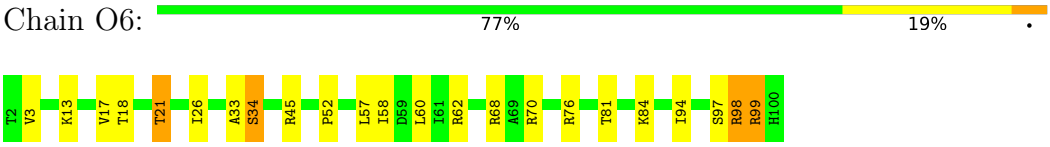
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



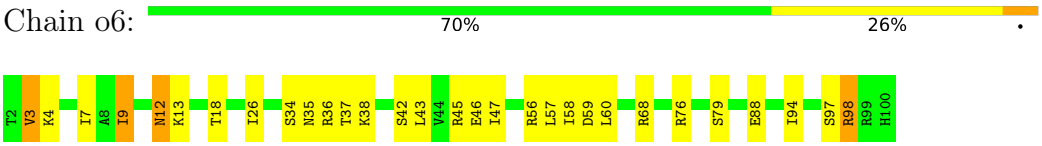
• Molecule 72: 60S ribosomal protein L36-A

Chain O6:



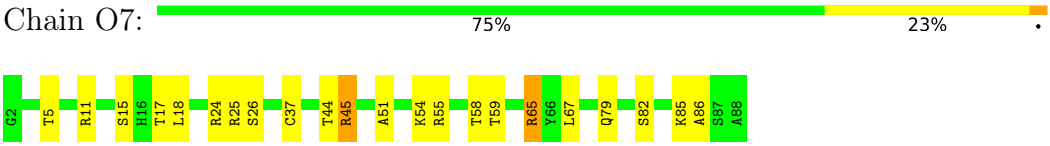
• Molecule 72: 60S ribosomal protein L36-A

Chain o6:



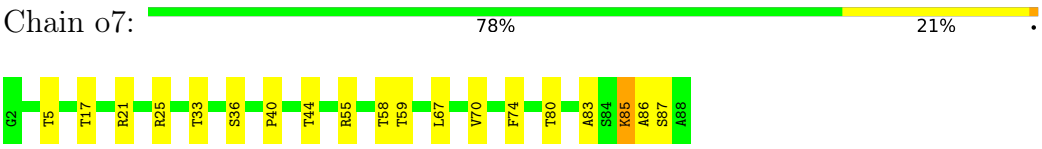
• Molecule 73: 60S ribosomal protein L37-A

Chain O7:



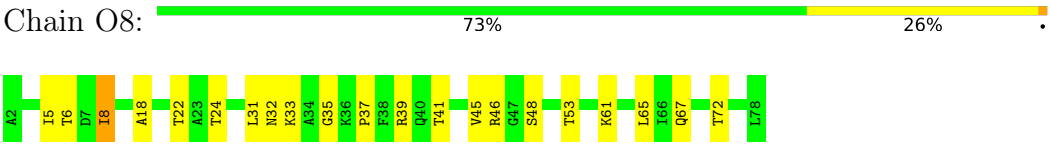
• Molecule 73: 60S ribosomal protein L37-A

Chain o7:



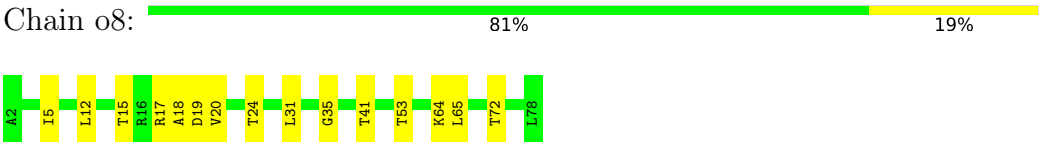
• Molecule 74: 60S ribosomal protein L38

Chain O8:



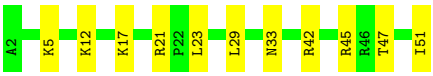
• Molecule 74: 60S ribosomal protein L38

Chain o8:



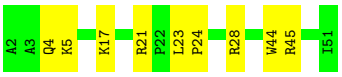
• Molecule 75: 60S ribosomal protein L39

Chain O9: 78% 22%



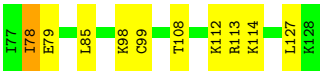
• Molecule 75: 60S ribosomal protein L39

Chain o9: 82% 18%



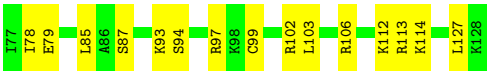
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0: 81% 17%



• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0: 71% 29%

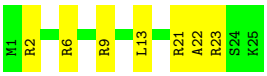


• Molecule 77: 60S ribosomal protein L41-A

Chain Q1: 56% 44%

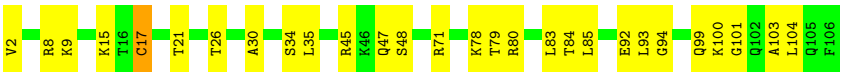
• Molecule 77: 60S ribosomal protein L41-A

Chain q1: 72% 28%



• Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 73% 26%



• Molecule 78: 60S ribosomal protein L42-A

Chain q2: 80% 19%

• Molecule 79: 60S ribosomal protein L43-A

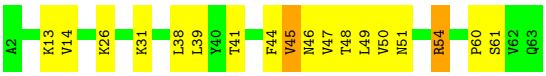
Chain Q3: 80% 19%

• Molecule 79: 60S ribosomal protein L43-A

Chain q3: 81% 19%

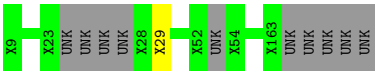
• Molecule 80: 40S ribosomal protein S30-A

Chain e0: 71% 26%



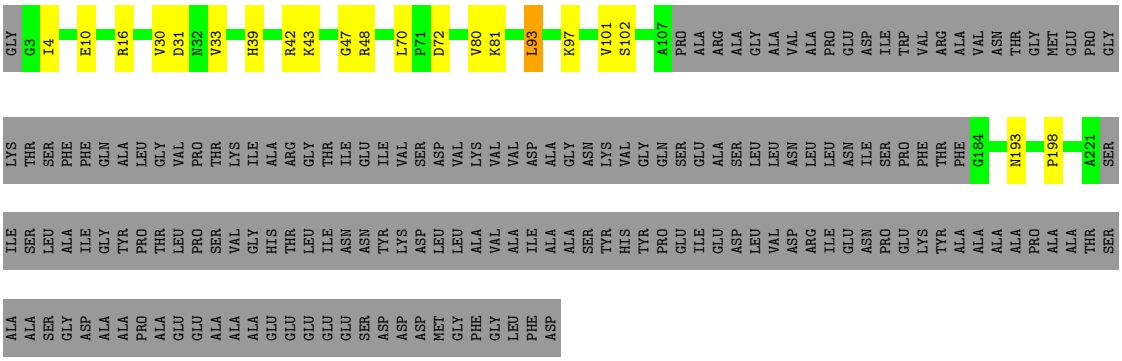
• Molecule 81: unknown protein chain m2

Chain m2: 93% 6%



• Molecule 82: 60S acidic ribosomal protein P0

Chain p0: 39% 6% 54%



• Molecule 83: unknown protein chain p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 84: unknown protein chain p2

Chain p2: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	436.92Å 288.52Å 305.75Å 90.00° 99.04° 90.00°	Depositor
Resolution (Å)	267.96 – 3.20	Depositor
% Data completeness (in resolution range)	100.0 (267.96-3.20)	Depositor
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.193 , 0.245	Depositor
Wilson B-factor (Å^2)	81.5	Xtriage
Anisotropy	0.087	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	411223	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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, MG, PCY, OHX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	2	0.79	6/41698 (0.0%)	1.36	368/64972 (0.6%)
1	6	0.95	31/42765 (0.1%)	1.47	608/66634 (0.9%)
2	S0	0.48	0/1617	0.69	0/2215
2	s0	0.53	0/1623	0.71	0/2222
3	S1	0.42	0/1735	0.70	1/2335 (0.0%)
3	s1	0.51	0/1748	0.70	1/2352 (0.0%)
4	S2	0.54	0/1665	0.69	0/2263
4	s2	0.64	0/1665	0.82	0/2263
5	S3	0.51	0/1759	0.71	1/2368 (0.0%)
5	s3	0.48	0/1759	0.63	0/2368
6	S4	0.51	0/2109	0.74	1/2839 (0.0%)
6	s4	0.60	0/2109	0.82	2/2839 (0.1%)
7	S5	0.43	0/1629	0.62	0/2202
7	s5	0.49	0/1629	0.67	0/2202
8	S6	0.49	0/1823	0.68	0/2439
8	s6	0.62	0/1779	0.74	0/2379
9	S7	0.46	0/1506	0.67	0/2028
9	s7	0.51	0/1516	0.71	2/2043 (0.1%)
10	S8	0.58	0/1514	0.77	1/2021 (0.0%)
10	s8	0.67	0/1514	0.80	1/2021 (0.0%)
11	S9	0.51	0/1519	0.68	0/2035
11	s9	0.62	0/1519	0.80	1/2035 (0.0%)
12	C0	0.45	0/790	0.65	1/1069 (0.1%)
12	c0	0.40	0/777	0.66	3/1049 (0.3%)
13	C1	0.64	0/1240	0.78	1/1675 (0.1%)
13	c1	0.70	1/1194 (0.1%)	0.81	0/1610
14	C2	0.38	0/900	0.61	0/1224
14	c2	0.29	0/900	0.58	1/1224 (0.1%)
15	C3	0.54	0/1215	0.71	1/1638 (0.1%)
15	c3	0.60	0/1215	0.74	0/1638
16	C4	0.46	0/901	0.69	0/1217
16	c4	0.55	0/960	0.77	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.48	0/998	0.69	0/1341
17	c5	0.51	0/1060	0.68	0/1426
18	C6	0.47	0/1125	0.71	2/1510 (0.1%)
18	c6	0.52	0/1131	0.73	0/1518
19	C7	0.46	0/935	0.67	0/1254
19	c7	0.53	0/914	0.73	0/1224
20	C8	0.48	0/1211	0.71	1/1628 (0.1%)
20	c8	0.52	0/1211	0.73	1/1628 (0.1%)
21	C9	0.47	0/1130	0.68	1/1517 (0.1%)
21	c9	0.56	0/1130	0.69	1/1517 (0.1%)
22	D0	0.48	0/865	0.68	0/1169
22	d0	0.53	0/892	0.68	0/1205
23	D1	0.51	0/693	0.67	0/935
23	d1	0.59	0/693	0.70	0/935
24	D2	0.53	0/1038	0.76	2/1395 (0.1%)
24	d2	0.66	0/1038	0.76	1/1395 (0.1%)
25	D3	0.65	0/1139	0.80	0/1518
25	d3	0.75	0/1139	0.87	1/1518 (0.1%)
26	D4	0.48	0/1087	0.67	0/1449
26	d4	0.59	0/1087	0.75	0/1449
27	D5	0.43	0/571	0.72	0/768
27	d5	0.49	0/566	0.75	0/761
28	D6	0.53	0/782	0.75	0/1047
28	d6	0.63	0/782	0.75	2/1047 (0.2%)
29	D7	0.47	0/620	0.71	0/838
29	d7	0.48	0/620	0.70	0/838
30	D8	0.40	0/499	0.64	0/670
30	d8	0.46	0/499	0.67	0/670
31	D9	0.55	0/452	0.80	1/600 (0.2%)
31	d9	0.57	0/452	0.68	0/600
32	E0	0.47	0/483	0.63	0/643
33	E1	0.47	0/577	0.76	0/770
33	e1	0.42	0/619	0.68	0/822
34	SR	0.44	0/2494	0.67	1/3393 (0.0%)
34	sR	0.42	0/2495	0.60	0/3395
35	SM	0.54	0/1113	0.76	2/1502 (0.1%)
35	sM	0.50	0/682	0.73	1/921 (0.1%)
36	1	1.21	245/75394 (0.3%)	1.71	2098/117545 (1.8%)
36	5	1.24	244/75414 (0.3%)	1.72	2161/117575 (1.8%)
37	3	1.00	5/2883 (0.2%)	1.48	35/4491 (0.8%)
37	7	1.20	3/2883 (0.1%)	1.74	84/4491 (1.9%)
38	4	1.17	3/3746 (0.1%)	1.66	91/5832 (1.6%)
38	8	1.05	3/3746 (0.1%)	1.57	70/5832 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	L2	0.77	0/1948	0.86	2/2617 (0.1%)
39	l2	0.76	0/1946	0.91	4/2614 (0.2%)
40	L3	0.78	2/3146 (0.1%)	0.84	1/4228 (0.0%)
40	l3	0.90	1/3146 (0.0%)	0.94	5/4228 (0.1%)
41	L4	0.86	2/2800 (0.1%)	0.95	6/3790 (0.2%)
41	l4	0.77	1/2800 (0.0%)	0.89	3/3790 (0.1%)
42	L5	0.62	1/2425 (0.0%)	0.72	1/3271 (0.0%)
42	l5	0.77	0/2408	0.83	2/3248 (0.1%)
43	L6	0.79	0/1260	0.86	0/1694
43	l6	0.81	0/1269	0.88	1/1705 (0.1%)
44	L7	0.81	0/1821	0.91	4/2451 (0.2%)
44	l7	0.88	0/1828	0.91	3/2461 (0.1%)
45	L8	0.59	0/1836	0.68	0/2481
45	l8	0.55	0/1795	0.72	1/2429 (0.0%)
46	L9	0.66	0/1539	0.75	0/2073
46	l9	0.84	0/1539	0.83	0/2073
47	M0	0.77	1/1741 (0.1%)	0.82	2/2335 (0.1%)
47	m0	0.81	0/1758	0.88	2/2358 (0.1%)
48	M1	0.52	0/1374	0.73	1/1842 (0.1%)
48	m1	0.68	0/1374	0.85	3/1842 (0.2%)
49	M3	0.79	0/1568	0.91	4/2106 (0.2%)
49	m3	0.70	0/1573	0.87	2/2113 (0.1%)
50	M4	0.80	0/1068	0.81	0/1438
50	m4	0.88	0/1074	0.90	2/1446 (0.1%)
51	M5	0.79	0/1757	0.87	2/2354 (0.1%)
51	m5	0.67	0/1757	0.83	3/2354 (0.1%)
52	M6	0.86	0/1585	0.94	4/2128 (0.2%)
52	m6	1.08	3/1585 (0.2%)	1.03	7/2128 (0.3%)
53	M7	0.82	0/1443	0.86	4/1944 (0.2%)
53	m7	0.94	0/1250	0.89	0/1683
54	M8	0.81	0/1465	0.93	2/1965 (0.1%)
54	m8	0.77	0/1465	0.90	0/1965
55	M9	0.58	0/1538	0.72	1/2050 (0.0%)
55	m9	0.65	0/1538	0.71	1/2050 (0.0%)
56	N0	0.77	0/1481	0.86	5/1990 (0.3%)
56	n0	0.94	0/1481	0.96	4/1990 (0.2%)
57	N1	0.87	0/1300	0.85	0/1743
57	n1	0.87	1/1300 (0.1%)	0.88	4/1743 (0.2%)
58	N2	0.46	0/812	0.63	0/1099
58	n2	0.53	0/794	0.70	0/1076
59	N3	0.73	0/1018	0.80	0/1369
59	n3	0.90	0/1018	0.94	3/1369 (0.2%)
60	N4	0.61	0/712	0.70	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	n4	0.76	0/1052	0.77	0/1398
61	N5	0.67	0/979	0.88	4/1321 (0.3%)
61	n5	0.69	0/974	0.82	1/1314 (0.1%)
62	N6	0.73	0/1004	0.87	0/1341
62	n6	0.68	0/1004	0.84	0/1341
63	N7	0.56	0/1118	0.70	0/1497
63	n7	0.53	0/1118	0.66	0/1497
64	N8	0.86	0/1204	0.97	1/1612 (0.1%)
64	n8	0.78	0/1204	0.91	1/1612 (0.1%)
65	N9	0.75	0/473	0.84	0/629
65	n9	0.80	0/473	1.02	1/629 (0.2%)
66	O0	0.52	0/751	0.70	0/1008
66	o0	0.50	0/775	0.67	1/1040 (0.1%)
67	O1	0.69	0/890	0.78	0/1196
67	o1	0.83	0/897	0.89	2/1205 (0.2%)
68	O2	0.87	0/1041	0.94	1/1394 (0.1%)
68	o2	0.83	0/1041	0.91	0/1394
69	O3	0.91	0/868	0.87	1/1168 (0.1%)
69	o3	0.93	0/868	0.98	1/1168 (0.1%)
70	O4	0.72	1/890 (0.1%)	0.90	3/1189 (0.3%)
70	o4	0.61	0/890	0.84	1/1189 (0.1%)
71	O5	0.74	0/978	0.82	0/1301
71	o5	0.63	0/974	0.72	0/1297
72	O6	0.67	0/778	0.78	0/1034
72	o6	0.59	0/777	0.73	0/1033
73	O7	0.84	0/696	1.08	6/923 (0.7%)
73	o7	0.74	0/696	0.81	0/923
74	O8	0.51	0/618	0.70	0/826
74	o8	0.49	0/614	0.67	0/822
75	O9	0.82	0/443	0.87	0/588
75	o9	0.68	0/443	0.81	0/588
76	Q0	0.67	0/423	0.79	0/562
76	q0	0.96	1/423 (0.2%)	0.97	3/562 (0.5%)
77	Q1	0.66	0/234	0.81	0/300
77	q1	0.77	0/234	0.91	0/300
78	Q2	0.88	1/860 (0.1%)	0.86	0/1136
78	q2	0.80	1/860 (0.1%)	0.77	0/1136
79	Q3	0.75	0/701	0.86	1/934 (0.1%)
79	q3	0.72	0/701	0.80	0/934
80	e0	0.59	0/499	0.77	0/665
82	p0	0.49	0/1091	0.67	0/1472
All	All	0.95	557/430072 (0.1%)	1.36	5668/631360 (0.9%)

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
9	s7	0	2
10	S8	0	2
16	C4	0	2
16	c4	0	1
17	c5	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	2
22	d0	0	1
25	d3	0	1
26	d4	0	1
27	D5	0	2
27	d5	0	1
28	D6	0	1
31	D9	0	1
34	SR	0	1
39	L2	0	1
39	l2	0	2
43	L6	0	1
44	l7	0	2
47	m0	0	1
51	m5	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
68	o2	0	2
73	o7	0	1
81	m2	0	1
All	All	0	46

All (557) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	13.06	2.04	1.82
36	5	1152	G	N9-C4	-11.97	1.28	1.38
78	q2	17	CYS	CB-SG	11.57	2.02	1.82
36	5	1152	G	N3-C4	-10.20	1.28	1.35
36	5	2971	A	N9-C4	9.62	1.43	1.37
36	1	3181	C	N3-C4	-9.18	1.27	1.33
36	1	2404	A	N3-C4	8.60	1.40	1.34
1	6	623	A	N9-C4	-8.40	1.32	1.37
36	1	2875	U	C2-N3	8.34	1.43	1.37
36	5	367	A	N9-C4	-8.19	1.32	1.37
36	1	1103	A	N3-C4	8.16	1.39	1.34
36	5	1143	A	N9-C4	-8.13	1.32	1.37
36	5	960	U	N1-C2	7.81	1.45	1.38
36	1	2946	A	N7-C5	-7.78	1.34	1.39
36	5	1152	G	C5-C6	-7.75	1.34	1.42
36	1	804	C	N1-C6	-7.71	1.32	1.37
36	5	917	A	N3-C4	-7.64	1.30	1.34
36	1	34	A	N9-C4	-7.61	1.33	1.37
1	6	46	A	N3-C4	-7.45	1.30	1.34
36	5	1307	G	C5-C4	-7.38	1.33	1.38
36	1	1116	G	N7-C5	-7.35	1.34	1.39
36	5	2943	G	N7-C5	-7.35	1.34	1.39
41	l4	94	CYS	CB-SG	-7.28	1.69	1.82
36	5	642	U	C2-N3	-7.27	1.32	1.37
36	5	2363	A	N7-C5	-7.26	1.34	1.39
36	5	2874	G	C5-C6	7.25	1.49	1.42
1	6	1537	C	C2-N3	7.24	1.41	1.35
36	5	1189	C	N1-C6	-7.24	1.32	1.37
36	1	2358	A	N3-C4	-7.23	1.30	1.34
36	1	1159	A	N3-C4	-7.22	1.30	1.34
1	6	1800	A	N9-C4	7.20	1.42	1.37
36	1	2617	U	N3-C4	-7.18	1.31	1.38
36	5	2954	U	N1-C2	7.17	1.45	1.38
36	1	1153	A	N7-C5	-7.14	1.34	1.39
1	6	1744	A	N9-C4	-7.14	1.33	1.37
36	5	2799	A	C6-N1	-7.14	1.30	1.35
36	5	3218	A	C5-C6	-7.13	1.34	1.41
36	5	2358	A	N9-C4	-7.12	1.33	1.37
1	6	163	G	N9-C4	-7.11	1.32	1.38
36	1	2326	A	N9-C4	-7.08	1.33	1.37
1	6	163	G	N3-C4	-7.07	1.30	1.35
36	5	3047	U	C2-N3	-7.02	1.32	1.37
36	5	2335	G	C5-C4	-6.97	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	1556	C	N1-C2	6.96	1.47	1.40
1	6	46	A	C6-N1	-6.96	1.30	1.35
36	5	40	A	N7-C5	-6.95	1.35	1.39
36	1	1153	A	N3-C4	-6.88	1.30	1.34
57	n1	104	GLU	CB-CG	6.88	1.65	1.52
36	5	1490	A	N7-C5	-6.87	1.35	1.39
52	m6	16	VAL	CB-CG2	-6.81	1.38	1.52
36	1	706	A	N9-C4	-6.75	1.33	1.37
1	2	992	A	N9-C4	-6.72	1.33	1.37
36	1	826	G	C5-C4	-6.70	1.33	1.38
36	1	1133	A	N9-C4	-6.70	1.33	1.37
36	1	1192	C	N1-C2	6.70	1.46	1.40
36	5	921	A	N7-C5	-6.70	1.35	1.39
36	1	49	A	N3-C4	-6.70	1.30	1.34
36	1	282	G	N7-C5	-6.67	1.35	1.39
36	5	3008	A	N9-C4	-6.64	1.33	1.37
36	1	913	A	N7-C5	-6.64	1.35	1.39
36	1	638	C	N1-C6	-6.63	1.33	1.37
36	5	420	G	C5-C4	-6.62	1.33	1.38
37	3	89	G	C5-C4	-6.62	1.33	1.38
36	5	2643	A	N9-C4	-6.61	1.33	1.37
36	1	1367	G	N7-C5	-6.58	1.35	1.39
36	1	3142	A	N3-C4	-6.58	1.30	1.34
36	1	2875	U	N1-C2	6.57	1.44	1.38
36	5	3006	A	N3-C4	-6.55	1.30	1.34
36	1	2276	G	N7-C5	-6.55	1.35	1.39
47	M0	127	ALA	CA-CB	-6.54	1.38	1.52
36	1	1150	A	N3-C4	-6.53	1.30	1.34
36	5	2610	G	N7-C5	-6.52	1.35	1.39
36	5	1200	A	N3-C4	-6.52	1.30	1.34
36	1	939	U	N1-C2	-6.51	1.32	1.38
36	1	1660	C	N1-C6	-6.48	1.33	1.37
36	1	1304	A	N9-C4	-6.47	1.33	1.37
36	1	928	C	N1-C6	-6.46	1.33	1.37
36	5	2996	U	N1-C2	6.46	1.44	1.38
36	5	1370	G	C6-N1	-6.46	1.35	1.39
36	1	287	G	N7-C5	-6.43	1.35	1.39
36	5	1338	C	N1-C6	-6.43	1.33	1.37
36	5	877	C	C4-N4	-6.41	1.28	1.33
36	5	953	G	C5-C4	-6.39	1.33	1.38
36	5	2626	A	N3-C4	-6.38	1.31	1.34
36	5	1112	A	N7-C5	-6.38	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	645	A	C6-N1	-6.37	1.31	1.35
36	1	638	C	N3-C4	-6.36	1.29	1.33
36	1	1158	A	N7-C5	-6.36	1.35	1.39
36	5	2913	C	N3-C4	-6.35	1.29	1.33
1	6	542	A	N7-C5	-6.33	1.35	1.39
36	1	2714	G	N9-C8	6.33	1.42	1.37
36	5	2659	G	N7-C5	-6.32	1.35	1.39
13	c1	128	CYS	CB-SG	-6.32	1.71	1.82
36	1	1850	A	N9-C4	-6.31	1.34	1.37
36	1	653	A	C6-N1	-6.30	1.31	1.35
38	4	15	G	C5-C4	-6.29	1.33	1.38
36	5	2141	U	N1-C2	-6.29	1.32	1.38
36	1	1429	G	N9-C8	-6.27	1.33	1.37
36	5	2404	A	N3-C4	6.27	1.38	1.34
36	1	345	G	N9-C8	-6.27	1.33	1.37
36	1	100	A	N3-C4	-6.26	1.31	1.34
36	5	2386	A	N7-C5	-6.25	1.35	1.39
36	1	1394	A	N9-C4	-6.25	1.34	1.37
36	1	656	A	C5-C4	-6.25	1.34	1.38
36	1	636	C	C4-C5	-6.24	1.38	1.43
36	5	981	U	N1-C2	6.24	1.44	1.38
36	5	2903	A	N9-C4	-6.23	1.34	1.37
40	L3	200	GLU	CG-CD	6.23	1.61	1.51
36	1	699	A	N9-C4	-6.22	1.34	1.37
36	5	869	G	C6-N1	-6.22	1.35	1.39
36	5	519	A	N7-C5	-6.21	1.35	1.39
36	5	872	U	N1-C6	-6.21	1.32	1.38
36	1	2305	G	N7-C5	-6.21	1.35	1.39
36	1	815	G	C6-N1	-6.20	1.35	1.39
36	5	367	A	N3-C4	-6.18	1.31	1.34
36	1	2419	A	N9-C4	-6.17	1.34	1.37
36	1	1793	C	N1-C6	-6.17	1.33	1.37
36	5	3141	A	N9-C8	-6.16	1.32	1.37
36	5	2134	G	C6-N1	-6.16	1.35	1.39
36	1	2616	C	N1-C6	-6.15	1.33	1.37
36	5	2639	G	N7-C5	-6.14	1.35	1.39
36	1	1308	A	N7-C5	-6.11	1.35	1.39
36	1	701	G	N3-C4	-6.11	1.31	1.35
36	1	920	A	N3-C4	-6.10	1.31	1.34
36	5	2954	U	C2-N3	6.10	1.42	1.37
36	1	504	A	N9-C4	-6.10	1.34	1.37
36	5	1143	A	N3-C4	-6.09	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	216	G	N7-C5	-6.08	1.35	1.39
70	O4	87	GLU	CG-CD	6.08	1.61	1.51
36	1	1153	A	C5-C4	-6.07	1.34	1.38
36	1	1153	A	C6-N1	-6.06	1.31	1.35
36	1	1399	A	N9-C4	-6.06	1.34	1.37
36	5	2703	A	N3-C4	-6.05	1.31	1.34
36	5	2954	U	C4-O4	6.05	1.28	1.23
36	1	1201	C	C2-N3	6.04	1.40	1.35
36	1	339	C	N3-C4	-6.03	1.29	1.33
36	1	409	A	C5-C4	-6.03	1.34	1.38
36	5	787	G	N7-C5	-6.03	1.35	1.39
36	5	2908	G	N3-C4	-6.02	1.31	1.35
36	1	1154	A	N7-C5	-6.02	1.35	1.39
36	1	1103	A	N7-C5	6.01	1.42	1.39
36	5	367	A	C5-C4	-6.01	1.34	1.38
36	1	1308	A	N3-C4	-6.01	1.31	1.34
36	1	2801	A	N3-C4	-6.00	1.31	1.34
36	1	2877	G	N3-C4	-5.99	1.31	1.35
36	5	2147	A	C5-C6	-5.99	1.35	1.41
36	1	2138	A	N9-C4	-5.98	1.34	1.37
36	1	1402	C	N3-C4	-5.98	1.29	1.33
36	5	923	C	N1-C6	-5.97	1.33	1.37
36	5	3218	A	N9-C4	-5.96	1.34	1.37
36	1	3130	A	N7-C5	-5.96	1.35	1.39
36	5	2279	A	N3-C4	-5.96	1.31	1.34
36	5	719	U	N1-C2	5.95	1.44	1.38
36	5	2335	G	N1-C2	-5.95	1.32	1.37
36	5	866	A	N9-C4	-5.95	1.34	1.37
36	1	3006	A	N9-C4	-5.94	1.34	1.37
36	1	2330	C	N1-C6	-5.93	1.33	1.37
36	5	1915	A	N9-C4	-5.93	1.34	1.37
36	1	699	A	N3-C4	-5.93	1.31	1.34
36	5	2911	A	N7-C5	-5.92	1.35	1.39
36	1	654	C	N1-C6	-5.92	1.33	1.37
36	1	659	G	C5-C4	-5.92	1.34	1.38
36	1	2647	A	N3-C4	-5.91	1.31	1.34
36	5	1332	A	C5-C4	-5.91	1.34	1.38
36	5	2726	C	N3-C4	-5.91	1.29	1.33
36	1	2621	G	N3-C4	-5.91	1.31	1.35
37	3	89	G	N9-C8	-5.91	1.33	1.37
36	5	859	G	N1-C2	-5.90	1.33	1.37
36	1	1606	U	N1-C2	-5.90	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2295	A	C5-C6	-5.90	1.35	1.41
36	5	1298	C	N3-C4	-5.89	1.29	1.33
36	1	34	A	N3-C4	-5.88	1.31	1.34
36	5	2627	C	N1-C6	-5.88	1.33	1.37
36	1	296	A	N9-C4	5.88	1.41	1.37
1	6	1765	A	N9-C4	-5.88	1.34	1.37
52	m6	80	PHE	CB-CG	-5.87	1.41	1.51
36	5	2392	C	C2-N3	-5.86	1.31	1.35
36	1	426	G	N1-C2	-5.86	1.33	1.37
36	5	649	A	N7-C5	-5.86	1.35	1.39
36	1	40	A	C8-N7	-5.83	1.27	1.31
36	5	2362	C	N3-C4	-5.83	1.29	1.33
36	1	980	A	C5-C4	5.83	1.42	1.38
36	5	1151	U	N1-C2	-5.83	1.33	1.38
36	5	2143	A	N9-C4	5.82	1.41	1.37
36	5	2910	A	N9-C4	-5.82	1.34	1.37
36	1	1143	A	N3-C4	-5.81	1.31	1.34
1	6	17	C	N3-C4	-5.81	1.29	1.33
36	5	576	C	N1-C6	-5.80	1.33	1.37
36	5	1177	G	N3-C4	-5.80	1.31	1.35
36	5	3209	A	C5-C4	5.80	1.42	1.38
36	5	2993	G	C5-C4	-5.79	1.34	1.38
36	1	1116	G	N9-C8	-5.79	1.33	1.37
36	1	3209	A	C5-C4	5.79	1.42	1.38
38	8	80	A	N9-C4	5.79	1.41	1.37
36	5	1902	G	N7-C5	-5.78	1.35	1.39
36	5	2341	A	C5-C4	-5.78	1.34	1.38
36	1	1143	A	N9-C4	-5.78	1.34	1.37
1	6	1655	A	C5-C4	-5.78	1.34	1.38
36	5	1178	G	N7-C5	-5.78	1.35	1.39
1	6	1773	C	C4-N4	5.78	1.39	1.33
36	1	925	A	N3-C4	-5.77	1.31	1.34
36	1	1395	G	C5-C4	-5.77	1.34	1.38
36	5	2819	A	N3-C4	-5.77	1.31	1.34
36	5	1148	G	N9-C8	-5.77	1.33	1.37
36	5	2941	A	N3-C4	-5.77	1.31	1.34
36	5	958	C	N1-C6	-5.76	1.33	1.37
36	1	2138	A	N3-C4	-5.75	1.31	1.34
1	6	437	A	N9-C4	-5.75	1.34	1.37
36	5	2147	A	C5-C4	-5.75	1.34	1.38
36	5	2943	G	C5-C6	-5.75	1.36	1.42
36	1	1137	C	N1-C6	-5.74	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	653	A	C5-C6	-5.73	1.35	1.41
36	1	2946	A	C5-C6	-5.73	1.35	1.41
36	5	3047	U	N3-C4	-5.73	1.33	1.38
36	1	2147	A	N9-C4	-5.73	1.34	1.37
36	5	609	G	N3-C4	-5.73	1.31	1.35
36	5	1304	A	N7-C5	-5.73	1.35	1.39
36	5	2286	U	C2-N3	-5.72	1.33	1.37
36	5	2934	A	C6-N1	-5.72	1.31	1.35
36	1	2326	A	N3-C4	-5.72	1.31	1.34
36	5	2364	G	N3-C4	-5.72	1.31	1.35
36	5	2703	A	N7-C5	-5.71	1.35	1.39
36	1	1452	A	N9-C4	-5.71	1.34	1.37
36	5	2954	U	N3-C4	5.70	1.43	1.38
36	5	2334	U	C4-O4	-5.70	1.19	1.23
36	1	627	U	N1-C2	-5.70	1.33	1.38
36	1	2357	A	N7-C5	-5.70	1.35	1.39
36	1	1406	A	C5-C6	-5.70	1.35	1.41
36	1	630	A	C6-N1	-5.69	1.31	1.35
36	5	1332	A	N7-C5	-5.69	1.35	1.39
36	1	707	U	N1-C2	-5.69	1.33	1.38
36	1	2971	A	N9-C4	5.68	1.41	1.37
36	5	2814	G	C5-C4	-5.68	1.34	1.38
36	5	3040	A	N7-C5	-5.67	1.35	1.39
36	5	2828	G	C6-N1	-5.66	1.35	1.39
40	L3	7	GLU	CG-CD	5.66	1.60	1.51
36	5	1149	G	N9-C8	-5.66	1.33	1.37
36	1	402	A	N3-C4	-5.65	1.31	1.34
36	1	884	A	N9-C4	-5.65	1.34	1.37
36	1	2714	G	N9-C4	-5.64	1.33	1.38
36	5	2354	C	N1-C6	-5.64	1.33	1.37
38	4	111	A	C5-C6	-5.64	1.35	1.41
36	1	716	A	C5-C6	-5.63	1.35	1.41
36	5	1103	A	N9-C4	5.63	1.41	1.37
1	6	1025	A	N3-C4	-5.62	1.31	1.34
36	5	423	A	N7-C5	-5.62	1.35	1.39
36	5	1332	A	N3-C4	-5.62	1.31	1.34
1	6	1537	C	N1-C6	5.61	1.40	1.37
36	5	631	U	C2-N3	-5.61	1.33	1.37
36	1	2401	A	C5-C4	5.60	1.42	1.38
36	1	3054	U	C4-O4	5.60	1.28	1.23
36	1	2355	G	N7-C5	-5.60	1.35	1.39
36	5	2617	U	N1-C2	-5.60	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	1025	A	N9-C4	-5.59	1.34	1.37
36	5	1178	G	C5-C6	-5.59	1.36	1.42
36	5	1874	A	N9-C4	-5.59	1.34	1.37
36	5	2291	A	N9-C4	-5.59	1.34	1.37
36	1	1103	A	N9-C4	5.59	1.41	1.37
36	1	646	A	N7-C5	-5.59	1.35	1.39
36	1	940	G	N9-C8	-5.59	1.33	1.37
36	5	34	A	N3-C4	-5.58	1.31	1.34
52	m6	40	GLU	CG-CD	5.58	1.60	1.51
36	1	1902	G	N7-C5	-5.58	1.35	1.39
36	1	2939	G	C5-C4	-5.58	1.34	1.38
1	6	1537	C	C5-C6	5.57	1.38	1.34
36	5	3305	A	N7-C5	-5.57	1.35	1.39
36	1	407	A	N7-C5	-5.57	1.35	1.39
36	5	848	A	N3-C4	-5.57	1.31	1.34
36	1	2733	A	C5-C6	-5.57	1.36	1.41
36	5	818	C	N1-C2	-5.57	1.34	1.40
36	1	1429	G	C8-N7	-5.57	1.27	1.30
36	5	49	A	N9-C4	-5.57	1.34	1.37
36	5	2913	C	N1-C2	-5.56	1.34	1.40
36	1	1394	A	N3-C4	-5.56	1.31	1.34
36	1	2368	A	C6-N1	-5.56	1.31	1.35
76	q0	99	CYS	CB-SG	-5.55	1.72	1.81
36	1	1489	A	C5-C6	-5.55	1.36	1.41
36	1	3319	U	N1-C2	5.55	1.43	1.38
36	5	953	G	N7-C5	-5.55	1.35	1.39
36	1	505	G	N3-C4	-5.54	1.31	1.35
1	6	321	C	N1-C2	5.54	1.45	1.40
36	5	861	C	N1-C6	-5.54	1.33	1.37
36	1	66	A	N9-C4	-5.54	1.34	1.37
36	5	2913	C	N1-C6	-5.54	1.33	1.37
36	5	650	C	N1-C6	-5.53	1.33	1.37
36	1	505	G	C6-N1	-5.53	1.35	1.39
36	5	1103	A	N3-C4	5.53	1.38	1.34
36	1	2368	A	N3-C4	-5.53	1.31	1.34
1	6	1756	A	N3-C4	5.52	1.38	1.34
36	1	3173	G	C8-N7	-5.52	1.27	1.30
36	1	2893	C	N3-C4	-5.51	1.30	1.33
36	5	2729	U	C2-N3	-5.51	1.33	1.37
36	1	984	G	N7-C5	-5.51	1.35	1.39
36	5	1189	C	N1-C2	-5.50	1.34	1.40
36	5	2280	A	N9-C4	-5.50	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2686	A	N3-C4	-5.50	1.31	1.34
36	5	420	G	N9-C8	-5.50	1.33	1.37
36	5	652	G	C5-C4	-5.50	1.34	1.38
36	1	1425	U	N3-C4	-5.50	1.33	1.38
36	1	3316	A	N9-C4	-5.50	1.34	1.37
36	5	2874	G	C6-O6	5.50	1.29	1.24
37	3	89	G	N7-C5	-5.49	1.35	1.39
36	5	1307	G	P-O5'	-5.49	1.54	1.59
1	6	1119	G	N7-C5	-5.49	1.35	1.39
36	1	2619	G	C5-C4	-5.49	1.34	1.38
36	1	1416	C	N3-C4	-5.48	1.30	1.33
36	1	2157	G	N7-C5	-5.48	1.35	1.39
36	5	1462	A	N9-C4	-5.48	1.34	1.37
36	1	2363	A	N9-C4	-5.48	1.34	1.37
36	1	2333	C	N3-C4	-5.48	1.30	1.33
36	5	2632	G	C6-N1	-5.47	1.35	1.39
36	1	2287	C	N1-C6	-5.47	1.33	1.37
36	5	2385	G	N9-C4	-5.47	1.33	1.38
36	5	2910	A	N3-C4	-5.47	1.31	1.34
37	3	88	G	C6-N1	-5.46	1.35	1.39
36	5	2892	A	N7-C5	-5.46	1.35	1.39
36	1	2426	U	C2-N3	-5.46	1.33	1.37
36	1	2379	U	N1-C2	-5.46	1.33	1.38
36	5	719	U	C2-O2	5.46	1.27	1.22
1	2	1730	A	N9-C4	-5.45	1.34	1.37
41	L4	199	TRP	CB-CG	-5.45	1.40	1.50
36	1	3005	A	N7-C5	-5.45	1.35	1.39
36	5	3335	A	C5-C6	-5.44	1.36	1.41
36	1	1902	G	C5-C6	-5.44	1.36	1.42
36	1	3209	A	C6-N1	5.44	1.39	1.35
36	5	1302	A	N3-C4	-5.43	1.31	1.34
36	5	417	A	C5-C4	-5.43	1.34	1.38
36	1	923	C	N1-C6	-5.43	1.33	1.37
36	5	824	C	N3-C4	-5.43	1.30	1.33
36	1	3008	A	N9-C4	-5.43	1.34	1.37
36	5	924	G	C2-N3	-5.43	1.28	1.32
36	5	2874	G	C5-C4	5.43	1.42	1.38
36	5	49	A	N3-C4	-5.43	1.31	1.34
36	1	656	A	N7-C5	-5.42	1.35	1.39
36	1	2187	G	N7-C5	-5.42	1.35	1.39
36	1	672	A	C5-C6	-5.42	1.36	1.41
38	4	111	A	N7-C5	-5.41	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2286	U	N3-C4	-5.41	1.33	1.38
36	1	1103	A	C6-N1	5.41	1.39	1.35
36	5	872	U	N1-C2	-5.41	1.33	1.38
36	5	1452	A	C5-C6	-5.40	1.36	1.41
40	l3	251	CYS	CB-SG	-5.40	1.73	1.81
36	1	1369	A	N7-C5	-5.39	1.36	1.39
36	5	1321	G	N9-C8	-5.39	1.34	1.37
36	1	2702	A	N7-C5	-5.39	1.36	1.39
36	5	426	G	C5-C4	-5.39	1.34	1.38
36	5	88	A	N9-C4	-5.38	1.34	1.37
36	1	636	C	N1-C6	-5.38	1.33	1.37
36	1	2409	G	C5-C4	-5.38	1.34	1.38
36	1	2615	G	C5-C6	-5.38	1.36	1.42
36	5	2610	G	C5-C4	-5.38	1.34	1.38
36	5	2941	A	N7-C5	-5.37	1.36	1.39
36	1	1415	U	C2-N3	-5.37	1.33	1.37
36	1	48	A	N7-C5	-5.36	1.36	1.39
36	1	343	U	N1-C6	-5.36	1.33	1.38
36	5	2137	U	N1-C6	-5.36	1.33	1.38
36	5	397	A	N3-C4	-5.36	1.31	1.34
36	1	1447	G	N3-C4	-5.36	1.31	1.35
36	1	2404	A	N7-C5	5.36	1.42	1.39
36	1	2180	G	N7-C5	-5.35	1.36	1.39
1	2	632	U	C2-N3	-5.35	1.34	1.37
36	5	2637	A	C5-C6	-5.34	1.36	1.41
36	5	824	C	N1-C6	-5.34	1.33	1.37
36	5	2303	A	N7-C5	-5.34	1.36	1.39
36	1	2657	A	N7-C5	-5.34	1.36	1.39
36	5	836	A	N9-C4	-5.34	1.34	1.37
36	5	657	A	N9-C4	-5.34	1.34	1.37
36	5	2627	C	N3-C4	-5.34	1.30	1.33
36	1	1332	A	N7-C5	-5.33	1.36	1.39
36	5	877	C	C4-C5	-5.33	1.38	1.43
36	1	1392	G	C5-C4	-5.33	1.34	1.38
36	1	504	A	N3-C4	-5.33	1.31	1.34
36	1	1367	G	C5-C4	-5.33	1.34	1.38
36	5	1145	G	N3-C4	-5.33	1.31	1.35
36	5	2650	U	C4-O4	-5.32	1.19	1.23
36	1	1140	G	N1-C2	-5.32	1.33	1.37
36	5	2318	U	C2-N3	-5.32	1.34	1.37
36	5	1159	A	N9-C4	-5.31	1.34	1.37
1	6	1124	A	N9-C4	-5.31	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2743	A	N9-C8	-5.31	1.33	1.37
36	5	657	A	C5-C6	-5.31	1.36	1.41
36	1	1133	A	N7-C5	-5.30	1.36	1.39
36	1	1406	A	N7-C5	-5.30	1.36	1.39
42	L5	62	CYS	CB-SG	-5.30	1.73	1.81
36	1	211	A	C6-N6	-5.30	1.29	1.33
36	5	2958	A	N9-C4	-5.29	1.34	1.37
36	5	2851	A	N3-C4	-5.29	1.31	1.34
41	L4	46	LYS	CE-NZ	5.29	1.62	1.49
36	1	61	A	N3-C4	-5.29	1.31	1.34
36	5	1133	A	N9-C4	-5.29	1.34	1.37
36	5	2138	A	N7-C5	-5.29	1.36	1.39
36	5	3316	A	N9-C4	-5.29	1.34	1.37
36	5	1133	A	N3-C4	-5.29	1.31	1.34
36	1	343	U	C2-N3	-5.28	1.34	1.37
36	1	1382	G	C5-C4	-5.28	1.34	1.38
36	5	890	C	N1-C6	-5.28	1.33	1.37
36	5	2329	C	N1-C6	-5.28	1.33	1.37
37	7	76	A	N9-C4	-5.28	1.34	1.37
1	6	119	A	N9-C4	-5.28	1.34	1.37
36	1	1313	G	N7-C5	-5.28	1.36	1.39
36	1	716	A	N9-C4	-5.27	1.34	1.37
36	1	29	C	N1-C6	-5.27	1.33	1.37
36	1	1099	A	N7-C5	-5.27	1.36	1.39
36	1	1377	G	N1-C2	-5.27	1.33	1.37
36	1	2404	A	C6-N1	5.27	1.39	1.35
36	5	1429	G	N9-C4	-5.27	1.33	1.38
36	1	915	A	N3-C4	-5.27	1.31	1.34
36	1	915	A	C6-N1	-5.27	1.31	1.35
36	5	2892	A	N3-C4	-5.27	1.31	1.34
36	5	1307	G	N9-C8	-5.26	1.34	1.37
36	1	2762	A	N3-C4	-5.26	1.31	1.34
36	5	922	U	N1-C2	5.26	1.43	1.38
36	5	1888	U	N1-C6	-5.26	1.33	1.38
36	5	2649	A	N7-C5	-5.26	1.36	1.39
36	1	189	G	C6-N1	-5.25	1.35	1.39
36	5	2640	A	N9-C4	-5.25	1.34	1.37
36	1	2692	A	N7-C5	-5.25	1.36	1.39
36	5	417	A	N3-C4	-5.25	1.31	1.34
1	2	119	A	N9-C4	-5.25	1.34	1.37
36	5	2138	A	N9-C4	-5.25	1.34	1.37
36	1	980	A	N9-C4	5.24	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2920	U	C2-N3	-5.24	1.34	1.37
1	6	65	A	N9-C4	-5.24	1.34	1.37
36	5	1851	G	N7-C5	-5.24	1.36	1.39
36	1	64	G	C6-N1	-5.23	1.35	1.39
36	5	2625	C	N1-C6	-5.23	1.34	1.37
36	1	92	G	C6-N1	-5.23	1.35	1.39
36	1	1099	A	C5-C6	-5.23	1.36	1.41
36	5	818	C	N3-C4	-5.23	1.30	1.33
37	7	103	A	C5-C6	-5.23	1.36	1.41
36	1	952	A	N7-C5	-5.23	1.36	1.39
36	5	2138	A	N3-C4	-5.22	1.31	1.34
36	5	2983	C	N1-C6	-5.22	1.34	1.37
37	7	89	G	N9-C8	-5.22	1.34	1.37
36	5	2333	C	N1-C6	-5.22	1.34	1.37
36	1	668	G	N7-C5	-5.21	1.36	1.39
36	1	2874	G	C5-C4	5.21	1.42	1.38
1	6	426	G	C6-N1	-5.21	1.35	1.39
1	6	538	A	N9-C4	5.20	1.41	1.37
36	1	1377	G	N3-C4	-5.20	1.31	1.35
36	1	2645	G	N9-C8	-5.20	1.34	1.37
36	5	2644	C	N1-C6	-5.20	1.34	1.37
36	1	865	U	C2-N3	-5.20	1.34	1.37
36	5	2873	U	C4-C5	5.20	1.48	1.43
36	5	980	A	N7-C5	5.19	1.42	1.39
36	1	1114	U	C2-N3	-5.19	1.34	1.37
36	1	2726	C	N3-C4	-5.19	1.30	1.33
36	1	2203	U	N1-C2	-5.19	1.33	1.38
36	1	1392	G	N7-C5	-5.18	1.36	1.39
36	1	3273	A	N3-C4	-5.18	1.31	1.34
36	5	1370	G	N1-C2	-5.18	1.33	1.37
36	5	1148	G	N7-C5	-5.18	1.36	1.39
36	1	2621	G	C5-C4	-5.18	1.34	1.38
37	3	66	A	N9-C4	-5.18	1.34	1.37
1	6	317	C	N1-C6	-5.18	1.34	1.37
36	1	2968	G	N3-C4	-5.18	1.31	1.35
36	5	3138	U	N1-C2	-5.18	1.33	1.38
36	1	653	A	N7-C5	-5.17	1.36	1.39
36	5	2980	U	C2-O2	-5.17	1.17	1.22
36	5	1177	G	C6-N1	-5.17	1.35	1.39
36	1	1377	G	N9-C4	-5.17	1.33	1.38
36	1	934	G	N7-C5	-5.17	1.36	1.39
36	1	2609	A	C6-N1	-5.17	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	65	A	N9-C4	-5.17	1.34	1.37
36	5	3017	A	N7-C5	-5.17	1.36	1.39
36	1	1153	A	C5-C6	-5.17	1.36	1.41
36	5	2982	A	N3-C4	-5.17	1.31	1.34
36	1	40	A	N7-C5	-5.16	1.36	1.39
36	1	1667	A	N3-C4	-5.16	1.31	1.34
36	5	609	G	C2-N3	-5.16	1.28	1.32
36	5	386	A	C6-N1	5.16	1.39	1.35
36	5	2305	G	N7-C5	-5.16	1.36	1.39
1	6	65	A	C5-C6	-5.16	1.36	1.41
36	1	1428	A	C5-C6	-5.15	1.36	1.41
36	1	2364	G	C5-C4	-5.15	1.34	1.38
36	1	317	A	N7-C5	-5.15	1.36	1.39
36	1	1156	C	N3-C4	-5.15	1.30	1.33
36	5	2858	U	C2-N3	-5.14	1.34	1.37
36	5	2937	G	C5-C4	-5.14	1.34	1.38
36	1	884	A	N7-C5	-5.14	1.36	1.39
36	1	423	A	N7-C5	-5.13	1.36	1.39
36	1	2368	A	N9-C4	-5.13	1.34	1.37
36	1	1330	A	N7-C5	-5.13	1.36	1.39
36	5	2279	A	N9-C4	-5.13	1.34	1.37
36	5	1870	C	N1-C6	-5.13	1.34	1.37
36	1	2760	C	N1-C6	-5.13	1.34	1.37
36	5	1309	U	N1-C2	-5.13	1.33	1.38
36	5	2139	A	N9-C4	-5.13	1.34	1.37
36	5	407	A	N7-C5	-5.12	1.36	1.39
1	2	377	G	N9-C4	-5.12	1.33	1.38
36	1	921	A	N7-C5	-5.12	1.36	1.39
36	1	2396	G	N7-C5	-5.12	1.36	1.39
36	5	1174	G	N3-C4	-5.11	1.31	1.35
36	5	2272	G	C6-N1	-5.11	1.35	1.39
36	1	1401	A	N7-C5	-5.11	1.36	1.39
38	8	106	C	N1-C6	-5.11	1.34	1.37
36	5	716	A	C5-C6	-5.11	1.36	1.41
36	1	1468	A	N9-C4	-5.10	1.34	1.37
36	5	1173	U	N1-C2	-5.10	1.33	1.38
36	5	1854	C	N3-C4	-5.10	1.30	1.33
36	5	2704	A	N9-C4	-5.10	1.34	1.37
36	5	1592	G	C6-O6	5.10	1.28	1.24
36	1	2797	C	N1-C6	-5.10	1.34	1.37
36	5	2647	A	N9-C4	-5.10	1.34	1.37
36	5	2993	G	C5-C6	-5.10	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2875	U	N1-C6	5.09	1.42	1.38
36	1	1164	G	N7-C5	-5.09	1.36	1.39
36	5	3275	U	N1-C2	5.09	1.43	1.38
36	1	1434	G	N9-C8	-5.09	1.34	1.37
36	1	1481	A	N7-C5	-5.08	1.36	1.39
36	5	2885	C	N1-C6	-5.08	1.34	1.37
36	5	2814	G	N7-C5	-5.08	1.36	1.39
36	1	402	A	C5-C4	-5.08	1.35	1.38
1	6	616	G	N7-C5	-5.08	1.36	1.39
36	1	958	C	N3-C4	-5.08	1.30	1.33
36	5	2903	A	N3-C4	-5.08	1.31	1.34
36	1	116	A	N7-C5	5.08	1.42	1.39
1	6	351	C	N1-C6	-5.08	1.34	1.37
36	5	642	U	N1-C2	-5.08	1.33	1.38
36	1	2605	G	C5-C4	-5.07	1.34	1.38
36	5	980	A	N9-C4	5.07	1.40	1.37
36	1	2363	A	N3-C4	-5.07	1.31	1.34
36	1	55	G	C5-C4	-5.07	1.34	1.38
36	1	1364	C	N1-C6	-5.07	1.34	1.37
38	8	41	A	N3-C4	-5.06	1.31	1.34
36	1	2598	G	C5-C4	-5.06	1.34	1.38
36	1	821	U	C2-N3	-5.06	1.34	1.37
36	1	1159	A	C6-N1	-5.06	1.32	1.35
36	1	1667	A	N9-C4	-5.05	1.34	1.37
36	5	3366	G	N7-C5	-5.05	1.36	1.39
36	5	2887	A	N3-C4	-5.05	1.31	1.34
36	5	2897	A	C5-C4	-5.05	1.35	1.38
36	5	34	A	C5-C4	-5.05	1.35	1.38
36	5	2326	A	N3-C4	-5.04	1.31	1.34
36	5	3245	A	C5-C6	-5.04	1.36	1.41
36	1	608	A	N7-C5	-5.04	1.36	1.39
36	1	2875	U	C2-O2	5.03	1.26	1.22
36	1	74	G	N7-C5	-5.03	1.36	1.39
36	1	1371	G	N9-C8	-5.03	1.34	1.37
36	5	2811	A	C6-N1	-5.03	1.32	1.35
36	5	820	A	N7-C5	-5.03	1.36	1.39
36	1	2167	A	N7-C5	-5.02	1.36	1.39
36	1	887	G	N9-C8	-5.02	1.34	1.37
36	1	2605	G	N9-C4	-5.02	1.33	1.38
36	5	1849	C	N1-C6	-5.02	1.34	1.37
36	1	1184	A	C6-N1	-5.02	1.32	1.35
36	1	2640	A	N3-C4	-5.01	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	973	A	N7-C5	-5.01	1.36	1.39
36	5	657	A	C5-C4	-5.01	1.35	1.38
36	5	1855	U	C2-N3	-5.01	1.34	1.37
36	1	2616	C	C4-C5	-5.01	1.39	1.43
1	2	1205	C	N1-C6	-5.01	1.34	1.37
36	5	3081	C	N3-C4	-5.01	1.30	1.33
36	5	1207	G	C5-C4	-5.01	1.34	1.38
36	5	1451	C	N1-C6	-5.01	1.34	1.37
36	5	2317	A	N3-C4	-5.00	1.31	1.34
36	5	3121	U	N1-C2	-5.00	1.34	1.38

