



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 06:18 PM BST

PDB ID : 4U4N
Title : Crystal structure of Edeine bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), 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) : 2.13

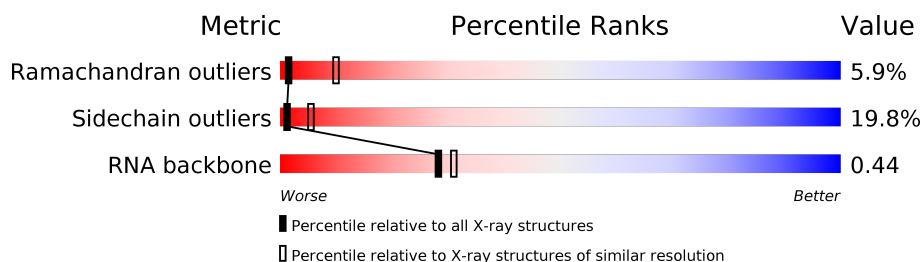
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)





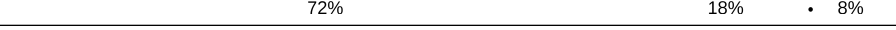
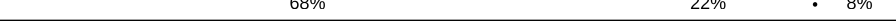

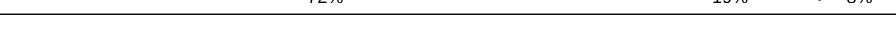
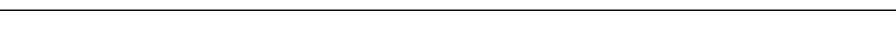
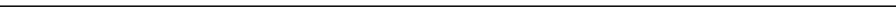















The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	62% 30% 5% .
1	6	1800	62% 32% 6%
2	S0	251	60% 21% . 18%
2	s0	251	63% 17% . 18%
3	S1	254	60% 20% . 16%
3	s1	254	67% 17% . 15%
4	S2	253	69% 16% . 14%
4	s2	253	66% 18% . 14%









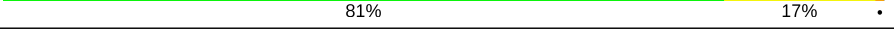


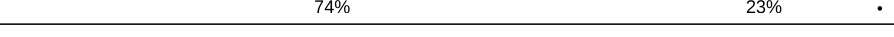

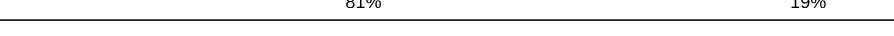


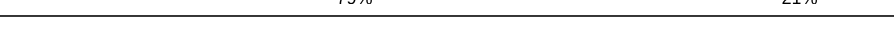

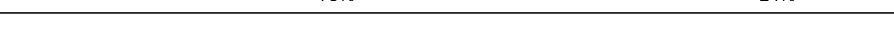
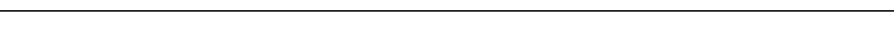

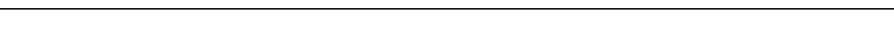
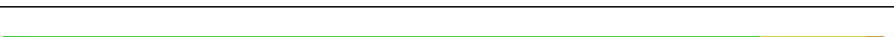


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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	
16	c4	136	
17	C5	141	














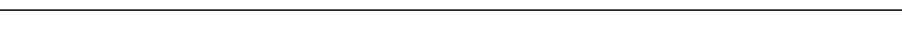











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Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	


























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Mol	Chain	Length	Quality of chain
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	















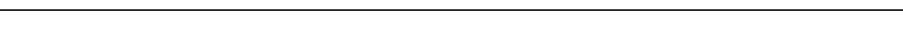




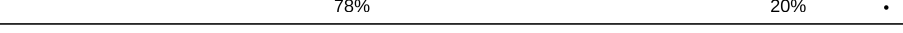





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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	















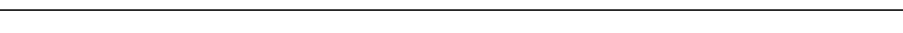




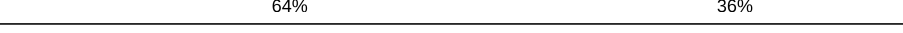





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Mol	Chain	Length	Quality of chain
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	

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Mol	Chain	Length	Quality of chain
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	e0	62	

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Mol	Chain	Length	Quality of chain
81	m2	160	<div><div></div><div>94%</div><div>6%</div></div>
82	p0	311	<div><div></div><div>38%</div><div>8%</div><div>54%</div></div>
83	p1	47	<div><div></div><div>100%</div></div>
84	p2	46	<div><div></div><div>100%</div></div>

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411258 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
1	2	1750	Total	C	N	O	P	0	0	0
			37283	16668	6591	12274	1750			
1	6	1795	Total	C	N	O	P	0	0	0
			38238	17095	6758	12590	1795			

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S0	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S1	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			773	500	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

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
13	C1	155	Total	C	N	O	S	0	0	0
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	12	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called Unknown protein m2.

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

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

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

- Molecule 83 is a protein called Unknown protein p1.

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

- Molecule 84 is a protein called Unknown protein p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	4	Total	Mg	0	0
			4	4		
85	m6	1	Total	Mg	0	0
			1	1		
85	n8	4	Total	Mg	0	0
			4	4		
85	o1	1	Total	Mg	0	0
			1	1		
85	N5	2	Total	Mg	0	0
			2	2		
85	6	146	Total	Mg	0	0
			146	146		
85	sM	2	Total	Mg	0	0
			2	2		
85	m5	2	Total	Mg	0	0
			2	2		
85	l3	2	Total	Mg	0	0
			2	2		
85	M1	1	Total	Mg	0	0
			1	1		
85	d6	1	Total	Mg	0	0
			1	1		
85	2	122	Total	Mg	0	0
			122	122		
85	n0	2	Total	Mg	0	0
			2	2		
85	L4	2	Total	Mg	0	0
			2	2		
85	l7	2	Total	Mg	0	0
			2	2		
85	M5	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	l4	1	Total 1	Mg 1	0	0
85	o0	1	Total 1	Mg 1	0	0
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	M0	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	n6	1	Total 1	Mg 1	0	0
85	5	508	Total 508	Mg 508	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	1	Total 1	Mg 1	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	n9	2	Total 2	Mg 2	0	0
85	1	475	Total 475	Mg 475	0	0
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	m1	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	q3	1	Total 1	Mg 1	0	0

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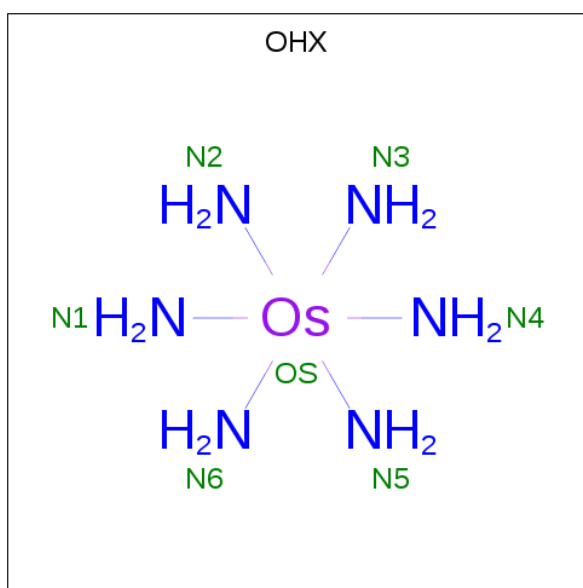
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	o3	1	Total 1	Mg 1	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	2	Total 2	Mg 2	0	0
85	4	23	Total 23	Mg 23	0	0
85	D4	1	Total 1	Mg 1	0	0
85	S4	1	Total 1	Mg 1	0	0
85	L2	1	Total 1	Mg 1	0	0
85	l5	2	Total 2	Mg 2	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	4	Total 4	Mg 4	0	0
85	N8	5	Total 5	Mg 5	0	0
85	s1	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0
85	O1	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	15	Total 15	Mg 15	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	2	Total 2	Mg 2	0	0
85	d4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	12	2	Total	Mg	0	0
			2	2		
85	8	13	Total	Mg	0	0
			13	13		
85	M6	1	Total	Mg	0	0
			1	1		
85	N0	1	Total	Mg	0	0
			1	1		
85	3	14	Total	Mg	0	0
			14	14		

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	L3	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
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86	L4	1	Total	N	Os	0	0
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86	M0	1	Total	N	Os	0	0
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86	M5	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M8	1	Total	N	Os	0	0
			7	6	1		
86	M9	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	N9	1	Total	N	Os	0	0
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86	O3	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	Q2	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	s9	1	Total	N	Os	0	0
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86	c3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		

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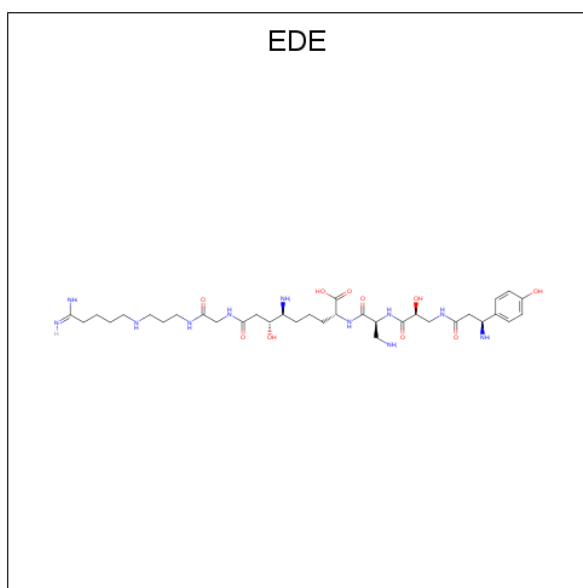
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	13	1	Total 7	N 6	Os 1	0	0
86	13	1	Total 7	N 6	Os 1	0	0
86	13	1	Total 7	N 6	Os 1	0	0
86	14	1	Total 7	N 6	Os 1	0	0
86	14	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	19	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m1	1	Total 7	N 6	Os 1	0	0
86	m4	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	n1	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is EDEINE B (three-letter code: EDE) (formula: $C_{34}H_{59}N_{11}O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
87	2	1	Total	C	N	O	0	0
			55	34	11	10		
87	6	1	Total	C	N	O	0	0
			55	34	11	10		