All (5668) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	C2-N3-C4	-24.18	99.81	111.90
36	5	1152	G	N3-C4-C5	20.67	138.94	128.60
36	5	1152	G	N3-C4-N9	-18.57	114.86	126.00
36	1	1902	G	N1-C6-O6	17.91	130.65	119.90
36	5	2893	C	N3-C4-C5	-17.30	114.98	121.90
1	6	1773	C	N3-C4-C5	-17.02	115.09	121.90
36	1	1902	G	C5-C6-O6	-15.94	119.04	128.60
36	5	1152	G	C5-N7-C8	-15.76	96.42	104.30
36	5	922	U	N3-C2-O2	-15.47	111.37	122.20
1	6	163	G	N3-C4-N9	-15.03	116.98	126.00
36	5	960	U	N1-C2-O2	15.01	133.31	122.80
36	1	2617	U	C5-C4-O4	14.87	134.82	125.90
1	6	1537	C	C6-N1-C2	-14.38	114.55	120.30
36	5	38	U	O5'-P-OP2	-14.33	92.80	105.70
36	5	3005	A	O5'-P-OP2	-14.10	93.01	105.70
36	5	877	C	N3-C4-C5	14.02	127.51	121.90
36	5	3218	A	N1-C6-N6	14.00	127.00	118.60
36	1	2714	G	N3-C4-C5	13.84	135.52	128.60
36	5	1006	A	O5'-P-OP2	-13.76	93.32	105.70
36	5	3245	A	C5-N7-C8	-13.44	97.18	103.90
36	5	1152	G	N1-C6-O6	13.36	127.92	119.90
36	1	2945	G	O5'-P-OP2	-13.34	93.70	105.70
36	1	608	A	N1-C6-N6	13.28	126.57	118.60
36	1	2714	G	N3-C4-N9	-13.19	118.09	126.00
36	1	1902	G	C4-C5-N7	13.14	116.06	110.80
36	5	3245	A	N7-C8-N9	13.10	120.35	113.80
36	1	1365	G	C8-N9-C4	-12.95	101.22	106.40
36	5	1902	G	N1-C6-O6	12.93	127.66	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	211	A	O5'-P-OP1	-12.83	94.15	105.70
36	1	645	A	N1-C6-N6	-12.80	110.92	118.60
36	1	1902	G	C6-C5-N7	-12.70	122.78	130.40
36	1	1308	A	C8-N9-C4	-12.63	100.75	105.80
36	5	1305	U	O5'-P-OP1	-12.53	94.43	105.70
36	5	1116	G	O5'-P-OP1	-12.51	94.45	105.70
1	2	553	G	N1-C6-O6	12.46	127.38	119.90
36	1	670	C	N3-C4-C5	-12.32	116.97	121.90
36	1	86	G	O5'-P-OP2	-12.16	94.76	105.70
36	1	716	A	N1-C6-N6	12.10	125.86	118.60
36	1	369	A	C8-N9-C4	-12.06	100.98	105.80
36	5	2899	C	C6-N1-C2	-12.04	115.48	120.30
36	5	960	U	N3-C2-O2	-11.93	113.85	122.20
36	5	994	G	O5'-P-OP2	-11.90	94.99	105.70
36	5	2893	C	C6-N1-C2	-11.88	115.55	120.30
36	5	398	A	O5'-P-OP2	-11.86	95.03	105.70
36	1	406	G	O4'-C1'-N9	11.85	117.68	108.20
36	5	1152	G	C4-C5-N7	11.83	115.53	110.80
36	5	2818	U	O5'-P-OP1	-11.80	95.08	105.70
36	5	1178	G	C6-C5-N7	-11.77	123.34	130.40
36	5	874	U	O5'-P-OP1	-11.69	95.17	105.70
36	1	2996	U	C2-N1-C1'	11.61	131.63	117.70
36	5	2372	A	C8-N9-C4	-11.53	101.19	105.80
36	1	3306	U	N3-C4-O4	-11.53	111.33	119.40
36	1	2884	C	N3-C4-C5	11.51	126.50	121.90
36	5	3245	A	C8-N9-C4	-11.40	101.24	105.80
36	1	1367	G	N1-C6-O6	11.30	126.68	119.90
36	1	2871	G	O5'-P-OP2	-11.29	95.54	105.70
36	5	957	C	C6-N1-C2	-11.29	115.78	120.30
36	1	672	A	N1-C6-N6	11.21	125.33	118.60
36	5	2283	G	N1-C6-O6	11.20	126.62	119.90
1	2	623	A	O5'-P-OP1	-11.19	95.63	105.70
36	5	1847	A	O5'-P-OP2	-11.18	95.63	105.70
36	1	2618	G	N1-C6-O6	-11.13	113.22	119.90
36	5	2176	U	N3-C2-O2	-11.12	114.41	122.20
36	5	2874	G	C5-C6-O6	11.09	135.25	128.60
36	5	2345	A	N1-C6-N6	11.08	125.25	118.60
36	1	1433	A	O5'-P-OP1	-11.06	95.75	105.70
36	1	652	G	O5'-P-OP2	-11.04	95.76	105.70
36	5	642	U	O5'-P-OP2	-11.04	95.76	105.70
36	5	222	A	O5'-P-OP2	-11.04	95.77	105.70
1	6	1537	C	N3-C4-C5	-11.02	117.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3245	A	C2-N3-C4	-11.00	105.10	110.60
36	1	2946	A	N1-C6-N6	10.95	125.17	118.60
36	1	2870	C	C2-N1-C1'	-10.94	106.77	118.80
36	1	1192	C	N1-C2-O2	10.93	125.45	118.90
36	1	636	C	C5-C4-N4	-10.91	112.56	120.20
36	1	2617	U	N1-C2-N3	10.86	121.42	114.90
36	5	2283	G	C5-C6-O6	-10.85	122.09	128.60
1	2	1200	G	N1-C6-O6	10.83	126.40	119.90
1	6	901	G	C4-C5-N7	10.83	115.13	110.80
36	5	3006	A	N1-C2-N3	10.82	134.71	129.30
36	5	2726	C	C5-C4-N4	10.82	127.77	120.20
36	1	1099	A	N1-C6-N6	10.82	125.09	118.60
36	5	1452	A	N1-C6-N6	10.81	125.09	118.60
37	7	101	G	N1-C6-O6	10.81	126.39	119.90
36	1	718	G	C4-C5-N7	10.79	115.12	110.80
1	6	901	G	N1-C6-O6	10.76	126.36	119.90
36	1	1437	C	C6-N1-C2	-10.74	116.00	120.30
36	5	2726	C	C6-N1-C2	-10.72	116.01	120.30
36	1	1132	C	O5'-P-OP1	-10.70	96.07	105.70
36	5	719	U	N1-C2-O2	10.69	130.28	122.80
36	1	2355	G	N1-C6-O6	10.68	126.31	119.90
36	5	776	U	C5-C6-N1	-10.68	117.36	122.70
36	5	1592	G	C8-N9-C4	-10.67	102.13	106.40
36	1	282	G	C8-N9-C4	-10.62	102.15	106.40
36	1	716	A	N9-C4-C5	-10.60	101.56	105.80
36	5	1902	G	C5-C6-O6	-10.51	122.29	128.60
36	1	2400	G	C4-C5-N7	10.49	114.99	110.80
36	1	920	A	N1-C2-N3	10.42	134.51	129.30
36	1	939	U	N1-C2-O2	-10.42	115.50	122.80
36	5	784	A	N1-C6-N6	10.42	124.85	118.60
36	1	2808	A	N1-C6-N6	10.38	124.83	118.60
36	5	2816	G	C8-N9-C4	10.38	110.55	106.40
36	5	1152	G	N1-C2-N3	10.37	130.12	123.90
36	1	3306	U	C5-C4-O4	10.35	132.11	125.90
36	1	960	U	C2-N1-C1'	-10.35	105.28	117.70
36	1	645	A	C6-N1-C2	-10.33	112.40	118.60
36	1	2408	U	O5'-P-OP1	-10.29	96.44	105.70
36	1	636	C	N3-C4-C5	10.29	126.02	121.90
36	5	2954	U	C2-N1-C1'	10.29	130.05	117.70
36	5	776	U	N1-C2-N3	10.28	121.07	114.90
36	1	2827	U	C5-C4-O4	10.28	132.07	125.90
1	2	639	U	N3-C2-O2	-10.22	115.05	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	776	U	C4-C5-C6	10.18	125.81	119.70
36	1	3181	C	C5-C4-N4	10.15	127.31	120.20
1	6	1773	C	C4-C5-C6	10.11	122.45	117.40
36	5	3197	G	N3-C2-N2	-10.11	112.83	119.90
37	7	49	G	N1-C6-O6	10.07	125.94	119.90
36	1	2283	G	N1-C6-O6	10.07	125.94	119.90
1	2	1039	A	O4'-C1'-N9	10.04	116.23	108.20
1	6	163	G	N9-C4-C5	10.04	109.42	105.40
1	6	338	C	C6-N1-C2	-10.04	116.29	120.30
36	5	2385	G	N3-C4-C5	10.03	133.61	128.60
1	6	1773	C	N3-C4-N4	10.02	125.01	118.00
36	5	56	G	N1-C6-O6	-10.00	113.90	119.90
36	5	3197	G	N3-C4-N9	-9.99	120.00	126.00
36	1	340	C	N3-C4-C5	9.99	125.90	121.90
1	6	1000	C	N3-C2-O2	-9.98	114.91	121.90
1	6	338	C	C5-C6-N1	9.98	125.99	121.00
36	5	1392	G	C8-N9-C4	9.97	110.39	106.40
36	1	2996	U	C6-N1-C1'	-9.97	107.24	121.20
1	6	163	G	N3-C4-C5	9.97	133.59	128.60
36	1	2777	G	N1-C6-O6	-9.94	113.93	119.90
36	5	1302	A	C8-N9-C4	-9.94	101.83	105.80
36	1	585	A	O5'-P-OP2	-9.94	96.76	105.70
36	5	2928	C	C6-N1-C2	-9.94	116.33	120.30
36	5	3218	A	C4-C5-N7	9.93	115.67	110.70
36	5	1178	G	C4-C5-N7	9.92	114.77	110.80
36	1	3181	C	N3-C4-N4	-9.92	111.06	118.00
1	6	1473	U	N3-C2-O2	-9.91	115.26	122.20
36	5	820	A	C8-N9-C4	-9.90	101.84	105.80
36	5	2403	G	O5'-P-OP2	-9.88	96.81	105.70
36	1	895	A	O5'-P-OP1	-9.86	96.83	105.70
36	5	2335	G	C5-C6-N1	9.84	116.42	111.50
36	5	800	G	N3-C2-N2	-9.82	113.03	119.90
1	6	337	G	C6-C5-N7	-9.76	124.54	130.40
40	l3	4	ARG	NE-CZ-NH1	9.76	125.18	120.30
36	1	3013	U	O5'-P-OP2	-9.76	96.92	105.70
36	5	2726	C	N3-C2-O2	-9.72	115.10	121.90
36	5	922	U	N1-C2-O2	9.71	129.60	122.80
36	5	965	A	O5'-P-OP2	-9.70	96.97	105.70
36	1	2726	C	N3-C2-O2	-9.69	115.11	121.90
36	5	1308	A	OP1-P-OP2	-9.68	105.08	119.60
1	2	1773	C	C6-N1-C2	-9.67	116.43	120.30
36	1	718	G	C6-C5-N7	-9.66	124.60	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3306	U	N3-C2-O2	-9.66	115.44	122.20
36	5	927	C	N1-C2-O2	-9.66	113.11	118.90
36	5	2700	G	C5-C6-O6	-9.64	122.82	128.60
36	1	949	C	C6-N1-C2	-9.63	116.45	120.30
36	5	957	C	N3-C2-O2	-9.62	115.17	121.90
36	1	1495	U	N1-C2-N3	9.62	120.67	114.90
36	1	776	U	C4-C5-C6	9.60	125.46	119.70
36	5	1834	U	N3-C4-C5	-9.59	108.84	114.60
36	5	2943	G	C6-C5-N7	-9.59	124.65	130.40
36	1	1495	U	C5-C6-N1	-9.56	117.92	122.70
36	5	2886	U	N3-C2-O2	-9.56	115.50	122.20
36	5	86	G	O5'-P-OP2	-9.56	97.09	105.70
36	1	1838	G	N1-C6-O6	9.56	125.64	119.90
36	5	3245	A	C4-C5-N7	9.54	115.47	110.70
1	6	1000	C	C2-N1-C1'	9.53	129.28	118.80
36	5	1447	G	O5'-P-OP1	-9.53	97.13	105.70
1	6	647	G	N3-C4-N9	-9.52	120.28	126.00
36	1	1115	G	C8-N9-C4	-9.52	102.59	106.40
1	2	992	A	C2-N3-C4	-9.50	105.85	110.60
37	7	101	G	C6-C5-N7	-9.49	124.70	130.40
36	1	350	C	C6-N1-C2	-9.49	116.50	120.30
36	1	646	A	C8-N9-C4	-9.48	102.01	105.80
36	1	917	A	O5'-P-OP2	-9.48	97.17	105.70
36	1	2818	U	O5'-P-OP1	-9.47	97.18	105.70
36	1	1365	G	N3-C4-C5	-9.47	123.87	128.60
36	1	670	C	C6-N1-C2	-9.46	116.52	120.30
36	1	653	A	O5'-P-OP2	-9.45	97.20	105.70
1	6	901	G	C5-C6-O6	-9.44	122.94	128.60
1	2	830	U	N3-C2-O2	-9.43	115.60	122.20
36	1	645	A	N9-C4-C5	9.43	109.57	105.80
36	1	2831	G	N1-C6-O6	9.43	125.56	119.90
1	6	1700	C	N1-C2-O2	9.43	124.56	118.90
36	5	1143	A	C2-N3-C4	-9.42	105.89	110.60
36	5	1604	G	N3-C4-N9	9.41	131.65	126.00
36	5	648	C	O5'-P-OP1	-9.41	97.23	105.70
36	1	1308	A	N7-C8-N9	9.41	118.50	113.80
36	1	3278	C	N1-C2-O2	9.41	124.54	118.90
36	5	2943	G	C4-C5-N7	9.40	114.56	110.80
36	5	776	U	N3-C2-O2	-9.40	115.62	122.20
36	5	3204	C	C6-N1-C2	9.40	124.06	120.30
36	5	712	G	O5'-P-OP2	-9.39	97.25	105.70
36	5	3305	A	N1-C6-N6	9.39	124.23	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2945	G	O5'-P-OP2	-9.36	97.27	105.70
36	5	2619	G	C5-C6-O6	-9.36	122.99	128.60
36	1	406	G	O5'-P-OP2	-9.32	97.31	105.70
36	5	2334	U	O5'-P-OP2	-9.29	97.34	105.70
73	O7	65	ARG	NE-CZ-NH1	9.28	124.94	120.30
37	7	45	A	O5'-P-OP2	-9.26	97.37	105.70
36	1	3005	A	C8-N9-C4	-9.25	102.10	105.80
36	5	1112	A	C4-C5-C6	9.25	121.63	117.00
36	1	937	G	O5'-P-OP2	-9.24	97.39	105.70
36	5	3218	A	N9-C4-C5	-9.24	102.11	105.80
36	5	877	C	C5-C4-N4	-9.23	113.74	120.20
36	5	1851	G	N1-C6-O6	9.23	125.44	119.90
36	1	718	G	C5-N7-C8	-9.22	99.69	104.30
36	1	1364	C	N3-C4-C5	9.22	125.59	121.90
36	5	873	C	C6-N1-C2	-9.22	116.61	120.30
36	1	1428	A	N1-C6-N6	9.21	124.13	118.60
38	4	14	C	O5'-P-OP2	-9.21	97.41	105.70
36	5	1390	A	N1-C6-N6	-9.21	113.07	118.60
36	1	104	G	C5-C6-O6	-9.20	123.08	128.60
36	1	339	C	N3-C4-N4	-9.19	111.56	118.00
36	5	1302	A	N9-C4-C5	9.19	109.48	105.80
1	2	794	U	N1-C2-O2	9.19	129.23	122.80
36	5	2799	A	N1-C6-N6	-9.18	113.09	118.60
36	5	780	A	O5'-P-OP1	-9.18	97.44	105.70
36	5	2395	G	O5'-P-OP2	-9.18	97.44	105.70
36	1	1385	C	N1-C2-O2	-9.16	113.41	118.90
36	5	1879	A	C5-N7-C8	-9.16	99.32	103.90
36	5	2763	U	C5-C4-O4	-9.13	120.42	125.90
36	5	1143	A	N1-C2-N3	9.12	133.86	129.30
36	1	2756	C	C6-N1-C2	-9.10	116.66	120.30
1	6	314	C	C6-N1-C2	-9.10	116.66	120.30
1	2	1773	C	N3-C4-C5	-9.09	118.27	121.90
36	5	3245	A	C6-C5-N7	-9.09	125.94	132.30
37	7	101	G	C5-C6-O6	-9.08	123.15	128.60
38	8	12	A	N1-C6-N6	9.08	124.05	118.60
36	5	283	G	C4-C5-N7	9.07	114.43	110.80
1	6	901	G	C6-C5-N7	-9.06	124.96	130.40
36	5	1440	G	C4-C5-N7	-9.06	107.18	110.80
36	5	2808	A	N1-C6-N6	9.05	124.03	118.60
1	2	448	C	C6-N1-C2	-9.04	116.68	120.30
36	1	645	A	N1-C2-N3	9.04	133.82	129.30
36	5	3093	C	C6-N1-C2	9.03	123.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1302	A	O5'-P-OP1	-9.03	97.58	105.70
36	1	984	G	N3-C2-N2	9.03	126.22	119.90
36	5	1152	G	N7-C8-N9	9.02	117.61	113.10
36	1	197	G	C5-C6-O6	-9.02	123.19	128.60
36	5	1452	A	C5-C6-N6	-9.01	116.49	123.70
36	5	2272	G	O4'-C1'-N9	9.01	115.41	108.20
38	8	12	A	C5-C6-N6	-9.01	116.50	123.70
36	1	3181	C	N3-C2-O2	-9.00	115.60	121.90
36	1	1343	A	N1-C6-N6	8.99	124.00	118.60
36	5	1473	G	C8-N9-C4	8.99	110.00	106.40
36	1	2636	A	C8-N9-C4	-8.99	102.20	105.80
1	2	1745	G	N3-C4-N9	8.98	131.39	126.00
1	6	1700	C	C2-N1-C1'	8.97	128.67	118.80
36	1	344	A	O5'-P-OP1	-8.96	97.63	105.70
36	1	2621	G	N3-C2-N2	-8.96	113.63	119.90
3	S1	218	LEU	CA-CB-CG	8.96	135.91	115.30
38	4	113	U	C5-C6-N1	-8.96	118.22	122.70
36	1	1416	C	N3-C4-N4	-8.95	111.73	118.00
36	5	1110	U	N1-C2-O2	8.94	129.06	122.80
36	5	2821	C	N1-C2-O2	-8.94	113.53	118.90
36	1	421	G	C8-N9-C4	8.94	109.97	106.40
36	5	2928	C	C2-N1-C1'	8.94	128.63	118.80
36	5	2351	U	N1-C2-N3	8.93	120.26	114.90
36	5	1115	G	C4-N9-C1'	8.93	138.10	126.50
36	5	1481	A	C8-N9-C4	-8.92	102.23	105.80
36	1	397	A	N1-C6-N6	-8.91	113.26	118.60
36	1	2252	A	C8-N9-C4	-8.91	102.24	105.80
1	2	1212	G	N1-C6-O6	8.90	125.24	119.90
36	5	429	U	O5'-P-OP2	-8.90	97.69	105.70
1	2	553	G	C5-C6-O6	-8.90	123.26	128.60
36	1	1367	G	C5-C6-O6	-8.87	123.28	128.60
36	5	2980	U	N1-C2-N3	8.87	120.22	114.90
36	5	2400	G	C8-N9-C4	8.87	109.95	106.40
36	1	611	A	O5'-P-OP2	-8.85	97.73	105.70
36	5	2398	A	N1-C2-N3	8.85	133.72	129.30
36	1	421	G	N9-C4-C5	-8.84	101.86	105.40
36	5	2572	C	N1-C2-O2	8.84	124.20	118.90
36	5	1181	U	C5-C6-N1	-8.84	118.28	122.70
36	1	2870	C	N3-C4-C5	8.82	125.43	121.90
36	5	2632	G	O5'-P-OP1	-8.82	97.76	105.70
36	5	2908	G	N9-C4-C5	8.80	108.92	105.40
36	5	1902	G	C6-C5-N7	-8.80	125.12	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1604	G	C8-N9-C1'	-8.80	115.57	127.00
36	5	2310	U	O5'-P-OP2	-8.79	97.79	105.70
36	1	2247	G	N1-C6-O6	8.78	125.17	119.90
1	6	610	G	C8-N9-C1'	-8.78	115.59	127.00
36	5	1152	G	N3-C2-N2	-8.77	113.76	119.90
36	5	2983	C	C4-C5-C6	8.77	121.78	117.40
1	2	453	U	C2-N1-C1'	8.76	128.21	117.70
36	5	2887	A	O5'-P-OP1	-8.76	97.81	105.70
36	5	3144	G	C8-N9-C4	-8.76	102.89	106.40
36	1	2601	A	C8-N9-C4	8.76	109.30	105.80
38	8	96	A	C8-N9-C4	8.76	109.30	105.80
36	5	2908	G	C8-N9-C4	-8.75	102.90	106.40
1	6	1	U	O4'-C1'-N1	8.75	115.20	108.20
36	5	2343	C	O5'-P-OP2	-8.72	97.85	105.70
36	1	439	C	C2-N1-C1'	8.71	128.38	118.80
36	5	682	U	C2-N1-C1'	-8.71	107.25	117.70
1	2	554	C	N1-C2-O2	8.71	124.12	118.90
36	5	2971	A	C2-N3-C4	8.70	114.95	110.60
36	5	2983	C	O5'-P-OP1	-8.70	97.87	105.70
11	s9	3	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	6	1129	U	C5-C4-O4	8.69	131.11	125.90
1	6	272	U	P-O3'-C3'	8.69	130.12	119.70
36	5	2400	G	C5-C6-O6	-8.68	123.39	128.60
36	1	2945	G	O5'-P-OP1	8.67	121.11	110.70
36	5	2345	A	C5-C6-N6	-8.67	116.76	123.70
36	5	3178	A	O5'-P-OP1	-8.67	97.89	105.70
36	1	2124	G	N1-C6-O6	8.67	125.10	119.90
36	5	705	A	O5'-P-OP2	-8.67	97.90	105.70
1	6	1629	G	O5'-P-OP2	-8.66	97.91	105.70
36	5	2945	G	O5'-P-OP1	8.66	121.09	110.70
36	5	1307	G	P-O3'-C3'	8.65	130.08	119.70
36	5	3154	C	C6-N1-C2	-8.65	116.84	120.30
36	1	1365	G	N7-C8-N9	8.65	117.42	113.10
36	1	2846	U	N3-C2-O2	-8.64	116.15	122.20
36	5	3218	A	C5-C6-N6	-8.64	116.79	123.70
38	8	80	A	C8-N9-C4	-8.64	102.34	105.80
1	2	577	G	C4-C5-N7	8.63	114.25	110.80
37	3	88	G	N1-C6-O6	-8.63	114.72	119.90
36	1	2968	G	C2-N3-C4	-8.62	107.59	111.90
1	6	390	G	O5'-P-OP2	-8.62	97.95	105.70
36	5	1042	U	N3-C4-C5	8.61	119.77	114.60
36	1	1849	C	N1-C2-O2	-8.61	113.73	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2359	C	N1-C2-O2	-8.60	113.74	118.90
36	5	2145	A	C6-N1-C2	-8.60	113.44	118.60
36	5	2186	U	N3-C2-O2	-8.59	116.19	122.20
36	5	881	C	N1-C2-O2	8.59	124.05	118.90
36	1	1216	C	C6-N1-C2	-8.58	116.87	120.30
36	1	339	C	C5-C4-N4	8.58	126.20	120.20
36	5	1152	G	C6-C5-N7	-8.57	125.26	130.40
36	5	966	U	N3-C2-O2	-8.57	116.20	122.20
36	1	3045	G	O5'-P-OP2	-8.56	97.99	105.70
1	2	1082	C	C6-N1-C2	-8.56	116.88	120.30
36	5	716	A	N1-C6-N6	8.56	123.73	118.60
36	5	2245	C	C6-N1-C2	-8.55	116.88	120.30
36	5	2820	A	N7-C8-N9	8.55	118.08	113.80
1	2	794	U	N3-C2-O2	-8.55	116.21	122.20
36	1	2400	G	C5-N7-C8	-8.55	100.03	104.30
36	5	2372	A	N7-C8-N9	8.55	118.08	113.80
36	1	3143	C	N3-C2-O2	8.55	127.88	121.90
36	1	969	C	N1-C2-O2	-8.55	113.77	118.90
36	5	2726	C	N3-C4-N4	-8.54	112.02	118.00
36	1	1158	A	C5-C6-N6	-8.54	116.87	123.70
36	1	2624	G	N1-C6-O6	8.54	125.02	119.90
36	5	1914	G	O5'-P-OP1	-8.54	98.02	105.70
36	1	1216	C	C5-C6-N1	8.53	125.26	121.00
36	1	984	G	N3-C4-C5	-8.52	124.34	128.60
38	4	24	G	C5-C6-O6	-8.51	123.50	128.60
36	1	54	C	N3-C4-C5	8.51	125.30	121.90
36	1	608	A	C6-C5-N7	-8.51	126.35	132.30
36	5	2996	U	N1-C2-O2	8.50	128.75	122.80
1	2	137	U	N3-C2-O2	-8.50	116.25	122.20
36	1	1829	G	C8-N9-C4	-8.50	103.00	106.40
36	1	1848	G	O5'-P-OP1	-8.50	98.05	105.70
36	1	2148	U	N3-C2-O2	8.50	128.15	122.20
36	5	426	G	C8-N9-C4	8.50	109.80	106.40
36	1	1447	G	N1-C6-O6	-8.50	114.80	119.90
36	1	2124	G	C5-C6-O6	-8.50	123.50	128.60
36	5	1834	U	C6-N1-C2	-8.50	115.90	121.00
36	5	3154	C	N1-C2-O2	8.50	124.00	118.90
36	1	2868	U	N1-C2-O2	8.49	128.74	122.80
36	1	940	G	O5'-P-OP1	-8.49	98.06	105.70
36	1	1481	A	C6-C5-N7	-8.48	126.36	132.30
36	1	1489	A	N1-C6-N6	8.48	123.69	118.60
1	6	610	G	C4-N9-C1'	8.48	137.53	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1370	G	N3-C4-N9	8.48	131.09	126.00
36	1	908	G	C5-C6-O6	-8.48	123.51	128.60
36	1	2714	G	C2-N3-C4	-8.48	107.66	111.90
36	5	3049	A	C8-N9-C4	8.48	109.19	105.80
36	1	1158	A	N1-C6-N6	8.46	123.68	118.60
36	1	3143	C	N1-C2-O2	-8.46	113.82	118.90
36	5	984	G	N3-C4-C5	-8.46	124.37	128.60
36	1	716	A	C4-C5-N7	8.46	114.93	110.70
36	5	2764	C	N3-C4-C5	8.45	125.28	121.90
36	1	2995	A	C8-N9-C4	8.45	109.18	105.80
1	6	144	U	N3-C2-O2	-8.45	116.29	122.20
36	1	2572	C	C2-N1-C1'	8.43	128.07	118.80
36	5	3218	A	C6-C5-N7	-8.43	126.40	132.30
36	1	2243	A	O5'-P-OP2	-8.42	98.12	105.70
36	5	2873	U	C4-C5-C6	8.41	124.75	119.70
36	1	1429	G	N3-C4-C5	-8.41	124.40	128.60
36	1	3362	A	N7-C8-N9	8.41	118.00	113.80
36	5	2893	C	N3-C4-N4	8.41	123.89	118.00
36	5	2385	G	O5'-P-OP1	-8.41	98.14	105.70
38	4	74	U	O5'-P-OP1	-8.40	98.14	105.70
36	1	647	A	C8-N9-C4	8.39	109.16	105.80
38	4	103	G	N3-C4-C5	-8.39	124.40	128.60
36	5	1184	A	N1-C6-N6	-8.39	113.57	118.60
36	1	952	A	C8-N9-C4	-8.39	102.45	105.80
36	5	2984	C	C2-N3-C4	-8.39	115.71	119.90
36	1	895	A	C4-C5-N7	8.38	114.89	110.70
36	5	578	A	N1-C6-N6	8.38	123.63	118.60
65	n9	23	LYS	C-N-CD	8.38	146.00	128.40
36	1	637	C	P-O3'-C3'	8.38	129.75	119.70
36	5	56	G	C5-C6-N1	8.37	115.69	111.50
36	1	2886	U	C5-C4-O4	-8.36	120.88	125.90
36	5	2145	A	N1-C6-N6	-8.36	113.58	118.60
36	5	1612	A	N1-C6-N6	-8.35	113.59	118.60
36	1	1166	G	C5-C6-O6	-8.35	123.59	128.60
36	1	1104	G	O5'-P-OP1	-8.34	98.19	105.70
36	5	2874	G	C4-C5-N7	-8.34	107.46	110.80
36	1	2311	G	O5'-P-OP1	-8.34	98.19	105.70
36	1	3206	C	N1-C2-O2	-8.34	113.90	118.90
36	5	1604	G	C4-N9-C1'	8.34	137.34	126.50
36	1	2714	G	C8-N9-C1'	8.33	137.83	127.00
1	6	151	G	N3-C4-N9	-8.33	121.00	126.00
38	8	18	U	O5'-P-OP2	-8.33	98.20	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1484	U	P-O3'-C3'	8.33	129.69	119.70
36	5	2893	C	C4-C5-C6	8.33	121.56	117.40
36	1	1741	A	C2-N3-C4	-8.32	106.44	110.60
36	5	945	C	C6-N1-C2	8.32	123.63	120.30
36	1	64	G	O5'-P-OP2	8.32	120.68	110.70
36	5	2978	U	O4'-C1'-N1	8.32	114.86	108.20
36	5	3078	U	N3-C2-O2	-8.32	116.38	122.20
36	1	1422	G	O5'-P-OP1	-8.32	98.22	105.70
1	6	1769	U	C6-N1-C2	8.32	125.99	121.00
36	5	2272	G	N1-C6-O6	-8.32	114.91	119.90
36	1	699	A	C2-N3-C4	-8.31	106.45	110.60
36	1	1902	G	C5-N7-C8	-8.31	100.15	104.30
36	1	500	C	C6-N1-C2	-8.30	116.98	120.30
36	5	2916	U	C4-C5-C6	8.30	124.68	119.70
36	5	838	G	C5-C6-O6	8.30	133.58	128.60
1	2	334	G	C2-N3-C4	-8.30	107.75	111.90
1	2	1291	G	N7-C8-N9	8.29	117.25	113.10
36	5	974	G	N3-C4-C5	-8.29	124.45	128.60
36	5	1903	U	O5'-P-OP2	8.29	120.65	110.70
36	1	3207	U	C2-N1-C1'	-8.29	107.76	117.70
36	1	913	A	C8-N9-C4	-8.28	102.49	105.80
36	1	1604	G	C8-N9-C4	-8.28	103.09	106.40
36	1	2819	A	O5'-P-OP2	-8.28	98.25	105.70
36	1	1364	C	C6-N1-C2	8.28	123.61	120.30
1	6	53	G	N3-C4-C5	-8.28	124.46	128.60
1	6	512	A	N1-C6-N6	8.28	123.57	118.60
36	5	3324	C	C6-N1-C2	8.28	123.61	120.30
36	1	1099	A	C5-C6-N6	-8.27	117.08	123.70
36	5	2760	C	N3-C4-C5	8.27	125.21	121.90
36	5	3050	U	C5-C4-O4	8.26	130.86	125.90
36	5	2136	C	C5-C6-N1	-8.26	116.87	121.00
36	1	1166	G	N1-C6-O6	8.25	124.85	119.90
36	1	421	G	N3-C4-N9	8.25	130.95	126.00
36	1	821	U	N3-C4-O4	-8.25	113.62	119.40
36	5	1158	A	N1-C6-N6	8.24	123.55	118.60
1	6	453	U	N3-C2-O2	-8.23	116.44	122.20
36	5	424	G	C5-C6-O6	-8.23	123.66	128.60
36	1	1154	A	C6-N1-C2	-8.23	113.66	118.60
36	5	2383	C	N1-C2-O2	-8.23	113.96	118.90
36	1	3362	A	C5-N7-C8	-8.22	99.79	103.90
36	1	2617	U	N3-C2-O2	-8.22	116.45	122.20
1	6	163	G	C2-N3-C4	-8.22	107.79	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1669	C	C6-N1-C2	8.21	123.59	120.30
1	2	577	G	C5-N7-C8	-8.21	100.19	104.30
36	1	1346	G	C2-N3-C4	-8.21	107.80	111.90
36	1	54	C	C6-N1-C2	8.20	123.58	120.30
38	8	84	C	C6-N1-C2	-8.19	117.02	120.30
36	5	3004	C	N3-C2-O2	8.19	127.63	121.90
36	5	2940	A	N1-C6-N6	8.18	123.51	118.60
1	2	1212	G	C5-C6-O6	-8.17	123.70	128.60
36	1	3217	C	C2-N1-C1'	8.17	127.79	118.80
36	5	2913	C	N1-C2-O2	-8.17	114.00	118.90
38	8	43	A	C8-N9-C4	-8.17	102.53	105.80
48	m1	112	LEU	CA-CB-CG	8.17	134.09	115.30
36	1	1116	G	C8-N9-C4	-8.16	103.13	106.40
36	1	1495	U	C4-C5-C6	8.16	124.60	119.70
36	1	1314	C	C6-N1-C2	-8.16	117.03	120.30
36	5	2353	G	C5-C6-O6	-8.16	123.70	128.60
36	5	2626	A	N1-C2-N3	8.16	133.38	129.30
36	1	2996	U	N1-C2-O2	8.16	128.51	122.80
36	5	1055	A	O5'-P-OP2	-8.16	98.36	105.70
36	1	608	A	C5-C6-N6	-8.15	117.18	123.70
36	5	923	C	C6-N1-C2	8.15	123.56	120.30
1	6	557	G	N3-C4-C5	-8.14	124.53	128.60
36	5	927	C	C5-C4-N4	-8.14	114.50	120.20
36	5	2700	G	N1-C6-O6	8.14	124.78	119.90
38	8	25	G	O5'-P-OP2	-8.14	98.38	105.70
36	1	105	C	C5-C4-N4	-8.12	114.51	120.20
36	1	3088	G	O5'-P-OP1	-8.12	98.39	105.70
36	1	3208	G	N9-C4-C5	8.12	108.65	105.40
36	5	580	C	C6-N1-C2	-8.12	117.05	120.30
36	5	3374	U	C6-N1-C2	8.12	125.87	121.00
38	8	80	A	N7-C8-N9	8.12	117.86	113.80
36	5	55	G	C8-N9-C4	8.12	109.65	106.40
36	5	3006	A	C2-N3-C4	-8.12	106.54	110.60
36	5	3154	C	C2-N1-C1'	8.12	127.73	118.80
36	1	1360	C	C6-N1-C2	8.11	123.54	120.30
70	O4	8	ARG	NE-CZ-NH1	8.10	124.35	120.30
36	1	2572	C	N1-C2-O2	8.10	123.76	118.90
36	1	50	U	N1-C2-N3	8.10	119.76	114.90
36	5	1154	A	C2-N3-C4	8.10	114.65	110.60
36	5	1200	A	C4-C5-C6	8.09	121.05	117.00
36	5	1187	C	N3-C4-C5	8.09	125.13	121.90
1	6	448	C	C6-N1-C2	-8.08	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2396	G	C8-N9-C4	-8.08	103.17	106.40
36	1	681	U	C5-C4-O4	-8.08	121.05	125.90
36	1	2777	G	C5-C6-O6	8.08	133.45	128.60
36	1	3344	A	N7-C8-N9	8.08	117.84	113.80
36	5	947	G	N3-C4-C5	-8.08	124.56	128.60
36	5	2293	C	N1-C2-O2	8.08	123.75	118.90
36	5	2278	C	C4-C5-C6	-8.07	113.36	117.40
36	1	1389	G	C5-C6-O6	-8.07	123.76	128.60
36	5	2144	A	O4'-C1'-N9	8.07	114.66	108.20
36	1	1149	G	C8-N9-C4	-8.06	103.17	106.40
1	6	387	A	O5'-P-OP2	-8.06	98.44	105.70
1	6	119	A	C2-N3-C4	-8.06	106.57	110.60
36	5	719	U	N3-C2-O2	-8.05	116.56	122.20
36	1	885	U	C5-C6-N1	-8.05	118.67	122.70
36	1	1447	G	N9-C4-C5	8.05	108.62	105.40
1	6	393	C	N3-C4-C5	8.05	125.12	121.90
36	1	439	C	N1-C2-O2	8.04	123.73	118.90
36	5	2893	C	N1-C2-O2	-8.04	114.07	118.90
1	6	4	C	N3-C4-C5	8.04	125.12	121.90
36	5	716	A	C5-C6-N6	-8.04	117.27	123.70
36	1	2376	G	N7-C8-N9	8.04	117.12	113.10
1	6	937	C	C6-N1-C2	-8.04	117.08	120.30
36	1	350	C	N3-C2-O2	-8.04	116.28	121.90
25	d3	16	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	2	1560	U	N3-C2-O2	-8.03	116.58	122.20
36	1	85	A	C2-N3-C4	-8.03	106.59	110.60
36	5	1124	U	N3-C4-C5	8.03	119.42	114.60
37	7	101	G	N9-C4-C5	-8.02	102.19	105.40
36	1	2615	G	C5-C6-O6	-8.02	123.79	128.60
36	5	1113	G	C2-N3-C4	-8.02	107.89	111.90
36	5	437	G	C8-N9-C4	-8.02	103.19	106.40
36	5	2660	G	O5'-P-OP2	-8.01	98.49	105.70
36	5	1390	A	N9-C4-C5	8.01	109.00	105.80
36	1	697	A	C8-N9-C4	8.01	109.00	105.80
36	1	2629	U	O5'-P-OP2	-8.01	98.50	105.70
1	6	1634	C	C2-N1-C1'	8.01	127.61	118.80
38	4	80	A	O5'-P-OP2	-8.00	98.50	105.70
36	5	1879	A	C4-C5-N7	8.00	114.70	110.70
1	6	1767	G	C8-N9-C4	8.00	109.60	106.40
36	5	2950	G	O4'-C1'-N9	8.00	114.60	108.20
36	1	1790	G	N1-C6-O6	8.00	124.70	119.90
36	5	1452	A	N9-C4-C5	-8.00	102.60	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1111	U	C5-C4-O4	-7.99	121.10	125.90
36	5	2715	A	C8-N9-C4	-7.99	102.60	105.80
36	1	2830	G	N3-C2-N2	-7.99	114.31	119.90
36	1	930	U	N1-C2-N3	7.99	119.69	114.90
36	1	2363	A	N9-C4-C5	7.98	108.99	105.80
36	5	1187	C	C6-N1-C2	7.98	123.49	120.30
36	1	2617	U	N3-C4-O4	-7.97	113.82	119.40
36	1	2873	U	N3-C2-O2	-7.97	116.62	122.20
1	6	1748	G	C8-N9-C4	7.96	109.58	106.40
1	6	542	A	N7-C8-N9	7.96	117.78	113.80
41	l4	339	LEU	CA-CB-CG	7.96	133.60	115.30
36	1	1159	A	O5'-P-OP2	-7.96	98.54	105.70
36	5	938	C	C5-C4-N4	-7.96	114.63	120.20
36	5	2849	C	N3-C2-O2	7.95	127.47	121.90
36	5	2916	U	N3-C4-O4	7.95	124.96	119.40
36	1	2946	A	N9-C4-C5	-7.95	102.62	105.80
36	5	1010	G	O5'-P-OP2	-7.95	98.55	105.70
36	5	2965	U	N1-C2-O2	-7.95	117.24	122.80
36	1	1406	A	N1-C6-N6	7.94	123.37	118.60
36	1	1300	G	N1-C6-O6	7.94	124.67	119.90
36	1	2846	U	C5-C4-O4	7.94	130.66	125.90
36	1	922	U	N1-C2-O2	7.94	128.35	122.80
36	1	1604	G	C4-N9-C1'	7.93	136.81	126.50
36	5	411	U	N1-C2-O2	-7.93	117.25	122.80
36	5	2136	C	C4-C5-C6	7.92	121.36	117.40
36	5	2899	C	N1-C2-N3	7.92	124.75	119.20
37	7	85	G	OP1-P-OP2	-7.92	107.71	119.60
1	2	73	U	O4'-C1'-N1	7.92	114.54	108.20
1	6	542	A	C6-C5-N7	-7.92	126.76	132.30
36	1	670	C	C4-C5-C6	7.92	121.36	117.40
36	5	2393	G	C5-C6-O6	-7.92	123.85	128.60
36	5	2285	C	C6-N1-C2	-7.92	117.13	120.30
36	5	3218	A	C5-N7-C8	-7.92	99.94	103.90
36	1	663	C	C2-N3-C4	-7.92	115.94	119.90
36	1	363	G	C5-C6-O6	-7.91	123.85	128.60
36	1	770	G	O4'-C1'-N9	7.91	114.53	108.20
36	5	63	A	N1-C6-N6	7.91	123.35	118.60
36	5	3218	A	C2-N3-C4	-7.91	106.65	110.60
36	5	1481	A	N7-C8-N9	7.90	117.75	113.80
36	5	2704	A	O5'-P-OP1	-7.90	98.59	105.70
36	5	2619	G	N1-C6-O6	7.90	124.64	119.90
36	1	758	C	C6-N1-C2	-7.89	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3204	C	N3-C4-C5	7.89	125.06	121.90
1	6	139	C	N3-C2-O2	-7.89	116.38	121.90
36	1	2808	A	N9-C4-C5	-7.89	102.65	105.80
36	5	2117	A	N1-C6-N6	-7.88	113.87	118.60
36	5	776	U	C5-C4-O4	7.88	130.63	125.90
36	1	716	A	C8-N9-C4	7.88	108.95	105.80
1	6	405	C	O5'-P-OP2	-7.88	98.61	105.70
36	5	1869	C	N3-C4-C5	7.88	125.05	121.90
36	1	2726	C	N3-C4-N4	-7.87	112.49	118.00
36	5	1468	A	N1-C6-N6	7.87	123.32	118.60
37	7	104	A	O5'-P-OP2	-7.87	98.62	105.70
37	3	94	C	N1-C2-O2	-7.86	114.18	118.90
1	2	287	G	O4'-C1'-N9	7.86	114.49	108.20
36	1	369	A	N7-C8-N9	7.86	117.73	113.80
36	5	1452	A	C4-C5-N7	7.86	114.63	110.70
36	5	348	A	N1-C6-N6	7.85	123.31	118.60
36	1	2679	A	O4'-C1'-N9	7.85	114.48	108.20
1	6	609	U	C5-C4-O4	7.85	130.61	125.90
36	5	2336	U	C5-C4-O4	-7.85	121.19	125.90
38	8	111	A	N1-C6-N6	7.84	123.31	118.60
36	1	2870	C	C6-N1-C1'	7.84	130.21	120.80
36	1	1425	U	N3-C2-O2	-7.84	116.71	122.20
36	1	1429	G	C4-C5-N7	-7.84	107.66	110.80
36	1	1495	U	C2-N1-C1'	-7.84	108.29	117.70
36	1	1307	G	C6-C5-N7	7.83	135.10	130.40
52	m6	78	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	2	830	U	N1-C2-O2	7.83	128.28	122.80
1	6	1100	G	N3-C4-C5	-7.83	124.69	128.60
36	5	2334	U	N1-C2-N3	7.83	119.59	114.90
36	5	2759	U	N3-C4-C5	-7.83	109.90	114.60
36	5	939	U	C5-C4-O4	-7.82	121.21	125.90
36	5	2751	G	C8-N9-C4	-7.82	103.27	106.40
36	5	437	G	N9-C4-C5	7.82	108.53	105.40
36	5	3004	C	N1-C2-O2	-7.82	114.21	118.90
36	1	709	A	C8-N9-C4	7.82	108.93	105.80
36	5	2954	U	O4'-C1'-N1	7.82	114.45	108.20
36	5	1178	G	N1-C6-O6	7.81	124.58	119.90
36	1	2418	G	OP1-P-O3'	7.80	122.37	105.20
36	5	1370	G	N3-C4-C5	-7.80	124.70	128.60
36	1	949	C	N1-C2-O2	-7.80	114.22	118.90
36	1	1902	G	N9-C4-C5	-7.80	102.28	105.40
36	1	843	A	N1-C6-N6	7.80	123.28	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2617	U	C4-C5-C6	7.80	124.38	119.70
36	1	2640	A	C6-N1-C2	-7.80	113.92	118.60
1	2	1745	G	N3-C4-C5	-7.79	124.70	128.60
36	5	2211	U	C4-C5-C6	7.79	124.38	119.70
1	2	75	U	N1-C2-O2	7.79	128.25	122.80
38	4	14	C	N3-C4-C5	7.79	125.02	121.90
36	5	784	A	C5-C6-N6	-7.79	117.47	123.70
38	4	111	A	N1-C6-N6	7.79	123.27	118.60
36	1	908	G	N1-C6-O6	7.79	124.57	119.90
36	1	1307	G	N1-C6-O6	-7.79	115.23	119.90
36	5	1199	C	C2-N3-C4	-7.79	116.01	119.90
36	5	41	G	C4-C5-N7	7.78	113.91	110.80
36	1	776	U	N1-C2-N3	7.78	119.57	114.90
36	1	3275	U	C5-C6-N1	7.78	126.59	122.70
36	5	716	A	C4-C5-N7	7.78	114.59	110.70
37	7	101	G	C4-C5-N7	7.78	113.91	110.80
36	5	1115	G	C8-N9-C4	-7.78	103.29	106.40
44	l7	229	PHE	CB-CG-CD1	7.77	126.24	120.80
36	5	2928	C	N3-C2-O2	-7.77	116.46	121.90
36	5	1075	A	C8-N9-C4	7.77	108.91	105.80
36	1	792	G	O5'-P-OP1	7.77	120.02	110.70
36	5	1158	A	O5'-P-OP2	-7.76	98.71	105.70
36	5	716	A	N9-C4-C5	-7.76	102.70	105.80
36	1	2121	G	N1-C6-O6	-7.76	115.24	119.90
36	5	1126	G	C8-N9-C4	-7.76	103.30	106.40
36	5	2308	C	N1-C2-O2	-7.75	114.25	118.90
1	6	1137	A	C8-N9-C4	7.75	108.90	105.80
36	1	330	G	O5'-P-OP1	-7.75	98.73	105.70
36	1	33	G	O5'-P-OP1	-7.75	98.73	105.70
36	5	940	G	N1-C6-O6	7.75	124.55	119.90
36	1	3092	C	C6-N1-C2	7.75	123.40	120.30
36	5	2796	G	O5'-P-OP2	-7.74	98.73	105.70
36	1	2884	C	C6-N1-C2	7.74	123.39	120.30
36	5	216	G	N1-C6-O6	7.74	124.54	119.90
36	1	2827	U	N1-C2-N3	7.73	119.54	114.90
36	5	1892	G	N1-C6-O6	-7.73	115.26	119.90
36	1	3201	C	N3-C4-C5	-7.73	118.81	121.90
36	1	2174	G	N1-C6-O6	7.72	124.53	119.90
36	5	1380	G	N9-C4-C5	-7.72	102.31	105.40
36	1	608	A	N9-C4-C5	-7.72	102.71	105.80
1	6	29	U	N3-C2-O2	-7.72	116.80	122.20
1	6	755	A	C8-N9-C4	-7.72	102.71	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1886	A	O5'-P-OP2	-7.71	98.76	105.70
36	1	343	U	N1-C2-N3	7.71	119.52	114.90
36	5	2953	U	N3-C4-O4	7.71	124.79	119.40
36	5	2821	C	C2-N1-C1'	-7.70	110.33	118.80
1	6	371	G	N3-C4-C5	-7.70	124.75	128.60
36	5	1909	A	C8-N9-C4	7.70	108.88	105.80
36	1	1493	G	C5-C6-O6	-7.69	123.98	128.60
36	1	2417	U	N1-C2-O2	-7.69	117.42	122.80
36	5	1333	C	C6-N1-C2	-7.69	117.22	120.30
36	5	921	A	N1-C6-N6	-7.69	113.98	118.60
36	5	2726	C	N1-C2-N3	7.69	124.58	119.20
1	6	453	U	N1-C2-O2	7.68	128.18	122.80
36	5	361	A	N1-C6-N6	-7.68	113.99	118.60
36	1	2374	C	O5'-P-OP2	-7.68	98.79	105.70
36	1	2983	C	C5-C6-N1	-7.68	117.16	121.00
1	2	402	C	O5'-P-OP1	-7.68	98.79	105.70
36	1	143	G	N1-C6-O6	-7.67	115.30	119.90
36	5	3043	C	N3-C4-C5	7.67	124.97	121.90
36	1	1346	G	C5-C6-N1	-7.67	107.66	111.50
1	2	1200	G	C5-C6-O6	-7.67	124.00	128.60
1	6	308	C	C5-C6-N1	-7.67	117.17	121.00
36	1	2400	G	C6-C5-N7	-7.67	125.80	130.40
36	1	2647	A	C6-N1-C2	-7.67	114.00	118.60
36	1	65	A	O5'-P-OP2	-7.66	98.80	105.70
36	1	2153	U	N1-C2-N3	7.66	119.50	114.90
1	2	728	U	C2-N1-C1'	7.66	126.89	117.70
36	1	359	U	N3-C4-C5	-7.66	110.00	114.60
36	5	65	A	O5'-P-OP2	-7.66	98.81	105.70
36	5	655	C	C6-N1-C2	-7.66	117.24	120.30
36	5	2920	U	N1-C2-N3	7.66	119.49	114.90
1	2	1291	G	C5-N7-C8	-7.65	100.47	104.30
1	6	308	C	C2-N1-C1'	-7.65	110.38	118.80
36	5	2335	G	C2-N3-C4	7.65	115.72	111.90
36	1	2944	U	N1-C2-O2	7.65	128.15	122.80
36	1	2249	G	N1-C6-O6	-7.64	115.31	119.90
36	5	2993	G	C4-C5-N7	7.64	113.86	110.80
36	5	75	G	C5-C6-O6	-7.64	124.02	128.60
36	5	352	A	O5'-P-OP1	-7.64	98.83	105.70
36	5	3078	U	N1-C2-O2	7.64	128.15	122.80
36	1	2814	G	C5-C6-O6	-7.63	124.02	128.60
36	1	2983	C	C4-C5-C6	7.63	121.22	117.40
36	5	922	U	C5-C6-N1	-7.63	118.88	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1838	G	C6-C5-N7	-7.63	125.82	130.40
36	1	1849	C	O5'-P-OP1	-7.63	98.83	105.70
36	1	1428	A	C5-C6-N6	-7.63	117.60	123.70
36	1	1481	A	C4-N9-C1'	7.63	140.03	126.30
36	1	2872	A	C8-N9-C4	7.62	108.85	105.80
36	5	2639	G	N1-C6-O6	7.62	124.47	119.90
36	1	890	C	C6-N1-C2	-7.62	117.25	120.30
36	5	1152	G	C5-C6-N1	-7.62	107.69	111.50
1	6	901	G	N9-C4-C5	-7.62	102.35	105.40
36	1	923	C	N3-C4-C5	-7.61	118.86	121.90
36	1	965	A	OP1-P-O3'	7.60	121.93	105.20
36	1	2827	U	C2-N1-C1'	-7.60	108.58	117.70
1	6	387	A	N9-C4-C5	7.60	108.84	105.80
36	5	921	A	N9-C4-C5	7.60	108.84	105.80
36	5	216	G	C5-C6-O6	-7.60	124.04	128.60
36	1	2827	U	C6-N1-C1'	7.60	131.84	121.20
36	5	1367	G	C5-C6-N1	-7.60	107.70	111.50
36	5	2659	G	N1-C6-O6	7.60	124.46	119.90
36	1	1116	G	N3-C4-C5	-7.59	124.80	128.60
38	8	99	C	C6-N1-C2	7.59	123.34	120.30
36	1	1428	A	C4-C5-N7	7.59	114.50	110.70
1	6	1140	G	C5-C6-O6	-7.59	124.05	128.60
36	1	1846	C	N3-C4-C5	-7.59	118.86	121.90
36	5	1367	G	N1-C6-O6	7.59	124.45	119.90
36	5	877	C	C4-C5-C6	-7.59	113.61	117.40
37	7	108	A	N1-C6-N6	7.59	123.15	118.60
36	5	1851	G	C5-C6-O6	-7.58	124.05	128.60
1	2	448	C	N3-C4-C5	-7.58	118.87	121.90
36	1	2620	G	C8-N9-C4	7.58	109.43	106.40
1	2	765	G	O4'-C1'-N9	-7.58	102.14	108.20
1	2	1291	G	N1-C2-N3	7.58	128.44	123.90
36	1	2714	G	C4-N9-C1'	-7.58	116.65	126.50
36	5	1178	G	C5-C6-O6	-7.57	124.06	128.60
36	5	2984	C	N1-C2-O2	-7.57	114.36	118.90
36	5	2356	A	C5-C6-N1	-7.57	113.92	117.70
36	1	1386	A	C6-N1-C2	-7.56	114.06	118.60
1	2	579	A	N1-C2-N3	7.56	133.08	129.30
1	6	1000	C	C4-C5-C6	7.56	121.18	117.40
36	5	2730	G	N1-C6-O6	7.56	124.44	119.90
1	2	402	C	C6-N1-C2	7.56	123.32	120.30
1	6	310	C	N1-C2-O2	-7.55	114.37	118.90
36	5	373	A	O5'-P-OP1	-7.55	98.90	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	802	C	C6-N1-C2	-7.55	117.28	120.30
36	5	2128	C	C5-C4-N4	-7.55	114.91	120.20
36	5	3216	G	C5-C6-O6	-7.55	124.07	128.60
37	3	86	U	O5'-P-OP2	-7.55	98.91	105.70
36	5	607	A	N1-C6-N6	-7.55	114.07	118.60
36	5	750	G	C5-C6-O6	-7.55	124.07	128.60
36	1	1556	C	N3-C2-O2	-7.55	116.62	121.90
36	5	2295	A	C5-C6-N6	-7.55	117.66	123.70
36	1	708	G	C8-N9-C4	-7.54	103.38	106.40
36	5	1688	U	N3-C2-O2	-7.54	116.92	122.20
36	5	2116	G	C6-C5-N7	-7.54	125.87	130.40
36	5	2354	C	N1-C2-O2	-7.54	114.38	118.90
36	1	645	A	C8-N9-C4	-7.54	102.78	105.80
1	6	321	C	N3-C2-O2	-7.54	116.62	121.90
36	1	2756	C	C2-N1-C1'	7.53	127.09	118.80
36	5	2954	U	N3-C4-O4	7.53	124.67	119.40
36	1	1836	C	N1-C2-O2	7.53	123.42	118.90
36	1	2870	C	N3-C4-N4	-7.53	112.73	118.00
36	1	3005	A	N9-C4-C5	7.53	108.81	105.80
36	1	645	A	C5-C6-N1	7.53	121.46	117.70
36	1	2376	G	C8-N9-C4	-7.53	103.39	106.40
36	1	3362	A	C6-C5-N7	-7.53	127.03	132.30
36	5	97	U	N3-C2-O2	7.53	127.47	122.20
36	1	3206	C	C2-N1-C1'	-7.52	110.53	118.80
36	5	1495	U	N3-C4-C5	-7.52	110.09	114.60
36	1	1481	A	N1-C6-N6	7.52	123.11	118.60
36	5	2950	G	C8-N9-C4	-7.52	103.39	106.40
1	2	1733	C	N3-C4-N4	7.52	123.26	118.00
36	5	2870	C	N3-C4-C5	7.52	124.91	121.90
36	1	984	G	N1-C2-N2	-7.51	109.44	116.20
36	1	2418	G	N3-C4-C5	-7.51	124.84	128.60
36	5	927	C	O5'-P-OP1	-7.51	98.94	105.70
36	5	1506	A	N9-C4-C5	7.51	108.80	105.80
38	4	13	A	O5'-P-OP1	-7.50	98.95	105.70
36	5	1513	G	N3-C4-C5	-7.50	124.85	128.60
36	1	979	U	N3-C2-O2	-7.50	116.95	122.20
36	5	947	G	C2-N3-C4	7.50	115.65	111.90
1	6	158	U	P-O3'-C3'	7.50	128.69	119.70
36	1	631	U	C5-C4-O4	-7.49	121.40	125.90
36	5	3115	C	N1-C2-O2	-7.49	114.40	118.90
1	2	453	U	N3-C2-O2	-7.49	116.96	122.20
36	5	2278	C	C5-C6-N1	7.49	124.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	647	A	C4-C5-C6	7.48	120.74	117.00
36	1	3369	G	C5-C6-O6	-7.48	124.11	128.60
36	1	1112	A	O5'-P-OP2	-7.48	98.97	105.70
36	1	511	G	C8-N9-C4	-7.48	103.41	106.40
36	1	2935	U	N3-C4-C5	-7.48	110.11	114.60
36	5	2284	C	C5-C4-N4	-7.48	114.97	120.20
36	1	2959	C	N1-C2-O2	-7.48	114.41	118.90
36	1	1345	G	O5'-P-OP2	-7.47	98.97	105.70
70	O4	8	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	6	323	A	N1-C6-N6	-7.47	114.12	118.60
36	5	417	A	N1-C6-N6	-7.47	114.12	118.60
37	7	44	C	N1-C2-O2	-7.47	114.42	118.90
36	5	1321	G	C8-N9-C4	7.47	109.39	106.40
1	2	553	G	C6-C5-N7	-7.46	125.92	130.40
36	5	2396	G	N9-C4-C5	7.46	108.38	105.40
36	1	663	C	C5-C6-N1	-7.46	117.27	121.00
36	1	2726	C	C6-N1-C2	-7.45	117.32	120.30
36	5	1199	C	C5-C6-N1	-7.45	117.27	121.00
36	1	2283	G	C5-C6-O6	-7.45	124.13	128.60
36	1	1151	U	N3-C4-O4	7.45	124.62	119.40
36	5	1208	U	N3-C2-O2	-7.45	116.98	122.20
36	1	80	G	C5-C6-O6	-7.45	124.13	128.60
36	5	2393	G	N1-C6-O6	7.45	124.37	119.90
36	1	2196	C	C5-C6-N1	7.45	124.72	121.00
1	2	1118	G	N1-C6-O6	7.44	124.37	119.90
36	1	25	U	N3-C4-O4	7.44	124.61	119.40
36	1	1402	C	N3-C4-N4	-7.44	112.79	118.00
36	5	1931	U	N1-C2-N3	7.44	119.37	114.90
36	1	2797	C	O5'-P-OP1	-7.44	99.00	105.70
36	1	1307	G	N9-C4-C5	7.44	108.38	105.40
36	1	3001	C	C6-N1-C2	7.44	123.28	120.30
36	5	1124	U	C4-C5-C6	-7.44	115.23	119.70
36	5	2659	G	C5-C6-O6	-7.44	124.14	128.60
38	4	38	U	N3-C2-O2	-7.44	116.99	122.20
36	5	2710	C	N3-C4-C5	-7.44	118.92	121.90
36	5	3093	C	C5-C6-N1	-7.44	117.28	121.00
36	1	3206	C	C6-N1-C1'	7.44	129.73	120.80
1	6	323	A	C8-N9-C4	-7.44	102.83	105.80
36	1	1441	G	O5'-P-OP2	-7.43	99.01	105.70
1	2	1654	G	N3-C4-N9	7.43	130.46	126.00
36	1	640	U	N3-C4-O4	7.43	124.60	119.40
36	5	1380	G	C8-N9-C4	7.43	109.37	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	805	U	C6-N1-C2	-7.43	116.54	121.00
1	2	639	U	N1-C2-O2	7.42	128.00	122.80
36	1	2968	G	C5-C6-N1	-7.42	107.79	111.50
36	1	2893	C	N3-C4-C5	7.41	124.86	121.90
36	1	2374	C	C6-N1-C2	-7.41	117.34	120.30
37	3	88	G	N3-C4-C5	-7.41	124.89	128.60
36	5	2392	C	N3-C4-C5	7.41	124.86	121.90
1	2	75	U	N3-C2-O2	-7.41	117.02	122.20
36	5	796	U	N1-C2-N3	7.41	119.34	114.90
36	5	942	U	N3-C4-O4	7.40	124.58	119.40
36	1	1180	A	O4'-C1'-N9	-7.40	102.28	108.20
1	6	1700	C	C6-N1-C1'	-7.40	111.92	120.80
36	1	359	U	C4-C5-C6	7.39	124.14	119.70
36	1	1346	G	N1-C6-O6	7.39	124.34	119.90
36	1	921	A	C8-N9-C4	-7.39	102.84	105.80
36	1	1838	G	C4-C5-N7	7.39	113.76	110.80
36	1	422	A	N1-C6-N6	-7.39	114.17	118.60
36	5	2147	A	N1-C6-N6	7.39	123.03	118.60
36	5	2935	U	O5'-P-OP2	-7.39	99.05	105.70
36	1	726	G	C8-N9-C4	-7.39	103.44	106.40
36	1	54	C	N3-C4-N4	-7.38	112.83	118.00
36	5	3362	A	N7-C8-N9	7.38	117.49	113.80
36	5	913	A	C8-N9-C4	-7.38	102.85	105.80
1	2	555	A	C8-N9-C4	-7.38	102.85	105.80
1	6	542	A	N1-C6-N6	7.38	123.03	118.60
36	5	2609	A	O5'-P-OP2	-7.38	99.06	105.70
36	1	2884	C	C4-C5-C6	-7.38	113.71	117.40
1	2	1486	G	C8-N9-C4	-7.38	103.45	106.40
36	1	645	A	C4-C5-N7	-7.37	107.01	110.70
36	1	2978	U	O4'-C1'-N1	7.37	114.10	108.20
36	5	2600	C	C6-N1-C2	-7.37	117.35	120.30
1	2	1280	C	N3-C4-C5	-7.37	118.95	121.90
36	1	695	C	C6-N1-C2	7.37	123.25	120.30
36	1	2700	G	N1-C6-O6	7.37	124.32	119.90
38	4	120	C	N1-C2-O2	-7.37	114.48	118.90
1	6	858	G	O4'-C1'-N9	7.37	114.09	108.20
36	1	895	A	C5-N7-C8	-7.37	100.22	103.90
36	1	2692	A	C8-N9-C4	-7.37	102.85	105.80
36	5	3143	C	N1-C2-O2	-7.37	114.48	118.90
36	1	3110	C	C6-N1-C2	-7.36	117.36	120.30
36	5	942	U	N1-C2-O2	-7.36	117.65	122.80
1	2	1761	U	C6-N1-C2	-7.36	116.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2621	G	N3-C2-N2	-7.36	114.75	119.90
36	5	641	C	C6-N1-C2	-7.35	117.36	120.30
36	5	1419	A	O5'-P-OP2	-7.35	99.08	105.70
36	1	709	A	N7-C8-N9	-7.35	110.12	113.80
36	5	2751	G	N7-C8-N9	7.34	116.77	113.10
36	1	211	A	C2-N3-C4	-7.33	106.93	110.60
36	5	2941	A	N9-C4-C5	7.33	108.73	105.80
36	5	2375	G	N1-C6-O6	-7.33	115.50	119.90
36	5	653	A	O5'-P-OP1	-7.33	99.10	105.70
36	5	1375	G	C2-N3-C4	7.33	115.56	111.90
36	1	39	A	O5'-P-OP2	-7.33	99.11	105.70
36	1	1154	A	C4-C5-C6	7.33	120.66	117.00
36	1	2946	A	C5-C6-N6	-7.33	117.84	123.70
36	5	1336	U	O5'-P-OP2	-7.32	99.11	105.70
36	1	2245	C	N3-C4-C5	-7.32	118.97	121.90
36	5	2799	A	C5-C6-N6	7.32	129.55	123.70
36	1	1349	G	N3-C4-N9	7.31	130.39	126.00
36	1	2700	G	C6-C5-N7	-7.31	126.01	130.40
1	2	610	G	C8-N9-C1'	-7.31	117.49	127.00
36	5	1390	A	C8-N9-C4	-7.31	102.88	105.80
36	5	1846	C	C6-N1-C2	7.31	123.22	120.30
36	5	3362	A	O4'-C1'-N9	7.31	114.05	108.20
36	1	1741	A	N1-C2-N3	7.31	132.95	129.30
37	7	87	G	C5-C6-O6	-7.31	124.22	128.60
36	5	2820	A	C8-N9-C4	-7.30	102.88	105.80
36	5	92	G	N3-C4-N9	7.30	130.38	126.00
37	7	103	A	N1-C6-N6	7.30	122.98	118.60
36	1	2196	C	C6-N1-C2	-7.30	117.38	120.30
36	1	3362	A	O4'-C1'-N9	7.30	114.04	108.20
36	5	1203	A	O5'-P-OP1	-7.30	99.13	105.70
36	5	2611	U	O5'-P-OP2	-7.30	99.13	105.70
36	5	1367	G	C4-C5-C6	7.29	123.18	118.80
36	5	2572	C	N3-C2-O2	-7.29	116.79	121.90
36	1	661	G	C8-N9-C4	-7.29	103.48	106.40
36	5	881	C	C5-C6-N1	7.29	124.65	121.00
1	6	47	A	O5'-P-OP1	-7.29	99.14	105.70
36	5	2709	C	N3-C4-C5	7.29	124.82	121.90
36	5	3305	A	C5-C6-N6	-7.29	117.87	123.70
36	1	672	A	C5-C6-N6	-7.29	117.87	123.70
36	1	678	G	N3-C2-N2	-7.29	114.80	119.90
1	6	913	G	N1-C6-O6	7.29	124.27	119.90
36	5	640	U	N3-C4-O4	7.29	124.50	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3209	A	O4'-C1'-N9	7.29	114.03	108.20
36	5	2399	A	C5-C6-N6	-7.28	117.87	123.70
36	1	2811	A	C6-N1-C2	-7.28	114.23	118.60
36	1	2400	G	N1-C6-O6	7.28	124.27	119.90
1	6	405	C	C6-N1-C2	7.28	123.21	120.30
36	5	1365	G	C8-N9-C4	-7.28	103.49	106.40
36	1	2395	G	O5'-P-OP2	-7.28	99.15	105.70
36	5	2405	C	N3-C2-O2	-7.28	116.81	121.90
36	5	2881	C	N3-C4-C5	7.27	124.81	121.90
36	1	2877	G	C4-C5-N7	-7.27	107.89	110.80
36	1	3344	A	C8-N9-C4	-7.27	102.89	105.80
38	4	20	U	O5'-P-OP2	-7.27	99.16	105.70
36	1	3201	C	C6-N1-C2	-7.27	117.39	120.30
36	5	2176	U	C2-N1-C1'	7.27	126.42	117.70
36	5	2993	G	C5-C6-O6	-7.27	124.24	128.60
1	6	826	U	C5-C6-N1	7.26	126.33	122.70
36	5	2858	U	N3-C2-O2	-7.26	117.11	122.20
36	5	2317	A	O5'-P-OP2	-7.26	99.16	105.70
36	1	1418	A	O5'-P-OP2	-7.26	99.16	105.70
36	5	1307	G	C2-N3-C4	7.26	115.53	111.90
38	4	79	A	C8-N9-C4	-7.26	102.90	105.80
36	5	663	C	C6-N1-C2	-7.26	117.40	120.30
36	5	869	G	N1-C6-O6	-7.26	115.54	119.90
36	5	961	C	N3-C4-C5	-7.26	119.00	121.90
36	1	189	G	N3-C4-C5	-7.26	124.97	128.60
36	1	127	G	N1-C6-O6	7.25	124.25	119.90
36	1	2153	U	C6-N1-C2	-7.25	116.65	121.00
36	1	1481	A	C5-N7-C8	-7.25	100.27	103.90
36	1	1383	G	C5-C6-O6	-7.25	124.25	128.60
36	5	804	C	N3-C4-C5	-7.25	119.00	121.90
1	6	577	G	C5-N7-C8	-7.25	100.68	104.30
36	1	3054	U	N3-C2-O2	-7.24	117.13	122.20
38	8	8	C	C6-N1-C2	-7.24	117.40	120.30
38	4	109	A	N1-C6-N6	7.24	122.94	118.60
36	1	776	U	C5-C6-N1	-7.24	119.08	122.70
36	1	1117	G	O5'-P-OP1	-7.24	99.19	105.70
36	1	2891	U	C5-C4-O4	-7.24	121.56	125.90
1	6	1000	C	C6-N1-C1'	-7.24	112.12	120.80
36	5	1361	U	N1-C2-O2	-7.24	117.73	122.80
36	1	2846	U	N1-C2-O2	7.24	127.86	122.80
36	5	2988	C	C2-N3-C4	-7.23	116.28	119.90
1	2	310	C	N3-C4-C5	-7.23	119.01	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1934	G	C8-N9-C4	-7.23	103.51	106.40
36	5	2140	U	N1-C2-N3	7.23	119.24	114.90
36	1	358	G	C5-C6-O6	-7.22	124.27	128.60
1	6	1773	C	C6-N1-C2	-7.22	117.41	120.30
1	6	609	U	N3-C4-O4	-7.22	114.34	119.40
36	5	1592	G	C5-C6-O6	7.22	132.93	128.60
36	5	3154	C	N3-C2-O2	-7.22	116.85	121.90
36	1	895	A	C2-N3-C4	-7.22	106.99	110.60
36	5	890	C	O5'-P-OP2	-7.21	99.22	105.70
36	5	1324	U	O5'-P-OP2	-7.21	99.21	105.70
36	5	844	G	C8-N9-C4	7.21	109.28	106.40
36	1	983	A	C6-N1-C2	-7.20	114.28	118.60
36	5	820	A	N7-C8-N9	7.20	117.40	113.80
1	6	1634	C	C6-N1-C2	-7.20	117.42	120.30
36	5	960	U	N3-C4-O4	-7.20	114.36	119.40
1	2	1389	C	N1-C2-O2	7.19	123.22	118.90
36	1	3101	G	C8-N9-C4	7.19	109.28	106.40
36	1	651	G	N3-C4-C5	-7.19	125.00	128.60
36	1	1906	G	C6-C5-N7	-7.19	126.08	130.40
1	6	1782	A	O5'-P-OP1	-7.19	99.23	105.70
37	7	49	G	C5-C6-O6	-7.19	124.29	128.60
36	1	1149	G	N9-C4-C5	7.19	108.28	105.40
36	5	2857	C	C5-C4-N4	-7.19	115.17	120.20
36	5	3214	U	C5-C4-O4	7.19	130.21	125.90
36	1	2827	U	N3-C4-O4	-7.18	114.37	119.40
1	6	272	U	N3-C2-O2	-7.18	117.17	122.20
36	5	784	A	N9-C4-C5	-7.18	102.93	105.80
36	1	959	C	C6-N1-C2	7.18	123.17	120.30
36	1	1325	U	C5-C4-O4	7.18	130.21	125.90
36	1	2869	U	OP2-P-O3'	7.18	121.00	105.20
36	5	2121	G	O5'-P-OP2	-7.18	99.24	105.70
36	5	3188	G	N1-C6-O6	-7.18	115.59	119.90
36	1	1371	G	C5-C6-N1	7.17	115.09	111.50
36	5	873	C	N3-C4-C5	-7.17	119.03	121.90
36	1	608	A	C4-C5-C6	7.17	120.58	117.00
1	6	310	C	N3-C4-C5	-7.17	119.03	121.90
36	1	1481	A	O5'-P-OP1	7.16	119.30	110.70
36	1	2884	C	C5-C4-N4	-7.16	115.19	120.20
36	5	592	A	C8-N9-C4	7.16	108.67	105.80
36	1	648	C	C2-N1-C1'	7.16	126.68	118.80
36	5	1155	C	N3-C4-C5	7.16	124.77	121.90
36	1	331	G	N1-C6-O6	-7.16	115.60	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2651	G	C4-C5-N7	-7.16	107.94	110.80
1	6	988	A	O5'-P-OP2	-7.16	99.26	105.70
36	1	1829	G	N9-C4-C5	7.16	108.26	105.40
1	6	453	U	C2-N1-C1'	7.16	126.29	117.70
36	5	1592	G	N7-C8-N9	7.16	116.68	113.10
36	5	2827	U	O4'-C1'-N1	7.16	113.92	108.20
36	1	340	C	C2-N3-C4	-7.15	116.33	119.90
36	1	1192	C	C2-N1-C1'	7.15	126.67	118.80
36	1	1412	G	C8-N9-C4	-7.15	103.54	106.40
36	5	3245	A	N1-C2-N3	7.15	132.87	129.30
36	1	3278	C	N3-C2-O2	-7.14	116.90	121.90
1	6	425	A	N1-C6-N6	-7.14	114.31	118.60
36	5	2186	U	N1-C2-O2	7.14	127.80	122.80
36	5	2650	U	C2-N3-C4	-7.14	122.72	127.00
36	5	2897	A	C6-N1-C2	-7.14	114.31	118.60
36	1	2916	U	N1-C2-N3	-7.14	110.62	114.90
1	6	1560	U	N3-C2-O2	-7.14	117.20	122.20
36	5	2849	C	N1-C2-O2	-7.14	114.62	118.90
36	5	1724	U	O4'-C1'-N1	7.13	113.91	108.20
36	5	2752	U	O5'-P-OP2	-7.13	99.28	105.70
50	m4	72	LEU	CA-CB-CG	7.13	131.71	115.30
36	5	1152	G	C5-C6-O6	-7.13	124.32	128.60
36	1	669	U	C5-C6-N1	-7.13	119.14	122.70
36	1	939	U	N3-C2-O2	7.13	127.19	122.20
36	1	1124	U	OP1-P-O3'	7.12	120.87	105.20
36	5	1516	C	N3-C4-C5	7.12	124.75	121.90
1	2	794	U	C2-N1-C1'	7.12	126.25	117.70
36	1	3207	U	C6-N1-C1'	7.12	131.17	121.20
1	2	1756	A	N7-C8-N9	7.12	117.36	113.80
36	1	2368	A	O5'-P-OP2	-7.12	99.29	105.70
36	5	1112	A	C6-C5-N7	-7.12	127.32	132.30
1	2	694	U	C2-N1-C1'	7.12	126.24	117.70
36	1	1165	A	C8-N9-C4	7.12	108.65	105.80
36	5	2873	U	C5-C6-N1	-7.11	119.14	122.70
36	5	1604	G	N3-C4-C5	-7.11	125.05	128.60
36	5	2610	G	O5'-P-OP1	7.11	119.23	110.70
36	1	2980	U	N1-C2-N3	7.11	119.17	114.90
36	5	609	G	N3-C2-N2	-7.11	114.92	119.90
1	2	597	G	N3-C4-C5	-7.11	125.05	128.60
36	1	2758	A	C8-N9-C4	7.11	108.64	105.80
36	5	2808	A	C4-C5-N7	7.11	114.25	110.70
36	1	2728	G	O5'-P-OP2	-7.10	99.31	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	310	C	C6-N1-C2	-7.10	117.46	120.30
1	2	577	G	N1-C6-O6	7.10	124.16	119.90
36	1	937	G	C8-N9-C4	7.10	109.24	106.40
38	4	40	A	C5-C6-N6	-7.10	118.02	123.70
36	5	645	A	N1-C2-N3	7.10	132.85	129.30
36	1	80	G	C6-N1-C2	-7.10	120.84	125.10
36	5	2398	A	C6-N1-C2	-7.10	114.34	118.60
36	5	2941	A	C8-N9-C4	-7.10	102.96	105.80
36	1	646	A	N7-C8-N9	7.09	117.35	113.80
36	5	2207	A	O4'-C1'-N9	7.09	113.88	108.20
36	5	2684	C	O5'-P-OP2	-7.09	99.32	105.70
36	5	2351	U	C6-N1-C2	-7.09	116.75	121.00
36	5	96	G	N1-C6-O6	7.08	124.15	119.90
36	5	2338	C	N3-C4-N4	7.08	122.96	118.00
36	5	2631	U	O5'-P-OP2	-7.08	99.33	105.70
36	1	890	C	N3-C2-O2	-7.08	116.94	121.90
36	1	651	G	N3-C4-N9	7.08	130.25	126.00
36	1	718	G	N7-C8-N9	7.08	116.64	113.10
36	1	1468	A	N1-C2-N3	7.08	132.84	129.30
1	6	371	G	N3-C4-N9	7.07	130.24	126.00
47	m0	48	LEU	CA-CB-CG	7.07	131.56	115.30
36	5	2851	A	C8-N9-C4	7.07	108.63	105.80
36	1	1441	G	C8-N9-C4	-7.07	103.57	106.40
36	1	2154	U	C5-C6-N1	7.07	126.23	122.70
36	1	3092	C	C2-N1-C1'	-7.07	111.03	118.80
36	1	1891	A	C8-N9-C4	7.07	108.63	105.80
38	4	28	C	C6-N1-C2	-7.06	117.47	120.30
36	1	1507	G	C5-C6-O6	-7.06	124.36	128.60
36	5	1115	G	N7-C8-N9	7.06	116.63	113.10
36	5	2407	C	O5'-P-OP2	-7.06	99.35	105.70
37	7	92	A	C8-N9-C4	7.06	108.62	105.80
36	5	1149	G	N1-C6-O6	7.06	124.13	119.90
38	4	38	U	N1-C2-O2	7.05	127.74	122.80
36	1	948	C	N1-C2-O2	-7.05	114.67	118.90
36	1	3209	A	N1-C6-N6	7.05	122.83	118.60
36	5	2353	G	N1-C6-O6	7.05	124.13	119.90
36	5	3049	A	N7-C8-N9	-7.05	110.28	113.80
1	2	1749	A	C2-N3-C4	-7.05	107.08	110.60
1	6	1742	U	O5'-P-OP2	-7.05	99.36	105.70
36	1	1152	G	O4'-C1'-N9	7.04	113.84	108.20
36	5	2632	G	N3-C4-C5	-7.04	125.08	128.60
1	2	942	G	N1-C6-O6	-7.04	115.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	967	A	N1-C2-N3	7.04	132.82	129.30
36	5	1132	C	O5'-P-OP1	-7.04	99.36	105.70
36	1	1389	G	C4-C5-N7	7.04	113.61	110.80
1	6	687	G	N3-C4-N9	-7.04	121.78	126.00
36	5	2373	A	O5'-P-OP1	-7.04	99.37	105.70
36	5	2830	G	OP2-P-O3'	7.03	120.67	105.20
36	1	859	G	N9-C4-C5	-7.03	102.59	105.40
36	1	1419	A	O5'-P-OP1	7.03	119.14	110.70
36	5	809	G	N1-C6-O6	7.03	124.12	119.90
36	1	2252	A	N7-C8-N9	7.03	117.31	113.80
36	1	702	C	N1-C2-O2	-7.03	114.69	118.90
38	4	108	C	C6-N1-C2	-7.03	117.49	120.30
1	2	1600	A	C5-C6-N1	-7.02	114.19	117.70
36	1	1171	G	O5'-P-OP1	-7.02	99.38	105.70
36	1	2868	U	N3-C2-O2	-7.02	117.29	122.20
36	1	3208	G	C4-C5-N7	-7.02	107.99	110.80
36	5	522	A	O5'-P-OP1	-7.02	99.38	105.70
36	5	1513	G	C8-N9-C4	-7.02	103.59	106.40
36	5	885	U	C5-C4-O4	-7.02	121.69	125.90
36	5	922	U	N3-C4-O4	-7.02	114.49	119.40
52	m6	41	LEU	CB-CG-CD2	-7.02	99.07	111.00
1	2	1272	U	N3-C2-O2	-7.01	117.29	122.20
36	5	3110	C	N1-C2-O2	-7.01	114.69	118.90
36	1	614	C	C5-C4-N4	-7.01	115.29	120.20
36	1	2937	G	N7-C8-N9	-7.01	109.59	113.10
36	5	1179	A	C4-C5-C6	7.01	120.51	117.00
36	1	2174	G	C5-C6-O6	-7.01	124.39	128.60
36	5	1834	U	C5-C4-O4	7.01	130.10	125.90
36	1	2169	G	N1-C6-O6	-7.01	115.69	119.90
36	1	2986	U	N1-C2-N3	7.01	119.10	114.90
1	6	10	G	C5-C6-O6	7.01	132.80	128.60
1	6	987	G	C5-C6-O6	-7.01	124.40	128.60
36	5	1150	A	O5'-P-OP2	-7.01	99.39	105.70
37	7	112	G	C8-N9-C4	-7.01	103.60	106.40
36	1	1316	C	N3-C4-N4	7.00	122.90	118.00
36	5	672	A	N1-C6-N6	7.00	122.80	118.60
36	5	2649	A	C8-N9-C4	-7.00	103.00	105.80
36	1	396	A	O5'-P-OP1	-7.00	99.40	105.70
36	5	1793	C	N3-C4-C5	-7.00	119.10	121.90
1	6	1764	C	C6-N1-C2	7.00	123.10	120.30
36	1	59	G	C6-C5-N7	-6.99	126.20	130.40
36	1	1373	A	C6-N1-C2	-6.99	114.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3057	U	C5-C4-O4	6.99	130.09	125.90
36	1	3369	G	N1-C6-O6	6.99	124.09	119.90
38	4	105	A	C8-N9-C4	-6.99	103.00	105.80
36	1	2409	G	N3-C4-C5	-6.99	125.11	128.60
36	5	3195	U	OP1-P-O3'	6.99	120.58	105.20
36	1	361	A	N1-C6-N6	-6.99	114.41	118.60
36	5	87	U	C5-C6-N1	6.99	126.19	122.70
36	5	1163	A	O5'-P-OP2	-6.99	99.41	105.70
36	5	1615	C	C6-N1-C2	-6.99	117.50	120.30
36	5	835	G	O4'-C1'-N9	6.98	113.79	108.20
36	5	2341	A	N7-C8-N9	-6.98	110.31	113.80
36	1	65	A	P-O3'-C3'	6.98	128.08	119.70
36	1	954	U	N1-C2-O2	-6.98	117.91	122.80
36	1	2615	G	C4-C5-N7	6.98	113.59	110.80
38	4	94	C	C6-N1-C2	6.98	123.09	120.30
36	5	2572	C	C2-N1-C1'	6.98	126.48	118.80
1	2	507	U	C2-N1-C1'	6.97	126.07	117.70
36	5	2761	G	C5-C6-O6	-6.97	124.42	128.60
38	8	86	U	C5-C6-N1	6.97	126.19	122.70
36	1	1361	U	O5'-P-OP1	-6.97	99.42	105.70
36	1	645	A	N3-C4-C5	-6.97	121.92	126.80
36	1	2369	G	N3-C4-C5	-6.97	125.11	128.60
36	5	2659	G	C6-C5-N7	-6.97	126.22	130.40
35	SM	167	PRO	N-CA-CB	6.97	111.66	103.30
1	6	438	A	N1-C6-N6	6.97	122.78	118.60
36	5	559	A	C8-N9-C4	-6.97	103.01	105.80
36	5	1000	C	C6-N1-C2	6.97	123.09	120.30
1	2	137	U	N1-C2-O2	6.97	127.68	122.80
36	5	1548	C	N1-C2-O2	-6.97	114.72	118.90
36	1	104	G	N1-C6-O6	6.97	124.08	119.90
36	1	429	U	O5'-P-OP1	-6.97	99.43	105.70
36	5	1181	U	C4-C5-C6	6.97	123.88	119.70
36	1	37	U	N1-C2-N3	6.96	119.08	114.90
1	6	1537	C	C6-N1-C1'	6.96	129.15	120.80
36	1	672	A	N9-C4-C5	-6.96	103.02	105.80
36	1	2194	G	C6-C5-N7	-6.96	126.22	130.40
1	6	163	G	C8-N9-C4	-6.96	103.62	106.40
1	6	1000	C	C2-N3-C4	-6.96	116.42	119.90
36	5	649	A	C8-N9-C4	-6.96	103.02	105.80
36	1	1116	G	C4-C5-C6	6.96	122.97	118.80
36	5	218	G	O5'-P-OP2	-6.96	99.44	105.70
36	5	1592	G	N9-C4-C5	6.96	108.18	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S3	182	LEU	CA-CB-CG	6.95	131.29	115.30
36	5	1399	A	N1-C6-N6	6.95	122.77	118.60
36	1	716	A	C5-C6-N6	-6.95	118.14	123.70
36	1	1307	G	P-O3'-C3'	6.95	128.04	119.70
37	3	99	G	O5'-P-OP2	-6.95	99.44	105.70
38	4	40	A	N1-C6-N6	6.95	122.77	118.60
1	6	1750	A	O5'-P-OP2	-6.95	99.44	105.70
36	5	1161	G	C5-C6-N1	6.95	114.97	111.50
36	5	2379	U	O5'-P-OP1	6.95	119.04	110.70
37	7	104	A	O5'-P-OP1	6.95	119.04	110.70
36	1	2550	U	N3-C2-O2	-6.95	117.34	122.20
36	1	2710	C	N1-C2-O2	-6.95	114.73	118.90
1	6	542	A	O4'-C1'-N9	6.95	113.76	108.20
36	1	1495	U	C5-C4-O4	6.95	130.07	125.90
1	6	120	U	N3-C2-O2	-6.95	117.34	122.20
1	2	580	A	C8-N9-C4	-6.95	103.02	105.80
36	1	1846	C	N1-C2-O2	-6.94	114.73	118.90
36	5	1112	A	N1-C6-N6	6.94	122.77	118.60
1	6	902	G	C5-C6-N1	-6.94	108.03	111.50
36	1	318	A	O5'-P-OP1	-6.94	99.45	105.70
36	5	2944	U	C6-N1-C2	-6.94	116.84	121.00
36	1	295	A	C8-N9-C4	-6.94	103.03	105.80
36	1	790	U	C5-C4-O4	6.94	130.06	125.90
36	1	2634	U	N1-C2-N3	6.93	119.06	114.90
36	5	2285	C	C5-C6-N1	6.93	124.47	121.00
36	5	3195	U	P-O3'-C3'	6.93	128.02	119.70
1	6	988	A	C8-N9-C4	-6.93	103.03	105.80
36	5	2954	U	C6-N1-C1'	-6.93	111.50	121.20
1	2	314	C	O5'-P-OP1	-6.93	99.47	105.70
36	5	411	U	N3-C2-O2	6.93	127.05	122.20
36	1	614	C	N3-C4-C5	6.93	124.67	121.90
36	5	645	A	C6-N1-C2	-6.93	114.44	118.60
36	5	1506	A	C8-N9-C4	-6.93	103.03	105.80
36	1	638	C	N3-C2-O2	-6.92	117.05	121.90
36	5	346	C	N1-C2-O2	6.92	123.05	118.90
1	6	622	A	O5'-P-OP2	6.92	119.00	110.70
36	5	1848	G	N1-C6-O6	6.92	124.05	119.90
36	5	2886	U	N1-C2-N3	6.92	119.05	114.90
1	2	1200	G	N3-C2-N2	-6.92	115.06	119.90
36	1	1103	A	N9-C4-C5	-6.92	103.03	105.80
1	6	1634	C	N3-C2-O2	-6.92	117.06	121.90
37	3	48	U	N3-C2-O2	-6.92	117.36	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	4	32	C	N3-C2-O2	6.92	126.74	121.90
36	5	2772	C	P-O3'-C3'	6.92	128.00	119.70
36	1	960	U	C5-C6-N1	-6.91	119.24	122.70
36	5	2128	C	N3-C4-N4	6.91	122.84	118.00
36	1	3219	G	O5'-P-OP2	-6.91	99.48	105.70
36	1	1943	C	C6-N1-C2	-6.91	117.54	120.30
36	1	2422	C	O5'-P-OP1	-6.91	99.48	105.70
1	6	17	C	C6-N1-C2	-6.91	117.54	120.30
1	2	554	C	C2-N1-C1'	6.91	126.40	118.80
38	8	111	A	O5'-P-OP2	-6.91	99.49	105.70
36	1	695	C	N3-C4-C5	6.90	124.66	121.90
36	1	1120	A	N1-C6-N6	-6.90	114.46	118.60
36	1	1513	G	C6-N1-C2	-6.90	120.96	125.10
36	5	1392	G	N7-C8-N9	-6.90	109.65	113.10
36	1	979	U	C6-N1-C2	-6.90	116.86	121.00
36	1	908	G	N1-C2-N2	6.90	122.41	116.20
36	5	1115	G	C6-C5-N7	-6.90	126.26	130.40
36	1	743	C	C6-N1-C2	6.90	123.06	120.30
36	1	3269	U	C5-C4-O4	6.90	130.04	125.90
36	1	1156	C	C5-C6-N1	-6.90	117.55	121.00
36	1	2355	G	C6-C5-N7	-6.90	126.26	130.40
36	1	3184	A	C8-N9-C4	6.90	108.56	105.80
36	1	658	G	C8-N9-C1'	-6.89	118.04	127.00
36	1	2174	G	C4-C5-N7	6.89	113.56	110.80
36	1	2314	U	C5-C4-O4	-6.89	121.76	125.90
36	5	700	C	C6-N1-C2	6.89	123.06	120.30
1	6	57	G	N3-C4-C5	-6.89	125.15	128.60
36	5	2419	A	C8-N9-C4	-6.89	103.04	105.80
36	1	1115	G	N7-C8-N9	6.89	116.55	113.10
36	1	3183	A	N1-C6-N6	6.89	122.73	118.60
1	2	1733	C	N3-C4-C5	-6.89	119.14	121.90
36	1	28	C	C6-N1-C2	6.89	123.06	120.30
36	1	984	G	N3-C4-N9	6.89	130.13	126.00
1	6	65	A	N1-C6-N6	6.89	122.73	118.60
36	5	3362	A	C2-N3-C4	-6.89	107.16	110.60
36	1	1495	U	C6-N1-C1'	6.89	130.84	121.20
36	1	2314	U	N3-C4-O4	6.89	124.22	119.40
38	8	68	G	C6-C5-N7	-6.89	126.27	130.40
36	5	1192	C	N3-C2-O2	-6.88	117.08	121.90
36	5	1657	C	N1-C2-O2	6.88	123.03	118.90
36	5	2868	U	N1-C2-O2	6.88	127.62	122.80
36	1	2960	C	C5-C6-N1	-6.88	117.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1361	U	C2-N1-C1'	6.88	125.95	117.70
36	1	54	C	C5-C6-N1	-6.88	117.56	121.00
36	1	931	C	C2-N3-C4	-6.88	116.46	119.90
36	1	1313	G	C5-C6-O6	-6.88	124.47	128.60
1	2	423	G	N1-C6-O6	-6.88	115.78	119.90
36	1	2174	G	C5-N7-C8	-6.88	100.86	104.30
36	1	2879	C	N1-C2-O2	-6.88	114.78	118.90
36	1	661	G	C5-C6-O6	6.87	132.72	128.60
36	5	1524	A	C8-N9-C4	6.87	108.55	105.80
36	5	3172	A	C2-N3-C4	-6.87	107.17	110.60
1	6	577	G	C4-C5-N7	6.87	113.55	110.80
36	5	372	A	O5'-P-OP2	-6.87	99.52	105.70
36	5	3362	A	C5-N7-C8	-6.87	100.47	103.90
36	5	217	U	OP1-P-O3'	6.87	120.30	105.20
36	5	682	U	C6-N1-C1'	6.87	130.81	121.20
1	2	610	G	C4-N9-C1'	6.86	135.42	126.50
36	1	3212	C	C6-N1-C2	6.86	123.05	120.30
1	6	901	G	C5-N7-C8	-6.86	100.87	104.30
36	5	1208	U	C5-C4-O4	6.86	130.02	125.90
36	1	2130	G	C5-C6-O6	6.86	132.72	128.60
36	1	1513	G	N3-C4-C5	-6.86	125.17	128.60
36	1	632	G	N9-C4-C5	-6.86	102.66	105.40
1	2	864	U	N3-C2-O2	-6.85	117.40	122.20
1	6	577	G	N7-C8-N9	6.85	116.53	113.10
1	6	1097	U	P-O3'-C3'	6.85	127.92	119.70
36	1	1435	A	O5'-P-OP2	6.85	118.92	110.70
36	1	2363	A	N1-C6-N6	-6.85	114.49	118.60
36	5	610	G	C8-N9-C4	-6.85	103.66	106.40
1	2	637	C	C6-N1-C2	6.85	123.04	120.30
36	1	721	G	C8-N9-C4	-6.85	103.66	106.40
36	1	2798	C	N3-C4-C5	-6.85	119.16	121.90
1	6	1634	C	N1-C2-O2	6.85	123.01	118.90
36	5	984	G	N3-C4-N9	6.85	130.11	126.00
36	5	1151	U	N3-C2-O2	6.85	126.99	122.20
36	1	2329	C	O5'-P-OP2	-6.85	99.54	105.70
36	1	957	C	O5'-P-OP2	-6.84	99.54	105.70
1	6	1614	A	N1-C6-N6	6.84	122.71	118.60
36	5	859	G	N3-C2-N2	6.84	124.69	119.90
36	5	3209	A	N7-C8-N9	6.84	117.22	113.80
36	5	1160	C	N1-C2-O2	-6.84	114.80	118.90
36	5	2354	C	N3-C2-O2	6.84	126.69	121.90
1	2	1568	C	P-O3'-C3'	6.84	127.91	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1100	U	C2-N3-C4	-6.84	122.90	127.00
36	5	1932	A	O5'-P-OP1	-6.84	99.55	105.70
36	1	2114	C	O5'-P-OP2	-6.84	99.55	105.70
36	1	362	U	O5'-P-OP1	-6.83	99.55	105.70
36	1	2777	G	C4-C5-N7	-6.83	108.07	110.80
36	5	521	A	N1-C6-N6	-6.83	114.50	118.60
36	5	922	U	N1-C2-N3	6.83	119.00	114.90
36	1	3269	U	O5'-P-OP2	-6.83	99.55	105.70
36	5	2191	U	N3-C4-O4	-6.83	114.62	119.40
1	2	377	G	N3-C4-C5	6.83	132.01	128.60
36	1	635	G	C5-C6-O6	-6.83	124.50	128.60
73	O7	65	ARG	NE-CZ-NH2	-6.83	116.89	120.30
36	1	2987	A	N1-C6-N6	6.83	122.70	118.60
36	1	3217	C	N1-C2-O2	6.82	122.99	118.90
36	5	2379	U	O5'-P-OP2	-6.82	99.56	105.70
36	5	3124	G	N3-C2-N2	-6.82	115.12	119.90
38	8	29	U	O5'-P-OP2	-6.82	99.56	105.70
36	1	644	G	C5-C6-N1	-6.82	108.09	111.50
36	5	3020	U	N3-C4-O4	6.82	124.17	119.40
36	1	671	U	O5'-P-OP2	-6.81	99.57	105.70
36	1	1353	U	N3-C2-O2	-6.81	117.43	122.20
36	1	1481	A	C8-N9-C1'	-6.81	115.44	127.70
36	5	1592	G	C5-C6-N1	-6.81	108.09	111.50
36	5	2992	U	C5-C6-N1	6.81	126.11	122.70
36	5	3374	U	N3-C4-C5	6.81	118.69	114.60
36	1	2197	C	C6-N1-C2	6.81	123.02	120.30
36	1	2870	C	C6-N1-C2	6.81	123.02	120.30
36	5	350	C	C6-N1-C2	-6.81	117.58	120.30
36	5	2183	A	N1-C6-N6	6.81	122.68	118.60
36	5	2399	A	N1-C6-N6	6.81	122.68	118.60
36	1	2714	G	C4-C5-C6	-6.80	114.72	118.80
36	1	32	U	O5'-P-OP2	-6.80	99.58	105.70
36	1	1480	G	N1-C6-O6	6.80	123.98	119.90
38	4	9	A	O5'-P-OP2	-6.80	99.58	105.70
36	5	1851	G	C6-C5-N7	-6.80	126.32	130.40
36	5	2385	G	C4-N9-C1'	-6.80	117.66	126.50
36	5	2617	U	N1-C2-O2	-6.80	118.04	122.80
36	1	2866	U	N1-C2-O2	6.80	127.56	122.80
36	1	835	G	O4'-C1'-N9	6.80	113.64	108.20
36	1	3034	C	N1-C2-O2	6.80	122.98	118.90
37	7	87	G	N1-C6-O6	6.80	123.98	119.90
36	1	859	G	N3-C4-N9	6.80	130.08	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	20	G	N1-C6-O6	6.79	123.98	119.90
1	6	696	C	O4'-C1'-N1	6.79	113.64	108.20
36	5	425	G	C8-N9-C4	6.79	109.12	106.40
36	1	984	G	C6-C5-N7	-6.79	126.33	130.40
36	1	3319	U	P-O3'-C3'	6.79	127.85	119.70
36	5	665	A	N1-C6-N6	6.79	122.67	118.60
36	5	1151	U	N3-C4-O4	6.79	124.15	119.40
36	5	3197	G	N3-C4-C5	6.79	131.99	128.60
36	5	1110	U	N3-C2-O2	-6.79	117.45	122.20
36	1	2968	G	N1-C6-O6	6.79	123.97	119.90
36	1	3207	U	C5-C4-O4	6.79	129.97	125.90
36	5	940	G	C5-C6-O6	-6.78	124.53	128.60
1	2	597	G	C4-N9-C1'	6.78	135.31	126.50
36	1	1366	A	C8-N9-C4	-6.78	103.09	105.80
36	1	2886	U	N3-C4-O4	6.78	124.15	119.40
36	5	1500	G	C8-N9-C4	6.78	109.11	106.40
36	5	2186	U	C5-C4-O4	6.78	129.97	125.90
1	2	1432	U	C6-N1-C2	6.78	125.07	121.00
36	1	2643	A	C8-N9-C4	6.78	108.51	105.80
1	6	1473	U	C5-C4-O4	6.78	129.97	125.90
36	5	2114	C	OP1-P-OP2	6.78	129.77	119.60
36	1	821	U	C5-C4-O4	6.78	129.97	125.90
36	5	1124	U	N3-C4-O4	-6.78	114.66	119.40
36	5	2142	A	C5-C6-N1	6.77	121.09	117.70
36	5	3141	A	C4-C5-C6	6.77	120.39	117.00
36	5	1321	G	N9-C4-C5	-6.77	102.69	105.40
1	2	1300	A	O5'-P-OP1	-6.77	99.61	105.70
36	1	67	A	O5'-P-OP1	-6.77	99.61	105.70
36	1	394	G	C8-N9-C4	-6.77	103.69	106.40
36	1	498	A	N1-C6-N6	-6.77	114.54	118.60
36	1	2808	A	C6-C5-N7	-6.77	127.56	132.30
36	1	2877	G	N9-C4-C5	6.77	108.11	105.40
1	6	139	C	C6-N1-C2	-6.77	117.59	120.30
1	6	687	G	N3-C2-N2	-6.77	115.16	119.90
1	6	1129	U	N3-C4-O4	-6.77	114.66	119.40
36	5	940	G	N3-C2-N2	-6.77	115.16	119.90
36	5	1483	G	O4'-C1'-N9	6.77	113.61	108.20
36	5	2968	G	N1-C6-O6	-6.77	115.84	119.90
1	2	1189	A	C8-N9-C4	6.77	108.51	105.80
36	1	1411	C	N3-C4-C5	6.77	124.61	121.90
1	6	577	G	N1-C6-O6	6.76	123.96	119.90
36	1	870	G	O5'-P-OP2	-6.76	99.61	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	960	U	N3-C4-O4	-6.76	114.67	119.40
36	1	1429	G	C6-N1-C2	-6.76	121.04	125.10
36	1	2343	C	N3-C4-C5	6.76	124.61	121.90
36	1	983	A	N1-C2-N3	6.76	132.68	129.30
36	5	437	G	N3-C2-N2	-6.76	115.17	119.90
36	5	1164	G	C8-N9-C4	6.76	109.10	106.40
36	5	3144	G	N3-C4-C5	-6.76	125.22	128.60
36	1	112	U	N3-C2-O2	-6.76	117.47	122.20
36	1	2369	G	C2-N3-C4	6.76	115.28	111.90
36	1	112	U	N1-C2-O2	6.75	127.53	122.80
36	1	2639	G	N1-C2-N3	6.75	127.95	123.90
36	1	439	C	C6-N1-C1'	-6.75	112.70	120.80
36	1	697	A	N9-C4-C5	-6.75	103.10	105.80
36	5	2283	G	O5'-P-OP2	-6.75	99.63	105.70
36	5	3362	A	C8-N9-C4	-6.75	103.10	105.80
36	5	821	U	N1-C2-N3	6.75	118.95	114.90
36	1	25	U	N3-C4-C5	-6.74	110.55	114.60
37	3	57	G	N1-C6-O6	-6.74	115.85	119.90
36	1	1849	C	N3-C2-O2	6.74	126.62	121.90
36	5	2661	G	N3-C4-C5	-6.74	125.23	128.60
36	1	221	A	C8-N9-C4	-6.74	103.10	105.80
1	6	172	C	C6-N1-C2	-6.74	117.60	120.30
36	5	838	G	N1-C6-O6	-6.74	115.86	119.90
36	1	2917	G	C2-N3-C4	6.74	115.27	111.90
1	6	1769	U	N3-C2-O2	6.74	126.92	122.20
36	5	1361	U	C6-N1-C2	-6.74	116.96	121.00
36	5	2663	G	O5'-P-OP2	-6.73	99.64	105.70
36	5	50	U	O5'-P-OP1	-6.73	99.64	105.70
36	5	922	U	C5-C4-O4	6.73	129.94	125.90
36	5	2691	A	C8-N9-C4	-6.73	103.11	105.80
36	5	1372	C	C6-N1-C2	6.73	122.99	120.30
36	5	1856	C	C6-N1-C2	-6.73	117.61	120.30
36	5	2756	C	OP2-P-O3'	6.73	120.00	105.20
36	5	2953	U	C5-C4-O4	-6.73	121.86	125.90
36	1	2423	U	O5'-P-OP2	-6.72	99.65	105.70
1	2	1595	U	O4'-C1'-N1	6.72	113.58	108.20
36	1	2651	G	C5-C6-O6	6.72	132.63	128.60
36	1	3045	G	C2-N3-C4	6.72	115.26	111.90
36	1	3057	U	N3-C4-O4	-6.72	114.69	119.40
1	6	371	G	C4-N9-C1'	6.72	135.24	126.50
1	6	1596	C	N3-C2-O2	-6.72	117.19	121.90
36	5	1367	G	C6-C5-N7	-6.72	126.37	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1150	G	C8-N9-C4	6.72	109.09	106.40
36	5	1155	C	O5'-P-OP1	-6.72	99.65	105.70
36	5	2639	G	C6-C5-N7	-6.72	126.37	130.40
36	5	2901	G	O5'-P-OP2	-6.72	99.65	105.70
36	1	2993	G	N9-C4-C5	-6.72	102.71	105.40
37	3	102	A	N1-C6-N6	6.72	122.63	118.60
36	1	81	C	C2-N3-C4	-6.72	116.54	119.90
36	1	2660	G	C5-C6-O6	-6.72	124.57	128.60
1	6	163	G	N3-C2-N2	-6.72	115.20	119.90
38	8	74	U	C5-C4-O4	-6.72	121.87	125.90
1	2	1493	A	O4'-C1'-N9	6.71	113.57	108.20
36	1	2937	G	C8-N9-C4	6.71	109.09	106.40
36	5	927	C	N3-C2-O2	6.71	126.60	121.90
36	5	1140	G	OP1-P-O3'	6.71	119.97	105.20
36	5	3177	G	C5-C6-O6	6.71	132.63	128.60
36	5	2710	C	N1-C2-O2	-6.71	114.87	118.90
1	6	1002	G	C5-C6-O6	-6.71	124.57	128.60
36	5	1370	G	N1-C2-N2	-6.71	110.16	116.20
36	5	3262	U	O5'-P-OP2	-6.71	99.66	105.70
36	1	968	G	C6-C5-N7	-6.71	126.38	130.40
36	1	3373	U	C5-C6-N1	-6.71	119.34	122.70
36	5	128	G	N1-C6-O6	6.71	123.92	119.90
36	5	337	G	C8-N9-C4	-6.71	103.72	106.40
36	5	2715	A	O5'-P-OP2	-6.71	99.66	105.70
36	1	2417	U	C2-N3-C4	-6.70	122.98	127.00
36	1	3103	A	O5'-P-OP2	-6.70	99.67	105.70
37	3	48	U	N1-C2-O2	6.70	127.49	122.80
36	1	1481	A	N7-C8-N9	6.70	117.15	113.80
36	1	2946	A	C4-C5-N7	6.70	114.05	110.70
51	M5	12	ARG	NE-CZ-NH1	-6.70	116.95	120.30
36	5	2429	G	C8-N9-C4	-6.70	103.72	106.40
36	5	3335	A	N1-C6-N6	6.70	122.62	118.60
1	6	296	U	O5'-P-OP1	6.70	118.73	110.70
36	5	995	U	O5'-P-OP1	-6.70	99.67	105.70
37	7	108	A	C5-C6-N6	-6.70	118.34	123.70
1	2	145	A	C8-N9-C4	-6.69	103.12	105.80
36	5	2350	C	O5'-P-OP1	6.69	118.73	110.70
38	8	109	A	C5-C6-N1	6.69	121.05	117.70
36	1	108	A	N1-C6-N6	-6.69	114.59	118.60
36	1	652	G	N1-C2-N2	-6.69	110.18	116.20
36	5	2403	G	O5'-P-OP1	6.69	118.73	110.70
36	1	2946	A	C6-C5-N7	-6.69	127.62	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2138	A	C5-N7-C8	-6.69	100.56	103.90
36	1	3217	C	N3-C2-O2	-6.69	117.22	121.90
36	1	920	A	C6-N1-C2	-6.69	114.59	118.60
36	1	3181	C	C6-N1-C2	-6.69	117.62	120.30
36	1	3344	A	O4'-C1'-N9	6.69	113.55	108.20
36	1	1789	G	C8-N9-C4	6.68	109.07	106.40
36	1	2798	C	C6-N1-C2	-6.68	117.63	120.30
36	5	3086	A	O5'-P-OP1	-6.68	99.69	105.70
1	2	992	A	N3-C4-C5	6.68	131.48	126.80
36	1	2983	C	C5-C4-N4	6.68	124.88	120.20
1	6	75	U	N1-C2-O2	6.68	127.48	122.80
1	6	512	A	C5-C6-N6	-6.68	118.36	123.70
36	5	1329	U	C2-N1-C1'	6.68	125.72	117.70
36	1	627	U	N3-C2-O2	6.68	126.87	122.20
36	1	1097	G	C8-N9-C4	-6.68	103.73	106.40
1	6	99	C	N3-C2-O2	-6.67	117.23	121.90
36	5	2751	G	C5-N7-C8	-6.67	100.96	104.30
36	1	1343	A	C5-C6-N6	-6.67	118.36	123.70
36	1	1901	A	N1-C6-N6	-6.67	114.60	118.60
36	1	2728	G	N3-C4-N9	6.67	130.00	126.00
36	5	3144	G	N7-C8-N9	6.67	116.44	113.10
36	1	1279	C	C6-N1-C2	-6.67	117.63	120.30
36	5	1043	C	N3-C2-O2	-6.67	117.23	121.90
36	5	2650	U	N3-C4-C5	6.67	118.60	114.60
37	7	37	G	N3-C4-N9	6.67	130.00	126.00
1	2	1329	A	N1-C6-N6	6.67	122.60	118.60
36	1	1131	G	C4-C5-N7	6.67	113.47	110.80
36	5	1127	G	O5'-P-OP2	-6.67	99.70	105.70
36	5	2798	C	N3-C4-N4	-6.67	113.33	118.00
1	2	1560	U	C5-C4-O4	6.67	129.90	125.90
36	5	1060	U	N3-C4-O4	-6.66	114.74	119.40
36	1	2728	G	C2-N3-C4	6.66	115.23	111.90
36	1	34	A	C5-N7-C8	-6.66	100.57	103.90
1	2	1241	G	O4'-C1'-N9	6.66	113.53	108.20
36	1	800	G	N3-C2-N2	-6.66	115.24	119.90
36	5	2174	G	N1-C6-O6	6.66	123.89	119.90
36	1	1382	G	C8-N9-C4	6.65	109.06	106.40
36	5	3293	U	C6-N1-C2	6.65	124.99	121.00
1	2	1596	C	N3-C2-O2	-6.65	117.24	121.90
36	1	372	A	O5'-P-OP2	-6.65	99.71	105.70
36	5	2940	A	C5-C6-N6	-6.65	118.38	123.70
36	5	831	G	C2-N3-C4	6.65	115.22	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2400	G	N9-C4-C5	-6.65	102.74	105.40
36	1	2147	A	C8-N9-C4	6.65	108.46	105.80
1	6	65	A	C2-N3-C4	-6.65	107.28	110.60
36	1	290	G	C8-N9-C4	-6.65	103.74	106.40
36	1	646	A	C2-N3-C4	-6.65	107.28	110.60
36	1	1425	U	N1-C2-N3	6.65	118.89	114.90
1	6	337	G	C4-N9-C1'	6.65	135.14	126.50
36	5	2824	G	C5-C6-O6	-6.65	124.61	128.60
36	5	2874	G	N1-C6-O6	-6.65	115.91	119.90
36	5	3223	A	N1-C6-N6	-6.65	114.61	118.60
36	1	659	G	C2-N3-C4	6.64	115.22	111.90
36	5	2841	G	OP1-P-OP2	6.64	129.57	119.60
36	1	915	A	N1-C6-N6	-6.64	114.61	118.60
36	1	1149	G	O4'-C1'-N9	6.64	113.51	108.20
1	6	542	A	C8-N9-C4	-6.64	103.14	105.80
36	1	648	C	O5'-P-OP1	-6.64	99.72	105.70
36	1	2756	C	N3-C4-N4	6.64	122.65	118.00
36	1	53	G	N3-C4-N9	6.64	129.98	126.00
36	1	107	A	N1-C6-N6	6.64	122.58	118.60
37	3	12	U	N3-C2-O2	6.64	126.84	122.20
1	6	75	U	N3-C2-O2	-6.64	117.56	122.20
36	5	2345	A	N9-C4-C5	-6.63	103.15	105.80
38	8	20	U	O5'-P-OP1	6.63	118.66	110.70
1	6	383	G	C8-N9-C4	-6.63	103.75	106.40
36	5	921	A	C8-N9-C4	-6.63	103.15	105.80
38	8	109	A	C5-C6-N6	-6.63	118.39	123.70
36	5	2831	G	C5-C6-O6	-6.63	124.62	128.60
36	1	590	G	C4-C5-N7	6.63	113.45	110.80
36	1	646	A	N1-C2-N3	6.63	132.61	129.30
36	1	424	G	C8-N9-C4	6.63	109.05	106.40
36	1	1296	C	C6-N1-C2	-6.63	117.65	120.30
38	8	125	U	N1-C2-O2	6.62	127.44	122.80
36	1	669	U	C6-N1-C2	6.62	124.97	121.00
36	5	2628	A	C6-N1-C2	-6.62	114.63	118.60
36	1	3107	U	O5'-P-OP2	-6.62	99.74	105.70
24	d2	93	LEU	CA-CB-CG	6.62	130.53	115.30
36	1	3214	U	O4'-C1'-N1	6.62	113.50	108.20
36	1	788	C	C2-N1-C1'	-6.62	111.52	118.80
36	1	1838	G	C5-C6-O6	-6.62	124.63	128.60
1	2	728	U	N1-C2-O2	6.62	127.43	122.80
36	5	2314	U	C5-C4-O4	-6.62	121.93	125.90
36	5	2696	A	OP2-P-O3'	6.62	119.76	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1149	G	C4-C5-C6	6.62	122.77	118.80
36	1	66	A	O5'-P-OP1	-6.61	99.75	105.70
36	1	1103	A	O5'-P-OP2	6.61	118.64	110.70
36	5	2623	G	N9-C4-C5	-6.61	102.75	105.40
36	5	2943	G	N1-C6-O6	6.61	123.87	119.90
1	2	1041	G	C8-N9-C4	-6.61	103.76	106.40
36	1	708	G	N7-C8-N9	6.61	116.41	113.10
36	5	2899	C	C2-N1-C1'	6.61	126.07	118.80
37	7	47	C	C2-N3-C4	-6.61	116.60	119.90
1	2	61	A	C5-N7-C8	-6.60	100.60	103.90
36	1	946	U	N1-C2-N3	6.60	118.86	114.90
36	1	1144	U	C5-C6-N1	-6.60	119.40	122.70
36	5	1378	U	C6-N1-C2	6.60	124.96	121.00
36	5	2341	A	C8-N9-C4	6.60	108.44	105.80
36	5	879	U	N1-C2-N3	6.60	118.86	114.90
31	D9	36	LEU	CA-CB-CG	6.60	130.48	115.30
36	1	3076	C	C6-N1-C2	-6.60	117.66	120.30
36	5	1481	A	P-O3'-C3'	6.60	127.62	119.70
36	1	1604	G	N7-C8-N9	6.60	116.40	113.10
44	L7	160	ARG	NE-CZ-NH2	-6.60	117.00	120.30
36	5	1848	G	C5-C6-O6	-6.60	124.64	128.60
36	5	2412	G	N3-C4-C5	-6.60	125.30	128.60
36	5	2976	A	N1-C6-N6	-6.60	114.64	118.60
36	1	1520	G	N7-C8-N9	-6.59	109.80	113.10
36	1	2298	U	N3-C4-O4	-6.59	114.78	119.40
1	6	1109	G	O5'-P-OP1	-6.59	99.77	105.70
36	5	1321	G	C8-N9-C1'	-6.59	118.43	127.00
36	5	3309	G	N3-C4-C5	-6.59	125.30	128.60
12	C0	88	PRO	N-CA-CB	6.59	111.21	103.30
36	1	1360	C	O5'-P-OP1	-6.59	99.77	105.70
36	5	2234	G	C5-C6-O6	-6.59	124.65	128.60
36	5	3335	A	C6-C5-N7	-6.59	127.69	132.30
36	1	1300	G	C5-C6-O6	-6.59	124.65	128.60
36	5	871	U	N1-C2-N3	6.59	118.85	114.90
36	1	895	A	N7-C8-N9	6.58	117.09	113.80
36	1	1390	A	N1-C2-N3	6.58	132.59	129.30
1	6	630	A	N1-C6-N6	6.58	122.55	118.60
36	5	2211	U	C5-C4-O4	6.58	129.85	125.90
36	5	2920	U	N1-C2-O2	-6.58	118.19	122.80
36	1	2629	U	O5'-P-OP1	6.58	118.60	110.70
36	5	942	U	N3-C2-O2	6.58	126.81	122.20
1	2	1778	G	C5-C6-O6	6.58	132.55	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1520	G	C5-N7-C8	6.58	107.59	104.30
36	5	2358	A	C8-N9-C4	6.58	108.43	105.80
1	2	447	U	C6-N1-C2	-6.58	117.06	121.00
36	1	388	G	N3-C2-N2	-6.58	115.30	119.90
36	1	685	G	N1-C6-O6	6.58	123.84	119.90
36	1	1428	A	C5-N7-C8	-6.58	100.61	103.90
36	5	227	G	O5'-P-OP2	-6.58	99.78	105.70
36	5	1189	C	N1-C2-O2	-6.57	114.96	118.90
36	5	1591	G	C8-N9-C4	-6.57	103.77	106.40
36	1	3195	U	N3-C2-O2	-6.57	117.60	122.20
49	m3	21	ARG	NE-CZ-NH1	-6.57	117.02	120.30
36	1	968	G	N3-C4-C5	-6.57	125.32	128.60
1	2	1486	G	N7-C8-N9	6.56	116.38	113.10
38	4	24	G	N1-C6-O6	6.56	123.84	119.90
36	1	290	G	N9-C4-C5	6.56	108.03	105.40
36	5	1786	G	N1-C6-O6	-6.56	115.96	119.90
37	7	104	A	N1-C6-N6	6.56	122.54	118.60
36	1	639	G	N1-C6-O6	6.56	123.84	119.90
36	1	658	G	C4-N9-C1'	6.56	135.03	126.50
36	1	1156	C	C2-N3-C4	-6.56	116.62	119.90
36	5	1115	G	C8-N9-C1'	-6.56	118.47	127.00
38	4	113	U	N1-C2-N3	6.56	118.83	114.90
1	6	1100	G	N3-C4-N9	6.56	129.93	126.00
36	5	3008	A	N1-C2-N3	6.56	132.58	129.30
36	1	2572	C	N3-C2-O2	-6.56	117.31	121.90
1	2	969	C	N1-C2-O2	-6.55	114.97	118.90
1	6	385	A	N1-C6-N6	-6.55	114.67	118.60
1	6	1019	A	C8-N9-C4	6.55	108.42	105.80
36	5	1894	U	N1-C2-O2	-6.55	118.21	122.80
36	5	1460	A	N1-C6-N6	6.55	122.53	118.60
36	5	2426	U	C5-C4-O4	6.55	129.83	125.90
36	1	229	G	N3-C2-N2	-6.55	115.31	119.90
36	5	1042	U	N3-C4-O4	-6.55	114.81	119.40
36	5	1520	G	C5-C6-O6	-6.55	124.67	128.60
38	8	33	A	N1-C6-N6	6.55	122.53	118.60
36	1	405	U	C5-C4-O4	-6.55	121.97	125.90
36	1	726	G	O5'-P-OP1	-6.55	99.81	105.70
36	1	1103	A	O5'-P-OP1	-6.55	99.81	105.70
36	5	2271	A	N7-C8-N9	-6.55	110.53	113.80
36	5	2385	G	C8-N9-C4	6.55	109.02	106.40
1	2	1654	G	N1-C2-N2	-6.55	110.31	116.20
36	1	2550	U	C5-C4-O4	6.55	129.83	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	216	G	C8-N9-C4	-6.55	103.78	106.40
36	1	961	C	C4-C5-C6	6.55	120.67	117.40
73	O7	45	ARG	NE-CZ-NH1	-6.55	117.03	120.30
36	5	2816	G	N9-C4-C5	-6.54	102.78	105.40
55	M9	138	LEU	CA-CB-CG	6.54	130.35	115.30
36	5	2315	G	O5'-P-OP1	-6.54	99.81	105.70
36	1	650	C	OP2-P-O3'	6.54	119.59	105.20
36	1	2309	A	N1-C6-N6	6.54	122.52	118.60
36	1	2869	U	O5'-P-OP1	-6.54	99.81	105.70
36	5	656	A	C8-N9-C4	6.54	108.42	105.80
36	1	188	U	N3-C4-C5	-6.54	110.68	114.60
36	1	197	G	C4-C5-N7	6.54	113.42	110.80
36	5	1152	G	C8-N9-C1'	6.54	135.50	127.00
36	1	997	A	C4-C5-C6	6.54	120.27	117.00
36	1	324	A	N1-C2-N3	6.53	132.57	129.30
36	1	426	G	N3-C4-N9	6.53	129.92	126.00
36	1	1429	G	C2-N3-C4	6.53	115.17	111.90
36	5	2382	G	N1-C6-O6	-6.53	115.98	119.90
36	5	2719	U	C2-N1-C1'	-6.53	109.86	117.70
36	1	581	U	OP2-P-O3'	6.53	119.56	105.20
36	1	1187	C	C6-N1-C2	6.53	122.91	120.30
36	1	614	C	C6-N1-C2	6.52	122.91	120.30
36	1	820	A	C8-N9-C4	-6.52	103.19	105.80
36	1	1481	A	C4-C5-N7	6.52	113.96	110.70
36	1	2244	A	O5'-P-OP2	-6.52	99.83	105.70
36	1	2306	C	N3-C4-N4	-6.52	113.44	118.00
36	5	2799	A	N9-C4-C5	6.52	108.41	105.80
36	5	2190	U	N1-C2-N3	6.52	118.81	114.90
36	5	1445	U	C2-N3-C4	-6.52	123.09	127.00
36	1	2816	G	C5-C6-O6	-6.51	124.69	128.60
36	1	1346	G	N3-C4-C5	6.51	131.86	128.60
36	1	1506	A	N1-C6-N6	-6.51	114.69	118.60
36	1	356	C	O5'-P-OP2	-6.51	99.84	105.70
36	1	2842	U	N1-C2-O2	6.51	127.36	122.80
1	6	557	G	N1-C6-O6	-6.51	116.00	119.90
36	5	927	C	N3-C4-N4	6.51	122.56	118.00
36	1	50	U	C6-N1-C2	-6.51	117.10	121.00
36	1	2355	G	C5-C6-N1	-6.51	108.25	111.50
36	5	1154	A	N9-C4-C5	6.51	108.40	105.80
36	5	3197	G	N9-C4-C5	6.51	108.00	105.40
38	8	54	A	N1-C6-N6	6.51	122.50	118.60
36	5	1192	C	N3-C4-C5	6.50	124.50	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1941	C	C6-N1-C2	-6.50	117.70	120.30
36	5	2411	U	C5-C6-N1	-6.50	119.45	122.70
12	c0	97	PRO	N-CA-CB	6.50	111.10	103.30
36	5	220	G	O5'-P-OP2	-6.50	99.85	105.70
36	5	1876	U	C5-C6-N1	-6.50	119.45	122.70
36	5	2943	G	N9-C4-C5	-6.50	102.80	105.40
36	1	197	G	N1-C6-O6	6.50	123.80	119.90
36	1	394	G	N9-C4-C5	6.50	108.00	105.40
35	sM	167	PRO	N-CA-CB	6.50	111.10	103.30
36	5	2327	U	C5-C6-N1	-6.50	119.45	122.70
38	8	20	U	O5'-P-OP2	-6.50	99.85	105.70
1	2	581	U	C2-N1-C1'	6.50	125.49	117.70
36	5	2356	A	C6-N1-C2	6.50	122.50	118.60
36	1	1317	A	C2-N3-C4	6.49	113.85	110.60
36	1	2601	A	N7-C8-N9	-6.49	110.55	113.80
1	6	1463	C	C6-N1-C2	6.49	122.90	120.30
1	6	1765	A	C8-N9-C4	6.49	108.40	105.80
36	5	2245	C	N3-C4-C5	-6.49	119.30	121.90
36	5	2645	G	C5-C6-N1	6.49	114.75	111.50
36	1	993	G	N3-C4-C5	-6.49	125.35	128.60
36	1	1154	A	N1-C2-N3	6.49	132.55	129.30
1	6	1022	C	O5'-P-OP1	-6.49	99.86	105.70
36	5	1313	G	O5'-P-OP2	-6.49	99.86	105.70
36	5	1321	G	N1-C6-O6	6.49	123.80	119.90
36	1	1412	G	OP1-P-OP2	-6.49	109.87	119.60
36	1	2859	U	O5'-P-OP1	-6.49	99.86	105.70
36	1	196	G	N9-C4-C5	-6.48	102.81	105.40
36	1	1428	A	C6-C5-N7	-6.48	127.76	132.30
36	1	1713	G	N3-C4-C5	6.48	131.84	128.60
36	1	2726	C	N1-C2-N3	6.48	123.74	119.20
1	6	321	C	N1-C2-O2	6.48	122.79	118.90
36	5	2759	U	C4-C5-C6	6.48	123.59	119.70
10	S8	29	LEU	CA-CB-CG	6.48	130.21	115.30
1	6	1619	C	C6-N1-C2	-6.48	117.71	120.30
36	5	2399	A	C8-N9-C4	6.48	108.39	105.80
36	5	1468	A	C6-C5-N7	-6.48	127.77	132.30
1	2	377	G	N3-C2-N2	-6.48	115.36	119.90
18	C6	40	GLU	C-N-CD	-6.48	106.35	120.60
1	6	558	U	P-O3'-C3'	6.48	127.47	119.70
1	6	1162	C	C6-N1-C2	-6.48	117.71	120.30
36	5	739	G	O5'-P-OP1	-6.48	99.87	105.70
36	5	2385	G	C2-N3-C4	-6.48	108.66	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	272	U	C2-N1-C1'	6.48	125.47	117.70
36	5	1302	A	O5'-P-OP2	6.48	118.47	110.70
36	5	2435	G	N1-C6-O6	6.48	123.79	119.90
36	1	1103	A	C8-N9-C4	6.47	108.39	105.80
36	5	2304	C	C6-N1-C2	-6.47	117.71	120.30
36	5	2624	G	C6-C5-N7	-6.47	126.52	130.40
37	7	49	G	C8-N9-C4	6.47	108.99	106.40
36	1	2618	G	C5-C6-O6	6.47	132.48	128.60
36	5	2267	C	N3-C4-C5	6.47	124.49	121.90
59	n3	87	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	2	354	C	C6-N1-C2	-6.47	117.71	120.30
56	N0	115	ARG	NE-CZ-NH2	-6.47	117.07	120.30
36	1	2899	C	N3-C2-O2	-6.46	117.38	121.90
36	1	3362	A	C4-C5-N7	6.46	113.93	110.70
36	5	1158	A	C5-C6-N6	-6.46	118.53	123.70
1	2	377	G	N3-C4-N9	-6.46	122.12	126.00
36	1	810	A	C6-N1-C2	-6.46	114.72	118.60
36	1	1370	G	C8-N9-C4	-6.46	103.82	106.40
1	6	1745	G	N3-C4-N9	6.46	129.88	126.00
36	5	1639	C	C6-N1-C2	-6.46	117.72	120.30
36	1	2610	G	C5-C6-O6	-6.46	124.73	128.60
36	5	1160	C	C2-N1-C1'	-6.46	111.70	118.80
36	5	2836	C	C4-C5-C6	6.46	120.63	117.40
36	5	3105	U	C2-N3-C4	-6.46	123.13	127.00
36	5	433	A	N1-C2-N3	6.46	132.53	129.30
36	5	2948	C	O5'-P-OP1	6.46	118.45	110.70
1	2	590	C	C2-N1-C1'	6.45	125.90	118.80
36	1	1585	C	N3-C4-C5	6.45	124.48	121.90
36	1	3212	C	O5'-P-OP1	6.45	118.44	110.70
36	5	656	A	O5'-P-OP2	-6.45	99.89	105.70
36	5	891	G	OP1-P-OP2	-6.45	109.92	119.60
36	1	2352	A	O5'-P-OP2	-6.45	99.89	105.70
36	1	3306	U	N1-C2-O2	6.45	127.31	122.80
36	5	350	C	N3-C2-O2	-6.45	117.39	121.90
36	1	2138	A	C8-N9-C4	-6.45	103.22	105.80
1	2	1199	G	C4-N9-C1'	6.45	134.88	126.50
1	2	1778	G	N1-C6-O6	-6.44	116.03	119.90
36	1	2393	G	C5-C6-O6	-6.44	124.73	128.60
36	5	884	A	N1-C6-N6	6.44	122.47	118.60
36	5	3216	G	N1-C6-O6	6.44	123.77	119.90
1	2	1744	A	O5'-P-OP1	-6.44	99.90	105.70
1	2	1761	U	P-O3'-C3'	6.44	127.43	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	637	C	O4'-C1'-N1	6.44	113.35	108.20
36	1	1367	G	C6-C5-N7	-6.44	126.53	130.40
36	5	1134	G	O5'-P-OP2	-6.44	99.90	105.70
21	C9	57	ARG	NE-CZ-NH1	6.44	123.52	120.30
36	1	721	G	N7-C8-N9	6.44	116.32	113.10
36	5	2345	A	C6-C5-N7	-6.44	127.79	132.30
36	5	2626	A	N9-C4-C5	6.44	108.38	105.80
36	5	639	G	O5'-P-OP1	6.44	118.42	110.70
13	C1	91	LEU	CA-CB-CG	6.43	130.10	115.30
36	1	1906	G	N1-C6-O6	6.43	123.76	119.90
36	1	3009	G	O5'-P-OP2	-6.43	99.91	105.70
36	5	2146	C	C6-N1-C2	6.43	122.87	120.30
36	1	2406	C	C6-N1-C2	6.43	122.87	120.30
36	1	2643	A	N9-C4-C5	-6.43	103.23	105.80
36	1	1495	U	N1-C2-O2	-6.43	118.30	122.80
36	5	1506	A	N1-C6-N6	-6.43	114.74	118.60
24	D2	93	LEU	CA-CB-CG	6.43	130.08	115.30
36	5	2774	C	C6-N1-C2	-6.43	117.73	120.30
36	1	2586	G	O5'-P-OP2	-6.42	99.92	105.70
36	1	2942	C	OP1-P-OP2	-6.42	109.96	119.60
36	1	2958	A	C5-C6-N1	6.42	120.91	117.70
36	5	91	G	C5-C6-O6	-6.42	124.75	128.60
36	5	429	U	C5-C6-N1	-6.42	119.49	122.70
36	1	1198	C	N1-C2-O2	-6.42	115.05	118.90
36	1	3362	A	N1-C6-N6	6.42	122.45	118.60
1	6	422	G	C8-N9-C4	-6.42	103.83	106.40
36	5	2364	G	N3-C4-N9	-6.42	122.15	126.00
36	1	2846	U	N3-C4-O4	-6.42	114.91	119.40
36	5	1542	G	C8-N9-C4	-6.42	103.83	106.40
36	1	780	A	C8-N9-C4	-6.42	103.23	105.80
36	5	1929	G	OP1-P-OP2	-6.42	109.97	119.60
1	6	163	G	C8-N9-C1'	6.42	135.34	127.00
36	1	155	G	N1-C6-O6	-6.42	116.05	119.90
1	6	1269	U	C6-N1-C2	-6.42	117.15	121.00
36	1	1099	A	C6-C5-N7	-6.41	127.81	132.30
36	1	2806	U	N1-C2-O2	-6.41	118.31	122.80
36	1	790	U	N1-C2-N3	6.41	118.75	114.90
36	1	1414	G	N1-C6-O6	6.41	123.75	119.90
1	6	3	U	C6-N1-C2	6.41	124.85	121.00
36	1	933	A	O5'-P-OP2	-6.41	99.93	105.70
36	1	2622	C	C6-N1-C2	-6.41	117.74	120.30
36	1	1343	A	C4-C5-N7	6.41	113.90	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	340	C	O5'-P-OP2	-6.41	99.94	105.70
36	5	2764	C	C5-C4-N4	-6.41	115.72	120.20
61	N5	113	LEU	CB-CG-CD2	-6.40	100.11	111.00
36	5	2406	C	N1-C2-O2	-6.40	115.06	118.90
36	5	1412	G	C8-N9-C4	-6.40	103.84	106.40
1	2	555	A	P-O3'-C3'	6.40	127.38	119.70
1	6	1112	G	C5-C6-N1	6.40	114.70	111.50
36	5	1390	A	C5-C6-N6	6.40	128.82	123.70
36	1	2620	G	N3-C2-N2	-6.40	115.42	119.90
37	7	98	C	O5'-P-OP2	-6.40	99.94	105.70
37	3	98	C	C2-N1-C1'	-6.40	111.76	118.80
1	6	303	U	C5-C4-O4	6.40	129.74	125.90
36	5	1476	G	C8-N9-C4	6.40	108.96	106.40
36	5	2964	G	O5'-P-OP2	-6.40	99.94	105.70
1	6	1600	A	C2-N3-C4	-6.40	107.40	110.60
36	5	346	C	N3-C2-O2	-6.40	117.42	121.90
36	5	864	G	N3-C4-C5	-6.39	125.40	128.60
36	1	3369	G	C4-C5-N7	6.39	113.36	110.80
1	6	339	C	N1-C2-O2	-6.39	115.06	118.90
36	1	2624	G	N7-C8-N9	6.39	116.30	113.10
1	6	976	G	C4-C5-N7	6.39	113.36	110.80
37	7	105	C	N3-C4-C5	-6.39	119.34	121.90
36	1	979	U	O4'-C1'-N1	6.38	113.31	108.20
36	1	1294	A	N1-C6-N6	-6.38	114.77	118.60
36	1	1379	G	N1-C2-N2	-6.38	110.45	116.20
36	1	1556	C	N1-C2-O2	6.38	122.73	118.90
36	1	2374	C	C4-C5-C6	6.38	120.59	117.40
36	5	388	G	N1-C6-O6	6.38	123.73	119.90
36	1	1368	U	O5'-P-OP1	-6.38	99.96	105.70
36	1	1789	G	C5-C6-O6	-6.38	124.77	128.60
1	6	385	A	C5-C6-N6	6.38	128.81	123.70
1	2	51	A	C8-N9-C4	6.38	108.35	105.80
36	1	1392	G	C2-N3-C4	6.38	115.09	111.90
36	1	2325	G	C8-N9-C4	-6.38	103.85	106.40
36	1	2416	U	N3-C4-O4	6.38	123.87	119.40
38	8	47	C	C5-C6-N1	-6.38	117.81	121.00
47	M0	24	ARG	NE-CZ-NH1	6.38	123.49	120.30
36	1	632	G	N3-C4-N9	6.38	129.83	126.00
36	5	942	U	C5-C4-O4	-6.38	122.07	125.90
36	5	2808	A	C6-C5-N7	-6.38	127.84	132.30
36	1	2640	A	C5-C6-N6	-6.38	118.60	123.70
1	6	610	G	N3-C4-N9	6.38	129.83	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1547	G	C8-N9-C4	6.38	108.95	106.40
36	1	232	G	C6-C5-N7	-6.38	126.58	130.40
38	4	99	C	C6-N1-C2	6.38	122.85	120.30
38	4	140	G	C8-N9-C4	-6.38	103.85	106.40
36	1	642	U	C5-C4-O4	6.37	129.72	125.90
36	5	2759	U	N1-C2-N3	6.37	118.72	114.90
36	1	3369	G	C6-C5-N7	-6.37	126.58	130.40
1	6	272	U	N1-C2-O2	6.37	127.26	122.80
36	5	1115	G	N1-C2-N2	-6.37	110.47	116.20
36	1	64	G	N1-C6-O6	-6.37	116.08	119.90
36	1	416	A	C8-N9-C4	6.37	108.35	105.80
1	6	542	A	C4-N9-C1'	6.37	137.76	126.30
36	5	644	G	C4-C5-N7	-6.37	108.25	110.80
36	5	1872	C	N3-C2-O2	-6.37	117.44	121.90
36	5	3046	A	C2-N3-C4	-6.37	107.42	110.60
36	1	716	A	C6-C5-N7	-6.36	127.85	132.30
36	1	1201	C	N3-C4-N4	6.36	122.45	118.00
36	5	634	C	C6-N1-C2	-6.36	117.75	120.30
36	5	1047	A	C5-C6-N6	-6.36	118.61	123.70
55	m9	5	ARG	NE-CZ-NH1	6.36	123.48	120.30
36	1	3078	U	N3-C2-O2	-6.36	117.75	122.20
36	1	1891	A	C2-N3-C4	-6.36	107.42	110.60
36	5	938	C	N3-C4-C5	6.36	124.44	121.90
36	5	2911	A	N1-C2-N3	-6.36	126.12	129.30
36	5	3028	G	O5'-P-OP1	-6.36	99.97	105.70
36	1	2283	G	N3-C2-N2	-6.36	115.45	119.90
36	1	3375	A	O5'-P-OP1	-6.36	99.98	105.70
37	7	22	A	O5'-P-OP1	-6.36	99.98	105.70
37	7	93	C	O5'-P-OP1	6.36	118.33	110.70
36	1	3373	U	C6-N1-C2	6.36	124.81	121.00
1	6	647	G	N9-C4-C5	6.36	107.94	105.40
1	2	144	U	N3-C2-O2	-6.35	117.75	122.20
36	1	2746	A	N1-C6-N6	-6.35	114.79	118.60
1	6	337	G	C4-C5-N7	6.35	113.34	110.80
36	5	3214	U	N3-C2-O2	-6.35	117.75	122.20
36	1	2704	A	C2-N3-C4	-6.35	107.42	110.60
36	1	718	G	N1-C6-O6	6.35	123.71	119.90
1	2	359	A	C8-N9-C4	6.35	108.34	105.80
36	1	1351	U	C2-N1-C1'	6.35	125.31	117.70
36	5	871	U	C5-C4-O4	6.35	129.71	125.90
36	1	2093	A	C2-N3-C4	6.34	113.77	110.60
36	1	2403	G	N3-C4-N9	6.34	129.81	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	647	G	N3-C4-C5	6.34	131.77	128.60
36	5	530	G	N1-C6-O6	-6.34	116.09	119.90
36	5	2283	G	C4-C5-N7	6.34	113.34	110.80
36	1	960	U	C6-N1-C1'	6.34	130.08	121.20
37	7	121	U	C2-N1-C1'	6.34	125.31	117.70
36	1	859	G	C6-C5-N7	-6.34	126.60	130.40
36	5	2635	A	O5'-P-OP2	-6.34	99.99	105.70
36	1	1425	U	C5-C4-O4	6.34	129.70	125.90
36	5	2709	C	C6-N1-C2	6.34	122.83	120.30
1	2	338	C	C6-N1-C2	-6.34	117.77	120.30
36	5	1164	G	N7-C8-N9	-6.34	109.93	113.10
36	5	2833	A	C8-N9-C4	6.34	108.33	105.80
1	2	1202	A	C8-N9-C4	-6.33	103.27	105.80