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

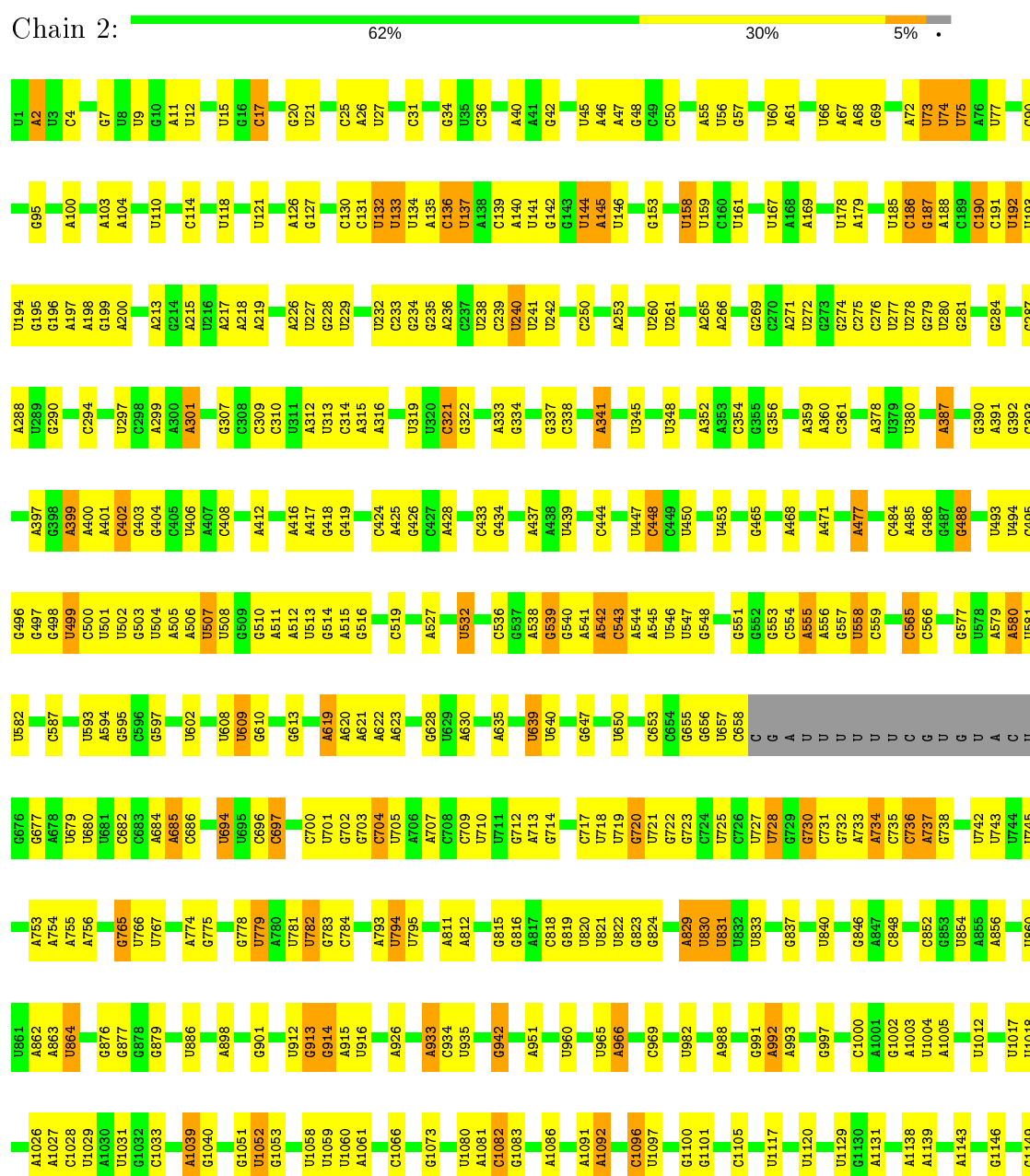
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	q0	1	Total	Zn	0	0
			1	1		
88	D6	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		
88	Q3	1	Total	Zn	0	0
			1	1		
88	D9	1	Total	Zn	0	0
			1	1		
88	E1	1	Total	Zn	0	0
			1	1		
88	Q0	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0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

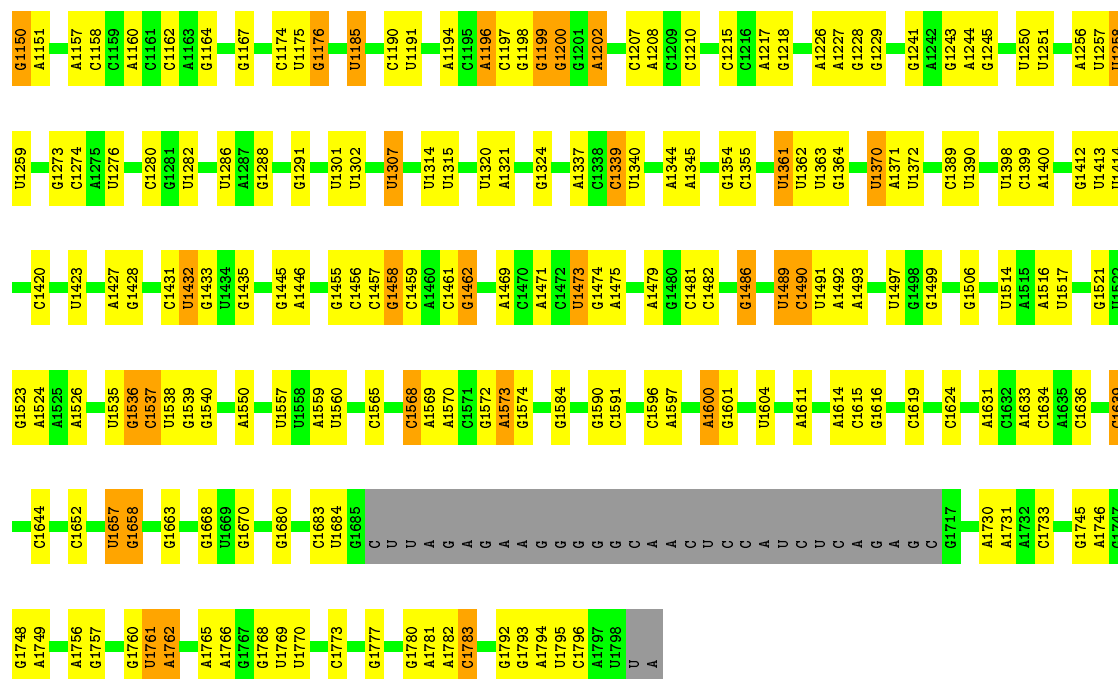
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