36	1	1364	C	OP2-P-O3'	6.33	119.14	105.20
36	1	1380	G	O5'-P-OP1	6.33	118.30	110.70
36	1	1480	G	C5-C6-O6	-6.33	124.80	128.60
36	1	1495	U	C2-N3-C4	-6.33	123.20	127.00
36	1	2669	G	C8-N9-C4	6.33	108.93	106.40
36	5	343	U	O5'-P-OP1	-6.33	100.00	105.70
36	5	809	G	C5-C6-O6	-6.33	124.80	128.60
36	5	810	A	C2-N3-C4	6.33	113.77	110.60
36	5	2811	A	N1-C6-N6	-6.33	114.80	118.60
38	4	19	C	C6-N1-C2	-6.33	117.77	120.30
36	1	2960	C	C2-N3-C4	-6.33	116.73	119.90
20	c8	116	LEU	CA-CB-CG	6.33	129.86	115.30
36	5	859	G	C5-C6-N1	6.33	114.67	111.50
36	1	3029	A	C8-N9-C4	-6.33	103.27	105.80
36	5	2412	G	N3-C4-N9	6.33	129.80	126.00
36	1	104	G	N3-C4-N9	6.33	129.80	126.00
36	1	417	A	O5'-P-OP2	-6.33	100.01	105.70
36	1	2865	U	N3-C4-C5	6.33	118.40	114.60
36	1	3022	G	O4'-C1'-N9	6.33	113.26	108.20
36	5	2305	G	C8-N9-C4	-6.33	103.87	106.40
36	1	54	C	C2-N3-C4	-6.33	116.74	119.90
36	1	1834	U	N3-C4-C5	-6.33	110.80	114.60
36	1	2197	C	N1-C2-N3	-6.33	114.77	119.20
1	2	1307	U	C2-N1-C1'	6.32	125.29	117.70
36	1	1381	A	OP1-P-O3'	6.32	119.11	105.20
1	6	542	A	C5-N7-C8	-6.32	100.74	103.90
36	5	1144	U	N1-C2-O2	-6.32	118.37	122.80
36	5	1115	G	N3-C4-C5	-6.32	125.44	128.60
36	1	2148	U	N1-C2-O2	-6.32	118.38	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2246	G	N3-C2-N2	-6.32	115.47	119.90
36	5	2920	U	C2-N3-C4	-6.32	123.21	127.00
36	5	3137	C	N3-C4-N4	-6.32	113.58	118.00
36	1	1392	G	N3-C4-C5	-6.32	125.44	128.60
36	1	1634	G	C8-N9-C4	-6.32	103.87	106.40
36	1	702	C	C5-C4-N4	-6.32	115.78	120.20
36	5	1862	U	O5'-P-OP1	-6.32	100.01	105.70
36	5	1879	A	N1-C6-N6	6.32	122.39	118.60
36	1	955	U	C2-N1-C1'	-6.32	110.12	117.70
1	6	151	G	C6-C5-N7	6.32	134.19	130.40
36	5	1370	G	C5-C6-N1	6.32	114.66	111.50
36	5	2851	A	N1-C2-N3	6.32	132.46	129.30
36	1	424	G	N7-C8-N9	-6.31	109.94	113.10
36	1	2689	A	N1-C6-N6	-6.31	114.81	118.60
36	5	1053	A	N1-C6-N6	-6.31	114.81	118.60
38	8	68	G	C4-N9-C1'	6.31	134.70	126.50
36	1	142	C	C5-C6-N1	6.31	124.16	121.00
36	5	948	C	C6-N1-C2	6.31	122.82	120.30
36	5	1909	A	O5'-P-OP2	-6.31	100.02	105.70
36	5	2857	C	N3-C4-C5	6.31	124.42	121.90
36	1	2850	G	C5-C6-O6	-6.30	124.82	128.60
36	5	1117	G	O5'-P-OP1	-6.30	100.03	105.70
36	1	1120	A	N1-C2-N3	6.30	132.45	129.30
38	8	98	U	N3-C4-C5	-6.30	110.82	114.60
1	2	577	G	C5-C6-O6	-6.30	124.82	128.60
36	1	1838	G	N9-C4-C5	-6.30	102.88	105.40
36	1	3362	A	C2-N3-C4	-6.30	107.45	110.60
36	5	2639	G	C5-C6-O6	-6.30	124.82	128.60
36	1	217	U	OP1-P-O3'	6.30	119.06	105.20
36	1	2764	C	C5-C6-N1	6.30	124.15	121.00
38	4	57	C	C6-N1-C2	6.30	122.82	120.30
36	5	873	C	P-O3'-C3'	6.30	127.26	119.70
36	5	961	C	C4-C5-C6	6.30	120.55	117.40
1	2	1761	U	C5-C4-O4	6.30	129.68	125.90
36	5	3343	G	N3-C4-N9	6.30	129.78	126.00
36	1	2943	G	C6-C5-N7	-6.30	126.62	130.40
36	5	3079	U	C5-C4-O4	6.29	129.68	125.90
36	1	420	G	N1-C6-O6	6.29	123.67	119.90
36	1	1177	G	N3-C2-N2	-6.29	115.50	119.90
36	5	632	G	N3-C4-C5	-6.29	125.45	128.60
36	5	2755	C	O5'-P-OP1	-6.29	100.04	105.70
36	1	3118	C	N3-C4-C5	-6.29	119.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	297	G	O4'-C1'-N9	6.29	113.23	108.20
36	5	2156	C	C6-N1-C2	6.29	122.81	120.30
36	1	968	G	N3-C4-N9	6.29	129.77	126.00
36	1	1366	A	C5-N7-C8	-6.29	100.76	103.90
36	1	2777	G	N9-C4-C5	6.29	107.91	105.40
1	6	1039	A	O4'-C1'-N9	6.29	113.23	108.20
36	5	2245	C	N3-C2-O2	-6.29	117.50	121.90
36	1	805	G	C8-N9-C4	6.28	108.91	106.40
1	6	1104	U	OP2-P-O3'	6.28	119.02	105.20
1	6	1129	U	C2-N1-C1'	-6.28	110.16	117.70
36	1	343	U	C6-N1-C2	-6.28	117.23	121.00
36	1	676	G	C8-N9-C4	-6.28	103.89	106.40
36	1	916	G	P-O3'-C3'	6.28	127.23	119.70
36	1	2424	A	N1-C2-N3	-6.28	126.16	129.30
1	2	581	U	C5-C6-N1	6.28	125.84	122.70
36	1	644	G	C8-N9-C4	-6.28	103.89	106.40
36	1	1416	C	N3-C4-C5	6.28	124.41	121.90
1	6	65	A	C4-C5-N7	6.28	113.84	110.70
1	6	609	U	C5-C6-N1	-6.28	119.56	122.70
36	5	998	A	O5'-P-OP1	-6.28	100.05	105.70
36	1	3344	A	C5-N7-C8	-6.27	100.76	103.90
1	6	1139	A	N1-C6-N6	-6.27	114.83	118.60
36	1	1116	G	OP2-P-O3'	6.27	119.00	105.20
56	n0	13	ARG	NE-CZ-NH1	6.27	123.44	120.30
38	4	103	G	C8-N9-C4	-6.27	103.89	106.40
1	6	438	A	N9-C4-C5	-6.27	103.29	105.80
1	6	1764	C	N3-C4-C5	6.27	124.41	121.90
36	5	984	G	C4-C5-C6	6.27	122.56	118.80
36	5	2116	G	N1-C6-O6	6.27	123.66	119.90
36	5	2808	A	N9-C4-C5	-6.27	103.29	105.80
36	5	2617	U	N3-C4-C5	-6.27	110.84	114.60
1	2	1199	G	C8-N9-C1'	-6.27	118.86	127.00
36	1	2191	U	O5'-P-OP2	-6.27	100.06	105.70
36	1	2639	G	C6-C5-N7	-6.27	126.64	130.40
36	5	2623	G	C8-N9-C4	6.27	108.91	106.40
36	1	2624	G	C6-C5-N7	-6.26	126.64	130.40
36	1	2831	G	C5-C6-N1	-6.26	108.37	111.50
36	1	2937	G	C4-C5-N7	-6.26	108.29	110.80
1	6	65	A	N9-C4-C5	-6.26	103.29	105.80
36	5	1834	U	N1-C2-N3	6.26	118.66	114.90
1	2	429	G	C8-N9-C4	-6.26	103.89	106.40
36	1	1099	A	N9-C4-C5	-6.26	103.30	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1933	A	O5'-P-OP1	-6.26	100.06	105.70
36	1	2298	U	O5'-P-OP2	-6.26	100.06	105.70
36	1	2624	G	C5-C6-O6	-6.26	124.84	128.60
36	5	1149	G	N9-C1'-C2'	-6.26	105.11	112.00
36	5	1199	C	C4-C5-C6	6.26	120.53	117.40
36	5	2143	A	C8-N9-C4	-6.26	103.30	105.80
36	5	2899	C	N3-C2-O2	-6.26	117.52	121.90
36	5	424	G	C4-C5-N7	6.26	113.30	110.80
36	5	807	A	N1-C6-N6	6.26	122.36	118.60
36	5	2350	C	C6-N1-C2	-6.26	117.80	120.30
36	1	1437	C	C2-N1-C1'	6.26	125.68	118.80
1	6	1087	A	C2-N3-C4	-6.26	107.47	110.60
1	6	1481	C	N3-C2-O2	-6.26	117.52	121.90
36	5	417	A	OP2-P-O3'	6.26	118.97	105.20
36	1	970	A	C5-N7-C8	-6.25	100.77	103.90
36	1	1116	G	C6-C5-N7	-6.25	126.65	130.40
36	1	1586	G	O5'-P-OP2	-6.25	100.07	105.70
36	5	817	A	C2-N3-C4	6.25	113.73	110.60
36	5	2400	G	N3-C4-C5	6.25	131.73	128.60
52	M6	84	LEU	CB-CG-CD2	-6.25	100.37	111.00
36	5	2411	U	N3-C4-C5	6.25	118.35	114.60
36	5	2821	C	N3-C2-O2	6.25	126.28	121.90
36	1	2403	G	O5'-P-OP1	-6.25	100.07	105.70
36	5	98	G	N3-C4-C5	6.25	131.73	128.60
36	5	881	C	C2-N1-C1'	6.25	125.68	118.80
36	5	2816	G	N7-C8-N9	-6.25	109.97	113.10
36	5	69	C	C6-N1-C2	-6.25	117.80	120.30
36	5	879	U	N3-C4-O4	6.25	123.78	119.40
36	5	1884	A	N1-C6-N6	6.25	122.35	118.60
36	1	919	U	O5'-P-OP1	6.25	118.20	110.70
36	1	1373	A	OP2-P-O3'	6.25	118.95	105.20
37	3	30	G	N3-C4-C5	-6.25	125.47	128.60
1	6	1535	U	C5-C6-N1	-6.25	119.58	122.70
36	5	2729	U	N1-C2-O2	6.25	127.17	122.80
36	5	1338	C	N3-C4-N4	6.25	122.37	118.00
36	5	2730	G	C5-C6-O6	-6.25	124.85	128.60
36	1	3184	A	N7-C8-N9	-6.24	110.68	113.80
38	4	113	U	C4-C5-C6	6.24	123.45	119.70
36	5	1770	G	C4-N9-C1'	6.24	134.62	126.50
1	2	390	G	N3-C2-N2	-6.24	115.53	119.90
36	1	809	G	C8-N9-C4	6.24	108.90	106.40
36	5	2750	U	N1-C2-O2	-6.24	118.43	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	933	A	N1-C2-N3	6.24	132.42	129.30
36	1	942	U	C2-N3-C4	-6.24	123.26	127.00
36	1	2197	C	C5-C4-N4	-6.24	115.83	120.20
1	6	59	C	C6-N1-C2	6.24	122.80	120.30
36	5	933	A	C6-N1-C2	-6.24	114.86	118.60
36	5	938	C	C4-C5-C6	-6.24	114.28	117.40
36	5	1336	U	O5'-P-OP1	6.24	118.19	110.70
1	2	1773	C	N3-C4-N4	6.24	122.37	118.00
36	1	2812	C	C5-C6-N1	-6.24	117.88	121.00
1	6	351	C	N3-C4-N4	6.24	122.36	118.00
1	2	1258	U	N3-C2-O2	-6.23	117.84	122.20
36	1	2374	C	N3-C2-O2	-6.23	117.54	121.90
1	6	128	U	C5-C6-N1	-6.23	119.58	122.70
59	n3	87	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	6	1535	U	N3-C2-O2	-6.23	117.84	122.20
36	5	3197	G	N1-C2-N2	6.23	121.81	116.20
1	6	1698	G	P-O3'-C3'	6.23	127.18	119.70
36	5	513	G	N1-C6-O6	-6.23	116.16	119.90
36	1	2355	G	C4-C5-C6	6.23	122.54	118.80
1	6	163	G	C5-C6-O6	6.23	132.34	128.60
36	5	1199	C	C6-N1-C2	6.23	122.79	120.30
1	2	831	U	C6-N1-C2	-6.23	117.26	121.00
36	1	37	U	N1-C2-O2	-6.23	118.44	122.80
36	1	1868	G	C8-N9-C4	-6.23	103.91	106.40
36	1	2374	C	N1-C2-N3	6.23	123.56	119.20
36	1	2714	G	C5-N7-C8	-6.22	101.19	104.30
1	6	992	A	O5'-P-OP1	-6.22	100.10	105.70
36	5	2849	C	N3-C4-N4	6.22	122.36	118.00
41	l4	327	LEU	CA-CB-CG	6.22	129.62	115.30
51	m5	183	THR	N-CA-C	6.22	127.81	111.00
36	1	51	A	N7-C8-N9	6.22	116.91	113.80
36	1	942	U	C5-C4-O4	-6.22	122.17	125.90
38	4	13	A	C8-N9-C4	-6.22	103.31	105.80
36	5	813	G	C8-N9-C4	-6.22	103.91	106.40
36	5	1637	A	N1-C6-N6	-6.22	114.87	118.60
36	5	2977	G	OP2-P-O3'	6.22	118.89	105.20
36	1	1792	C	N1-C2-O2	-6.22	115.17	118.90
1	6	113	U	O5'-P-OP2	-6.22	100.10	105.70
1	6	1665	U	C5-C6-N1	-6.22	119.59	122.70
36	5	3380	U	C5-C4-O4	6.22	129.63	125.90
36	5	2887	A	C4-C5-C6	6.22	120.11	117.00
36	5	3150	A	C2-N3-C4	-6.22	107.49	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1404	G	C8-N9-C4	6.22	108.89	106.40
1	6	421	A	C8-N9-C4	6.22	108.29	105.80
36	5	1869	C	C4-C5-C6	-6.22	114.29	117.40
36	1	1151	U	N3-C4-C5	-6.21	110.87	114.60
36	5	1113	G	C5-C6-N1	-6.21	108.39	111.50
36	5	3141	A	N1-C2-N3	6.21	132.41	129.30
36	1	1053	A	O5'-P-OP2	-6.21	100.11	105.70
36	1	1517	G	N1-C6-O6	-6.21	116.17	119.90
1	6	119	A	N1-C2-N3	6.21	132.41	129.30
1	6	523	G	C8-N9-C4	6.21	108.88	106.40
1	6	577	G	C6-C5-N7	-6.21	126.67	130.40
1	6	1150	G	N3-C4-C5	6.21	131.71	128.60
36	5	85	A	N1-C6-N6	-6.21	114.87	118.60
36	5	1307	G	C2'-C3'-O3'	6.21	123.64	113.70
36	5	2331	C	N3-C4-C5	-6.21	119.42	121.90
36	1	1859	A	O5'-P-OP2	-6.21	100.11	105.70
1	6	351	C	C2-N1-C1'	6.21	125.63	118.80
36	5	11	A	O5'-P-OP2	-6.21	100.11	105.70
36	5	43	A	N1-C6-N6	6.21	122.32	118.60
36	5	2375	G	N9-C4-C5	6.21	107.88	105.40
36	1	2800	G	N1-C2-N2	-6.20	110.62	116.20
36	1	2808	A	O4'-C1'-N9	-6.20	103.24	108.20
36	5	2147	A	C8-N9-C4	6.20	108.28	105.80
36	1	699	A	N1-C2-N3	6.20	132.40	129.30
36	1	1351	U	N1-C2-O2	6.20	127.14	122.80
36	1	1389	G	N1-C6-O6	6.20	123.62	119.90
36	1	2687	G	N1-C6-O6	-6.20	116.18	119.90
36	1	2823	G	N3-C2-N2	-6.20	115.56	119.90
1	6	308	C	C6-N1-C1'	6.20	128.24	120.80
36	5	645	A	C8-N9-C4	-6.20	103.32	105.80
36	1	1371	G	C8-N9-C4	6.20	108.88	106.40
36	1	2836	C	C4-C5-C6	6.20	120.50	117.40
36	5	938	C	C6-N1-C2	6.20	122.78	120.30
36	1	1381	A	O5'-P-OP2	6.20	118.14	110.70
36	1	2610	G	C6-C5-N7	-6.20	126.68	130.40
36	1	2719	U	N1-C2-O2	-6.20	118.46	122.80
36	5	1285	G	C8-N9-C4	6.20	108.88	106.40
36	5	2145	A	C5-C6-N1	6.20	120.80	117.70
36	5	2820	A	C5-C6-N6	-6.20	118.74	123.70
36	5	2820	A	C5-N7-C8	-6.20	100.80	103.90
36	5	834	U	C6-N1-C2	6.19	124.72	121.00
1	2	1274	C	C6-N1-C2	-6.19	117.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	69	C	N3-C4-C5	-6.19	119.42	121.90
1	6	1109	G	C8-N9-C4	-6.19	103.92	106.40
36	1	343	U	O5'-P-OP2	-6.19	100.13	105.70
36	1	667	C	N3-C4-N4	-6.19	113.67	118.00
36	1	1430	U	O5'-P-OP2	-6.19	100.13	105.70
36	1	2138	A	C2-N3-C4	-6.19	107.50	110.60
1	6	90	C	N3-C2-O2	-6.19	117.57	121.90
36	5	939	U	N3-C2-O2	6.19	126.53	122.20
36	1	2651	G	N3-C4-N9	-6.19	122.29	126.00
36	5	3308	C	N1-C2-O2	-6.19	115.19	118.90
36	1	30	G	N1-C2-N3	6.19	127.61	123.90
36	1	1365	G	N1-C2-N2	-6.19	110.63	116.20
36	1	1489	A	C6-C5-N7	-6.19	127.97	132.30
36	1	1507	G	N1-C6-O6	6.19	123.61	119.90
36	5	1392	G	N9-C4-C5	-6.19	102.92	105.40
70	O4	51	LEU	CA-CB-CG	6.19	129.53	115.30
36	5	346	C	C2-N1-C1'	6.19	125.61	118.80
1	2	783	G	N9-C4-C5	-6.18	102.93	105.40
36	1	1581	C	N1-C2-O2	6.18	122.61	118.90
36	1	2200	U	C6-N1-C2	-6.18	117.29	121.00
36	5	1305	U	N3-C4-O4	6.18	123.73	119.40
36	5	2980	U	C6-N1-C2	-6.18	117.29	121.00
36	5	3245	A	N1-C6-N6	6.18	122.31	118.60
37	7	44	C	N3-C2-O2	6.18	126.23	121.90
67	o1	51	LEU	CA-CB-CG	6.18	129.53	115.30
36	1	104	G	C4-C5-N7	6.18	113.27	110.80
36	1	3367	C	N3-C4-C5	6.18	124.37	121.90
36	1	104	G	C6-C5-N7	-6.18	126.69	130.40
36	5	641	C	C5-C6-N1	6.18	124.09	121.00
36	5	1589	A	C5-C6-N6	-6.18	118.76	123.70
36	1	114	A	O5'-P-OP1	-6.18	100.14	105.70
36	1	420	G	C5-C6-O6	-6.18	124.89	128.60
36	1	421	G	C5-C6-O6	-6.18	124.89	128.60
37	3	61	G	C4-C5-N7	6.18	113.27	110.80
1	6	681	U	N3-C2-O2	-6.17	117.88	122.20
37	7	12	U	C5-C4-O4	-6.17	122.19	125.90
36	1	331	G	C2-N3-C4	6.17	114.99	111.90
38	4	15	G	C5-C6-N1	6.17	114.59	111.50
36	5	339	C	C6-N1-C2	-6.17	117.83	120.30
36	1	511	G	N7-C8-N9	6.17	116.19	113.10
36	1	1190	A	C6-C5-N7	-6.17	127.98	132.30
36	5	1048	A	C2-N3-C4	-6.17	107.51	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1298	C	C6-N1-C2	-6.17	117.83	120.30
36	5	3001	C	C4-C5-C6	6.17	120.49	117.40
36	1	1585	C	O5'-P-OP1	-6.17	100.15	105.70
36	5	960	U	N3-C4-C5	6.17	118.30	114.60
36	1	2585	G	N3-C4-C5	-6.17	125.52	128.60
36	1	3034	C	O5'-P-OP2	-6.17	100.15	105.70
36	1	3235	C	C6-N1-C2	-6.17	117.83	120.30
1	6	1019	A	N7-C8-N9	-6.17	110.72	113.80
36	5	404	G	O5'-P-OP2	-6.17	100.15	105.70
36	5	1178	G	C5-N7-C8	-6.17	101.22	104.30
1	6	1472	C	C2-N1-C1'	-6.17	112.02	118.80
36	1	953	G	N3-C4-N9	-6.16	122.30	126.00
36	5	370	U	N3-C2-O2	-6.16	117.89	122.20
36	5	684	G	N1-C6-O6	6.16	123.60	119.90
36	5	1377	G	C5-C6-O6	-6.16	124.90	128.60
36	1	2376	G	N3-C4-C5	-6.16	125.52	128.60
36	5	2683	U	N1-C2-O2	6.16	127.11	122.80
37	7	84	A	C8-N9-C4	-6.16	103.33	105.80
1	2	1633	A	N1-C6-N6	-6.16	114.90	118.60
36	1	2830	G	N1-C6-O6	6.16	123.60	119.90
1	6	323	A	N9-C4-C5	6.16	108.26	105.80
1	6	400	A	N1-C6-N6	6.16	122.30	118.60
36	5	1154	A	N1-C6-N6	-6.16	114.90	118.60
36	5	1430	U	C6-N1-C2	6.16	124.70	121.00
36	5	1788	C	C6-N1-C2	-6.16	117.84	120.30
36	1	1124	U	C5-C6-N1	6.16	125.78	122.70
36	1	2984	C	C5-C4-N4	6.16	124.51	120.20
36	5	2400	G	N1-C6-O6	6.16	123.59	119.90
36	1	2643	A	O5'-P-OP1	-6.15	100.16	105.70
36	5	1181	U	N1-C2-N3	6.15	118.59	114.90
36	1	810	A	C5-C6-N1	6.15	120.78	117.70
36	1	952	A	N9-C4-C5	6.15	108.26	105.80
36	1	2191	U	N1-C2-O2	6.15	127.11	122.80
36	5	1181	U	N3-C2-O2	-6.15	117.89	122.20
36	5	1368	U	C5-C4-O4	-6.15	122.21	125.90
1	2	1600	A	C2-N3-C4	-6.15	107.53	110.60
1	6	65	A	N3-C4-C5	6.15	131.10	126.80
1	6	1340	U	N1-C2-O2	6.15	127.11	122.80
36	5	2176	U	N1-C2-N3	6.15	118.59	114.90
1	2	13	C	O5'-P-OP2	-6.15	100.17	105.70
1	6	354	C	C5-C6-N1	6.15	124.07	121.00
69	o3	99	ARG	NE-CZ-NH1	-6.15	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1342	C	N3-C4-C5	6.15	124.36	121.90
20	C8	3	LEU	CA-CB-CG	6.14	129.43	115.30
36	1	2279	A	N9-C4-C5	-6.14	103.34	105.80
36	1	2309	A	C5-C6-N6	-6.14	118.78	123.70
1	6	151	G	C4-N9-C1'	-6.14	118.51	126.50
36	1	2193	U	N1-C2-O2	6.14	127.10	122.80
36	5	1440	G	C5-C6-O6	6.14	132.29	128.60
36	5	3308	C	C4-C5-C6	6.14	120.47	117.40
1	2	312	A	N1-C6-N6	-6.14	114.92	118.60
36	5	952	A	O5'-P-OP2	-6.14	100.17	105.70
36	1	1820	U	P-O3'-C3'	6.14	127.07	119.70
1	2	334	G	N3-C4-C5	6.14	131.67	128.60
1	2	359	A	C4-C5-C6	-6.14	113.93	117.00
36	1	912	G	OP2-P-O3'	6.14	118.70	105.20
36	1	2409	G	C8-N9-C4	-6.14	103.95	106.40
36	1	2879	C	N3-C4-C5	-6.14	119.44	121.90
1	6	1796	C	N3-C4-N4	-6.14	113.70	118.00
36	5	91	G	N9-C4-C5	-6.14	102.94	105.40
36	5	1205	A	C5-C6-N1	6.14	120.77	117.70
36	5	1007	U	N1-C2-O2	-6.13	118.51	122.80
36	1	2917	G	N3-C4-C5	-6.13	125.53	128.60
36	5	683	U	N3-C4-C5	-6.13	110.92	114.60
37	7	47	C	C5-C6-N1	-6.13	117.93	121.00
36	1	1360	C	N3-C2-O2	6.13	126.19	121.90
36	1	56	G	C5-C6-O6	-6.13	124.92	128.60
36	1	1163	A	N1-C2-N3	6.13	132.36	129.30
36	1	2403	G	N9-C4-C5	-6.13	102.95	105.40
1	6	44	U	N1-C2-O2	-6.13	118.51	122.80
36	1	331	G	C5-C6-N1	6.13	114.56	111.50
36	5	146	U	N3-C4-O4	-6.13	115.11	119.40
36	5	2524	A	O4'-C1'-N9	6.13	113.10	108.20
36	1	343	U	N3-C4-C5	-6.12	110.92	114.60
36	1	1049	C	C6-N1-C2	-6.12	117.85	120.30
36	5	806	A	O5'-P-OP1	-6.12	100.19	105.70
1	2	933	A	C8-N9-C4	-6.12	103.35	105.80
1	2	1012	U	C2-N3-C4	6.12	130.67	127.00
36	5	1496	C	C2-N1-C1'	6.12	125.54	118.80
36	5	2147	A	N9-C4-C5	-6.12	103.35	105.80
36	5	2295	A	C4-C5-N7	6.12	113.76	110.70
36	5	3374	U	C5-C6-N1	-6.12	119.64	122.70
36	1	1201	C	C5-C4-N4	-6.12	115.91	120.20
36	1	3054	U	C5-C4-O4	6.12	129.57	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1643	U	C2-N3-C4	-6.12	123.33	127.00
36	5	1130	A	C2-N3-C4	6.12	113.66	110.60
36	5	2278	C	N3-C4-C5	6.12	124.35	121.90
36	1	843	A	C2-N3-C4	-6.12	107.54	110.60
36	5	2157	G	N9-C4-C5	-6.12	102.95	105.40
36	5	3018	C	O5'-P-OP2	-6.12	100.19	105.70
36	5	2687	G	N3-C4-N9	6.12	129.67	126.00
36	1	2639	G	C8-N9-C1'	-6.12	119.05	127.00
36	1	189	G	N1-C6-O6	-6.11	116.23	119.90
36	1	2660	G	C4-C5-N7	6.11	113.25	110.80
1	6	1737	G	C5-C6-O6	-6.11	124.93	128.60
36	1	810	A	C8-N9-C4	-6.11	103.36	105.80
36	5	283	G	C5-C6-O6	-6.11	124.93	128.60
36	5	684	G	C5-C6-O6	-6.11	124.93	128.60
36	5	2287	C	C2-N3-C4	-6.11	116.84	119.90
36	5	1897	G	C5-C6-O6	-6.11	124.94	128.60
36	5	3118	C	C6-N1-C2	-6.11	117.86	120.30
37	7	89	G	C5-C6-N1	6.11	114.55	111.50
48	m1	60	ARG	NE-CZ-NH2	6.11	123.36	120.30
36	1	859	G	C8-N9-C1'	-6.11	119.06	127.00
1	2	1291	G	C2-N3-C4	-6.11	108.85	111.90
36	1	1192	C	C6-N1-C1'	-6.11	113.47	120.80
36	1	1419	A	C5'-C4'-O4'	6.11	116.43	109.10
36	5	1405	U	C2-N3-C4	-6.11	123.34	127.00
36	5	1446	A	C8-N9-C4	6.11	108.24	105.80
36	5	1492	G	N1-C6-O6	-6.11	116.24	119.90
36	5	2794	G	O5'-P-OP2	-6.11	100.20	105.70
36	1	573	C	C6-N1-C2	6.10	122.74	120.30
1	6	1793	G	C4-C5-N7	-6.10	108.36	110.80
36	5	2689	A	O4'-C1'-N9	6.10	113.08	108.20
36	5	1017	C	C2-N1-C1'	6.10	125.51	118.80
36	5	2349	U	C6-N1-C2	-6.10	117.34	121.00
1	2	602	U	O5'-P-OP1	-6.10	100.21	105.70
36	1	1724	U	O4'-C1'-N1	6.10	113.08	108.20
1	6	29	U	C5-C4-O4	6.10	129.56	125.90
36	5	645	A	N9-C4-C5	6.10	108.24	105.80
36	5	3362	A	N1-C2-N3	6.10	132.35	129.30
1	2	1486	G	C5-N7-C8	-6.10	101.25	104.30
36	1	2241	U	C5-C4-O4	6.10	129.56	125.90
36	1	2783	U	OP1-P-O3'	6.10	118.61	105.20
36	5	1125	U	OP1-P-OP2	-6.10	110.45	119.60
36	1	1884	A	C8-N9-C4	6.10	108.24	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1307	G	N9-C4-C5	6.10	107.84	105.40
36	5	2338	C	N3-C4-C5	-6.10	119.46	121.90
36	5	2615	G	N9-C4-C5	-6.10	102.96	105.40
36	5	2808	A	C5-C6-N6	-6.10	118.82	123.70
1	2	985	G	C5-C6-O6	-6.09	124.94	128.60
36	1	1140	G	N3-C2-N2	6.09	124.17	119.90
36	1	1337	A	C5-C6-N1	6.09	120.75	117.70
36	1	2572	C	C6-N1-C1'	-6.09	113.48	120.80
36	5	2286	U	N3-C2-O2	-6.09	117.93	122.20
36	1	681	U	N3-C4-O4	6.09	123.66	119.40
36	1	1414	G	C5-C6-O6	-6.09	124.94	128.60
36	1	2174	G	C6-C5-N7	-6.09	126.75	130.40
36	5	3136	G	C2-N3-C4	-6.09	108.85	111.90
1	2	1157	A	P-O3'-C3'	6.09	127.01	119.70
36	5	283	G	C5-N7-C8	-6.09	101.25	104.30
36	5	3137	C	OP1-P-O3'	6.09	118.60	105.20
1	6	1129	U	C6-N1-C1'	6.09	129.72	121.20
36	5	3270	U	O5'-P-OP1	-6.09	100.22	105.70
36	1	695	C	C5-C6-N1	-6.09	117.96	121.00
36	1	1929	G	N9-C4-C5	-6.09	102.97	105.40
36	1	2343	C	OP2-P-O3'	6.09	118.59	105.20
36	5	879	U	C2-N1-C1'	6.09	125.00	117.70
36	5	1490	A	C8-N9-C4	-6.09	103.36	105.80
36	1	93	C	C6-N1-C2	-6.08	117.87	120.30
36	5	2419	A	N7-C8-N9	6.08	116.84	113.80
36	1	3277	U	N3-C2-O2	-6.08	117.94	122.20
36	5	649	A	C2-N3-C4	6.08	113.64	110.60
36	5	2385	G	N3-C4-N9	-6.08	122.35	126.00
36	5	2717	U	N1-C2-O2	-6.08	118.54	122.80
1	2	969	C	N3-C2-O2	6.08	126.16	121.90
36	1	395	A	C8-N9-C4	-6.08	103.37	105.80
36	5	504	A	C8-N9-C4	6.08	108.23	105.80
36	5	2327	U	C6-N1-C2	6.08	124.65	121.00
36	1	941	G	C5-C6-N1	6.08	114.54	111.50
36	1	1138	U	N1-C2-N3	6.08	118.55	114.90
36	5	3294	A	N9-C4-C5	6.08	108.23	105.80
36	1	636	C	C2-N3-C4	-6.08	116.86	119.90
36	5	2172	A	N1-C6-N6	6.08	122.25	118.60
36	5	2320	A	C5-C6-N1	-6.08	114.66	117.70
36	1	785	G	C2-N3-C4	6.08	114.94	111.90
36	1	2335	G	N1-C6-O6	-6.08	116.25	119.90
12	c0	83	PRO	N-CA-CB	6.08	110.59	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	392	G	C5-C6-O6	-6.08	124.95	128.60
36	1	2412	G	C5-C6-O6	-6.08	124.95	128.60
36	1	1141	C	N3-C4-N4	6.07	122.25	118.00
36	1	2817	A	C5-C6-N1	6.07	120.74	117.70
1	6	393	C	C5-C4-N4	-6.07	115.95	120.20
1	6	352	A	N7-C8-N9	-6.07	110.76	113.80
36	1	2980	U	C4-C5-C6	6.07	123.34	119.70
36	5	406	G	O4'-C1'-N9	6.07	113.06	108.20
36	5	2197	C	C6-N1-C2	6.07	122.73	120.30
36	1	1507	G	N3-C2-N2	-6.07	115.65	119.90
1	2	1196	A	P-O3'-C3'	6.07	126.98	119.70
36	1	2418	G	N3-C4-N9	6.07	129.64	126.00
36	1	3092	C	O4'-C1'-N1	6.07	113.05	108.20
36	5	414	U	N3-C4-O4	6.07	123.65	119.40
36	5	1443	G	C8-N9-C4	6.07	108.83	106.40
36	5	2943	G	C5-N7-C8	-6.07	101.27	104.30
36	1	1366	A	N7-C8-N9	6.07	116.83	113.80
36	1	2133	U	C2-N1-C1'	-6.07	110.42	117.70
36	1	3049	A	C8-N9-C4	6.07	108.23	105.80
36	5	92	G	C5-C6-N1	6.07	114.53	111.50
36	5	1846	C	C2-N3-C4	-6.07	116.87	119.90
37	7	103	A	C5-C6-N6	-6.07	118.85	123.70
36	1	2554	A	P-O3'-C3'	6.06	126.98	119.70
36	1	3212	C	C2-N1-C1'	-6.06	112.13	118.80
36	5	934	G	N3-C4-N9	6.06	129.64	126.00
36	1	1192	C	N3-C2-O2	-6.06	117.66	121.90
36	1	2395	G	C5-C6-N1	6.06	114.53	111.50
36	5	800	G	C6-N1-C2	-6.06	121.46	125.10
36	1	2705	A	C2-N3-C4	6.06	113.63	110.60
38	4	85	G	C4-C5-N7	6.06	113.22	110.80
36	5	1937	U	C5-C6-N1	-6.06	119.67	122.70
36	5	2817	A	C2-N3-C4	6.06	113.63	110.60
36	1	32	U	C5-C6-N1	-6.06	119.67	122.70
1	6	1472	C	N3-C4-N4	-6.06	113.76	118.00
37	7	112	G	C5-C6-O6	6.06	132.23	128.60
36	1	3298	C	C6-N1-C2	6.06	122.72	120.30
36	1	959	C	N3-C4-C5	6.05	124.32	121.90
36	5	1480	G	O4'-C1'-N9	6.05	113.04	108.20
36	5	2211	U	N3-C2-O2	-6.05	117.96	122.20
36	5	3054	U	N3-C4-C5	-6.05	110.97	114.60
36	1	287	G	C6-C5-N7	-6.05	126.77	130.40
1	6	1118	G	C2-N3-C4	-6.05	108.87	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	369	A	N3-C4-C5	-6.05	122.56	126.80
36	5	2635	A	N1-C6-N6	-6.05	114.97	118.60
36	5	2808	A	O5'-P-OP2	-6.05	100.25	105.70
36	5	3305	A	N9-C4-C5	-6.05	103.38	105.80
1	2	694	U	N1-C2-O2	6.05	127.03	122.80
36	5	998	A	OP2-P-O3'	6.05	118.50	105.20
36	5	3009	G	N3-C4-C5	-6.05	125.58	128.60
36	1	670	C	N1-C2-N3	6.05	123.43	119.20
36	1	2831	G	C6-C5-N7	-6.04	126.77	130.40
36	1	2983	C	N1-C2-N3	6.04	123.43	119.20
1	6	805	U	N3-C4-C5	-6.04	110.97	114.60
36	5	1846	C	C5-C6-N1	-6.04	117.98	121.00
1	2	779	U	O4'-C1'-N1	6.04	113.03	108.20
36	1	2617	U	C5-C6-N1	-6.04	119.68	122.70
1	6	634	G	N1-C6-O6	6.04	123.53	119.90
36	1	218	G	O5'-P-OP1	-6.04	100.26	105.70
36	1	895	A	C6-C5-N7	-6.04	128.07	132.30
36	1	942	U	N1-C2-O2	-6.04	118.57	122.80
36	1	1133	A	C5-C6-N6	-6.04	118.87	123.70
36	5	1200	A	N3-C4-C5	-6.04	122.57	126.80
36	5	41	G	C5-C6-O6	-6.04	124.98	128.60
1	2	794	U	P-O3'-C3'	6.04	126.94	119.70
1	2	992	A	N1-C2-N3	6.04	132.32	129.30
1	2	1756	A	N1-C6-N6	6.04	122.22	118.60
36	1	2306	C	N3-C2-O2	-6.04	117.68	121.90
36	1	80	G	C5-C6-N1	6.03	114.52	111.50
49	M3	70	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	6	338	C	C2-N1-C1'	6.03	125.44	118.80
36	5	201	A	C2-N3-C4	-6.03	107.58	110.60
36	5	693	A	O5'-P-OP2	6.03	117.94	110.70
36	5	1057	A	C5-N7-C8	-6.03	100.88	103.90
36	1	2694	A	O5'-P-OP1	-6.03	100.27	105.70
1	6	543	C	C6-N1-C2	-6.03	117.89	120.30
36	5	2644	C	O5'-P-OP1	-6.03	100.27	105.70
36	1	1182	A	C8-N9-C4	6.03	108.21	105.80
36	5	1902	G	N3-C2-N2	-6.03	115.68	119.90
1	6	151	G	N3-C2-N2	-6.03	115.68	119.90
36	5	1859	A	O5'-P-OP2	-6.03	100.28	105.70
36	5	2248	C	OP1-P-O3'	6.03	118.45	105.20
1	6	1726	G	OP2-P-O3'	6.02	118.45	105.20
36	5	2397	A	C8-N9-C4	6.02	108.21	105.80
36	1	199	A	O4'-C1'-N9	6.02	113.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	435	C	C6-N1-C2	6.02	122.71	120.30
36	1	1364	C	C2-N3-C4	-6.02	116.89	119.90
36	1	2874	G	C5-C6-N1	-6.02	108.49	111.50
36	5	593	C	OP2-P-O3'	6.02	118.45	105.20
36	1	672	A	C4-C5-N7	6.02	113.71	110.70
36	5	2097	U	C5-C6-N1	6.02	125.71	122.70
36	1	1114	U	O5'-P-OP2	-6.02	100.28	105.70
36	5	2191	U	C5-C4-O4	6.02	129.51	125.90
37	7	121	U	N3-C2-O2	-6.02	117.99	122.20
36	1	1412	G	N7-C8-N9	6.02	116.11	113.10
36	1	2639	G	N1-C2-N2	-6.02	110.78	116.20
36	1	3101	G	N7-C8-N9	-6.02	110.09	113.10
1	2	1727	G	N3-C4-C5	-6.02	125.59	128.60
36	5	2351	U	N3-C2-O2	-6.02	117.99	122.20
36	5	3174	A	C5-N7-C8	-6.02	100.89	103.90
36	1	2612	U	N3-C4-C5	6.01	118.21	114.60
38	4	24	G	C4-C5-N7	6.01	113.21	110.80
36	5	1042	U	C6-N1-C2	6.01	124.61	121.00
36	1	947	G	C8-N9-C1'	-6.01	119.19	127.00
36	5	889	U	N3-C4-C5	6.01	118.21	114.60
36	5	1327	C	N3-C4-C5	6.01	124.30	121.90
36	5	2838	A	C5-C6-N6	-6.01	118.89	123.70
36	5	1184	A	N9-C4-C5	6.01	108.20	105.80
36	5	1900	A	OP1-P-OP2	6.01	128.62	119.60
36	5	2981	U	C2-N1-C1'	6.01	124.91	117.70
36	5	3339	A	N1-C6-N6	6.01	122.20	118.60
36	1	589	A	N7-C8-N9	-6.01	110.80	113.80
36	5	28	C	C6-N1-C2	6.01	122.70	120.30
1	6	1514	U	C5-C4-O4	6.01	129.50	125.90
36	5	91	G	N1-C6-O6	6.01	123.50	119.90
36	5	1855	U	N1-C2-N3	6.00	118.50	114.90
36	5	2884	C	C5-C4-N4	-6.00	116.00	120.20
36	1	2305	G	C5-C6-O6	-6.00	125.00	128.60
1	6	405	C	C5-C6-N1	-6.00	118.00	121.00
37	7	1	G	C6-C5-N7	-6.00	126.80	130.40
36	1	1520	G	C8-N9-C4	6.00	108.80	106.40
44	L7	163	LEU	CA-CB-CG	-6.00	101.50	115.30
1	6	93	A	O5'-P-OP2	-6.00	100.30	105.70
1	6	782	U	C2-N1-C1'	6.00	124.90	117.70
1	6	864	U	N3-C2-O2	-6.00	118.00	122.20
1	6	1574	G	N1-C6-O6	-6.00	116.30	119.90
36	5	53	G	N1-C6-O6	-6.00	116.30	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	645	A	C4-C5-N7	-6.00	107.70	110.70
36	5	3285	C	N1-C2-O2	6.00	122.50	118.90
36	1	2993	G	N3-C4-N9	6.00	129.60	126.00
1	6	1473	U	N1-C2-N3	6.00	118.50	114.90
36	5	1443	G	C8-N9-C1'	-6.00	119.20	127.00
36	1	117	U	N1-C2-O2	-6.00	118.60	122.80
36	1	1300	G	C6-C5-N7	-6.00	126.80	130.40
36	1	1671	C	C6-N1-C2	-6.00	117.90	120.30
36	5	88	A	C8-N9-C4	6.00	108.20	105.80
36	1	2953	U	N3-C4-O4	6.00	123.60	119.40
39	L2	191	LEU	CA-CB-CG	-6.00	101.51	115.30
36	5	805	G	C8-N9-C4	6.00	108.80	106.40
36	5	2332	A	C8-N9-C4	6.00	108.20	105.80
36	5	3043	C	C6-N1-C2	6.00	122.70	120.30
1	6	973	A	C4-C5-C6	6.00	120.00	117.00
36	5	1716	U	P-O3'-C3'	6.00	126.89	119.70
36	5	2798	C	C2-N1-C1'	-6.00	112.20	118.80
1	2	1027	A	N1-C6-N6	5.99	122.20	118.60
1	6	1185	U	N3-C2-O2	-5.99	118.00	122.20
36	5	2186	U	O5'-P-OP2	-5.99	100.31	105.70
36	5	2917	G	N3-C4-N9	5.99	129.60	126.00
36	1	2309	A	N9-C4-C5	-5.99	103.40	105.80
36	1	296	A	C2-N3-C4	5.99	113.59	110.60
36	1	3326	G	C8-N9-C4	5.99	108.80	106.40
36	1	54	C	C2-N1-C1'	-5.99	112.21	118.80
36	1	984	G	C4-C5-C6	5.99	122.39	118.80
36	1	2610	G	C4-C5-N7	5.99	113.20	110.80
36	1	2728	G	N3-C4-C5	-5.99	125.61	128.60
37	7	77	G	C5-C6-O6	-5.99	125.01	128.60
36	1	2300	G	N9-C4-C5	5.99	107.80	105.40
36	1	776	U	C5-C4-O4	5.99	129.49	125.90
36	5	2147	A	C5-C6-N6	-5.99	118.91	123.70
1	2	1756	A	C5-N7-C8	-5.98	100.91	103.90
36	5	3004	C	N3-C4-N4	5.98	122.19	118.00
1	2	728	U	N3-C2-O2	-5.98	118.01	122.20
36	1	2400	G	C2-N3-C4	-5.98	108.91	111.90
1	6	543	C	C5-C6-N1	5.98	123.99	121.00
36	5	417	A	C5-C6-N1	5.98	120.69	117.70
36	5	1473	G	N7-C8-N9	-5.98	110.11	113.10
36	5	2375	G	C5-C6-O6	5.98	132.19	128.60
36	1	2802	A	OP2-P-O3'	5.98	118.36	105.20
53	M7	138	LYS	CD-CE-NZ	5.98	125.45	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	776	U	C2-N3-C4	-5.98	123.41	127.00
36	5	1710	C	N3-C4-C5	5.98	124.29	121.90
36	5	938	C	N3-C2-O2	5.98	126.08	121.90
1	2	1456	C	N3-C2-O2	-5.98	117.72	121.90
36	5	218	G	OP1-P-OP2	5.98	128.57	119.60
36	5	1192	C	N1-C2-O2	5.98	122.49	118.90
36	5	1886	A	N1-C2-N3	-5.98	126.31	129.30
36	5	1909	A	N7-C8-N9	-5.98	110.81	113.80
36	5	3372	A	C8-N9-C4	-5.97	103.41	105.80
38	8	39	G	N3-C4-C5	-5.97	125.61	128.60
38	8	86	U	C6-N1-C2	-5.97	117.42	121.00
36	1	2406	C	N3-C2-O2	5.97	126.08	121.90
36	5	1939	G	OP2-P-O3'	5.97	118.34	105.20
36	5	2943	G	C5-C6-O6	-5.97	125.02	128.60
36	1	2891	U	N3-C4-O4	5.97	123.58	119.40
36	5	1049	C	C5-C6-N1	5.97	123.99	121.00
36	5	1881	A	C5-C6-N6	-5.97	118.92	123.70
36	1	39	A	O5'-P-OP1	5.97	117.86	110.70
1	6	1748	G	OP2-P-O3'	5.97	118.33	105.20
36	5	2176	U	N1-C2-O2	5.97	126.98	122.80
36	5	2621	G	N1-C2-N2	5.97	121.57	116.20
36	5	1464	G	N9-C4-C5	-5.97	103.01	105.40
37	7	75	G	C6-C5-N7	-5.97	126.82	130.40
36	1	1790	G	C5-C6-N1	-5.97	108.52	111.50
36	1	1791	C	C5-C6-N1	-5.97	118.02	121.00
36	1	3218	A	N9-C4-C5	5.97	108.19	105.80
1	6	151	G	C8-N9-C1'	5.97	134.75	127.00
36	5	1345	G	N1-C6-O6	5.97	123.48	119.90
36	1	590	G	C5-C6-O6	-5.96	125.02	128.60
36	5	200	C	N3-C4-N4	5.96	122.18	118.00
36	5	567	G	C6-C5-N7	-5.96	126.82	130.40
36	5	2615	G	O5'-P-OP2	-5.96	100.33	105.70
36	5	1365	G	N7-C8-N9	5.96	116.08	113.10
36	1	2434	U	C5-C4-O4	5.96	129.48	125.90
1	6	1537	C	C4-C5-C6	5.96	120.38	117.40
37	7	12	U	C4-C5-C6	-5.96	116.12	119.70
36	1	652	G	N3-C2-N2	5.96	124.07	119.90
1	6	1781	A	C5-C6-N1	-5.96	114.72	117.70
36	1	397	A	C5-C6-N1	5.96	120.68	117.70
36	1	688	G	C6-C5-N7	-5.96	126.83	130.40
36	1	1513	G	C5-C6-N1	5.96	114.48	111.50
1	2	829	A	C2-N3-C4	5.96	113.58	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1663	G	C8-N9-C4	-5.96	104.02	106.40
36	5	2617	U	N1-C2-N3	5.96	118.47	114.90
36	5	2825	C	C6-N1-C2	5.96	122.68	120.30
1	2	554	C	C6-N1-C1'	-5.95	113.66	120.80
36	1	634	C	C5-C6-N1	-5.95	118.02	121.00
1	6	1428	G	O5'-P-OP1	-5.95	100.34	105.70
1	6	1473	U	C6-N1-C2	-5.95	117.43	121.00
36	5	1157	G	N1-C6-O6	-5.95	116.33	119.90
36	5	810	A	N1-C2-N3	-5.95	126.32	129.30
36	1	358	G	N9-C4-C5	-5.95	103.02	105.40
36	1	981	U	C5-C6-N1	5.95	125.67	122.70
36	1	2137	U	N1-C2-O2	5.95	126.97	122.80
36	5	1155	C	C4-C5-C6	-5.95	114.42	117.40
36	1	359	U	N1-C2-N3	5.95	118.47	114.90
36	1	619	A	N9-C4-C5	-5.95	103.42	105.80
36	1	1500	G	C5-C6-O6	-5.95	125.03	128.60
36	1	3181	C	N1-C2-O2	5.95	122.47	118.90
36	5	718	G	O4'-C1'-N9	5.95	112.96	108.20
36	5	1666	G	C8-N9-C4	5.95	108.78	106.40
36	5	2272	G	C5-C6-O6	5.95	132.17	128.60
36	5	3216	G	C6-C5-N7	-5.95	126.83	130.40
1	2	1654	G	N3-C4-C5	-5.95	125.63	128.60
36	1	1854	C	N1-C2-O2	5.95	122.47	118.90
36	1	1406	A	C6-C5-N7	-5.95	128.14	132.30
36	1	1556	C	P-O3'-C3'	5.95	126.83	119.70
36	5	224	C	N1-C2-O2	5.95	122.47	118.90
36	5	875	G	N1-C6-O6	-5.95	116.33	119.90
36	5	2411	U	C6-N1-C2	5.95	124.57	121.00
36	5	3136	G	N1-C2-N2	-5.95	110.85	116.20
36	5	2752	U	O5'-P-OP1	5.94	117.83	110.70
36	1	1456	A	OP1-P-O3'	5.94	118.27	105.20
36	1	2814	G	O5'-P-OP2	5.94	117.83	110.70
38	4	113	U	N3-C2-O2	-5.94	118.04	122.20
51	M5	22	LEU	CA-CB-CG	5.94	128.97	115.30
1	6	404	G	O5'-P-OP1	-5.94	100.35	105.70
36	5	1464	G	N3-C4-N9	5.94	129.56	126.00
36	5	2677	G	N1-C6-O6	5.94	123.47	119.90
36	5	2870	C	O4'-C1'-N1	5.94	112.95	108.20
36	1	913	A	N9-C4-C5	5.94	108.18	105.80
49	M3	141	ALA	N-CA-C	-5.94	94.96	111.00
36	5	2765	C	C5-C6-N1	5.94	123.97	121.00
36	5	2819	A	O5'-P-OP2	-5.94	100.35	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	197	G	C6-C5-N7	-5.94	126.84	130.40
36	1	624	G	C8-N9-C4	-5.94	104.02	106.40
36	1	2814	G	N1-C6-O6	5.94	123.46	119.90
1	6	1354	G	C4-N9-C1'	5.94	134.22	126.50
37	7	85	G	O5'-P-OP2	5.94	117.83	110.70
36	1	1151	U	N1-C2-O2	-5.94	118.64	122.80
1	6	85	A	C8-N9-C4	-5.94	103.42	105.80
1	6	1679	G	N1-C6-O6	-5.94	116.34	119.90
36	5	770	G	C8-N9-C4	5.94	108.78	106.40
36	1	587	U	N1-C2-O2	-5.94	118.64	122.80
36	1	2400	G	C5-C6-O6	-5.94	125.04	128.60
37	7	1	G	C4-N9-C1'	5.94	134.22	126.50
36	1	1371	G	C2-N3-C4	5.93	114.87	111.90
36	1	2726	C	C5-C4-N4	5.93	124.35	120.20
36	1	2823	G	N9-C4-C5	5.93	107.77	105.40
36	1	3380	U	O5'-P-OP2	-5.93	100.36	105.70
36	5	2666	C	N1-C2-O2	-5.93	115.34	118.90
36	1	1382	G	N7-C8-N9	-5.93	110.13	113.10
36	1	2169	G	N3-C4-C5	-5.93	125.63	128.60
36	5	417	A	C6-N1-C2	-5.93	115.04	118.60
36	5	1149	G	C5-C6-O6	-5.93	125.04	128.60
36	1	207	U	N1-C2-O2	-5.93	118.65	122.80
36	1	2723	U	N1-C2-O2	-5.93	118.65	122.80
36	1	2369	G	C5-C6-N1	5.93	114.47	111.50
41	L4	139	GLY	N-CA-C	-5.93	98.28	113.10
36	5	607	A	N9-C4-C5	5.93	108.17	105.80
36	5	2288	G	C8-N9-C1'	-5.93	119.29	127.00
36	5	2361	A	C8-N9-C4	-5.93	103.43	105.80
36	5	3004	C	C5-C4-N4	-5.93	116.05	120.20
36	5	3120	C	C5-C4-N4	5.93	124.35	120.20
36	1	42	C	OP2-P-O3'	5.93	118.24	105.20
36	1	2385	G	N3-C4-C5	5.93	131.56	128.60
36	1	3269	U	N3-C2-O2	-5.93	118.05	122.20
1	6	99	C	N1-C2-O2	5.93	122.46	118.90
36	5	585	A	O5'-P-OP2	-5.93	100.36	105.70
36	1	92	G	N1-C6-O6	-5.92	116.34	119.90
36	1	2980	U	C6-N1-C2	-5.92	117.44	121.00
1	6	795	U	N3-C2-O2	-5.92	118.05	122.20
36	5	514	G	C5-C6-O6	-5.92	125.05	128.60
36	5	2148	U	N1-C2-O2	-5.92	118.65	122.80
36	5	3001	C	C5-C6-N1	-5.92	118.04	121.00
38	8	125	U	C2-N1-C1'	5.92	124.81	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	386	A	N1-C6-N6	5.92	122.15	118.60
36	5	3197	G	O5'-P-OP2	5.92	117.81	110.70
1	2	73	U	OP1-P-O3'	5.92	118.22	105.20
36	1	124	U	N1-C2-O2	5.92	126.94	122.80
36	1	2943	G	N1-C6-O6	5.92	123.45	119.90
36	5	1285	G	N7-C8-N9	-5.92	110.14	113.10
36	5	1445	U	N1-C2-O2	-5.92	118.66	122.80
40	l3	4	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	2	1215	C	C6-N1-C2	-5.92	117.93	120.30
36	1	427	C	N1-C2-O2	-5.92	115.35	118.90
36	1	2816	G	O4'-C1'-N9	5.92	112.93	108.20
36	1	2968	G	N3-C4-C5	5.92	131.56	128.60
1	6	610	G	N3-C4-C5	-5.92	125.64	128.60
36	5	1284	C	C6-N1-C2	-5.92	117.93	120.30
36	5	2820	A	N1-C6-N6	5.92	122.15	118.60
37	7	84	A	OP1-P-O3'	5.92	118.21	105.20
36	1	2130	G	N1-C6-O6	-5.91	116.35	119.90
36	1	2407	C	C5-C4-N4	-5.91	116.06	120.20
36	1	2418	G	C4-N9-C1'	5.91	134.19	126.50
36	1	2617	U	C6-N1-C2	-5.91	117.45	121.00
36	1	2960	C	N3-C4-C5	5.91	124.27	121.90
36	5	961	C	C2-N1-C1'	5.91	125.31	118.80
36	1	1378	U	C2-N1-C1'	5.91	124.80	117.70
36	1	2400	G	N9-C4-C5	-5.91	103.03	105.40
44	L7	207	LEU	CB-CG-CD1	-5.91	100.95	111.00
37	7	10	C	C6-N1-C1'	-5.91	113.71	120.80
36	1	664	U	C5-C4-O4	-5.91	122.35	125.90
36	1	1131	G	O5'-P-OP2	-5.91	100.38	105.70
36	1	3268	A	C4-C5-C6	5.91	119.96	117.00
36	5	2396	G	N3-C2-N2	-5.91	115.76	119.90
36	1	1396	C	C6-N1-C2	5.91	122.66	120.30
36	1	3215	A	C2-N3-C4	-5.91	107.65	110.60
36	5	1300	G	C5-C6-O6	-5.91	125.05	128.60
36	5	1405	U	N1-C2-N3	5.91	118.44	114.90
36	5	2358	A	N3-C4-C5	5.91	130.94	126.80
36	1	3055	U	C5-C4-O4	-5.91	122.36	125.90
36	5	410	U	N3-C4-C5	-5.91	111.06	114.60
36	5	3144	G	N1-C2-N3	5.91	127.44	123.90
36	1	282	G	C2'-C3'-O3'	5.91	123.15	113.70
36	1	2639	G	C4-N9-C1'	5.91	134.18	126.50
36	5	2626	A	C2-N3-C4	-5.91	107.65	110.60
36	1	2383	C	C5-C4-N4	-5.90	116.07	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1643	U	C2-N1-C1'	-5.90	110.62	117.70
36	1	2883	U	C5-C6-N1	5.90	125.65	122.70
36	1	171	G	N1-C6-O6	5.90	123.44	119.90
1	6	1100	G	C2-N3-C4	5.90	114.85	111.90
1	6	1140	G	C5-C6-N1	5.90	114.45	111.50
36	5	2295	A	C5-C6-N1	5.90	120.65	117.70
36	5	2896	A	O5'-P-OP2	-5.90	100.39	105.70
36	1	332	C	C5-C6-N1	-5.90	118.05	121.00
36	1	934	G	C4-N9-C1'	5.90	134.17	126.50
36	5	2305	G	C6-C5-N7	-5.90	126.86	130.40
36	5	947	G	N3-C4-N9	5.90	129.54	126.00
36	5	2434	U	C5-C4-O4	5.90	129.44	125.90
36	5	3060	C	C4-C5-C6	-5.90	114.45	117.40
36	1	305	U	N3-C2-O2	-5.89	118.07	122.20
36	1	1390	A	C6-N1-C2	-5.89	115.06	118.60
36	1	2610	G	N1-C6-O6	5.89	123.44	119.90
36	1	1100	U	C5-C6-N1	-5.89	119.75	122.70
36	1	2397	A	O5'-P-OP2	-5.89	100.40	105.70
1	6	101	U	N1-C2-O2	5.89	126.92	122.80
1	6	418	G	O5'-P-OP1	-5.89	100.40	105.70
36	5	1825	G	N9-C4-C5	5.89	107.76	105.40
36	5	2411	U	C2-N3-C4	-5.89	123.47	127.00
1	2	121	U	N3-C2-O2	-5.89	118.08	122.20
36	1	652	G	N3-C4-N9	5.89	129.53	126.00
36	1	1097	G	P-O3'-C3'	5.89	126.77	119.70
1	2	879	G	O5'-P-OP2	-5.89	100.40	105.70
1	2	1269	U	C2-N1-C1'	5.89	124.77	117.70
36	1	2163	C	N1-C2-O2	-5.89	115.37	118.90
36	1	2336	U	N3-C2-O2	-5.89	118.08	122.20
36	5	749	C	C6-N1-C2	-5.89	117.94	120.30
36	5	1376	C	OP1-P-OP2	5.89	128.43	119.60
36	5	2116	G	C4-C5-C6	5.89	122.33	118.80
36	1	339	C	OP1-P-OP2	-5.89	110.77	119.60
36	1	2118	C	C5-C6-N1	5.89	123.94	121.00
36	1	2306	C	C6-N1-C2	-5.89	117.94	120.30
38	4	113	U	C2-N3-C4	-5.89	123.47	127.00
1	2	639	U	C2-N1-C1'	5.88	124.76	117.70
1	2	1736	G	O5'-P-OP2	-5.88	100.40	105.70
36	1	584	G	N9-C4-C5	5.88	107.75	105.40
36	1	1131	G	N9-C4-C5	-5.88	103.05	105.40
36	1	2639	G	N3-C4-N9	5.88	129.53	126.00
36	5	189	G	N1-C6-O6	-5.88	116.37	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1115	G	N3-C4-N9	5.88	129.53	126.00
36	1	47	C	N1-C2-O2	-5.88	115.37	118.90
36	1	1307	G	C4-C5-N7	-5.88	108.45	110.80
36	1	2247	G	C5-C6-O6	-5.88	125.07	128.60
36	1	2358	A	C8-N9-C4	5.88	108.15	105.80
1	6	1539	G	N3-C4-N9	-5.88	122.47	126.00
36	5	2159	U	N3-C2-O2	-5.88	118.08	122.20
36	5	2245	C	C2-N1-C1'	5.88	125.27	118.80
36	1	426	G	N3-C4-C5	-5.88	125.66	128.60
36	1	2790	A	O5'-P-OP2	-5.88	100.41	105.70
36	1	3204	C	N1-C2-O2	5.88	122.43	118.90
1	6	53	G	C4-C5-C6	5.88	122.33	118.80
1	6	1091	A	N1-C2-N3	5.88	132.24	129.30
36	1	1151	U	C5-C6-N1	5.88	125.64	122.70
36	1	1308	A	C4-C5-C6	5.88	119.94	117.00
1	6	647	G	N3-C2-N2	-5.88	115.79	119.90
36	5	694	C	N1-C2-N3	5.88	123.31	119.20
36	5	881	C	C2-N3-C4	5.88	122.84	119.90
36	5	1398	U	C5-C4-O4	5.88	129.43	125.90
36	5	3065	G	O5'-P-OP1	-5.88	100.41	105.70
36	1	958	C	C2-N3-C4	-5.87	116.96	119.90
1	6	48	G	O5'-P-OP2	-5.87	100.41	105.70
36	5	996	A	N1-C6-N6	-5.87	115.08	118.60
36	1	373	A	OP2-P-O3'	5.87	118.12	105.20
36	1	716	A	C2-N3-C4	-5.87	107.66	110.60
36	1	2206	G	C5-C6-O6	-5.87	125.08	128.60
36	5	1446	A	N7-C8-N9	-5.87	110.86	113.80
36	5	1497	C	O5'-P-OP1	-5.87	100.42	105.70
36	5	2220	A	C8-N9-C4	-5.87	103.45	105.80
38	8	81	U	P-O3'-C3'	5.87	126.75	119.70
56	n0	82	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	2	1432	U	C5-C6-N1	-5.87	119.77	122.70
1	6	75	U	C2-N1-C1'	5.87	124.74	117.70
1	6	1539	G	N3-C4-C5	5.87	131.53	128.60
36	5	1182	A	C8-N9-C4	5.87	108.15	105.80
36	1	346	C	C5-C6-N1	-5.87	118.07	121.00
36	1	1546	A	C2-N3-C4	5.87	113.53	110.60
36	1	1789	G	N9-C4-C5	-5.87	103.05	105.40
1	6	938	G	O5'-P-OP2	-5.87	100.42	105.70
36	5	504	A	N9-C4-C5	-5.87	103.45	105.80
36	5	3099	C	C4-C5-C6	5.87	120.33	117.40
36	5	3154	C	C5-C6-N1	5.87	123.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1007	U	C5-C4-O4	-5.87	122.38	125.90
36	1	1589	A	O4'-C1'-N9	-5.87	103.51	108.20
36	1	2603	G	C4-C5-N7	5.87	113.15	110.80
36	5	822	G	O5'-P-OP1	-5.87	100.42	105.70
36	5	1863	G	C5-C6-N1	5.87	114.43	111.50
36	1	1320	C	N3-C4-C5	-5.87	119.55	121.90
36	5	2984	C	N1-C2-N3	5.87	123.31	119.20
36	1	2634	U	C2-N3-C4	-5.86	123.48	127.00
36	1	2967	A	C8-N9-C4	5.86	108.15	105.80
1	6	1340	U	N3-C2-O2	-5.86	118.10	122.20
56	n0	99	ARG	NE-CZ-NH1	-5.86	117.37	120.30
36	1	2924	U	C5-C6-N1	-5.86	119.77	122.70
36	5	2627	C	N3-C2-O2	-5.86	117.80	121.90
36	1	2806	U	N1-C2-N3	5.86	118.42	114.90
36	5	2383	C	N3-C4-C5	-5.86	119.56	121.90
1	2	874	C	N3-C2-O2	5.86	126.00	121.90
36	5	2984	C	C5-C6-N1	-5.86	118.07	121.00
1	2	1596	C	N1-C2-O2	5.86	122.41	118.90
36	1	1103	A	P-O3'-C3'	5.86	126.73	119.70
36	1	1493	G	O4'-C1'-N9	5.86	112.89	108.20
36	1	2922	G	OP1-P-O3'	5.86	118.09	105.20
36	5	691	A	C2-N3-C4	-5.86	107.67	110.60
36	5	811	U	C2-N3-C4	-5.86	123.48	127.00
1	6	269	G	C8-N9-C4	5.86	108.74	106.40
12	c0	88	PRO	N-CA-CB	5.86	110.33	103.30
36	5	2888	U	N1-C2-O2	5.86	126.90	122.80
36	1	345	G	C4-C5-C6	5.85	122.31	118.80
36	1	2284	C	C2-N1-C1'	5.85	125.24	118.80
36	1	3344	A	C2-N3-C4	-5.85	107.67	110.60
36	5	96	G	C2-N3-C4	-5.85	108.97	111.90
36	5	961	C	C6-N1-C2	-5.85	117.96	120.30
36	1	344	A	N1-C6-N6	-5.85	115.09	118.60
36	1	2636	A	N7-C8-N9	5.85	116.73	113.80
37	3	102	A	C8-N9-C4	5.85	108.14	105.80
36	1	1152	G	OP1-P-OP2	5.85	128.38	119.60
36	1	1851	G	C8-N9-C4	-5.85	104.06	106.40
36	1	2984	C	C6-N1-C2	-5.85	117.96	120.30
38	4	74	U	N1-C2-O2	-5.85	118.70	122.80
36	1	1468	A	C2-N3-C4	-5.85	107.67	110.60
36	1	1951	C	C2-N1-C1'	5.85	125.23	118.80
1	6	1150	G	C2-N3-C4	-5.85	108.98	111.90
36	5	2632	G	OP1-P-O3'	5.85	118.07	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	7	41	G	C8-N9-C4	5.85	108.74	106.40
1	2	1782	A	C5-C6-N6	5.85	128.38	123.70
52	M6	172	ARG	NE-CZ-NH2	-5.85	117.38	120.30
36	5	2851	A	C2-N3-C4	-5.85	107.68	110.60
37	7	103	A	N9-C4-C5	-5.85	103.46	105.80
1	2	99	C	N3-C2-O2	-5.85	117.81	121.90
36	1	1386	A	C5-C6-N6	-5.85	119.02	123.70
1	2	1600	A	N1-C6-N6	5.84	122.11	118.60
36	1	14	U	O5'-P-OP2	-5.84	100.44	105.70
36	1	2823	G	C4-C5-N7	-5.84	108.46	110.80
1	6	18	C	C6-N1-C2	-5.84	117.96	120.30
36	5	205	C	N1-C2-O2	5.84	122.41	118.90
1	2	443	C	C6-N1-C2	-5.84	117.96	120.30
1	2	61	A	N7-C8-N9	5.84	116.72	113.80
1	2	720	G	P-O3'-C3'	5.84	126.71	119.70
6	S4	3	ARG	NE-CZ-NH1	-5.84	117.38	120.30
36	1	3244	A	O5'-P-OP2	-5.84	100.44	105.70
36	5	2724	U	N3-C2-O2	-5.84	118.11	122.20
1	2	1740	A	N1-C6-N6	5.84	122.10	118.60
36	5	1115	G	OP1-P-O3'	5.84	118.05	105.20
36	5	1208	U	N1-C2-N3	5.84	118.40	114.90
36	5	2611	U	C4-C5-C6	5.84	123.20	119.70
36	5	2700	G	C6-C5-N7	-5.84	126.90	130.40
36	5	2899	C	O5'-P-OP1	5.84	117.71	110.70
36	1	2976	A	C5-C6-N6	-5.84	119.03	123.70
1	6	371	G	C8-N9-C1'	-5.84	119.41	127.00
36	1	64	G	C5-C6-O6	5.84	132.10	128.60
38	8	20	U	N1-C2-O2	-5.84	118.71	122.80
36	5	2724	U	C6-N1-C2	-5.83	117.50	121.00
36	1	2222	A	N9-C4-C5	5.83	108.13	105.80
36	1	2403	G	OP1-P-O3'	5.83	118.03	105.20
1	6	539	G	N3-C4-N9	-5.83	122.50	126.00
1	2	380	U	N1-C2-O2	5.83	126.88	122.80
36	1	176	G	N3-C4-N9	5.83	129.50	126.00
36	1	658	G	C4-C5-C6	5.83	122.30	118.80
36	1	901	G	N1-C6-O6	5.83	123.40	119.90
36	1	1316	C	N1-C2-O2	-5.83	115.40	118.90
41	L4	206	LEU	CA-CB-CG	5.83	128.71	115.30
36	5	614	C	C6-N1-C2	5.83	122.63	120.30
36	5	2283	G	N3-C2-N2	-5.83	115.82	119.90
36	1	155	G	N3-C2-N2	5.83	123.98	119.90
36	1	295	A	N7-C8-N9	5.83	116.71	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1159	A	O5'-P-OP1	5.83	117.69	110.70
36	1	2373	A	C8-N9-C4	-5.83	103.47	105.80
38	4	85	G	C6-C5-N7	-5.83	126.90	130.40
1	6	337	G	N1-C6-O6	5.83	123.40	119.90
36	5	519	A	N1-C6-N6	5.83	122.10	118.60
36	5	767	U	O4'-C1'-N1	5.83	112.86	108.20
36	5	2811	A	N1-C2-N3	5.83	132.22	129.30
36	5	3006	A	C6-N1-C2	-5.83	115.10	118.60
36	1	1184	A	N9-C4-C5	5.83	108.13	105.80
1	6	387	A	C4-C5-N7	-5.83	107.79	110.70
1	6	1280	C	N3-C4-C5	-5.83	119.57	121.90
36	1	648	C	C6-N1-C1'	-5.82	113.81	120.80
36	1	2664	C	C6-N1-C2	-5.82	117.97	120.30
36	5	275	U	C5-C4-O4	5.82	129.39	125.90
36	5	2404	A	O4'-C1'-N9	5.82	112.86	108.20
37	7	46	A	OP2-P-O3'	5.82	118.01	105.20
38	8	140	G	C5-C6-N1	-5.82	108.59	111.50
36	1	233	C	C6-N1-C2	5.82	122.63	120.30
1	6	767	U	N3-C2-O2	-5.82	118.12	122.20
36	5	1420	C	OP2-P-O3'	5.82	118.01	105.20
1	2	577	G	C6-C5-N7	-5.82	126.91	130.40
36	5	1429	G	C2-N3-C4	-5.82	108.99	111.90
36	5	1866	C	C5-C4-N4	-5.82	116.13	120.20
36	5	1925	U	C5-C6-N1	5.82	125.61	122.70
36	1	707	U	N1-C2-O2	-5.82	118.73	122.80
36	1	968	G	C5-C6-O6	-5.82	125.11	128.60
36	1	1196	C	C6-N1-C2	5.82	122.63	120.30
1	6	1700	C	N3-C2-O2	-5.82	117.83	121.90
36	5	1304	A	C8-N9-C4	-5.82	103.47	105.80
1	2	302	U	C5-C6-N1	5.82	125.61	122.70
1	2	1559	A	O4'-C1'-N9	5.82	112.85	108.20
36	1	1925	U	N1-C2-O2	-5.82	118.73	122.80
36	1	2165	G	O5'-P-OP2	-5.82	100.46	105.70
36	1	2621	G	N9-C4-C5	5.82	107.73	105.40
36	1	2866	U	C2-N1-C1'	5.82	124.68	117.70
36	1	3214	U	C5-C4-O4	5.82	129.39	125.90
36	1	3217	C	C6-N1-C1'	-5.82	113.82	120.80
36	5	964	G	C8-N9-C4	-5.82	104.07	106.40
36	5	2197	C	N3-C4-C5	5.82	124.23	121.90
36	5	3174	A	N7-C8-N9	5.82	116.71	113.80
36	1	221	A	N9-C4-C5	5.82	108.13	105.80
36	1	1355	A	P-O3'-C3'	5.82	126.68	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	448	C	OP1-P-O3'	5.82	118.00	105.20
36	5	75	G	N1-C6-O6	5.82	123.39	119.90
36	5	281	G	N3-C2-N2	-5.82	115.83	119.90
36	5	1119	C	OP2-P-O3'	5.81	117.99	105.20
36	5	1209	G	C5-C6-O6	-5.81	125.11	128.60
36	1	2142	A	N3-C4-C5	-5.81	122.73	126.80
36	1	2585	G	C2-N3-C4	5.81	114.81	111.90
1	6	608	U	N3-C2-O2	-5.81	118.13	122.20
36	5	1323	G	C8-N9-C4	-5.81	104.08	106.40
36	5	1790	G	C4-C5-C6	5.81	122.29	118.80
36	5	1838	G	OP1-P-O3'	5.81	117.99	105.20
36	5	2937	G	C6-C5-N7	-5.81	126.91	130.40
36	5	2944	U	C5-C6-N1	5.81	125.61	122.70
44	l7	83	LEU	CA-CB-CG	5.81	128.67	115.30
36	1	1011	A	C8-N9-C4	5.81	108.12	105.80
1	6	308	C	C4-C5-C6	5.81	120.31	117.40
36	5	704	U	N3-C4-O4	5.81	123.47	119.40
36	5	2435	G	C4-C5-N7	5.81	113.12	110.80
1	2	403	G	O5'-P-OP2	-5.81	100.47	105.70
36	1	1845	G	C8-N9-C4	-5.81	104.08	106.40
42	L5	115	LEU	CA-CB-CG	5.81	128.66	115.30
36	5	1900	A	O5'-P-OP1	-5.81	100.47	105.70
1	2	323	A	C8-N9-C4	-5.81	103.48	105.80
1	6	334	G	N3-C2-N2	5.81	123.97	119.90
36	5	2679	A	C8-N9-C4	5.81	108.12	105.80
36	5	3042	U	N1-C2-N3	5.81	118.38	114.90
36	5	2552	C	C2-N1-C1'	5.81	125.19	118.80
1	2	1654	G	C6-C5-N7	-5.80	126.92	130.40
36	5	2892	A	C6-C5-N7	-5.80	128.24	132.30
1	2	1789	G	C8-N9-C1'	-5.80	119.46	127.00
1	6	1677	C	N1-C2-O2	-5.80	115.42	118.90
36	1	909	G	C8-N9-C4	5.80	108.72	106.40
36	1	3079	U	C2-N1-C1'	-5.80	110.74	117.70
36	5	2145	A	N1-C2-N3	5.80	132.20	129.30
36	5	2376	G	C8-N9-C4	-5.80	104.08	106.40
36	5	2371	G	C8-N9-C4	5.80	108.72	106.40
36	5	2666	C	N3-C4-C5	-5.80	119.58	121.90
36	5	3306	U	C5-C4-O4	-5.80	122.42	125.90
36	5	1047	A	C5-C6-N1	5.80	120.60	117.70
36	1	417	A	C5-C6-N6	-5.80	119.06	123.70
36	1	2300	G	OP2-P-O3'	5.80	117.95	105.20
36	1	2429	G	N1-C6-O6	-5.80	116.42	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	425	A	O5'-P-OP1	5.80	117.66	110.70
1	6	1002	G	N1-C6-O6	5.80	123.38	119.90
1	6	1269	U	N3-C2-O2	-5.80	118.14	122.20
36	5	922	U	C4-C5-C6	5.80	123.18	119.70
36	5	1306	G	C5-C6-O6	-5.80	125.12	128.60
36	5	2163	C	N3-C2-O2	-5.80	117.84	121.90
36	5	2361	A	OP2-P-O3'	5.80	117.95	105.20
36	1	51	A	C8-N9-C4	-5.79	103.48	105.80
1	6	350	U	C5-C6-N1	-5.79	119.80	122.70
36	5	966	U	N1-C2-O2	5.79	126.86	122.80
36	5	1902	G	C4-C5-C6	5.79	122.28	118.80
36	5	2801	A	C8-N9-C4	5.79	108.12	105.80
36	5	3006	A	C5-N7-C8	-5.79	101.00	103.90
1	6	609	U	N3-C2-O2	-5.79	118.14	122.20
36	5	410	U	O5'-P-OP1	-5.79	100.49	105.70
36	5	2222	A	OP2-P-O3'	5.79	117.95	105.20
36	5	2735	U	C6-N1-C2	-5.79	117.52	121.00
36	1	153	U	N3-C4-C5	-5.79	111.12	114.60
36	5	187	A	C6-N1-C2	-5.79	115.12	118.60
36	5	388	G	C5-C6-O6	-5.79	125.12	128.60
36	5	903	U	OP1-P-O3'	5.79	117.94	105.20
36	5	2971	A	N3-C4-N9	5.79	132.03	127.40
36	5	3174	A	O4'-C1'-N9	5.79	112.83	108.20
1	2	416	A	C8-N9-C4	5.79	108.12	105.80
36	1	3028	G	C4-C5-N7	5.79	113.12	110.80
36	5	3343	G	N3-C2-N2	5.79	123.95	119.90
37	7	86	U	O5'-P-OP2	-5.79	100.49	105.70
1	2	1291	G	C6-C5-N7	-5.79	126.93	130.40
36	1	363	G	N1-C6-O6	5.79	123.37	119.90
36	1	1344	G	N9-C4-C5	-5.79	103.08	105.40
49	M3	85	LEU	CA-CB-CG	5.79	128.61	115.30
1	6	1736	G	N1-C6-O6	5.79	123.37	119.90
36	5	2883	U	N3-C2-O2	-5.79	118.15	122.20
37	7	101	G	N3-C4-N9	5.79	129.47	126.00
36	5	1367	G	C4-N9-C1'	5.79	134.02	126.50
36	1	1041	U	C6-N1-C2	5.79	124.47	121.00
1	6	1	U	N3-C2-O2	-5.79	118.15	122.20
36	5	2112	U	C6-N1-C2	-5.79	117.53	121.00
36	5	2299	A	O5'-P-OP2	-5.79	100.49	105.70
36	1	25	U	C4-C5-C6	5.78	123.17	119.70
36	1	2700	G	C5-C6-O6	-5.78	125.13	128.60
37	3	48	U	C2-N1-C1'	5.78	124.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1472	C	C5-C4-N4	5.78	124.25	120.20
36	5	2940	A	C6-C5-N7	-5.78	128.25	132.30
36	5	3285	C	C2-N1-C1'	5.78	125.16	118.80
36	5	2346	C	N1-C2-O2	-5.78	115.43	118.90
1	2	615	A	C5-C6-N1	5.78	120.59	117.70
36	1	1509	A	C2-N3-C4	-5.78	107.71	110.60
36	5	888	A	C8-N9-C4	-5.78	103.49	105.80
67	o1	90	PHE	CB-CA-C	-5.78	98.84	110.40
36	1	2111	G	C5-C6-O6	5.78	132.07	128.60
57	n1	88	ARG	NE-CZ-NH1	-5.78	117.41	120.30
36	1	3210	A	O5'-P-OP2	-5.78	100.50	105.70
36	5	1889	G	C2-N3-C4	5.78	114.79	111.90
37	7	73	C	C5-C6-N1	5.78	123.89	121.00
1	2	55	A	C8-N9-C4	-5.78	103.49	105.80
36	1	959	C	C5-C4-N4	-5.78	116.16	120.20
56	n0	13	ARG	NE-CZ-NH2	-5.78	117.41	120.30
36	1	941	G	OP1-P-O3'	5.77	117.90	105.20
36	1	961	C	C2-N3-C4	-5.77	117.01	119.90
1	2	1456	C	C6-N1-C2	-5.77	117.99	120.30
36	1	1503	A	C2-N3-C4	-5.77	107.71	110.60
36	1	2733	A	C5-C6-N6	-5.77	119.08	123.70
1	6	350	U	N1-C2-N3	5.77	118.36	114.90
36	5	1147	G	N3-C2-N2	-5.77	115.86	119.90
36	5	1309	U	N1-C2-N3	5.77	118.36	114.90
36	5	2354	C	N3-C4-C5	-5.77	119.59	121.90
36	1	1343	A	N9-C4-C5	-5.77	103.49	105.80
36	1	105	C	N3-C4-N4	5.77	122.04	118.00
36	1	2758	A	N7-C8-N9	-5.77	110.92	113.80
36	1	3109	G	C8-N9-C4	5.77	108.71	106.40
36	5	2340	U	O5'-P-OP1	-5.77	100.51	105.70
36	5	3392	U	C5-C4-O4	5.77	129.36	125.90
36	1	1008	U	C2-N1-C1'	-5.77	110.78	117.70
36	1	1640	G	N3-C4-N9	5.77	129.46	126.00
36	1	2409	G	C6-C5-N7	-5.77	126.94	130.40
36	5	1662	G	N1-C6-O6	5.77	123.36	119.90
36	5	1724	U	N1-C2-N3	5.77	118.36	114.90
36	5	2173	U	C5-C4-O4	5.77	129.36	125.90
1	2	338	C	N1-C2-O2	-5.77	115.44	118.90
36	5	3311	C	N3-C4-C5	-5.77	119.59	121.90
36	5	859	G	C4-C5-N7	5.76	113.11	110.80
36	5	864	G	C2-N3-C4	5.76	114.78	111.90
36	5	3118	C	C5-C6-N1	5.76	123.88	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	139	C	P-O3'-C3'	5.76	126.61	119.70
36	1	593	C	C2-N1-C1'	5.76	125.14	118.80
36	1	1893	A	C2-N3-C4	-5.76	107.72	110.60
36	5	269	G	C8-N9-C4	5.76	108.70	106.40
36	5	1872	C	N1-C2-O2	5.76	122.36	118.90
36	5	2425	G	C8-N9-C4	-5.76	104.09	106.40
36	5	2886	U	C4-C5-C6	5.76	123.16	119.70
36	5	3050	U	N3-C4-O4	-5.76	115.37	119.40
37	3	86	U	OP1-P-O3'	5.76	117.87	105.20
37	3	98	C	N1-C2-O2	-5.76	115.44	118.90
36	5	1178	G	N9-C4-C5	-5.76	103.10	105.40
1	6	1793	G	N1-C6-O6	-5.76	116.44	119.90
36	5	815	G	C4-N9-C1'	5.76	133.99	126.50
36	5	1112	A	C6-N1-C2	-5.76	115.14	118.60
36	1	1313	G	C4-C5-N7	5.76	113.10	110.80
36	1	2605	G	OP1-P-OP2	-5.76	110.97	119.60
36	5	3050	U	N3-C2-O2	-5.76	118.17	122.20
45	l8	69	LEU	CA-CB-CG	5.76	128.54	115.30
36	1	980	A	C5-C6-N1	-5.75	114.82	117.70
36	5	1117	G	N1-C6-O6	-5.75	116.45	119.90
36	1	1114	U	C5-C4-O4	5.75	129.35	125.90
36	1	2376	G	C5-N7-C8	-5.75	101.42	104.30
38	4	111	A	C6-C5-N7	-5.75	128.27	132.30
1	6	565	C	C6-N1-C2	5.75	122.60	120.30
36	1	1796	G	C8-N9-C4	-5.75	104.10	106.40
36	1	2418	G	C2-N3-C4	5.75	114.78	111.90
39	L2	25	GLY	N-CA-C	-5.75	98.72	113.10
36	1	718	G	N9-C4-C5	-5.75	103.10	105.40
36	1	2130	G	C4-C5-N7	-5.75	108.50	110.80
36	1	3344	A	C6-C5-N7	-5.75	128.28	132.30
36	5	1468	A	C4-C5-C6	5.75	119.88	117.00
1	2	747	C	C2-N1-C1'	5.75	125.12	118.80
36	1	1175	C	C5-C6-N1	-5.75	118.13	121.00
36	5	2821	C	C6-N1-C2	5.75	122.60	120.30
36	5	2934	A	N1-C6-N6	-5.75	115.15	118.60
36	5	3243	A	C4-C5-C6	5.75	119.87	117.00
36	1	2337	C	C6-N1-C2	-5.75	118.00	120.30
36	1	2633	U	N3-C2-O2	-5.75	118.18	122.20
1	6	467	G	N3-C4-N9	5.75	129.45	126.00
36	5	1431	G	C4-C5-N7	-5.75	108.50	110.80
36	1	1190	A	C4-N9-C1'	5.75	136.64	126.30
36	5	622	A	N1-C6-N6	5.75	122.05	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1396	C	C6-N1-C2	5.75	122.60	120.30
36	5	1419	A	O5'-P-OP1	5.75	117.59	110.70
1	2	551	G	C8-N9-C4	-5.74	104.10	106.40
36	1	2332	A	N1-C6-N6	5.74	122.05	118.60
36	1	3062	G	C5-C6-O6	-5.74	125.15	128.60
36	5	1210	U	N3-C4-O4	-5.74	115.38	119.40
36	5	2256	A	C8-N9-C4	5.74	108.10	105.80
1	6	1767	G	N3-C4-C5	5.74	131.47	128.60
36	5	974	G	N3-C4-N9	5.74	129.44	126.00
36	5	2283	G	N9-C4-C5	-5.74	103.10	105.40
1	2	1537	C	C5-C6-N1	5.74	123.87	121.00
36	1	1099	A	C4-C5-N7	5.74	113.57	110.70
36	1	1116	G	N1-C6-O6	5.74	123.34	119.90
36	5	1226	G	N9-C4-C5	-5.74	103.10	105.40
36	5	1490	A	C6-C5-N7	-5.74	128.28	132.30
36	5	3043	C	C2-N3-C4	-5.74	117.03	119.90
36	5	3188	G	C4-C5-N7	-5.74	108.50	110.80
36	5	784	A	C6-C5-N7	-5.74	128.28	132.30
36	5	2379	U	C5-C6-N1	-5.74	119.83	122.70
36	5	2614	G	C8-N9-C1'	-5.74	119.54	127.00
36	5	2757	U	N3-C4-O4	5.74	123.42	119.40
36	5	2960	C	C2-N3-C4	-5.74	117.03	119.90
36	1	3109	G	O5'-P-OP2	5.74	117.58	110.70
36	5	631	U	N3-C4-O4	-5.74	115.38	119.40
36	5	1912	U	N3-C2-O2	5.74	126.22	122.20
1	2	597	G	C8-N9-C1'	-5.74	119.55	127.00
1	2	1370	U	P-O3'-C3'	5.74	126.58	119.70
36	1	1868	G	N7-C8-N9	5.74	115.97	113.10
36	1	1931	U	C2-N1-C1'	-5.74	110.82	117.70
38	4	48	A	C5-C6-N6	-5.74	119.11	123.70
36	5	2917	G	C6-C5-N7	-5.74	126.96	130.40
36	1	1116	G	C6-N1-C2	-5.73	121.66	125.10
1	6	957	G	N1-C6-O6	5.73	123.34	119.90
36	5	40	A	N7-C8-N9	5.73	116.67	113.80
36	5	97	U	OP2-P-O3'	5.73	117.81	105.20
36	5	658	G	C8-N9-C4	-5.73	104.11	106.40
36	5	1493	G	O4'-C1'-N9	5.73	112.79	108.20
1	6	337	G	C8-N9-C1'	-5.73	119.55	127.00
1	6	350	U	N1-C2-O2	-5.73	118.79	122.80
1	6	630	A	C2-N3-C4	-5.73	107.73	110.60
36	5	2339	C	N3-C2-O2	-5.73	117.89	121.90
36	1	1489	A	C5-C6-N6	-5.73	119.12	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2112	U	C2-N1-C1'	5.73	124.57	117.70
36	1	2279	A	C8-N9-C4	5.73	108.09	105.80
36	5	2713	U	N3-C2-O2	-5.73	118.19	122.20
36	5	3366	G	N3-C4-C5	-5.73	125.74	128.60
36	1	957	C	N1-C2-O2	-5.73	115.46	118.90
36	1	2719	U	C2-N1-C1'	-5.73	110.83	117.70
38	4	32	C	C2-N1-C1'	-5.73	112.50	118.80
1	2	830	U	C2-N1-C1'	5.72	124.57	117.70
36	1	947	G	C4-N9-C1'	5.72	133.94	126.50
36	1	1175	C	C2-N3-C4	-5.72	117.04	119.90
38	4	50	C	C6-N1-C2	-5.72	118.01	120.30
36	5	2531	C	C2-N1-C1'	5.72	125.10	118.80
36	5	3209	A	C8-N9-C4	-5.72	103.51	105.80
36	1	2636	A	N9-C4-C5	5.72	108.09	105.80
1	6	409	C	N1-C2-O2	-5.72	115.47	118.90
38	8	38	U	C4-C5-C6	5.72	123.13	119.70
36	1	70	A	C2-N3-C4	-5.72	107.74	110.60
1	6	579	A	P-O3'-C3'	5.72	126.56	119.70
36	5	568	G	C5-C6-O6	-5.72	125.17	128.60
36	5	2419	A	C2-N3-C4	-5.72	107.74	110.60
36	5	2886	U	C5-C4-O4	5.72	129.33	125.90
36	1	931	C	N3-C4-C5	5.72	124.19	121.90
1	6	1124	A	C8-N9-C4	5.72	108.09	105.80
36	5	1151	U	O5'-P-OP2	-5.72	100.55	105.70
36	1	1308	A	N9-C4-C5	5.72	108.09	105.80
1	2	507	U	N1-C2-O2	5.71	126.80	122.80
36	1	967	A	OP2-P-O3'	5.71	117.77	105.20
1	6	1002	G	C6-C5-N7	-5.71	126.97	130.40
1	6	1552	U	N3-C2-O2	5.71	126.20	122.20
1	2	377	G	C4-N9-C1'	-5.71	119.07	126.50
36	1	29	C	N3-C4-C5	5.71	124.19	121.90
36	5	2868	U	C5-C6-N1	5.71	125.56	122.70
36	1	3210	A	N1-C6-N6	-5.71	115.17	118.60
36	5	410	U	N3-C4-O4	5.71	123.40	119.40
36	5	2113	A	C8-N9-C4	5.71	108.08	105.80
37	7	10	C	C2-N1-C1'	5.71	125.08	118.80
36	5	941	G	OP1-P-O3'	5.71	117.76	105.20
36	5	1598	G	C8-N9-C4	5.71	108.68	106.40
36	1	2355	G	N3-C2-N2	-5.71	115.90	119.90
36	1	2630	C	N3-C4-C5	-5.71	119.62	121.90
36	5	2211	U	N3-C4-C5	-5.71	111.17	114.60
36	5	2611	U	O5'-P-OP1	5.71	117.55	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3207	U	C2-N1-C1'	-5.71	110.85	117.70
36	1	652	G	N3-C4-C5	-5.71	125.75	128.60
38	4	151	C	N3-C4-C5	-5.71	119.62	121.90
36	5	1659	U	N3-C2-O2	-5.71	118.21	122.20
36	5	2899	C	N3-C4-C5	-5.71	119.62	121.90
36	5	3060	C	C5-C6-N1	5.71	123.85	121.00
1	2	694	U	C5-C6-N1	5.71	125.55	122.70
36	1	2374	C	N3-C4-C5	-5.71	119.62	121.90
36	1	663	C	C6-N1-C2	5.70	122.58	120.30
36	1	1322	U	N3-C2-O2	5.70	126.19	122.20
38	4	47	C	C5-C6-N1	-5.70	118.15	121.00
36	5	398	A	OP1-P-OP2	5.70	128.16	119.60
36	5	666	A	C6-N1-C2	-5.70	115.18	118.60
38	4	140	G	N3-C2-N2	-5.70	115.91	119.90
36	5	2183	A	C5-C6-N6	-5.70	119.14	123.70
36	5	3137	C	C2-N1-C1'	-5.70	112.53	118.80
36	1	939	U	C5'-C4'-O4'	-5.70	102.26	109.10
36	5	75	G	O5'-P-OP2	-5.70	100.57	105.70
36	5	3183	A	N1-C6-N6	5.70	122.02	118.60
36	1	32	U	O5'-P-OP1	5.70	117.54	110.70
36	5	2618	G	C5-C6-N1	5.70	114.35	111.50
36	5	3145	C	C6-N1-C2	5.70	122.58	120.30
36	5	3269	U	P-O3'-C3'	5.70	126.54	119.70
36	1	2725	U	C5-C4-O4	5.70	129.32	125.90
36	1	2968	G	C6-C5-N7	-5.70	126.98	130.40
36	5	974	G	C2-N3-C4	5.70	114.75	111.90
36	5	2719	U	C6-N1-C1'	5.70	129.18	121.20
1	2	5	U	N3-C2-O2	-5.70	118.21	122.20
36	1	1190	A	N1-C6-N6	5.70	122.02	118.60
36	1	2237	C	N1-C2-O2	5.70	122.32	118.90
36	1	2379	U	O5'-P-OP2	-5.70	100.58	105.70
36	5	2377	G	N3-C2-N2	5.70	123.89	119.90
36	5	3343	G	N1-C2-N2	-5.70	111.07	116.20
36	5	1370	G	C6-N1-C2	-5.69	121.68	125.10
36	5	2136	C	C2-N3-C4	-5.69	117.05	119.90
36	5	2145	A	N9-C4-C5	5.69	108.08	105.80
1	2	73	U	P-O3'-C3'	5.69	126.53	119.70
36	1	2385	G	N1-C6-O6	5.69	123.31	119.90
37	3	61	G	N1-C6-O6	5.69	123.32	119.90
36	5	69	C	N3-C4-C5	-5.69	119.62	121.90
36	5	3129	A	C5-C6-N1	5.69	120.55	117.70
1	2	426	G	C4-N9-C1'	5.69	133.90	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2996	U	C5-C6-N1	5.69	125.55	122.70
38	4	111	A	C5-C6-N6	-5.69	119.15	123.70
36	5	3015	G	C4-C5-N7	-5.69	108.52	110.80
36	5	3204	C	C5-C6-N1	-5.69	118.16	121.00
1	2	941	A	N1-C6-N6	5.69	122.01	118.60
1	6	1540	G	N1-C6-O6	-5.69	116.49	119.90
36	1	585	A	C2-N3-C4	-5.69	107.76	110.60
36	1	1180	A	N9-C4-C5	5.69	108.08	105.80
36	1	1846	C	C6-N1-C2	-5.69	118.03	120.30
36	1	3057	U	N1-C2-N3	5.69	118.31	114.90
48	M1	112	LEU	CA-CB-CG	5.69	128.38	115.30
1	6	25	C	N1-C2-O2	-5.69	115.49	118.90
36	5	1181	U	C5-C4-O4	5.69	129.31	125.90
36	5	1375	G	C8-N9-C4	-5.69	104.12	106.40
36	5	2824	G	N3-C2-N2	-5.69	115.92	119.90
51	m5	96	ARG	NE-CZ-NH2	-5.69	117.46	120.30
36	1	1665	C	C5-C4-N4	-5.69	116.22	120.20
36	1	3006	A	C2-N3-C4	-5.69	107.76	110.60
36	5	281	G	C5-C6-O6	-5.69	125.19	128.60
36	5	671	U	C5-C6-N1	-5.69	119.86	122.70
36	5	796	U	N3-C2-O2	-5.69	118.22	122.20
36	5	936	A	P-O3'-C3'	5.69	126.52	119.70
36	1	2373	A	O5'-P-OP1	-5.68	100.58	105.70
36	5	922	U	C2-N3-C4	-5.68	123.59	127.00
36	5	1149	G	C6-C5-N7	-5.68	126.99	130.40
36	5	2297	U	O5'-P-OP2	-5.68	100.58	105.70
36	5	2647	A	C5-C6-N1	5.68	120.54	117.70
1	2	831	U	N3-C2-O2	-5.68	118.22	122.20
36	1	1918	C	C6-N1-C2	-5.68	118.03	120.30
36	1	2413	A	C5-C6-N1	5.68	120.54	117.70
1	6	323	A	O5'-P-OP2	-5.68	100.59	105.70
36	5	43	A	O4'-C1'-N9	5.68	112.75	108.20
36	5	70	A	C8-N9-C4	-5.68	103.53	105.80
36	5	2895	G	N3-C4-C5	-5.68	125.76	128.60
36	1	2811	A	N1-C2-N3	5.68	132.14	129.30
36	5	2930	A	C5-C6-N1	5.68	120.54	117.70
36	1	1154	A	N3-C4-C5	-5.68	122.83	126.80
36	1	1336	U	OP2-P-O3'	5.68	117.70	105.20
36	1	2984	C	N1-C2-N3	5.68	123.18	119.20
36	5	2410	U	O5'-P-OP1	-5.68	100.59	105.70
36	5	2435	G	C5-C6-O6	-5.68	125.19	128.60
36	5	3093	C	N1-C2-O2	-5.68	115.49	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1212	G	C6-C5-N7	-5.68	126.99	130.40
36	1	2815	G	C8-N9-C4	5.68	108.67	106.40
36	1	3112	G	OP1-P-O3'	5.68	117.69	105.20
1	6	447	U	N1-C2-N3	5.68	118.31	114.90
1	6	555	A	C8-N9-C4	-5.68	103.53	105.80
36	5	819	U	OP2-P-O3'	5.68	117.69	105.20
38	8	111	A	C5-C6-N6	-5.68	119.16	123.70
1	2	1202	A	C2-N3-C4	5.68	113.44	110.60
36	1	2541	U	P-O3'-C3'	5.68	126.51	119.70
36	1	2604	U	N3-C2-O2	-5.68	118.23	122.20
36	1	2624	G	C8-N9-C4	-5.68	104.13	106.40
38	4	40	A	C6-C5-N7	-5.68	128.33	132.30
36	5	332	C	N3-C2-O2	-5.68	117.93	121.90
36	5	640	U	N1-C2-O2	-5.68	118.83	122.80
36	5	977	C	N1-C2-O2	5.68	122.31	118.90
1	6	387	A	N1-C6-N6	-5.67	115.19	118.60
36	5	1112	A	N3-C4-C5	-5.67	122.83	126.80
36	5	2615	G	C6-C5-N7	-5.67	127.00	130.40
36	1	3179	U	N3-C4-O4	-5.67	115.43	119.40
1	6	634	G	C5-C6-O6	-5.67	125.20	128.60
36	5	361	A	C4-C5-N7	-5.67	107.86	110.70
1	2	778	G	C5-C6-O6	-5.67	125.20	128.60
36	1	1115	G	OP1-P-O3'	5.67	117.68	105.20
1	6	187	G	P-O3'-C3'	5.67	126.51	119.70
36	5	426	G	N7-C8-N9	-5.67	110.26	113.10
36	5	1389	G	C5-C6-O6	-5.67	125.20	128.60
36	5	1449	A	O5'-P-OP1	5.67	117.50	110.70
36	5	2724	U	N1-C2-N3	5.67	118.30	114.90
36	5	3164	C	O4'-C1'-N1	5.67	112.74	108.20
38	8	111	A	C6-C5-N7	-5.67	128.33	132.30
1	2	308	C	C2-N3-C4	-5.67	117.06	119.90
36	1	895	A	C8-N9-C4	-5.67	103.53	105.80
36	1	2923	U	C5-C4-O4	-5.67	122.50	125.90
36	5	2919	A	N1-C2-N3	5.67	132.13	129.30
1	2	412	A	N1-C6-N6	5.67	122.00	118.60
1	2	973	A	O5'-P-OP2	-5.67	100.60	105.70
36	1	2114	C	OP1-P-OP2	5.67	128.10	119.60
1	6	646	C	C6-N1-C2	-5.67	118.03	120.30
1	2	1558	U	N3-C2-O2	-5.67	118.23	122.20
36	1	611	A	O5'-P-OP1	5.67	117.50	110.70
36	1	1789	G	C5-C6-N1	5.67	114.33	111.50
36	5	2715	A	N9-C4-C5	5.67	108.07	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2820	A	C2-N3-C4	5.67	113.43	110.60
1	2	241	U	O5'-P-OP2	-5.67	100.60	105.70
36	1	107	A	N9-C4-C5	-5.67	103.53	105.80
36	1	701	G	OP2-P-O3'	5.67	117.66	105.20
36	1	2935	U	C6-N1-C2	-5.67	117.60	121.00
36	5	3092	C	O4'-C1'-N1	5.67	112.73	108.20
1	2	297	U	N3-C2-O2	-5.66	118.23	122.20
1	2	1200	G	N1-C2-N2	5.66	121.30	116.20
36	1	2647	A	N1-C2-N3	5.66	132.13	129.30
36	5	1589	A	C5-C6-N1	5.66	120.53	117.70
36	5	1879	A	C6-C5-N7	-5.66	128.34	132.30
36	5	2334	U	N3-C2-O2	-5.66	118.24	122.20
36	5	2700	G	N3-C4-N9	5.66	129.40	126.00
36	1	908	G	O4'-C1'-N9	-5.66	103.67	108.20
38	4	94	C	N3-C4-C5	5.66	124.17	121.90
36	5	2615	G	N3-C4-N9	5.66	129.40	126.00
36	1	949	C	N3-C4-C5	-5.66	119.64	121.90
36	5	573	C	N1-C2-O2	-5.66	115.50	118.90
36	5	1302	A	N7-C8-N9	5.66	116.63	113.80
36	5	3015	G	OP2-P-O3'	5.66	117.65	105.20
36	5	3004	C	C6-N1-C2	5.66	122.56	120.30
36	1	53	G	N3-C4-C5	-5.65	125.77	128.60
36	1	906	A	C8-N9-C4	-5.65	103.54	105.80
36	5	1464	G	C5-C6-O6	-5.65	125.21	128.60
36	5	2293	C	C2-N1-C1'	5.65	125.02	118.80
36	5	2634	U	C2-N3-C4	-5.65	123.61	127.00
36	5	2715	A	OP2-P-O3'	5.65	117.63	105.20
36	1	3197	G	N3-C4-C5	5.65	131.42	128.60
36	5	3259	U	N1-C2-O2	-5.65	118.85	122.80
36	1	2148	U	C5-C4-O4	-5.65	122.51	125.90
1	6	17	C	O5'-P-OP2	-5.65	100.62	105.70
1	6	1111	G	C6-C5-N7	-5.65	127.01	130.40
1	6	1652	C	N3-C4-C5	5.65	124.16	121.90
36	5	1106	G	C2-N3-C4	5.65	114.72	111.90
36	5	1437	C	C2-N1-C1'	5.65	125.01	118.80
36	5	2645	G	C2-N3-C4	5.65	114.72	111.90
36	5	3319	U	C2-N1-C1'	5.65	124.48	117.70
41	l4	134	LEU	CA-CB-CG	5.65	128.29	115.30
1	2	1745	G	C5-C6-O6	-5.65	125.21	128.60
36	5	561	C	C6-N1-C2	-5.65	118.04	120.30
1	2	296	U	N3-C2-O2	5.64	126.15	122.20
36	1	1458	U	C5-C6-N1	-5.64	119.88	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1746	A	O5'-P-OP1	-5.64	100.62	105.70
36	5	92	G	N9-C4-C5	-5.64	103.14	105.40
36	5	341	G	N3-C4-C5	5.64	131.42	128.60
36	5	1496	C	N1-C2-O2	5.64	122.29	118.90
37	7	83	U	C5-C4-O4	5.64	129.29	125.90
36	1	325	A	OP1-P-O3'	5.64	117.61	105.20
36	1	949	C	OP2-P-O3'	5.64	117.61	105.20
36	1	1314	C	C5-C6-N1	5.64	123.82	121.00
36	1	2124	G	C6-C5-N7	-5.64	127.01	130.40
36	1	2893	C	N3-C4-N4	-5.64	114.05	118.00
1	6	305	C	N1-C2-O2	-5.64	115.51	118.90
36	5	80	G	C5-C6-O6	-5.64	125.21	128.60
36	5	1113	G	N1-C2-N3	5.64	127.29	123.90
36	5	2169	G	C5-C6-N1	5.64	114.32	111.50
36	5	3188	G	C5-C6-O6	5.64	131.99	128.60
36	1	2879	C	N3-C2-O2	5.64	125.85	121.90
53	M7	131	ARG	NE-CZ-NH1	-5.64	117.48	120.30
36	5	3305	A	C6-C5-N7	-5.64	128.35	132.30
36	1	369	A	C2-N3-C4	5.64	113.42	110.60
36	1	665	A	C5-C6-N1	5.64	120.52	117.70
36	5	1113	G	N3-C4-N9	-5.64	122.62	126.00
36	5	2305	G	N7-C8-N9	5.64	115.92	113.10
36	1	2624	G	C4-C5-N7	5.64	113.06	110.80
36	1	2169	G	C2-N3-C4	5.64	114.72	111.90
36	5	128	G	C6-C5-N7	-5.64	127.02	130.40
36	1	200	C	C2-N3-C4	-5.63	117.08	119.90
36	1	2306	C	C5-C4-N4	5.63	124.14	120.20
36	5	2699	G	C5-C6-O6	-5.63	125.22	128.60
38	8	10	A	N1-C6-N6	5.63	121.98	118.60
36	1	329	U	C6-N1-C2	-5.63	117.62	121.00
36	1	1604	G	C8-N9-C1'	-5.63	119.68	127.00
1	6	858	G	C4-C5-N7	5.63	113.05	110.80
36	5	2393	G	N1-C2-N2	5.63	121.27	116.20
1	2	453	U	N1-C2-O2	5.63	126.74	122.80
36	1	1405	U	C6-N1-C2	5.63	124.38	121.00
36	1	3362	A	C8-N9-C4	-5.63	103.55	105.80
1	6	547	U	N3-C4-O4	-5.63	115.46	119.40
36	5	2189	U	O5'-P-OP1	-5.63	100.63	105.70
37	7	78	U	O5'-P-OP2	-5.63	100.63	105.70
36	1	1385	C	N3-C2-O2	5.63	125.84	121.90
36	1	2325	G	O5'-P-OP2	-5.63	100.63	105.70
36	5	915	A	C2-N3-C4	5.63	113.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3093	C	C2-N1-C1'	-5.63	112.61	118.80
36	5	58	G	C8-N9-C4	-5.63	104.15	106.40
36	5	1229	G	C8-N9-C4	5.63	108.65	106.40
36	5	2643	A	C5-N7-C8	-5.63	101.09	103.90
36	5	2661	G	C5-C6-N1	5.63	114.31	111.50
36	1	994	G	N3-C4-C5	-5.63	125.79	128.60
36	1	2720	G	N3-C4-N9	5.63	129.38	126.00
36	1	2976	A	C5-C6-N1	5.63	120.51	117.70
36	5	989	A	C5-C6-N1	5.63	120.51	117.70
36	5	1723	A	C8-N9-C4	-5.63	103.55	105.80
36	5	3174	A	C6-C5-N7	-5.63	128.36	132.30
36	1	2276	G	C8-N9-C4	-5.62	104.15	106.40
36	1	3044	G	N1-C6-O6	-5.62	116.53	119.90
36	5	1910	A	OP2-P-O3'	5.62	117.58	105.20
1	2	380	U	N3-C2-O2	-5.62	118.26	122.20
36	1	324	A	C6-N1-C2	-5.62	115.23	118.60
36	1	2101	C	P-O3'-C3'	5.62	126.45	119.70
36	5	2619	G	C4-C5-N7	5.62	113.05	110.80
36	5	3026	G	C5-C6-O6	-5.62	125.23	128.60
36	1	1484	U	C2-N1-C1'	5.62	124.44	117.70
54	M8	178	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	6	1000	C	N1-C2-O2	5.62	122.27	118.90
36	5	2816	G	OP1-P-O3'	5.62	117.57	105.20
36	1	3316	A	N3-C4-C5	5.62	130.73	126.80
36	1	2812	C	C6-N1-C2	5.62	122.55	120.30
36	1	3275	U	C6-N1-C2	-5.62	117.63	121.00
36	1	421	G	C8-N9-C1'	-5.62	119.70	127.00
36	1	778	U	N3-C4-O4	-5.62	115.47	119.40
36	1	2937	G	N3-C2-N2	-5.62	115.97	119.90
1	2	457	G	N3-C4-C5	-5.62	125.79	128.60
36	1	1709	C	N1-C2-O2	-5.62	115.53	118.90
38	4	109	A	C5-C6-N6	-5.62	119.21	123.70
73	O7	11	ARG	NE-CZ-NH1	-5.62	117.49	120.30
36	5	2119	A	C8-N9-C4	-5.62	103.55	105.80
36	5	2357	A	C5-C6-N1	5.62	120.51	117.70
36	5	2858	U	C6-N1-C2	-5.62	117.63	121.00
1	6	1672	G	C4-N9-C1'	5.61	133.80	126.50
1	6	1782	A	C5-C6-N6	5.61	128.19	123.70
36	5	607	A	C5-C6-N6	5.61	128.19	123.70
36	5	962	A	C5-C6-N6	-5.61	119.21	123.70
36	5	1803	C	C6-N1-C2	5.61	122.55	120.30
36	5	2861	U	O5'-P-OP2	5.61	117.44	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1115	G	P-O3'-C3'	5.61	126.43	119.70
36	1	1901	A	C5-C6-N1	5.61	120.50	117.70
36	1	2309	A	C8-N9-C4	5.61	108.04	105.80
1	6	151	G	N9-C4-C5	5.61	107.64	105.40
1	6	429	G	N1-C2-N3	5.61	127.27	123.90
36	5	607	A	C8-N9-C4	-5.61	103.56	105.80
36	5	671	U	C6-N1-C2	5.61	124.37	121.00
36	5	2356	A	C2-N3-C4	-5.61	107.80	110.60
36	5	2964	G	O4'-C1'-N9	5.61	112.69	108.20
64	n8	73	LEU	CA-CB-CG	5.61	128.20	115.30
36	1	188	U	C4-C5-C6	5.61	123.06	119.70
1	2	1212	G	C4-C5-N7	5.61	113.04	110.80
36	1	942	U	OP1-P-OP2	-5.61	111.19	119.60
36	1	1050	U	N1-C2-O2	5.61	126.72	122.80
36	1	1308	A	N1-C2-N3	5.61	132.10	129.30
1	6	542	A	C4-C5-N7	5.61	113.50	110.70
36	5	1348	U	O4'-C1'-N1	5.61	112.69	108.20
1	2	811	A	N3-C4-C5	-5.61	122.88	126.80
1	2	1004	U	N3-C2-O2	-5.61	118.28	122.20
36	1	2316	G	N3-C4-N9	5.61	129.36	126.00
36	1	2936	A	O5'-P-OP1	-5.61	100.66	105.70
1	6	590	C	C6-N1-C2	-5.61	118.06	120.30
36	5	880	G	C8-N9-C4	5.61	108.64	106.40
1	2	1490	C	C6-N1-C2	-5.60	118.06	120.30
36	1	922	U	N3-C2-O2	-5.60	118.28	122.20
36	1	1383	G	N1-C6-O6	5.60	123.26	119.90
36	5	2723	U	O5'-P-OP2	-5.60	100.66	105.70
1	2	448	C	C5-C6-N1	5.60	123.80	121.00
1	2	1426	C	C4-C5-C6	-5.60	114.60	117.40
36	1	2899	C	C4-C5-C6	5.60	120.20	117.40
36	5	2399	A	C6-N1-C2	-5.60	115.24	118.60
36	1	716	A	C5-N7-C8	-5.60	101.10	103.90
1	6	66	U	P-O3'-C3'	5.60	126.42	119.70
36	5	45	A	C6-N1-C2	-5.60	115.24	118.60
36	5	2639	G	C4-C5-C6	5.60	122.16	118.80
36	5	2831	G	C5-C6-N1	5.60	114.30	111.50
38	8	113	U	N3-C2-O2	-5.60	118.28	122.20
36	1	155	G	C5-C6-N1	5.60	114.30	111.50
36	1	967	A	C2-N3-C4	-5.60	107.80	110.60
36	1	1101	G	N3-C4-N9	-5.60	122.64	126.00
36	1	1396	C	N3-C4-C5	5.60	124.14	121.90
1	6	935	U	N3-C4-C5	-5.60	111.24	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1051	G	N1-C6-O6	-5.60	116.54	119.90
36	5	947	G	C4-N9-C1'	5.60	133.78	126.50
36	5	3129	A	C8-N9-C4	5.60	108.04	105.80
36	1	589	A	C8-N9-C4	5.60	108.04	105.80
38	4	2	A	OP2-P-O3'	5.60	117.51	105.20
1	6	53	G	C4-N9-C1'	5.60	133.78	126.50
36	5	1189	C	N3-C2-O2	5.60	125.82	121.90
36	5	1637	A	N9-C4-C5	5.60	108.04	105.80
36	5	2916	U	N3-C4-C5	-5.60	111.24	114.60
36	1	3212	C	O5'-P-OP2	-5.59	100.67	105.70
1	6	1584	G	OP1-P-O3'	5.59	117.51	105.20
1	6	1678	A	N1-C6-N6	5.59	121.96	118.60
36	1	1344	G	N1-C6-O6	5.59	123.26	119.90
36	5	3024	A	C8-N9-C4	-5.59	103.56	105.80
1	6	1481	C	N1-C2-O2	5.59	122.25	118.90
3	s1	61	LEU	CA-CB-CG	5.59	128.16	115.30
36	5	2624	G	C5-C6-N1	-5.59	108.70	111.50
38	8	4	C	N1-C2-O2	5.59	122.25	118.90
1	2	176	C	N1-C2-O2	5.59	122.25	118.90
36	1	158	G	C2-N3-C4	-5.59	109.11	111.90
36	1	2651	G	N9-C4-C5	5.59	107.64	105.40
36	5	3143	C	N3-C2-O2	5.59	125.81	121.90
54	M8	180	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	6	403	G	C2-N3-C4	-5.59	109.11	111.90
36	5	536	U	C5-C6-N1	-5.59	119.91	122.70
1	2	1428	G	N3-C4-C5	5.59	131.39	128.60
36	1	85	A	C5-C6-N1	-5.59	114.91	117.70
36	1	980	A	C4-C5-C6	5.59	119.79	117.00
36	1	1116	G	O5'-P-OP1	-5.59	100.67	105.70
36	1	3344	A	N1-C2-N3	5.59	132.09	129.30
36	5	1306	G	C5-N7-C8	-5.59	101.51	104.30
36	5	2148	U	N3-C2-O2	5.59	126.11	122.20
36	5	3179	U	N3-C4-O4	5.59	123.31	119.40
1	2	1745	G	C2-N3-C4	5.58	114.69	111.90
36	1	1150	A	N9-C4-C5	5.58	108.03	105.80
36	5	3123	A	C8-N9-C4	5.58	108.03	105.80
1	2	377	G	N1-C2-N2	5.58	121.22	116.20
36	1	1157	G	OP2-P-O3'	5.58	117.48	105.20
36	1	2618	G	C5-C6-N1	5.58	114.29	111.50
36	1	2785	A	O5'-P-OP2	-5.58	100.67	105.70
1	6	426	G	O5'-P-OP2	-5.58	100.67	105.70
36	5	715	A	O4'-C1'-N9	5.58	112.67	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1364	C	OP2-P-O3'	5.58	117.48	105.20
1	2	158	U	P-O3'-C3'	5.58	126.40	119.70
36	1	577	C	C4-C5-C6	5.58	120.19	117.40
36	1	1897	G	N1-C6-O6	5.58	123.25	119.90
36	1	1905	G	N3-C4-N9	-5.58	122.65	126.00
36	1	2892	A	O5'-P-OP2	-5.58	100.68	105.70
1	6	1640	C	C2-N1-C1'	5.58	124.94	118.80
1	6	1766	A	O5'-P-OP2	-5.58	100.68	105.70
38	8	7	U	O5'-P-OP2	-5.58	100.68	105.70
36	1	2939	G	C5-N7-C8	5.58	107.09	104.30
1	6	43	A	O5'-P-OP1	-5.58	100.68	105.70
36	5	1112	A	C5-C6-N6	-5.58	119.24	123.70
36	5	1152	G	C8-N9-C4	-5.58	104.17	106.40
36	5	2961	G	O5'-P-OP1	5.58	117.40	110.70
36	5	397	A	N9-C4-C5	5.58	108.03	105.80
36	5	408	A	C6-N1-C2	-5.58	115.25	118.60
36	5	534	U	O5'-P-OP2	-5.58	100.68	105.70
36	5	1652	G	C5-N7-C8	5.58	107.09	104.30
36	1	1305	U	O5'-P-OP1	-5.58	100.68	105.70
1	2	1241	G	C4-C5-N7	5.58	113.03	110.80
36	1	1115	G	C4-N9-C1'	5.58	133.75	126.50
36	1	1120	A	C6-N1-C2	-5.58	115.25	118.60
36	1	1791	C	N1-C2-O2	-5.58	115.56	118.90
36	5	1176	C	N3-C4-C5	5.58	124.13	121.90
36	5	2190	U	C6-N1-C2	-5.58	117.65	121.00
36	1	2122	G	N3-C4-N9	-5.57	122.66	126.00
1	6	866	G	C8-N9-C4	5.57	108.63	106.40
36	5	935	U	N3-C4-O4	5.57	123.30	119.40
36	5	2166	A	N1-C6-N6	5.57	121.94	118.60
36	1	2651	G	C6-C5-N7	5.57	133.74	130.40
1	2	901	G	O4'-C1'-N9	5.57	112.66	108.20
36	5	1123	U	C4-C5-C6	5.57	123.04	119.70
21	c9	57	ARG	NE-CZ-NH2	-5.57	117.52	120.30
36	5	96	G	C5-C6-O6	-5.57	125.26	128.60
36	5	716	A	C5-N7-C8	-5.57	101.11	103.90
36	5	807	A	OP1-P-O3'	5.57	117.45	105.20
36	1	41	G	OP2-P-O3'	5.57	117.45	105.20
36	1	650	C	O4'-C1'-N1	-5.57	103.75	108.20
36	1	895	A	N1-C6-N6	5.57	121.94	118.60
36	1	1344	G	C4-C5-N7	5.57	113.03	110.80
36	1	2351	U	N3-C2-O2	-5.57	118.30	122.20
36	1	2600	C	N3-C2-O2	-5.57	118.00	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	4	105	A	N7-C8-N9	5.57	116.58	113.80
36	5	212	G	OP1-P-O3'	5.57	117.45	105.20
36	5	1128	U	C2-N3-C4	-5.57	123.66	127.00
70	o4	10	ARG	NE-CZ-NH2	-5.57	117.52	120.30
36	1	2598	G	C2-N3-C4	5.57	114.68	111.90
16	c4	35	GLY	N-CA-C	5.57	127.01	113.10
36	5	831	G	N1-C2-N3	-5.57	120.56	123.90
36	5	2659	G	N9-C4-C5	-5.57	103.17	105.40
36	5	2817	A	N1-C6-N6	5.57	121.94	118.60
1	6	512	A	C4-C5-N7	5.56	113.48	110.70
1	6	1614	A	C4-C5-N7	5.56	113.48	110.70
36	5	1598	G	C5-C6-N1	5.56	114.28	111.50
36	1	284	A	O4'-C1'-N9	5.56	112.65	108.20
36	1	397	A	C6-N1-C2	-5.56	115.26	118.60
36	1	964	G	N3-C2-N2	-5.56	116.01	119.90
36	1	3002	C	C6-N1-C2	5.56	122.53	120.30
1	6	1537	C	N1-C2-O2	-5.56	115.56	118.90
36	5	43	A	C5-C6-N6	-5.56	119.25	123.70
36	5	919	U	C6-N1-C2	-5.56	117.66	121.00
36	1	672	A	C6-C5-N7	-5.56	128.41	132.30
36	1	1425	U	OP1-P-O3'	5.56	117.43	105.20
36	1	2304	C	N3-C4-C5	-5.56	119.68	121.90
36	1	2179	C	OP2-P-O3'	5.56	117.43	105.20
36	1	2399	A	C5-C6-N6	-5.56	119.25	123.70
56	N0	115	ARG	NE-CZ-NH1	5.56	123.08	120.30
36	5	1825	G	C4-C5-N7	-5.56	108.58	110.80
1	2	778	G	C4-C5-N7	5.56	113.02	110.80
36	1	3193	C	C6-N1-C2	-5.56	118.08	120.30
38	4	64	U	N3-C2-O2	-5.56	118.31	122.20
1	6	1081	A	O4'-C1'-N9	5.56	112.64	108.20
1	2	1199	G	C6-C5-N7	-5.55	127.07	130.40
38	4	147	U	C2-N1-C1'	5.55	124.36	117.70
36	5	410	U	N1-C2-O2	-5.55	118.91	122.80
36	5	2377	G	N1-C6-O6	-5.55	116.57	119.90
36	5	3204	C	C2-N3-C4	-5.55	117.12	119.90
36	5	3309	G	C5-C6-O6	5.55	131.93	128.60
1	2	111	U	N1-C2-N3	5.55	118.23	114.90
1	2	1611	A	N7-C8-N9	5.55	116.58	113.80
1	2	1633	A	N9-C4-C5	5.55	108.02	105.80
36	1	1371	G	N3-C4-N9	5.55	129.33	126.00
36	1	1940	G	N1-C2-N2	-5.55	111.20	116.20
1	6	125	U	N3-C2-O2	5.55	126.09	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1539	G	O5'-P-OP1	-5.55	100.70	105.70
36	5	1371	G	N1-C6-O6	-5.55	116.57	119.90
36	1	2760	C	N3-C4-N4	5.55	121.88	118.00
36	1	2808	A	C5-C6-N1	-5.55	114.92	117.70
36	5	895	A	C2-N3-C4	-5.55	107.83	110.60
36	5	1869	C	N3-C4-N4	-5.55	114.12	118.00
1	6	136	C	C2-N1-C1'	5.55	124.90	118.80
38	8	33	A	C5-C6-N6	-5.55	119.26	123.70
36	1	131	C	C6-N1-C2	-5.54	118.08	120.30
1	6	1662	G	C8-N9-C4	5.54	108.62	106.40
36	5	2145	A	N3-C4-C5	-5.54	122.92	126.80
37	7	88	G	N1-C6-O6	-5.54	116.57	119.90
36	1	608	A	N3-C4-N9	5.54	131.83	127.40
36	1	730	C	C6-N1-C2	5.54	122.52	120.30
36	1	1433	A	C8-N9-C4	-5.54	103.58	105.80
36	1	2131	A	OP1-P-O3'	5.54	117.39	105.20
1	6	287	G	C5-C6-O6	-5.54	125.27	128.60
1	6	438	A	O4'-C1'-N9	-5.54	103.76	108.20
1	6	914	G	C5-C6-O6	-5.54	125.27	128.60
1	6	1091	A	C2-N3-C4	-5.54	107.83	110.60
36	5	1361	U	C5-C6-N1	5.54	125.47	122.70
36	5	1652	G	C4-C5-N7	-5.54	108.58	110.80
36	5	2287	C	C6-N1-C2	-5.54	118.08	120.30
36	5	2991	A	N1-C6-N6	-5.54	115.27	118.60
36	1	91	G	C5-C6-N1	5.54	114.27	111.50
36	1	292	U	N1-C2-N3	5.54	118.22	114.90
36	5	1396	C	OP2-P-O3'	5.54	117.39	105.20
36	5	2403	G	N3-C4-N9	5.54	129.32	126.00
36	5	2404	A	O5'-P-OP1	5.54	117.35	110.70
1	6	755	A	N7-C8-N9	5.54	116.57	113.80
1	6	1121	C	O5'-P-OP2	-5.54	100.71	105.70
36	1	2862	U	O5'-P-OP2	-5.54	100.72	105.70
36	1	189	G	C5-C6-N1	5.54	114.27	111.50
36	1	1128	U	N3-C4-C5	5.54	117.92	114.60
36	1	1346	G	N3-C2-N2	-5.54	116.02	119.90
36	5	2971	A	N3-C4-C5	-5.54	122.92	126.80
36	1	142	C	C5-C4-N4	-5.54	116.33	120.20
36	1	2247	G	C6-C5-N7	-5.54	127.08	130.40
36	5	2970	C	O5'-P-OP1	-5.54	100.72	105.70
76	q0	103	LEU	CB-CG-CD2	-5.54	101.59	111.00
36	1	1003	A	N1-C6-N6	5.53	121.92	118.60
1	6	1134	C	C6-N1-C2	-5.53	118.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2790	A	O5'-P-OP2	-5.53	100.72	105.70
36	5	2818	U	N3-C4-C5	5.53	117.92	114.60
36	1	100	A	C4-C5-C6	5.53	119.77	117.00
36	1	320	G	O5'-P-OP2	-5.53	100.72	105.70
1	6	813	U	C2-N1-C1'	5.53	124.34	117.70
6	s4	51	ARG	NE-CZ-NH1	-5.53	117.53	120.30
36	5	2123	G	O5'-P-OP1	-5.53	100.72	105.70
1	2	579	A	P-O3'-C3'	5.53	126.34	119.70
36	1	943	U	N1-C2-N3	5.53	118.22	114.90
36	1	1113	G	C8-N9-C4	-5.53	104.19	106.40
36	1	1365	G	N9-C4-C5	5.53	107.61	105.40
37	3	98	C	C5-C6-N1	-5.53	118.23	121.00
38	4	40	A	C4-C5-N7	5.53	113.47	110.70
1	6	614	C	C2-N3-C4	5.53	122.67	119.90
36	5	1316	C	N1-C2-O2	-5.53	115.58	118.90
36	5	2120	A	O5'-P-OP2	-5.53	100.72	105.70
1	2	1291	G	C4-C5-N7	5.53	113.01	110.80
36	1	278	U	N3-C4-O4	5.53	123.27	119.40
36	1	811	U	O5'-P-OP2	-5.53	100.72	105.70
36	5	2808	A	C5-N7-C8	-5.53	101.14	103.90
36	1	84	U	C6-N1-C2	5.53	124.32	121.00
1	6	337	G	C4-C5-C6	5.53	122.12	118.80
36	5	631	U	C5-C4-O4	5.53	129.22	125.90
36	1	589	A	C5-N7-C8	5.53	106.66	103.90
36	1	2917	G	C5-C6-O6	-5.53	125.28	128.60
36	5	1392	G	N3-C4-N9	5.53	129.31	126.00
36	5	1863	G	N1-C6-O6	-5.53	116.58	119.90
36	1	107	A	C5-C6-N6	-5.52	119.28	123.70
36	1	1514	G	C5-C6-N1	5.52	114.26	111.50
36	5	1547	G	O5'-P-OP1	-5.52	100.73	105.70
36	5	2334	U	C6-N1-C2	-5.52	117.69	121.00
36	1	1932	A	C5-C6-N6	-5.52	119.28	123.70
68	O2	19	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	6	1200	G	N1-C6-O6	5.52	123.21	119.90
36	5	875	G	O5'-P-OP2	-5.52	100.73	105.70
36	5	2938	G	OP2-P-O3'	5.52	117.35	105.20
36	1	287	G	C4-C5-C6	5.52	122.11	118.80
36	1	859	G	N3-C2-N2	5.52	123.76	119.90
36	1	863	C	N1-C2-O2	-5.52	115.59	118.90
36	1	1294	A	O4'-C1'-N9	5.52	112.62	108.20
36	1	1550	C	N1-C2-O2	-5.52	115.59	118.90
36	1	1581	C	N3-C2-O2	-5.52	118.04	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1948	G	N1-C6-O6	5.52	123.21	119.90
1	6	558	U	C2-N1-C1'	5.52	124.32	117.70
1	6	647	G	C8-N9-C1'	5.52	134.18	127.00
36	5	1380	G	C5-C6-O6	-5.52	125.29	128.60
36	5	2271	A	C8-N9-C4	5.52	108.01	105.80
36	5	2364	G	N9-C4-C5	5.52	107.61	105.40
36	5	3177	G	C5-N7-C8	5.52	107.06	104.30
1	6	557	G	P-O3'-C3'	5.52	126.32	119.70
28	d6	10	ARG	NE-CZ-NH2	5.52	123.06	120.30
36	5	1424	C	N3-C2-O2	5.52	125.76	121.90
36	5	1433	A	O4'-C1'-N9	-5.52	103.79	108.20
36	5	2350	C	OP1-P-OP2	-5.52	111.32	119.60
36	1	678	G	N1-C6-O6	5.52	123.21	119.90
36	5	1476	G	N3-C4-C5	5.52	131.36	128.60
1	6	351	C	C6-N1-C1'	-5.51	114.18	120.80
36	5	1457	U	O5'-P-OP1	-5.51	100.74	105.70
36	5	2290	C	C5-C4-N4	-5.51	116.34	120.20
36	5	2392	C	C2-N3-C4	-5.51	117.14	119.90
36	5	3101	G	O5'-P-OP1	-5.51	100.74	105.70
36	1	2933	A	C4-C5-C6	-5.51	114.24	117.00
37	3	102	A	N9-C4-C5	-5.51	103.59	105.80
36	5	878	G	C8-N9-C4	-5.51	104.19	106.40
36	1	780	A	N1-C2-N3	5.51	132.06	129.30
36	1	933	A	C6-N1-C2	-5.51	115.29	118.60
36	1	1160	C	N3-C4-C5	-5.51	119.69	121.90
36	5	1321	G	C5-C6-N1	-5.51	108.74	111.50
36	5	2687	G	N3-C4-C5	-5.51	125.84	128.60
36	5	2832	C	O5'-P-OP2	-5.51	100.74	105.70
1	2	422	G	C6-C5-N7	-5.51	127.09	130.40
1	2	986	G	N3-C4-N9	5.51	129.31	126.00
36	1	1370	G	C5-C6-N1	5.51	114.25	111.50
36	5	416	A	N1-C6-N6	5.51	121.91	118.60
36	5	1891	A	C6-N1-C2	-5.51	115.29	118.60
36	5	3216	G	C8-N9-C1'	-5.51	119.84	127.00
36	1	189	G	N3-C4-N9	5.51	129.30	126.00
36	1	663	C	N1-C2-O2	-5.51	115.60	118.90
36	1	2894	C	N3-C2-O2	-5.51	118.05	121.90
36	1	2935	U	C5-C6-N1	5.51	125.45	122.70
1	6	151	G	N3-C4-C5	5.51	131.35	128.60
36	5	2291	A	OP1-P-OP2	-5.51	111.34	119.60
42	l5	152	ARG	NE-CZ-NH2	-5.51	117.55	120.30
36	1	2281	A	C8-N9-C4	5.50	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1510	G	N3-C4-N9	5.50	129.30	126.00
36	1	2242	A	C4-C5-C6	5.50	119.75	117.00
1	6	1537	C	C2-N3-C4	5.50	122.65	119.90
36	5	1178	G	N3-C4-N9	5.50	129.30	126.00
36	5	2157	G	C8-N9-C4	5.50	108.60	106.40
36	5	2391	G	C5-C6-N1	5.50	114.25	111.50
36	5	2753	G	N7-C8-N9	5.50	115.85	113.10
36	5	2951	G	O5'-P-OP1	-5.50	100.75	105.70
1	2	1274	C	C5-C4-N4	5.50	124.05	120.20
37	3	61	G	C5-N7-C8	-5.50	101.55	104.30
36	5	2753	G	C8-N9-C4	-5.50	104.20	106.40
37	7	77	G	N1-C6-O6	5.50	123.20	119.90
36	1	1380	G	N3-C4-C5	5.50	131.35	128.60
1	6	1293	U	C5-C6-N1	-5.50	119.95	122.70
36	5	534	U	N1-C2-O2	5.50	126.65	122.80
36	5	2885	C	C2-N3-C4	-5.50	117.15	119.90
36	1	1365	G	N1-C6-O6	-5.50	116.60	119.90
36	5	408	A	N1-C2-N3	5.50	132.05	129.30
36	5	873	C	O5'-P-OP1	5.50	117.30	110.70
36	5	1335	C	N1-C2-O2	-5.50	115.60	118.90
36	5	1460	A	C5-C6-N6	-5.50	119.30	123.70
38	8	54	A	C4-C5-N7	5.50	113.45	110.70
42	l5	110	LEU	CA-CB-CG	5.50	127.94	115.30
36	1	1128	U	N1-C2-O2	5.50	126.65	122.80
36	5	1909	A	N9-C4-C5	-5.50	103.60	105.80
1	2	1745	G	C6-C5-N7	-5.50	127.10	130.40
36	1	304	G	N3-C2-N2	-5.50	116.05	119.90
36	5	1196	C	C6-N1-C1'	-5.50	114.20	120.80
52	m6	69	GLY	N-CA-C	-5.50	99.36	113.10
36	1	1060	U	C5-C6-N1	-5.49	119.95	122.70
36	1	1402	C	C5-C4-N4	5.49	124.05	120.20
36	1	1898	G	N1-C6-O6	5.49	123.20	119.90
36	1	3172	A	C8-N9-C4	5.49	108.00	105.80
37	3	28	C	N3-C4-N4	5.49	121.84	118.00
36	5	348	A	N9-C4-C5	-5.49	103.60	105.80
36	5	1402	C	OP2-P-O3'	5.49	117.29	105.20
1	6	583	C	C2-N1-C1'	5.49	124.84	118.80
1	6	1745	G	C5-C6-N1	5.49	114.25	111.50
36	5	3197	G	C8-N9-C1'	5.49	134.14	127.00
1	2	786	C	C6-N1-C2	-5.49	118.10	120.30
36	1	906	A	C6-N1-C2	-5.49	115.31	118.60
36	1	2187	G	C4-C5-C6	5.49	122.09	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	892	U	C2-N1-C1'	-5.49	111.11	117.70
36	5	1839	A	O5'-P-OP1	-5.49	100.76	105.70
36	5	2799	A	C4-C5-N7	-5.49	107.95	110.70
36	5	2821	C	C5-C6-N1	-5.49	118.25	121.00
36	1	1313	G	N1-C6-O6	5.49	123.19	119.90
1	6	6	G	N1-C6-O6	5.49	123.19	119.90
1	6	1308	G	C6-C5-N7	-5.49	127.11	130.40
1	6	1600	A	N1-C6-N6	5.49	121.89	118.60
36	5	1852	G	N7-C8-N9	5.49	115.84	113.10
36	5	2634	U	C5-C4-O4	-5.49	122.61	125.90
36	5	3305	A	C4-C5-N7	5.49	113.44	110.70
36	1	2733	A	C4-C5-N7	5.49	113.44	110.70
1	6	335	U	N3-C2-O2	-5.49	118.36	122.20
36	5	1147	G	C5-C6-O6	-5.49	125.31	128.60
37	7	88	G	N3-C4-C5	-5.49	125.86	128.60
36	5	368	G	C8-N9-C4	-5.48	104.21	106.40
36	1	908	G	N3-C2-N2	-5.48	116.06	119.90
1	6	1000	C	O4'-C1'-N1	5.48	112.59	108.20
1	6	1100	G	C5-C6-N1	5.48	114.24	111.50
36	5	859	G	C8-N9-C4	-5.48	104.21	106.40
36	1	356	C	O5'-P-OP1	5.48	117.28	110.70
36	1	2376	G	C6-N1-C2	-5.48	121.81	125.10
36	1	2618	G	C6-C5-N7	5.48	133.69	130.40
1	6	1560	U	N1-C2-O2	5.48	126.64	122.80
36	5	283	G	C6-C5-N7	-5.48	127.11	130.40
36	1	2720	G	C8-N9-C1'	-5.48	119.88	127.00
36	1	2983	C	N3-C4-N4	-5.48	114.17	118.00
36	1	3209	A	N9-C4-C5	-5.48	103.61	105.80
36	1	944	C	C5-C6-N1	5.48	123.74	121.00
36	1	1518	U	C5-C6-N1	-5.48	119.96	122.70
69	O3	67	MET	CG-SD-CE	-5.48	91.44	100.20
1	6	565	C	C2-N3-C4	-5.48	117.16	119.90
36	5	2552	C	N1-C2-O2	5.48	122.19	118.90
36	5	2888	U	C2-N1-C1'	5.48	124.27	117.70
1	2	1733	C	C2-N3-C4	5.48	122.64	119.90
36	1	142	C	C2-N1-C1'	5.48	124.82	118.80
36	1	719	U	C6-N1-C2	5.48	124.28	121.00
36	1	3172	A	O5'-P-OP1	5.48	117.27	110.70
36	5	2336	U	C5-C6-N1	5.48	125.44	122.70
36	5	3141	A	C4-C5-N7	-5.48	107.96	110.70
36	1	619	A	C8-N9-C4	5.47	107.99	105.80
36	1	1442	U	N3-C4-O4	5.47	123.23	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2414	G	C5-C6-O6	5.47	131.88	128.60
36	1	2418	G	C8-N9-C1'	-5.47	119.88	127.00
36	1	2731	U	OP2-P-O3'	5.47	117.24	105.20
38	4	38	U	C2-N1-C1'	5.47	124.27	117.70
1	6	542	A	C4-C5-C6	5.47	119.74	117.00
36	5	2887	A	C6-C5-N7	-5.47	128.47	132.30
36	5	2887	A	N1-C6-N6	5.47	121.88	118.60
1	2	1536	G	N3-C4-N9	5.47	129.28	126.00
36	1	1454	A	O5'-P-OP1	-5.47	100.77	105.70
36	1	3374	U	C5-C4-O4	-5.47	122.62	125.90
1	6	273	G	O5'-P-OP1	-5.47	100.77	105.70
36	5	792	G	C2-N3-C4	-5.47	109.16	111.90
36	5	961	C	N3-C4-N4	5.47	121.83	118.00
36	5	1370	G	N1-C2-N3	5.47	127.18	123.90
36	5	1930	A	N1-C6-N6	5.47	121.88	118.60
36	1	369	A	N9-C4-C5	5.47	107.99	105.80
36	1	640	U	C5-C4-O4	-5.47	122.62	125.90
36	1	960	U	C6-N1-C2	5.47	124.28	121.00
36	1	999	G	C5-C6-O6	-5.47	125.32	128.60
1	6	317	C	C5-C6-N1	-5.47	118.27	121.00
36	5	2754	G	N1-C2-N2	-5.47	111.28	116.20
1	6	343	C	N1-C2-O2	-5.47	115.62	118.90
1	6	999	U	C4-C5-C6	-5.47	116.42	119.70
36	5	922	U	O5'-P-OP2	-5.47	100.78	105.70
36	1	2300	G	C8-N9-C4	-5.47	104.21	106.40
36	1	2944	U	N3-C2-O2	-5.47	118.37	122.20
36	1	2949	U	N1-C2-N3	-5.47	111.62	114.90
37	3	15	C	C6-N1-C2	5.47	122.49	120.30
36	5	2376	G	N7-C8-N9	5.47	115.83	113.10
15	C3	22	ALA	C-N-CD	-5.46	108.58	120.60
36	1	3324	C	C6-N1-C2	5.46	122.48	120.30
1	6	453	U	C5-C4-O4	5.46	129.18	125.90
36	5	2286	U	N3-C4-O4	-5.46	115.58	119.40
36	5	2287	C	N1-C2-N3	5.46	123.03	119.20
36	5	2400	G	C4-C5-N7	5.46	112.99	110.80
36	5	2837	A	O5'-P-OP1	-5.46	100.78	105.70
1	2	1082	C	N3-C2-O2	-5.46	118.08	121.90
36	1	97	U	OP2-P-O3'	5.46	117.22	105.20
36	1	2556	C	C6-N1-C2	5.46	122.48	120.30
36	5	2295	A	N1-C2-N3	-5.46	126.57	129.30
36	5	2360	C	N3-C4-N4	5.46	121.82	118.00
36	5	2661	G	N3-C4-N9	5.46	129.28	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	3209	A	C6-C5-N7	-5.46	128.48	132.30
36	1	1310	G	C8-N9-C4	-5.46	104.22	106.40
1	6	1572	G	N7-C8-N9	5.46	115.83	113.10
36	5	2675	C	O5'-P-OP1	-5.46	100.78	105.70
1	2	829	A	P-O3'-C3'	5.46	126.25	119.70
38	4	108	C	C2-N1-C1'	5.46	124.81	118.80
1	6	1697	G	N3-C4-C5	-5.46	125.87	128.60
36	5	599	C	N1-C2-O2	-5.46	115.62	118.90
36	5	906	A	C6-N1-C2	-5.46	115.32	118.60
36	5	1879	A	O5'-P-OP1	5.46	117.25	110.70
36	5	3321	C	C6-N1-C2	5.46	122.48	120.30
36	1	1056	U	C5-C6-N1	5.46	125.43	122.70
36	1	1517	G	O5'-P-OP2	-5.46	100.79	105.70
36	1	2637	A	O5'-P-OP1	-5.46	100.79	105.70
1	6	1572	G	C8-N9-C4	-5.46	104.22	106.40
36	1	983	A	C4-C5-C6	5.46	119.73	117.00
36	1	1789	G	C4-C5-N7	5.46	112.98	110.80
36	1	2246	G	N1-C2-N2	5.46	121.11	116.20
36	1	2760	C	N1-C2-O2	-5.46	115.63	118.90
36	5	699	A	C2-N3-C4	-5.46	107.87	110.60
36	5	1561	G	O4'-C1'-N9	5.46	112.56	108.20
36	5	1858	A	N7-C8-N9	5.46	116.53	113.80
36	5	2317	A	C8-N9-C4	-5.46	103.62	105.80
36	5	2398	A	C4-C5-C6	5.46	119.73	117.00
36	5	2630	C	OP2-P-O3'	5.46	117.21	105.20
36	5	2861	U	N3-C4-O4	-5.46	115.58	119.40
36	5	2932	U	C2-N3-C4	-5.46	123.73	127.00
39	l2	242	ARG	NE-CZ-NH2	-5.46	117.57	120.30
36	5	1060	U	C5-C6-N1	-5.46	119.97	122.70
36	5	2363	A	C6-C5-N7	-5.46	128.48	132.30
36	1	1429	G	C5-N7-C8	5.45	107.03	104.30
53	M7	41	LEU	CA-CB-CG	5.45	127.84	115.30
1	6	1735	U	N3-C2-O2	-5.45	118.38	122.20
36	5	1440	G	C5-N7-C8	5.45	107.03	104.30
36	5	1720	U	C5-C6-N1	-5.45	119.97	122.70
36	5	3188	G	N9-C4-C5	5.45	107.58	105.40
36	5	3209	A	C5-N7-C8	-5.45	101.17	103.90
1	2	1657	U	C5-C4-O4	5.45	129.17	125.90
36	1	368	G	C2-N3-C4	-5.45	109.17	111.90
36	5	665	A	C5-C6-N6	-5.45	119.34	123.70
40	l3	251	CYS	CA-CB-SG	-5.45	104.19	114.00
36	1	115	A	N9-C4-C5	5.45	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	148	G	N1-C6-O6	5.45	123.17	119.90
36	1	2364	G	C6-N1-C2	-5.45	121.83	125.10
36	1	2640	A	C5-C6-N1	5.45	120.42	117.70
36	1	3218	A	N1-C6-N6	-5.45	115.33	118.60
36	5	710	A	C5-C6-N1	5.45	120.42	117.70
36	5	974	G	C5-C6-N1	5.45	114.23	111.50
36	5	2893	C	C2-N3-C4	5.45	122.62	119.90
36	5	2906	C	O5'-P-OP1	5.45	117.24	110.70
36	5	2940	A	C4-C5-C6	5.45	119.73	117.00
36	1	877	C	C5-C4-N4	-5.45	116.39	120.20
36	1	2282	U	C2-N3-C4	-5.45	123.73	127.00
36	5	280	U	O5'-P-OP2	-5.45	100.80	105.70
36	5	585	A	C2-N3-C4	-5.45	107.88	110.60
36	5	722	G	C5-C6-O6	5.45	131.87	128.60
36	5	1834	U	C4-C5-C6	5.45	122.97	119.70
36	1	3302	U	C5-C6-N1	-5.45	119.98	122.70
36	5	977	C	N3-C2-O2	-5.45	118.09	121.90
36	5	1177	G	N1-C6-O6	-5.45	116.63	119.90
36	1	872	U	O5'-P-OP2	-5.45	100.80	105.70
36	1	910	G	C5-C6-N1	-5.45	108.78	111.50
36	1	973	A	C2-N3-C4	-5.45	107.88	110.60
36	1	1468	A	OP1-P-OP2	5.45	127.77	119.60
36	1	3205	G	C2-N3-C4	-5.45	109.18	111.90
1	6	1493	A	N1-C6-N6	5.45	121.87	118.60
36	5	289	A	C6-N1-C2	-5.45	115.33	118.60
36	5	425	G	N7-C8-N9	-5.45	110.38	113.10
36	5	2754	G	N3-C2-N2	5.45	123.71	119.90
1	6	1305	U	N1-C2-O2	-5.44	118.99	122.80
36	5	421	G	C8-N9-C4	-5.44	104.22	106.40
36	5	889	U	C5-C4-O4	-5.44	122.63	125.90
36	5	1159	A	N3-C4-C5	5.44	130.61	126.80
36	1	1131	G	C5-C6-O6	-5.44	125.33	128.60
36	1	1875	G	N7-C8-N9	-5.44	110.38	113.10
36	5	2759	U	C6-N1-C2	-5.44	117.73	121.00
37	7	2	G	C8-N9-C4	-5.44	104.22	106.40
1	2	89	G	C8-N9-C4	5.44	108.58	106.40
36	1	124	U	N3-C2-O2	-5.44	118.39	122.20
36	1	283	G	O4'-C1'-N9	-5.44	103.85	108.20
1	6	354	C	C6-N1-C2	-5.44	118.12	120.30
36	5	408	A	O5'-P-OP1	-5.44	100.80	105.70
36	5	1312	C	C6-N1-C2	-5.44	118.12	120.30
36	5	1461	A	C8-N9-C4	5.44	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1786	G	C5-C6-N1	5.44	114.22	111.50
36	5	2887	A	C6-N1-C2	-5.44	115.34	118.60
1	6	978	A	N9-C4-C5	5.44	107.97	105.80
36	5	3311	C	N1-C2-O2	-5.44	115.64	118.90
36	1	90	C	O5'-P-OP2	-5.44	100.81	105.70
36	1	2215	A	C8-N9-C4	5.44	107.97	105.80
36	5	1126	G	N9-C4-C5	5.44	107.58	105.40
36	5	1148	G	C5-C6-O6	-5.44	125.34	128.60
36	5	2345	A	C4-C5-N7	5.44	113.42	110.70
1	2	942	G	C5-C6-N1	5.43	114.22	111.50
36	1	785	G	N3-C4-C5	-5.43	125.88	128.60
36	1	797	U	OP2-P-O3'	5.43	117.16	105.20
56	N0	106	LEU	CA-CB-CG	5.43	127.80	115.30
61	N5	113	LEU	CA-CB-CG	5.43	127.80	115.30
1	6	1398	U	N3-C2-O2	-5.43	118.40	122.20
36	5	1239	C	C5-C6-N1	5.43	123.72	121.00
36	5	1304	A	C2-N3-C4	5.43	113.32	110.60
36	5	1462	A	C2-N3-C4	-5.43	107.88	110.60
36	5	3351	U	N3-C2-O2	-5.43	118.40	122.20
37	7	92	A	N1-C6-N6	5.43	121.86	118.60
36	1	2322	C	OP2-P-O3'	5.43	117.15	105.20
38	4	4	C	N1-C2-O2	-5.43	115.64	118.90
1	6	36	C	C6-N1-C2	5.43	122.47	120.30
36	5	386	A	N9-C4-C5	-5.43	103.63	105.80
36	5	964	G	N7-C8-N9	5.43	115.82	113.10
36	5	2158	A	N1-C6-N6	-5.43	115.34	118.60
36	5	2659	G	C4-C5-N7	5.43	112.97	110.80
52	m6	84	LEU	CA-CB-CG	-5.43	102.80	115.30
36	1	3318	G	C4-N9-C1'	5.43	133.56	126.50
1	2	240	U	OP2-P-O3'	5.43	117.14	105.20
36	1	332	C	C4-C5-C6	5.43	120.11	117.40
36	1	1343	A	C6-C5-N7	-5.43	128.50	132.30
36	1	2192	C	C5-C6-N1	-5.43	118.28	121.00
1	6	467	G	N3-C4-C5	-5.43	125.89	128.60
1	6	542	A	P-O3'-C3'	5.43	126.22	119.70
1	6	1672	G	C6-C5-N7	-5.43	127.14	130.40
36	5	3177	G	C4-C5-N7	-5.43	108.63	110.80
52	m6	10	ASP	CB-CG-OD1	5.43	123.19	118.30
1	2	608	U	N1-C2-N3	5.43	118.16	114.90
36	5	796	U	C5-C4-O4	5.43	129.16	125.90
36	5	3006	A	C8-N9-C4	-5.43	103.63	105.80
36	1	105	C	C2-N3-C4	-5.43	117.19	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	Q3	29	LEU	CA-CB-CG	-5.43	102.82	115.30
1	6	1600	A	C4-C5-N7	5.43	113.41	110.70
36	5	919	U	N1-C2-N3	5.43	118.16	114.90
36	5	984	G	C6-C5-N7	-5.43	127.14	130.40
1	2	747	C	C6-N1-C2	-5.42	118.13	120.30
1	2	1756	A	C8-N9-C4	-5.42	103.63	105.80
36	1	628	A	N1-C2-N3	5.42	132.01	129.30
38	4	46	G	N1-C6-O6	-5.42	116.64	119.90
36	5	682	U	N1-C2-O2	-5.42	119.00	122.80
36	5	2334	U	O5'-P-OP1	5.42	117.21	110.70
1	2	988	A	C2-N3-C4	-5.42	107.89	110.60
36	1	155	G	N3-C4-N9	5.42	129.25	126.00
36	1	933	A	C4-C5-C6	5.42	119.71	117.00
36	1	1421	G	OP1-P-OP2	-5.42	111.47	119.60
36	1	1429	G	N3-C4-N9	5.42	129.25	126.00
36	1	1929	G	C8-N9-C4	5.42	108.57	106.40
36	5	2257	C	C6-N1-C2	-5.42	118.13	120.30
1	2	1662	G	C5-C6-N1	5.42	114.21	111.50
36	1	695	C	N3-C4-N4	-5.42	114.21	118.00
36	1	1055	A	O5'-P-OP1	-5.42	100.82	105.70
1	6	767	U	C6-N1-C2	-5.42	117.75	121.00
36	1	820	A	N9-C4-C5	5.42	107.97	105.80
36	1	1083	G	N3-C4-C5	-5.42	125.89	128.60
36	1	1884	A	N9-C4-C5	-5.42	103.63	105.80
36	1	648	C	C5-C4-N4	-5.42	116.41	120.20
36	1	1795	U	C2-N1-C1'	5.42	124.20	117.70
36	1	2279	A	O4'-C1'-N9	5.42	112.53	108.20
1	6	569	C	N3-C4-C5	-5.42	119.73	121.90
36	5	1163	A	N1-C6-N6	-5.42	115.35	118.60
36	5	2820	A	OP2-P-O3'	5.42	117.12	105.20
36	1	930	U	N1-C2-O2	-5.42	119.01	122.80
1	6	404	G	N9-C4-C5	5.42	107.57	105.40
1	6	941	A	N1-C6-N6	-5.42	115.35	118.60
1	6	1349	G	N1-C6-O6	5.42	123.15	119.90
36	5	2178	A	C8-N9-C4	5.42	107.97	105.80
36	5	2329	C	C2-N3-C4	-5.42	117.19	119.90
36	5	2664	C	N3-C2-O2	5.42	125.69	121.90
36	1	3208	G	N1-C6-O6	-5.42	116.65	119.90
36	5	40	A	C6-C5-N7	-5.42	128.51	132.30
36	5	590	G	C5-C6-O6	-5.42	125.35	128.60
36	5	852	U	OP2-P-O3'	5.42	117.11	105.20
1	2	1486	G	N3-C4-N9	-5.41	122.75	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	958	C	N3-C4-C5	5.41	124.06	121.90
37	3	38	U	N3-C2-O2	5.41	125.99	122.20
1	6	780	A	N1-C2-N3	5.41	132.01	129.30
36	5	845	G	OP1-P-O3'	5.41	117.11	105.20
38	8	74	U	N3-C4-O4	5.41	123.19	119.40
36	1	881	C	N3-C4-C5	5.41	124.06	121.90
36	1	2881	C	N1-C2-O2	5.41	122.15	118.90
64	N8	4	ARG	NE-CZ-NH1	-5.41	117.59	120.30
36	5	1189	C	N3-C4-N4	5.41	121.79	118.00
36	5	2234	G	C8-N9-C4	5.41	108.56	106.40
36	5	2365	C	C6-N1-C2	5.41	122.47	120.30
36	5	2435	G	N9-C4-C5	-5.41	103.23	105.40
1	2	542	A	O4'-C1'-N9	5.41	112.53	108.20
1	2	1765	A	O5'-P-OP1	-5.41	100.83	105.70
36	1	955	U	N3-C4-O4	-5.41	115.61	119.40
36	1	1520	G	C2-N3-C4	5.41	114.61	111.90
36	1	2373	A	C5'-C4'-O4'	-5.41	102.61	109.10
1	6	385	A	C4-C5-N7	-5.41	108.00	110.70
36	5	2134	G	C4-N9-C1'	5.41	133.53	126.50
36	5	2896	A	C8-N9-C4	5.41	107.96	105.80
1	2	1503	A	C5-N7-C8	-5.41	101.20	103.90
36	1	1180	A	C4-C5-C6	5.41	119.70	117.00
36	1	1851	G	C6-C5-N7	-5.41	127.16	130.40
36	1	2308	C	C6-N1-C2	5.41	122.46	120.30
36	1	2617	U	N3-C4-C5	-5.41	111.35	114.60
44	L7	129	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	6	337	G	N7-C8-N9	5.41	115.81	113.10
1	6	634	G	O5'-P-OP2	-5.41	100.83	105.70
1	6	687	G	C8-N9-C1'	5.41	134.03	127.00
36	5	224	C	N3-C2-O2	-5.41	118.11	121.90
36	5	2310	U	O5'-P-OP1	5.41	117.19	110.70
36	1	2173	U	C6-N1-C2	-5.41	117.76	121.00
36	5	787	G	N1-C6-O6	5.41	123.14	119.90
1	2	312	A	C8-N9-C4	-5.41	103.64	105.80
1	2	1273	G	C8-N9-C4	-5.41	104.24	106.40
36	1	143	G	C5-C6-N1	5.41	114.20	111.50
36	1	1184	A	C8-N9-C4	-5.41	103.64	105.80
36	1	1480	G	C4-C5-N7	5.41	112.96	110.80
1	6	1028	C	N3-C4-C5	5.41	124.06	121.90
36	5	746	A	N1-C2-N3	5.41	132.00	129.30
36	5	1820	U	O4'-C1'-N1	5.41	112.52	108.20
1	2	92	A	N1-C6-N6	-5.40	115.36	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1098	A	C8-N9-C4	-5.40	103.64	105.80
1	6	1800	A	C8-N9-C4	-5.40	103.64	105.80
36	1	368	G	N9-C4-C5	-5.40	103.24	105.40
36	1	2430	A	C4-C5-C6	5.40	119.70	117.00
36	1	3101	G	C5-C6-N1	5.40	114.20	111.50
36	5	1183	C	OP2-P-O3'	5.40	117.08	105.20
36	5	1534	A	C6-N1-C2	-5.40	115.36	118.60
36	5	2659	G	N3-C4-N9	5.40	129.24	126.00
36	5	2765	C	C6-N1-C2	-5.40	118.14	120.30
1	2	1273	G	N9-C4-C5	5.40	107.56	105.40
36	1	930	U	C2-N3-C4	-5.40	123.76	127.00
36	1	970	A	N7-C8-N9	5.40	116.50	113.80
36	1	1041	U	C5-C6-N1	-5.40	120.00	122.70
36	1	1157	G	C4-C5-N7	-5.40	108.64	110.80
37	3	57	G	C5-C6-O6	5.40	131.84	128.60
1	6	1141	G	C8-N9-C4	5.40	108.56	106.40
36	5	75	G	N3-C4-N9	5.40	129.24	126.00
36	5	424	G	N1-C6-O6	5.40	123.14	119.90
36	5	583	G	N1-C6-O6	-5.40	116.66	119.90
36	5	3085	G	OP1-P-O3'	5.40	117.08	105.20
38	8	68	G	N1-C6-O6	5.40	123.14	119.90
47	M0	57	LEU	CA-CB-CG	5.40	127.72	115.30
1	2	1171	A	N1-C6-N6	-5.40	115.36	118.60
36	1	59	G	N1-C6-O6	5.40	123.14	119.90
36	1	1891	A	N9-C4-C5	-5.40	103.64	105.80
36	1	2190	U	OP2-P-O3'	5.40	117.07	105.20
36	1	2419	A	C5-N7-C8	-5.40	101.20	103.90
1	6	687	G	C6-C5-N7	5.40	133.64	130.40
36	5	55	G	N7-C8-N9	-5.40	110.40	113.10
36	5	1147	G	N1-C6-O6	5.40	123.14	119.90
36	5	2339	C	O5'-P-OP1	-5.40	100.84	105.70
36	5	2890	A	C4-C5-C6	5.40	119.70	117.00
38	8	4	C	N3-C2-O2	-5.40	118.12	121.90
36	1	3056	U	C2-N1-C1'	-5.40	111.22	117.70
1	2	254	A	C8-N9-C4	5.39	107.96	105.80
36	1	2237	C	C6-N1-C2	5.39	122.46	120.30
36	1	2856	G	N1-C6-O6	5.39	123.14	119.90
38	4	14	C	C2-N3-C4	-5.39	117.20	119.90
41	L4	190	GLY	N-CA-C	5.39	126.58	113.10
36	5	1331	U	C5-C6-N1	-5.39	120.00	122.70
1	2	1196	A	C8-N9-C4	-5.39	103.64	105.80
36	5	809	G	N9-C4-C5	-5.39	103.24	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1208	U	C6-N1-C2	-5.39	117.76	121.00
36	5	2116	G	C5-C6-N1	-5.39	108.80	111.50
36	5	2195	C	N1-C2-O2	-5.39	115.66	118.90
36	1	388	G	C8-N9-C4	-5.39	104.24	106.40
36	1	2242	A	N1-C6-N6	5.39	121.83	118.60
36	1	2888	U	C5-C4-O4	-5.39	122.67	125.90
36	1	3309	G	C8-N9-C4	-5.39	104.24	106.40
36	5	1303	A	N1-C6-N6	5.39	121.83	118.60
36	1	1166	G	C8-N9-C4	5.39	108.56	106.40
36	5	2377	G	N3-C4-N9	5.39	129.23	126.00
36	1	836	A	C6-N1-C2	-5.39	115.37	118.60
36	1	1421	G	OP2-P-O3'	5.39	117.05	105.20
38	4	40	A	C5-N7-C8	-5.39	101.21	103.90
36	5	805	G	N7-C8-N9	-5.39	110.41	113.10
36	5	2116	G	C4-N9-C1'	5.39	133.50	126.50
1	2	266	A	C8-N9-C4	5.38	107.95	105.80
36	1	1620	U	C2-N1-C1'	5.38	124.16	117.70
36	5	2103	U	N3-C2-O2	-5.38	118.43	122.20
36	5	2292	U	C4-C5-C6	5.38	122.93	119.70
36	1	1174	G	C8-N9-C1'	-5.38	120.00	127.00
36	5	1460	A	C5-N7-C8	-5.38	101.21	103.90
36	1	915	A	N1-C2-N3	5.38	131.99	129.30
36	1	2777	G	N3-C4-C5	-5.38	125.91	128.60
36	1	3216	G	N9-C4-C5	5.38	107.55	105.40
36	5	583	G	C4-C5-N7	-5.38	108.65	110.80
36	5	677	A	C2-N3-C4	-5.38	107.91	110.60
36	5	912	G	C5-C6-N1	5.38	114.19	111.50
36	5	1790	G	C4-N9-C1'	5.38	133.50	126.50
36	1	2640	A	C4-N9-C1'	5.38	135.98	126.30
1	6	353	A	C2-N3-C4	5.38	113.29	110.60
1	6	569	C	C4-C5-C6	5.38	120.09	117.40
50	m4	106	ARG	NE-CZ-NH1	5.38	122.99	120.30
36	1	3377	G	OP2-P-O3'	5.38	117.03	105.20
1	2	337	G	C6-C5-N7	-5.38	127.17	130.40
36	1	498	A	C5-C6-N6	5.38	128.00	123.70
36	1	646	A	C4-C5-C6	5.38	119.69	117.00
36	1	3375	A	C8-N9-C4	-5.38	103.65	105.80
36	5	66	A	N1-C6-N6	5.38	121.83	118.60
36	5	1323	G	N3-C4-C5	-5.38	125.91	128.60
48	m1	12	LEU	CA-CB-CG	5.38	127.67	115.30
1	6	426	G	N1-C6-O6	-5.38	116.67	119.90
36	5	1879	A	N7-C8-N9	5.38	116.49	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	647	G	N3-C4-N9	-5.37	122.78	126.00
1	2	934	C	C2-N1-C1'	5.37	124.71	118.80
36	1	584	G	C8-N9-C4	-5.37	104.25	106.40
36	1	922	U	C2-N1-C1'	5.37	124.15	117.70
36	1	2877	G	N3-C2-N2	-5.37	116.14	119.90
1	6	1472	C	C6-N1-C1'	5.37	127.25	120.80
36	5	1646	G	C5-C6-O6	-5.37	125.38	128.60
36	5	2850	G	C5-C6-O6	-5.37	125.38	128.60
36	1	879	U	C5-C4-O4	5.37	129.12	125.90
1	6	1031	U	C6-N1-C2	5.37	124.22	121.00
36	5	1741	A	C8-N9-C4	-5.37	103.65	105.80
36	5	2174	G	C5-C6-O6	-5.37	125.38	128.60
36	5	145	G	N3-C4-N9	-5.37	122.78	126.00
36	5	968	G	C8-N9-C1'	-5.37	120.02	127.00
36	5	1513	G	N7-C8-N9	5.37	115.78	113.10
36	1	2984	C	N3-C4-N4	-5.37	114.24	118.00
36	1	343	U	OP2-P-O3'	5.37	117.00	105.20
36	1	1365	G	N3-C2-N2	5.37	123.66	119.90
36	1	2624	G	C5-N7-C8	-5.37	101.62	104.30
36	5	798	G	C8-N9-C4	-5.37	104.25	106.40
36	5	1200	A	C6-N1-C2	-5.37	115.38	118.60
36	1	2808	A	C4-C5-N7	5.36	113.38	110.70
1	6	307	G	C4-C5-N7	-5.36	108.66	110.80
1	6	565	C	C5-C6-N1	-5.36	118.32	121.00
1	6	957	G	C5-C6-N1	-5.36	108.82	111.50
36	5	2908	G	N3-C2-N2	-5.36	116.15	119.90
36	1	3000	A	C8-N9-C4	5.36	107.94	105.80
1	6	577	G	C8-N9-C4	-5.36	104.25	106.40
1	2	1685	G	C8-N9-C4	-5.36	104.26	106.40
36	1	53	G	C8-N9-C1'	-5.36	120.03	127.00
36	1	785	G	N3-C4-N9	5.36	129.22	126.00
36	1	1124	U	N3-C4-O4	-5.36	115.65	119.40
38	4	48	A	N1-C6-N6	5.36	121.82	118.60
1	6	1020	A	C8-N9-C4	-5.36	103.66	105.80
1	6	1051	G	N9-C4-C5	5.36	107.54	105.40
6	s4	38	LEU	CA-CB-CG	5.36	127.63	115.30
36	5	414	U	N1-C2-O2	-5.36	119.05	122.80
36	5	838	G	C2-N3-C4	-5.36	109.22	111.90
36	5	1888	U	C2-N3-C4	-5.36	123.78	127.00
36	5	1893	A	C8-N9-C4	5.36	107.94	105.80
36	5	2211	U	N1-C2-N3	5.36	118.12	114.90
36	5	2344	U	N3-C2-O2	-5.36	118.45	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	201	A	C5-N7-C8	-5.36	101.22	103.90
36	5	2757	U	N1-C2-O2	-5.36	119.05	122.80
36	5	3311	C	C6-N1-C2	-5.36	118.16	120.30
38	8	54	A	C5-N7-C8	-5.36	101.22	103.90
36	1	1307	G	C5-C6-O6	5.36	131.81	128.60
36	1	2339	C	OP1-P-O3'	5.36	116.99	105.20
36	1	2642	A	C5-C6-N1	-5.36	115.02	117.70
52	M6	16	VAL	CB-CA-C	-5.36	101.22	111.40
36	5	101	G	O4'-C1'-N9	5.36	112.49	108.20
36	5	861	C	C6-N1-C2	5.36	122.44	120.30
36	5	890	C	O5'-P-OP1	5.36	117.13	110.70
36	5	3144	G	N9-C4-C5	5.36	107.54	105.40
36	1	816	A	C8-N9-C4	-5.36	103.66	105.80
36	1	865	U	OP2-P-O3'	5.36	116.98	105.20
36	1	1180	A	C4-C5-N7	-5.36	108.02	110.70
1	6	1764	C	N3-C4-N4	-5.36	114.25	118.00
36	5	971	G	C6-N1-C2	-5.36	121.89	125.10
36	5	1348	U	C6-N1-C2	-5.36	117.79	121.00
36	5	1378	U	N3-C4-C5	5.36	117.81	114.60
36	5	2420	C	N1-C2-O2	-5.36	115.69	118.90
38	8	96	A	N7-C8-N9	-5.36	111.12	113.80
1	6	455	C	C5-C4-N4	-5.35	116.45	120.20
36	5	214	G	N7-C8-N9	-5.35	110.42	113.10
36	5	1169	A	O5'-P-OP2	-5.35	100.88	105.70
36	5	2693	C	C2-N1-C1'	-5.35	112.91	118.80
1	2	720	G	OP1-P-O3'	5.35	116.98	105.20
1	2	1121	C	N3-C4-N4	-5.35	114.25	118.00
36	1	1392	G	C5-N7-C8	5.35	106.98	104.30
36	1	1660	C	N1-C2-O2	-5.35	115.69	118.90
36	1	2165	G	N1-C6-O6	5.35	123.11	119.90
36	5	3206	C	N3-C2-O2	-5.35	118.15	121.90
38	8	20	U	N1-C2-N3	5.35	118.11	114.90
36	1	2723	U	C5-C4-O4	-5.35	122.69	125.90
1	6	308	C	N3-C4-N4	-5.35	114.25	118.00
36	5	1376	C	O5'-P-OP2	-5.35	100.89	105.70
1	2	7	G	N1-C6-O6	-5.35	116.69	119.90
1	2	811	A	C8-N9-C4	-5.35	103.66	105.80
1	2	1205	C	C6-N1-C1'	-5.35	114.38	120.80
36	1	78	U	N1-C2-N3	5.35	118.11	114.90
36	1	942	U	N3-C4-O4	5.35	123.14	119.40
36	1	1481	A	C4-C5-C6	5.35	119.67	117.00
1	6	1662	G	N7-C8-N9	-5.35	110.42	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2283	G	C8-N9-C4	5.35	108.54	106.40
36	5	2645	G	N1-C6-O6	-5.35	116.69	119.90
36	5	3049	A	C6-N1-C2	5.35	121.81	118.60
36	1	50	U	N3-C2-O2	-5.35	118.46	122.20
36	1	2959	C	OP2-P-O3'	5.35	116.96	105.20
1	6	1574	G	C4-C5-N7	-5.35	108.66	110.80
36	5	128	G	C8-N9-C1'	-5.35	120.05	127.00
36	5	694	C	C4-C5-C6	5.35	120.07	117.40
36	5	1392	G	C8-N9-C1'	-5.35	120.05	127.00
36	5	2194	G	N1-C2-N2	-5.35	111.39	116.20
1	6	297	U	N3-C4-O4	5.35	123.14	119.40
1	6	1126	G	C5-C6-O6	5.35	131.81	128.60
36	5	866	A	N1-C6-N6	5.35	121.81	118.60
36	1	53	G	N1-C2-N2	-5.34	111.39	116.20
36	1	205	C	C5-C6-N1	-5.34	118.33	121.00
36	1	2836	C	N3-C4-C5	-5.34	119.76	121.90
36	5	1051	U	OP1-P-O3'	5.34	116.96	105.20
36	5	1604	G	N9-C4-C5	-5.34	103.26	105.40
36	1	1176	C	N1-C2-O2	-5.34	115.69	118.90
36	1	1379	G	N1-C2-N3	5.34	127.11	123.90
36	1	1405	U	N3-C4-C5	5.34	117.81	114.60
36	5	1494	U	C2-N1-C1'	-5.34	111.29	117.70
36	5	2989	U	C5-C6-N1	-5.34	120.03	122.70
36	1	609	G	O5'-P-OP2	-5.34	100.89	105.70
36	1	894	G	OP1-P-O3'	5.34	116.95	105.20
36	1	1545	A	C8-N9-C4	-5.34	103.66	105.80
37	3	117	A	C2-N3-C4	-5.34	107.93	110.60
41	L4	327	LEU	CA-CB-CG	5.34	127.58	115.30
1	6	514	G	C8-N9-C4	5.34	108.53	106.40
36	5	824	C	N3-C2-O2	-5.34	118.16	121.90
36	5	882	A	N1-C2-N3	5.34	131.97	129.30
36	1	2425	G	O5'-P-OP1	5.34	117.11	110.70
36	5	2205	U	O4'-C1'-N1	5.34	112.47	108.20
1	2	9	U	O5'-P-OP1	-5.34	100.90	105.70
1	6	1791	A	N1-C6-N6	5.34	121.80	118.60
36	5	1371	G	C5-C6-N1	5.34	114.17	111.50
36	5	1452	A	C6-C5-N7	-5.34	128.56	132.30
36	5	1491	A	C4-C5-C6	5.34	119.67	117.00
36	5	343	U	OP1-P-O3'	5.33	116.94	105.20
36	5	2144	A	OP1-P-O3'	5.33	116.94	105.20
1	2	394	C	N1-C2-O2	5.33	122.10	118.90
73	O7	67	LEU	CA-CB-CG	5.33	127.57	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1549	C	C4-C5-C6	5.33	120.07	117.40
36	5	997	A	C8-N9-C4	-5.33	103.67	105.80
36	5	1481	A	O4'-C1'-N9	5.33	112.47	108.20
36	5	2719	U	N1-C2-O2	-5.33	119.07	122.80
36	5	2815	G	N7-C8-N9	-5.33	110.43	113.10
36	5	2874	G	C5-C6-N1	-5.33	108.83	111.50
38	8	1	A	O5'-P-OP2	-5.33	100.90	105.70
38	8	34	U	N1-C2-N3	5.33	118.10	114.90
38	8	56	G	C5-C6-O6	-5.33	125.40	128.60
36	1	2222	A	C8-N9-C4	-5.33	103.67	105.80
1	6	989	U	O5'-P-OP1	-5.33	100.90	105.70
1	6	1745	G	C5-C6-O6	-5.33	125.40	128.60
36	5	91	G	C4-C5-N7	5.33	112.93	110.80
52	M6	172	ARG	NE-CZ-NH1	5.33	122.97	120.30
36	5	48	A	O5'-P-OP2	-5.33	100.90	105.70
36	5	1770	G	C8-N9-C1'	-5.33	120.07	127.00
18	C6	40	GLU	C-N-CA	5.33	144.38	122.00
36	1	429	U	N1-C2-O2	5.33	126.53	122.80
36	1	1316	C	N3-C4-C5	-5.33	119.77	121.90
36	1	3135	U	C5-C6-N1	-5.33	120.03	122.70
37	3	61	G	C5-C6-O6	-5.33	125.40	128.60
36	5	800	G	N1-C2-N2	5.33	121.00	116.20
36	5	2690	G	C4-C5-N7	5.33	112.93	110.80
36	5	2975	U	N1-C2-O2	5.33	126.53	122.80
36	5	3027	A	N1-C6-N6	5.33	121.80	118.60
36	5	3209	A	N1-C6-N6	5.33	121.80	118.60
38	8	156	U	C2-N1-C1'	5.33	124.09	117.70
1	2	73	U	N3-C2-O2	-5.33	118.47	122.20
36	1	145	G	C5-C6-O6	-5.33	125.40	128.60
36	1	3215	A	C8-N9-C4	5.33	107.93	105.80
1	6	561	G	C8-N9-C4	-5.33	104.27	106.40
36	5	1054	A	O5'-P-OP2	-5.33	100.91	105.70
36	5	2134	G	N1-C2-N2	-5.33	111.41	116.20
36	5	2323	G	OP1-P-OP2	-5.33	111.61	119.60
36	1	1169	A	C8-N9-C4	-5.33	103.67	105.80
36	1	2388	U	OP2-P-O3'	5.33	116.92	105.20
36	5	659	G	P-O3'-C3'	5.33	126.09	119.70
36	5	3299	A	O5'-P-OP1	-5.33	100.91	105.70
36	1	1445	U	C2-N1-C1'	-5.32	111.31	117.70
36	1	1483	G	N1-C6-O6	-5.32	116.71	119.90
36	1	1876	U	C2-N1-C1'	5.32	124.09	117.70
36	1	2314	U	N3-C2-O2	5.32	125.93	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	858	G	C4-N9-C1'	5.32	133.42	126.50
1	6	1653	C	C4-C5-C6	5.32	120.06	117.40
36	5	283	G	C4-N9-C1'	5.32	133.42	126.50
36	5	622	A	N9-C4-C5	-5.32	103.67	105.80
36	5	873	C	O5'-P-OP2	-5.32	100.91	105.70
36	5	966	U	C6-N1-C2	-5.32	117.81	121.00
36	5	1790	G	C6-C5-N7	-5.32	127.21	130.40
36	1	1827	C	C6-N1-C2	-5.32	118.17	120.30
37	3	85	G	OP2-P-O3'	5.32	116.91	105.20
38	4	46	G	N3-C4-C5	-5.32	125.94	128.60
1	6	144	U	N1-C2-N3	5.32	118.09	114.90
1	6	475	A	N1-C6-N6	5.32	121.79	118.60
36	5	2167	A	N3-C4-C5	-5.32	123.08	126.80
36	1	127	G	C5-C6-O6	-5.32	125.41	128.60
36	1	906	A	N3-C4-C5	-5.32	123.08	126.80
36	1	1101	G	C6-C5-N7	5.32	133.59	130.40
36	1	2842	U	N3-C2-O2	-5.32	118.48	122.20
38	4	13	A	N7-C8-N9	5.32	116.46	113.80
36	5	1312	C	N1-C2-O2	-5.32	115.71	118.90
36	5	1710	C	C6-N1-C2	5.32	122.43	120.30
36	1	894	G	C6-C5-N7	-5.32	127.21	130.40
36	1	1310	G	N1-C6-O6	-5.32	116.71	119.90
36	5	2129	U	O5'-P-OP1	-5.32	100.91	105.70
36	5	2434	U	N1-C2-N3	5.32	118.09	114.90
36	1	2104	A	C8-N9-C4	5.32	107.93	105.80
36	1	2165	G	C5-C6-O6	-5.32	125.41	128.60
36	1	2369	G	C6-N1-C2	-5.32	121.91	125.10
36	1	2388	U	N1-C2-O2	-5.32	119.08	122.80
36	1	2880	U	OP2-P-O3'	5.32	116.90	105.20
36	5	583	G	C5-C6-O6	5.32	131.79	128.60
36	5	609	G	N3-C4-N9	-5.32	122.81	126.00
36	5	934	G	C4-N9-C1'	5.32	133.41	126.50
36	5	2764	C	C4-C5-C6	-5.32	114.74	117.40
37	7	85	G	OP2-P-O3'	5.32	116.90	105.20
1	2	281	G	N1-C6-O6	-5.32	116.71	119.90
36	1	1948	G	C6-C5-N7	-5.32	127.21	130.40
1	6	747	C	N1-C2-O2	-5.32	115.71	118.90
1	6	956	C	C6-N1-C2	5.32	122.43	120.30
36	5	2132	C	C6-N1-C2	-5.32	118.17	120.30
36	1	808	A	C6-N1-C2	-5.31	115.41	118.60
36	1	2710	C	N3-C2-O2	5.31	125.62	121.90
1	6	1014	G	N1-C2-N2	-5.31	111.42	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2399	A	N9-C4-C5	-5.31	103.67	105.80
36	5	2615	G	C4-C5-N7	5.31	112.93	110.80
1	2	396	G	N9-C1'-C2'	-5.31	106.16	112.00
41	L4	313	LEU	CA-CB-CG	5.31	127.52	115.30
1	6	1097	U	N1-C2-N3	5.31	118.09	114.90
36	5	1161	G	C2-N3-C4	5.31	114.56	111.90
36	5	1405	U	C5-C6-N1	-5.31	120.04	122.70
36	5	1519	G	N1-C6-O6	5.31	123.09	119.90
36	5	1680	G	N3-C4-N9	-5.31	122.81	126.00
36	5	2164	A	C8-N9-C4	-5.31	103.67	105.80
37	7	2	G	N7-C8-N9	5.31	115.76	113.10
36	1	2976	A	C6-N1-C2	-5.31	115.41	118.60
14	c2	58	LEU	CA-CB-CG	5.31	127.51	115.30
36	5	400	G	N3-C4-N9	-5.31	122.81	126.00
36	5	1199	C	N1-C2-O2	-5.31	115.71	118.90
36	5	2928	C	N3-C4-N4	5.31	121.72	118.00
36	5	2983	C	OP1-P-OP2	5.31	127.57	119.60
38	8	32	C	N1-C2-O2	-5.31	115.71	118.90
38	8	38	U	N1-C2-N3	5.31	118.09	114.90
36	1	2878	G	C8-N9-C4	5.31	108.52	106.40
36	5	1169	A	N1-C2-N3	5.31	131.96	129.30
36	5	1792	C	O5'-P-OP2	-5.31	100.92	105.70
36	5	2293	C	N3-C2-O2	-5.31	118.18	121.90
36	1	726	G	N7-C8-N9	5.31	115.75	113.10
36	1	931	C	C5-C6-N1	-5.31	118.35	121.00
36	1	1179	A	C2-N3-C4	-5.31	107.95	110.60
1	6	616	G	C2-N3-C4	5.31	114.55	111.90
36	5	339	C	N1-C2-O2	-5.31	115.72	118.90
36	5	3197	G	C6-C5-N7	5.31	133.59	130.40
57	n1	55	LYS	CD-CE-NZ	-5.31	99.49	111.70
1	6	1373	C	N1-C2-O2	5.31	122.08	118.90
36	5	911	C	C5-C6-N1	-5.31	118.35	121.00
36	5	1379	G	C8-N9-C1'	-5.31	120.10	127.00
36	5	1379	G	N3-C4-N9	5.31	129.18	126.00
36	5	1594	A	N9-C4-C5	5.31	107.92	105.80
36	1	1795	U	N1-C2-O2	5.30	126.51	122.80
1	6	1565	C	N3-C4-C5	5.30	124.02	121.90
36	5	815	G	N3-C4-C5	-5.30	125.95	128.60
36	5	1345	G	N3-C4-C5	5.30	131.25	128.60
1	6	144	U	C6-N1-C2	-5.30	117.82	121.00
1	6	352	A	C8-N9-C4	5.30	107.92	105.80
1	6	622	A	O5'-P-OP1	-5.30	100.93	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	s7	131	PHE	C-N-CD	5.30	139.54	128.40
36	5	1116	G	OP2-P-O3'	5.30	116.87	105.20
36	1	228	U	N1-C2-N3	5.30	118.08	114.90
36	1	325	A	C5-C6-N1	5.30	120.35	117.70
36	1	2130	G	N1-C2-N2	-5.30	111.43	116.20
36	1	2537	U	P-O3'-C3'	5.30	126.06	119.70
36	1	2653	C	N3-C4-N4	-5.30	114.29	118.00
36	5	1749	A	C8-N9-C4	5.30	107.92	105.80
36	1	702	C	N3-C4-N4	5.30	121.71	118.00
36	1	1515	A	OP2-P-O3'	5.30	116.86	105.20
36	1	2811	A	C5-C6-N1	5.30	120.35	117.70
1	6	139	C	O4'-C1'-N1	5.30	112.44	108.20
36	5	895	A	C8-N9-C4	5.30	107.92	105.80
36	5	1592	G	N3-C4-C5	-5.30	125.95	128.60
36	5	1603	A	N1-C2-N3	5.30	131.95	129.30
36	5	2318	U	N3-C4-O4	-5.30	115.69	119.40
36	5	2372	A	C5-N7-C8	-5.30	101.25	103.90
1	2	213	A	C8-N9-C4	5.30	107.92	105.80
36	1	954	U	N1-C2-N3	5.30	118.08	114.90
36	1	2621	G	N1-C2-N2	5.30	120.97	116.20
36	1	3338	C	C6-N1-C2	-5.30	118.18	120.30
1	6	259	U	OP2-P-O3'	5.30	116.86	105.20
1	6	351	C	C5-C4-N4	-5.30	116.49	120.20
36	5	1214	U	C5-C6-N1	5.30	125.35	122.70
36	5	1329	U	N3-C2-O2	-5.30	118.49	122.20
36	5	2861	U	C5-C4-O4	5.30	129.08	125.90
36	5	2954	U	N3-C4-C5	-5.30	111.42	114.60
36	1	282	G	N7-C8-N9	5.30	115.75	113.10
36	1	1371	G	N7-C8-N9	-5.30	110.45	113.10
36	1	2800	G	O5'-P-OP1	5.30	117.06	110.70
36	1	3157	U	N3-C4-O4	-5.30	115.69	119.40
1	6	1117	U	N3-C4-O4	5.30	123.11	119.40
36	5	652	G	C5-C6-O6	-5.30	125.42	128.60
36	5	876	A	N1-C2-N3	5.30	131.95	129.30
37	7	93	C	N3-C2-O2	-5.30	118.19	121.90
36	1	1346	G	N3-C4-N9	-5.29	122.82	126.00
49	M3	67	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	6	247	A	N1-C6-N6	5.29	121.78	118.60
36	5	1043	C	O5'-P-OP1	5.29	117.05	110.70
36	5	2376	G	C5-N7-C8	-5.29	101.65	104.30
37	7	77	G	N9-C4-C5	-5.29	103.28	105.40
36	1	3130	A	C4-C5-C6	5.29	119.65	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	4	56	G	C8-N9-C4	5.29	108.52	106.40
36	5	411	U	C2-N1-C1'	-5.29	111.35	117.70
36	5	947	G	C8-N9-C1'	-5.29	120.12	127.00
36	5	1210	U	C5-C4-O4	5.29	129.08	125.90
36	5	3182	G	OP1-P-OP2	-5.29	111.66	119.60
37	7	22	A	N1-C6-N6	5.29	121.78	118.60
36	1	2419	A	OP2-P-O3'	5.29	116.84	105.20
36	1	2555	G	O5'-P-OP2	-5.29	100.94	105.70
1	6	1210	C	C6-N1-C2	-5.29	118.18	120.30
1	6	1481	C	OP1-P-O3'	5.29	116.84	105.20
36	5	217	U	C5-C6-N1	-5.29	120.06	122.70
36	5	816	A	N9-C4-C5	5.29	107.92	105.80
36	5	944	C	OP2-P-O3'	5.29	116.84	105.20
36	5	1628	C	C6-N1-C2	-5.29	118.18	120.30
36	5	2334	U	C2-N3-C4	-5.29	123.83	127.00
36	5	2633	U	C5-C6-N1	-5.29	120.05	122.70
36	5	3354	U	N3-C2-O2	-5.29	118.50	122.20
38	8	36	G	O5'-P-OP1	-5.29	100.94	105.70
36	1	2138	A	N7-C8-N9	5.29	116.44	113.80
36	1	3058	U	C2-N1-C1'	5.29	124.05	117.70
61	n5	115	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	2	1608	U	O5'-P-OP1	-5.29	100.94	105.70
36	1	802	C	O5'-P-OP2	5.29	117.05	110.70
36	5	1239	C	C2-N1-C1'	5.29	124.62	118.80
36	5	2234	G	C6-N1-C2	-5.29	121.93	125.10
36	5	2772	C	OP2-P-O3'	5.29	116.84	105.20
36	1	2636	A	N1-C6-N6	-5.29	115.43	118.60
36	1	2796	G	N7-C8-N9	5.29	115.74	113.10
36	1	2899	C	C2-N1-C1'	5.29	124.61	118.80
36	5	706	A	C8-N9-C4	5.29	107.92	105.80
36	5	1160	C	C2-N3-C4	-5.29	117.26	119.90
36	5	3295	A	OP2-P-O3'	5.29	116.83	105.20
1	2	1241	G	C4-N9-C1'	5.29	133.37	126.50
36	1	937	G	OP1-P-OP2	5.29	127.53	119.60
36	1	994	G	N3-C4-N9	5.29	129.17	126.00
36	1	2753	G	C2-N3-C4	5.29	114.54	111.90
36	1	2772	C	O4'-C1'-N1	5.29	112.43	108.20
36	1	3034	C	C6-N1-C2	-5.29	118.19	120.30
38	4	96	A	N1-C6-N6	5.29	121.77	118.60
1	6	217	A	P-O3'-C3'	5.29	126.04	119.70
1	6	1361	U	C6-N1-C1'	-5.29	113.80	121.20
36	5	92	G	C5-C6-O6	-5.29	125.43	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1788	C	O5'-P-OP2	-5.29	100.94	105.70
36	5	2816	G	C5-C6-O6	-5.29	125.43	128.60
36	5	3044	G	C8-N9-C4	-5.29	104.29	106.40
38	8	93	U	N1-C2-N3	5.29	118.07	114.90
76	q0	102	ARG	NE-CZ-NH1	-5.29	117.66	120.30
36	1	71	A	N9-C4-C5	5.28	107.91	105.80
36	1	619	A	N1-C6-N6	5.28	121.77	118.60
36	1	793	C	C6-N1-C2	-5.28	118.19	120.30
36	1	1657	C	C2-N3-C4	5.28	122.54	119.90
36	1	2193	U	N3-C2-O2	-5.28	118.50	122.20
36	1	2866	U	N3-C2-O2	-5.28	118.50	122.20
36	5	1881	A	N1-C6-N6	5.28	121.77	118.60
36	5	2690	G	C5-C6-O6	-5.28	125.43	128.60
36	5	2702	A	C4-C5-C6	5.28	119.64	117.00
36	5	3296	A	O5'-P-OP2	-5.28	100.95	105.70
36	1	325	A	C6-N1-C2	-5.28	115.43	118.60
36	1	1716	U	P-O3'-C3'	5.28	126.04	119.70
36	1	2774	C	C2-N3-C4	-5.28	117.26	119.90
1	6	1003	A	O5'-P-OP2	5.28	117.04	110.70
36	5	2134	G	N1-C6-O6	-5.28	116.73	119.90
36	5	2292	U	N3-C4-O4	5.28	123.10	119.40
36	5	3272	C	N1-C2-O2	-5.28	115.73	118.90
36	1	644	G	O5'-P-OP1	-5.28	100.95	105.70
36	1	2412	G	N1-C6-O6	5.28	123.07	119.90
40	L3	4	ARG	NE-CZ-NH2	-5.28	117.66	120.30
36	5	3033	A	N1-C6-N6	5.28	121.77	118.60
36	1	961	C	C5-C6-N1	-5.28	118.36	121.00
36	1	1435	A	OP1-P-OP2	-5.28	111.68	119.60
36	1	1604	G	N3-C4-C5	-5.28	125.96	128.60
36	1	1838	G	C5-N7-C8	-5.28	101.66	104.30
1	6	1619	C	C5-C6-N1	5.28	123.64	121.00
36	1	27	C	OP1-P-OP2	5.28	127.52	119.60
36	1	1140	G	N1-C2-N2	-5.28	111.45	116.20
36	1	1798	A	C2-N3-C4	-5.28	107.96	110.60
36	1	2950	G	O4'-C1'-N9	5.28	112.42	108.20
1	6	334	G	N9-C4-C5	-5.28	103.29	105.40
1	6	1274	C	N1-C2-O2	5.28	122.07	118.90
36	5	88	A	N7-C8-N9	-5.28	111.16	113.80
36	5	1908	A	C8-N9-C4	-5.28	103.69	105.80
1	2	453	U	C6-N1-C1'	-5.28	113.81	121.20
1	2	1182	U	N1-C2-O2	5.28	126.49	122.80
36	1	680	G	O5'-P-OP2	-5.28	100.95	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1578	C	C2-N1-C1'	5.28	124.60	118.80
36	1	2637	A	C8-N9-C4	-5.28	103.69	105.80
36	1	3303	G	O4'-C1'-N9	5.28	112.42	108.20
56	N0	155	ARG	NE-CZ-NH1	-5.28	117.66	120.30
36	5	2283	G	N3-C4-C5	5.28	131.24	128.60
37	7	27	A	OP1-P-O3'	5.28	116.81	105.20
38	8	96	A	N9-C4-C5	-5.28	103.69	105.80
36	1	941	G	C8-N9-C4	-5.27	104.29	106.40
36	1	2174	G	N7-C8-N9	5.27	115.74	113.10
36	1	2409	G	C4-C5-C6	5.27	121.96	118.80
38	4	100	U	C2-N1-C1'	5.27	124.03	117.70
36	5	1668	G	C6-C5-N7	-5.27	127.24	130.40
1	2	404	G	N9-C4-C5	-5.27	103.29	105.40
36	1	3215	A	N3-C4-C5	5.27	130.49	126.80
1	6	584	C	N1-C2-O2	5.27	122.06	118.90
36	5	1003	A	OP1-P-O3'	5.27	116.80	105.20
36	5	1193	A	C4-C5-C6	5.27	119.64	117.00
36	5	1380	G	C4-C5-N7	5.27	112.91	110.80
36	5	3099	C	C5-C6-N1	-5.27	118.36	121.00
36	1	1506	A	O5'-P-OP2	-5.27	100.96	105.70
1	6	1582	U	C5-C6-N1	-5.27	120.06	122.70
1	2	1093	A	C8-N9-C4	5.27	107.91	105.80
36	1	3183	A	OP2-P-O3'	5.27	116.79	105.20
36	5	957	C	N1-C2-N3	5.27	122.89	119.20
36	1	793	C	N1-C2-O2	-5.27	115.74	118.90
36	1	1373	A	N1-C2-N3	5.27	131.93	129.30
36	1	2363	A	OP2-P-O3'	5.27	116.79	105.20
36	1	3062	G	N1-C6-O6	5.27	123.06	119.90
36	1	651	G	OP2-P-O3'	5.26	116.78	105.20
36	5	1113	G	N3-C4-C5	5.26	131.23	128.60
36	5	3100	U	N3-C2-O2	-5.26	118.52	122.20
38	8	63	G	N1-C6-O6	-5.26	116.74	119.90
36	1	1333	C	O5'-P-OP2	-5.26	100.96	105.70
1	6	543	C	N3-C4-N4	-5.26	114.32	118.00
36	5	1837	U	OP2-P-O3'	5.26	116.78	105.20
36	5	2744	U	C6-N1-C2	-5.26	117.84	121.00
36	5	3091	A	N1-C6-N6	-5.26	115.44	118.60
1	2	142	G	N3-C4-N9	-5.26	122.84	126.00
1	2	783	G	C8-N9-C4	5.26	108.50	106.40
36	1	984	G	C4-N9-C1'	5.26	133.34	126.50
36	1	2640	A	C5-N7-C8	-5.26	101.27	103.90
1	6	1058	U	P-O3'-C3'	5.26	126.02	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	1672	G	N3-C4-N9	5.26	129.16	126.00
9	s7	67	LEU	CA-CB-CG	5.26	127.40	115.30
36	5	1106	G	N3-C4-C5	-5.26	125.97	128.60
36	1	59	G	C4-C5-N7	5.26	112.90	110.80
36	1	1143	A	N1-C2-N3	5.26	131.93	129.30
36	1	1213	G	C5'-C4'-O4'	-5.26	102.79	109.10
36	1	1411	C	OP1-P-O3'	5.26	116.77	105.20
36	1	2355	G	C5-C6-O6	-5.26	125.44	128.60
36	1	2371	G	O5'-P-OP2	-5.26	100.97	105.70
1	6	114	C	C2-N1-C1'	5.26	124.58	118.80
1	6	606	A	C8-N9-C4	5.26	107.90	105.80
36	5	82	C	N3-C4-C5	-5.26	119.80	121.90
36	5	931	C	N3-C4-C5	5.26	124.00	121.90
36	5	1133	A	N9-C4-C5	5.26	107.90	105.80
36	5	1723	A	N1-C6-N6	-5.26	115.44	118.60
1	6	557	G	C4-N9-C1'	5.26	133.34	126.50
1	6	1124	A	N9-C4-C5	-5.26	103.70	105.80
1	6	1672	G	C8-N9-C1'	-5.26	120.17	127.00
36	5	2826	U	O5'-P-OP2	-5.26	100.97	105.70
24	D2	127	GLY	N-CA-C	5.26	126.24	113.10
36	1	627	U	N1-C2-O2	-5.26	119.12	122.80
36	1	1144	U	C2-N3-C4	-5.26	123.85	127.00
36	1	1406	A	C5-C6-N6	-5.26	119.50	123.70
36	1	2958	A	OP2-P-O3'	5.26	116.76	105.20
36	1	3268	A	N1-C2-N3	5.26	131.93	129.30
1	6	1614	A	C5-N7-C8	-5.26	101.27	103.90
36	5	2648	G	C5-C6-N1	5.26	114.13	111.50
36	5	3039	C	C6-N1-C2	-5.26	118.20	120.30
37	7	83	U	N3-C4-O4	-5.26	115.72	119.40
36	1	3172	A	O5'-P-OP2	-5.25	100.97	105.70
38	4	28	C	OP2-P-O3'	5.25	116.76	105.20
36	5	388	G	C6-C5-N7	-5.25	127.25	130.40
1	2	772	G	N1-C6-O6	5.25	123.05	119.90
35	SM	134	ASP	CB-CG-OD2	5.25	123.03	118.30
36	1	1834	U	C4-C5-C6	5.25	122.85	119.70
36	1	1916	U	C2-N3-C4	-5.25	123.85	127.00
36	1	2154	U	C2-N1-C1'	5.25	124.00	117.70
36	1	3195	U	N1-C2-O2	5.25	126.48	122.80
38	4	16	G	O4'-C1'-N9	5.25	112.40	108.20
1	6	1140	G	O5'-P-OP1	-5.25	100.97	105.70
36	5	425	G	O5'-P-OP1	5.25	117.00	110.70
36	5	1004	U	O5'-P-OP1	-5.25	100.97	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2874	G	C5-C6-O6	5.25	131.75	128.60
36	5	665	A	C6-C5-N7	-5.25	128.62	132.30
36	5	2758	A	O4'-C1'-N9	5.25	112.40	108.20
36	5	2965	U	N3-C2-O2	5.25	125.88	122.20
1	2	1453	G	C4-N9-C1'	-5.25	119.67	126.50
36	1	1615	C	C4-C5-C6	5.25	120.03	117.40
36	1	2643	A	N1-C6-N6	5.25	121.75	118.60
36	5	1380	G	N1-C6-O6	5.25	123.05	119.90
36	1	1379	G	C8-N9-C4	5.25	108.50	106.40
36	5	676	G	OP2-P-O3'	5.25	116.75	105.20
36	5	1158	A	O5'-P-OP1	5.25	117.00	110.70
1	2	1273	G	O5'-P-OP1	-5.25	100.98	105.70
36	1	155	G	N3-C4-C5	-5.25	125.98	128.60
36	1	501	A	OP2-P-O3'	5.25	116.74	105.20
36	1	701	G	N3-C2-N2	-5.25	116.23	119.90
1	6	18	C	N3-C4-C5	-5.25	119.80	121.90
1	6	1123	C	C5-C6-N1	5.25	123.62	121.00
36	5	204	A	N1-C6-N6	5.25	121.75	118.60
36	5	437	G	N3-C4-N9	-5.25	122.85	126.00
36	5	3293	U	C5-C6-N1	-5.25	120.08	122.70
36	5	811	U	C5-C6-N1	-5.25	120.08	122.70
36	5	1495	U	O4'-C1'-N1	5.25	112.40	108.20
36	5	1615	C	N3-C2-O2	-5.25	118.23	121.90
36	5	2108	C	N1-C2-O2	-5.25	115.75	118.90
1	2	17	C	C6-N1-C2	-5.24	118.20	120.30
1	2	21	U	C5-C6-N1	5.24	125.32	122.70
36	1	817	A	N1-C6-N6	-5.24	115.45	118.60
36	1	1141	C	N1-C2-O2	-5.24	115.75	118.90
36	1	2300	G	N3-C2-N2	-5.24	116.23	119.90
36	5	804	C	N3-C4-N4	5.24	121.67	118.00
36	5	838	G	N1-C2-N2	-5.24	111.48	116.20
36	5	1329	U	C6-N1-C1'	-5.24	113.86	121.20
36	5	1431	G	C6-C5-N7	5.24	133.55	130.40
36	5	2383	C	C4-C5-C6	5.24	120.02	117.40
36	5	2865	U	N1-C2-O2	5.24	126.47	122.80
36	5	3129	A	N1-C2-N3	-5.24	126.68	129.30
38	8	110	C	OP2-P-O3'	5.24	116.73	105.20
1	2	1324	G	N3-C4-N9	-5.24	122.86	126.00
36	1	1305	U	C5-C4-O4	5.24	129.04	125.90
36	1	3127	A	C5-C6-N6	-5.24	119.51	123.70
1	6	512	A	C6-C5-N7	-5.24	128.63	132.30
36	5	2288	G	C4-N9-C1'	5.24	133.31	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	339	C	C6-N1-C2	-5.24	118.20	120.30
1	2	1745	G	N3-C2-N2	5.24	123.57	119.90
36	1	35	A	N1-C6-N6	5.24	121.74	118.60
36	1	2234	G	O5'-P-OP1	-5.24	100.98	105.70
1	6	1744	A	C8-N9-C4	5.24	107.90	105.80
36	5	639	G	O5'-P-OP2	-5.24	100.98	105.70
36	5	2134	G	N3-C2-N2	5.24	123.57	119.90
1	2	501	U	OP1-P-O3'	5.24	116.72	105.20
1	2	1600	A	N9-C4-C5	-5.24	103.70	105.80
36	1	1905	G	N3-C4-C5	5.24	131.22	128.60
38	4	4	C	C5-C4-N4	-5.24	116.53	120.20
36	5	945	C	C5-C6-N1	-5.24	118.38	121.00
1	2	398	G	C8-N9-C4	-5.24	104.31	106.40
36	5	784	A	C4-C5-N7	5.24	113.32	110.70
36	5	2777	G	P-O3'-C3'	5.24	125.98	119.70
36	1	86	G	N9-C4-C5	5.24	107.49	105.40
36	1	218	G	OP1-P-OP2	5.24	127.45	119.60
36	1	941	G	C5-C6-O6	-5.24	125.46	128.60
37	3	81	U	C6-N1-C2	5.24	124.14	121.00
1	6	939	A	C5-C6-N6	-5.24	119.51	123.70
36	5	439	C	C6-N1-C2	-5.24	118.20	120.30
36	5	1306	G	N3-C2-N2	-5.24	116.23	119.90
36	5	2724	U	N3-C4-C5	-5.24	111.46	114.60
36	1	89	A	N1-C6-N6	-5.23	115.46	118.60
36	1	100	A	N1-C2-N3	5.23	131.92	129.30
36	5	1355	A	P-O3'-C3'	5.23	125.98	119.70
36	5	2293	C	N3-C4-C5	5.23	123.99	121.90
1	2	1620	C	C6-N1-C2	-5.23	118.21	120.30
36	1	76	G	C8-N9-C4	-5.23	104.31	106.40
36	1	609	G	C2-N3-C4	5.23	114.52	111.90
36	1	632	G	N3-C2-N2	5.23	123.56	119.90
36	1	1049	C	C2-N1-C1'	5.23	124.56	118.80
36	1	2627	C	C2-N3-C4	-5.23	117.28	119.90
36	1	3000	A	N7-C8-N9	-5.23	111.18	113.80
37	3	13	A	C5'-C4'-C3'	-5.23	107.63	116.00
1	6	63	G	C5-C6-O6	-5.23	125.46	128.60
36	5	96	G	N3-C4-C5	5.23	131.22	128.60
36	5	1321	G	C6-C5-N7	-5.23	127.26	130.40
36	5	2372	A	P-O3'-C3'	5.23	125.98	119.70
1	2	1340	U	N3-C2-O2	-5.23	118.54	122.20
1	2	1777	G	OP2-P-O3'	5.23	116.71	105.20
36	1	108	A	C5-C6-N1	5.23	120.31	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2247	G	N3-C2-N2	-5.23	116.24	119.90
36	1	2378	C	N3-C4-N4	5.23	121.66	118.00
36	1	2848	G	C5-C6-N1	5.23	114.11	111.50
36	1	2973	G	N1-C6-O6	5.23	123.04	119.90
1	6	1540	G	C5-C6-O6	5.23	131.74	128.60
36	5	2314	U	N3-C4-O4	5.23	123.06	119.40
36	5	2385	G	N1-C6-O6	5.23	123.04	119.90
36	1	646	A	C6-C5-N7	-5.23	128.64	132.30
36	1	2859	U	N1-C2-O2	-5.23	119.14	122.80
36	5	1487	G	N3-C4-C5	-5.23	125.99	128.60
1	2	635	A	N1-C6-N6	5.23	121.74	118.60
36	1	153	U	C6-N1-C2	-5.23	117.86	121.00
36	1	1880	U	N3-C2-O2	5.23	125.86	122.20
1	6	273	G	C4-C5-N7	5.23	112.89	110.80
36	5	1108	U	C5-C4-O4	5.23	129.04	125.90
36	5	1115	G	P-O3'-C3'	5.23	125.97	119.70
36	5	2584	G	OP2-P-O3'	5.23	116.70	105.20
38	8	125	U	N3-C2-O2	-5.23	118.54	122.20
36	1	2298	U	C5-C6-N1	-5.23	120.09	122.70
36	1	2728	G	C5-C6-O6	-5.23	125.47	128.60
36	5	945	C	C6-N1-C1'	-5.23	114.53	120.80
36	5	960	U	OP2-P-O3'	5.23	116.70	105.20
36	5	1307	G	N1-C6-O6	-5.23	116.77	119.90
1	2	1134	C	C6-N1-C2	-5.22	118.21	120.30
1	2	1535	U	C2-N1-C1'	5.22	123.97	117.70
36	1	196	G	C5-C6-O6	-5.22	125.47	128.60
36	1	2184	U	C5-C6-N1	5.22	125.31	122.70
36	1	2402	A	O4'-C1'-N9	5.22	112.38	108.20
36	1	2582	C	N3-C2-O2	-5.22	118.24	121.90
36	1	2640	A	C6-C5-N7	-5.22	128.64	132.30
1	6	1123	C	C5-C4-N4	-5.22	116.54	120.20
36	5	644	G	N9-C4-C5	5.22	107.49	105.40
36	5	2307	G	N3-C2-N2	5.22	123.56	119.90
36	5	3130	A	C6-N1-C2	-5.22	115.47	118.60
37	7	88	G	C5-C6-O6	5.22	131.74	128.60
1	2	1591	C	N3-C2-O2	-5.22	118.24	121.90
36	1	2325	G	C6-C5-N7	-5.22	127.27	130.40
36	5	3374	U	N3-C4-O4	-5.22	115.74	119.40
36	1	881	C	N1-C2-O2	5.22	122.03	118.90
36	1	907	G	N3-C4-N9	5.22	129.13	126.00
36	1	2156	C	C5-C6-N1	-5.22	118.39	121.00
1	6	1640	C	C5-C4-N4	-5.22	116.55	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1370	G	O5'-P-OP1	-5.22	101.00	105.70
36	5	2743	A	C4-C5-C6	5.22	119.61	117.00
36	1	1416	C	C5-C4-N4	5.22	123.85	120.20
36	1	1495	U	O4'-C1'-N1	5.22	112.38	108.20
38	4	88	A	N1-C6-N6	5.22	121.73	118.60
36	5	424	G	O5'-P-OP2	-5.22	101.00	105.70
1	2	1747	G	N1-C6-O6	5.22	123.03	119.90
1	6	245	U	O5'-P-OP1	-5.22	101.00	105.70
1	6	541	A	P-O3'-C3'	-5.22	113.44	119.70
36	5	91	G	C8-N9-C4	5.22	108.49	106.40
36	5	1495	U	OP1-P-O3'	5.22	116.68	105.20
36	5	2859	U	N1-C2-N3	5.22	118.03	114.90
1	2	4	C	C2-N1-C1'	5.22	124.54	118.80
1	2	1611	A	C5-N7-C8	-5.22	101.29	103.90
36	1	2121	G	C5-C6-O6	5.22	131.73	128.60
36	1	2184	U	OP2-P-O3'	5.22	116.68	105.20
1	6	536	C	C6-N1-C2	-5.22	118.21	120.30
1	6	1735	U	N1-C2-O2	5.22	126.45	122.80
36	5	934	G	C8-N9-C1'	-5.22	120.22	127.00
36	5	1891	A	N1-C2-N3	5.22	131.91	129.30
39	l2	246	LEU	CA-CB-CG	5.22	127.30	115.30
36	1	22	G	N9-C4-C5	5.21	107.49	105.40
36	1	1920	U	N3-C2-O2	-5.21	118.55	122.20
36	1	2604	U	OP1-P-O3'	5.21	116.67	105.20
1	6	314	C	C2-N1-C1'	5.21	124.54	118.80
36	5	128	G	C5-C6-O6	-5.21	125.47	128.60
36	1	2298	U	C5-C4-O4	5.21	129.03	125.90
1	6	911	U	C6-N1-C2	-5.21	117.87	121.00
36	5	1064	A	P-O3'-C3'	5.21	125.96	119.70
36	1	43	A	N1-C6-N6	-5.21	115.47	118.60
36	1	338	A	OP2-P-O3'	5.21	116.66	105.20
36	1	1447	G	C5-C6-O6	5.21	131.73	128.60
36	1	1788	C	C5-C4-N4	-5.21	116.55	120.20
36	1	2235	C	N1-C2-O2	5.21	122.03	118.90
36	1	2727	A	N1-C6-N6	-5.21	115.47	118.60
36	1	2827	U	C5-C6-N1	-5.21	120.09	122.70
38	4	111	A	C4-C5-C6	5.21	119.61	117.00
36	5	2598	G	N1-C6-O6	5.21	123.03	119.90
36	5	2931	C	OP1-P-O3'	5.21	116.67	105.20
36	1	73	C	N1-C2-O2	-5.21	115.77	118.90
36	1	1595	U	C2-N1-C1'	-5.21	111.45	117.70
36	1	1741	A	C6-C5-N7	-5.21	128.65	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2253	G	C8-N9-C4	-5.21	104.32	106.40
36	1	101	G	N3-C2-N2	-5.21	116.25	119.90
36	1	1449	A	C5-C6-N1	5.21	120.31	117.70
36	1	3075	G	O5'-P-OP1	-5.21	101.01	105.70
36	1	3361	G	N3-C4-N9	5.21	129.13	126.00
53	M7	135	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	6	687	G	C4-N9-C1'	-5.21	119.73	126.50
36	5	907	G	N9-C4-C5	-5.21	103.32	105.40
36	5	1411	C	N1-C2-O2	-5.21	115.78	118.90
1	2	1734	U	C2-N1-C1'	-5.21	111.45	117.70
36	1	359	U	N3-C4-O4	5.21	123.04	119.40
36	1	587	U	N1-C2-N3	5.21	118.02	114.90
36	1	2270	A	OP1-P-OP2	5.21	127.41	119.60
36	5	87	U	C6-N1-C2	-5.21	117.88	121.00
36	5	96	G	C4-C5-N7	5.21	112.88	110.80
36	5	1510	G	N1-C2-N3	5.21	127.02	123.90
39	l2	179	LEU	CA-CB-CG	5.21	127.27	115.30
1	2	1768	G	C4-N9-C1'	-5.21	119.73	126.50
36	1	693	A	C8-N9-C4	-5.21	103.72	105.80
36	1	2935	U	C2-N3-C4	5.21	130.12	127.00
36	5	1178	G	C4-N9-C1'	5.21	133.27	126.50
1	2	359	A	C4-N9-C1'	-5.20	116.93	126.30
36	1	843	A	C6-C5-N7	-5.20	128.66	132.30
36	1	1190	A	C4-C5-C6	5.20	119.60	117.00
36	1	1646	G	O4'-C1'-N9	5.20	112.36	108.20
1	6	29	U	C4-C5-C6	5.20	122.82	119.70
1	6	1527	C	O5'-P-OP2	-5.20	101.02	105.70
36	5	2895	G	N3-C4-N9	5.20	129.12	126.00
36	5	923	C	C5-C4-N4	-5.20	116.56	120.20
36	1	290	G	N3-C4-N9	-5.20	122.88	126.00
1	6	1112	G	O5'-P-OP2	5.20	116.94	110.70
36	5	2204	C	C6-N1-C2	-5.20	118.22	120.30
36	5	2363	A	N1-C6-N6	5.20	121.72	118.60
36	5	3020	U	C5-C4-O4	-5.20	122.78	125.90
36	5	3129	A	C4-C5-C6	-5.20	114.40	117.00
1	2	90	C	N3-C4-C5	-5.20	119.82	121.90
36	1	673	U	N3-C4-O4	-5.20	115.76	119.40
36	1	981	U	C6-N1-C2	-5.20	117.88	121.00
36	1	1118	C	N1-C2-O2	-5.20	115.78	118.90
36	1	2156	C	C6-N1-C2	5.20	122.38	120.30
37	3	30	G	N3-C4-N9	5.20	129.12	126.00
36	5	530	G	C6-C5-N7	5.20	133.52	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1076	C	N3-C2-O2	-5.20	118.26	121.90
36	5	1370	G	N1-C6-O6	-5.20	116.78	119.90
36	5	2294	U	N1-C2-N3	5.20	118.02	114.90
36	5	2306	C	OP2-P-O3'	5.20	116.64	105.20
36	5	2367	A	N1-C6-N6	-5.20	115.48	118.60
36	5	2531	C	O4'-C1'-N1	5.20	112.36	108.20
1	6	297	U	C5-C6-N1	5.20	125.30	122.70
1	6	975	C	O5'-P-OP2	-5.20	101.02	105.70
36	5	2649	A	N7-C8-N9	5.20	116.40	113.80
36	1	424	G	O5'-P-OP2	-5.20	101.03	105.70
36	1	799	G	N1-C2-N2	-5.20	111.52	116.20
36	1	1407	A	N1-C6-N6	-5.20	115.48	118.60
36	1	1741	A	C5-N7-C8	-5.20	101.30	103.90
38	4	32	C	N3-C4-C5	5.20	123.98	121.90
38	4	89	A	C8-N9-C4	5.20	107.88	105.80
36	5	1667	A	N9-C4-C5	-5.20	103.72	105.80
36	5	1844	C	N1-C2-O2	-5.20	115.78	118.90
36	1	799	G	N1-C2-N3	5.19	127.02	123.90
36	1	50	U	C5-C4-O4	5.19	129.02	125.90
36	1	1069	C	C6-N1-C2	-5.19	118.22	120.30
36	1	2310	U	C5-C4-O4	5.19	129.02	125.90
38	4	109	A	N9-C4-C5	-5.19	103.72	105.80
36	5	406	G	N1-C6-O6	-5.19	116.78	119.90
36	5	1482	A	O5'-P-OP2	-5.19	101.03	105.70
37	7	78	U	C6-N1-C2	-5.19	117.88	121.00
39	l2	238	ILE	CG1-CB-CG2	-5.19	99.98	111.40
1	2	360	A	N1-C6-N6	5.19	121.71	118.60
36	1	589	A	C4-C5-N7	-5.19	108.11	110.70
36	1	920	A	C2-N3-C4	-5.19	108.00	110.60
36	1	1124	U	N1-C2-O2	5.19	126.43	122.80
36	1	2960	C	C6-N1-C2	5.19	122.38	120.30
1	6	1037	C	C6-N1-C2	5.19	122.38	120.30
1	6	1354	G	N7-C8-N9	5.19	115.69	113.10
36	5	98	G	N3-C4-N9	-5.19	122.89	126.00
36	5	1496	C	C6-N1-C1'	-5.19	114.57	120.80
36	5	2693	C	N3-C4-C5	5.19	123.98	121.90
36	5	2968	G	C4-C5-N7	-5.19	108.72	110.80
38	8	3	A	C5-C6-N1	5.19	120.30	117.70
36	5	885	U	N3-C4-O4	5.19	123.03	119.40
1	2	507	U	N3-C2-O2	-5.19	118.57	122.20
1	2	1241	G	C6-C5-N7	-5.19	127.29	130.40
36	1	601	U	N1-C2-O2	5.19	126.43	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1279	C	C5-C6-N1	5.19	123.59	121.00
36	1	2130	G	N1-C2-N3	5.19	127.01	123.90
36	1	2132	C	O5'-P-OP2	-5.19	101.03	105.70
38	4	13	A	C6-C5-N7	-5.19	128.67	132.30
1	6	416	A	C2-N3-C4	-5.19	108.01	110.60
36	5	214	G	C8-N9-C4	5.19	108.47	106.40
36	5	776	U	O4'-C1'-N1	5.19	112.35	108.20
36	5	984	G	C4-N9-C1'	5.19	133.24	126.50
36	5	1392	G	OP2-P-O3'	5.19	116.61	105.20
36	5	1790	G	N3-C4-C5	-5.19	126.01	128.60
36	5	3309	G	N1-C2-N2	-5.19	111.53	116.20
36	5	3309	G	N1-C6-O6	-5.19	116.79	119.90
36	1	1878	G	O4'-C1'-N9	-5.19	104.05	108.20
1	6	308	C	C5-C4-N4	5.19	123.83	120.20
1	6	353	A	N1-C6-N6	-5.19	115.49	118.60
1	6	1389	C	C2-N1-C1'	5.19	124.50	118.80
36	5	1098	A	N1-C6-N6	5.19	121.71	118.60
36	5	1160	C	C5-C6-N1	-5.19	118.41	121.00
36	5	1589	A	C2-N3-C4	5.19	113.19	110.60
1	2	1118	G	C5-C6-O6	-5.18	125.49	128.60
1	6	400	A	C5-C6-N6	-5.18	119.55	123.70
1	6	1058	U	OP1-P-O3'	5.18	116.60	105.20
1	6	1407	U	O5'-P-OP1	-5.18	101.03	105.70
36	5	342	A	C2-N3-C4	5.18	113.19	110.60
36	5	1475	A	N1-C2-N3	5.18	131.89	129.30
36	5	2167	A	C2-N3-C4	5.18	113.19	110.60
36	5	3027	A	N1-C2-N3	5.18	131.89	129.30
36	1	665	A	N1-C6-N6	-5.18	115.49	118.60
36	1	2124	G	C4-C5-N7	5.18	112.87	110.80
36	5	530	G	O4'-C1'-N9	5.18	112.34	108.20
36	5	690	A	C8-N9-C4	5.18	107.87	105.80
36	5	2134	G	C8-N9-C1'	-5.18	120.26	127.00
36	5	2617	U	O5'-P-OP2	-5.18	101.03	105.70
36	5	2887	A	O4'-C1'-N9	-5.18	104.05	108.20
1	2	334	G	N9-C4-C5	-5.18	103.33	105.40
36	5	888	A	C5-N7-C8	-5.18	101.31	103.90
36	5	2917	G	C4-N9-C1'	5.18	133.24	126.50
36	5	2941	A	OP1-P-O3'	5.18	116.60	105.20
36	1	857	G	C5-C6-N1	-5.18	108.91	111.50
36	1	1298	C	O5'-P-OP1	-5.18	101.04	105.70
36	1	2796	G	C8-N9-C4	-5.18	104.33	106.40
1	6	541	A	OP1-P-O3'	5.18	116.59	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	878	G	C6-C5-N7	-5.18	127.29	130.40
40	l3	334	ARG	NE-CZ-NH1	-5.18	117.71	120.30
36	5	2377	G	N1-C2-N2	-5.18	111.54	116.20
36	5	2388	U	N3-C4-O4	5.18	123.03	119.40
1	2	1636	C	C6-N1-C2	-5.18	118.23	120.30
36	1	884	A	N1-C6-N6	5.18	121.70	118.60
36	1	1525	G	C8-N9-C4	-5.18	104.33	106.40
36	1	2887	A	C4-C5-N7	5.18	113.29	110.70
36	1	2940	A	C6-N1-C2	-5.18	115.49	118.60
36	1	3368	U	C2-N1-C1'	-5.18	111.49	117.70
1	6	448	C	N3-C4-C5	-5.18	119.83	121.90
36	5	424	G	N1-C2-N3	-5.18	120.79	123.90
36	5	2627	C	C6-N1-C2	-5.18	118.23	120.30
36	5	2699	G	N3-C4-N9	5.18	129.11	126.00
36	5	3062	G	C2-N3-C4	5.18	114.49	111.90
36	5	3200	G	N1-C6-O6	5.18	123.00	119.90
38	8	140	G	N1-C6-O6	5.18	123.01	119.90
36	5	116	A	O4'-C1'-N9	5.17	112.34	108.20
36	5	1825	G	C5-C6-O6	5.17	131.71	128.60
36	5	3131	U	N1-C2-O2	5.17	126.42	122.80
1	2	606	A	N1-C6-N6	5.17	121.70	118.60
36	1	158	G	C6-C5-N7	-5.17	127.30	130.40
36	1	2618	G	C4-C5-N7	-5.17	108.73	110.80
36	5	40	A	N1-C6-N6	5.17	121.70	118.60
36	5	41	G	OP2-P-O3'	5.17	116.58	105.20
36	5	1187	C	N1-C2-O2	5.17	122.00	118.90
36	5	2287	C	N1-C2-O2	-5.17	115.80	118.90
36	5	2650	U	N1-C2-O2	-5.17	119.18	122.80
36	5	3180	A	C6-N1-C2	-5.17	115.50	118.60
36	1	176	G	C4-N9-C1'	5.17	133.22	126.50
36	1	368	G	N3-C2-N2	5.17	123.52	119.90
36	1	2660	G	N3-C4-N9	5.17	129.10	126.00
1	6	1123	C	O5'-P-OP1	-5.17	101.05	105.70
36	5	1471	U	N3-C4-O4	-5.17	115.78	119.40
36	5	2875	U	P-O3'-C3'	-5.17	113.50	119.70
1	2	1600	A	P-O3'-C3'	5.17	125.90	119.70
36	1	1226	G	N3-C4-C5	5.17	131.18	128.60
36	1	2571	U	N3-C2-O2	-5.17	118.58	122.20
36	1	2650	U	OP1-P-O3'	5.17	116.57	105.20
36	5	2821	C	C6-N1-C1'	5.17	127.00	120.80
36	5	2996	U	N3-C2-O2	-5.17	118.58	122.20
36	1	359	U	C6-N1-C2	-5.17	117.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	917	A	O5'-P-OP1	5.17	116.90	110.70
38	4	32	C	C6-N1-C1'	5.17	127.00	120.80
1	6	1639	C	N3-C4-C5	5.17	123.97	121.90
36	5	366	A	C2-N3-C4	-5.17	108.02	110.60
36	5	1513	G	N3-C4-N9	5.17	129.10	126.00
36	5	2700	G	C4-C5-N7	5.17	112.87	110.80
37	7	83	U	C2-N1-C1'	-5.17	111.50	117.70
36	1	1417	G	C8-N9-C4	5.17	108.47	106.40
1	6	1514	U	N3-C4-O4	-5.17	115.78	119.40
36	5	1542	G	N7-C8-N9	5.17	115.68	113.10
36	5	1695	U	N3-C2-O2	-5.17	118.58	122.20
36	5	2246	G	C2-N3-C4	5.17	114.48	111.90
36	1	35	A	C4-C5-N7	5.16	113.28	110.70
36	1	1179	A	OP2-P-O3'	5.16	116.56	105.20
36	1	2795	U	OP1-P-OP2	5.16	127.34	119.60
36	1	3271	G	N1-C6-O6	5.16	123.00	119.90
1	6	1484	G	N3-C4-C5	-5.16	126.02	128.60
36	5	3060	C	C5-C4-N4	-5.16	116.58	120.20
36	5	3099	C	C6-N1-C2	5.16	122.36	120.30
36	1	1351	U	N3-C2-O2	-5.16	118.59	122.20
36	1	2147	A	C5-C6-N1	5.16	120.28	117.70
57	n1	17	ARG	NE-CZ-NH2	-5.16	117.72	120.30
36	1	794	U	O5'-P-OP2	-5.16	101.06	105.70
36	1	2939	G	OP2-P-O3'	5.16	116.55	105.20
1	6	72	A	C8-N9-C4	-5.16	103.73	105.80
1	6	1000	C	N1-C2-N3	5.16	122.81	119.20
36	5	86	G	O4'-C1'-N9	5.16	112.33	108.20
36	5	2981	U	N3-C2-O2	-5.16	118.59	122.20
36	5	3373	U	N1-C2-N3	5.16	118.00	114.90
37	7	104	A	C5-C6-N1	-5.16	115.12	117.70
36	1	3134	A	N9-C4-C5	-5.16	103.74	105.80
36	1	3140	G	N3-C4-N9	5.16	129.09	126.00
1	6	606	A	N9-C4-C5	-5.16	103.74	105.80
1	6	1137	A	N9-C4-C5	-5.16	103.74	105.80
1	6	1361	U	N1-C2-O2	5.16	126.41	122.80
1	6	1550	A	C5-N7-C8	-5.16	101.32	103.90
36	5	20	A	N1-C6-N6	5.16	121.70	118.60
36	5	934	G	N3-C4-C5	-5.16	126.02	128.60
36	5	1192	C	C2-N1-C1'	5.16	124.47	118.80
37	7	75	G	C4-C5-C6	5.16	121.89	118.80
36	1	765	C	N1-C2-O2	5.16	121.99	118.90
36	1	2366	C	O5'-P-OP2	-5.16	101.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	3	1	G	C4-C5-N7	5.16	112.86	110.80
36	5	2407	C	C5-C4-N4	-5.16	116.59	120.20
36	1	1522	U	N3-C4-O4	5.16	123.01	119.40
36	5	973	A	C5-C6-N6	-5.16	119.58	123.70
36	5	1017	C	N1-C2-O2	5.16	121.99	118.90
36	5	2703	A	N9-C4-C5	5.16	107.86	105.80
36	5	2817	A	OP2-P-O3'	5.16	116.54	105.20
36	5	3088	G	N1-C6-O6	5.16	122.99	119.90
1	6	1458	G	C4-N9-C1'	5.15	133.20	126.50
36	5	1612	A	C5-C6-N6	5.15	127.82	123.70
36	5	1877	U	N3-C4-O4	5.15	123.01	119.40
36	5	2284	C	N3-C4-C5	5.15	123.96	121.90
36	5	2687	G	C5-C6-N1	5.15	114.08	111.50
1	2	1739	C	OP2-P-O3'	5.15	116.54	105.20
36	1	198	A	C8-N9-C4	-5.15	103.74	105.80
36	1	205	C	C2-N3-C4	-5.15	117.32	119.90
1	6	75	U	O4'-C1'-N1	5.15	112.32	108.20
1	6	937	C	N3-C4-C5	-5.15	119.84	121.90
1	6	1266	U	C5-C6-N1	5.15	125.28	122.70
36	5	838	G	N1-C2-N3	5.15	126.99	123.90
36	5	1368	U	N3-C2-O2	5.15	125.81	122.20
36	1	960	U	O4'-C1'-N1	5.15	112.32	108.20
36	1	1329	U	OP1-P-O3'	5.15	116.53	105.20
36	1	3034	C	N3-C2-O2	-5.15	118.30	121.90
1	6	410	A	C5-C6-N1	5.15	120.28	117.70
36	5	1284	C	C5-C6-N1	5.15	123.58	121.00
36	5	3057	U	C5-C4-O4	-5.15	122.81	125.90
37	7	63	A	C8-N9-C4	5.15	107.86	105.80
1	2	1121	C	C2-N3-C4	-5.15	117.33	119.90
36	1	3269	U	P-O3'-C3'	5.15	125.88	119.70
37	3	94	C	N3-C2-O2	5.15	125.50	121.90
1	6	1140	G	C2-N3-C4	5.15	114.47	111.90
36	5	2988	C	C5-C6-N1	-5.15	118.42	121.00
36	1	857	G	N1-C6-O6	5.15	122.99	119.90
36	1	2110	G	O5'-P-OP1	-5.15	101.07	105.70
36	1	2621	G	C4-C5-N7	-5.15	108.74	110.80
1	6	455	C	N3-C4-N4	5.15	121.60	118.00
36	5	883	A	O5'-P-OP2	5.15	116.88	110.70
36	5	892	U	C5-C4-O4	5.15	128.99	125.90
36	5	2350	C	N3-C2-O2	-5.15	118.30	121.90
1	2	1756	A	C5-C6-N6	-5.15	119.58	123.70
36	5	1303	A	C5-C6-N6	-5.15	119.58	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1793	C	O5'-P-OP1	-5.15	101.07	105.70
36	5	2739	A	C8-N9-C4	5.15	107.86	105.80
36	5	3115	C	N1-C2-N3	5.15	122.80	119.20
1	2	1536	G	C4-N9-C1'	5.14	133.19	126.50
1	2	1774	G	N3-C4-C5	-5.14	126.03	128.60
36	1	1844	C	C5-C6-N1	-5.14	118.43	121.00
36	1	2407	C	C2-N3-C4	-5.14	117.33	119.90
38	4	61	A	OP2-P-O3'	5.14	116.52	105.20
1	6	1552	U	N1-C2-O2	-5.14	119.20	122.80
36	5	915	A	N3-C4-C5	-5.14	123.20	126.80
36	5	933	A	N1-C2-N3	5.14	131.87	129.30
36	5	2295	A	N1-C6-N6	5.14	121.69	118.60
1	2	34	G	N1-C6-O6	-5.14	116.81	119.90
36	1	519	A	N1-C6-N6	5.14	121.69	118.60
38	4	102	U	C5-C6-N1	5.14	125.27	122.70
1	6	363	G	C8-N9-C4	5.14	108.46	106.40
1	6	416	A	N1-C6-N6	5.14	121.69	118.60
36	5	622	A	C8-N9-C4	5.14	107.86	105.80
36	5	630	A	C2-N3-C4	-5.14	108.03	110.60
36	5	833	G	N1-C2-N3	5.14	126.99	123.90
36	5	2628	A	C5-C6-N1	5.14	120.27	117.70
36	1	1157	G	C5-C6-O6	5.14	131.69	128.60
36	1	2977	G	C2-N3-C4	5.14	114.47	111.90
36	1	3326	G	N7-C8-N9	-5.14	110.53	113.10
1	2	1536	G	C8-N9-C1'	-5.14	120.32	127.00
36	1	1114	U	N1-C2-O2	5.14	126.40	122.80
36	1	2850	G	C6-C5-N7	-5.14	127.32	130.40
36	5	723	U	C6-N1-C2	-5.14	117.92	121.00
36	5	2617	U	C6-N1-C2	-5.14	117.92	121.00
38	8	32	C	N3-C2-O2	5.14	125.50	121.90
36	1	725	G	OP1-P-O3'	5.14	116.50	105.20
36	5	1178	G	C4-C5-C6	5.14	121.88	118.80
1	2	1168	U	OP1-P-O3'	5.14	116.50	105.20
1	2	1291	G	N1-C6-O6	5.14	122.98	119.90
1	2	1598	U	N1-C2-O2	-5.14	119.20	122.80
1	2	1731	A	C8-N9-C4	5.14	107.86	105.80
36	1	1000	C	C6-N1-C1'	-5.14	114.64	120.80
36	1	1361	U	C5-C4-O4	-5.14	122.82	125.90
36	1	2733	A	N1-C6-N6	5.14	121.68	118.60
38	4	13	A	C5-C6-N6	-5.14	119.59	123.70
36	5	1112	A	C4-N9-C1'	5.14	135.54	126.30
36	5	1147	G	N1-C2-N2	5.14	120.82	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1378	U	C5-C6-N1	-5.14	120.13	122.70
36	5	1779	C	C6-N1-C2	5.14	122.35	120.30
1	2	426	G	C8-N9-C1'	-5.13	120.32	127.00
1	2	610	G	C6-C5-N7	-5.13	127.32	130.40
36	1	95	A	OP1-P-O3'	5.13	116.50	105.20
36	1	1530	U	N1-C1'-C2'	-5.13	106.35	112.00
36	1	2142	A	C2-N3-C4	5.13	113.17	110.60
36	1	3318	G	C6-C5-N7	-5.13	127.32	130.40
1	6	1614	A	O4'-C1'-N9	5.13	112.31	108.20
36	5	359	U	OP2-P-O3'	5.13	116.50	105.20
36	5	1200	A	N1-C2-N3	5.13	131.87	129.30
36	5	3011	A	OP1-P-O3'	5.13	116.50	105.20
47	m0	88	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	2	312	A	N9-C4-C5	5.13	107.85	105.80
1	2	747	C	N1-C2-O2	5.13	121.98	118.90
36	1	70	A	N1-C2-N3	5.13	131.87	129.30
36	1	147	U	N1-C2-N3	5.13	117.98	114.90
1	6	1535	U	N1-C2-N3	5.13	117.98	114.90
36	5	1366	A	C5-C6-N6	5.13	127.81	123.70
38	8	68	G	C8-N9-C1'	-5.13	120.33	127.00
36	1	1381	A	O5'-P-OP1	-5.13	101.08	105.70
36	1	1449	A	C6-N1-C2	-5.13	115.52	118.60
36	1	1466	G	C8-N9-C1'	-5.13	120.33	127.00
36	1	3277	U	P-O3'-C3'	5.13	125.86	119.70
38	4	108	C	N3-C4-C5	-5.13	119.85	121.90
1	6	1573	A	P-O3'-C3'	5.13	125.86	119.70
1	6	1633	A	N1-C6-N6	-5.13	115.52	118.60
1	6	1782	A	C5-C6-N1	-5.13	115.14	117.70
36	5	273	A	C8-N9-C4	5.13	107.85	105.80
36	5	2281	A	OP1-P-O3'	5.13	116.49	105.20
36	1	358	G	C5-C6-N1	5.13	114.06	111.50
36	1	678	G	C5-C6-O6	-5.13	125.52	128.60
36	1	1001	G	N1-C6-O6	5.13	122.98	119.90
36	1	1169	A	C4-C5-C6	5.13	119.56	117.00
38	4	7	U	N1-C2-O2	-5.13	119.21	122.80
1	6	615	A	N1-C2-N3	5.13	131.87	129.30
36	5	3207	U	C6-N1-C1'	5.13	128.38	121.20
66	o0	41	LEU	CA-CB-CG	5.13	127.10	115.30
1	2	1768	G	C8-N9-C1'	5.13	133.67	127.00
36	1	2631	U	N3-C4-C5	5.13	117.68	114.60
1	6	423	G	N3-C2-N2	-5.13	116.31	119.90
1	6	904	G	C6-C5-N7	-5.13	127.32	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1077	U	N1-C2-O2	-5.13	119.21	122.80
36	1	2287	C	N1-C2-O2	-5.13	115.82	118.90
36	1	2400	G	N3-C4-C5	5.13	131.16	128.60
38	4	82	U	P-O3'-C3'	5.13	125.85	119.70
1	6	1767	G	N7-C8-N9	-5.13	110.54	113.10
36	5	75	G	N9-C4-C5	-5.13	103.35	105.40
36	5	2361	A	C5-C6-N1	5.13	120.26	117.70
36	5	2767	U	C5-C4-O4	5.13	128.98	125.90
51	m5	187	ARG	NE-CZ-NH1	-5.13	117.74	120.30
52	m6	141	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	2	549	G	C8-N9-C4	-5.12	104.35	106.40
36	1	94	G	C2-N3-C4	-5.12	109.34	111.90
36	1	1660	C	N3-C4-N4	5.12	121.59	118.00
1	6	568	G	N1-C6-O6	-5.12	116.83	119.90
36	5	1226	G	N1-C6-O6	5.12	122.97	119.90
36	5	2848	G	C6-C5-N7	-5.12	127.33	130.40
36	1	1821	U	C5-C4-O4	-5.12	122.83	125.90
36	1	1888	U	C5-C6-N1	-5.12	120.14	122.70
38	4	73	U	N3-C4-C5	5.12	117.67	114.60
1	6	362	G	N1-C2-N2	-5.12	111.59	116.20
1	6	1288	G	O5'-P-OP2	-5.12	101.09	105.70
36	5	951	A	C5-N7-C8	-5.12	101.34	103.90
36	5	1200	A	P-O3'-C3'	5.12	125.85	119.70
36	5	1316	C	N3-C4-C5	-5.12	119.85	121.90
36	5	1352	A	P-O3'-C3'	5.12	125.85	119.70
36	5	1855	U	N3-C2-O2	-5.12	118.61	122.20
36	5	2550	U	C5-C4-O4	5.12	128.97	125.90
36	5	2763	U	N3-C2-O2	5.12	125.79	122.20
36	5	3220	G	N1-C2-N3	5.12	126.97	123.90
36	1	707	U	C2-N1-C1'	-5.12	111.55	117.70
36	1	2987	A	C6-C5-N7	-5.12	128.71	132.30
36	5	672	A	C6-C5-N7	-5.12	128.72	132.30
36	5	1059	G	N3-C4-N9	5.12	129.07	126.00
36	5	1475	A	C2-N3-C4	-5.12	108.04	110.60
36	5	1914	G	O5'-P-OP2	5.12	116.85	110.70
36	5	2107	A	O5'-P-OP1	-5.12	101.09	105.70
1	2	1789	G	N3-C4-N9	5.12	129.07	126.00
36	1	2344	U	O5'-P-OP1	5.12	116.84	110.70
36	5	3006	A	C6-C5-N7	-5.12	128.72	132.30
1	2	1273	G	N1-C6-O6	-5.12	116.83	119.90
36	1	943	U	N1-C2-O2	-5.12	119.22	122.80
1	6	10	G	N9-C4-C5	5.12	107.45	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6	54	C	N3-C4-C5	5.12	123.95	121.90
1	6	103	A	C8-N9-C4	-5.12	103.75	105.80
1	6	402	C	C5-C4-N4	-5.12	116.62	120.20
36	5	533	A	O5'-P-OP1	-5.12	101.09	105.70
36	5	1294	A	C5-C6-N1	5.12	120.26	117.70
36	5	3140	G	C4-C5-N7	5.12	112.85	110.80
36	1	2419	A	N7-C8-N9	5.12	116.36	113.80
1	6	311	U	N3-C4-C5	-5.12	111.53	114.60
1	6	1651	A	O5'-P-OP2	-5.12	101.09	105.70
37	7	8	G	N3-C4-C5	-5.12	126.04	128.60
1	2	323	A	N7-C8-N9	5.12	116.36	113.80
36	1	1360	C	N1-C2-O2	-5.12	115.83	118.90
36	1	1447	G	C2-N3-C4	5.12	114.46	111.90
36	1	2921	U	N1-C2-N3	5.12	117.97	114.90
1	6	913	G	C5-C6-O6	-5.12	125.53	128.60
1	6	1465	C	N1-C2-O2	-5.12	115.83	118.90
36	5	1482	A	C6-N1-C2	-5.12	115.53	118.60
44	l7	229	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	2	1100	G	C8-N9-C4	-5.11	104.35	106.40
36	1	1515	A	C4-C5-C6	5.11	119.56	117.00
36	1	1904	C	O5'-P-OP1	5.11	116.84	110.70
36	1	2369	G	C5-C6-O6	-5.11	125.53	128.60
36	1	2726	C	C2-N3-C4	-5.11	117.34	119.90
36	1	2993	G	C5-C6-O6	-5.11	125.53	128.60
36	1	3028	G	C6-C5-N7	-5.11	127.33	130.40
1	6	959	U	C5-C4-O4	-5.11	122.83	125.90
1	6	1183	A	C8-N9-C4	-5.11	103.75	105.80
1	6	1746	A	N9-C4-C5	5.11	107.85	105.80
1	6	1765	A	O5'-P-OP1	-5.11	101.10	105.70
36	5	809	G	C4-C5-N7	5.11	112.85	110.80
36	1	2873	U	N1-C2-O2	5.11	126.38	122.80
36	5	2377	G	C5-C6-N1	5.11	114.06	111.50
36	1	1107	C	C5-C4-N4	-5.11	116.62	120.20
36	1	1307	G	N3-C4-N9	-5.11	122.93	126.00
36	1	1443	G	N7-C8-N9	5.11	115.66	113.10
1	6	314	C	N3-C4-N4	5.11	121.58	118.00
36	5	75	G	C4-C5-N7	5.11	112.84	110.80
36	5	884	A	C5-C6-N6	-5.11	119.61	123.70
52	m6	78	ARG	NE-CZ-NH2	-5.11	117.75	120.30
36	1	944	C	C6-N1-C2	-5.11	118.26	120.30
1	6	1457	C	O4'-C1'-N1	5.11	112.29	108.20
36	1	1189	C	N1-C2-O2	-5.11	115.83	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2856	G	C5-C6-O6	-5.11	125.54	128.60
36	1	3142	A	N1-C2-N3	5.11	131.85	129.30
1	6	904	G	N3-C4-N9	5.11	129.06	126.00
1	6	1127	G	N1-C2-N3	5.11	126.97	123.90
36	5	39	A	N1-C6-N6	5.11	121.66	118.60
36	5	821	U	C2-N3-C4	-5.11	123.94	127.00
36	5	1723	A	N9-C4-C5	5.11	107.84	105.80
36	5	1866	C	O4'-C1'-N1	-5.11	104.11	108.20
36	5	2882	U	N1-C2-N3	5.11	117.97	114.90
43	l6	173	MET	CB-CG-SD	-5.11	97.08	112.40
1	2	423	G	C4-C5-N7	-5.11	108.76	110.80
36	1	213	A	C5-N7-C8	-5.11	101.35	103.90
36	1	1187	C	N3-C4-N4	-5.11	114.43	118.00
36	1	1344	G	OP2-P-O3'	5.11	116.43	105.20
36	1	2246	G	N9-C4-C5	5.11	107.44	105.40
1	6	1399	C	N1-C2-O2	5.11	121.96	118.90
36	5	96	G	C5-N7-C8	-5.11	101.75	104.30
36	5	2147	A	N7-C8-N9	-5.11	111.25	113.80
36	1	2154	U	C6-N1-C2	-5.10	117.94	121.00
36	1	2367	A	C4-C5-C6	5.10	119.55	117.00
36	5	1890	U	C6-N1-C2	-5.10	117.94	121.00
36	1	395	A	N9-C4-C5	5.10	107.84	105.80
36	1	1399	A	O5'-P-OP2	-5.10	101.11	105.70
36	1	2836	C	C5-C4-N4	5.10	123.77	120.20
1	6	1327	C	OP2-P-O3'	5.10	116.42	105.20
36	5	41	G	C5-N7-C8	-5.10	101.75	104.30
36	5	1876	U	C2-N3-C4	-5.10	123.94	127.00
36	5	1888	U	C4-C5-C6	5.10	122.76	119.70
36	5	2158	A	C5-C6-N1	5.10	120.25	117.70
36	5	2365	C	C5-C6-N1	-5.10	118.45	121.00
36	5	2632	G	N3-C4-N9	5.10	129.06	126.00
36	5	3215	A	N1-C6-N6	5.10	121.66	118.60
36	5	3223	A	C5-C6-N1	5.10	120.25	117.70
36	5	3308	C	OP2-P-O3'	5.10	116.42	105.20
37	7	101	G	C8-N9-C1'	-5.10	120.37	127.00
76	q0	97	ARG	NE-CZ-NH1	-5.10	117.75	120.30
36	1	1434	G	N3-C4-N9	5.10	129.06	126.00
36	1	2313	A	C5-N7-C8	-5.10	101.35	103.90
36	1	2760	C	N3-C4-C5	-5.10	119.86	121.90
1	6	935	U	C6-N1-C2	-5.10	117.94	121.00
36	5	1900	A	C5-C6-N1	5.10	120.25	117.70
36	5	2420	C	N3-C2-O2	5.10	125.47	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	411	U	N3-C4-C5	-5.10	111.54	114.60
36	1	1129	A	N1-C6-N6	5.10	121.66	118.60
36	1	2146	C	N3-C4-N4	-5.10	114.43	118.00
36	5	392	G	C5-C6-O6	-5.10	125.54	128.60
36	5	1170	A	OP2-P-O3'	5.10	116.42	105.20
36	5	3137	C	C6-N1-C1'	5.10	126.92	120.80
1	2	1027	A	C6-C5-N7	-5.10	128.73	132.30
36	1	145	G	C4-C5-N7	5.10	112.84	110.80
36	1	793	C	C5-C4-N4	-5.10	116.63	120.20
36	1	994	G	N1-C6-O6	-5.10	116.84	119.90
36	1	1556	C	C4-C5-C6	5.10	119.95	117.40
36	1	2200	U	N1-C2-N3	5.10	117.96	114.90
1	6	630	A	N9-C4-C5	-5.10	103.76	105.80
1	6	1021	C	N3-C4-C5	-5.10	119.86	121.90
36	5	2970	C	C4-C5-C6	5.10	119.95	117.40
36	1	921	A	N9-C4-C5	5.10	107.84	105.80
36	1	2287	C	C4-C5-C6	5.10	119.95	117.40
1	6	681	U	N1-C2-O2	5.10	126.37	122.80
36	5	196	G	N3-C2-N2	5.10	123.47	119.90
1	2	307	G	C8-N9-C4	5.09	108.44	106.40
36	1	667	C	N3-C4-C5	5.09	123.94	121.90
36	1	1507	G	O5'-P-OP2	-5.09	101.11	105.70
36	1	1587	A	C6-N1-C2	5.09	121.66	118.60
36	1	2789	U	N1-C2-N3	5.09	117.96	114.90
36	1	3355	U	C2-N1-C1'	5.09	123.81	117.70
36	5	859	G	N3-C4-N9	5.09	129.06	126.00
36	5	1001	G	C5-C6-O6	-5.09	125.54	128.60
36	5	2110	G	C4-C5-N7	5.09	112.84	110.80
36	5	1057	A	C4-C5-N7	5.09	113.25	110.70
36	5	2151	C	C6-N1-C2	5.09	122.34	120.30
36	1	1545	A	N7-C8-N9	5.09	116.35	113.80
36	1	1760	A	C8-N9-C4	-5.09	103.76	105.80
36	1	2359	C	C2-N3-C4	-5.09	117.35	119.90
36	1	2395	G	OP2-P-O3'	5.09	116.40	105.20
1	6	616	G	C8-N9-C4	-5.09	104.36	106.40
1	6	951	A	C8-N9-C4	5.09	107.84	105.80
1	6	1773	C	N1-C2-O2	-5.09	115.84	118.90
36	5	576	C	N3-C4-N4	5.09	121.56	118.00
36	5	1592	G	C4-C5-C6	5.09	121.86	118.80
36	5	2352	A	C4-C5-C6	5.09	119.55	117.00
36	1	1380	G	C2-N3-C4	-5.09	109.36	111.90
36	1	1587	A	C4-C5-C6	-5.09	114.45	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2953	U	N1-C2-O2	-5.09	119.24	122.80
38	4	85	G	C5-C6-O6	-5.09	125.55	128.60
1	6	272	U	OP2-P-O3'	5.09	116.40	105.20
10	s8	8	ARG	NE-CZ-NH2	-5.09	117.75	120.30
36	5	1120	A	OP2-P-O3'	5.09	116.39	105.20
36	5	2416	U	N1-C2-N3	5.09	117.95	114.90
36	1	155	G	N1-C2-N2	-5.09	111.62	116.20
36	1	388	G	N9-C4-C5	5.09	107.44	105.40
36	1	1547	G	N3-C4-N9	5.09	129.05	126.00
36	5	1429	G	C5-N7-C8	-5.09	101.76	104.30
36	1	370	U	C6-N1-C2	-5.09	117.95	121.00
36	1	786	A	C5-N7-C8	5.09	106.44	103.90
36	1	788	C	O5'-P-OP1	-5.09	101.12	105.70
36	1	2409	G	C6-N1-C2	-5.09	122.05	125.10
36	1	3041	U	C6-N1-C2	-5.09	117.95	121.00
1	6	162	A	N1-C6-N6	-5.09	115.55	118.60
1	6	338	C	N3-C4-N4	5.09	121.56	118.00
1	6	459	G	C5-C6-N1	-5.09	108.96	111.50
36	5	2142	A	C6-N1-C2	-5.09	115.55	118.60
36	5	2913	C	N3-C2-O2	5.09	125.46	121.90
1	2	1291	G	C8-N9-C4	-5.08	104.37	106.40
36	5	996	A	OP2-P-O3'	5.08	116.39	105.20
36	5	1641	U	C6-N1-C2	5.08	124.05	121.00
1	2	1547	A	N1-C6-N6	-5.08	115.55	118.60
36	1	104	G	N9-C4-C5	-5.08	103.37	105.40
36	1	153	U	C4-C5-C6	5.08	122.75	119.70
36	1	635	G	C6-N1-C2	-5.08	122.05	125.10
36	1	718	G	C5-C6-O6	-5.08	125.55	128.60
36	1	982	C	C5-C6-N1	-5.08	118.46	121.00
36	1	2920	U	C2-N3-C4	-5.08	123.95	127.00
36	1	3252	G	C8-N9-C4	5.08	108.43	106.40
36	5	824	C	C4-C5-C6	5.08	119.94	117.40
36	5	1300	G	OP1-P-O3'	5.08	116.38	105.20
36	5	1892	G	C5-C6-N1	5.08	114.04	111.50
36	5	3125	U	O5'-P-OP1	-5.08	101.13	105.70
36	1	2627	C	N1-C2-O2	-5.08	115.85	118.90
36	1	2995	A	C2-N3-C4	-5.08	108.06	110.60
36	5	75	G	C6-C5-N7	-5.08	127.35	130.40
36	5	739	G	N1-C6-O6	-5.08	116.85	119.90
1	2	624	G	N1-C6-O6	-5.08	116.85	119.90
36	1	427	C	N3-C4-C5	-5.08	119.87	121.90
36	1	2817	A	C5-C6-N6	-5.08	119.64	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1112	A	N3-C4-N9	5.08	131.46	127.40
36	5	2361	A	C6-N1-C2	-5.08	115.55	118.60
36	1	2698	G	C5-C6-N1	5.08	114.04	111.50
36	1	2983	C	O4'-C1'-N1	5.08	112.26	108.20
1	6	1605	G	C8-N9-C4	-5.08	104.37	106.40
36	5	404	G	C4-N9-C1'	5.08	133.10	126.50
36	5	2704	A	OP1-P-OP2	5.08	127.22	119.60
36	5	3342	A	N1-C2-N3	5.08	131.84	129.30
1	2	610	G	N1-C6-O6	5.08	122.95	119.90
34	SR	161	LYS	N-CA-C	5.08	124.71	111.00
36	1	368	G	C4-C5-N7	5.08	112.83	110.80
36	1	1269	U	C2-N1-C1'	5.08	123.79	117.70
36	1	2924	U	N1-C2-O2	-5.08	119.25	122.80
36	5	1432	C	O5'-P-OP2	-5.08	101.13	105.70
36	5	1851	G	C4-C5-N7	5.08	112.83	110.80
37	7	51	A	C8-N9-C4	-5.08	103.77	105.80
36	1	404	G	C5-C6-N1	-5.08	108.96	111.50
36	1	1002	A	C4-C5-C6	-5.08	114.46	117.00
36	1	1198	C	N1-C2-N3	5.08	122.75	119.20
36	1	1834	U	N1-C2-N3	5.08	117.95	114.90
36	1	1888	U	N1-C2-N3	5.08	117.95	114.90
36	1	2180	G	O5'-P-OP1	-5.08	101.13	105.70
1	6	163	G	C5-C6-N1	-5.08	108.96	111.50
1	6	540	G	C2-N3-C4	5.08	114.44	111.90
36	5	2677	G	C5-C6-O6	-5.08	125.56	128.60
37	7	22	A	C4-N9-C1'	5.08	135.44	126.30
36	1	693	A	N7-C8-N9	5.07	116.34	113.80
36	1	1127	G	C5-C6-O6	-5.07	125.56	128.60
36	1	1396	C	N3-C2-O2	5.07	125.45	121.90
36	1	1493	G	C6-N1-C2	-5.07	122.06	125.10
36	1	1795	U	N3-C2-O2	-5.07	118.65	122.20
1	6	687	G	N9-C4-C5	5.07	107.43	105.40
36	5	210	U	C5-C6-N1	-5.07	120.16	122.70
36	5	957	C	N1-C2-O2	5.07	121.94	118.90
36	5	2117	A	C5-C6-N6	5.07	127.76	123.70
1	2	1235	C	C2-N1-C1'	-5.07	113.22	118.80
36	1	1551	C	N1-C2-O2	5.07	121.94	118.90
36	1	2968	G	O5'-P-OP1	-5.07	101.14	105.70
36	1	2993	G	C4-C5-N7	5.07	112.83	110.80
1	6	1596	C	C6-N1-C2	-5.07	118.27	120.30
1	6	1678	A	C6-C5-N7	-5.07	128.75	132.30
36	5	2345	A	C8-N9-C4	5.07	107.83	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	647	G	N9-C4-C5	5.07	107.43	105.40
36	1	91	G	C5-C6-O6	-5.07	125.56	128.60
36	1	337	G	N1-C2-N2	5.07	120.76	116.20
36	1	1585	C	C6-N1-C2	5.07	122.33	120.30
37	3	61	G	C6-C5-N7	-5.07	127.36	130.40
1	6	1002	G	C4-C5-N7	5.07	112.83	110.80
36	5	659	G	OP2-P-O3'	5.07	116.36	105.20
36	5	1116	G	N3-C4-C5	-5.07	126.06	128.60
36	5	1154	A	C8-N9-C4	-5.07	103.77	105.80
36	5	2914	G	C4-N9-C1'	5.07	133.09	126.50
36	5	2916	U	OP1-P-O3'	5.07	116.36	105.20
36	1	91	G	N3-C4-N9	5.07	129.04	126.00
36	1	2395	G	C5-C6-O6	-5.07	125.56	128.60
1	6	334	G	N1-C2-N2	-5.07	111.64	116.20
36	5	586	C	N3-C2-O2	5.07	125.45	121.90
1	2	901	G	C4-N9-C1'	5.07	133.09	126.50
36	1	1489	A	C4-C5-N7	5.07	113.23	110.70
36	1	2617	U	C6-N1-C1'	5.07	128.29	121.20
1	6	1672	G	N3-C4-C5	-5.07	126.07	128.60
28	d6	10	ARG	NE-CZ-NH1	-5.07	117.77	120.30
36	5	56	G	C6-C5-N7	5.07	133.44	130.40
36	5	957	C	C2-N1-C1'	5.07	124.37	118.80
36	5	985	U	C6-N1-C2	5.07	124.04	121.00
36	5	1047	A	C5-N7-C8	-5.07	101.37	103.90
36	5	2619	G	C5-N7-C8	-5.07	101.77	104.30
36	5	2787	G	OP1-P-OP2	5.07	127.20	119.60
36	5	2815	G	C5-N7-C8	5.07	106.83	104.30
36	5	2980	U	C2-N3-C4	-5.07	123.96	127.00
36	5	3006	A	N7-C8-N9	5.07	116.33	113.80
36	1	34	A	N7-C8-N9	5.07	116.33	113.80
36	1	80	G	N3-C4-N9	5.07	129.04	126.00
36	1	649	A	N1-C6-N6	-5.07	115.56	118.60
36	1	709	A	O5'-P-OP2	5.07	116.78	110.70
36	1	1892	G	C5-C6-O6	-5.07	125.56	128.60
61	N5	133	LEU	CA-CB-CG	5.07	126.95	115.30
1	6	813	U	C6-N1-C1'	-5.07	114.11	121.20
36	5	438	A	C8-N9-C4	5.07	107.83	105.80
49	m3	46	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	2	1767	G	O4'-C1'-N9	5.06	112.25	108.20
36	1	59	G	OP1-P-O3'	5.06	116.34	105.20
36	1	2334	U	O5'-P-OP2	-5.06	101.14	105.70
1	6	1746	A	C8-N9-C4	-5.06	103.77	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1157	G	C5-C6-O6	5.06	131.64	128.60
36	5	1604	G	C6-C5-N7	-5.06	127.36	130.40
36	5	2277	C	OP2-P-O3'	5.06	116.34	105.20
37	7	39	C	N3-C4-C5	5.06	123.93	121.90
1	2	572	C	O5'-P-OP1	-5.06	101.14	105.70
1	6	901	G	O4'-C1'-N9	5.06	112.25	108.20
1	6	1595	U	O4'-C1'-N1	5.06	112.25	108.20
1	6	1672	G	C4-C5-C6	5.06	121.84	118.80
36	5	645	A	N3-C4-C5	-5.06	123.26	126.80
36	5	921	A	C5-C6-N6	5.06	127.75	123.70
36	5	1603	A	C8-N9-C4	-5.06	103.78	105.80
36	5	2142	A	OP1-P-OP2	-5.06	112.00	119.60
36	5	2552	C	N3-C2-O2	-5.06	118.36	121.90
36	5	2763	U	N3-C4-C5	5.06	117.64	114.60
36	5	2950	G	OP1-P-O3'	5.06	116.34	105.20
36	5	3131	U	C4-C5-C6	-5.06	116.66	119.70
37	7	103	A	C4-C5-N7	5.06	113.23	110.70
38	8	43	A	N9-C4-C5	5.06	107.83	105.80
36	1	799	G	C2-N3-C4	-5.06	109.37	111.90
36	1	1130	A	N1-C6-N6	5.06	121.64	118.60
36	5	831	G	C5-C6-O6	-5.06	125.56	128.60
36	5	1157	G	OP2-P-O3'	5.06	116.33	105.20
36	5	2363	A	C4-C5-C6	5.06	119.53	117.00
1	2	1560	U	C6-N1-C2	-5.06	117.96	121.00
36	1	1904	C	C5-C6-N1	5.06	123.53	121.00
36	1	2378	C	C5-C4-N4	-5.06	116.66	120.20
36	1	2950	G	C5-C6-N1	5.06	114.03	111.50
1	6	1716	C	O4'-C1'-N1	5.06	112.25	108.20
36	5	363	G	OP1-P-O3'	5.06	116.33	105.20
36	5	672	A	C5-C6-N6	-5.06	119.65	123.70
36	5	1620	U	C2-N1-C1'	5.06	123.77	117.70
36	5	3278	C	N3-C4-N4	5.06	121.54	118.00
59	n3	89	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	2	453	U	C6-N1-C2	-5.06	117.97	121.00
36	1	326	U	N3-C4-O4	5.06	122.94	119.40
36	1	805	G	OP1-P-O3'	5.06	116.32	105.20
37	3	65	G	C8-N9-C4	5.06	108.42	106.40
36	5	1456	A	OP1-P-O3'	5.06	116.33	105.20
36	5	1496	C	O5'-P-OP2	-5.06	101.15	105.70
36	5	2798	C	OP1-P-O3'	5.06	116.33	105.20
36	5	2983	C	N1-C2-O2	-5.06	115.87	118.90
36	5	3182	G	C4-C5-N7	-5.06	108.78	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	7	75	G	O5'-P-OP1	5.06	116.77	110.70
36	1	1314	C	C2-N1-C1'	5.06	124.36	118.80
36	1	2192	C	C4-C5-C6	5.06	119.93	117.40
36	1	2407	C	N3-C4-N4	5.06	121.54	118.00
1	6	433	C	C2-N1-C1'	5.06	124.36	118.80
36	5	974	G	C6-N1-C2	-5.06	122.07	125.10
36	5	3309	G	N3-C4-N9	5.06	129.03	126.00
1	2	1796	C	C4-C5-C6	5.05	119.93	117.40
36	1	68	C	N3-C2-O2	-5.05	118.36	121.90
36	1	410	U	C5-C6-N1	5.05	125.23	122.70
36	1	1116	G	N9-C4-C5	5.05	107.42	105.40
36	1	1143	A	C2-N3-C4	-5.05	108.07	110.60
36	1	1166	G	N9-C4-C5	-5.05	103.38	105.40
36	1	1405	U	C2-N3-C4	-5.05	123.97	127.00
36	1	1414	G	C6-C5-N7	-5.05	127.37	130.40
36	1	2585	G	C8-N9-C4	-5.05	104.38	106.40
36	1	2817	A	OP2-P-O3'	5.05	116.32	105.20
36	1	2968	G	C4-C5-N7	5.05	112.82	110.80
38	4	16	G	C8-N9-C4	5.05	108.42	106.40
38	4	65	A	C5-N7-C8	-5.05	101.37	103.90
1	6	576	G	C5-C6-O6	-5.05	125.57	128.60
1	6	1354	G	C8-N9-C4	-5.05	104.38	106.40
1	6	1535	U	C2-N3-C4	-5.05	123.97	127.00
36	5	614	C	C2-N1-C1'	-5.05	113.24	118.80
36	5	822	G	N3-C4-C5	5.05	131.13	128.60
36	5	1513	G	C2-N3-C4	5.05	114.43	111.90
36	5	2801	A	N7-C8-N9	-5.05	111.27	113.80
38	8	47	C	C2-N3-C4	-5.05	117.37	119.90
40	l3	17	LEU	CA-CB-CG	5.05	126.92	115.30
36	1	225	C	C6-N1-C2	-5.05	118.28	120.30
36	1	1127	G	N1-C6-O6	5.05	122.93	119.90
1	6	273	G	C6-C5-N7	-5.05	127.37	130.40
36	5	586	C	N1-C2-O2	-5.05	115.87	118.90
36	5	2130	G	N9-C1'-C2'	-5.05	106.44	112.00
36	5	2231	C	O4'-C1'-N1	5.05	112.24	108.20
36	5	2639	G	C8-N9-C4	-5.05	104.38	106.40
36	5	2919	A	C5-C6-N1	-5.05	115.17	117.70
36	1	225	C	C2-N1-C1'	5.05	124.36	118.80
36	1	659	G	N3-C4-C5	-5.05	126.08	128.60
36	1	3006	A	N1-C2-N3	5.05	131.83	129.30
36	1	3340	G	C8-N9-C4	-5.05	104.38	106.40
41	L4	212	ASP	CB-CG-OD1	5.05	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	341	G	N3-C4-N9	-5.05	122.97	126.00
36	5	1083	G	OP1-P-OP2	5.05	127.18	119.60
36	5	2333	C	C5-C4-N4	-5.05	116.66	120.20
36	5	2777	G	OP1-P-O3'	5.05	116.31	105.20
36	1	573	C	C5-C6-N1	-5.05	118.47	121.00
36	1	2985	C	C6-N1-C2	-5.05	118.28	120.30
36	1	3050	U	N1-C2-O2	5.05	126.33	122.80
1	6	49	C	N3-C4-C5	5.05	123.92	121.90
1	6	813	U	N1-C2-O2	5.05	126.33	122.80
36	5	2888	U	C6-N1-C1'	-5.05	114.13	121.20
38	8	12	A	C4-C5-N7	5.05	113.22	110.70
38	8	68	G	C4-C5-C6	5.05	121.83	118.80
36	1	1420	C	OP2-P-O3'	5.05	116.31	105.20
38	4	30	C	O5'-P-OP1	-5.05	101.16	105.70
38	4	41	A	N1-C2-N3	5.05	131.82	129.30
1	2	831	U	C2-N1-C1'	5.05	123.75	117.70
1	6	87	C	C6-N1-C2	-5.05	118.28	120.30
1	6	826	U	C6-N1-C2	-5.05	117.97	121.00
36	5	750	G	N1-C6-O6	5.05	122.93	119.90
36	5	810	A	C5-C6-N1	5.05	120.22	117.70
36	5	964	G	OP2-P-O3'	5.05	116.30	105.20
36	5	1846	C	N3-C4-C5	5.05	123.92	121.90
36	5	2904	U	N1-C2-N3	5.05	117.93	114.90
36	5	3021	A	C2-N3-C4	5.05	113.12	110.60
36	5	3136	G	N1-C2-N3	5.05	126.93	123.90
1	6	426	G	C4-N9-C1'	5.04	133.06	126.50
36	1	693	A	C4-C5-C6	5.04	119.52	117.00
36	1	1151	U	C6-N1-C2	-5.04	117.97	121.00
36	1	2968	G	C5-N7-C8	-5.04	101.78	104.30
36	1	3095	U	O5'-P-OP1	-5.04	101.16	105.70
1	6	136	C	N1-C2-O2	5.04	121.93	118.90
1	6	1305	U	N1-C2-N3	5.04	117.93	114.90
36	5	195	U	N1-C2-N3	5.04	117.93	114.90
36	5	3372	A	N7-C8-N9	5.04	116.32	113.80
36	1	1307	G	C8-N9-C1'	5.04	133.55	127.00
36	1	1876	U	N3-C4-O4	5.04	122.93	119.40
36	1	2376	G	C5-C6-N1	5.04	114.02	111.50
36	5	418	A	N1-C6-N6	5.04	121.62	118.60
36	5	2140	U	C6-N1-C2	-5.04	117.97	121.00
36	1	675	C	C6-N1-C2	-5.04	118.28	120.30
36	5	2937	G	N1-C6-O6	5.04	122.92	119.90
1	2	401	A	OP2-P-O3'	5.04	116.29	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	336	A	N3-C4-N9	5.04	131.43	127.40
36	1	695	C	C2-N3-C4	-5.04	117.38	119.90
36	1	2953	U	N3-C4-C5	-5.04	111.58	114.60
36	1	3121	U	N1-C2-N3	5.04	117.92	114.90
36	5	58	G	N7-C8-N9	5.04	115.62	113.10
36	5	93	C	O5'-P-OP1	-5.04	101.17	105.70
36	5	951	A	N7-C8-N9	5.04	116.32	113.80
36	5	1054	A	C8-N9-C4	5.04	107.81	105.80
36	5	3209	A	C4-N9-C1'	5.04	135.37	126.30
37	7	12	U	N3-C4-C5	5.04	117.62	114.60
36	1	780	A	N9-C4-C5	5.04	107.81	105.80
36	1	1410	U	OP2-P-O3'	5.04	116.28	105.20
36	1	2332	A	C2-N3-C4	-5.04	108.08	110.60
36	1	2986	U	C6-N1-C2	-5.04	117.98	121.00
1	2	1768	G	C4-C5-N7	-5.04	108.78	110.80
36	1	90	C	C2-N1-C1'	5.04	124.34	118.80
36	1	285	A	C5-C6-N6	-5.04	119.67	123.70
36	1	1332	A	N7-C8-N9	5.04	116.32	113.80
36	1	1343	A	C5-N7-C8	-5.04	101.38	103.90
36	1	1405	U	N3-C2-O2	5.04	125.72	122.20
36	1	1836	C	N3-C2-O2	-5.04	118.38	121.90
36	1	2429	G	C5-C6-O6	5.04	131.62	128.60
36	1	2787	G	C8-N9-C4	-5.04	104.39	106.40
36	1	3079	U	C6-N1-C1'	5.04	128.25	121.20
36	1	3079	U	O5'-P-OP1	-5.04	101.17	105.70
73	O7	18	LEU	CB-CG-CD2	-5.04	102.44	111.00
1	6	1094	G	C2-N3-C4	5.04	114.42	111.90
36	5	1152	G	C4-N9-C1'	-5.04	119.95	126.50
36	5	1912	U	C6-N1-C2	5.04	124.02	121.00
36	1	1227	C	C5-C6-N1	5.03	123.52	121.00
36	1	1371	G	N1-C6-O6	-5.03	116.88	119.90
36	5	1117	G	OP2-P-O3'	5.03	116.27	105.20
36	5	1158	A	C6-C5-N7	-5.03	128.78	132.30
57	n1	17	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	2	551	G	N7-C8-N9	5.03	115.62	113.10
36	1	36	C	N3-C4-C5	-5.03	119.89	121.90
36	1	1156	C	N3-C4-N4	-5.03	114.48	118.00
36	1	1371	G	N3-C4-C5	-5.03	126.08	128.60
36	1	2257	C	O4'-C1'-N1	5.03	112.22	108.20
36	5	971	G	C5-N7-C8	5.03	106.82	104.30
36	5	1849	C	C5-C4-N4	-5.03	116.68	120.20
36	1	796	U	N1-C2-N3	5.03	117.92	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2147	A	O5'-P-OP1	-5.03	101.17	105.70
36	1	2242	A	O4'-C1'-N9	-5.03	104.18	108.20
38	4	113	U	C5-C4-O4	5.03	128.92	125.90
1	6	524	U	N1-C2-N3	5.03	117.92	114.90
1	6	1651	A	P-O3'-C3'	5.03	125.74	119.70
1	6	1697	G	N3-C4-N9	5.03	129.02	126.00
36	5	2140	U	N1-C2-O2	-5.03	119.28	122.80
1	2	1365	C	C6-N1-C2	-5.03	118.29	120.30
36	1	2194	G	C4-N9-C1'	5.03	133.04	126.50
36	1	3218	A	C5-C6-N6	5.03	127.72	123.70
1	6	1754	A	N9-C4-C5	5.03	107.81	105.80
36	1	633	C	C5-C6-N1	-5.03	118.49	121.00
36	1	1592	G	OP2-P-O3'	5.03	116.26	105.20
36	1	2372	A	OP1-P-O3'	5.03	116.26	105.20
36	1	2582	C	N1-C2-O2	5.03	121.92	118.90
36	5	55	G	OP2-P-O3'	5.03	116.26	105.20
36	5	635	G	C4-C5-N7	5.03	112.81	110.80
36	5	1858	A	O4'-C1'-N9	5.03	112.22	108.20
36	5	2143	A	N3-C4-C5	-5.03	123.28	126.80
36	5	2342	U	OP2-P-O3'	5.03	116.26	105.20
37	7	1	G	C8-N9-C1'	-5.03	120.46	127.00
37	7	22	A	C8-N9-C1'	-5.03	118.65	127.70
36	1	633	C	N1-C2-O2	-5.03	115.89	118.90
36	1	889	U	C2-N3-C4	-5.03	123.98	127.00
36	1	1742	U	N3-C4-O4	5.03	122.92	119.40
36	1	2151	C	C5-C6-N1	5.03	123.51	121.00
36	5	946	U	C4-C5-C6	5.03	122.72	119.70
36	5	1292	C	O5'-P-OP1	-5.03	101.18	105.70
36	5	1524	A	N7-C8-N9	-5.03	111.29	113.80
36	5	2134	G	N3-C4-C5	-5.03	126.09	128.60
36	5	2352	A	N1-C2-N3	5.03	131.81	129.30
36	5	2988	C	N1-C2-O2	-5.03	115.88	118.90
36	5	3380	U	C6-N1-C2	-5.03	117.98	121.00
36	1	1490	A	C5-N7-C8	-5.02	101.39	103.90
36	1	1934	G	N7-C8-N9	5.02	115.61	113.10
36	1	2828	G	C4-N9-C1'	5.02	133.03	126.50
1	6	1697	G	C4-N9-C1'	5.02	133.03	126.50
36	5	3294	A	N1-C6-N6	-5.02	115.58	118.60
1	2	1789	G	C4-N9-C1'	5.02	133.03	126.50
36	1	1101	G	N9-C4-C5	5.02	107.41	105.40
36	1	1349	G	N9-C4-C5	-5.02	103.39	105.40
36	1	1606	U	C2-N1-C1'	-5.02	111.67	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	1925	U	N3-C2-O2	5.02	125.72	122.20
36	1	2870	C	C2-N3-C4	-5.02	117.39	119.90
36	5	1108	U	N1-C2-N3	5.02	117.91	114.90
36	5	2889	C	N3-C4-C5	5.02	123.91	121.90
36	5	3110	C	C2-N3-C4	-5.02	117.39	119.90
37	7	77	G	N3-C4-N9	5.02	129.01	126.00
36	1	600	G	C4-N9-C1'	5.02	133.03	126.50
38	4	138	A	N1-C2-N3	5.02	131.81	129.30
36	5	986	U	N3-C2-O2	-5.02	118.69	122.20
36	5	987	U	N3-C2-O2	-5.02	118.69	122.20
36	5	3137	C	C5-C4-N4	5.02	123.72	120.20
38	8	2	A	N1-C6-N6	-5.02	115.59	118.60
36	1	1326	A	C8-N9-C4	5.02	107.81	105.80
36	1	1475	A	C5-C6-N1	5.02	120.21	117.70
1	6	913	G	N9-C4-C5	-5.02	103.39	105.40
36	5	1328	C	C4-C5-C6	5.02	119.91	117.40
36	5	3216	G	N3-C4-N9	5.02	129.01	126.00
1	2	1778	G	N9-C4-C5	5.02	107.41	105.40
36	1	2417	U	C5-C6-N1	-5.02	120.19	122.70
1	6	768	C	C6-N1-C2	5.02	122.31	120.30
36	5	86	G	O5'-P-OP1	5.02	116.72	110.70
36	5	703	G	O5'-P-OP1	-5.02	101.18	105.70
36	5	3244	A	OP1-P-OP2	5.02	127.13	119.60
37	7	7	G	C2-N3-C4	5.02	114.41	111.90
38	8	16	G	N1-C6-O6	5.02	122.91	119.90
36	1	413	U	C5-C6-N1	-5.02	120.19	122.70
36	1	671	U	OP2-P-O3'	5.02	116.24	105.20
36	1	1158	A	N9-C4-C5	-5.02	103.79	105.80
36	1	1472	U	C6-N1-C2	5.02	124.01	121.00
36	1	2906	C	N1-C2-N3	5.02	122.71	119.20
36	1	2917	G	C5-C6-N1	5.02	114.01	111.50
37	7	91	G	C5-C6-N1	5.02	114.01	111.50
36	1	647	A	N7-C8-N9	-5.01	111.29	113.80
56	N0	167	ARG	C-N-CD	5.01	138.93	128.40
1	6	96	G	N3-C4-C5	-5.01	126.09	128.60
36	5	1086	C	C2-N3-C4	5.01	122.41	119.90
36	5	3115	C	C2-N3-C4	-5.01	117.39	119.90
36	5	3366	G	C4-N9-C1'	5.01	133.02	126.50
36	5	637	C	O5'-P-OP2	-5.01	101.19	105.70
36	5	888	A	C4-C5-N7	5.01	113.21	110.70
36	5	2205	U	C2-N1-C1'	5.01	123.72	117.70
36	5	2892	A	C8-N9-C4	-5.01	103.80	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	2207	A	O4'-C1'-N9	5.01	112.21	108.20
36	5	1205	A	C5-C6-N6	-5.01	119.69	123.70
36	5	2664	C	N1-C2-O2	-5.01	115.89	118.90
36	5	3335	A	C4-C5-N7	5.01	113.21	110.70
36	1	2177	G	C5-C6-N1	5.01	114.00	111.50
36	1	2404	A	C5-C6-N1	5.01	120.20	117.70
36	1	2572	C	C6-N1-C2	-5.01	118.30	120.30
36	1	3101	G	C2-N3-C4	5.01	114.40	111.90
1	6	29	U	N1-C2-N3	5.01	117.91	114.90
1	6	978	A	N1-C6-N6	-5.01	115.59	118.60
1	6	1025	A	C8-N9-C4	5.01	107.80	105.80
1	6	1055	U	C6-N1-C2	-5.01	117.99	121.00
1	6	1629	G	OP2-P-O3'	5.01	116.22	105.20
36	5	359	U	N1-C2-O2	-5.01	119.29	122.80
36	5	912	G	N1-C6-O6	-5.01	116.89	119.90
36	5	1476	G	C2-N3-C4	-5.01	109.39	111.90
36	5	2981	U	C5-C4-O4	-5.01	122.89	125.90
36	1	2278	C	C5-C6-N1	5.01	123.50	121.00
36	1	3269	U	N3-C4-O4	-5.01	115.89	119.40
36	5	1416	C	N3-C4-C5	5.01	123.90	121.90
1	2	1212	G	N9-C4-C5	-5.01	103.40	105.40
36	1	687	U	C5-C4-O4	5.01	128.90	125.90
36	1	2327	U	C5-C6-N1	5.01	125.20	122.70
36	1	3028	G	N3-C4-N9	5.01	129.00	126.00
1	6	20	G	C5-C6-O6	-5.01	125.60	128.60
36	5	882	A	C6-N1-C2	-5.01	115.60	118.60
36	5	1192	C	C2-N3-C4	-5.01	117.40	119.90
36	5	1213	G	C5-C6-N1	5.01	114.00	111.50
36	5	1399	A	N9-C4-C5	-5.01	103.80	105.80
1	2	36	C	C6-N1-C2	5.00	122.30	120.30
36	1	999	G	N9-C4-C5	-5.00	103.40	105.40
36	1	2634	U	C5-C6-N1	-5.00	120.20	122.70
36	5	2189	U	N3-C4-O4	5.00	122.90	119.40
1	2	124	A	O5'-P-OP2	-5.00	101.20	105.70
1	2	549	G	N7-C8-N9	5.00	115.60	113.10
1	2	647	G	N3-C2-N2	-5.00	116.40	119.90
1	2	1773	C	C5-C6-N1	5.00	123.50	121.00
36	1	709	A	C5-N7-C8	5.00	106.40	103.90
36	1	902	G	N1-C6-O6	5.00	122.90	119.90
36	1	942	U	O5'-P-OP1	5.00	116.70	110.70
36	1	1325	U	C2-N1-C1'	-5.00	111.70	117.70
61	N5	38	LEU	CA-CB-CG	5.00	126.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	504	A	N1-C2-N3	-5.00	126.80	129.30
36	5	567	G	N3-C4-N9	5.00	129.00	126.00
36	5	1162	U	C5-C4-O4	5.00	128.90	125.90
36	5	2892	A	C4-C5-C6	5.00	119.50	117.00
36	1	75	G	C6-C5-N7	-5.00	127.40	130.40
36	1	1002	A	C8-N9-C4	5.00	107.80	105.80
36	1	2794	G	C6-N1-C2	-5.00	122.10	125.10
36	1	2865	U	OP2-P-O3'	5.00	116.20	105.20
1	6	564	G	C8-N9-C4	-5.00	104.40	106.40
1	6	1736	G	C5-C6-N1	-5.00	109.00	111.50
36	5	861	C	N3-C4-C5	-5.00	119.90	121.90
36	5	2316	G	OP2-P-O3'	5.00	116.20	105.20