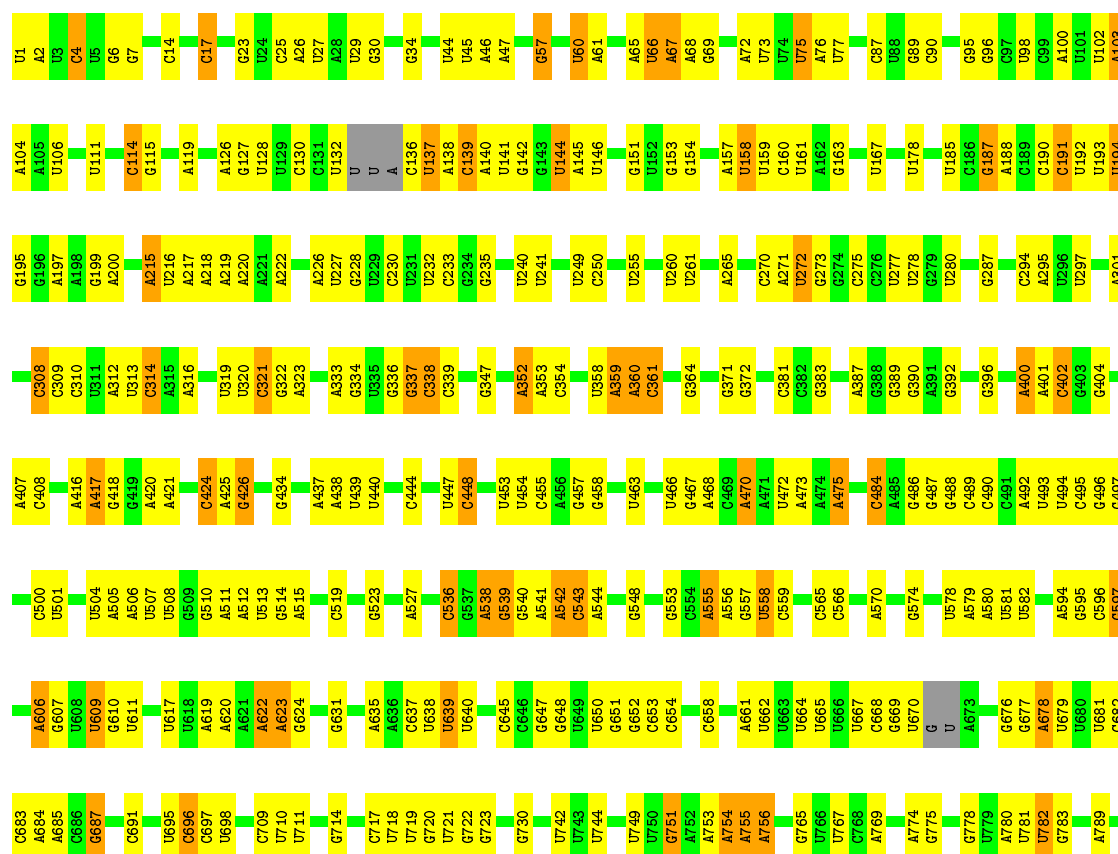
• Molecule 1: 18S ribosomal RNA

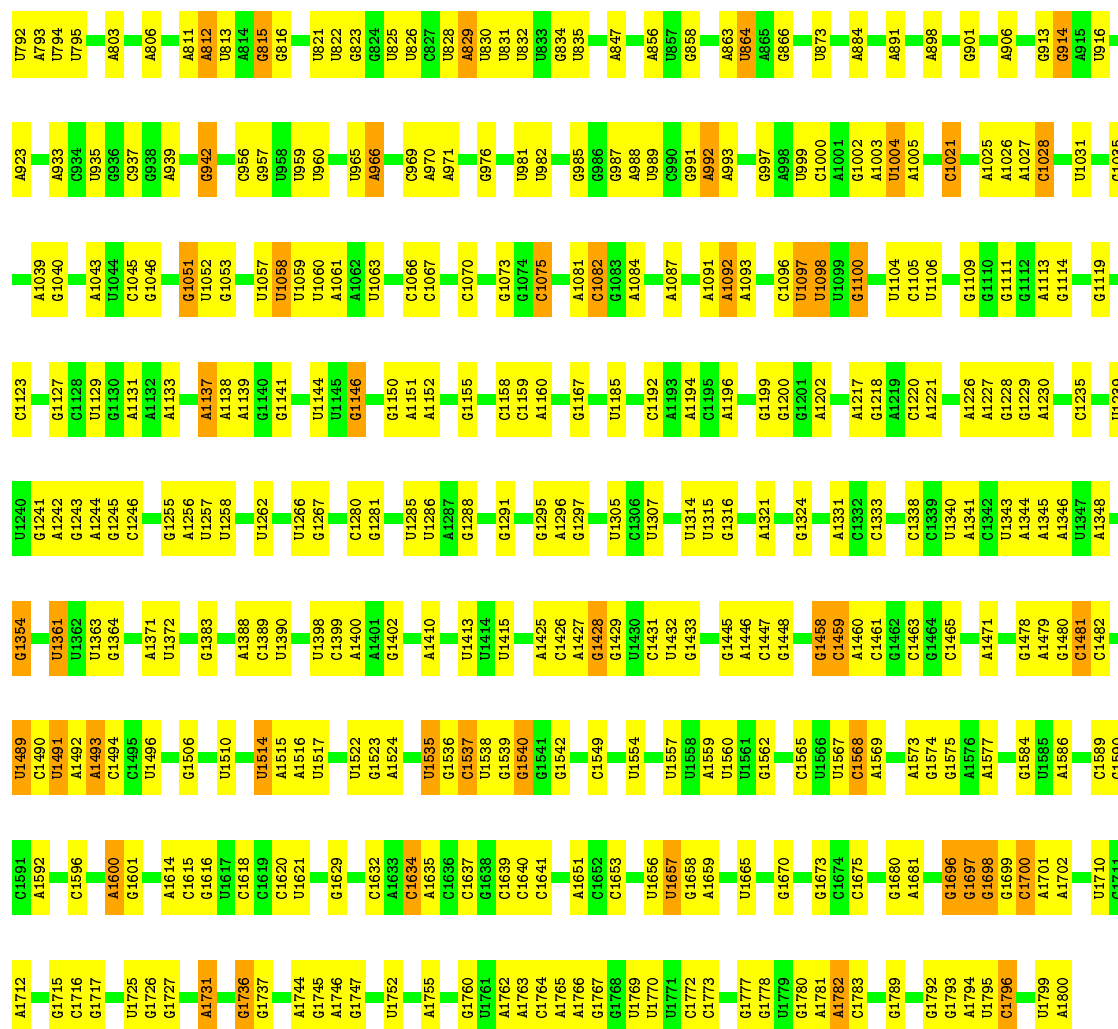




• Molecule 1: 18S ribosomal RNA

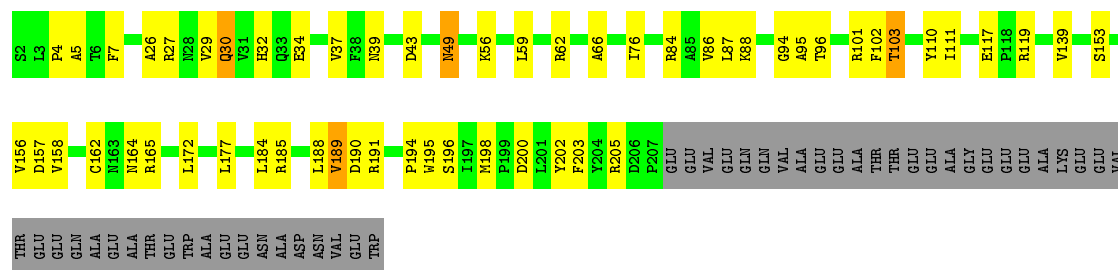
Chain 6: 62% 32% 6%





- Molecule 2: 40S ribosomal protein S0-A

Chain S0:  60% 21% • 18%

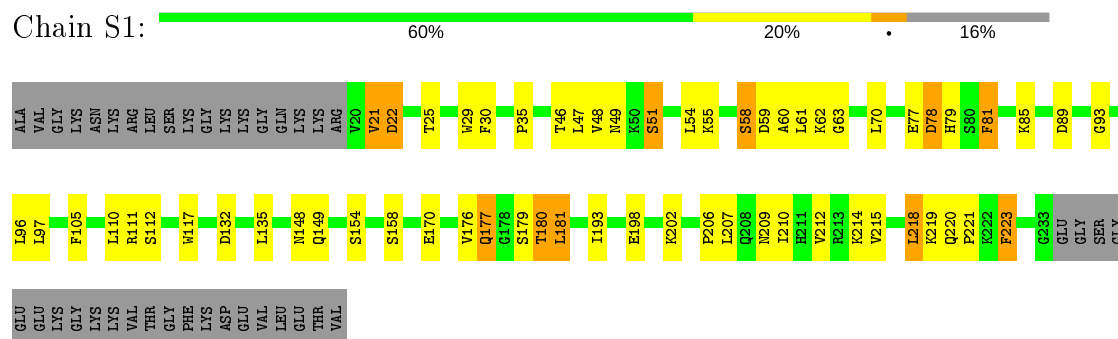


- Molecule 2: 40S ribosomal protein S0-A

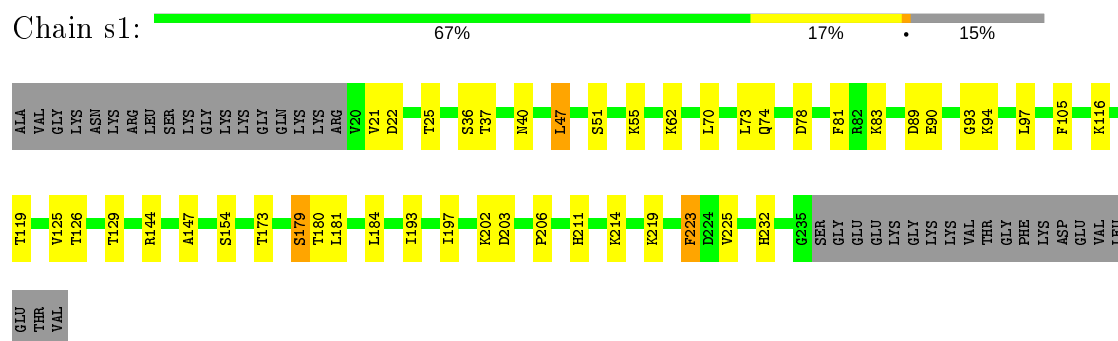
Chain s0:  63% 17% • 18%



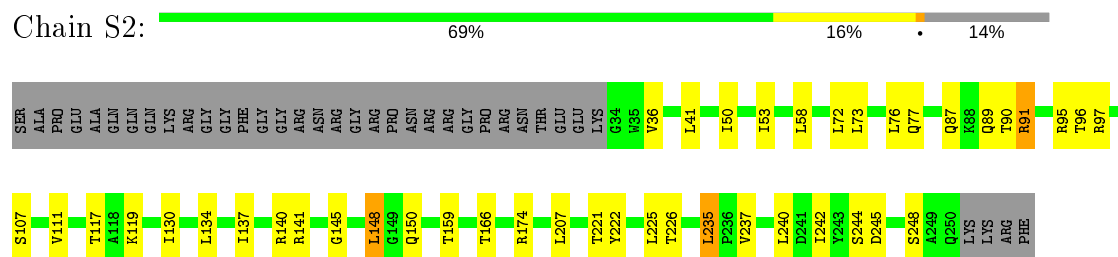
- Molecule 3: 40S ribosomal protein S1-A



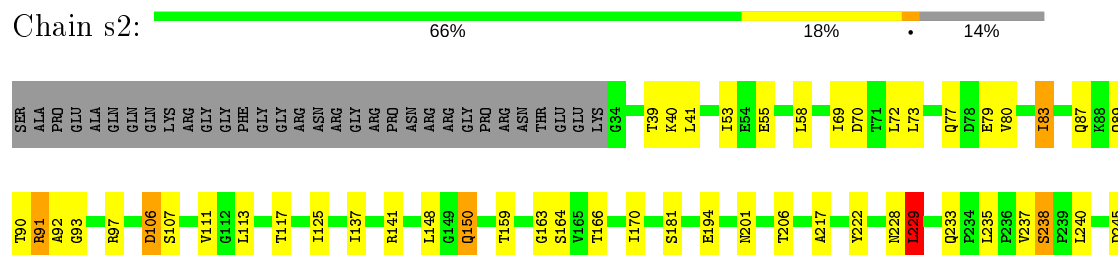
- Molecule 3: 40S ribosomal protein S1-A



- Molecule 4: 40S ribosomal protein S2



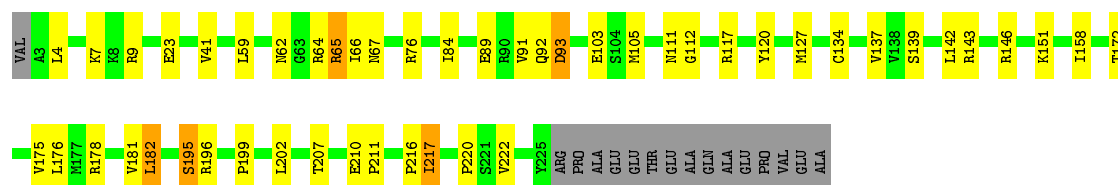
- Molecule 4: 40S ribosomal protein S2





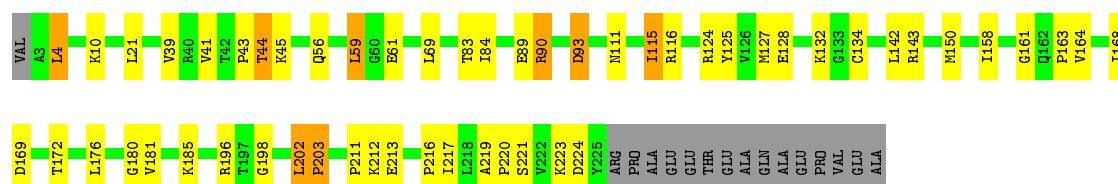
- Molecule 5: 40S ribosomal protein S3

Chain S3: 73% 18% 7%



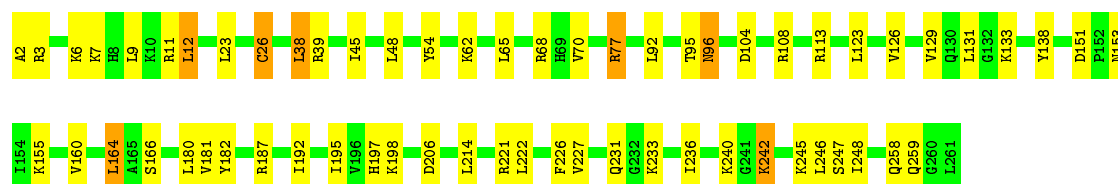
- Molecule 5: 40S ribosomal protein S3

Chain s3: 71% 19% 7%



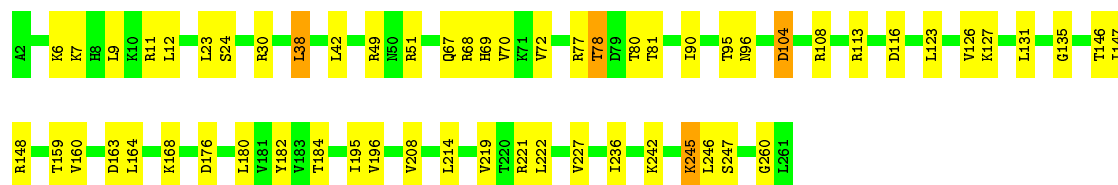
- Molecule 6: 40S ribosomal protein S4-A

Chain S4: 76% 21%



- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 77% 21%



- Molecule 7: 40S ribosomal protein S5

Chain S5: 72% 18% 8%





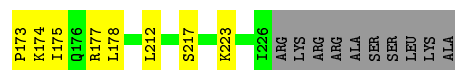
• Molecule 7: 40S ribosomal protein S5

Chain s5: 68% 22% 8%



• Molecule 8: 40S ribosomal protein S6-A

Chain S6: 78% 17%



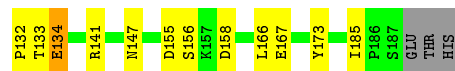
• Molecule 8: 40S ribosomal protein S6-A

Chain s6: 72% 19% 8%



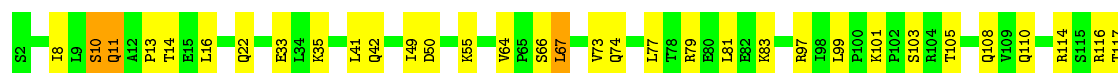
• Molecule 9: 40S ribosomal protein S7-A

Chain S7: 74% 22%



• Molecule 9: 40S ribosomal protein S7-A

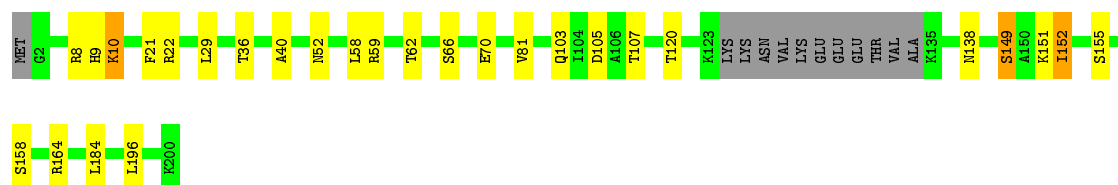
Chain s7: 76% 21%





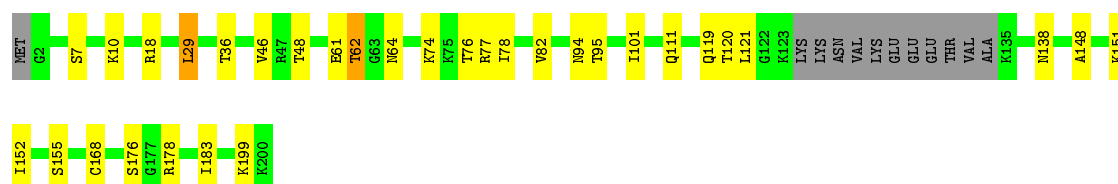
- Molecule 10: 40S ribosomal protein S8-A

Chain S8: 80% 13% 6%



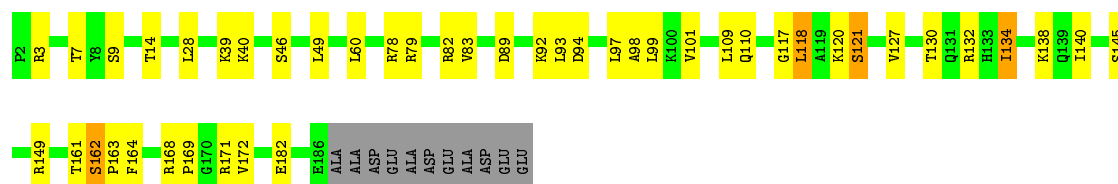
- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 78% 15% 6%



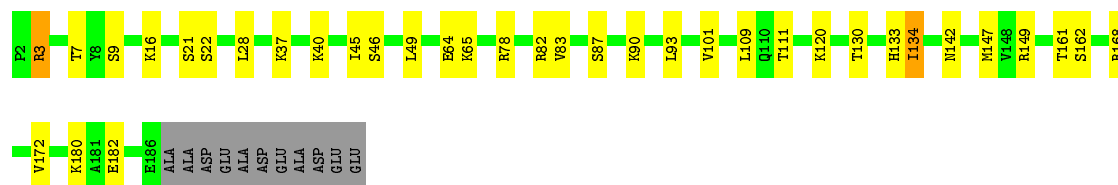
- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 71% 21% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 76% 17% 6%



- Molecule 12: 40S ribosomal protein S10-A

Chain C0: 72% 17% 9%




- Molecule 12: 40S ribosomal protein S10-A

Chain c0:  72% 16% 9%



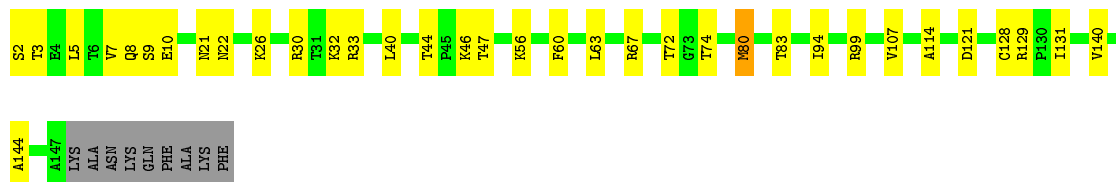
- Molecule 13: 40S ribosomal protein S11-A

Chain C1:  79% 20%



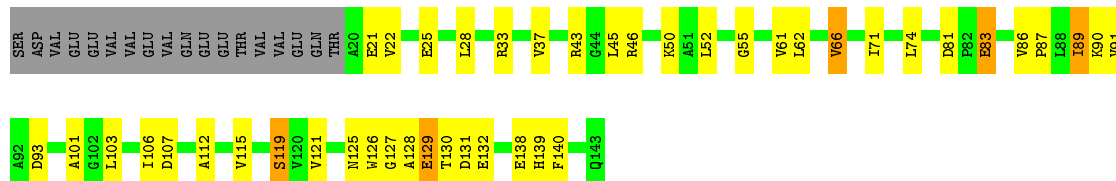
- Molecule 13: 40S ribosomal protein S11-A

Chain c1:  72% 22% 6%



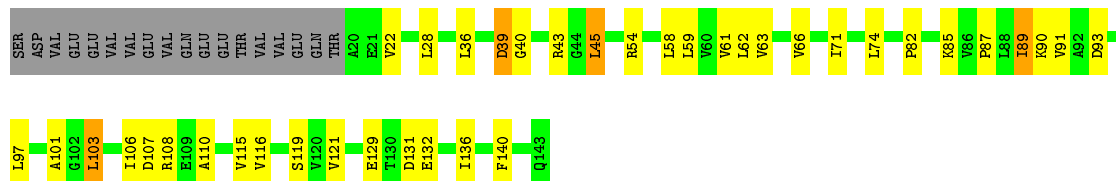
- Molecule 14: 40S ribosomal protein S12

Chain C2:  56% 27% 13%




- Molecule 14: 40S ribosomal protein S12

Chain c2:  60% 25% 13%



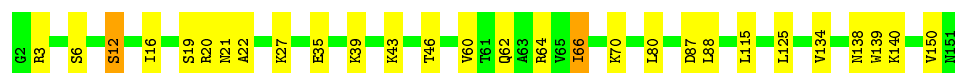
- Molecule 15: 40S ribosomal protein S13

Chain C3:  79% 19%



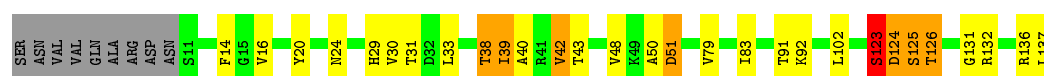
- Molecule 15: 40S ribosomal protein S13

Chain c3: 81% 17%



- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 72% 15% 5% 7%



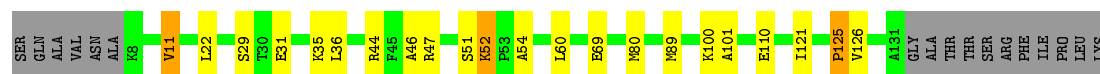
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 73% 20% 6%



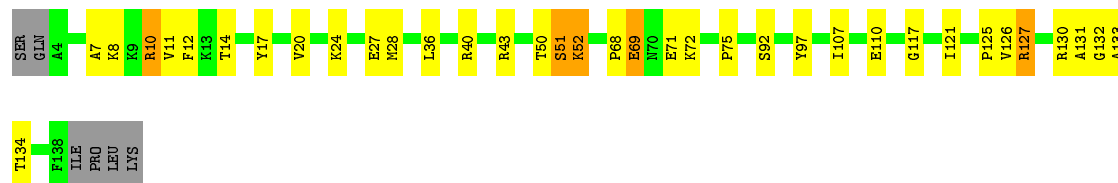
- Molecule 17: 40S ribosomal protein S15

Chain C5: 72% 13% 12%



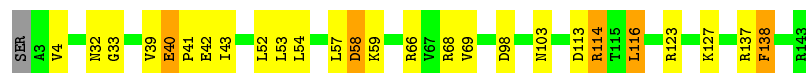
- Molecule 17: 40S ribosomal protein S15

Chain c5: 70% 22%

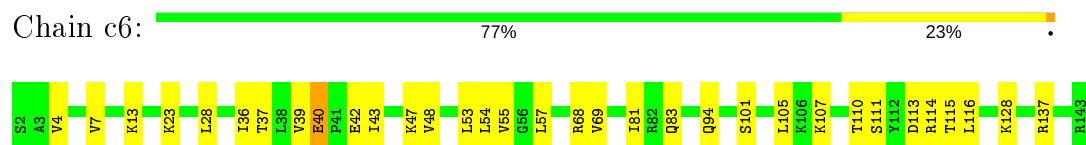


- Molecule 18: 40S ribosomal protein S16-A

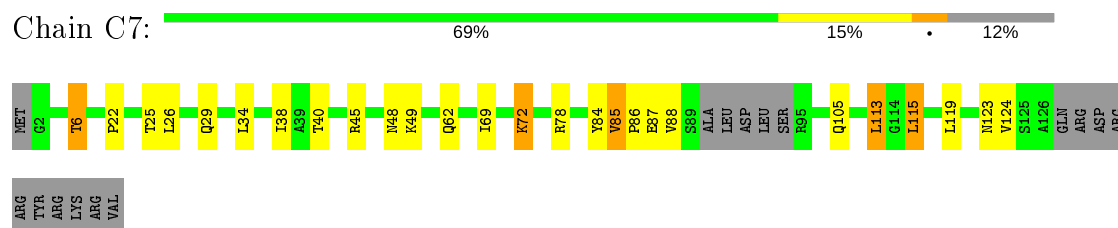
Chain C6: 81% 15%



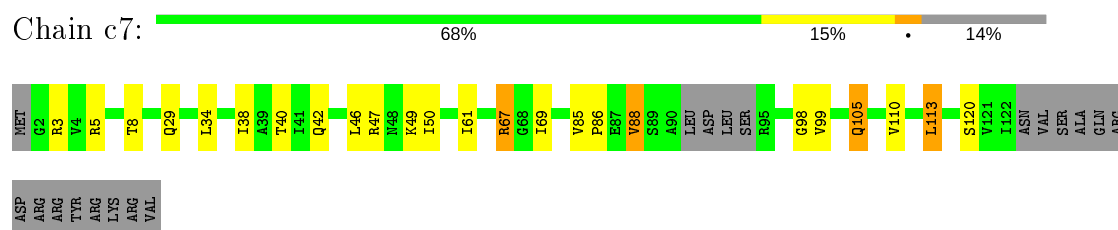
- Molecule 18: 40S ribosomal protein S16-A