There are no chirality outliers.

All (46) 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	84	VAL	Peptide
31	D9	9	SER	Peptide
39	L2	19	HIS	Peptide
43	L6	51	ARG	Peptide
52	M6	110	PRO	Peptide
56	N0	22	PRO	Peptide
65	N9	20	GLY	Peptide
67	O1	5	LYS	Peptide
9	S7	131	PHE	Peptide
10	S8	79	ALA	Peptide
10	S8	8	ARG	Peptide
34	SR	71	CYS	Peptide
16	c4	124	ASP	Peptide
17	c5	52	LYS	Peptide
18	c6	41	PRO	Peptide
19	c7	66	VAL	Peptide
19	c7	96	SER	Peptide
22	d0	70	THR	Peptide
25	d3	44	GLY	Peptide

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Mol	Chain	Res	Type	Group
26	d4	29	HIS	Peptide
27	d5	85	LYS	Peptide
39	l2	141	PRO	Peptide
39	l2	143	GLU	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
47	m0	168	SER	Peptide
81	m2	29	UNK	Peptide
51	m5	182	ASN	Peptide
52	m6	110	PRO	Peptide
64	n8	46	ASP	Peptide
64	n8	66	ALA	Peptide
65	n9	19	ASN	Peptide
67	o1	90	PHE	Peptide
68	o2	15	LYS	Peptide
68	o2	4	LEU	Peptide
73	o7	83	ALA	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide
9	s7	130	VAL	Peptide
9	s7	30	SER	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%)	148 (72%)	34 (17%)	22 (11%)	0 2
2	s0	204/251 (81%)	155 (76%)	31 (15%)	18 (9%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S1	212/254 (84%)	143 (68%)	36 (17%)	33 (16%)	0	1
3	s1	214/254 (84%)	168 (78%)	30 (14%)	16 (8%)	1	7
4	S2	215/253 (85%)	176 (82%)	24 (11%)	15 (7%)	1	8
4	s2	215/253 (85%)	178 (83%)	24 (11%)	13 (6%)	1	12
5	S3	221/239 (92%)	182 (82%)	31 (14%)	8 (4%)	3	23
5	s3	221/239 (92%)	172 (78%)	31 (14%)	18 (8%)	1	5
6	S4	258/260 (99%)	208 (81%)	27 (10%)	23 (9%)	1	4
6	s4	258/260 (99%)	200 (78%)	36 (14%)	22 (8%)	1	4
7	S5	204/224 (91%)	154 (76%)	29 (14%)	21 (10%)	0	3
7	s5	204/224 (91%)	158 (78%)	26 (13%)	20 (10%)	0	3
8	S6	224/236 (95%)	185 (83%)	22 (10%)	17 (8%)	1	7
8	s6	216/236 (92%)	187 (87%)	19 (9%)	10 (5%)	2	18
9	S7	182/189 (96%)	134 (74%)	23 (13%)	25 (14%)	0	1
9	s7	184/189 (97%)	145 (79%)	27 (15%)	12 (6%)	1	10
10	S8	184/200 (92%)	149 (81%)	24 (13%)	11 (6%)	1	12
10	s8	184/200 (92%)	159 (86%)	19 (10%)	6 (3%)	4	25
11	S9	183/196 (93%)	143 (78%)	29 (16%)	11 (6%)	1	12
11	s9	183/196 (93%)	148 (81%)	25 (14%)	10 (6%)	2	14
12	C0	94/105 (90%)	74 (79%)	10 (11%)	10 (11%)	0	2
12	c0	92/105 (88%)	63 (68%)	15 (16%)	14 (15%)	0	1
13	C1	153/155 (99%)	118 (77%)	20 (13%)	15 (10%)	0	3
13	c1	144/155 (93%)	117 (81%)	19 (13%)	8 (6%)	2	14
14	C2	122/142 (86%)	75 (62%)	26 (21%)	21 (17%)	0	0
14	c2	122/142 (86%)	69 (57%)	34 (28%)	19 (16%)	0	1
15	C3	148/150 (99%)	120 (81%)	20 (14%)	8 (5%)	2	14
15	c3	148/150 (99%)	120 (81%)	18 (12%)	10 (7%)	1	9
16	C4	125/136 (92%)	94 (75%)	21 (17%)	10 (8%)	1	6
16	c4	126/136 (93%)	92 (73%)	22 (18%)	12 (10%)	0	3
17	C5	122/141 (86%)	90 (74%)	18 (15%)	14 (12%)	0	2
17	c5	133/141 (94%)	86 (65%)	23 (17%)	24 (18%)	0	0
18	C6	139/142 (98%)	116 (84%)	13 (9%)	10 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	c6	140/142 (99%)	115 (82%)	18 (13%)	7 (5%)	2	16
19	C7	116/136 (85%)	86 (74%)	18 (16%)	12 (10%)	0	3
19	c7	113/136 (83%)	87 (77%)	12 (11%)	14 (12%)	0	2
20	C8	143/145 (99%)	110 (77%)	22 (15%)	11 (8%)	1	6
20	c8	143/145 (99%)	111 (78%)	22 (15%)	10 (7%)	1	8
21	C9	141/143 (99%)	113 (80%)	25 (18%)	3 (2%)	7	37
21	c9	141/143 (99%)	116 (82%)	18 (13%)	7 (5%)	2	16
22	D0	105/120 (88%)	83 (79%)	19 (18%)	3 (3%)	4	28
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	0	3
23	D1	85/87 (98%)	65 (76%)	14 (16%)	6 (7%)	1	8
23	d1	85/87 (98%)	74 (87%)	7 (8%)	4 (5%)	2	17
24	D2	127/129 (98%)	108 (85%)	12 (9%)	7 (6%)	2	14
24	d2	127/129 (98%)	114 (90%)	9 (7%)	4 (3%)	4	26
25	D3	142/144 (99%)	107 (75%)	22 (16%)	13 (9%)	1	3
25	d3	142/144 (99%)	116 (82%)	19 (13%)	7 (5%)	2	17
26	D4	132/134 (98%)	102 (77%)	23 (17%)	7 (5%)	2	15
26	d4	132/134 (98%)	101 (76%)	21 (16%)	10 (8%)	1	7
27	D5	68/107 (64%)	43 (63%)	14 (21%)	11 (16%)	0	0
27	d5	67/107 (63%)	50 (75%)	14 (21%)	3 (4%)	2	18
28	D6	95/97 (98%)	56 (59%)	19 (20%)	20 (21%)	0	0
28	d6	95/97 (98%)	73 (77%)	13 (14%)	9 (10%)	0	3
29	D7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	3	22
29	d7	79/81 (98%)	60 (76%)	15 (19%)	4 (5%)	2	15
30	D8	61/66 (92%)	50 (82%)	7 (12%)	4 (7%)	1	9
30	d8	61/66 (92%)	44 (72%)	10 (16%)	7 (12%)	0	2
31	D9	51/55 (93%)	43 (84%)	7 (14%)	1 (2%)	7	38
31	d9	51/55 (93%)	39 (76%)	8 (16%)	4 (8%)	1	6
32	E0	58/60 (97%)	49 (84%)	6 (10%)	3 (5%)	2	15
33	E1	69/76 (91%)	33 (48%)	15 (22%)	21 (30%)	0	0
33	e1	74/76 (97%)	33 (45%)	24 (32%)	17 (23%)	0	0
34	SR	316/318 (99%)	244 (77%)	52 (16%)	20 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	sR	316/318 (99%)	259 (82%)	43 (14%)	14 (4%)	2	19
35	SM	155/273 (57%)	114 (74%)	23 (15%)	18 (12%)	0	2
35	sM	98/273 (36%)	61 (62%)	21 (21%)	16 (16%)	0	0
39	L2	250/253 (99%)	218 (87%)	26 (10%)	6 (2%)	6	34
39	l2	250/253 (99%)	203 (81%)	36 (14%)	11 (4%)	2	19
40	L3	384/386 (100%)	336 (88%)	30 (8%)	18 (5%)	2	17
40	l3	384/386 (100%)	329 (86%)	42 (11%)	13 (3%)	3	24
41	L4	359/361 (99%)	303 (84%)	37 (10%)	19 (5%)	2	15
41	l4	359/361 (99%)	297 (83%)	43 (12%)	19 (5%)	2	15
42	L5	294/296 (99%)	244 (83%)	31 (10%)	19 (6%)	1	10
42	l5	292/296 (99%)	250 (86%)	30 (10%)	12 (4%)	3	21
43	L6	152/175 (87%)	129 (85%)	19 (12%)	4 (3%)	5	31
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	5	31
44	L7	220/243 (90%)	183 (83%)	28 (13%)	9 (4%)	3	21
44	l7	221/243 (91%)	191 (86%)	24 (11%)	6 (3%)	5	30
45	L8	231/255 (91%)	185 (80%)	37 (16%)	9 (4%)	3	22
45	l8	229/255 (90%)	175 (76%)	32 (14%)	22 (10%)	0	3
46	L9	189/191 (99%)	161 (85%)	24 (13%)	4 (2%)	7	37
46	l9	189/191 (99%)	165 (87%)	18 (10%)	6 (3%)	4	26
47	M0	207/220 (94%)	168 (81%)	33 (16%)	6 (3%)	4	28
47	m0	209/220 (95%)	175 (84%)	20 (10%)	14 (7%)	1	9
48	M1	167/173 (96%)	135 (81%)	18 (11%)	14 (8%)	1	5
48	m1	167/173 (96%)	132 (79%)	20 (12%)	15 (9%)	1	4
49	M3	191/198 (96%)	161 (84%)	21 (11%)	9 (5%)	2	17
49	m3	192/198 (97%)	154 (80%)	19 (10%)	19 (10%)	0	3
50	M4	134/137 (98%)	119 (89%)	8 (6%)	7 (5%)	2	15
50	m4	135/137 (98%)	118 (87%)	15 (11%)	2 (2%)	10	44
51	M5	201/203 (99%)	184 (92%)	11 (6%)	6 (3%)	4	28
51	m5	201/203 (99%)	181 (90%)	15 (8%)	5 (2%)	5	32
52	M6	195/198 (98%)	176 (90%)	16 (8%)	3 (2%)	10	44
52	m6	195/198 (98%)	175 (90%)	15 (8%)	5 (3%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	M7	181/183 (99%)	154 (85%)	22 (12%)	5 (3%)	5	29
53	m7	153/183 (84%)	131 (86%)	19 (12%)	3 (2%)	7	38
54	M8	183/185 (99%)	157 (86%)	19 (10%)	7 (4%)	3	22
54	m8	183/185 (99%)	148 (81%)	29 (16%)	6 (3%)	4	25
55	M9	186/188 (99%)	165 (89%)	17 (9%)	4 (2%)	6	35
55	m9	186/188 (99%)	162 (87%)	20 (11%)	4 (2%)	6	35
56	N0	170/172 (99%)	152 (89%)	15 (9%)	3 (2%)	8	41
56	n0	170/172 (99%)	154 (91%)	13 (8%)	3 (2%)	8	41
57	N1	157/159 (99%)	136 (87%)	13 (8%)	8 (5%)	2	15
57	n1	157/159 (99%)	139 (88%)	16 (10%)	2 (1%)	12	47
58	N2	98/120 (82%)	77 (79%)	15 (15%)	6 (6%)	1	12
58	n2	96/120 (80%)	75 (78%)	19 (20%)	2 (2%)	7	37
59	N3	134/136 (98%)	119 (89%)	15 (11%)	0	100	100
59	n3	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	10	44
60	N4	96/155 (62%)	72 (75%)	18 (19%)	6 (6%)	1	10
60	n4	133/155 (86%)	111 (84%)	15 (11%)	7 (5%)	2	15
61	N5	119/141 (84%)	106 (89%)	9 (8%)	4 (3%)	3	24
61	n5	118/141 (84%)	96 (81%)	15 (13%)	7 (6%)	1	12
62	N6	124/126 (98%)	110 (89%)	8 (6%)	6 (5%)	2	17
62	n6	124/126 (98%)	108 (87%)	11 (9%)	5 (4%)	3	21
63	N7	133/135 (98%)	112 (84%)	14 (10%)	7 (5%)	2	15
63	n7	133/135 (98%)	108 (81%)	20 (15%)	5 (4%)	3	22
64	N8	146/148 (99%)	124 (85%)	18 (12%)	4 (3%)	5	30
64	n8	146/148 (99%)	120 (82%)	16 (11%)	10 (7%)	1	9
65	N9	56/58 (97%)	44 (79%)	10 (18%)	2 (4%)	3	23
65	n9	56/58 (97%)	41 (73%)	10 (18%)	5 (9%)	1	4
66	O0	95/104 (91%)	83 (87%)	10 (10%)	2 (2%)	7	37
66	o0	98/104 (94%)	86 (88%)	9 (9%)	3 (3%)	4	26
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	2	17
67	o1	107/112 (96%)	91 (85%)	12 (11%)	4 (4%)	3	22
68	O2	125/129 (97%)	109 (87%)	13 (10%)	3 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	o2	125/129 (97%)	102 (82%)	18 (14%)	5 (4%)	3	21
69	O3	104/106 (98%)	93 (89%)	10 (10%)	1 (1%)	15	54
69	o3	104/106 (98%)	90 (86%)	11 (11%)	3 (3%)	4	28
70	O4	110/120 (92%)	92 (84%)	16 (14%)	2 (2%)	8	41
70	o4	110/120 (92%)	92 (84%)	12 (11%)	6 (6%)	2	14
71	O5	117/119 (98%)	103 (88%)	8 (7%)	6 (5%)	2	15
71	o5	117/119 (98%)	97 (83%)	13 (11%)	7 (6%)	1	12
72	O6	97/99 (98%)	76 (78%)	11 (11%)	10 (10%)	0	3
72	o6	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	7
73	O7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	6	34
73	o7	85/87 (98%)	69 (81%)	13 (15%)	3 (4%)	3	24
74	O8	75/77 (97%)	61 (81%)	9 (12%)	5 (7%)	1	9
74	o8	75/77 (97%)	59 (79%)	11 (15%)	5 (7%)	1	9
75	O9	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
75	o9	48/50 (96%)	41 (85%)	5 (10%)	2 (4%)	3	20
76	Q0	50/52 (96%)	43 (86%)	5 (10%)	2 (4%)	3	21
76	q0	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	7	38
77	Q1	23/25 (92%)	23 (100%)	0	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	20
78	Q2	103/105 (98%)	78 (76%)	16 (16%)	9 (9%)	1	4
78	q2	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	8	39
79	Q3	89/91 (98%)	75 (84%)	10 (11%)	4 (4%)	2	18
79	q3	89/91 (98%)	76 (85%)	12 (14%)	1 (1%)	14	51
80	e0	60/62 (97%)	48 (80%)	5 (8%)	7 (12%)	0	2
82	p0	139/311 (45%)	111 (80%)	23 (16%)	5 (4%)	3	23
All	All	22333/24143 (92%)	18179 (81%)	2816 (13%)	1338 (6%)	1	12