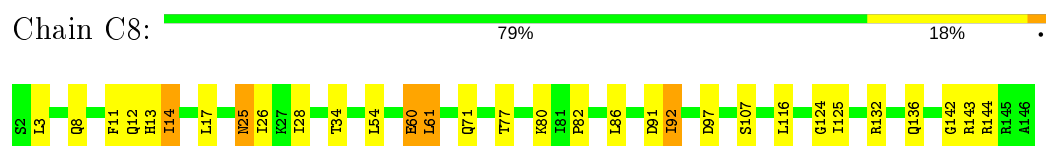
- Molecule 19: 40S ribosomal protein S17-A



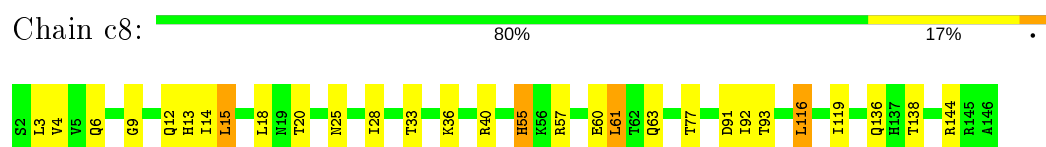
- Molecule 19: 40S ribosomal protein S17-A



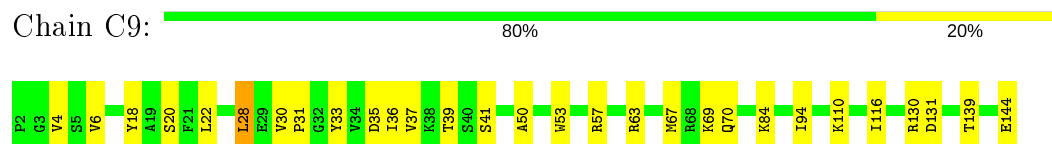
- Molecule 20: 40S ribosomal protein S18-A



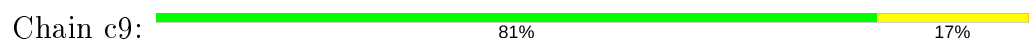
- Molecule 20: 40S ribosomal protein S18-A



- Molecule 21: 40S ribosomal protein S19-A

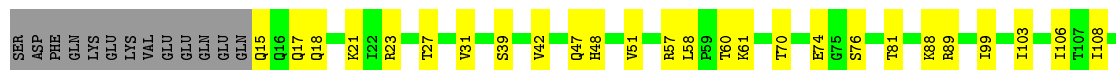


- Molecule 21: 40S ribosomal protein S19-A

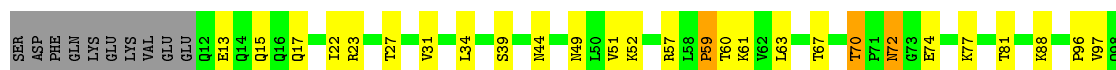




- Molecule 22: 40S ribosomal protein S20



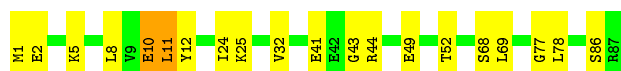
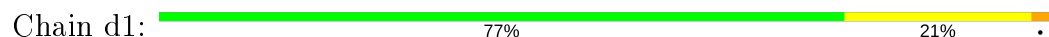
- Molecule 22: 40S ribosomal protein S20



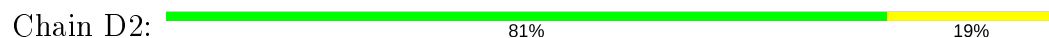
- Molecule 23: 40S ribosomal protein S21-A



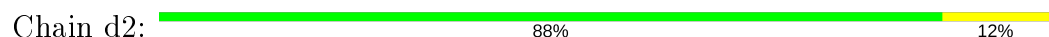
- Molecule 23: 40S ribosomal protein S21-A

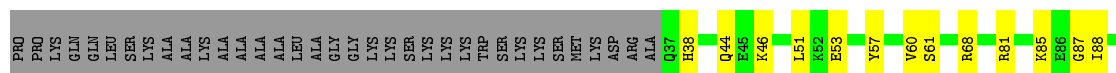


- Molecule 24: 40S ribosomal protein S22-A



- Molecule 24: 40S ribosomal protein S22-A







- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 66% 26% 8%



- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 74% 26%



- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 85% 12% •



- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 75% 25%



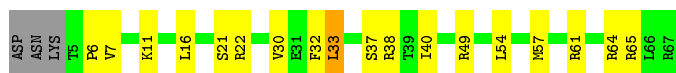
- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 71% 23% • 5%



- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 68% 26% • 5%

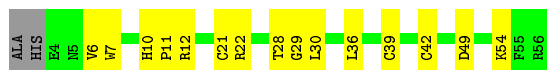


- Molecule 31: 40S ribosomal protein S29-A

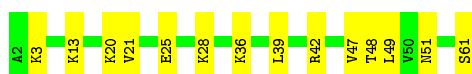
Chain D9: 71% 22% • •



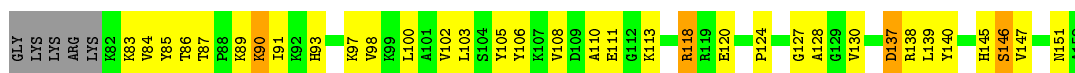
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A



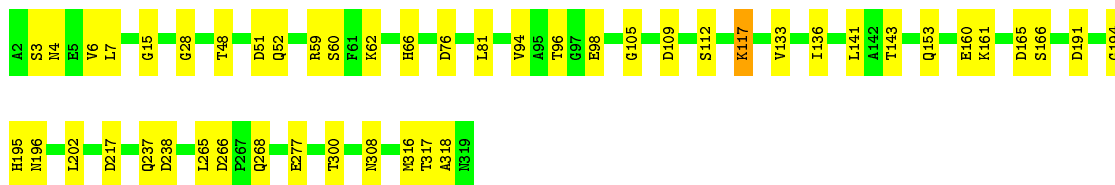
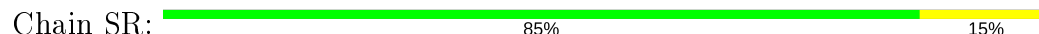
- Molecule 33: Ubiquitin-40S ribosomal protein S31



- Molecule 33: Ubiquitin-40S ribosomal protein S31



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

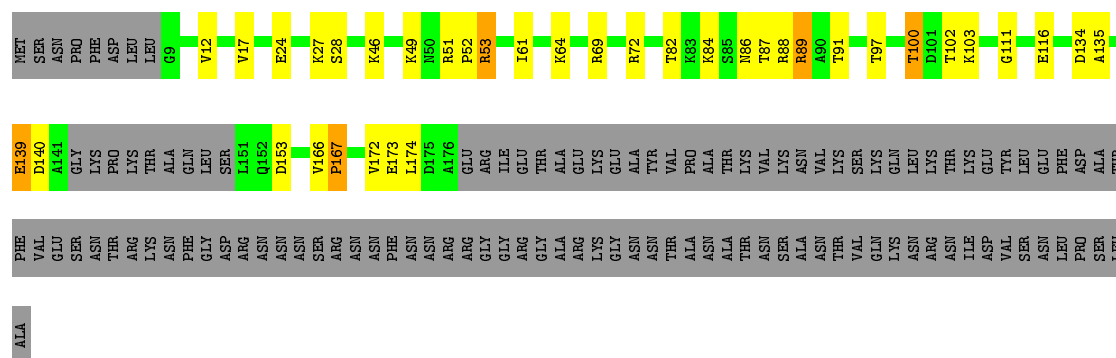


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



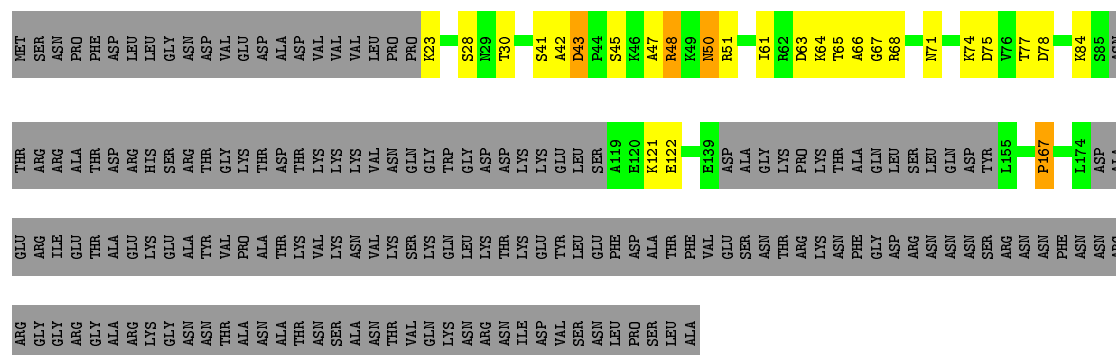
- Molecule 35: Suppressor protein STM1

Chain SM: 



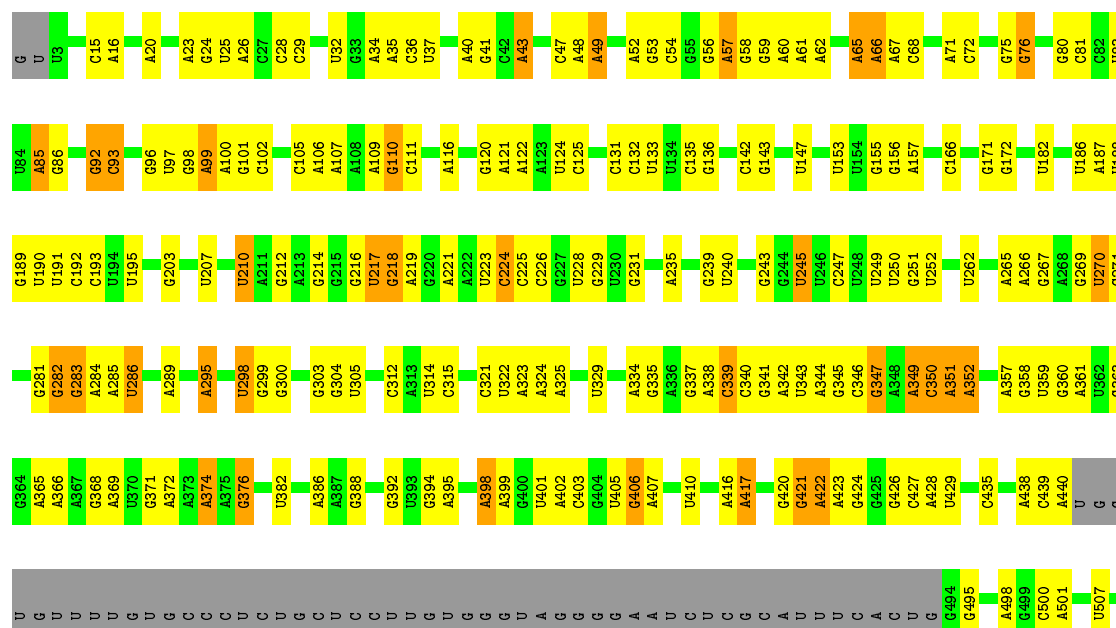
• Molecule 35: Suppressor protein STM1

Chain sM: 