All (1338) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	66	ALA
2	S0	158	VAL
2	S0	191	ARG

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Mol	Chain	Res	Type
2	S0	194	PRO
3	S1	40	ASN
3	S1	49	ASN
3	S1	90	GLU
3	S1	132	ASP
3	S1	181	LEU
3	S1	182	ALA
3	S1	206	PRO
3	S1	213	ARG
3	S1	221	PRO
3	S1	223	PHE
4	S2	48	GLY
4	S2	148	LEU
5	S3	93	ASP
5	S3	137	VAL
5	S3	216	PRO
5	S3	220	PRO
6	S4	3	ARG
6	S4	12	LEU
6	S4	38	LEU
6	S4	39	ARG
6	S4	79	ASP
6	S4	96	ASN
6	S4	104	ASP
6	S4	142	HIS
6	S4	188	ASN
6	S4	227	VAL
6	S4	242	LYS
7	S5	26	ALA
7	S5	35	GLN
7	S5	36	ALA
7	S5	39	GLU
7	S5	43	PHE
7	S5	63	GLN
7	S5	81	ARG
7	S5	101	GLY
7	S5	154	ALA
8	S6	122	GLU
8	S6	173	PRO
8	S6	174	LYS
9	S7	31	SER
9	S7	32	PRO

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Mol	Chain	Res	Type
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	134	GLU
10	S8	120	THR
10	S8	149	SER
10	S8	153	GLU
11	S9	98	ALA
11	S9	134	ILE
11	S9	164	PHE
11	S9	169	PRO
12	C0	60	SER
12	C0	88	PRO
12	C0	94	GLU
13	C1	7	VAL
13	C1	29	LYS
13	C1	96	LYS
13	C1	139	VAL
13	C1	140	VAL
14	C2	101	ALA
16	C4	50	ALA
16	C4	124	ASP
16	C4	125	SER
16	C4	126	THR
17	C5	11	VAL
17	C5	125	PRO
17	C5	126	VAL
18	C6	39	VAL
18	C6	41	PRO
18	C6	58	ASP
18	C6	114	ARG
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
20	C8	14	ILE
20	C8	60	GLU
20	C8	91	ASP
20	C8	144	ARG
21	C9	31	PRO

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Mol	Chain	Res	Type
21	C9	53	TRP
23	D1	4	ASP
23	D1	82	VAL
24	D2	83	ILE
24	D2	127	GLY
25	D3	54	LEU
25	D3	138	GLU
25	D3	144	ARG
26	D4	6	THR
27	D5	37	GLN
28	D6	18	VAL
28	D6	45	VAL
28	D6	46	GLU
28	D6	47	ALA
28	D6	61	GLU
28	D6	65	PRO
28	D6	66	LYS
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
28	D6	88	SER
29	D7	38	PRO
29	D7	62	ILE
32	E0	47	VAL
33	E1	84	VAL
33	E1	98	VAL
33	E1	102	VAL
33	E1	103	LEU
34	SR	24	ALA
34	SR	155	ARG
34	SR	161	LYS
34	SR	188	ILE
34	SR	201	THR
34	SR	231	MET
35	SM	42	ALA
35	SM	102	THR
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
39	L2	144	ASN
39	L2	246	LEU
40	L3	3	HIS

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Mol	Chain	Res	Type
40	L3	5	LYS
40	L3	140	ASP
40	L3	347	SER
40	L3	386	ASP
41	L4	4	PRO
41	L4	131	VAL
41	L4	311	HIS
41	L4	338	LYS
42	L5	57	ASN
42	L5	178	ASN
42	L5	234	ASP
42	L5	258	LYS
43	L6	98	VAL
44	L7	24	GLU
45	L8	25	PRO
46	L9	2	LYS
47	M0	189	GLU
47	M0	207	GLU
47	M0	219	ALA
48	M1	8	PRO
48	M1	9	MET
48	M1	140	ARG
48	M1	145	LYS
48	M1	165	GLN
49	M3	13	HIS
49	M3	47	ALA
49	M3	129	ASN
49	M3	192	GLU
50	M4	9	ALA
50	M4	10	SER
51	M5	74	PRO
52	M6	110	PRO
52	M6	111	PRO
53	M7	157	VAL
54	M8	41	ASP
54	M8	98	LYS
54	M8	99	THR
56	N0	2	ALA
57	N1	122	GLN
57	N1	124	VAL
57	N1	126	VAL
58	N2	31	ALA

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Mol	Chain	Res	Type
58	N2	44	GLU
60	N4	76	VAL
60	N4	81	PRO
61	N5	44	PRO
62	N6	52	ARG
63	N7	3	LYS
63	N7	59	ALA
64	N8	76	ASP
67	O1	6	ASP
68	O2	127	ALA
71	O5	96	GLU
71	O5	119	LYS
72	O6	33	ALA
72	O6	34	SER
72	O6	52	PRO
72	O6	98	ARG
72	O6	99	ARG
74	O8	18	ALA
78	Q2	100	LYS
2	s0	29	VAL
2	s0	30	GLN
2	s0	111	ILE
2	s0	158	VAL
2	s0	164	ASN
2	s0	167	LYS
2	s0	186	GLY
2	s0	189	VAL
2	s0	206	ASP
3	s1	206	PRO
3	s1	232	HIS
4	s2	92	ALA
5	s3	61	GLU
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	12	LEU
6	s4	24	SER
6	s4	57	ASN
6	s4	90	ILE
6	s4	95	THR
6	s4	104	ASP

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Mol	Chain	Res	Type
6	s4	196	VAL
7	s5	28	PRO
7	s5	29	ILE
7	s5	36	ALA
7	s5	151	GLY
7	s5	184	PHE
7	s5	209	TYR
8	s6	70	PRO
8	s6	122	GLU
8	s6	153	VAL
8	s6	154	ARG
8	s6	173	PRO
9	s7	64	VAL
9	s7	74	GLN
9	s7	131	PHE
9	s7	163	ASP
9	s7	185	ILE
10	s8	62	THR
10	s8	137	LYS
11	s9	65	LYS
11	s9	162	SER
12	c0	73	VAL
12	c0	83	PRO
12	c0	88	PRO
12	c0	94	GLU
12	c0	97	PRO
13	c1	129	ARG
13	c1	144	ALA
14	c2	22	VAL
14	c2	130	THR
14	c2	131	ASP
15	c3	19	SER
15	c3	29	SER
15	c3	66	ILE
16	c4	35	GLY
16	c4	91	THR
16	c4	98	GLY
16	c4	126	THR
17	c5	11	VAL
17	c5	20	VAL
17	c5	50	THR
17	c5	51	SER

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Mol	Chain	Res	Type
17	c5	68	PRO
17	c5	125	PRO
17	c5	127	ARG
18	c6	42	GLU
18	c6	113	ASP
18	c6	115	THR
18	c6	116	LEU
19	c7	63	LYS
19	c7	98	GLY
19	c7	104	ASN
19	c7	105	GLN
20	c8	91	ASP
20	c8	92	ILE
21	c9	29	GLU
21	c9	33	TYR
22	d0	15	GLN
22	d0	49	ASN
22	d0	51	VAL
22	d0	52	LYS
22	d0	97	VAL
23	d1	4	ASP
24	d2	56	HIS
26	d4	30	PRO
26	d4	33	ALA
26	d4	35	VAL
27	d5	104	ALA
29	d7	3	LEU
29	d7	59	CYS
31	d9	6	VAL
31	d9	7	TRP
80	e0	45	VAL
80	e0	51	ASN
80	e0	60	PRO
33	e1	84	VAL
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	103	LEU
33	e1	106	TYR
33	e1	111	GLU
34	sR	4	ASN
34	sR	149	ASP

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Mol	Chain	Res	Type
34	sR	165	ASP
34	sR	297	ASP
34	sR	318	ALA
35	sM	172	VAL
39	l2	24	GLN
39	l2	56	ALA
39	l2	104	LEU
39	l2	238	ILE
39	l2	249	SER
40	l3	129	ALA
40	l3	140	ASP
40	l3	142	ALA
40	l3	188	ILE
41	l4	14	GLU
41	l4	15	ALA
41	l4	90	PHE
41	l4	132	ALA
41	l4	301	PRO
41	l4	329	PRO
41	l4	330	TYR
41	l4	342	LYS
42	l5	260	PHE
42	l5	269	SER
42	l5	270	LYS
43	l6	98	VAL
45	l8	25	PRO
45	l8	81	THR
45	l8	120	LYS
45	l8	122	LYS
45	l8	123	GLN
46	l9	144	ILE
46	l9	167	VAL
47	m0	25	ALA
47	m0	82	ARG
47	m0	170	LYS
47	m0	220	GLN
48	m1	8	PRO
48	m1	10	ARG
48	m1	108	GLU
48	m1	115	LYS
49	m3	47	ALA
49	m3	50	PRO

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Mol	Chain	Res	Type
49	m3	76	THR
49	m3	93	ILE
49	m3	134	GLU
49	m3	135	ALA
49	m3	152	THR
49	m3	193	ALA
50	m4	135	LEU
50	m4	136	ALA
51	m5	76	PRO
51	m5	81	TYR
51	m5	182	ASN
51	m5	183	THR
52	m6	16	VAL
52	m6	110	PRO
52	m6	111	PRO
54	m8	99	THR
55	m9	36	ASN
57	n1	122	GLN
58	n2	50	LEU
60	n4	63	ILE
60	n4	76	VAL
62	n6	83	ASP
62	n6	126	LEU
63	n7	56	LYS
64	n8	28	HIS
64	n8	76	ASP
65	n9	5	LYS
65	n9	21	ILE
65	n9	23	LYS
65	n9	39	PHE
67	o1	84	ASP
68	o2	5	PRO
70	o4	79	SER
71	o5	82	ALA
72	o6	98	ARG
74	o8	17	ARG
74	o8	18	ALA
74	o8	19	ASP
76	q0	78	ILE
82	p0	93	LEU
82	p0	102	SER
2	S0	5	ALA

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Mol	Chain	Res	Type
2	S0	30	GLN
2	S0	49	ASN
2	S0	94	GLY
2	S0	95	ALA
2	S0	111	ILE
2	S0	139	VAL
2	S0	162	CYS
2	S0	192	THR
3	S1	26	ARG
3	S1	51	SER
3	S1	58	SER
3	S1	63	GLY
3	S1	93	GLY
3	S1	105	PHE
3	S1	148	ASN
3	S1	179	SER
3	S1	224	ASP
4	S2	107	SER
4	S2	248	SER
5	S3	218	LEU
6	S4	26	CYS
6	S4	175	PHE
6	S4	195	ILE
6	S4	228	ILE
6	S4	245	LYS
7	S5	45	LYS
7	S5	127	GLN
8	S6	54	GLY
8	S6	111	LEU
8	S6	123	GLY
9	S7	5	GLN
9	S7	29	ASN
9	S7	30	SER
9	S7	35	LYS
9	S7	67	LEU
9	S7	73	VAL
9	S7	155	ASP
9	S7	156	SER
9	S7	159	VAL
9	S7	163	ASP
10	S8	22	ARG
10	S8	52	ASN

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Mol	Chain	Res	Type
11	S9	163	PRO
12	C0	81	ASN
13	C1	55	ASP
13	C1	95	PRO
14	C2	25	GLU
14	C2	91	VAL
14	C2	126	TRP
14	C2	127	GLY
14	C2	130	THR
15	C3	12	SER
15	C3	22	ALA
15	C3	24	ALA
15	C3	68	GLY
16	C4	40	ALA
16	C4	42	VAL
16	C4	132	ARG
17	C5	22	LEU
17	C5	51	SER
18	C6	59	LYS
19	C7	113	LEU
19	C7	115	LEU
19	C7	122	ILE
20	C8	7	GLU
22	D0	49	ASN
23	D1	43	GLY
24	D2	66	ASN
24	D2	78	ARG
25	D3	128	SER
25	D3	131	SER
27	D5	39	ALA
27	D5	43	ASP
27	D5	44	GLN
27	D5	55	PRO
27	D5	56	THR
27	D5	97	LYS
28	D6	3	LYS
28	D6	63	ALA
28	D6	86	VAL
31	D9	6	VAL
32	E0	51	ASN
33	E1	83	LYS
33	E1	93	HIS

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Mol	Chain	Res	Type
33	E1	99	LYS
33	E1	110	ALA
33	E1	111	GLU
33	E1	128	ALA
33	E1	138	ARG
34	SR	3	SER
34	SR	160	GLU
34	SR	194	GLY
34	SR	269	TYR
35	SM	52	PRO
35	SM	87	THR
35	SM	89	ARG
35	SM	139	GLU
35	SM	154	TYR
35	SM	165	LYS
39	L2	70	ARG
39	L2	127	ALA
40	L3	138	ALA
40	L3	142	ALA
40	L3	351	LEU
41	L4	72	ALA
41	L4	130	ALA
41	L4	190	GLY
41	L4	291	ASN
42	L5	58	LYS
42	L5	148	ILE
42	L5	215	ASP
42	L5	253	PHE
43	L6	108	LYS
44	L7	25	GLN
44	L7	32	ALA
44	L7	175	LYS
45	L8	36	ILE
45	L8	122	LYS
45	L8	135	GLY
45	L8	156	ASP
47	M0	117	GLY
47	M0	145	LYS
48	M1	115	LYS
48	M1	151	SER
49	M3	141	ALA
49	M3	163	GLY

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Mol	Chain	Res	Type
50	M4	8	LYS
50	M4	36	VAL
52	M6	16	VAL
53	M7	161	ALA
54	M8	24	VAL
55	M9	112	ALA
55	M9	133	LYS
57	N1	159	PHE
58	N2	51	GLY
60	N4	97	LYS
61	N5	45	LYS
62	N6	53	ASP
62	N6	84	LYS
62	N6	92	GLY
63	N7	125	GLY
64	N8	66	ALA
65	N9	53	ALA
66	O0	71	GLN
68	O2	27	ARG
70	O4	74	ARG
70	O4	77	GLY
71	O5	97	ALA
72	O6	3	VAL
72	O6	97	SER
73	O7	86	ALA
76	Q0	78	ILE
78	Q2	30	ALA
78	Q2	94	GLY
2	s0	44	GLY
2	s0	139	VAL
3	s1	39	GLU
3	s1	61	LEU
3	s1	147	ALA
3	s1	233	GLY
4	s2	91	ARG
4	s2	107	SER
4	s2	163	GLY
5	s3	161	GLY
5	s3	179	GLN
6	s4	164	LEU
6	s4	195	ILE
6	s4	245	LYS

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Mol	Chain	Res	Type
7	s5	40	ILE
7	s5	43	PHE
7	s5	56	ALA
7	s5	101	GLY
7	s5	102	ARG
7	s5	204	GLY
8	s6	68	LEU
9	s7	7	LYS
9	s7	67	LEU
10	s8	149	SER
11	s9	147	MET
11	s9	183	ALA
12	c0	32	HIS
12	c0	82	LEU
12	c0	92	ILE
13	c1	80	MET
13	c1	121	ASP
14	c2	45	LEU
14	c2	89	ILE
14	c2	90	LYS
14	c2	106	ILE
14	c2	119	SER
15	c3	60	VAL
15	c3	87	ASP
15	c3	139	TRP
16	c4	58	TYR
16	c4	97	GLY
16	c4	109	GLY
17	c5	9	LYS
17	c5	14	THR
17	c5	49	MET
17	c5	65	LEU
17	c5	133	ALA
18	c6	39	VAL
18	c6	97	VAL
19	c7	113	LEU
19	c7	120	SER
20	c8	29	VAL
20	c8	135	GLY
21	c9	34	VAL
22	d0	118	VAL
24	d2	68	ARG

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Mol	Chain	Res	Type
25	d3	66	SER
25	d3	131	SER
26	d4	53	ASP
27	d5	103	ARG
28	d6	35	ALA
28	d6	45	VAL
28	d6	46	GLU
30	d8	33	LEU
30	d8	57	MET
30	d8	61	ARG
31	d9	11	PRO
33	e1	83	LYS
33	e1	102	VAL
33	e1	127	GLY
34	sR	96	THR
34	sR	160	GLU
34	sR	237	GLN
35	sM	47	ALA
35	sM	50	ASN
35	sM	66	ALA
35	sM	121	LYS
39	l2	32	LEU
39	l2	80	GLU
39	l2	130	SER
39	l2	194	ASN
40	l3	3	HIS
40	l3	22	ALA
40	l3	155	ALA
40	l3	239	PRO
40	l3	289	ASP
40	l3	347	SER
41	l4	43	ASN
41	l4	190	GLY
41	l4	311	HIS
42	l5	258	LYS
42	l5	277	LEU
42	l5	279	LYS
43	l6	97	ASN
44	l7	130	ILE
45	l8	39	ALA
45	l8	82	LEU
45	l8	109	LEU

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Mol	Chain	Res	Type
45	l8	133	LYS
45	l8	202	GLU
45	l8	223	ALA
45	l8	239	GLY
46	l9	109	ALA
46	l9	110	LYS
47	m0	100	ASN
47	m0	204	GLY
48	m1	9	MET
48	m1	39	GLN
48	m1	94	ARG
48	m1	116	TYR
48	m1	153	LYS
49	m3	44	ALA
49	m3	51	LEU
49	m3	129	ASN
49	m3	141	ALA
49	m3	150	PRO
52	m6	13	GLY
53	m7	67	ILE
54	m8	74	GLU
54	m8	108	ALA
54	m8	109	GLY
54	m8	147	ARG
55	m9	156	ASN
59	n3	134	GLY
60	n4	77	LYS
61	n5	25	LYS
62	n6	84	LYS
63	n7	16	GLY
63	n7	134	LEU
64	n8	120	ASN
67	o1	45	GLY
67	o1	83	GLU
68	o2	27	ARG
68	o2	124	GLY
69	o3	33	GLU
71	o5	29	ALA
71	o5	39	PRO
71	o5	119	LYS
72	o6	12	ASN
72	o6	13	LYS

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Mol	Chain	Res	Type
73	o7	87	SER
82	p0	33	VAL
82	p0	47	GLY
82	p0	198	PRO
2	S0	4	PRO
2	S0	39	ASN
3	S1	35	PRO
3	S1	54	LEU
3	S1	78	ASP
3	S1	79	HIS
3	S1	147	ALA
3	S1	158	SER
3	S1	209	ASN
3	S1	226	GLY
4	S2	39	THR
4	S2	47	ALA
4	S2	106	ASP
4	S2	236	PRO
5	S3	44	THR
6	S4	32	SER
6	S4	164	LEU
6	S4	200	ARG
6	S4	258	GLN
7	S5	51	VAL
7	S5	153	GLY
7	S5	206	SER
8	S6	39	GLU
8	S6	146	GLY
8	S6	148	SER
8	S6	152	ASP
8	S6	154	ARG
9	S7	98	ILE
10	S8	105	ASP
10	S8	152	ILE
10	S8	154	SER
11	S9	89	ASP
11	S9	150	LEU
12	C0	86	ILE
12	C0	87	VAL
13	C1	4	GLU
13	C1	72	THR
13	C1	145	ALA

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Mol	Chain	Res	Type
13	C1	146	ALA
13	C1	154	ALA
14	C2	21	GLU
14	C2	22	VAL
14	C2	83	GLU
14	C2	92	ALA
14	C2	106	ILE
14	C2	107	ASP
14	C2	112	ALA
15	C3	31	GLU
17	C5	54	ALA
17	C5	80	MET
17	C5	101	ALA
18	C6	116	LEU
19	C7	123	ASN
20	C8	61	LEU
20	C8	83	ALA
20	C8	92	ILE
23	D1	7	GLN
25	D3	3	LYS
25	D3	40	SER
25	D3	41	SER
25	D3	53	VAL
25	D3	70	LYS
25	D3	112	LYS
26	D4	97	ALA
26	D4	133	ASN
27	D5	93	SER
28	D6	55	GLU
29	D7	57	GLU
30	D8	14	LYS
33	E1	90	LYS
33	E1	118	ARG
34	SR	70	ASP
34	SR	114	ASP
34	SR	153	GLN
34	SR	189	GLU
34	SR	318	ALA
35	SM	88	ARG
35	SM	155	LEU
35	SM	174	LEU
39	L2	250	GLN

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Mol	Chain	Res	Type
40	L3	155	ALA
40	L3	185	GLY
41	L4	15	ALA
41	L4	90	PHE
41	L4	232	SER
42	L5	7	ALA
42	L5	260	PHE
43	L6	7	PRO
44	L7	164	SER
45	L8	39	ALA
48	M1	114	ILE
48	M1	117	ASP
48	M1	167	TYR
48	M1	173	ASP
49	M3	136	GLU
49	M3	165	SER
50	M4	6	ILE
50	M4	29	ALA
51	M5	75	VAL
53	M7	156	ALA
53	M7	164	LYS
55	M9	111	ASP
56	N0	170	THR
57	N1	114	ALA
57	N1	120	LYS
57	N1	125	ALA
58	N2	11	ILE
60	N4	64	THR
60	N4	69	LYS
63	N7	33	SER
63	N7	102	GLU
63	N7	103	GLN
64	N8	47	LYS
67	O1	60	TRP
67	O1	82	GLU
67	O1	84	ASP
69	O3	59	VAL
71	O5	10	ARG
71	O5	27	GLU
73	O7	51	ALA
74	O8	33	LYS
78	Q2	15	LYS

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Mol	Chain	Res	Type
78	Q2	34	SER
78	Q2	103	ALA
79	Q3	84	ARG
2	s0	8	ASP
2	s0	92	HIS
2	s0	94	GLY
2	s0	95	ALA
3	s1	26	ARG
3	s1	106	THR
3	s1	160	HIS
3	s1	161	ILE
4	s2	106	ASP
4	s2	234	PRO
5	s3	160	SER
5	s3	180	GLY
6	s4	3	ARG
6	s4	11	ARG
6	s4	189	LEU
6	s4	213	SER
7	s5	35	GLN
8	s6	152	ASP
8	s6	156	PHE
9	s7	6	ALA
11	s9	121	SER
11	s9	161	THR
11	s9	167	ALA
12	c0	3	MET
14	c2	21	GLU
14	c2	58	LEU
14	c2	93	ASP
14	c2	103	LEU
14	c2	108	ARG
15	c3	43	LYS
15	c3	137	PRO
15	c3	140	LYS
16	c4	32	ASP
16	c4	125	SER
17	c5	7	ALA
17	c5	10	ARG
17	c5	66	ALA
17	c5	126	VAL
17	c5	136	SER

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Mol	Chain	Res	Type
19	c7	15	ALA
19	c7	99	VAL
19	c7	116	LYS
20	c8	61	LEU
21	c9	119	LYS
22	d0	17	GLN
22	d0	96	PRO
23	d1	43	GLY
25	d3	119	GLY
25	d3	134	ALA
26	d4	36	SER
26	d4	58	PHE
26	d4	78	SER
27	d5	85	LYS
28	d6	8	ASN
28	d6	13	LYS
28	d6	34	LYS
28	d6	47	ALA
29	d7	38	PRO
31	d9	16	LYS
33	e1	81	LYS
33	e1	85	TYR
33	e1	128	ALA
34	sR	161	LYS
34	sR	163	ASP
34	sR	186	PHE
34	sR	279	ALA
35	sM	39	PRO
35	sM	42	ALA
35	sM	63	ASP
39	l2	215	ASN
40	l3	139	GLN
41	l4	232	SER
41	l4	302	ALA
42	l5	265	TYR
42	l5	266	ALA
43	l6	10	TYR
44	l7	129	LEU
44	l7	158	LYS
44	l7	191	VAL
45	l8	203	VAL
45	l8	209	ALA

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Mol	Chain	Res	Type
45	l8	237	ILE
47	m0	143	SER
47	m0	176	LEU
47	m0	194	GLY
47	m0	207	GLU
48	m1	167	TYR
49	m3	60	ALA
49	m3	130	GLY
55	m9	47	ASN
55	m9	155	LEU
56	n0	2	ALA
58	n2	27	VAL
60	n4	64	THR
61	n5	24	LEU
61	n5	40	LEU
61	n5	44	PRO
61	n5	45	LYS
61	n5	47	ALA
63	n7	127	ASN
65	n9	24	PRO
67	o1	86	LYS
69	o3	88	ASN
71	o5	43	LYS
73	o7	86	ALA
78	q2	74	CYS
2	S0	33	GLN
2	S0	36	TYR
2	S0	44	GLY
2	S0	103	THR
2	S0	190	ASP
3	S1	55	LYS
3	S1	81	PHE
4	S2	91	ARG
4	S2	145	GLY
4	S2	150	GLN
4	S2	183	ALA
4	S2	247	ALA
5	S3	89	GLU
5	S3	217	ILE
6	S4	5	PRO
6	S4	17	HIS
7	S5	58	LEU

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Mol	Chain	Res	Type
8	S6	112	VAL
8	S6	138	ALA
8	S6	149	LYS
9	S7	132	PRO
9	S7	186	PRO
11	S9	120	LYS
12	C0	34	GLU
12	C0	93	GLN
14	C2	66	VAL
14	C2	87	PRO
14	C2	119	SER
14	C2	125	ASN
14	C2	131	ASP
15	C3	3	ARG
15	C3	23	PRO
16	C4	24	ASN
16	C4	79	VAL
17	C5	52	LYS
17	C5	69	GLU
18	C6	33	GLY
18	C6	113	ASP
18	C6	142	TYR
19	C7	23	LYS
20	C8	139	LYS
21	C9	29	GLU
23	D1	10	GLU
25	D3	11	SER
25	D3	37	ALA
26	D4	5	VAL
26	D4	58	PHE
28	D6	5	ARG
28	D6	64	LEU
30	D8	16	LEU
30	D8	61	ARG
33	E1	85	TYR
33	E1	86	THR
33	E1	94	LYS
33	E1	137	ASP
34	SR	112	SER
34	SR	242	SER
34	SR	244	ALA
35	SM	10	ASN

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Mol	Chain	Res	Type
35	SM	173	GLU
40	L3	139	GLN
40	L3	348	ARG
40	L3	378	ALA
41	L4	5	GLN
41	L4	140	HIS
41	L4	233	LEU
41	L4	270	SER
42	L5	137	ASP
42	L5	221	GLU
42	L5	259	LYS
44	L7	91	GLY
44	L7	159	GLN
45	L8	47	SER
45	L8	138	HIS
45	L8	157	VAL
46	L9	164	ILE
48	M1	94	ARG
48	M1	108	GLU
49	M3	76	THR
51	M5	181	ASN
54	M8	91	ALA
54	M8	162	ALA
55	M9	53	LYS
57	N1	133	ALA
60	N4	91	LYS
61	N5	25	LYS
61	N5	128	ALA
71	O5	75	TYR
72	O6	13	LYS
72	O6	21	THR
76	Q0	79	GLU
78	Q2	8	ARG
78	Q2	17	CYS
79	Q3	85	ARG
2	s0	103	THR
3	s1	93	GLY
4	s2	144	TRP
4	s2	150	GLN
4	s2	235	LEU
4	s2	238	SER
5	s3	43	PRO

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Mol	Chain	Res	Type
5	s3	45	LYS
5	s3	76	ARG
6	s4	31	PRO
6	s4	168	LYS
6	s4	171	ASP
6	s4	255	ARG
7	s5	21	THR
7	s5	45	LYS
7	s5	60	ASP
7	s5	98	MET
9	s7	106	SER
10	s8	52	ASN
11	s9	55	ALA
12	c0	25	LYS
12	c0	95	ARG
13	c1	7	VAL
13	c1	146	ALA
17	c5	6	ASN
17	c5	17	TYR
17	c5	52	LYS
17	c5	69	GLU
17	c5	80	MET
20	c8	60	GLU
23	d1	10	GLU
24	d2	24	GLN
26	d4	11	LYS
26	d4	52	LYS
28	d6	59	TYR
30	d8	6	PRO
30	d8	64	ARG
30	d8	65	ARG
80	e0	61	SER
33	e1	124	PRO
33	e1	137	ASP
34	sR	250	TYR
35	sM	65	THR
35	sM	67	GLY
41	l4	233	LEU
41	l4	258	LEU
41	l4	272	VAL
45	l8	240	ASN
46	l9	31	ARG

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Mol	Chain	Res	Type
47	m0	102	MET
47	m0	193	ASP
47	m0	219	ALA
48	m1	117	ASP
49	m3	13	HIS
49	m3	45	LYS
49	m3	140	SER
49	m3	162	ASN
51	m5	11	GLN
52	m6	4	GLU
60	n4	71	ARG
61	n5	87	SER
62	n6	75	ARG
63	n7	125	GLY
64	n8	17	ALA
64	n8	24	LYS
64	n8	47	LYS
64	n8	129	PHE
66	o0	46	ALA
68	o2	6	HIS
68	o2	12	LYS
70	o4	78	GLY
70	o4	82	ALA
71	o5	83	LYS
71	o5	84	LYS
72	o6	4	LYS
73	o7	85	LYS
74	o8	15	THR
75	o9	44	TRP
78	q2	17	CYS
2	S0	195	TRP
3	S1	38	PHE
3	S1	154	SER
4	S2	36	VAL
4	S2	182	PRO
7	S5	21	THR
7	S5	54	LYS
7	S5	64	VAL
7	S5	156	ARG
9	S7	36	ALA
10	S8	59	ARG
10	S8	81	VAL

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Mol	Chain	Res	Type
10	S8	82	VAL
12	C0	27	PHE
13	C1	30	ARG
13	C1	71	LEU
14	C2	37	VAL
14	C2	108	ARG
15	C3	29	SER
17	C5	68	PRO
17	C5	130	ARG
20	C8	8	GLN
22	D0	16	GLN
22	D0	17	GLN
23	D1	12	TYR
24	D2	57	ARG
28	D6	11	ASN
33	E1	100	LEU
34	SR	217	ASP
35	SM	12	VAL
35	SM	53	ARG
40	L3	317	ILE
41	L4	223	PRO
42	L5	188	GLU
42	L5	214	ASP
42	L5	233	ALA
42	L5	295	GLY
43	L6	6	ALA
44	L7	217	PRO
47	M0	208	ASN
48	M1	95	ASN
51	M5	81	TYR
51	M5	183	THR
53	M7	160	ALA
58	N2	52	ASN
63	N7	128	GLN
66	O0	20	SER
67	O1	7	VAL
79	Q3	7	LYS
79	Q3	45	LYS
3	s1	129	THR
3	s1	177	GLN
3	s1	234	GLU
5	s3	81	PRO

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Mol	Chain	Res	Type
5	s3	142	LEU
5	s3	163	PRO
5	s3	203	PRO
5	s3	219	ALA
6	s4	96	ASN
6	s4	119	ALA
6	s4	163	ASP
7	s5	152	GLY
8	s6	69	LEU
8	s6	150	GLU
9	s7	10	SER
9	s7	11	GLN
9	s7	133	THR
10	s8	142	LYS
11	s9	169	PRO
12	c0	30	ALA
12	c0	35	ILE
13	c1	55	ASP
14	c2	87	PRO
14	c2	118	ALA
16	c4	92	LYS
16	c4	100	ALA
17	c5	100	LYS
17	c5	128	HIS
18	c6	4	VAL
19	c7	68	GLY
19	c7	97	ASN
20	c8	9	GLY
20	c8	14	ILE
23	d1	6	GLY
24	d2	31	SER
25	d3	29	TYR
25	d3	101	GLU
25	d3	133	LEU
29	d7	12	ALA
30	d8	62	GLU
80	e0	50	VAL
35	sM	43	ASP
35	sM	52	PRO
35	sM	68	ARG
35	sM	84	LYS
41	l4	5	GLN

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Mol	Chain	Res	Type
41	l4	257	LYS
41	l4	328	ASN
42	l5	178	ASN
44	l7	178	ILE
45	l8	76	ALA
45	l8	79	GLN
45	l8	117	ALA
45	l8	121	SER
45	l8	124	ASP
45	l8	196	ALA
47	m0	101	LYS
48	m1	114	ILE
53	m7	25	SER
53	m7	134	GLY
54	m8	112	ALA
57	n1	121	ALA
64	n8	48	TYR
64	n8	56	VAL
70	o4	47	CYS
72	o6	97	SER
77	q1	22	ALA
79	q3	51	ALA
2	S0	188	LEU
3	S1	22	ASP
3	S1	210	ILE
6	S4	53	LYS
8	S6	117	GLY
9	S7	14	THR
11	S9	118	LEU
11	S9	147	MET
11	S9	162	SER
13	C1	113	PRO
17	C5	29	SER
17	C5	53	PRO
19	C7	72	LYS
19	C7	84	TYR
19	C7	124	VAL
20	C8	125	ILE
24	D2	100	GLY
26	D4	60	PHE
28	D6	36	ILE
30	D8	35	ASP

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Mol	Chain	Res	Type
32	E0	50	VAL
33	E1	107	LYS
33	E1	148	TYR
40	L3	37	ARG
40	L3	300	ARG
41	L4	14	GLU
41	L4	79	GLY
42	L5	115	LEU
44	L7	178	ILE
46	L9	108	GLY
50	M4	28	SER
51	M5	94	TYR
58	N2	70	LYS
62	N6	125	LYS
68	O2	125	ARG
74	O8	8	ILE
74	O8	35	GLY
2	s0	4	PRO
2	s0	10	THR
3	s1	22	ASP
3	s1	207	LEU
4	s2	164	SER
6	s4	30	ARG
7	s5	100	ASN
7	s5	154	ALA
10	s8	78	ILE
12	c0	23	ALA
14	c2	26	ASP
15	c3	22	ALA
16	c4	114	ARG
19	c7	102	VAL
20	c8	94	ASP
21	c9	3	GLY
21	c9	28	LEU
21	c9	118	PRO
22	d0	45	ALA
80	e0	54	ARG
33	e1	126	CYS
33	e1	148	TYR
34	sR	185	GLN
40	l3	362	ALA
43	l6	30	LEU

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Mol	Chain	Res	Type
46	l9	85	GLY
48	m1	7	ASN
48	m1	38	GLU
48	m1	152	HIS
56	n0	129	ILE
60	n4	83	THR
62	n6	65	GLY
69	o3	59	VAL
70	o4	77	GLY
72	o6	9	ILE
75	o9	24	PRO
7	S5	187	ILE
8	S6	69	LEU
27	D5	54	VAL
41	L4	146	PRO
54	M8	183	GLY
74	O8	37	PRO
4	s2	83	ILE
80	e0	47	VAL
35	sM	166	VAL
40	l3	185	GLY
60	n4	98	PRO
14	C2	115	VAL
18	C6	97	VAL
19	C7	38	ILE
39	L2	13	GLY
56	N0	153	PRO
65	N9	21	ILE
72	O6	94	ILE
11	s9	185	GLY
14	c2	40	GLY
14	c2	82	PRO
19	c7	88	VAL
20	c8	28	ILE
35	sM	51	ARG
42	l5	135	VAL
56	n0	51	VAL
64	n8	110	GLY
74	o8	35	GLY
7	S5	151	GLY
8	S6	165	GLY
12	C0	92	ILE

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Mol	Chain	Res	Type
16	C4	75	GLY
34	SR	113	VAL
40	L3	141	GLY
42	L5	125	VAL
78	Q2	101	GLY
22	d0	19	ILE
26	d4	29	HIS
28	d6	58	VAL
42	l5	286	VAL
44	l7	193	PRO
66	o0	96	GLY
72	o6	3	VAL
9	S7	63	PRO
24	D2	77	PRO
27	D5	41	ILE
27	D5	88	ILE
33	E1	87	THR
40	L3	166	ILE
46	L9	98	PRO
62	N6	45	ILE
5	s3	199	PRO
14	c2	115	VAL
19	c7	117	LEU
39	l2	103	PRO
42	l5	125	VAL
59	n3	16	GLY
66	o0	100	ILE
70	o4	100	ILE
26	D4	75	VAL
28	D6	59	TYR
64	N8	70	LYS
4	s2	93	GLY
13	c1	113	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%)	129 (79%)	35 (21%)	1	5
2	s0	165/209 (79%)	129 (78%)	36 (22%)	1	5
3	S1	191/223 (86%)	150 (78%)	41 (22%)	1	5
3	s1	192/223 (86%)	150 (78%)	42 (22%)	1	5
4	S2	176/204 (86%)	142 (81%)	34 (19%)	1	8
4	s2	176/204 (86%)	124 (70%)	52 (30%)	0	1
5	S3	182/194 (94%)	140 (77%)	42 (23%)	1	3
5	s3	182/194 (94%)	146 (80%)	36 (20%)	1	7
6	S4	221/221 (100%)	167 (76%)	54 (24%)	0	2
6	s4	221/221 (100%)	180 (81%)	41 (19%)	1	8
7	S5	173/190 (91%)	141 (82%)	32 (18%)	1	8
7	s5	173/190 (91%)	142 (82%)	31 (18%)	2	9
8	S6	188/201 (94%)	156 (83%)	32 (17%)	2	10
8	s6	187/201 (93%)	151 (81%)	36 (19%)	1	8
9	S7	165/169 (98%)	137 (83%)	28 (17%)	2	10
9	s7	165/169 (98%)	137 (83%)	28 (17%)	2	10
10	S8	150/161 (93%)	125 (83%)	25 (17%)	2	10
10	s8	150/161 (93%)	119 (79%)	31 (21%)	1	6
11	S9	158/165 (96%)	122 (77%)	36 (23%)	1	4
11	s9	158/165 (96%)	123 (78%)	35 (22%)	1	4
12	C0	77/98 (79%)	61 (79%)	16 (21%)	1	6
12	c0	73/98 (74%)	64 (88%)	9 (12%)	4	21
13	C1	129/136 (95%)	108 (84%)	21 (16%)	2	11
13	c1	129/136 (95%)	104 (81%)	25 (19%)	1	7
14	C2	88/118 (75%)	64 (73%)	24 (27%)	0	1
14	c2	88/118 (75%)	63 (72%)	25 (28%)	0	1
15	C3	127/127 (100%)	102 (80%)	25 (20%)	1	7
15	c3	127/127 (100%)	102 (80%)	25 (20%)	1	7
16	C4	81/104 (78%)	57 (70%)	24 (30%)	0	1
16	c4	97/104 (93%)	73 (75%)	24 (25%)	0	2
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1	6
17	c5	103/117 (88%)	84 (82%)	19 (18%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1	7
18	c6	118/118 (100%)	99 (84%)	19 (16%)	2	11
19	C7	94/124 (76%)	74 (79%)	20 (21%)	1	5
19	c7	92/124 (74%)	73 (79%)	19 (21%)	1	6
20	C8	128/128 (100%)	98 (77%)	30 (23%)	1	3
20	c8	128/128 (100%)	102 (80%)	26 (20%)	1	6
21	C9	115/115 (100%)	88 (76%)	27 (24%)	1	3
21	c9	115/115 (100%)	95 (83%)	20 (17%)	2	10
22	D0	100/113 (88%)	75 (75%)	25 (25%)	0	2
22	d0	103/113 (91%)	74 (72%)	29 (28%)	0	1
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	5
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	5
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	6
24	d2	110/110 (100%)	94 (86%)	16 (14%)	3	15
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2	9
25	d3	119/119 (100%)	100 (84%)	19 (16%)	2	11
26	D4	112/112 (100%)	90 (80%)	22 (20%)	1	7
26	d4	112/112 (100%)	94 (84%)	18 (16%)	2	11
27	D5	61/88 (69%)	46 (75%)	15 (25%)	0	2
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	11
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1	6
28	d6	83/83 (100%)	70 (84%)	13 (16%)	2	12
29	D7	70/70 (100%)	63 (90%)	7 (10%)	7	30
29	d7	70/70 (100%)	60 (86%)	10 (14%)	3	15
30	D8	56/59 (95%)	42 (75%)	14 (25%)	0	2
30	d8	56/59 (95%)	42 (75%)	14 (25%)	0	2
31	D9	47/48 (98%)	41 (87%)	6 (13%)	4	20
31	d9	47/48 (98%)	35 (74%)	12 (26%)	0	2
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1	7
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	1
33	e1	66/66 (100%)	46 (70%)	20 (30%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	SR	260/261 (100%)	219 (84%)	41 (16%)	2	12
34	sR	260/261 (100%)	229 (88%)	31 (12%)	5	22
35	SM	97/228 (42%)	77 (79%)	20 (21%)	1	6
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	1
39	L2	193/195 (99%)	154 (80%)	39 (20%)	1	6
39	l2	192/195 (98%)	161 (84%)	31 (16%)	2	11
40	L3	321/322 (100%)	245 (76%)	76 (24%)	1	3
40	l3	321/322 (100%)	257 (80%)	64 (20%)	1	6
41	L4	288/288 (100%)	231 (80%)	57 (20%)	1	7
41	l4	288/288 (100%)	232 (81%)	56 (19%)	1	7
42	L5	244/244 (100%)	199 (82%)	45 (18%)	1	8
42	l5	243/244 (100%)	192 (79%)	51 (21%)	1	6
43	L6	134/152 (88%)	116 (87%)	18 (13%)	4	18
43	l6	135/152 (89%)	113 (84%)	22 (16%)	2	11
44	L7	186/204 (91%)	156 (84%)	30 (16%)	2	11
44	l7	187/204 (92%)	159 (85%)	28 (15%)	3	14
45	L8	187/207 (90%)	150 (80%)	37 (20%)	1	7
45	l8	177/207 (86%)	141 (80%)	36 (20%)	1	6
46	L9	171/171 (100%)	138 (81%)	33 (19%)	1	8
46	l9	171/171 (100%)	131 (77%)	40 (23%)	1	3
47	M0	177/186 (95%)	142 (80%)	35 (20%)	1	7
47	m0	179/186 (96%)	138 (77%)	41 (23%)	1	4
48	M1	147/150 (98%)	112 (76%)	35 (24%)	0	3
48	m1	147/150 (98%)	114 (78%)	33 (22%)	1	4
49	M3	154/158 (98%)	129 (84%)	25 (16%)	2	11
49	m3	154/158 (98%)	128 (83%)	26 (17%)	2	10
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	9
50	m4	108/108 (100%)	81 (75%)	27 (25%)	0	2
51	M5	175/175 (100%)	146 (83%)	29 (17%)	2	10
51	m5	175/175 (100%)	144 (82%)	31 (18%)	2	9
52	M6	160/161 (99%)	134 (84%)	26 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	m6	160/161 (99%)	123 (77%)	37 (23%)	1 3
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1 4
53	m7	125/145 (86%)	101 (81%)	24 (19%)	1 8
54	M8	150/150 (100%)	126 (84%)	24 (16%)	2 11
54	m8	150/150 (100%)	115 (77%)	35 (23%)	1 3
55	M9	153/153 (100%)	123 (80%)	30 (20%)	1 7
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1 4
56	N0	156/156 (100%)	127 (81%)	29 (19%)	1 8
56	n0	156/156 (100%)	118 (76%)	38 (24%)	0 2
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1 3
57	n1	136/136 (100%)	110 (81%)	26 (19%)	1 8
58	N2	87/106 (82%)	69 (79%)	18 (21%)	1 6
58	n2	85/106 (80%)	67 (79%)	18 (21%)	1 5
59	N3	104/104 (100%)	81 (78%)	23 (22%)	1 4
59	n3	104/104 (100%)	87 (84%)	17 (16%)	2 11
60	N4	57/129 (44%)	49 (86%)	8 (14%)	3 16
60	n4	100/129 (78%)	86 (86%)	14 (14%)	3 16
61	N5	104/117 (89%)	79 (76%)	25 (24%)	0 3
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1 6
62	N6	109/109 (100%)	84 (77%)	25 (23%)	1 4
62	n6	109/109 (100%)	85 (78%)	24 (22%)	1 5
63	N7	115/115 (100%)	92 (80%)	23 (20%)	1 6
63	n7	115/115 (100%)	88 (76%)	27 (24%)	1 3
64	N8	118/118 (100%)	98 (83%)	20 (17%)	2 10
64	n8	118/118 (100%)	98 (83%)	20 (17%)	2 10
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1 5
65	n9	46/46 (100%)	34 (74%)	12 (26%)	0 2
66	O0	81/87 (93%)	64 (79%)	17 (21%)	1 6
66	o0	84/87 (97%)	65 (77%)	19 (23%)	1 4
67	O1	92/96 (96%)	65 (71%)	27 (29%)	0 1
67	o1	94/96 (98%)	70 (74%)	24 (26%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	O2	109/110 (99%)	90 (83%)	19 (17%)	2	10
68	o2	109/110 (99%)	81 (74%)	28 (26%)	0	2
69	O3	90/90 (100%)	76 (84%)	14 (16%)	2	12
69	o3	90/90 (100%)	76 (84%)	14 (16%)	2	12
70	O4	95/102 (93%)	80 (84%)	15 (16%)	2	12
70	o4	95/102 (93%)	76 (80%)	19 (20%)	1	6
71	O5	104/104 (100%)	82 (79%)	22 (21%)	1	5
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1	6
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1	6
72	o6	80/81 (99%)	53 (66%)	27 (34%)	0	0
73	O7	70/70 (100%)	53 (76%)	17 (24%)	0	2
73	o7	70/70 (100%)	54 (77%)	16 (23%)	1	4
74	O8	68/68 (100%)	51 (75%)	17 (25%)	0	2
74	o8	67/68 (98%)	57 (85%)	10 (15%)	3	14
75	O9	45/45 (100%)	34 (76%)	11 (24%)	0	2
75	o9	45/45 (100%)	38 (84%)	7 (16%)	2	12
76	Q0	47/47 (100%)	38 (81%)	9 (19%)	1	8
76	q0	47/47 (100%)	37 (79%)	10 (21%)	1	5
77	Q1	23/23 (100%)	12 (52%)	11 (48%)	0	0
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0	2
78	Q2	90/90 (100%)	71 (79%)	19 (21%)	1	6
78	q2	90/90 (100%)	71 (79%)	19 (21%)	1	6
79	Q3	71/71 (100%)	57 (80%)	14 (20%)	1	7
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1	4
80	e0	53/53 (100%)	40 (76%)	13 (24%)	0	2
82	p0	105/253 (42%)	89 (85%)	16 (15%)	3	13
All	All	18730/20241 (92%)	14956 (80%)	3774 (20%)	1	6

All (3774) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	6	THR
2	S0	7	PHE

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Mol	Chain	Res	Type
2	S0	28	ASN
2	S0	30	GLN
2	S0	32	HIS
2	S0	34	GLU
2	S0	37	VAL
2	S0	39	ASN
2	S0	43	ASP
2	S0	50	VAL
2	S0	72	ASP
2	S0	74	VAL
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	101	ARG
2	S0	103	THR
2	S0	110	TYR
2	S0	112	THR
2	S0	113	ARG
2	S0	123	VAL
2	S0	127	ARG
2	S0	131	GLN
2	S0	135	GLU
2	S0	154	GLU
2	S0	157	ASP
2	S0	165	ARG
2	S0	170	ILE
2	S0	172	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	189	VAL
2	S0	196	SER
2	S0	200	ASP
3	S1	21	VAL
3	S1	22	ASP
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	39	GLU
3	S1	43	VAL
3	S1	46	THR
3	S1	47	LEU

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Mol	Chain	Res	Type
3	S1	61	LEU
3	S1	65	VAL
3	S1	68	VAL
3	S1	70	LEU
3	S1	77	GLU
3	S1	81	PHE
3	S1	85	LYS
3	S1	89	ASP
3	S1	96	LEU
3	S1	97	LEU
3	S1	105	PHE
3	S1	107	THR
3	S1	108	ASP
3	S1	110	LEU
3	S1	115	ARG
3	S1	117	TRP
3	S1	135	LEU
3	S1	153	HIS
3	S1	154	SER
3	S1	180	THR
3	S1	181	LEU
3	S1	186	SER
3	S1	198	GLU
3	S1	202	LYS
3	S1	214	LYS
3	S1	215	VAL
3	S1	217	LEU
3	S1	218	LEU
3	S1	223	PHE
3	S1	229	MET
3	S1	231	LEU
3	S1	232	HIS
4	S2	41	LEU
4	S2	50	ILE
4	S2	58	LEU
4	S2	64	LYS
4	S2	69	ILE
4	S2	72	LEU
4	S2	73	LEU
4	S2	76	LEU
4	S2	87	GLN
4	S2	89	GLN

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Mol	Chain	Res	Type
4	S2	91	ARG
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	111	VAL
4	S2	113	LEU
4	S2	134	LEU
4	S2	137	ILE
4	S2	140	ARG
4	S2	141	ARG
4	S2	148	LEU
4	S2	153	SER
4	S2	166	THR
4	S2	170	ILE
4	S2	181	SER
4	S2	207	LEU
4	S2	221	THR
4	S2	222	TYR
4	S2	224	PHE
4	S2	226	THR
4	S2	235	LEU
4	S2	237	VAL
4	S2	246	GLU
4	S2	250	GLN
5	S3	6	SER
5	S3	7	LYS
5	S3	9	ARG
5	S3	21	LEU
5	S3	23	GLU
5	S3	37	VAL
5	S3	65	ARG
5	S3	66	ILE
5	S3	74	GLN
5	S3	76	ARG
5	S3	78	LYS
5	S3	84	ILE
5	S3	89	GLU
5	S3	92	GLN
5	S3	93	ASP
5	S3	94	ARG
5	S3	111	ASN
5	S3	113	LEU

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Mol	Chain	Res	Type
5	S3	117	ARG
5	S3	120	TYR
5	S3	124	ARG
5	S3	134	CYS
5	S3	136	VAL
5	S3	142	LEU
5	S3	143	ARG
5	S3	146	ARG
5	S3	151	LYS
5	S3	158	ILE
5	S3	168	ILE
5	S3	170	THR
5	S3	172	THR
5	S3	175	VAL
5	S3	176	LEU
5	S3	178	ARG
5	S3	181	VAL
5	S3	182	LEU
5	S3	188	ILE
5	S3	202	LEU
5	S3	207	THR
5	S3	212	LYS
5	S3	217	ILE
5	S3	218	LEU
6	S4	6	LYS
6	S4	9	LEU
6	S4	12	LEU
6	S4	21	ASP
6	S4	23	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	39	ARG
6	S4	45	ILE
6	S4	49	ARG
6	S4	52	LEU
6	S4	54	TYR
6	S4	56	LEU
6	S4	65	LEU
6	S4	68	ARG
6	S4	69	HIS
6	S4	76	VAL
6	S4	77	ARG

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Mol	Chain	Res	Type
6	S4	78	THR
6	S4	93	ASP
6	S4	95	THR
6	S4	108	ARG
6	S4	115	THR
6	S4	116	ASP
6	S4	117	GLU
6	S4	123	LEU
6	S4	126	VAL
6	S4	128	LYS
6	S4	131	LEU
6	S4	133	LYS
6	S4	141	THR
6	S4	155	LYS
6	S4	164	LEU
6	S4	170	THR
6	S4	180	LEU
6	S4	181	VAL
6	S4	182	TYR
6	S4	187	ARG
6	S4	191	ARG
6	S4	192	ILE
6	S4	206	ASP
6	S4	215	ASP
6	S4	220	THR
6	S4	221	ARG
6	S4	222	LEU
6	S4	226	PHE
6	S4	228	ILE
6	S4	236	ILE
6	S4	240	LYS
6	S4	246	LEU
6	S4	247	SER
6	S4	248	ILE
6	S4	258	GLN
6	S4	259	GLN
7	S5	25	LEU
7	S5	32	GLU
7	S5	38	THR
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS

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Mol	Chain	Res	Type
7	S5	48	PHE
7	S5	49	GLU
7	S5	53	VAL
7	S5	66	GLN
7	S5	76	ARG
7	S5	81	ARG
7	S5	84	LYS
7	S5	89	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	97	LEU
7	S5	99	MET
7	S5	119	ASP
7	S5	121	ILE
7	S5	147	THR
7	S5	156	ARG
7	S5	157	ARG
7	S5	162	VAL
7	S5	163	SER
7	S5	166	ARG
7	S5	184	PHE
7	S5	190	ILE
7	S5	194	LEU
7	S5	211	ILE
7	S5	224	ASN
7	S5	225	ARG
8	S6	3	LEU
8	S6	6	SER
8	S6	13	GLN
8	S6	14	LYS
8	S6	25	ARG
8	S6	43	ASP
8	S6	45	PHE
8	S6	51	LYS
8	S6	58	LYS
8	S6	67	VAL
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	82	SER
8	S6	98	ARG
8	S6	109	LEU

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Mol	Chain	Res	Type
8	S6	113	ILE
8	S6	120	GLU
8	S6	122	GLU
8	S6	127	THR
8	S6	128	THR
8	S6	132	ARG
8	S6	133	LEU
8	S6	154	ARG
8	S6	155	ASP
8	S6	162	VAL
8	S6	170	THR
8	S6	175	ILE
8	S6	201	GLN
8	S6	211	LEU
8	S6	212	LEU
8	S6	223	LYS
9	S7	7	LYS
9	S7	9	LEU
9	S7	14	THR
9	S7	24	PHE
9	S7	28	GLU
9	S7	42	GLN
9	S7	50	ASP
9	S7	51	VAL
9	S7	67	LEU
9	S7	74	GLN
9	S7	76	LYS
9	S7	77	LEU
9	S7	79	ARG
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG
9	S7	104	ARG
9	S7	106	SER
9	S7	114	ARG
9	S7	123	ASP
9	S7	126	LEU
9	S7	144	VAL
9	S7	147	ASN
9	S7	156	SER
9	S7	163	ASP
9	S7	167	GLU

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Mol	Chain	Res	Type
9	S7	176	LEU
9	S7	186	PRO
10	S8	7	SER
10	S8	8	ARG
10	S8	21	PHE
10	S8	22	ARG
10	S8	36	THR
10	S8	37	LYS
10	S8	46	VAL
10	S8	49	ARG
10	S8	56	ARG
10	S8	58	LEU
10	S8	60	ILE
10	S8	66	SER
10	S8	70	GLU
10	S8	74	LYS
10	S8	93	THR
10	S8	123	LYS
10	S8	135	LYS
10	S8	138	ASN
10	S8	151	LYS
10	S8	152	ILE
10	S8	155	SER
10	S8	158	SER
10	S8	161	SER
10	S8	184	LEU
10	S8	195	ARG
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR
11	S9	14	THR
11	S9	21	SER
11	S9	28	LEU
11	S9	30	LEU
11	S9	40	LYS
11	S9	46	SER
11	S9	49	LEU
11	S9	64	GLU
11	S9	78	ARG
11	S9	82	ARG
11	S9	92	LYS
11	S9	93	LEU

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Mol	Chain	Res	Type
11	S9	94	ASP
11	S9	95	TYR
11	S9	97	LEU
11	S9	99	LEU
11	S9	101	VAL
11	S9	106	GLU
11	S9	110	GLN
11	S9	115	LYS
11	S9	121	SER
11	S9	123	HIS
11	S9	134	ILE
11	S9	138	LYS
11	S9	140	ILE
11	S9	149	ARG
11	S9	161	THR
11	S9	162	SER
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	175	ARG
11	S9	182	GLU
12	C0	5	LYS
12	C0	6	GLU
12	C0	13	GLN
12	C0	27	PHE
12	C0	28	ASN
12	C0	40	LEU
12	C0	46	LEU
12	C0	49	LEU
12	C0	55	VAL
12	C0	56	LYS
12	C0	76	LEU
12	C0	78	GLU
12	C0	79	TYR
12	C0	80	LEU
12	C0	81	ASN
12	C0	82	LEU
13	C1	21	ASN
13	C1	25	VAL
13	C1	29	LYS
13	C1	30	ARG
13	C1	31	THR

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Mol	Chain	Res	Type
13	C1	40	LEU
13	C1	43	LYS
13	C1	44	THR
13	C1	63	LEU
13	C1	64	VAL
13	C1	67	ARG
13	C1	69	LYS
13	C1	74	THR
13	C1	80	MET
13	C1	91	LEU
13	C1	107	VAL
13	C1	127	GLN
13	C1	131	ILE
13	C1	138	ASN
13	C1	140	VAL
13	C1	141	LYS
14	C2	33	ARG
14	C2	37	VAL
14	C2	43	ARG
14	C2	45	LEU
14	C2	46	ARG
14	C2	49	THR
14	C2	50	LYS
14	C2	52	LEU
14	C2	54	ARG
14	C2	59	LEU
14	C2	62	LEU
14	C2	66	VAL
14	C2	71	ILE
14	C2	74	LEU
14	C2	86	VAL
14	C2	89	ILE
14	C2	90	LYS
14	C2	103	LEU
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	135	MET
14	C2	139	HIS
14	C2	140	PHE
15	C3	3	ARG
15	C3	6	SER

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Mol	Chain	Res	Type
15	C3	16	ILE
15	C3	27	LYS
15	C3	32	SER
15	C3	39	LYS
15	C3	43	LYS
15	C3	45	LEU
15	C3	61	THR
15	C3	64	ARG
15	C3	66	ILE
15	C3	72	MET
15	C3	76	LYS
15	C3	80	LEU
15	C3	83	GLU
15	C3	96	VAL
15	C3	102	LEU
15	C3	105	ASN
15	C3	114	ARG
15	C3	115	LEU
15	C3	125	LEU
15	C3	131	THR
15	C3	134	VAL
15	C3	145	THR
15	C3	147	SER
16	C4	16	VAL
16	C4	26	THR
16	C4	30	VAL
16	C4	31	THR
16	C4	38	THR
16	C4	39	ILE
16	C4	42	VAL
16	C4	46	MET
16	C4	48	VAL
16	C4	55	SER
16	C4	76	ILE
16	C4	84	ARG
16	C4	89	THR
16	C4	92	LYS
16	C4	93	THR
16	C4	103	ARG
16	C4	114	ARG
16	C4	118	VAL
16	C4	119	THR

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Mol	Chain	Res	Type
16	C4	123	SER
16	C4	125	SER
16	C4	126	THR
16	C4	132	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	14	THR
17	C5	22	LEU
17	C5	28	MET
17	C5	29	SER
17	C5	34	VAL
17	C5	36	LEU
17	C5	40	ARG
17	C5	44	ARG
17	C5	52	LYS
17	C5	80	MET
17	C5	89	MET
17	C5	92	SER
17	C5	98	ASN
17	C5	105	VAL
17	C5	106	GLU
17	C5	110	GLU
17	C5	116	LEU
17	C5	121	ILE
17	C5	124	THR
17	C5	125	PRO
18	C6	14	LYS
18	C6	19	VAL
18	C6	28	LEU
18	C6	43	ILE
18	C6	52	LEU
18	C6	53	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	59	LYS
18	C6	66	ARG
18	C6	69	VAL
18	C6	98	ASP
18	C6	104	GLU
18	C6	105	LEU
18	C6	106	LYS
18	C6	116	LEU

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Mol	Chain	Res	Type
18	C6	117	LEU
18	C6	118	ILE
18	C6	123	ARG
18	C6	128	LYS
18	C6	136	SER
18	C6	137	ARG
18	C6	143	ARG
19	C7	5	ARG
19	C7	6	THR
19	C7	25	THR
19	C7	36	ASP
19	C7	38	ILE
19	C7	40	THR
19	C7	46	LEU
19	C7	49	LYS
19	C7	54	THR
19	C7	69	ILE
19	C7	72	LYS
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	88	VAL
19	C7	104	ASN
19	C7	105	GLN
19	C7	108	ASP
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	6	GLN
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	18	LEU
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	34	THR
20	C8	60	GLU
20	C8	61	LEU
20	C8	71	GLN

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Mol	Chain	Res	Type
20	C8	72	ILE
20	C8	80	LYS
20	C8	92	ILE
20	C8	93	THR
20	C8	97	ASP
20	C8	101	LEU
20	C8	108	LYS
20	C8	114	GLU
20	C8	116	LEU
20	C8	120	ARG
20	C8	132	ARG
20	C8	136	GLN
20	C8	138	THR
20	C8	141	THR
20	C8	143	ARG
21	C9	4	VAL
21	C9	6	VAL
21	C9	13	ASP
21	C9	18	TYR
21	C9	22	LEU
21	C9	27	LYS
21	C9	28	LEU
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	39	THR
21	C9	57	ARG
21	C9	67	MET
21	C9	68	ARG
21	C9	70	GLN
21	C9	71	VAL
21	C9	94	ILE
21	C9	111	ILE
21	C9	122	ARG
21	C9	124	ILE
21	C9	126	GLU
21	C9	130	ARG
21	C9	131	ASP
21	C9	132	LEU
21	C9	139	THR
21	C9	144	GLU

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Mol	Chain	Res	Type
22	D0	15	GLN
22	D0	18	GLN
22	D0	19	ILE
22	D0	20	ILE
22	D0	23	ARG
22	D0	27	THR
22	D0	31	VAL
22	D0	34	LEU
22	D0	39	SER
22	D0	40	ASN
22	D0	41	ILE
22	D0	49	ASN
22	D0	51	VAL
22	D0	57	ARG
22	D0	58	LEU
22	D0	61	LYS
22	D0	68	ARG
22	D0	74	GLU
22	D0	76	SER
22	D0	81	THR
22	D0	89	ARG
22	D0	99	ILE
22	D0	103	ILE
22	D0	106	ILE
22	D0	121	ASN
23	D1	1	MET
23	D1	3	ASN
23	D1	7	GLN
23	D1	9	VAL
23	D1	11	LEU
23	D1	12	TYR
23	D1	18	SER
23	D1	27	ASP
23	D1	36	VAL
23	D1	41	GLU
23	D1	52	THR
23	D1	68	SER
23	D1	69	LEU
23	D1	78	LEU
23	D1	82	VAL
23	D1	87	ARG
24	D2	2	THR

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Mol	Chain	Res	Type
24	D2	7	LEU
24	D2	12	ASN
24	D2	22	LYS
24	D2	23	ARG
24	D2	24	GLN
24	D2	25	VAL
24	D2	26	LEU
24	D2	31	SER
24	D2	49	GLU
24	D2	53	ILE
24	D2	56	HIS
24	D2	65	LEU
24	D2	70	ASN
24	D2	76	SER
24	D2	97	ARG
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	121	VAL
24	D2	126	LEU
24	D2	129	VAL
25	D3	7	ARG
25	D3	9	LEU
25	D3	16	ARG
25	D3	19	ARG
25	D3	28	ASN
25	D3	31	LYS
25	D3	36	THR
25	D3	40	SER
25	D3	47	SER
25	D3	52	ILE
25	D3	63	GLN
25	D3	72	VAL
25	D3	75	GLN
25	D3	84	THR
25	D3	103	LEU
25	D3	107	PHE
25	D3	109	ARG
25	D3	114	LYS
25	D3	117	ILE
25	D3	120	VAL
25	D3	132	LEU

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Mol	Chain	Res	Type
26	D4	13	ILE
26	D4	21	LYS
26	D4	28	LEU
26	D4	29	HIS
26	D4	34	ASN
26	D4	36	SER
26	D4	40	LEU
26	D4	51	GLU
26	D4	52	LYS
26	D4	57	VAL
26	D4	61	ARG
26	D4	62	THR
26	D4	63	GLN
26	D4	70	VAL
26	D4	79	VAL
26	D4	96	LEU
26	D4	102	LYS
26	D4	124	ARG
26	D4	127	LYS
26	D4	131	ARG
26	D4	132	ARG
26	D4	133	ASN
27	D5	40	VAL
27	D5	42	LEU
27	D5	48	ASP
27	D5	58	ARG
27	D5	63	SER
27	D5	67	ASP
27	D5	71	ILE
27	D5	75	LEU
27	D5	83	LEU
27	D5	85	LYS
27	D5	90	LYS
27	D5	92	ILE
27	D5	95	HIS
27	D5	96	SER
27	D5	100	ILE
28	D6	10	ARG
28	D6	27	SER
28	D6	36	ILE
28	D6	37	LYS
28	D6	39	MET

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Mol	Chain	Res	Type
28	D6	41	ILE
28	D6	44	ILE
28	D6	57	SER
28	D6	61	GLU
28	D6	64	LEU
28	D6	68	TYR
28	D6	70	LYS
28	D6	76	SER
28	D6	82	ARG
28	D6	83	ILE
28	D6	84	VAL
28	D6	85	ARG
29	D7	3	LEU
29	D7	29	ARG
29	D7	33	LEU
29	D7	42	ASN
29	D7	60	SER
29	D7	64	CYS
29	D7	75	GLU
30	D8	13	ILE
30	D8	15	VAL
30	D8	19	THR
30	D8	32	PHE
30	D8	36	THR
30	D8	38	ARG
30	D8	39	THR
30	D8	41	VAL
30	D8	49	ARG
30	D8	51	ASN
30	D8	58	GLU
30	D8	61	ARG
30	D8	64	ARG
30	D8	65	ARG
31	D9	5	ASN
31	D9	12	ARG
31	D9	22	ARG
31	D9	28	THR
31	D9	32	ARG
31	D9	36	LEU
32	E0	3	LYS
32	E0	26	LYS
32	E0	31	LYS

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Mol	Chain	Res	Type
32	E0	42	ARG
32	E0	43	ARG
32	E0	47	VAL
32	E0	48	THR
32	E0	49	LEU
32	E0	50	VAL
32	E0	54	ARG
33	E1	89	LYS
33	E1	90	LYS
33	E1	91	ILE
33	E1	97	LYS
33	E1	108	VAL
33	E1	109	ASP
33	E1	111	GLU
33	E1	113	LYS
33	E1	115	THR
33	E1	118	ARG
33	E1	120	GLU
33	E1	130	VAL
33	E1	137	ASP
33	E1	145	HIS
33	E1	146	SER
33	E1	150	VAL
33	E1	151	ASN
34	SR	6	VAL
34	SR	7	LEU
34	SR	21	THR
34	SR	37	SER
34	SR	48	THR
34	SR	50	ASP
34	SR	52	GLN
34	SR	59	ARG
34	SR	60	SER
34	SR	70	ASP
34	SR	76	ASP
34	SR	96	THR
34	SR	116	ASP
34	SR	117	LYS
34	SR	133	VAL
34	SR	136	ILE
34	SR	137	LYS
34	SR	141	LEU

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Mol	Chain	Res	Type
34	SR	143	THR
34	SR	144	LEU
34	SR	149	ASP
34	SR	153	GLN
34	SR	159	ASN
34	SR	199	ILE
34	SR	200	ASN
34	SR	202	LEU
34	SR	207	ASP
34	SR	231	MET
34	SR	232	TYR
34	SR	238	ASP
34	SR	241	PHE
34	SR	258	THR
34	SR	266	ASP
34	SR	268	GLN
34	SR	269	TYR
34	SR	277	GLU
34	SR	300	THR
34	SR	312	VAL
34	SR	314	GLN
34	SR	317	THR
34	SR	319	ASN
35	SM	27	LYS
35	SM	30	THR
35	SM	34	LYS
35	SM	37	VAL
35	SM	41	SER
35	SM	43	ASP
35	SM	45	SER
35	SM	61	ILE
35	SM	64	LYS
35	SM	72	ARG
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	101	ASP
35	SM	115	LYS
35	SM	131	ILE

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Mol	Chain	Res	Type
35	SM	139	GLU
39	L2	18	SER
39	L2	28	LYS
39	L2	32	LEU
39	L2	36	GLU
39	L2	37	ARG
39	L2	44	ILE
39	L2	45	VAL
39	L2	47	GLN
39	L2	48	ILE
39	L2	62	VAL
39	L2	71	LEU
39	L2	73	GLU
39	L2	95	SER
39	L2	96	LEU
39	L2	97	ASN
39	L2	101	VAL
39	L2	104	LEU
39	L2	114	SER
39	L2	116	VAL
39	L2	137	ILE
39	L2	139	HIS
39	L2	143	GLU
39	L2	149	ARG
39	L2	157	VAL
39	L2	163	ARG
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	191	LEU
39	L2	193	ARG
39	L2	202	VAL
39	L2	207	VAL
39	L2	227	ARG
39	L2	230	VAL
39	L2	241	ARG
39	L2	252	THR
40	L3	3	HIS
40	L3	7	GLU

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Mol	Chain	Res	Type
40	L3	10	ARG
40	L3	17	LEU
40	L3	19	ARG
40	L3	21	ARG
40	L3	24	SER
40	L3	25	ILE
40	L3	30	LYS
40	L3	37	ARG
40	L3	47	LEU
40	L3	56	ILE
40	L3	66	LYS
40	L3	70	ARG
40	L3	73	VAL
40	L3	79	VAL
40	L3	81	THR
40	L3	84	VAL
40	L3	85	VAL
40	L3	87	VAL
40	L3	100	ARG
40	L3	102	LEU
40	L3	103	THR
40	L3	114	VAL
40	L3	116	ARG
40	L3	126	LYS
40	L3	128	LYS
40	L3	134	SER
40	L3	139	GLN
40	L3	146	ARG
40	L3	148	LEU
40	L3	153	LYS
40	L3	157	VAL
40	L3	160	VAL
40	L3	165	GLN
40	L3	166	ILE
40	L3	167	ARG
40	L3	169	THR
40	L3	187	SER
40	L3	188	ILE
40	L3	189	SER
40	L3	192	VAL
40	L3	196	ARG
40	L3	200	GLU

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Mol	Chain	Res	Type
40	L3	201	LYS
40	L3	202	THR
40	L3	208	VAL
40	L3	210	GLU
40	L3	212	ASN
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	238	LEU
40	L3	241	LYS
40	L3	252	ILE
40	L3	264	VAL
40	L3	266	ARG
40	L3	274	SER
40	L3	284	ARG
40	L3	305	ILE
40	L3	308	MET
40	L3	320	ASP
40	L3	324	VAL
40	L3	328	ILE
40	L3	332	ARG
40	L3	338	LEU
40	L3	341	SER
40	L3	343	TYR
40	L3	347	SER
40	L3	353	GLU
40	L3	354	VAL
40	L3	355	SER
40	L3	364	LYS
40	L3	382	THR
40	L3	385	LYS
40	L3	387	LEU
41	L4	2	SER
41	L4	6	VAL
41	L4	16	THR
41	L4	20	LEU
41	L4	37	THR
41	L4	40	THR
41	L4	64	SER
41	L4	71	VAL
41	L4	74	ILE
41	L4	93	MET

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Mol	Chain	Res	Type
41	L4	99	MET
41	L4	112	LYS
41	L4	117	GLU
41	L4	120	TYR
41	L4	124	SER
41	L4	133	SER
41	L4	136	LEU
41	L4	148	ILE
41	L4	150	LEU
41	L4	152	VAL
41	L4	156	LEU
41	L4	179	LEU
41	L4	186	LYS
41	L4	187	LEU
41	L4	188	ARG
41	L4	193	LYS
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	206	LEU
41	L4	211	GLU
41	L4	220	ARG
41	L4	222	VAL
41	L4	223	PRO
41	L4	230	VAL
41	L4	258	LEU
41	L4	259	ASP
41	L4	267	VAL
41	L4	270	SER
41	L4	284	SER
41	L4	287	THR
41	L4	289	ILE
41	L4	292	SER
41	L4	295	ILE
41	L4	306	THR
41	L4	307	GLN
41	L4	308	LYS
41	L4	313	LEU
41	L4	323	VAL
41	L4	327	LEU
41	L4	333	VAL
41	L4	338	LYS

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Mol	Chain	Res	Type
41	L4	343	LYS
41	L4	346	LYS
41	L4	349	THR
41	L4	350	LYS
41	L4	359	LEU
42	L5	4	GLN
42	L5	22	ARG
42	L5	23	ARG
42	L5	27	LYS
42	L5	34	LYS
42	L5	41	LYS
42	L5	43	LYS
42	L5	65	ILE
42	L5	66	SER
42	L5	70	THR
42	L5	75	LEU
42	L5	105	ILE
42	L5	109	THR
42	L5	112	LYS
42	L5	115	LEU
42	L5	118	THR
42	L5	131	LEU
42	L5	132	THR
42	L5	137	ASP
42	L5	140	ARG
42	L5	146	LEU
42	L5	148	ILE
42	L5	151	GLN
42	L5	152	ARG
42	L5	155	THR
42	L5	158	ARG
42	L5	159	VAL
42	L5	163	LEU
42	L5	185	PHE
42	L5	186	GLU
42	L5	188	GLU
42	L5	196	ARG
42	L5	217	GLU
42	L5	218	ARG
42	L5	220	SER
42	L5	222	LEU
42	L5	227	LEU

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Mol	Chain	Res	Type
42	L5	232	ASP
42	L5	242	SER
42	L5	257	GLU
42	L5	259	LYS
42	L5	263	GLU
42	L5	273	ARG
42	L5	275	THR
42	L5	290	ILE
43	L6	5	LYS
43	L6	15	VAL
43	L6	18	LEU
43	L6	21	THR
43	L6	48	ARG
43	L6	52	VAL
43	L6	64	LEU
43	L6	65	ILE
43	L6	79	VAL
43	L6	84	VAL
43	L6	89	THR
43	L6	90	LYS
43	L6	94	GLU
43	L6	98	VAL
43	L6	134	ARG
43	L6	155	LEU
43	L6	162	SER
43	L6	166	LYS
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	33	ARG
44	L7	38	LYS
44	L7	40	LYS
44	L7	59	GLU
44	L7	60	ARG
44	L7	77	VAL
44	L7	82	LYS
44	L7	89	ILE
44	L7	93	ASN
44	L7	98	LYS
44	L7	110	ARG
44	L7	118	LYS
44	L7	120	THR

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Mol	Chain	Res	Type
44	L7	124	LEU
44	L7	128	LYS
44	L7	158	LYS
44	L7	161	VAL
44	L7	164	SER
44	L7	175	LYS
44	L7	179	LEU
44	L7	182	ASP
44	L7	184	LEU
44	L7	206	LYS
44	L7	224	ILE
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	50	VAL
45	L8	63	LYS
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	81	THR
45	L8	82	LEU
45	L8	84	ARG
45	L8	95	ASN
45	L8	101	THR
45	L8	106	LYS
45	L8	118	GLU
45	L8	132	VAL
45	L8	136	LEU
45	L8	149	LYS
45	L8	150	LEU
45	L8	156	ASP
45	L8	163	VAL
45	L8	169	LEU
45	L8	172	LYS
45	L8	181	LYS
45	L8	185	ARG
45	L8	189	LEU
45	L8	197	VAL
45	L8	203	VAL

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Mol	Chain	Res	Type
45	L8	206	GLU
45	L8	211	LEU
45	L8	219	ASP
45	L8	221	ASN
45	L8	232	HIS
45	L8	238	LEU
45	L8	241	LYS
45	L8	246	MET
45	L8	248	LYS
46	L9	5	GLN
46	L9	6	THR
46	L9	14	GLU
46	L9	18	VAL
46	L9	20	ILE
46	L9	22	SER
46	L9	34	LEU
46	L9	36	LYS
46	L9	41	ILE
46	L9	48	VAL
46	L9	52	LEU
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	72	LYS
46	L9	78	MET
46	L9	82	VAL
46	L9	115	ARG
46	L9	123	ILE
46	L9	124	ARG
46	L9	135	GLU
46	L9	138	THR
46	L9	139	ASN
46	L9	147	SER
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	173	ARG
46	L9	177	ASP
46	L9	189	GLU

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Mol	Chain	Res	Type
47	M0	3	ARG
47	M0	21	ARG
47	M0	24	ARG
47	M0	26	VAL
47	M0	30	LYS
47	M0	31	ILE
47	M0	32	ARG
47	M0	33	ILE
47	M0	39	LYS
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	63	GLU
47	M0	87	LEU
47	M0	102	MET
47	M0	128	ARG
47	M0	130	ASP
47	M0	133	GLN
47	M0	138	VAL
47	M0	139	ARG
47	M0	146	ASP
47	M0	163	GLN
47	M0	165	ILE
47	M0	166	ILE
47	M0	174	THR
47	M0	175	ASN
47	M0	176	LEU
47	M0	177	ASP
47	M0	178	ARG
47	M0	180	GLU
47	M0	184	LYS
47	M0	191	LYS
47	M0	203	LYS
47	M0	205	SER
47	M0	207	GLU
48	M1	6	GLN
48	M1	9	MET
48	M1	10	ARG
48	M1	11	ASP
48	M1	12	LEU
48	M1	13	LYS
48	M1	26	SER

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Mol	Chain	Res	Type
48	M1	28	ASP
48	M1	34	SER
48	M1	38	GLU
48	M1	40	LEU
48	M1	44	THR
48	M1	46	VAL
48	M1	52	TYR
48	M1	63	GLU
48	M1	65	ILE
48	M1	71	VAL
48	M1	77	GLU
48	M1	80	LEU
48	M1	82	ARG
48	M1	94	ARG
48	M1	95	ASN
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	130	VAL
48	M1	137	ARG
48	M1	140	ARG
48	M1	142	LYS
48	M1	155	THR
48	M1	158	ASP
48	M1	161	SER
48	M1	165	GLN
48	M1	166	LYS
48	M1	171	VAL
49	M3	23	LYS
49	M3	35	ARG
49	M3	54	LEU
49	M3	55	ARG
49	M3	57	VAL
49	M3	58	VAL
49	M3	59	ARG
49	M3	62	THR
49	M3	67	ARG
49	M3	69	VAL
49	M3	80	VAL
49	M3	85	LEU
49	M3	107	GLU
49	M3	114	GLN

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Mol	Chain	Res	Type
49	M3	122	LYS
49	M3	124	ILE
49	M3	131	LYS
49	M3	136	GLU
49	M3	144	THR
49	M3	147	ILE
49	M3	164	GLU
49	M3	168	ARG
49	M3	169	THR
49	M3	171	ARG
49	M3	190	LYS
50	M4	5	SER
50	M4	8	LYS
50	M4	19	ARG
50	M4	20	VAL
50	M4	23	ILE
50	M4	27	GLN
50	M4	38	ILE
50	M4	50	LYS
50	M4	53	VAL
50	M4	64	VAL
50	M4	66	THR
50	M4	72	LEU
50	M4	90	VAL
50	M4	91	CYS
50	M4	102	LYS
50	M4	105	GLN
50	M4	108	ARG
50	M4	121	MET
50	M4	135	LEU
51	M5	10	LEU
51	M5	13	LYS
51	M5	18	VAL
51	M5	22	LEU
51	M5	24	ARG
51	M5	38	ARG
51	M5	68	ARG
51	M5	80	THR
51	M5	83	LYS
51	M5	85	THR
51	M5	96	ARG
51	M5	105	ARG

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Mol	Chain	Res	Type
51	M5	106	VAL
51	M5	109	ARG
51	M5	117	ASN
51	M5	124	ASP
51	M5	133	ILE
51	M5	138	GLN
51	M5	142	ILE
51	M5	144	ARG
51	M5	151	ILE
51	M5	153	ASP
51	M5	159	ARG
51	M5	167	THR
51	M5	175	ASN
51	M5	182	ASN
51	M5	184	LYS
51	M5	190	THR
51	M5	204	LYS
52	M6	6	VAL
52	M6	33	ILE
52	M6	36	VAL
52	M6	50	ASN
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	89	SER
52	M6	106	GLU
52	M6	110	PRO
52	M6	116	LYS
52	M6	117	ARG
52	M6	122	GLN
52	M6	124	LEU
52	M6	128	ARG
52	M6	134	LYS
52	M6	143	THR
52	M6	151	ASP
52	M6	164	SER
52	M6	184	THR
52	M6	190	VAL

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Mol	Chain	Res	Type
52	M6	192	LYS
53	M7	3	ARG
53	M7	9	THR
53	M7	16	SER
53	M7	18	ARG
53	M7	23	ARG
53	M7	24	VAL
53	M7	32	THR
53	M7	36	ILE
53	M7	40	GLU
53	M7	41	LEU
53	M7	52	LEU
53	M7	56	ARG
53	M7	69	ARG
53	M7	78	VAL
53	M7	79	THR
53	M7	87	SER
53	M7	107	LEU
53	M7	118	GLN
53	M7	119	VAL
53	M7	120	ASN
53	M7	126	ARG
53	M7	127	ARG
53	M7	128	ARG
53	M7	138	LYS
53	M7	142	SER
53	M7	144	SER
53	M7	148	LEU
53	M7	157	VAL
53	M7	171	ARG
53	M7	180	LYS
53	M7	181	ARG
54	M8	22	ASP
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	41	ASP
54	M8	49	LEU
54	M8	50	LYS
54	M8	63	SER
54	M8	67	ILE
54	M8	69	ARG

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Mol	Chain	Res	Type
54	M8	73	GLN
54	M8	74	GLU
54	M8	80	THR
54	M8	104	LEU
54	M8	111	ARG
54	M8	113	LYS
54	M8	127	LEU
54	M8	129	VAL
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	161	LYS
54	M8	174	ARG
54	M8	179	ARG
55	M9	5	ARG
55	M9	10	LEU
55	M9	29	THR
55	M9	31	GLU
55	M9	34	GLN
55	M9	37	SER
55	M9	41	ILE
55	M9	44	LEU
55	M9	55	VAL
55	M9	60	LYS
55	M9	61	SER
55	M9	63	THR
55	M9	74	ARG
55	M9	86	GLU
55	M9	91	SER
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	116	ASP
55	M9	134	HIS
55	M9	138	LEU
55	M9	139	VAL
55	M9	150	GLN
55	M9	153	LYS
55	M9	156	ASN
55	M9	164	LEU
55	M9	165	LYS
55	M9	175	GLN

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Mol	Chain	Res	Type
55	M9	176	ARG
55	M9	181	ARG
56	N0	1	MET
56	N0	8	GLN
56	N0	45	LEU
56	N0	46	GLN
56	N0	51	VAL
56	N0	52	LYS
56	N0	57	GLU
56	N0	85	SER
56	N0	87	THR
56	N0	92	LYS
56	N0	99	ARG
56	N0	100	VAL
56	N0	104	GLU
56	N0	106	LEU
56	N0	113	ARG
56	N0	115	ARG
56	N0	117	ARG
56	N0	122	HIS
56	N0	125	LYS
56	N0	132	THR
56	N0	136	LYS
56	N0	137	ARG
56	N0	142	GLN
56	N0	144	LEU
56	N0	155	ARG
56	N0	156	VAL
56	N0	162	THR
56	N0	171	PHE
56	N0	172	TYR
57	N1	12	ARG
57	N1	18	ASP
57	N1	25	VAL
57	N1	26	HIS
57	N1	27	LEU
57	N1	32	LYS
57	N1	36	VAL
57	N1	55	LYS
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET

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Mol	Chain	Res	Type
57	N1	80	VAL
57	N1	83	ARG
57	N1	87	LYS
57	N1	88	ARG
57	N1	89	LEU
57	N1	92	ARG
57	N1	96	ILE
57	N1	102	ARG
57	N1	106	LEU
57	N1	110	LYS
57	N1	118	GLU
57	N1	122	GLN
57	N1	124	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	139	ARG
57	N1	143	THR
57	N1	149	GLN
57	N1	158	THR
57	N1	159	PHE
57	N1	160	ILE
58	N2	10	LYS
58	N2	14	THR
58	N2	16	THR
58	N2	32	SER
58	N2	39	ASP
58	N2	43	VAL
58	N2	50	LEU
58	N2	52	ASN
58	N2	54	VAL
58	N2	59	ASP
58	N2	61	THR
58	N2	66	VAL
58	N2	70	LYS
58	N2	74	LYS
58	N2	88	GLN
58	N2	93	ILE
58	N2	99	LYS
58	N2	100	THR
59	N3	9	THR
59	N3	12	ARG
59	N3	13	ILE

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Mol	Chain	Res	Type
59	N3	14	SER
59	N3	32	ARG
59	N3	40	LYS
59	N3	42	SER
59	N3	44	SER
59	N3	46	LEU
59	N3	48	ARG
59	N3	54	LEU
59	N3	69	LEU
59	N3	73	VAL
59	N3	78	VAL
59	N3	83	LYS
59	N3	88	ARG
59	N3	91	VAL
59	N3	102	ILE
59	N3	110	LYS
59	N3	125	LEU
59	N3	131	SER
59	N3	135	VAL
59	N3	137	VAL
60	N4	2	LYS
60	N4	5	ILE
60	N4	19	THR
60	N4	34	SER
60	N4	39	LEU
60	N4	43	ARG
60	N4	47	ARG
60	N4	64	THR
61	N5	26	VAL
61	N5	27	ARG
61	N5	28	THR
61	N5	34	LEU
61	N5	36	LYS
61	N5	38	LEU
61	N5	42	ARG
61	N5	48	SER
61	N5	49	LYS
61	N5	63	ILE
61	N5	71	THR
61	N5	75	LYS
61	N5	86	VAL
61	N5	88	MET

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Mol	Chain	Res	Type
61	N5	92	LYS
61	N5	102	LEU
61	N5	108	LEU
61	N5	113	LEU
61	N5	115	ARG
61	N5	125	ARG
61	N5	127	THR
61	N5	133	LEU
61	N5	135	ILE
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	4	GLN
62	N6	9	SER
62	N6	13	ARG
62	N6	17	LYS
62	N6	31	LEU
62	N6	36	SER
62	N6	37	LYS
62	N6	38	GLU
62	N6	42	GLN
62	N6	45	ILE
62	N6	50	ILE
62	N6	56	VAL
62	N6	57	LEU
62	N6	60	ARG
62	N6	62	SER
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	83	ASP
62	N6	115	ARG
62	N6	122	LYS
62	N6	125	LYS
62	N6	126	LEU
62	N6	127	GLU
63	N7	14	VAL
63	N7	21	LYS
63	N7	24	VAL
63	N7	34	LYS
63	N7	46	ILE
63	N7	52	LYS

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Mol	Chain	Res	Type
63	N7	64	LYS
63	N7	72	ILE
63	N7	74	VAL
63	N7	75	VAL
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	87	LEU
63	N7	95	VAL
63	N7	99	GLU
63	N7	102	GLU
63	N7	106	GLN
63	N7	109	GLU
63	N7	121	ARG
63	N7	134	LEU
63	N7	135	ARG
63	N7	136	PHE
64	N8	4	ARG
64	N8	8	THR
64	N8	10	LYS
64	N8	29	PRO
64	N8	32	ARG
64	N8	34	MET
64	N8	42	ARG
64	N8	47	LYS
64	N8	60	TYR
64	N8	64	GLN
64	N8	65	GLN
64	N8	78	LEU
64	N8	88	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	137	LYS
65	N9	6	ASN
65	N9	13	THR
65	N9	14	ARG
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	50	THR
65	N9	59	LYS
66	O0	12	GLN
66	O0	14	LEU
66	O0	16	LEU
66	O0	20	SER
66	O0	22	LYS
66	O0	24	THR
66	O0	36	GLN
66	O0	40	LYS
66	O0	41	LEU
66	O0	54	SER
66	O0	61	MET
66	O0	65	THR
66	O0	79	THR
66	O0	81	VAL
66	O0	83	LYS
66	O0	87	VAL
66	O0	101	LEU
67	O1	6	ASP
67	O1	8	VAL
67	O1	13	THR
67	O1	16	LEU
67	O1	26	LYS
67	O1	28	ARG
67	O1	42	LEU
67	O1	46	THR
67	O1	53	PRO
67	O1	55	LEU
67	O1	64	VAL
67	O1	68	GLU
67	O1	73	LEU
67	O1	76	SER
67	O1	79	ARG
67	O1	82	GLU
67	O1	83	GLU
67	O1	84	ASP
67	O1	86	LYS
67	O1	87	ASN

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Mol	Chain	Res	Type
67	O1	94	GLU
67	O1	96	VAL
67	O1	102	LYS
67	O1	104	LEU
67	O1	105	GLN
67	O1	106	THR
67	O1	110	GLU
68	O2	4	LEU
68	O2	19	ARG
68	O2	33	ARG
68	O2	51	SER
68	O2	54	LYS
68	O2	66	LEU
68	O2	73	THR
68	O2	82	LEU
68	O2	84	THR
68	O2	87	MET
68	O2	91	THR
68	O2	101	SER
68	O2	103	LYS
68	O2	106	VAL
68	O2	109	LEU
68	O2	120	THR
68	O2	125	ARG
68	O2	126	LEU
68	O2	128	LEU
69	O3	15	SER
69	O3	20	LYS
69	O3	21	ARG
69	O3	24	ASN
69	O3	49	ILE
69	O3	63	LYS
69	O3	70	LYS
69	O3	74	THR
69	O3	80	VAL
69	O3	86	ARG
69	O3	90	PRO
69	O3	98	VAL
69	O3	105	SER
69	O3	106	ASN
70	O4	8	ARG
70	O4	20	ILE

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Mol	Chain	Res	Type
70	O4	21	LYS
70	O4	23	VAL
70	O4	49	SER
70	O4	51	LEU
70	O4	58	ARG
70	O4	65	VAL
70	O4	71	THR
70	O4	79	SER
70	O4	81	CYS
70	O4	86	LYS
70	O4	88	ARG
70	O4	102	LYS
70	O4	104	VAL
71	O5	15	GLU
71	O5	20	GLN
71	O5	21	LEU
71	O5	27	GLU
71	O5	41	LEU
71	O5	46	THR
71	O5	48	ARG
71	O5	49	LYS
71	O5	50	SER
71	O5	62	GLN
71	O5	69	LEU
71	O5	71	LYS
71	O5	74	LYS
71	O5	89	ARG
71	O5	90	ARG
71	O5	101	THR
71	O5	102	GLU
71	O5	103	LYS
71	O5	104	GLN
71	O5	105	ARG
71	O5	107	LYS
71	O5	119	LYS
72	O6	17	VAL
72	O6	18	THR
72	O6	21	THR
72	O6	26	ILE
72	O6	34	SER
72	O6	45	ARG
72	O6	57	LEU

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Mol	Chain	Res	Type
72	O6	58	ILE
72	O6	60	LEU
72	O6	62	ARG
72	O6	68	ARG
72	O6	70	ARG
72	O6	76	ARG
72	O6	81	THR
72	O6	84	LYS
72	O6	98	ARG
72	O6	99	ARG
73	O7	5	THR
73	O7	15	SER
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	26	SER
73	O7	37	CYS
73	O7	44	THR
73	O7	45	ARG
73	O7	54	LYS
73	O7	55	ARG
73	O7	58	THR
73	O7	59	THR
73	O7	65	ARG
73	O7	79	GLN
73	O7	82	SER
73	O7	85	LYS
74	O8	5	ILE
74	O8	6	THR
74	O8	8	ILE
74	O8	22	THR
74	O8	24	THR
74	O8	31	LEU
74	O8	32	ASN
74	O8	39	ARG
74	O8	41	THR
74	O8	45	VAL
74	O8	46	ARG
74	O8	48	SER
74	O8	53	THR
74	O8	61	LYS
74	O8	65	LEU

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Mol	Chain	Res	Type
74	O8	67	GLN
74	O8	72	THR
75	O9	5	LYS
75	O9	12	LYS
75	O9	17	LYS
75	O9	21	ARG
75	O9	23	LEU
75	O9	29	LEU
75	O9	33	ASN
75	O9	42	ARG
75	O9	45	ARG
75	O9	47	THR
75	O9	51	ILE
76	Q0	78	ILE
76	Q0	85	LEU
76	Q0	98	LYS
76	Q0	99	CYS
76	Q0	108	THR
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	127	LEU
77	Q1	1	MET
77	Q1	2	ARG
77	Q1	6	ARG
77	Q1	9	ARG
77	Q1	10	THR
77	Q1	11	ARG
77	Q1	13	LEU
77	Q1	16	LYS
77	Q1	19	LYS
77	Q1	20	VAL
77	Q1	21	ARG
78	Q2	2	VAL
78	Q2	9	LYS
78	Q2	21	THR
78	Q2	26	THR
78	Q2	35	LEU
78	Q2	45	ARG
78	Q2	47	GLN
78	Q2	48	SER
78	Q2	71	ARG

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Mol	Chain	Res	Type
78	Q2	78	LYS
78	Q2	79	THR
78	Q2	80	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	92	GLU
78	Q2	93	LEU
78	Q2	99	GLN
78	Q2	104	LEU
79	Q3	5	THR
79	Q3	11	THR
79	Q3	25	GLN
79	Q3	27	LYS
79	Q3	31	ILE
79	Q3	32	GLN
79	Q3	40	SER
79	Q3	45	LYS
79	Q3	49	ARG
79	Q3	54	ILE
79	Q3	60	CYS
79	Q3	78	THR
79	Q3	90	VAL
79	Q3	91	GLU
2	s0	9	LEU
2	s0	10	THR
2	s0	12	GLU
2	s0	27	ARG
2	s0	29	VAL
2	s0	32	HIS
2	s0	39	ASN
2	s0	41	ARG
2	s0	43	ASP
2	s0	57	LEU
2	s0	59	LEU
2	s0	62	ARG
2	s0	72	ASP
2	s0	87	LEU
2	s0	93	THR
2	s0	96	THR
2	s0	106	SER
2	s0	110	TYR

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Mol	Chain	Res	Type
2	s0	119	ARG
2	s0	124	THR
2	s0	131	GLN
2	s0	137	SER
2	s0	144	ILE
2	s0	153	SER
2	s0	154	GLU
2	s0	156	VAL
2	s0	157	ASP
2	s0	165	ARG
2	s0	167	LYS
2	s0	172	LEU
2	s0	179	ARG
2	s0	183	ARG
2	s0	185	ARG
2	s0	189	VAL
2	s0	198	MET
2	s0	200	ASP
3	s1	21	VAL
3	s1	25	THR
3	s1	37	THR
3	s1	40	ASN
3	s1	47	LEU
3	s1	51	SER
3	s1	54	LEU
3	s1	55	LYS
3	s1	62	LYS
3	s1	66	VAL
3	s1	70	LEU
3	s1	73	LEU
3	s1	83	LYS
3	s1	84	ILE
3	s1	90	GLU
3	s1	91	VAL
3	s1	105	PHE
3	s1	119	THR
3	s1	125	VAL
3	s1	131	ASP
3	s1	137	ILE
3	s1	154	SER
3	s1	158	SER
3	s1	159	SER

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Mol	Chain	Res	Type
3	s1	164	ILE
3	s1	169	SER
3	s1	175	GLU
3	s1	177	GLN
3	s1	180	THR
3	s1	181	LEU
3	s1	188	LEU
3	s1	193	ILE
3	s1	195	LYS
3	s1	202	LYS
3	s1	206	PRO
3	s1	211	HIS
3	s1	215	VAL
3	s1	219	LYS
3	s1	222	LYS
3	s1	225	VAL
3	s1	228	LEU
3	s1	231	LEU
4	s2	41	LEU
4	s2	46	LYS
4	s2	51	THR
4	s2	53	ILE
4	s2	54	GLU
4	s2	55	GLU
4	s2	58	LEU
4	s2	60	SER
4	s2	61	LEU
4	s2	69	ILE
4	s2	73	LEU
4	s2	80	VAL
4	s2	83	ILE
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	97	ARG
4	s2	106	ASP
4	s2	108	ASN
4	s2	111	VAL
4	s2	113	LEU
4	s2	117	THR
4	s2	120	GLU

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Mol	Chain	Res	Type
4	s2	134	LEU
4	s2	137	ILE
4	s2	139	ILE
4	s2	140	ARG
4	s2	141	ARG
4	s2	146	THR
4	s2	148	LEU
4	s2	150	GLN
4	s2	153	SER
4	s2	159	THR
4	s2	164	SER
4	s2	166	THR
4	s2	170	ILE
4	s2	179	VAL
4	s2	181	SER
4	s2	182	PRO
4	s2	185	LYS
4	s2	186	LYS
4	s2	190	LEU
4	s2	194	GLU
4	s2	195	ASP
4	s2	206	THR
4	s2	207	LEU
4	s2	212	LYS
4	s2	225	LEU
4	s2	229	LEU
4	s2	246	GLU
4	s2	248	SER
5	s3	4	LEU
5	s3	9	ARG
5	s3	10	LYS
5	s3	11	LEU
5	s3	21	LEU
5	s3	26	THR
5	s3	32	GLU
5	s3	37	VAL
5	s3	40	ARG
5	s3	44	THR
5	s3	59	LEU
5	s3	61	GLU
5	s3	65	ARG
5	s3	69	LEU

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Mol	Chain	Res	Type
5	s3	76	ARG
5	s3	83	THR
5	s3	94	ARG
5	s3	103	GLU
5	s3	115	ILE
5	s3	124	ARG
5	s3	128	GLU
5	s3	139	SER
5	s3	142	LEU
5	s3	146	ARG
5	s3	158	ILE
5	s3	164	VAL
5	s3	172	THR
5	s3	181	VAL
5	s3	195	SER
5	s3	196	ARG
5	s3	202	LEU
5	s3	209	ILE
5	s3	210	GLU
5	s3	212	LYS
5	s3	217	ILE
5	s3	223	LYS
6	s4	6	LYS
6	s4	7	LYS
6	s4	12	LEU
6	s4	20	LEU
6	s4	23	LEU
6	s4	24	SER
6	s4	38	LEU
6	s4	42	LEU
6	s4	49	ARG
6	s4	56	LEU
6	s4	69	HIS
6	s4	70	VAL
6	s4	77	ARG
6	s4	78	THR
6	s4	89	VAL
6	s4	104	ASP
6	s4	115	THR
6	s4	116	ASP
6	s4	117	GLU
6	s4	123	LEU

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Mol	Chain	Res	Type
6	s4	127	LYS
6	s4	128	LYS
6	s4	146	THR
6	s4	148	ARG
6	s4	159	THR
6	s4	176	ASP
6	s4	180	LEU
6	s4	182	TYR
6	s4	184	THR
6	s4	200	ARG
6	s4	214	LEU
6	s4	221	ARG
6	s4	222	LEU
6	s4	223	ASN
6	s4	227	VAL
6	s4	236	ILE
6	s4	237	SER
6	s4	242	LYS
6	s4	245	LYS
6	s4	248	ILE
6	s4	254	ARG
7	s5	23	VAL
7	s5	24	VAL
7	s5	25	LEU
7	s5	31	GLU
7	s5	33	VAL
7	s5	38	THR
7	s5	45	LYS
7	s5	50	GLU
7	s5	59	VAL
7	s5	63	GLN
7	s5	64	VAL
7	s5	68	ILE
7	s5	76	ARG
7	s5	79	ASN
7	s5	83	ARG
7	s5	93	LEU
7	s5	102	ARG
7	s5	119	ASP
7	s5	124	LEU
7	s5	128	ASN
7	s5	146	THR

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Mol	Chain	Res	Type
7	s5	156	ARG
7	s5	157	ARG
7	s5	167	ARG
7	s5	190	ILE
7	s5	192	GLU
7	s5	194	LEU
7	s5	205	SER
7	s5	213	LYS
7	s5	216	GLU
7	s5	219	ARG
8	s6	21	GLU
8	s6	22	HIS
8	s6	30	LYS
8	s6	31	ARG
8	s6	63	MET
8	s6	69	LEU
8	s6	71	THR
8	s6	73	ILE
8	s6	76	LEU
8	s6	78	THR
8	s6	79	LYS
8	s6	89	ASP
8	s6	93	LYS
8	s6	96	SER
8	s6	98	ARG
8	s6	108	VAL
8	s6	109	LEU
8	s6	120	GLU
8	s6	121	LEU
8	s6	125	THR
8	s6	126	ASP
8	s6	127	THR
8	s6	129	VAL
8	s6	143	LYS
8	s6	151	ASP
8	s6	153	VAL
8	s6	154	ARG
8	s6	155	ASP
8	s6	166	GLU
8	s6	168	THR
8	s6	171	LYS
8	s6	177	ARG

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Mol	Chain	Res	Type
8	s6	182	GLN
8	s6	193	LEU
8	s6	197	ASN
8	s6	215	ARG
9	s7	9	LEU
9	s7	17	GLU
9	s7	24	PHE
9	s7	26	GLU
9	s7	28	GLU
9	s7	35	LYS
9	s7	42	GLN
9	s7	49	ILE
9	s7	50	ASP
9	s7	77	LEU
9	s7	78	THR
9	s7	79	ARG
9	s7	80	GLU
9	s7	86	GLN
9	s7	97	ARG
9	s7	110	GLN
9	s7	114	ARG
9	s7	115	SER
9	s7	117	THR
9	s7	119	THR
9	s7	122	HIS
9	s7	129	LEU
9	s7	143	LEU
9	s7	144	VAL
9	s7	149	ILE
9	s7	162	ILE
9	s7	185	ILE
9	s7	187	SER
10	s8	7	SER
10	s8	9	HIS
10	s8	22	ARG
10	s8	25	ARG
10	s8	29	LEU
10	s8	32	GLN
10	s8	36	THR
10	s8	54	LYS
10	s8	59	ARG
10	s8	61	GLU

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Mol	Chain	Res	Type
10	s8	62	THR
10	s8	64	ASN
10	s8	72	ILE
10	s8	74	LYS
10	s8	76	THR
10	s8	77	ARG
10	s8	89	GLU
10	s8	110	ARG
10	s8	119	GLN
10	s8	120	THR
10	s8	121	LEU
10	s8	138	ASN
10	s8	141	ARG
10	s8	149	SER
10	s8	151	LYS
10	s8	152	ILE
10	s8	155	SER
10	s8	158	SER
10	s8	176	SER
10	s8	183	ILE
10	s8	199	LYS
11	s9	3	ARG
11	s9	7	THR
11	s9	10	LYS
11	s9	16	LYS
11	s9	20	GLU
11	s9	28	LEU
11	s9	37	LYS
11	s9	49	LEU
11	s9	53	ARG
11	s9	60	LEU
11	s9	89	ASP
11	s9	90	LYS
11	s9	92	LYS
11	s9	93	LEU
11	s9	96	VAL
11	s9	101	VAL
11	s9	105	LEU
11	s9	109	LEU
11	s9	111	THR
11	s9	113	VAL
11	s9	120	LYS

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Mol	Chain	Res	Type
11	s9	126	ARG
11	s9	127	VAL
11	s9	130	THR
11	s9	132	ARG
11	s9	134	ILE
11	s9	142	ASN
11	s9	149	ARG
11	s9	150	LEU
11	s9	152	SER
11	s9	164	PHE
11	s9	168	ARG
11	s9	172	VAL
11	s9	179	ARG
11	s9	180	LYS
12	c0	2	LEU
12	c0	5	LYS
12	c0	20	VAL
12	c0	22	VAL
12	c0	40	LEU
12	c0	55	VAL
12	c0	57	THR
12	c0	73	VAL
12	c0	76	LEU
13	c1	5	LEU
13	c1	6	THR
13	c1	10	GLU
13	c1	21	ASN
13	c1	24	LYS
13	c1	27	THR
13	c1	30	ARG
13	c1	32	LYS
13	c1	40	LEU
13	c1	44	THR
13	c1	56	LYS
13	c1	60	PHE
13	c1	67	ARG
13	c1	69	LYS
13	c1	74	THR
13	c1	77	SER
13	c1	80	MET
13	c1	82	ARG
13	c1	87	ARG

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Mol	Chain	Res	Type
13	c1	107	VAL
13	c1	119	VAL
13	c1	129	ARG
13	c1	138	ASN
13	c1	140	VAL
13	c1	143	SER
14	c2	26	ASP
14	c2	28	LEU
14	c2	30	VAL
14	c2	36	LEU
14	c2	37	VAL
14	c2	38	HIS
14	c2	39	ASP
14	c2	45	LEU
14	c2	52	LEU
14	c2	58	LEU
14	c2	61	VAL
14	c2	67	THR
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	89	ILE
14	c2	97	LEU
14	c2	103	LEU
14	c2	121	VAL
14	c2	129	GLU
14	c2	132	GLU
14	c2	136	ILE
14	c2	140	PHE
14	c2	142	GLN
15	c3	3	ARG
15	c3	6	SER
15	c3	12	SER
15	c3	14	SER
15	c3	20	ARG
15	c3	21	ASN
15	c3	27	LYS
15	c3	29	SER
15	c3	35	GLU
15	c3	64	ARG
15	c3	66	ILE

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Mol	Chain	Res	Type
15	c3	70	LYS
15	c3	84	ILE
15	c3	87	ASP
15	c3	97	SER
15	c3	102	LEU
15	c3	104	ARG
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	131	THR
15	c3	134	VAL
15	c3	138	ASN
15	c3	139	TRP
15	c3	151	ASN
16	c4	18	ARG
16	c4	20	TYR
16	c4	23	PHE
16	c4	26	THR
16	c4	31	THR
16	c4	33	LEU
16	c4	43	THR
16	c4	49	LYS
16	c4	51	ASP
16	c4	52	ARG
16	c4	58	TYR
16	c4	62	LEU
16	c4	70	LYS
16	c4	81	VAL
16	c4	92	LYS
16	c4	102	LEU
16	c4	107	ARG
16	c4	114	ARG
16	c4	119	THR
16	c4	123	SER
16	c4	132	ARG
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
17	c5	12	PHE
17	c5	13	LYS
17	c5	22	LEU
17	c5	24	LYS

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Mol	Chain	Res	Type
17	c5	27	GLU
17	c5	36	LEU
17	c5	40	ARG
17	c5	51	SER
17	c5	68	PRO
17	c5	69	GLU
17	c5	71	GLU
17	c5	92	SER
17	c5	107	ILE
17	c5	110	GLU
17	c5	111	MET
17	c5	121	ILE
17	c5	124	THR
17	c5	127	ARG
17	c5	134	THR
18	c6	23	LYS
18	c6	26	LYS
18	c6	28	LEU
18	c6	37	THR
18	c6	43	ILE
18	c6	48	VAL
18	c6	53	LEU
18	c6	57	LEU
18	c6	66	ARG
18	c6	68	ARG
18	c6	69	VAL
18	c6	83	GLN
18	c6	94	GLN
18	c6	110	THR
18	c6	114	ARG
18	c6	118	ILE
18	c6	137	ARG
18	c6	140	LYS
18	c6	143	ARG
19	c7	3	ARG
19	c7	5	ARG
19	c7	8	THR
19	c7	26	LEU
19	c7	34	LEU
19	c7	38	ILE
19	c7	46	LEU
19	c7	47	ARG