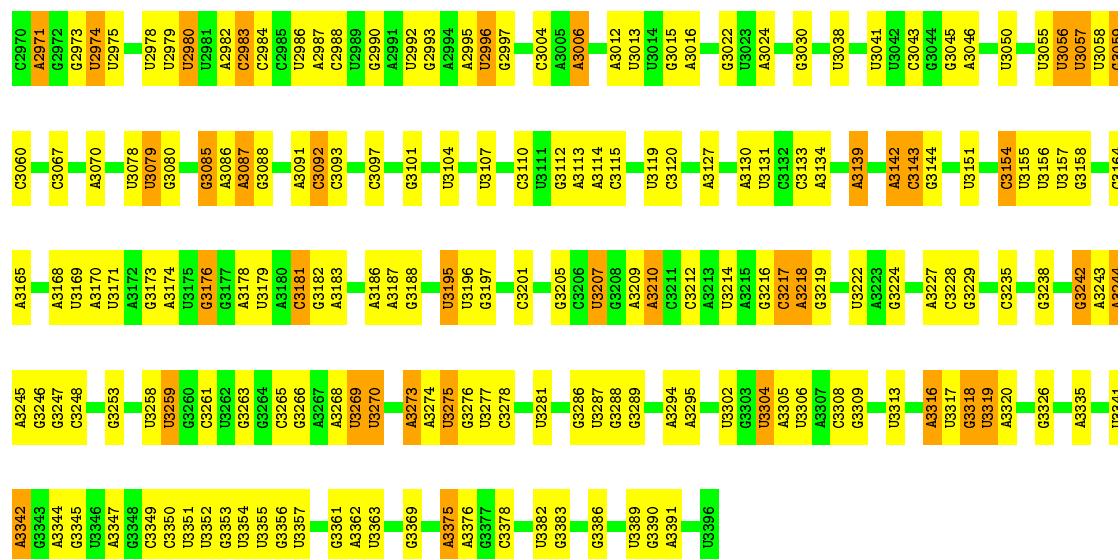
• Molecule 36: 25S ribosomal RNA

Chain 1: 



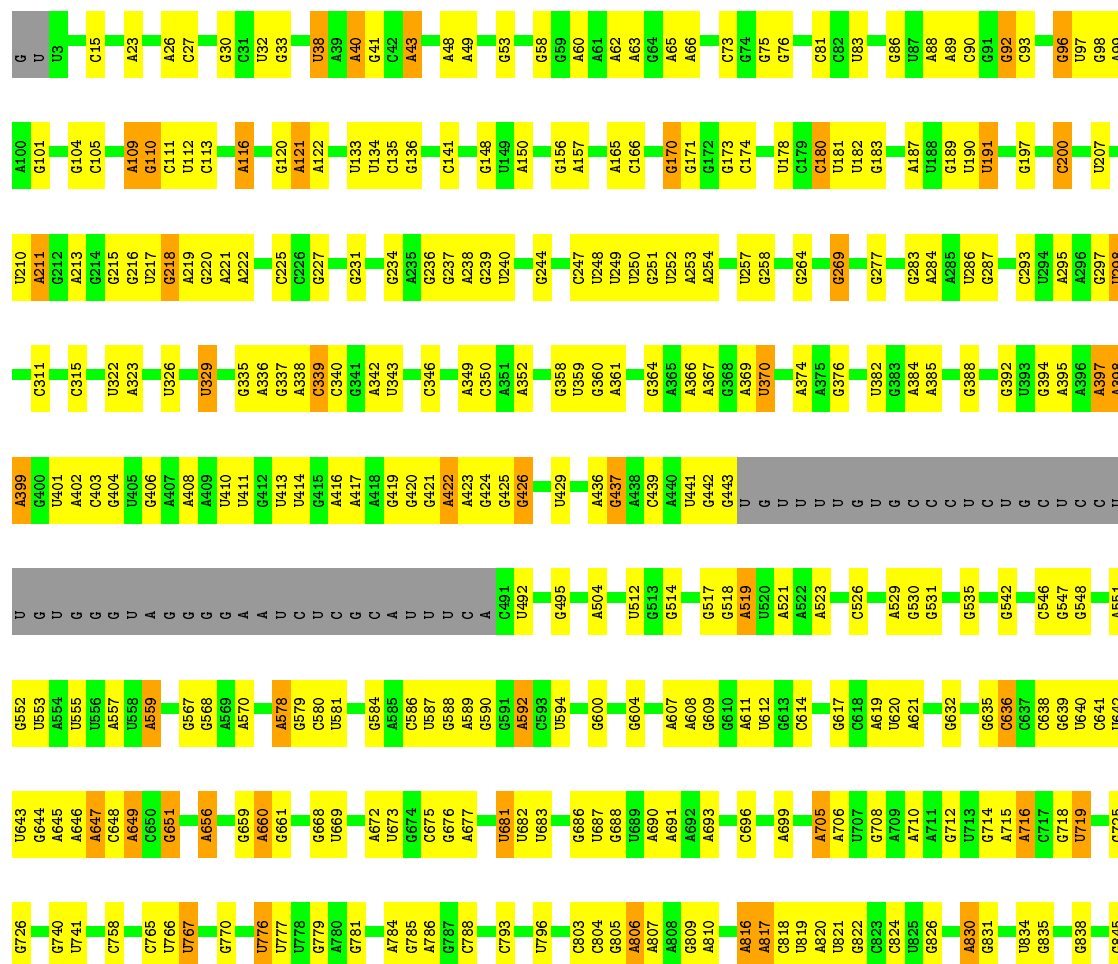
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G1669	G1670	G1671	G1672	G1673	G1674	G1675	G1676	G1677	G1678	G1558	A1465	A1386	U1321	G1249	U1174	C1107	G1019	G941	C868	U681	U612	C515
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G1769	G1770	G1771	G1772	G1773	G1774	G1775	G1776	G1777	G1778	G1568	A1487	A1402	C1340	U1267	U1188	U1121	U1043	U956	C696	U620	U620	A521
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			U2613	U2613	U2514	G2377	A2303	A2223	A2145	C	G	U1819	
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			G2616	G2616	A2523	U2380	G2306	C2227	U2148	G	C	G1822	
			U2617	U2617			C2307	C2228		U	U		
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			A2696	A2696				A2233	A2158	A	U	A1835	
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			G2620	G2620	G2533	A2389	A2313	C2237	G2160	G	U	U1837	
			G2621	G2621	G2534	A2390	G2314		G2161	U	G	U1840	
			G2622	G2622		G2391	G2315		C2162	C	U	A1841	
			G2623	G2623	U2537	C2392	G2316	U2241	C2163	G	U	A1842	
			G2624	G2624	A2538	G2393		A2242	A2164	C	A		
			C2625	A2626	G2539	G2394	A2320	A2243	G2165	U	G	G1845	
			A2627	A2627	A2540	G2395	A2321	A2244	A2166	U	G	C1846	
			A2628	A2628	U2541	G2396	C2322	G2245	A2167	G	C	A1847	
			U2629	U2629	U2542	G2397	G2323	G2246	A2168	C	C	G1848	
			C2630	C2630	U2543	A2398	A2324	G2247	G2169	U	G	A1849	
			U2631	U2631		A2399	G2325	G2248	U2170	A	U	A1850	
			G2632	G2632	A2547	G2400	A2326	G2249	G2171	C	U	G1851	
			C2548	C2548	C2548			G2250		A	U		
			G2549	G2549	U2550	A2401	C2331	G2253	G2174	A	A	U1855	
			U2551	U2551	C2551	G2402	A2332	U2254	G2177	U	C	G1856	
			C2552	C2552	U2553	G2403	C2333	A2255	A2178	U	U	C1857	
			U2553	U2553	A2554	C2405	U2334	A2256	C2179	A	U	A1864	
			A2554	A2554	C2555	C2406	G2335			C	G	A1865	
			G2555	G2555	G2555	C2407	U2336	U2268	A2182	C	A	C1866	
			A2561	A2561		G2408	C2337	U2269	G2187	U	U	A1867	
						U2410	A2341	A2270	U2186	G	C	G1868	
			C2568	C2568	U2411	U2411	U2342	A2271	G2187	C	A	G1869	
			A2569	A2569	G2412	G2412	C2343	G2272	A2188	C	G	G1870	
			U2570	U2570	G2413	G2413	U2344	U2273		U	U	U1871	
			U2571	U2571	A2414	A2414	G2345	G2274	C2192	C	C		
			C2572	C2572	G2415	G2415	A2346	A2275	U2193	G	G	U1876	

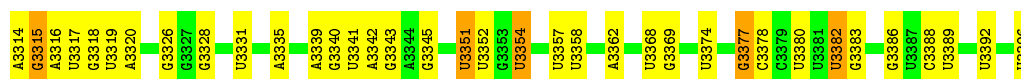


• Molecule 36: 25S ribosomal RNA

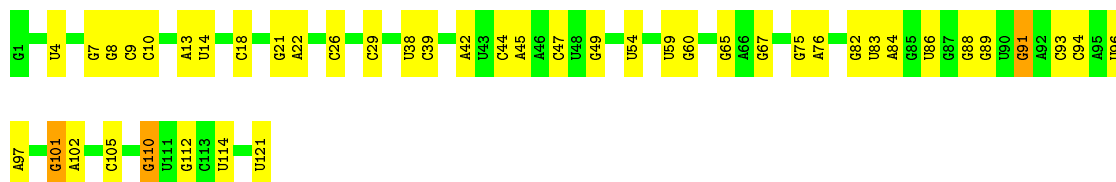
Chain 5: 49% 37% 7% 7%



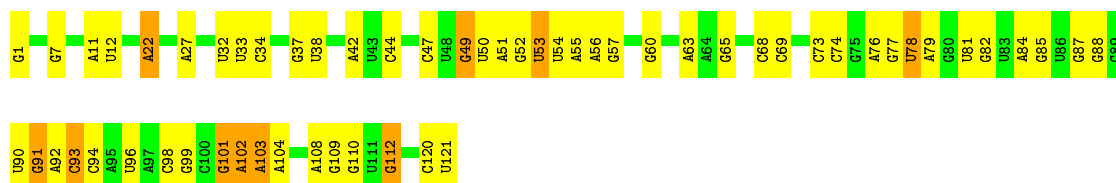
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U	U1938	A1847	U1724	G1590	A1515	G1434	C1358	U1258	A1163	A1093	C1000	A933	
G	U1939	G1848	C1725	G1591	G1517	C1437	C1359		G1164	U1094	A1001	G934	C851
C	C1941	C1849		G1592	U1518	U1438	A1363	G1262	A1170	U1095	A1003	A936	G857
G		A1850	G1730	A1593	U1519	U1439	G1364	U1263	U1173	U1096	A1006	G937	A858
U	G1947	G1851	G1736	G1598	G1520	G1440	G1365	U1264	G1174	A1097	U1007	C938	G859
U		G1852			G1521		A1366	U1265	U1175	A1098	U1008		A858
A		U1853		A1602	U1522	G1443	G1367	G1266	U1176	A1099	U1009	G941	G860
G	G1952	C1854		G1603	U1526	U1445	U1368		G1177	U1100	A1010	U942	U861
A	G1953	U1855	A1741	G1604	U1527	U1446	U1369	C1284	G1178	U1101	A1011	G944	C862
C		C1856	A1750	A1605	G1528		U1370	G1285	U1179	A1102	G1012	C945	
C	U	C1857	G1751	U1606	A1529	A1446	G1371		A1180	A1103	G1013	C946	G869
U	A	A1858		U1607			C1372	C1292	U1181	G1104	U1014	U947	G870
G			A1757	C1608	U1533	G1450	A1373		A1182		U1015	G948	U871
C	U	C1865		C1609	U1534	G1451	G1374	U1299	U1183	U1110	U1016	G949	U872
C	U	C1866		C1609	U1535	A1452	G1375	A1300	C1183	U1111	C1017	C949	C873
C	A	A1867	C1762	C1615	U1536	A1453	C1376	A1301	C1184	A1112	C1017	G950	U874
U	G	G1868	U1763	G1615	U1537	A1454	G1377	A1302	C1185	G1113	G1018	U875	G875
U	G	C1869	U1764	G1616	G1541	U1455	U1378	A1303	G1186	U1114	G1019	A851	A876
G	C	C1870	U1765	A1618	G1542	U1456	G1379	A1304	C1187	G1115	G1020	A852	C877
C	C		G1766	A1619			G1380	U1305	U1188	G1116	G1021	G953	G878
U	C	U1874	G1770	U1620	A1546	A1460		G1306	U1189	G1117		U955	U879
A	U				G1547	A1461	U1384	G1307	A1190	C1118	U1024	U956	G880
C	U	G1878		C1628	G1548	A1462	C1385	A1308	U1191	C1119	A1025	C957	C881
C	U	A1879	G1780	U1629	U1549	A1463	A1386	U1309	C1192		A1026	C958	A882
A	G	U1880				G1464	G1387		A1193	U1123	A1027	C959	A883
U	U		C1788	G1635	U1553	A1465		G1310	U1194	U1124	U1028	U960	U884
U	C	U1885	G1789	U1636	U1554	G1466	G1388	G1311	A1195	U1125	G1029	C961	U885
U	A	A1886	G1790	C1639	U1555	A1467	G1389	C1312	C1196	G1126		A962	C886
U	G	G1887	C1791	G1640	U1556	A1468	G1390	C1313	A1200	A1129	G1035	G963	
C	A	A1891	U1795	U1641	C1556	A1469	A1392	C1314	A1201	A1130	U1041	G964	U889
C	C	G1892	G1796	A1842	A1557	C1469	A1393	U1315	A1202	A1131	U1042	A965	C890
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U	C	U1894		C1644	G1560	G1473	C1395	A1317	A1204	A1133	A1048	G968	A896
C	A		U1645	U1645	G1561	G1476	C1396	A1318	G1207	G1134	C1049	A970	U897
C	G	G1897	A1800	C1562	C1562				U1208	A1135			
U	C			C1563	U1564	G1476	A1399	G1321	G1209	G1140	A1054	G971	U905
U	G	G1898	A1810	G1568	U1564	G1480	G1400	U1322	U1209		U1060	A972	A906
G	G	U1903	G1811	U1569	G1565	A1481		G1323	G1209	A1143	A1064	G974	G907
U	U	C1904	G1812	A1566	A1566	A1482	U1405	G1323	U1208	G1144	A1065	A980	G908
U	C	G1905	A1813	G1661	U1567	G1483	U1405		G1209	G1145	A1066	C975	G909
G	G	G1906	A1814	G1662	U1568	G1488	G1408	U1329	G1209	G1147	A1067	G979	G910
U	U	C1907	U1815	U1569	U1569	A1489	G1409	U1330	G1209	G1148	A1068	A981	C911
A	U	A1908	A1816	C1665	U1570	A1490	U1410	U1331	G1209	G1149	C1069	A982	A913
G	C	A1909	G1817		A1571		C1411	A1332	G1209	A1150	U1070	C982	A914
A	U		U1818	G1680	U1572	U1495	G1412		G1209	G1151	U1071	A953	A915
C	U	U1911	U1819	A1583	G1573	C1496	G1413	C1335	G1209	G1152	A1075	G984	A917
G	U	U1912	U1820	G1583	C1574		G1414	C1336	G1209	A1153	A1076	U979	
G	U	A1913	U1821	U1588	A1575	C1496	G1415	U1337	G1209	A1154	A1077	A980	G912
C	G	G1914			G1576	C1499	G1416	C1338	G1209	G1155	A1078	A981	A913
C	G		G1833	U1688	G1577	G1500	G1417	C1339	G1209	G1156	A1079	A982	A914
U	A	C1918	U1834	C1698	C1578	A1418	A1418	U1348	G1209	G1157	A1080	G993	G924
U	U			C1698	C1579	A1419	A1419	G1349	G1209	A1158	A1081	G994	
G	U	C1701	A1839	A1580	A1504	A1503	G1420	U1350	A1240	A1159	A1082	U995	C927
G	U	U1930	U1840	C1581	A1505	A1506	G1421	U1351	A1241	A1160	A1083	A998	C931
U	C	U1931	A1841	C1582	A1506	A1507	A1428	U1352	G1242	G1157	A1084		
A	U		A1842	A1583	G1507	C1508	G1429	U1353	G1243	U1157	A1085		
U	U	G1934	C1843	A1587	C1508		U1430	G1354	A1244	A1159	A1086		
G	U	G1935		U1716			G1431	A1355	A1245	A1160	A1087		
U	G	A1936	G1845	A1588	A1588	G1513	C1432	U1356	G1246	G1161			



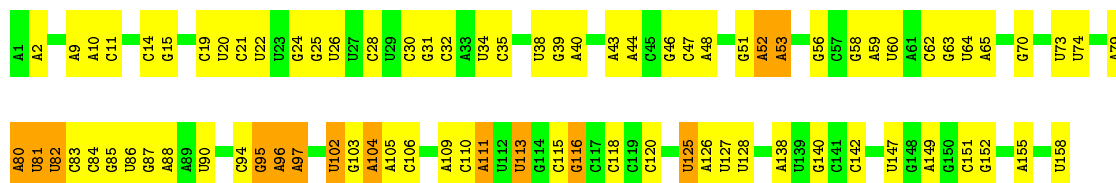
• Molecule 37: 5S ribosomal RNA



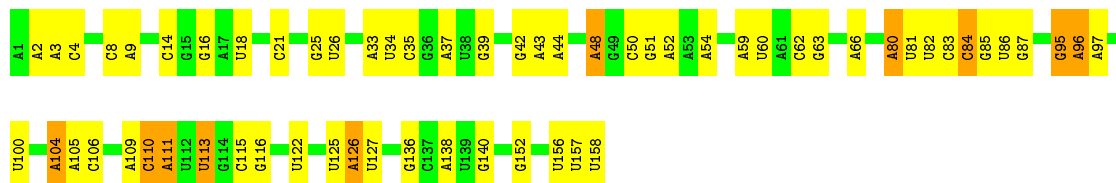
• Molecule 37: 5S ribosomal RNA



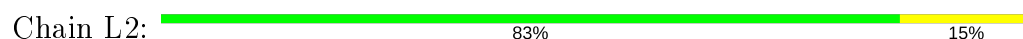
• Molecule 38: 5.8S ribosomal RNA



• Molecule 38: 5.8S ribosomal RNA



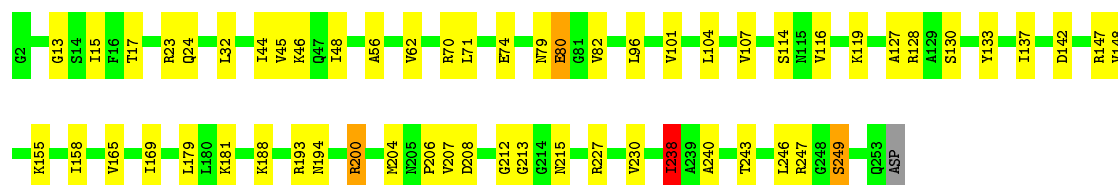
• Molecule 39: 60S ribosomal protein L2-A





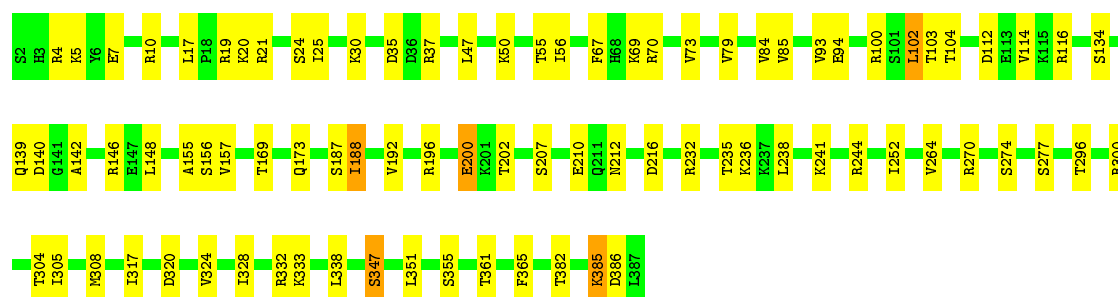
- Molecule 39: 60S ribosomal protein L2-A