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Mol	Chain	Res	Type
19	c7	61	ILE
19	c7	62	GLN
19	c7	63	LYS
19	c7	69	ILE
19	c7	72	LYS
19	c7	83	GLN
19	c7	85	VAL
19	c7	87	GLU
19	c7	105	GLN
19	c7	112	SER
19	c7	113	LEU
20	c8	2	SER
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	7	GLU
20	c8	8	GLN
20	c8	12	GLN
20	c8	20	THR
20	c8	25	ASN
20	c8	28	ILE
20	c8	29	VAL
20	c8	33	THR
20	c8	34	THR
20	c8	40	ARG
20	c8	46	VAL
20	c8	57	ARG
20	c8	61	LEU
20	c8	63	GLN
20	c8	66	LEU
20	c8	80	LYS
20	c8	105	VAL
20	c8	116	LEU
20	c8	119	ILE
20	c8	143	ARG
20	c8	144	ARG
21	c9	6	VAL
21	c9	28	LEU
21	c9	34	VAL
21	c9	37	VAL
21	c9	41	SER

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Mol	Chain	Res	Type
21	c9	51	GLU
21	c9	68	ARG
21	c9	70	GLN
21	c9	71	VAL
21	c9	86	ARG
21	c9	91	TYR
21	c9	102	ARG
21	c9	116	ILE
21	c9	123	ARG
21	c9	126	GLU
21	c9	131	ASP
21	c9	133	ASP
21	c9	139	THR
21	c9	141	GLU
21	c9	142	GLU
22	d0	13	GLU
22	d0	16	GLN
22	d0	23	ARG
22	d0	25	THR
22	d0	27	THR
22	d0	30	LYS
22	d0	31	VAL
22	d0	34	LEU
22	d0	44	ASN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	61	LYS
22	d0	63	LEU
22	d0	70	THR
22	d0	72	ASN
22	d0	74	GLU
22	d0	77	LYS
22	d0	81	THR
22	d0	88	LYS
22	d0	89	ARG
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	105	GLN
22	d0	107	THR
22	d0	113	ASP

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Mol	Chain	Res	Type
22	d0	115	GLU
22	d0	121	ASN
23	d1	2	GLU
23	d1	3	ASN
23	d1	5	LYS
23	d1	11	LEU
23	d1	12	TYR
23	d1	25	LYS
23	d1	32	VAL
23	d1	38	LYS
23	d1	44	ARG
23	d1	50	TYR
23	d1	52	THR
23	d1	68	SER
23	d1	69	LEU
23	d1	75	ASN
23	d1	78	LEU
23	d1	81	ASN
24	d2	7	LEU
24	d2	20	THR
24	d2	23	ARG
24	d2	25	VAL
24	d2	26	LEU
24	d2	37	PHE
24	d2	65	LEU
24	d2	68	ARG
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	105	THR
24	d2	117	ARG
24	d2	119	LYS
24	d2	124	LYS
24	d2	129	VAL
25	d3	9	LEU
25	d3	14	LYS
25	d3	16	ARG
25	d3	19	ARG
25	d3	28	ASN
25	d3	34	LEU
25	d3	40	SER
25	d3	52	ILE

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Mol	Chain	Res	Type
25	d3	73	ARG
25	d3	78	LYS
25	d3	83	VAL
25	d3	84	THR
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	121	ARG
25	d3	125	VAL
25	d3	128	SER
25	d3	133	LEU
26	d4	6	THR
26	d4	10	ARG
26	d4	21	LYS
26	d4	36	SER
26	d4	43	LYS
26	d4	46	GLU
26	d4	47	VAL
26	d4	49	LYS
26	d4	62	THR
26	d4	83	LYS
26	d4	88	THR
26	d4	91	LEU
26	d4	100	VAL
26	d4	121	THR
26	d4	125	LEU
26	d4	127	LYS
26	d4	128	LYS
26	d4	133	ASN
27	d5	41	ILE
27	d5	43	ASP
27	d5	51	LEU
27	d5	52	LYS
27	d5	60	VAL
27	d5	71	ILE
27	d5	75	LEU
27	d5	81	ARG
27	d5	88	ILE
27	d5	90	LYS
28	d6	4	LYS
28	d6	10	ARG
28	d6	15	ARG

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Mol	Chain	Res	Type
28	d6	25	ASN
28	d6	41	ILE
28	d6	44	ILE
28	d6	53	LEU
28	d6	54	SER
28	d6	55	GLU
28	d6	67	THR
28	d6	82	ARG
28	d6	85	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	4	VAL
29	d7	15	GLU
29	d7	26	GLN
29	d7	36	LYS
29	d7	43	ILE
29	d7	52	THR
29	d7	72	LYS
29	d7	74	SER
29	d7	77	THR
30	d8	8	THR
30	d8	11	LYS
30	d8	19	THR
30	d8	22	ARG
30	d8	30	VAL
30	d8	32	PHE
30	d8	33	LEU
30	d8	39	THR
30	d8	40	ILE
30	d8	49	ARG
30	d8	54	LEU
30	d8	58	GLU
30	d8	61	ARG
30	d8	66	LEU
31	d9	6	VAL
31	d9	10	HIS
31	d9	12	ARG
31	d9	19	ARG
31	d9	25	SER
31	d9	26	SER
31	d9	30	LEU
31	d9	31	ILE

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Mol	Chain	Res	Type
31	d9	32	ARG
31	d9	36	LEU
31	d9	39	CYS
31	d9	54	LYS
80	e0	13	LYS
80	e0	14	VAL
80	e0	26	LYS
80	e0	31	LYS
80	e0	38	LEU
80	e0	39	LEU
80	e0	41	THR
80	e0	44	PHE
80	e0	45	VAL
80	e0	46	ASN
80	e0	48	THR
80	e0	49	LEU
80	e0	54	ARG
33	e1	80	ARG
33	e1	84	VAL
33	e1	86	THR
33	e1	96	LYS
33	e1	97	LYS
33	e1	100	LEU
33	e1	106	TYR
33	e1	109	ASP
33	e1	113	LYS
33	e1	115	THR
33	e1	116	LYS
33	e1	118	ARG
33	e1	119	ARG
33	e1	130	VAL
33	e1	135	HIS
33	e1	138	ARG
33	e1	147	VAL
33	e1	148	TYR
33	e1	150	VAL
33	e1	151	ASN
34	sR	13	LEU
34	sR	21	THR
34	sR	23	LEU
34	sR	29	GLN
34	sR	50	ASP

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Mol	Chain	Res	Type
34	sR	52	GLN
34	sR	58	VAL
34	sR	64	HIS
34	sR	65	SER
34	sR	66	HIS
34	sR	72	THR
34	sR	76	ASP
34	sR	82	SER
34	sR	96	THR
34	sR	98	GLU
34	sR	166	SER
34	sR	167	VAL
34	sR	176	LYS
34	sR	178	VAL
34	sR	185	GLN
34	sR	197	SER
34	sR	209	THR
34	sR	232	TYR
34	sR	237	GLN
34	sR	258	THR
34	sR	266	ASP
34	sR	275	ARG
34	sR	286	GLU
34	sR	297	ASP
34	sR	310	ILE
34	sR	314	GLN
35	sM	23	LYS
35	sM	24	GLU
35	sM	28	SER
35	sM	29	ASN
35	sM	41	SER
35	sM	43	ASP
35	sM	48	ARG
35	sM	61	ILE
35	sM	68	ARG
35	sM	72	ARG
35	sM	74	LYS
35	sM	75	ASP
35	sM	77	THR
35	sM	79	SER
35	sM	82	THR
39	l2	15	ILE

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Mol	Chain	Res	Type
39	l2	32	LEU
39	l2	41	ILE
39	l2	44	ILE
39	l2	45	VAL
39	l2	48	ILE
39	l2	61	VAL
39	l2	62	VAL
39	l2	68	LYS
39	l2	82	VAL
39	l2	101	VAL
39	l2	109	GLU
39	l2	114	SER
39	l2	116	VAL
39	l2	123	ARG
39	l2	126	LEU
39	l2	137	ILE
39	l2	142	ASP
39	l2	157	VAL
39	l2	177	LYS
39	l2	179	LEU
39	l2	191	LEU
39	l2	193	ARG
39	l2	194	ASN
39	l2	204	MET
39	l2	206	PRO
39	l2	227	ARG
39	l2	230	VAL
39	l2	241	ARG
39	l2	245	LEU
39	l2	246	LEU
40	l3	3	HIS
40	l3	4	ARG
40	l3	10	ARG
40	l3	17	LEU
40	l3	19	ARG
40	l3	20	LYS
40	l3	21	ARG
40	l3	24	SER
40	l3	30	LYS
40	l3	38	SER
40	l3	44	THR
40	l3	56	ILE

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Mol	Chain	Res	Type
40	l3	60	LEU
40	l3	66	LYS
40	l3	74	GLU
40	l3	77	THR
40	l3	79	VAL
40	l3	81	THR
40	l3	85	VAL
40	l3	87	VAL
40	l3	103	THR
40	l3	114	VAL
40	l3	126	LYS
40	l3	132	LYS
40	l3	139	GLN
40	l3	140	ASP
40	l3	146	ARG
40	l3	148	LEU
40	l3	150	ARG
40	l3	156	SER
40	l3	157	VAL
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	208	VAL
40	l3	211	GLN
40	l3	221	THR
40	l3	232	ARG
40	l3	235	THR
40	l3	237	LYS
40	l3	238	LEU
40	l3	242	THR
40	l3	244	ARG
40	l3	252	ILE
40	l3	264	VAL
40	l3	266	ARG
40	l3	274	SER
40	l3	284	ARG
40	l3	297	SER

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Mol	Chain	Res	Type
40	l3	304	THR
40	l3	308	MET
40	l3	317	ILE
40	l3	328	ILE
40	l3	332	ARG
40	l3	338	LEU
40	l3	346	THR
40	l3	359	ILE
40	l3	363	SER
40	l3	382	THR
41	l4	3	ARG
41	l4	6	VAL
41	l4	25	VAL
41	l4	47	ARG
41	l4	52	VAL
41	l4	53	SER
41	l4	55	LYS
41	l4	69	ARG
41	l4	73	ARG
41	l4	90	PHE
41	l4	93	MET
41	l4	98	ARG
41	l4	112	LYS
41	l4	120	TYR
41	l4	122	THR
41	l4	129	THR
41	l4	144	LYS
41	l4	156	LEU
41	l4	172	VAL
41	l4	176	SER
41	l4	177	ASP
41	l4	179	LEU
41	l4	182	LEU
41	l4	186	LYS
41	l4	187	LEU
41	l4	203	ARG
41	l4	206	LEU
41	l4	215	ILE
41	l4	222	VAL
41	l4	226	GLU
41	l4	230	VAL
41	l4	233	LEU

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Mol	Chain	Res	Type
41	l4	287	THR
41	l4	291	ASN
41	l4	299	ILE
41	l4	300	ARG
41	l4	301	PRO
41	l4	304	GLN
41	l4	306	THR
41	l4	307	GLN
41	l4	310	THR
41	l4	313	LEU
41	l4	319	LYS
41	l4	323	VAL
41	l4	327	LEU
41	l4	333	VAL
41	l4	338	LYS
41	l4	339	LEU
41	l4	342	LYS
41	l4	345	GLU
41	l4	346	LYS
41	l4	347	THR
41	l4	349	THR
41	l4	356	THR
41	l4	357	GLU
41	l4	359	LEU
42	l5	9	SER
42	l5	10	SER
42	l5	15	ARG
42	l5	34	LYS
42	l5	35	ARG
42	l5	41	LYS
42	l5	51	LEU
42	l5	61	ILE
42	l5	68	THR
42	l5	70	THR
42	l5	73	VAL
42	l5	74	VAL
42	l5	75	LEU
42	l5	109	THR
42	l5	110	LEU
42	l5	112	LYS
42	l5	113	LEU
42	l5	115	LEU

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Mol	Chain	Res	Type
42	l5	118	THR
42	l5	120	LYS
42	l5	131	LEU
42	l5	133	GLU
42	l5	135	VAL
42	l5	140	ARG
42	l5	144	VAL
42	l5	146	LEU
42	l5	148	ILE
42	l5	152	ARG
42	l5	155	THR
42	l5	164	LYS
42	l5	176	SER
42	l5	183	TRP
42	l5	185	PHE
42	l5	187	THR
42	l5	194	LEU
42	l5	211	LEU
42	l5	218	ARG
42	l5	227	LEU
42	l5	230	ASP
42	l5	236	LEU
42	l5	238	ASP
42	l5	239	ILE
42	l5	254	LYS
42	l5	258	LYS
42	l5	259	LYS
42	l5	262	LYS
42	l5	268	GLU
42	l5	271	LYS
42	l5	275	THR
42	l5	279	LYS
42	l5	293	LEU
43	l6	8	LYS
43	l6	14	ASP
43	l6	15	VAL
43	l6	20	LYS
43	l6	21	THR
43	l6	31	ARG
43	l6	46	ARG
43	l6	64	LEU
43	l6	65	ILE

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Mol	Chain	Res	Type
43	l6	78	ARG
43	l6	82	ARG
43	l6	89	THR
43	l6	91	VAL
43	l6	98	VAL
43	l6	99	GLU
43	l6	131	LYS
43	l6	133	GLU
43	l6	150	LYS
43	l6	152	THR
43	l6	155	LEU
43	l6	170	LYS
43	l6	175	LYS
44	l7	24	GLU
44	l7	30	ARG
44	l7	41	ARG
44	l7	45	LEU
44	l7	54	GLU
44	l7	60	ARG
44	l7	82	LYS
44	l7	83	LEU
44	l7	88	ARG
44	l7	94	LYS
44	l7	100	ARG
44	l7	121	LYS
44	l7	124	LEU
44	l7	130	ILE
44	l7	156	ILE
44	l7	158	LYS
44	l7	159	GLN
44	l7	173	LEU
44	l7	178	ILE
44	l7	179	LEU
44	l7	181	ILE
44	l7	184	LEU
44	l7	193	PRO
44	l7	219	LYS
44	l7	229	PHE
44	l7	239	LEU
44	l7	242	SER
44	l7	244	ASN
45	l8	29	SER

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Mol	Chain	Res	Type
45	l8	40	VAL
45	l8	41	GLN
45	l8	46	LEU
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	82	LEU
45	l8	83	ASP
45	l8	85	ASN
45	l8	93	LEU
45	l8	95	ASN
45	l8	111	LYS
45	l8	128	LYS
45	l8	132	VAL
45	l8	136	LEU
45	l8	147	LYS
45	l8	149	LYS
45	l8	153	ILE
45	l8	160	ILE
45	l8	163	VAL
45	l8	164	VAL
45	l8	169	LEU
45	l8	183	LYS
45	l8	200	LEU
45	l8	208	GLU
45	l8	211	LEU
45	l8	213	LYS
45	l8	214	LEU
45	l8	224	ASP
45	l8	231	LYS
45	l8	245	LYS
45	l8	248	LYS
46	l9	5	GLN
46	l9	6	THR
46	l9	16	VAL
46	l9	18	VAL
46	l9	19	SER
46	l9	31	ARG
46	l9	33	THR

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Mol	Chain	Res	Type
46	l9	37	ASN
46	l9	43	VAL
46	l9	44	THR
46	l9	51	GLN
46	l9	52	LEU
46	l9	55	VAL
46	l9	62	ARG
46	l9	68	LEU
46	l9	69	ARG
46	l9	70	THR
46	l9	80	THR
46	l9	82	VAL
46	l9	92	TYR
46	l9	115	ARG
46	l9	118	LEU
46	l9	121	LYS
46	l9	122	LYS
46	l9	123	ILE
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	162	GLN
46	l9	163	GLN
46	l9	166	ARG
46	l9	167	VAL
46	l9	173	ARG
46	l9	179	ILE
46	l9	191	LEU
47	m0	4	ARG
47	m0	24	ARG
47	m0	28	ASP
47	m0	36	LEU
47	m0	42	THR
47	m0	44	ASP
47	m0	48	LEU
47	m0	50	VAL
47	m0	52	LEU

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Mol	Chain	Res	Type
47	m0	57	LEU
47	m0	58	GLU
47	m0	63	GLU
47	m0	71	CYS
47	m0	77	THR
47	m0	78	THR
47	m0	83	ASP
47	m0	87	LEU
47	m0	91	VAL
47	m0	99	ILE
47	m0	101	LYS
47	m0	129	VAL
47	m0	135	ILE
47	m0	139	ARG
47	m0	143	SER
47	m0	144	ASN
47	m0	145	LYS
47	m0	156	ARG
47	m0	169	LYS
47	m0	170	LYS
47	m0	176	LEU
47	m0	177	ASP
47	m0	182	LEU
47	m0	185	ARG
47	m0	197	VAL
47	m0	200	LEU
47	m0	202	LYS
47	m0	205	SER
47	m0	206	LEU
47	m0	210	ILE
47	m0	211	ARG
47	m0	212	GLU
48	m1	6	GLN
48	m1	10	ARG
48	m1	11	ASP
48	m1	12	LEU
48	m1	13	LYS
48	m1	16	LYS
48	m1	23	VAL
48	m1	37	LEU
48	m1	44	THR
48	m1	46	VAL

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Mol	Chain	Res	Type
48	m1	49	LYS
48	m1	60	ARG
48	m1	65	ILE
48	m1	78	GLU
48	m1	80	LEU
48	m1	87	LYS
48	m1	99	THR
48	m1	106	ILE
48	m1	107	ASP
48	m1	112	LEU
48	m1	122	ILE
48	m1	129	VAL
48	m1	130	VAL
48	m1	137	ARG
48	m1	138	VAL
48	m1	140	ARG
48	m1	142	LYS
48	m1	147	THR
48	m1	152	HIS
48	m1	154	THR
48	m1	158	ASP
48	m1	159	THR
48	m1	171	VAL
49	m3	28	GLN
49	m3	31	LYS
49	m3	36	ARG
49	m3	54	LEU
49	m3	55	ARG
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	103	ASN
49	m3	104	ARG
49	m3	107	GLU
49	m3	124	ILE
49	m3	131	LYS
49	m3	149	GLN
49	m3	152	THR

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Mol	Chain	Res	Type
49	m3	157	ARG
49	m3	165	SER
49	m3	171	ARG
49	m3	175	SER
49	m3	176	GLU
49	m3	184	GLU
49	m3	194	GLU
50	m4	2	SER
50	m4	3	THR
50	m4	4	ASP
50	m4	6	ILE
50	m4	13	ARG
50	m4	15	VAL
50	m4	16	GLU
50	m4	24	LYS
50	m4	27	GLN
50	m4	28	SER
50	m4	53	VAL
50	m4	58	ILE
50	m4	62	GLN
50	m4	63	VAL
50	m4	64	VAL
50	m4	66	THR
50	m4	72	LEU
50	m4	80	THR
50	m4	82	SER
50	m4	85	TRP
50	m4	105	GLN
50	m4	106	ARG
50	m4	107	GLU
50	m4	124	ARG
50	m4	130	THR
50	m4	133	LYS
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	27	VAL
51	m5	49	ARG
51	m5	50	ARG

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Mol	Chain	Res	Type
51	m5	66	VAL
51	m5	67	ARG
51	m5	68	ARG
51	m5	76	PRO
51	m5	80	THR
51	m5	85	THR
51	m5	92	LEU
51	m5	96	ARG
51	m5	97	SER
51	m5	105	ARG
51	m5	109	ARG
51	m5	117	ASN
51	m5	138	GLN
51	m5	142	ILE
51	m5	152	CYS
51	m5	153	ASP
51	m5	159	ARG
51	m5	165	THR
51	m5	170	LYS
51	m5	171	SER
51	m5	184	LYS
51	m5	190	THR
51	m5	204	LYS
52	m6	3	VAL
52	m6	4	GLU
52	m6	12	LYS
52	m6	34	VAL
52	m6	46	GLU
52	m6	51	LYS
52	m6	58	LEU
52	m6	59	ARG
52	m6	66	LYS
52	m6	67	THR
52	m6	74	ARG
52	m6	78	ARG
52	m6	79	ILE
52	m6	84	LEU
52	m6	85	ARG
52	m6	89	SER
52	m6	94	ARG
52	m6	100	GLU
52	m6	106	GLU

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Mol	Chain	Res	Type
52	m6	108	ILE
52	m6	110	PRO
52	m6	117	ARG
52	m6	122	GLN
52	m6	124	LEU
52	m6	128	ARG
52	m6	129	LEU
52	m6	130	LYS
52	m6	134	LYS
52	m6	144	SER
52	m6	151	ASP
52	m6	152	VAL
52	m6	160	ARG
52	m6	171	LYS
52	m6	175	THR
52	m6	182	ASN
52	m6	184	THR
52	m6	197	LEU
53	m7	7	THR
53	m7	9	THR
53	m7	20	SER
53	m7	23	ARG
53	m7	29	THR
53	m7	32	THR
53	m7	52	LEU
53	m7	79	THR
53	m7	82	ARG
53	m7	87	SER
53	m7	89	LYS
53	m7	110	THR
53	m7	112	LEU
53	m7	114	VAL
53	m7	119	VAL
53	m7	126	ARG
53	m7	127	ARG
53	m7	136	ILE
53	m7	138	LYS
53	m7	140	GLU
53	m7	144	SER
53	m7	150	VAL
53	m7	153	LYS
53	m7	155	GLU

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Mol	Chain	Res	Type
54	m8	3	ILE
54	m8	7	SER
54	m8	12	ARG
54	m8	22	ASP
54	m8	24	VAL
54	m8	26	LEU
54	m8	27	LYS
54	m8	31	LYS
54	m8	32	LEU
54	m8	34	THR
54	m8	40	THR
54	m8	46	LYS
54	m8	49	LEU
54	m8	57	ILE
54	m8	63	SER
54	m8	64	VAL
54	m8	80	THR
54	m8	81	VAL
54	m8	86	THR
54	m8	93	ILE
54	m8	98	LYS
54	m8	113	LYS
54	m8	127	LEU
54	m8	129	VAL
54	m8	135	GLN
54	m8	146	SER
54	m8	147	ARG
54	m8	165	ILE
54	m8	170	ARG
54	m8	171	LYS
54	m8	174	ARG
54	m8	176	ARG
54	m8	178	ARG
54	m8	180	ARG
54	m8	186	VAL
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

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Mol	Chain	Res	Type
55	m9	31	GLU
55	m9	36	ASN
55	m9	43	LYS
55	m9	49	THR
55	m9	56	THR
55	m9	57	VAL
55	m9	63	THR
55	m9	70	LYS
55	m9	74	ARG
55	m9	76	SER
55	m9	88	ARG
55	m9	98	ARG
55	m9	99	LEU
55	m9	111	ASP
55	m9	117	LYS
55	m9	138	LEU
55	m9	152	GLU
55	m9	153	LYS
55	m9	156	ASN
55	m9	158	GLU
55	m9	164	LEU
55	m9	165	LYS
55	m9	167	ARG
55	m9	170	ARG
55	m9	173	ARG
55	m9	177	VAL
55	m9	180	LYS
56	n0	13	ARG
56	n0	16	THR
56	n0	23	LYS
56	n0	24	LEU
56	n0	32	SER
56	n0	45	LEU
56	n0	50	LYS
56	n0	52	LYS
56	n0	53	LYS
56	n0	60	SER
56	n0	62	ASN
56	n0	63	GLN
56	n0	70	THR
56	n0	71	LYS
56	n0	73	LYS

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Mol	Chain	Res	Type
56	n0	87	THR
56	n0	97	VAL
56	n0	100	VAL
56	n0	104	GLU
56	n0	105	THR
56	n0	115	ARG
56	n0	117	ARG
56	n0	120	SER
56	n0	130	GLU
56	n0	136	LYS
56	n0	137	ARG
56	n0	145	THR
56	n0	148	LEU
56	n0	149	LYS
56	n0	155	ARG
56	n0	160	THR
56	n0	161	LYS
56	n0	162	THR
56	n0	164	SER
56	n0	166	LYS
56	n0	167	ARG
56	n0	169	SER
56	n0	172	TYR
57	n1	12	ARG
57	n1	17	ARG
57	n1	26	HIS
57	n1	27	LEU
57	n1	35	LYS
57	n1	47	SER
57	n1	55	LYS
57	n1	68	THR
57	n1	71	SER
57	n1	75	ILE
57	n1	78	LYS
57	n1	80	VAL
57	n1	83	ARG
57	n1	88	ARG
57	n1	89	LEU
57	n1	96	ILE
57	n1	97	LYS
57	n1	102	ARG
57	n1	127	GLN

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Mol	Chain	Res	Type
57	n1	130	ARG
57	n1	139	ARG
57	n1	140	ILE
57	n1	141	VAL
57	n1	143	THR
57	n1	149	GLN
57	n1	150	THR
58	n2	11	ILE
58	n2	16	THR
58	n2	23	THR
58	n2	27	VAL
58	n2	37	LEU
58	n2	38	ILE
58	n2	43	VAL
58	n2	50	LEU
58	n2	54	VAL
58	n2	55	THR
58	n2	58	GLU
58	n2	62	VAL
58	n2	63	VAL
58	n2	68	THR
58	n2	90	ARG
58	n2	92	TRP
58	n2	94	ARG
58	n2	98	THR
59	n3	4	ASN
59	n3	13	ILE
59	n3	14	SER
59	n3	15	LEU
59	n3	42	SER
59	n3	45	ARG
59	n3	48	ARG
59	n3	63	LYS
59	n3	66	LYS
59	n3	72	LYS
59	n3	79	VAL
59	n3	83	LYS
59	n3	88	ARG
59	n3	91	VAL
59	n3	93	LEU
59	n3	115	THR
59	n3	120	LYS

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Mol	Chain	Res	Type
60	n4	1	MET
60	n4	19	THR
60	n4	39	LEU
60	n4	54	LEU
60	n4	57	LYS
60	n4	63	ILE
60	n4	87	LEU
60	n4	96	LEU
60	n4	97	LYS
60	n4	100	VAL
60	n4	104	ASN
60	n4	107	GLU
60	n4	127	LYS
60	n4	135	SER
61	n5	27	ARG
61	n5	37	THR
61	n5	40	LEU
61	n5	46	TYR
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	71	THR
61	n5	74	LYS
61	n5	78	ASP
61	n5	86	VAL
61	n5	108	LEU
61	n5	109	LYS
61	n5	115	ARG
61	n5	117	ASN
61	n5	119	THR
61	n5	125	ARG
61	n5	133	LEU
61	n5	134	ASP
61	n5	135	ILE
61	n5	142	ILE
62	n6	4	GLN
62	n6	12	ARG
62	n6	13	ARG
62	n6	17	LYS
62	n6	25	SER
62	n6	37	LYS
62	n6	45	ILE

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Mol	Chain	Res	Type
62	n6	51	ARG
62	n6	52	ARG
62	n6	53	ASP
62	n6	57	LEU
62	n6	62	SER
62	n6	64	LYS
62	n6	66	GLN
62	n6	74	TYR
62	n6	80	VAL
62	n6	83	ASP
62	n6	86	THR
62	n6	88	GLU
62	n6	89	LYS
62	n6	108	LYS
62	n6	112	ASP
62	n6	120	GLN
62	n6	127	GLU
63	n7	3	LYS
63	n7	5	LEU
63	n7	14	VAL
63	n7	15	ARG
63	n7	17	ARG
63	n7	21	LYS
63	n7	24	VAL
63	n7	26	VAL
63	n7	36	HIS
63	n7	46	ILE
63	n7	52	LYS
63	n7	65	ARG
63	n7	72	ILE
63	n7	81	LEU
63	n7	83	THR
63	n7	86	THR
63	n7	88	ASP
63	n7	90	GLU
63	n7	92	PHE
63	n7	94	SER
63	n7	98	THR
63	n7	102	GLU
63	n7	103	GLN
63	n7	105	SER
63	n7	126	LYS

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Mol	Chain	Res	Type
63	n7	134	LEU
63	n7	135	ARG
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	10	LYS
64	n8	14	HIS
64	n8	42	ARG
64	n8	46	ASP
64	n8	60	TYR
64	n8	64	GLN
64	n8	65	GLN
64	n8	70	LYS
64	n8	76	ASP
64	n8	78	LEU
64	n8	82	ILE
64	n8	91	LEU
64	n8	98	THR
64	n8	115	LYS
64	n8	124	ILE
64	n8	133	LEU
64	n8	146	GLU
65	n9	3	LYS
65	n9	5	LYS
65	n9	12	GLN
65	n9	19	ASN
65	n9	21	ILE
65	n9	22	LYS
65	n9	23	LYS
65	n9	35	VAL
65	n9	38	LYS
65	n9	54	LEU
65	n9	58	LYS
65	n9	59	LYS
66	o0	9	SER
66	o0	10	ILE
66	o0	12	GLN
66	o0	18	ILE
66	o0	32	LYS
66	o0	33	SER
66	o0	34	LEU
66	o0	40	LYS

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Mol	Chain	Res	Type
66	o0	43	ILE
66	o0	44	ILE
66	o0	48	THR
66	o0	50	VAL
66	o0	55	GLU
66	o0	61	MET
66	o0	68	TYR
66	o0	74	ASN
66	o0	81	VAL
66	o0	86	ARG
66	o0	87	VAL
67	o1	6	ASP
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	31	ARG
67	o1	34	LYS
67	o1	38	LYS
67	o1	44	MET
67	o1	48	ASP
67	o1	61	LYS
67	o1	68	GLU
67	o1	76	SER
67	o1	82	GLU
67	o1	83	GLU
67	o1	89	LEU
67	o1	90	PHE
67	o1	93	VAL
67	o1	102	LYS
67	o1	104	LEU
67	o1	106	THR
67	o1	107	VAL
67	o1	110	GLU
67	o1	112	ASP
68	o2	5	PRO
68	o2	6	HIS
68	o2	16	LYS
68	o2	19	ARG
68	o2	21	HIS
68	o2	24	ARG
68	o2	31	ASN

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Mol	Chain	Res	Type
68	o2	33	ARG
68	o2	35	GLN
68	o2	51	SER
68	o2	52	GLN
68	o2	54	LYS
68	o2	61	LYS
68	o2	62	LYS
68	o2	71	HIS
68	o2	73	THR
68	o2	75	LEU
68	o2	81	ASP
68	o2	82	LEU
68	o2	84	THR
68	o2	86	THR
68	o2	87	MET
68	o2	91	THR
68	o2	101	SER
68	o2	106	VAL
68	o2	113	LYS
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	10	LYS
69	o3	31	LYS
69	o3	49	ILE
69	o3	56	SER
69	o3	59	VAL
69	o3	70	LYS
69	o3	74	THR
69	o3	84	THR
69	o3	92	LYS
69	o3	93	THR
69	o3	97	SER
69	o3	98	VAL
69	o3	107	ILE
70	o4	5	VAL
70	o4	8	ARG
70	o4	9	ARG
70	o4	20	ILE
70	o4	21	LYS
70	o4	23	VAL
70	o4	29	ILE

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Mol	Chain	Res	Type
70	o4	31	ARG
70	o4	38	LEU
70	o4	47	CYS
70	o4	58	ARG
70	o4	65	VAL
70	o4	68	THR
70	o4	79	SER
70	o4	85	VAL
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	21	LEU
71	o5	27	GLU
71	o5	28	LEU
71	o5	36	LEU
71	o5	37	SER
71	o5	40	SER
71	o5	47	VAL
71	o5	48	ARG
71	o5	57	VAL
71	o5	63	ARG
71	o5	81	ARG
71	o5	85	THR
71	o5	89	ARG
71	o5	90	ARG
71	o5	101	THR
71	o5	105	ARG
71	o5	107	LYS
71	o5	108	GLN
72	o6	3	VAL
72	o6	7	ILE
72	o6	9	ILE
72	o6	12	ASN
72	o6	18	THR
72	o6	26	ILE
72	o6	34	SER
72	o6	35	ASN
72	o6	36	ARG

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Mol	Chain	Res	Type
72	o6	37	THR
72	o6	38	LYS
72	o6	42	SER
72	o6	43	LEU
72	o6	45	ARG
72	o6	46	GLU
72	o6	47	ILE
72	o6	56	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	59	ASP
72	o6	60	LEU
72	o6	68	ARG
72	o6	76	ARG
72	o6	79	SER
72	o6	88	GLU
72	o6	94	ILE
72	o6	98	ARG
73	o7	5	THR
73	o7	17	THR
73	o7	21	ARG
73	o7	25	ARG
73	o7	33	THR
73	o7	36	SER
73	o7	40	PRO
73	o7	44	THR
73	o7	55	ARG
73	o7	58	THR
73	o7	59	THR
73	o7	67	LEU
73	o7	70	VAL
73	o7	74	PHE
73	o7	80	THR
73	o7	85	LYS
74	o8	5	ILE
74	o8	12	LEU
74	o8	20	VAL
74	o8	24	THR
74	o8	31	LEU
74	o8	41	THR
74	o8	53	THR
74	o8	64	LYS

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Mol	Chain	Res	Type
74	o8	65	LEU
74	o8	72	THR
75	o9	4	GLN
75	o9	5	LYS
75	o9	17	LYS
75	o9	21	ARG
75	o9	23	LEU
75	o9	28	ARG
75	o9	45	ARG
76	q0	79	GLU
76	q0	85	LEU
76	q0	87	SER
76	q0	93	LYS
76	q0	94	SER
76	q0	106	ARG
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	127	LEU
77	q1	2	ARG
77	q1	6	ARG
77	q1	9	ARG
77	q1	13	LEU
77	q1	21	ARG
77	q1	23	ARG
78	q2	2	VAL
78	q2	6	LYS
78	q2	7	THR
78	q2	8	ARG
78	q2	26	THR
78	q2	38	GLN
78	q2	45	ARG
78	q2	46	LYS
78	q2	48	SER
78	q2	61	LYS
78	q2	68	VAL
78	q2	71	ARG
78	q2	78	LYS
78	q2	79	THR
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU

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Mol	Chain	Res	Type
78	q2	93	LEU
78	q2	100	LYS
79	q3	3	LYS
79	q3	10	ILE
79	q3	20	SER
79	q3	24	ARG
79	q3	40	SER
79	q3	42	CYS
79	q3	48	LYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	57	CYS
79	q3	70	THR
79	q3	73	THR
79	q3	81	SER
79	q3	90	VAL
79	q3	91	GLU
82	p0	4	ILE
82	p0	10	GLU
82	p0	30	VAL
82	p0	31	ASP
82	p0	39	HIS
82	p0	42	ARG
82	p0	43	LYS
82	p0	48	ARG
82	p0	70	LEU
82	p0	72	ASP
82	p0	80	VAL
82	p0	81	LYS
82	p0	93	LEU
82	p0	97	LYS
82	p0	101	VAL
82	p0	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
2	S0	168	HIS
3	S1	232	HIS
6	S4	67	GLN
7	S5	103	ASN

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Mol	Chain	Res	Type
7	S5	139	ASN
9	S7	170	GLN
9	S7	174	ASN
12	C0	12	HIS
22	D0	40	ASN
22	D0	121	ASN
23	D1	70	ASN
24	D2	56	HIS
27	D5	95	HIS
29	D7	26	GLN
29	D7	49	HIS
39	L2	209	HIS
42	L5	40	HIS
42	L5	264	GLN
43	L6	28	GLN
44	L7	25	GLN
44	L7	244	ASN
45	L8	38	GLN
46	L9	8	GLN
46	L9	59	ASN
47	M0	59	GLN
47	M0	144	ASN
49	M3	25	HIS
50	M4	126	GLN
55	M9	34	GLN
57	N1	98	HIS
59	N3	98	ASN
61	N5	80	ASN
63	N7	127	ASN
72	O6	63	ASN
78	Q2	22	GLN
78	Q2	99	GLN
78	Q2	102	GLN
2	s0	21	ASN
3	s1	149	GLN
5	s3	74	GLN
7	s5	104	ASN
9	s7	110	GLN
9	s7	122	HIS
9	s7	174	ASN
11	s9	142	ASN
15	c3	49	GLN

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Mol	Chain	Res	Type
26	d4	22	GLN
39	l2	50	HIS
44	l7	186	HIS
54	m8	58	ASN
58	n2	101	ASN
61	n5	111	ASN
63	n7	57	HIS
64	n8	49	HIS
75	o9	4	GLN
75	o9	38	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	480 (27%)	50 (2%)
1	6	1792/1800 (99%)	484 (27%)	49 (2%)
36	1	3145/3396 (92%)	690 (21%)	93 (2%)
36	5	3145/3396 (92%)	693 (22%)	78 (2%)
37	3	120/121 (99%)	17 (14%)	1 (0%)
37	7	120/121 (99%)	20 (16%)	1 (0%)
38	4	157/158 (99%)	40 (25%)	6 (3%)
38	8	157/158 (99%)	38 (24%)	1 (0%)
All	All	10383/10950 (94%)	2462 (23%)	279 (2%)

All (2462) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	45	U
1	2	46	A
1	2	47	A
1	2	57	G
1	2	60	U
1	2	66	U
1	2	67	A

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Mol	Chain	Res	Type
1	2	68	A
1	2	69	G
1	2	71	A
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	95	G
1	2	104	A
1	2	114	C
1	2	115	G
1	2	126	A
1	2	127	G
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	167	U
1	2	169	A
1	2	178	U
1	2	185	U
1	2	186	C
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

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Mol	Chain	Res	Type
1	2	200	A
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	226	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	231	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	236	A
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U
1	2	250	C
1	2	257	A
1	2	260	U
1	2	261	U
1	2	262	U
1	2	265	A
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	302	U
1	2	314	C
1	2	316	A
1	2	319	U

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Mol	Chain	Res	Type
1	2	321	C
1	2	322	G
1	2	337	G
1	2	338	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	381	C
1	2	387	A
1	2	397	A
1	2	400	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	418	G
1	2	419	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	434	G
1	2	437	A
1	2	439	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	454	U
1	2	464	A
1	2	468	A
1	2	477	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

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Mol	Chain	Res	Type
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	519	C
1	2	520	A
1	2	527	A
1	2	534	A
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
1	2	548	G
1	2	555	A
1	2	556	A
1	2	558	U
1	2	559	C
1	2	565	C
1	2	566	C
1	2	579	A
1	2	580	A
1	2	594	A
1	2	595	G
1	2	597	G
1	2	606	A
1	2	609	U
1	2	611	U
1	2	617	U
1	2	619	A
1	2	620	A

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Mol	Chain	Res	Type
1	2	621	A
1	2	622	A
1	2	623	A
1	2	630	A
1	2	639	U
1	2	640	U
1	2	645	C
1	2	648	G
1	2	650	U
1	2	653	C
1	2	655	G
1	2	656	G
1	2	658	C
1	2	677	G
1	2	680	U
1	2	682	C
1	2	684	A
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	711	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	722	G
1	2	723	G
1	2	724	C
1	2	725	U
1	2	727	U

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Mol	Chain	Res	Type
1	2	728	U
1	2	729	G
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	744	U
1	2	753	A
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	785	U
1	2	789	A
1	2	794	U
1	2	795	U
1	2	806	A
1	2	811	A
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G

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Mol	Chain	Res	Type
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	841	U
1	2	846	G
1	2	854	U
1	2	856	A
1	2	861	U
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	904	G
1	2	911	U
1	2	912	U
1	2	913	G
1	2	914	G
1	2	916	U
1	2	921	U
1	2	933	A
1	2	935	U
1	2	942	G
1	2	944	A
1	2	951	A
1	2	960	U
1	2	961	U
1	2	966	A
1	2	984	G
1	2	987	G
1	2	992	A
1	2	993	A
1	2	995	A
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1026	A

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Mol	Chain	Res	Type
1	2	1028	C
1	2	1031	U
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1075	C
1	2	1079	U
1	2	1081	A
1	2	1082	C
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1101	G
1	2	1111	G
1	2	1117	U
1	2	1121	C
1	2	1138	A
1	2	1143	A
1	2	1149	G
1	2	1150	G
1	2	1151	A
1	2	1157	A
1	2	1158	C
1	2	1159	C
1	2	1160	A
1	2	1163	A
1	2	1166	A
1	2	1167	G
1	2	1168	U
1	2	1176	G
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A

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Mol	Chain	Res	Type
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1207	C
1	2	1217	A
1	2	1218	G
1	2	1226	A
1	2	1227	A
1	2	1228	G
1	2	1235	C
1	2	1241	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1258	U
1	2	1284	C
1	2	1286	U
1	2	1287	A
1	2	1290	U
1	2	1314	U
1	2	1315	U
1	2	1321	A
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1342	C
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1361	U
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1367	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1383	G
1	2	1388	A

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Mol	Chain	Res	Type
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1412	G
1	2	1413	U
1	2	1414	U
1	2	1415	U
1	2	1424	A
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1433	G
1	2	1445	G
1	2	1446	A
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1461	C
1	2	1469	A
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1478	G
1	2	1481	C
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	1501	C
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	1540	G
1	2	1556	A
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1573	A
1	2	1574	G
1	2	1584	G
1	2	1590	G
1	2	1591	C
1	2	1596	C
1	2	1600	A
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1619	C
1	2	1631	A
1	2	1634	C
1	2	1637	C
1	2	1657	U
1	2	1658	G
1	2	1663	G
1	2	1680	G
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1685	G
1	2	1719	A
1	2	1731	A
1	2	1747	G
1	2	1756	A
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1768	G
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G

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Mol	Chain	Res	Type
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	13	A
36	1	15	C
36	1	16	A
36	1	26	A
36	1	33	G
36	1	40	A
36	1	45	A
36	1	49	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	74	G
36	1	76	G
36	1	83	U
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	116	A
36	1	117	U
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	147	U
36	1	156	G
36	1	157	A
36	1	165	A
36	1	166	C
36	1	169	U
36	1	187	A
36	1	190	U
36	1	191	U

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Mol	Chain	Res	Type
36	1	192	C
36	1	210	U
36	1	218	G
36	1	219	A
36	1	224	C
36	1	237	G
36	1	240	U
36	1	241	G
36	1	243	G
36	1	245	U
36	1	247	C
36	1	248	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	270	U
36	1	282	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	305	U
36	1	311	C
36	1	315	C
36	1	323	A
36	1	329	U
36	1	339	C
36	1	344	A
36	1	349	A
36	1	350	C
36	1	376	G
36	1	397	A
36	1	398	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	412	G
36	1	417	A
36	1	421	G

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Mol	Chain	Res	Type
36	1	422	A
36	1	438	A
36	1	439	C
36	1	440	A
36	1	495	G
36	1	498	A
36	1	507	U
36	1	520	U
36	1	521	A
36	1	535	G
36	1	541	U
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G
36	1	549	U
36	1	551	A
36	1	552	G
36	1	555	U
36	1	556	U
36	1	557	A
36	1	559	A
36	1	560	G
36	1	578	A
36	1	579	G
36	1	585	A
36	1	592	A
36	1	600	G
36	1	604	G
36	1	607	A
36	1	609	G
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A
36	1	636	C
36	1	638	C
36	1	640	U
36	1	649	A
36	1	660	A
36	1	661	G
36	1	677	A

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Mol	Chain	Res	Type
36	1	681	U
36	1	683	U
36	1	691	A
36	1	705	A
36	1	712	G
36	1	715	A
36	1	716	A
36	1	725	G
36	1	726	G
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	781	G
36	1	785	G
36	1	806	A
36	1	811	U
36	1	816	A
36	1	817	A
36	1	830	A
36	1	837	A
36	1	849	C
36	1	859	G
36	1	860	G
36	1	861	C
36	1	874	U
36	1	879	U
36	1	882	A
36	1	890	C
36	1	896	A
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	937	G
36	1	939	U

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Mol	Chain	Res	Type
36	1	943	U
36	1	944	C
36	1	959	C
36	1	960	U
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	993	G
36	1	994	G
36	1	1001	G
36	1	1002	A
36	1	1003	A
36	1	1006	A
36	1	1010	G
36	1	1013	G
36	1	1015	U
36	1	1016	C
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1021	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1037	C
36	1	1042	U
36	1	1045	C
36	1	1047	A
36	1	1049	C
36	1	1064	A
36	1	1065	A
36	1	1068	C
36	1	1069	C
36	1	1072	G
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1087	G
36	1	1093	A
36	1	1094	U

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Mol	Chain	Res	Type
36	1	1095	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1111	U
36	1	1117	G
36	1	1128	U
36	1	1131	G
36	1	1149	G
36	1	1150	A
36	1	1153	A
36	1	1159	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1191	U
36	1	1192	C
36	1	1197	A
36	1	1201	C
36	1	1209	G
36	1	1213	G
36	1	1216	C
36	1	1218	U
36	1	1222	G
36	1	1225	A
36	1	1226	G
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1235	U
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1253	U
36	1	1258	U
36	1	1259	A

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Mol	Chain	Res	Type
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1267	U
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1274	A
36	1	1278	A
36	1	1279	C
36	1	1280	C
36	1	1285	G
36	1	1287	A
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1314	C
36	1	1317	A
36	1	1323	G
36	1	1324	U
36	1	1330	A
36	1	1331	U
36	1	1336	U
36	1	1345	G
36	1	1348	U
36	1	1349	G
36	1	1350	A
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1354	G
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1367	G
36	1	1386	A
36	1	1392	G
36	1	1399	A
36	1	1400	G
36	1	1417	G

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Mol	Chain	Res	Type
36	1	1418	A
36	1	1419	A
36	1	1433	A
36	1	1434	G
36	1	1437	C
36	1	1446	A
36	1	1450	G
36	1	1454	A
36	1	1455	U
36	1	1462	A
36	1	1465	A
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1502	C
36	1	1508	C
36	1	1516	C
36	1	1527	C
36	1	1529	A
36	1	1531	C
36	1	1533	U
36	1	1536	G
36	1	1549	U
36	1	1555	U
36	1	1556	C
36	1	1557	A
36	1	1559	A
36	1	1560	G
36	1	1561	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1571	A
36	1	1572	U
36	1	1579	C
36	1	1580	A
36	1	1581	C

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Mol	Chain	Res	Type
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1605	A
36	1	1620	U
36	1	1621	A
36	1	1629	U
36	1	1630	U
36	1	1633	C
36	1	1639	C
36	1	1643	A
36	1	1654	A
36	1	1657	C
36	1	1677	G
36	1	1683	A
36	1	1688	U
36	1	1713	G
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1736	G
36	1	1750	A
36	1	1751	G
36	1	1760	A
36	1	1761	C
36	1	1762	C
36	1	1763	U
36	1	1764	U
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1769	G
36	1	1770	G
36	1	1780	G
36	1	1781	C
36	1	1783	U
36	1	1797	A
36	1	1809	A
36	1	1810	A
36	1	1814	A
36	1	1816	A

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Mol	Chain	Res	Type
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1825	G
36	1	1834	U
36	1	1839	A
36	1	1841	A
36	1	1842	A
36	1	1845	G
36	1	1846	C
36	1	1847	A
36	1	1849	C
36	1	1850	A
36	1	1855	U
36	1	1866	C
36	1	1871	U
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1895	A
36	1	1897	G
36	1	1901	A
36	1	1906	G
36	1	1908	A
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	1954	G
36	1	2094	C
36	1	2097	U
36	1	2101	C
36	1	2102	U
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2115	G
36	1	2116	G
36	1	2121	G
36	1	2122	G
36	1	2131	A
36	1	2134	G

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Mol	Chain	Res	Type
36	1	2140	U
36	1	2144	A
36	1	2158	A
36	1	2169	G
36	1	2173	U
36	1	2184	U
36	1	2185	G
36	1	2187	G
36	1	2193	U
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	2234	G
36	1	2239	G
36	1	2244	A
36	1	2245	C
36	1	2249	G
36	1	2250	G
36	1	2252	A
36	1	2255	A
36	1	2256	A
36	1	2262	A
36	1	2272	G
36	1	2273	G
36	1	2281	A
36	1	2282	U
36	1	2284	C
36	1	2299	A
36	1	2303	A
36	1	2304	C
36	1	2306	C
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2315	G
36	1	2317	A
36	1	2334	U
36	1	2336	U
36	1	2362	C

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Mol	Chain	Res	Type
36	1	2366	C
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2388	U
36	1	2392	C
36	1	2393	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2405	C
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2435	G
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2504	U
36	1	2509	U
36	1	2514	U
36	1	2515	A
36	1	2522	G
36	1	2523	A
36	1	2532	U
36	1	2533	G
36	1	2534	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2544	U
36	1	2549	G
36	1	2552	C
36	1	2554	A

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Mol	Chain	Res	Type
36	1	2555	G
36	1	2561	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2582	C
36	1	2585	G
36	1	2586	G
36	1	2593	A
36	1	2594	C
36	1	2595	A
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2617	U
36	1	2618	G
36	1	2628	A
36	1	2637	A
36	1	2638	C
36	1	2652	U
36	1	2656	A
36	1	2672	G
36	1	2674	A
36	1	2677	G
36	1	2689	A
36	1	2691	A
36	1	2694	A
36	1	2696	A
36	1	2705	A
36	1	2714	G
36	1	2728	G
36	1	2729	U
36	1	2752	U
36	1	2753	G
36	1	2762	A
36	1	2771	U
36	1	2772	C
36	1	2773	C
36	1	2777	G

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Mol	Chain	Res	Type
36	1	2778	G
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2803	A
36	1	2810	C
36	1	2817	A
36	1	2818	U
36	1	2822	U
36	1	2827	U
36	1	2829	U
36	1	2836	C
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2846	U
36	1	2847	A
36	1	2856	G
36	1	2860	U
36	1	2863	G
36	1	2871	G
36	1	2872	A
36	1	2886	U
36	1	2887	A
36	1	2889	C
36	1	2898	G
36	1	2899	C
36	1	2900	A
36	1	2911	A
36	1	2914	G
36	1	2923	U
36	1	2927	C
36	1	2932	U
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	2956	A

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Mol	Chain	Res	Type
36	1	2971	A
36	1	2974	U
36	1	2977	G
36	1	2979	U
36	1	2983	C
36	1	2990	G
36	1	2992	U
36	1	2997	G
36	1	3012	A
36	1	3030	G
36	1	3034	C
36	1	3040	A
36	1	3058	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3080	G
36	1	3086	A
36	1	3087	A
36	1	3092	C
36	1	3104	U
36	1	3113	A
36	1	3119	U
36	1	3122	A
36	1	3130	A
36	1	3131	U
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3164	C
36	1	3165	A
36	1	3167	A
36	1	3168	A
36	1	3169	U
36	1	3170	A
36	1	3171	U
36	1	3173	G

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Mol	Chain	Res	Type
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	3195	U
36	1	3196	U
36	1	3198	U
36	1	3207	U
36	1	3210	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3229	G
36	1	3235	C
36	1	3243	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3265	C
36	1	3266	G
36	1	3268	A
36	1	3269	U
36	1	3270	U
36	1	3273	A
36	1	3276	G
36	1	3280	U
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3288	G
36	1	3289	G
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

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Mol	Chain	Res	Type
36	1	3319	U
36	1	3320	A
36	1	3335	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
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	3363	U
36	1	3369	G
36	1	3375	A
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
36	1	3390	G
36	1	3396	U
37	3	11	A
37	3	13	A
37	3	14	U
37	3	22	A
37	3	23	A
37	3	42	A
37	3	54	U
37	3	59	U
37	3	60	G
37	3	64	A
37	3	65	G
37	3	74	C
37	3	75	G
37	3	76	A
37	3	91	G
37	3	102	A
37	3	112	G
38	4	2	A
38	4	9	A
38	4	26	U

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Mol	Chain	Res	Type
38	4	34	U
38	4	35	C
38	4	48	A
38	4	52	A
38	4	58	G
38	4	59	A
38	4	62	C
38	4	63	G
38	4	69	U
38	4	70	G
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	97	A
38	4	104	A
38	4	105	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	122	U
38	4	125	U
38	4	126	A
38	4	127	U
38	4	128	U
38	4	133	G
38	4	138	A
38	4	152	G
38	4	155	A
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	10	G
1	6	17	C
1	6	25	C

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Mol	Chain	Res	Type
1	6	26	A
1	6	27	U
1	6	34	G
1	6	42	G
1	6	47	A
1	6	57	G
1	6	60	U
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	78	A
1	6	103	A
1	6	104	A
1	6	114	C
1	6	115	G
1	6	127	G
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	144	U
1	6	145	A
1	6	153	G
1	6	158	U
1	6	159	U
1	6	166	C
1	6	175	G
1	6	178	U
1	6	181	A
1	6	182	A
1	6	185	U
1	6	187	G
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U

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Mol	Chain	Res	Type
1	6	193	U
1	6	194	U
1	6	195	G
1	6	196	G
1	6	197	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	222	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	234	G
1	6	235	G
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	260	U
1	6	261	U
1	6	265	A
1	6	270	C
1	6	271	A
1	6	272	U
1	6	273	G
1	6	275	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	287	G
1	6	299	A
1	6	304	U
1	6	308	C
1	6	313	U

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Mol	Chain	Res	Type
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	337	G
1	6	338	C
1	6	359	A
1	6	360	A
1	6	361	C
1	6	370	A
1	6	393	C
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	428	A
1	6	434	G
1	6	437	A
1	6	439	U
1	6	444	C
1	6	448	C
1	6	468	A
1	6	475	A
1	6	477	A
1	6	480	G
1	6	482	U
1	6	484	C
1	6	486	G
1	6	487	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U

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Mol	Chain	Res	Type
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	507	U
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	515	A
1	6	518	A
1	6	519	C
1	6	524	U
1	6	527	A
1	6	536	C
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	557	G
1	6	558	U
1	6	559	C
1	6	564	G
1	6	565	C
1	6	566	C
1	6	574	G
1	6	578	U
1	6	579	A
1	6	580	A
1	6	582	U
1	6	594	A
1	6	595	G
1	6	609	U
1	6	610	G
1	6	611	U

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Mol	Chain	Res	Type
1	6	617	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	630	A
1	6	637	C
1	6	639	U
1	6	640	U
1	6	645	C
1	6	648	G
1	6	650	U
1	6	652	G
1	6	653	C
1	6	658	C
1	6	659	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	669	G
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	680	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C
1	6	710	U
1	6	711	U
1	6	714	G
1	6	717	C
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U

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Mol	Chain	Res	Type
1	6	722	G
1	6	723	G
1	6	726	C
1	6	730	G
1	6	733	A
1	6	751	G
1	6	753	A
1	6	754	A
1	6	755	A
1	6	756	A
1	6	762	A
1	6	765	G
1	6	766	U
1	6	774	A
1	6	775	G
1	6	777	C
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G
1	6	789	A
1	6	792	U
1	6	793	A
1	6	794	U
1	6	806	A
1	6	811	A
1	6	812	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	822	U
1	6	823	G
1	6	825	U
1	6	826	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	842	C

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Mol	Chain	Res	Type
1	6	862	A
1	6	863	A
1	6	864	U
1	6	865	A
1	6	873	U
1	6	881	A
1	6	898	A
1	6	906	A
1	6	912	U
1	6	913	G
1	6	914	G
1	6	916	U
1	6	928	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	945	U
1	6	959	U
1	6	960	U
1	6	966	A
1	6	969	C
1	6	970	A
1	6	971	A
1	6	983	A
1	6	989	U
1	6	991	G
1	6	992	A
1	6	993	A
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1008	G
1	6	1021	C
1	6	1026	A
1	6	1028	C
1	6	1029	U
1	6	1039	A
1	6	1040	G
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U

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Mol	Chain	Res	Type
1	6	1059	U
1	6	1060	U
1	6	1074	G
1	6	1081	A
1	6	1082	C
1	6	1091	A
1	6	1092	A
1	6	1093	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1101	G
1	6	1104	U
1	6	1105	C
1	6	1109	G
1	6	1137	A
1	6	1138	A
1	6	1139	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	1164	G
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	1203	A
1	6	1207	C
1	6	1208	A
1	6	1216	C
1	6	1217	A
1	6	1218	G
1	6	1220	C
1	6	1227	A
1	6	1228	G

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Mol	Chain	Res	Type
1	6	1229	G
1	6	1230	A
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	1254	U
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1259	U
1	6	1261	G
1	6	1275	A
1	6	1276	U
1	6	1284	C
1	6	1286	U
1	6	1288	G
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1318	G
1	6	1319	A
1	6	1321	A
1	6	1327	C
1	6	1338	C
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1347	U
1	6	1349	G
1	6	1354	G
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1367	G
1	6	1371	A
1	6	1372	U
1	6	1373	C

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Mol	Chain	Res	Type
1	6	1377	U
1	6	1383	G
1	6	1388	A
1	6	1390	U
1	6	1391	A
1	6	1396	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1413	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1429	G
1	6	1433	G
1	6	1445	G
1	6	1446	A
1	6	1447	C
1	6	1448	G
1	6	1458	G
1	6	1459	C
1	6	1461	C
1	6	1471	A
1	6	1481	C
1	6	1482	C
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1496	U
1	6	1506	G
1	6	1514	U
1	6	1516	A
1	6	1517	U
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1531	G
1	6	1535	U
1	6	1536	G

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Mol	Chain	Res	Type
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1548	G
1	6	1549	C
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1571	C
1	6	1572	G
1	6	1573	A
1	6	1574	G
1	6	1575	G
1	6	1582	U
1	6	1584	G
1	6	1590	G
1	6	1601	G
1	6	1616	G
1	6	1621	U
1	6	1631	A
1	6	1634	C
1	6	1637	C
1	6	1638	G
1	6	1654	G
1	6	1656	U
1	6	1657	U
1	6	1658	G
1	6	1678	A
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1703	C
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1731	A
1	6	1736	G
1	6	1755	A
1	6	1760	G

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Mol	Chain	Res	Type
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1779	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
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	11	A
36	5	14	U
36	5	15	C
36	5	26	A
36	5	33	G
36	5	40	A
36	5	44	U
36	5	49	A
36	5	59	G
36	5	60	A
36	5	62	A
36	5	65	A
36	5	66	A
36	5	73	C
36	5	74	G
36	5	76	G
36	5	87	U
36	5	91	G
36	5	92	G
36	5	93	C
36	5	94	G
36	5	96	G
36	5	99	A
36	5	109	A
36	5	110	G

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Mol	Chain	Res	Type
36	5	113	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	130	A
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	142	C
36	5	151	A
36	5	152	U
36	5	156	G
36	5	157	A
36	5	161	G
36	5	165	A
36	5	166	C
36	5	169	U
36	5	170	G
36	5	171	G
36	5	172	G
36	5	173	G
36	5	174	C
36	5	180	C
36	5	182	U
36	5	183	G
36	5	184	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	210	U
36	5	211	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	236	G
36	5	237	G
36	5	239	G
36	5	240	U
36	5	243	G
36	5	244	G

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Mol	Chain	Res	Type
36	5	246	U
36	5	247	C
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	258	G
36	5	259	C
36	5	265	A
36	5	269	G
36	5	274	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	315	C
36	5	322	U
36	5	323	A
36	5	329	U
36	5	334	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	351	A
36	5	370	U
36	5	372	A
36	5	376	G
36	5	397	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	404	G
36	5	419	G
36	5	421	G
36	5	422	A
36	5	436	A
36	5	438	A
36	5	439	C

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Mol	Chain	Res	Type
36	5	440	A
36	5	442	G
36	5	492	U
36	5	507	U
36	5	520	U
36	5	521	A
36	5	530	G
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	554	A
36	5	557	A
36	5	559	A
36	5	570	A
36	5	578	A
36	5	579	G
36	5	592	A
36	5	594	U
36	5	595	G
36	5	600	G
36	5	604	G
36	5	607	A
36	5	609	G
36	5	611	A
36	5	619	A
36	5	621	A
36	5	636	C
36	5	649	A
36	5	651	G
36	5	660	A
36	5	661	G
36	5	677	A
36	5	681	U
36	5	683	U
36	5	685	G
36	5	689	U
36	5	691	A
36	5	705	A

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Mol	Chain	Res	Type
36	5	712	G
36	5	715	A
36	5	716	A
36	5	718	G
36	5	719	U
36	5	725	G
36	5	750	G
36	5	765	C
36	5	766	U
36	5	767	U
36	5	768	C
36	5	769	G
36	5	776	U
36	5	777	U
36	5	781	G
36	5	785	G
36	5	786	A
36	5	806	A
36	5	817	A
36	5	830	A
36	5	859	G
36	5	861	C
36	5	869	G
36	5	874	U
36	5	876	A
36	5	879	U
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	931	C
36	5	937	G
36	5	938	C
36	5	944	C
36	5	953	G

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Mol	Chain	Res	Type
36	5	959	C
36	5	960	U
36	5	964	G
36	5	979	U
36	5	990	U
36	5	993	G
36	5	994	G
36	5	1001	G
36	5	1002	A
36	5	1003	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	1028	U
36	5	1029	G
36	5	1032	C
36	5	1035	G
36	5	1041	U
36	5	1047	A
36	5	1049	C
36	5	1052	U
36	5	1064	A
36	5	1065	A
36	5	1071	U
36	5	1072	G
36	5	1081	U
36	5	1082	U
36	5	1083	G
36	5	1085	A
36	5	1087	G
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U

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Mol	Chain	Res	Type
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1117	G
36	5	1121	U
36	5	1131	G
36	5	1153	A
36	5	1159	A
36	5	1164	G
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1190	A
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1201	C
36	5	1208	U
36	5	1209	G
36	5	1222	G
36	5	1232	C
36	5	1235	U
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1243	G
36	5	1244	A
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	1285	G
36	5	1307	G

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Mol	Chain	Res	Type
36	5	1308	A
36	5	1309	U
36	5	1313	G
36	5	1314	C
36	5	1321	G
36	5	1330	A
36	5	1331	U
36	5	1348	U
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1379	G
36	5	1386	A
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1421	G
36	5	1431	G
36	5	1433	A
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1465	A
36	5	1476	G
36	5	1481	A
36	5	1482	A
36	5	1490	A
36	5	1508	C
36	5	1509	A
36	5	1519	G
36	5	1527	C
36	5	1528	G
36	5	1533	U
36	5	1536	G
36	5	1539	A
36	5	1541	G

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Mol	Chain	Res	Type
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	1565	G
36	5	1566	A
36	5	1567	U
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1573	G
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1593	A
36	5	1620	U
36	5	1621	A
36	5	1629	U
36	5	1630	U
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1657	C
36	5	1663	C
36	5	1683	A
36	5	1713	G
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1725	C
36	5	1750	A

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Mol	Chain	Res	Type
36	5	1751	G
36	5	1756	C
36	5	1759	C
36	5	1760	A
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1770	G
36	5	1775	G
36	5	1778	G
36	5	1780	G
36	5	1793	C
36	5	1797	A
36	5	1810	A
36	5	1812	G
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
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1849	C
36	5	1850	A
36	5	1858	A
36	5	1864	A
36	5	1866	C
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1886	A
36	5	1891	A
36	5	1901	A
36	5	1906	G
36	5	1914	G
36	5	1935	G
36	5	1947	G

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Mol	Chain	Res	Type
36	5	1952	G
36	5	1953	G
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2111	G
36	5	2112	U
36	5	2113	A
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2133	U
36	5	2138	A
36	5	2158	A
36	5	2169	G
36	5	2170	U
36	5	2192	C
36	5	2198	A
36	5	2205	U
36	5	2209	U
36	5	2210	G
36	5	2215	A
36	5	2222	A
36	5	2223	A
36	5	2228	A
36	5	2229	A
36	5	2234	G
36	5	2244	A
36	5	2246	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	2273	G
36	5	2278	C
36	5	2279	A
36	5	2280	A
36	5	2281	A
36	5	2282	U
36	5	2288	G

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Mol	Chain	Res	Type
36	5	2303	A
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2319	U
36	5	2324	A
36	5	2331	C
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2352	A
36	5	2372	A
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	2397	A
36	5	2401	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2410	U
36	5	2411	U
36	5	2412	G
36	5	2418	G
36	5	2419	A
36	5	2435	G
36	5	2437	G
36	5	2439	A
36	5	2441	A
36	5	2443	A
36	5	2504	U
36	5	2505	U
36	5	2506	U
36	5	2507	C
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2513	U

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Mol	Chain	Res	Type
36	5	2514	U
36	5	2515	A
36	5	2522	G
36	5	2523	A
36	5	2524	A
36	5	2525	G
36	5	2526	C
36	5	2530	G
36	5	2535	A
36	5	2536	A
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2549	G
36	5	2552	C
36	5	2555	G
36	5	2562	A
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2580	A
36	5	2585	G
36	5	2588	U
36	5	2589	G
36	5	2593	A
36	5	2594	C
36	5	2598	G
36	5	2599	U
36	5	2606	G
36	5	2607	G
36	5	2614	G
36	5	2636	A
36	5	2638	C
36	5	2643	A
36	5	2652	U

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Mol	Chain	Res	Type
36	5	2656	A
36	5	2674	A
36	5	2677	G
36	5	2681	U
36	5	2683	U
36	5	2689	A
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2707	C
36	5	2714	G
36	5	2720	G
36	5	2728	G
36	5	2729	U
36	5	2742	C
36	5	2752	U
36	5	2753	G
36	5	2754	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	2779	A
36	5	2780	A
36	5	2796	G
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2810	C
36	5	2817	A
36	5	2818	U
36	5	2822	U
36	5	2829	U
36	5	2839	G
36	5	2840	C
36	5	2842	U
36	5	2843	U
36	5	2845	A
36	5	2849	C

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Mol	Chain	Res	Type
36	5	2853	A
36	5	2871	G
36	5	2872	A
36	5	2875	U
36	5	2880	U
36	5	2881	C
36	5	2887	A
36	5	2889	C
36	5	2899	C
36	5	2900	A
36	5	2902	A
36	5	2904	U
36	5	2921	U
36	5	2922	G
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2939	G
36	5	2942	C
36	5	2947	G
36	5	2971	A
36	5	2972	G
36	5	2979	U
36	5	2980	U
36	5	2983	C
36	5	2990	G
36	5	2992	U
36	5	2993	G
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3028	G
36	5	3030	G
36	5	3048	A
36	5	3056	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3092	C
36	5	3094	A
36	5	3101	G

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Mol	Chain	Res	Type
36	5	3102	G
36	5	3119	U
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	3154	C
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3164	C
36	5	3165	A
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3179	U
36	5	3180	A
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3198	U
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3227	A
36	5	3228	C
36	5	3229	G
36	5	3238	G
36	5	3239	G
36	5	3244	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3259	U

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Mol	Chain	Res	Type
36	5	3263	G
36	5	3269	U
36	5	3270	U
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	3284	G
36	5	3285	C
36	5	3286	G
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3307	A
36	5	3313	U
36	5	3316	A
36	5	3319	U
36	5	3332	U
36	5	3333	G
36	5	3335	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	3369	G
36	5	3378	C
36	5	3382	U
36	5	3389	U
36	5	3390	G
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	27	A
37	7	29	C

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Mol	Chain	Res	Type
37	7	33	U
37	7	38	U
37	7	41	G
37	7	54	U
37	7	60	G
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	92	A
37	7	93	C
37	7	99	G
37	7	101	G
37	7	102	A
37	7	103	A
37	7	112	G
38	8	9	A
38	8	18	U
38	8	21	C
38	8	34	U
38	8	35	C
38	8	48	A
38	8	49	G
38	8	51	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
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	85	G
38	8	86	U
38	8	87	G
38	8	95	G
38	8	96	A
38	8	97	A
38	8	104	A

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Mol	Chain	Res	Type
38	8	105	A
38	8	106	C
38	8	108	C
38	8	111	A
38	8	113	U
38	8	125	U
38	8	126	A
38	8	152	G
38	8	155	A
38	8	156	U
38	8	157	U
38	8	158	U

All (279) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	73	U
1	2	103	A
1	2	114	C
1	2	126	A
1	2	130	C
1	2	131	C
1	2	139	C
1	2	144	U
1	2	158	U
1	2	192	U
1	2	217	A
1	2	232	U
1	2	240	U
1	2	280	U
1	2	400	A
1	2	417	A
1	2	499	U
1	2	501	U
1	2	503	G
1	2	510	G
1	2	512	A
1	2	555	A
1	2	558	U
1	2	704	C

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Mol	Chain	Res	Type
1	2	720	G
1	2	721	U
1	2	755	A
1	2	794	U
1	2	811	A
1	2	815	G
1	2	823	G
1	2	829	A
1	2	1058	U
1	2	1150	G
1	2	1157	A
1	2	1196	A
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1489	U
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1657	U
1	2	1761	U
36	1	65	A
36	1	210	U
36	1	217	U
36	1	223	U
36	1	239	G
36	1	264	G
36	1	282	G
36	1	369	A
36	1	397	A
36	1	406	G
36	1	547	G
36	1	556	U
36	1	588	G
36	1	594	U
36	1	620	U
36	1	637	C
36	1	647	A
36	1	719	U

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Mol	Chain	Res	Type
36	1	726	G
36	1	763	G
36	1	896	A
36	1	916	G
36	1	937	G
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1181	U
36	1	1196	C
36	1	1273	A
36	1	1307	G
36	1	1329	U
36	1	1352	A
36	1	1355	A
36	1	1419	A
36	1	1484	U
36	1	1554	U
36	1	1556	C
36	1	1562	C
36	1	1568	U
36	1	1580	A
36	1	1582	C
36	1	1589	A
36	1	1643	A
36	1	1716	U
36	1	1751	G
36	1	1815	U
36	1	1816	A
36	1	1820	U
36	1	1841	A
36	1	1842	A
36	1	1849	C
36	1	2101	C
36	1	2112	U
36	1	2116	G
36	1	2209	U
36	1	2227	C
36	1	2249	G

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Mol	Chain	Res	Type
36	1	2281	A
36	1	2372	A
36	1	2374	C
36	1	2418	G
36	1	2523	A
36	1	2537	U
36	1	2538	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2728	G
36	1	2772	C
36	1	2801	A
36	1	2817	A
36	1	2818	U
36	1	2842	U
36	1	2859	U
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3169	U
36	1	3195	U
36	1	3217	C
36	1	3228	C
36	1	3269	U
36	1	3275	U
36	1	3278	C
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3355	U
37	3	13	A
38	4	82	U
38	4	85	G
38	4	111	A
38	4	125	U
38	4	126	A
38	4	157	U
1	6	25	C
1	6	66	U

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Mol	Chain	Res	Type
1	6	103	A
1	6	114	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	272	U
1	6	277	U
1	6	313	U
1	6	400	A
1	6	417	A
1	6	512	A
1	6	542	A
1	6	557	G
1	6	558	U
1	6	651	G
1	6	664	U
1	6	667	U
1	6	717	C
1	6	755	A
1	6	829	A
1	6	834	G
1	6	1051	G
1	6	1058	U
1	6	1097	U
1	6	1098	U
1	6	1137	A
1	6	1207	C
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1346	A
1	6	1398	U
1	6	1481	C
1	6	1489	U
1	6	1535	U
1	6	1572	G
1	6	1573	A
1	6	1574	G
1	6	1600	A
1	6	1615	C

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Mol	Chain	Res	Type
1	6	1620	C
1	6	1657	U
1	6	1698	G
1	6	1700	C
1	6	1754	A
36	5	122	A
36	5	151	A
36	5	183	G
36	5	210	U
36	5	217	U
36	5	221	A
36	5	238	A
36	5	264	G
36	5	269	G
36	5	374	A
36	5	397	A
36	5	647	A
36	5	765	C
36	5	816	A
36	5	873	C
36	5	896	A
36	5	916	G
36	5	937	G
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1181	U
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1317	A
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1370	G
36	5	1392	G
36	5	1481	A
36	5	1514	G

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Mol	Chain	Res	Type
36	5	1554	U
36	5	1560	G
36	5	1580	A
36	5	1716	U
36	5	1750	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1841	A
36	5	1846	C
36	5	2101	C
36	5	2112	U
36	5	2204	C
36	5	2209	U
36	5	2255	A
36	5	2257	C
36	5	2372	A
36	5	2373	A
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2572	C
36	5	2585	G
36	5	2593	A
36	5	2682	C
36	5	2728	G
36	5	2772	C
36	5	2818	U
36	5	2887	A
36	5	2971	A
36	5	3078	U
36	5	3154	C
36	5	3167	A
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3269	U
36	5	3275	U
36	5	3289	G
36	5	3340	G
36	5	3341	U
37	7	76	A

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Mol	Chain	Res	Type
38	8	111	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2558 ligands modelled in this entry, 1426 are monoatomic - leaving 1132 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4197	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	7	215	-	0,6,6	-	-	-		
86	OHX	m0	301	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	5	4179	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	1	4116	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	5	4238	-	0,6,6	-	-	-		
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	Q2	503	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	1	4179	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	O7	104	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	M7	206	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	5	4228	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	5	4194	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	5	4230	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	n9	102	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	5	4218	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	1	4176	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	5	4195	-	0,6,6	-	-	-		
86	OHX	1	4119	-	0,6,6	-	-	-		
86	OHX	m7	206	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	1	4211	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	5	4181	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	8	231	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	5	3943	86	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	S8	302	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	5	4232	-	0,6,6	-	-	-		
86	OHX	o7	503	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	5	4233	86	0,6,6	-	-	-		
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	5	4250	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	L4	403	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	1	4170	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	1	3863	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	6	2202	-	0,6,6	-	-	-		
86	OHX	4	222	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	l5	303	-	0,6,6	-	-	-		
86	OHX	l9	600	-	0,6,6	-	-	-		
86	OHX	o3	202	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	1	4204	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	N1	201	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	5	4226	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	1	4161	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	5	4249	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	7	216	-	0,6,6	-	-	-		
86	OHX	L3	405	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	1	4194	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	D3	202	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	1	4168	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	o2	201	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	M7	205	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		
86	OHX	2	2158	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	q1	102	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	6	2190	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	5	4251	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	n9	101	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	l3	404	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	m5	305	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
87	PCY	2	2178	-	36,42,42	0.45	0	41,65,65	0.86	2 (4%)
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	l5	304	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	7	225	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	M9	204	-	0,6,6	-	-	-		
86	OHX	1	4212	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	5	4223	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	m1	203	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	2	2168	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	6	2046	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	6	2203	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	8	232	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	3	224	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	S6	301	-	0,6,6	-	-	-		
86	OHX	6	2187	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	6	2201	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	5	4216	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	1	4130	-	0,6,6	-	-	-		
86	OHX	1	3867	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	n3	203	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	O3	202	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
87	PCY	6	2204	-	36,42,42	0.60	1 (2%)	41,65,65	0.91	1 (2%)
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	1	4117	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	l4	402	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	7	217	-	0,6,6	-	-	-		
86	OHX	5	4178	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	1	4188	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		
86	OHX	l5	305	-	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	m6	203	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	3	226	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	5	4197	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	3	225	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	1	4210	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	5	4248	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	l3	403	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	1	4209	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	1	4213	-	0,6,6	-	-	-		
86	OHX	4	238	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	5	4246	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		
86	OHX	1	3864	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		
86	OHX	5	4175	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	4	237	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	N9	102	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	1	4150	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	l4	403	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	1	4200	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	1	4208	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	1	4043	-	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
87	PCY	6	2204	-	-	10/33/67/67	0/3/3/3
87	PCY	2	2178	-	-	6/33/67/67	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	6	2204	PCY	C24-C28	2.12	1.42	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	2	2178	PCY	O14-C7-C13	-2.92	102.82	109.09
87	2	2178	PCY	O5-C1-N2	2.62	126.12	121.05
87	6	2204	PCY	O5-C1-N2	2.58	126.04	121.05

There are no chirality outliers.

All (16) torsion outliers are listed below:

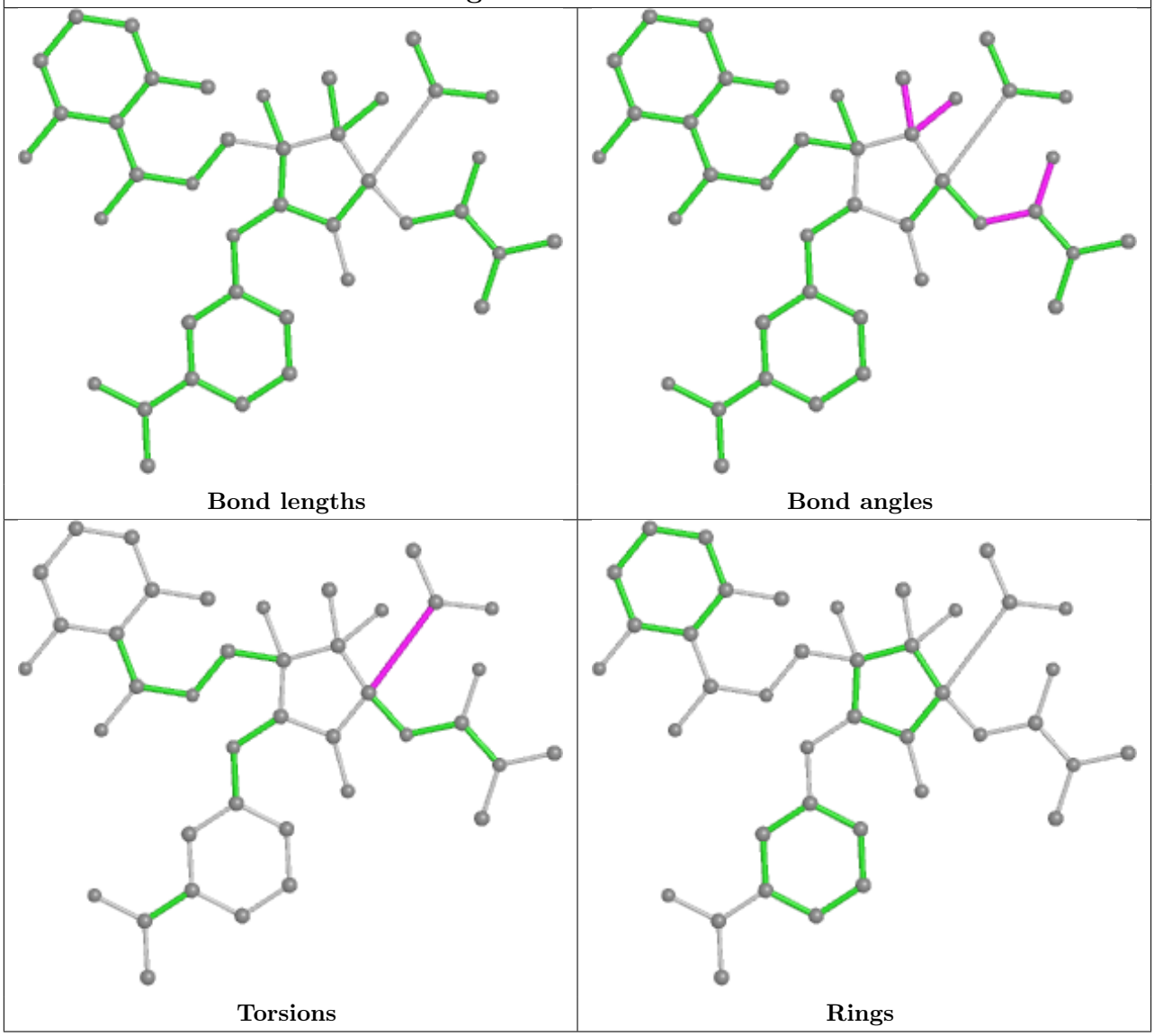
Mol	Chain	Res	Type	Atoms
87	2	2178	PCY	N2-C3-C6-C11
87	2	2178	PCY	N2-C3-C6-O12
87	2	2178	PCY	C7-C3-C6-C11
87	2	2178	PCY	C8-C3-C6-C11
87	6	2204	PCY	N2-C3-C6-C11
87	6	2204	PCY	N2-C3-C6-O12
87	6	2204	PCY	C7-C3-C6-C11
87	6	2204	PCY	C7-C3-C6-O12
87	6	2204	PCY	C8-C3-C6-C11
87	6	2204	PCY	C8-C3-C6-O12
87	6	2204	PCY	C7-C15-C18-O21
87	6	2204	PCY	O19-C15-C18-O21
87	6	2204	PCY	O26-C23-C27-C30
87	2	2178	PCY	C8-C3-C6-O12
87	2	2178	PCY	C7-C3-C6-O12
87	6	2204	PCY	O21-C23-C27-C30

There are no ring outliers.

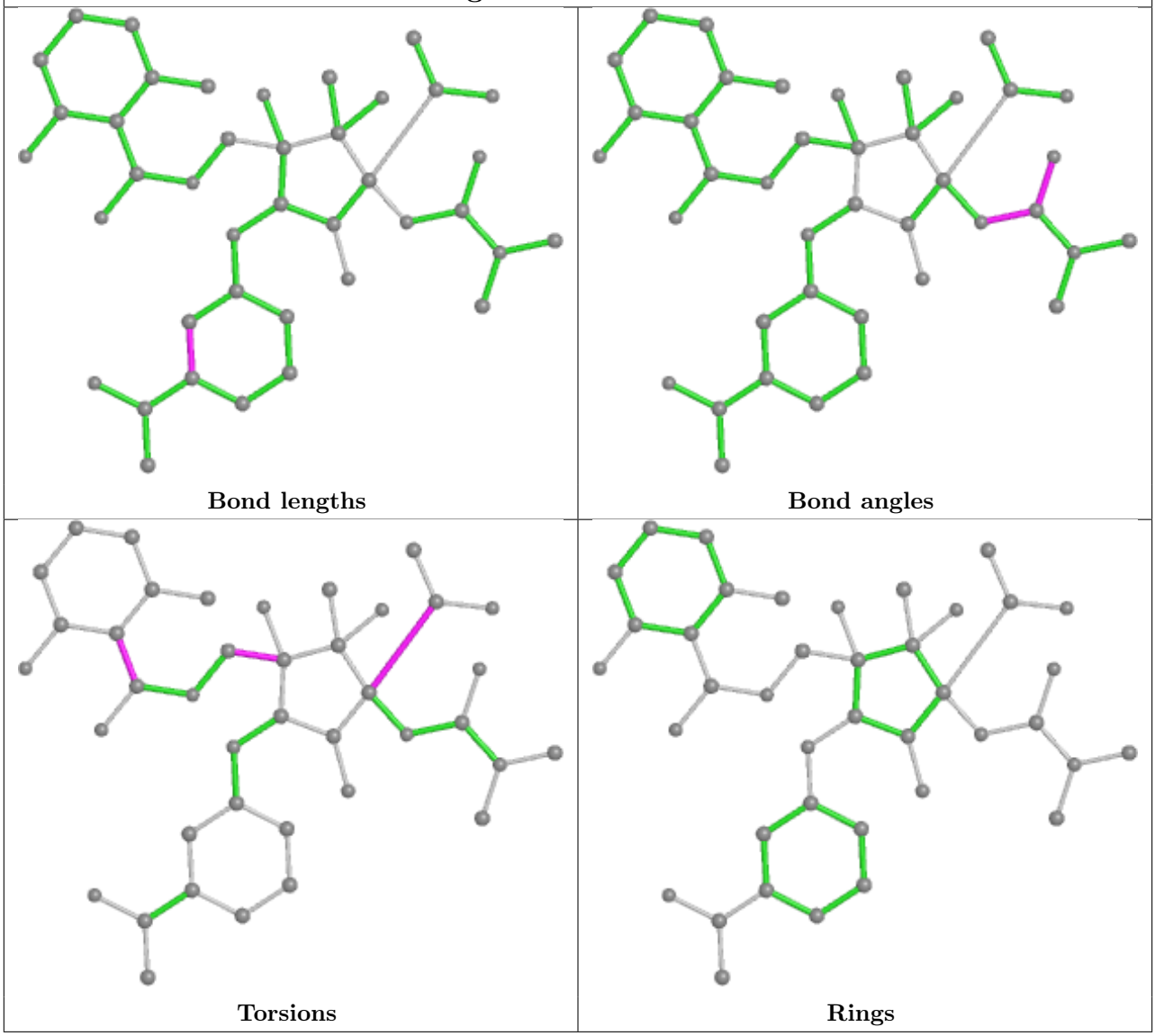
No monomer is involved in short contacts.

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 PCY 2 2178



Ligand PCY 6 2204



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.