Chain l2: 77% 21%



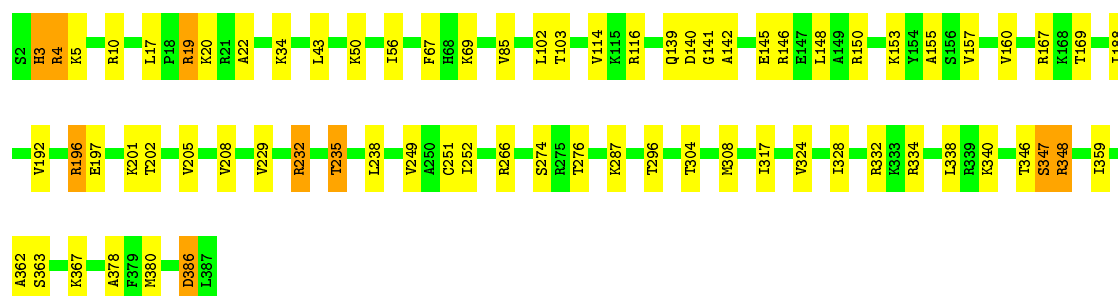
- Molecule 40: 60S ribosomal protein L3

Chain L3: 78% 21%



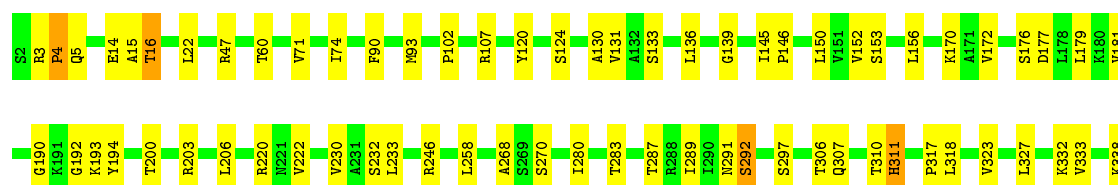
- Molecule 40: 60S ribosomal protein L3

Chain l3: 81% 16%



- Molecule 41: 60S ribosomal protein L4-A

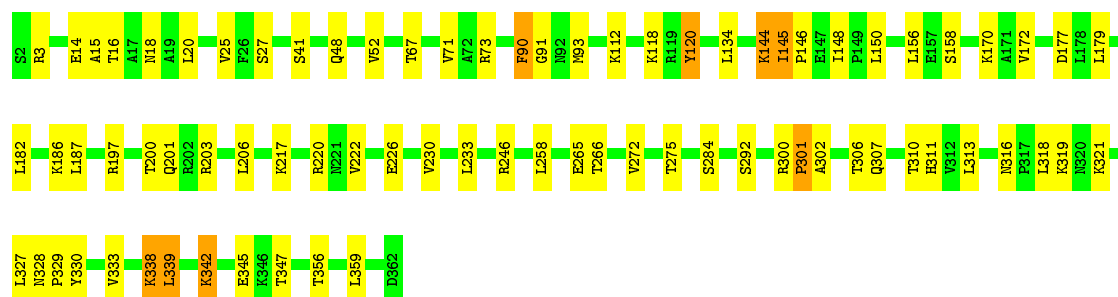
Chain L4: 80% 19%





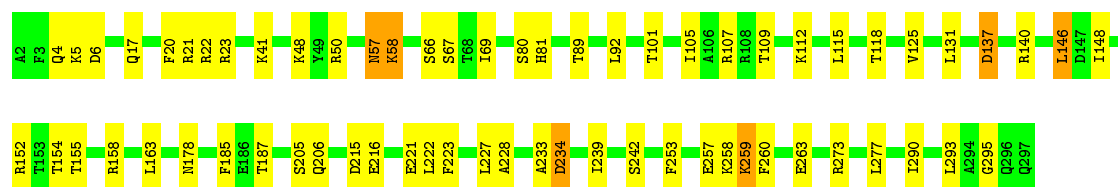
- Molecule 41: 60S ribosomal protein L4-A

Chain 14: 78% 19% •



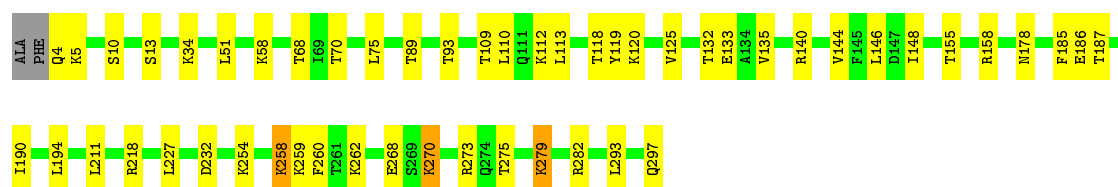
- Molecule 42: 60S ribosomal protein L5

Chain L5: 78% 20% •



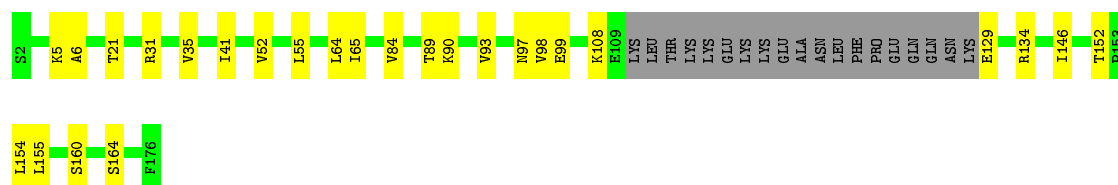
- Molecule 42: 60S ribosomal protein L5

Chain 15: 82% 17% ••



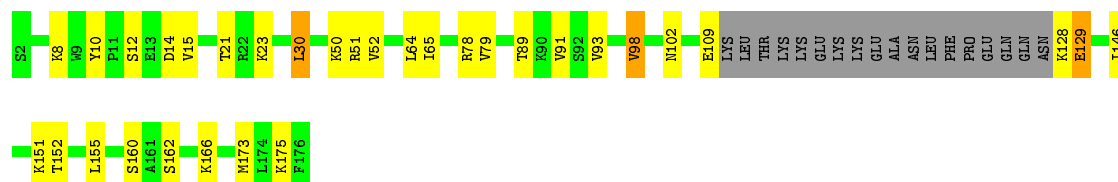
- Molecule 43: 60S ribosomal protein L6-A

Chain L6: 74% 15% 11%



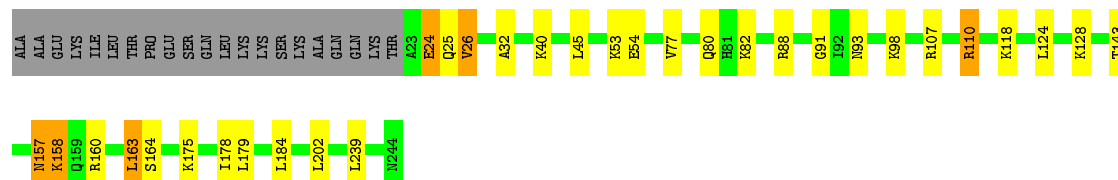
- Molecule 43: 60S ribosomal protein L6-A

Chain 16: 71% 17% • 10%



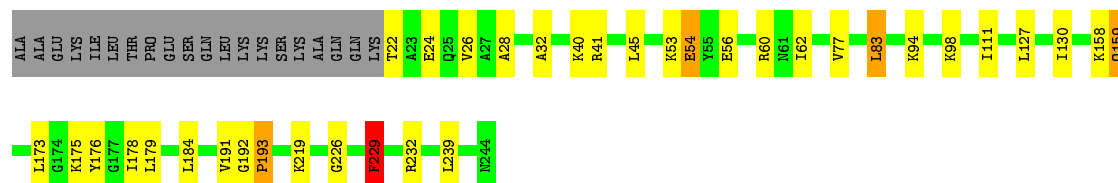
- Molecule 44: 60S ribosomal protein L7-A

Chain L7: 78% 11% 9%



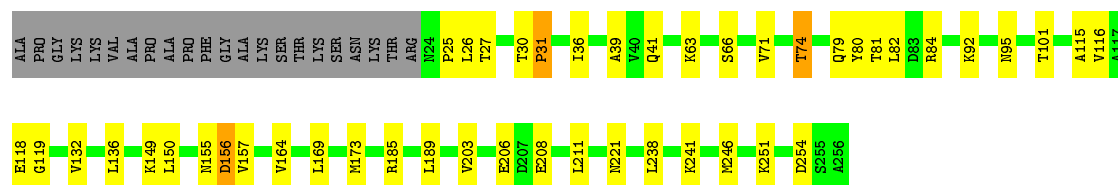
- Molecule 44: 60S ribosomal protein L7-A

Chain L7: 77% 13% 8%



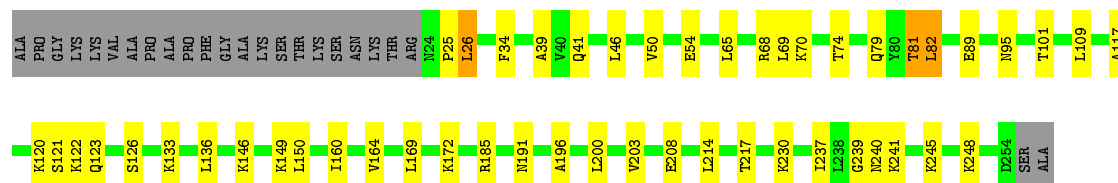
- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 73% 17% 9%



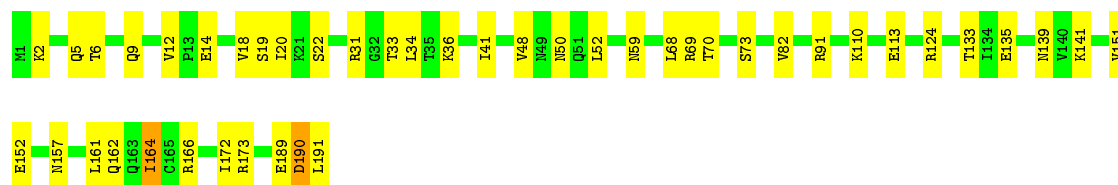
- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 71% 18% 9%



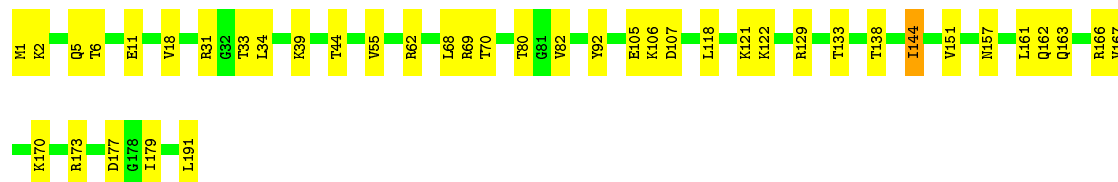
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 77% 22% 1%



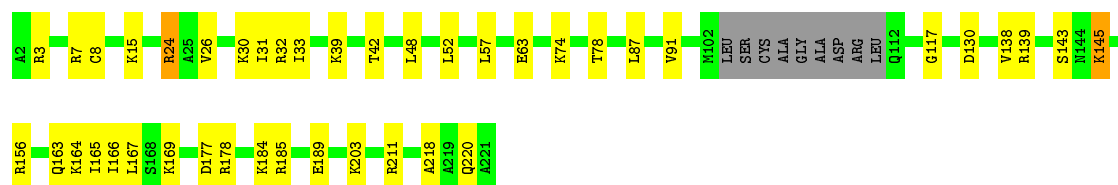
- Molecule 46: 60S ribosomal protein L9-A

Chain 19: 79% 21% .



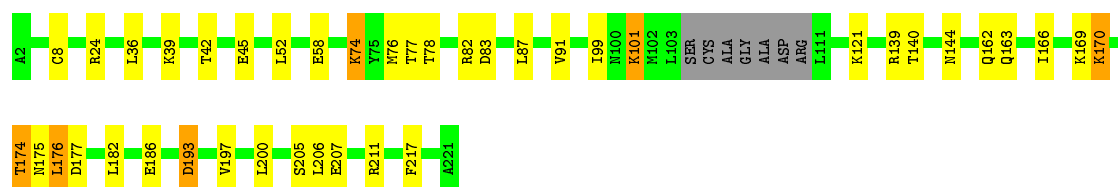
- Molecule 47: 60S ribosomal protein L10

Chain M0: 77% 18% . .



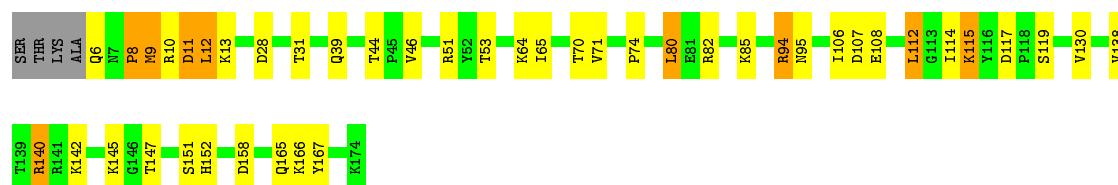
- Molecule 47: 60S ribosomal protein L10

Chain m0: 78% 16% . .



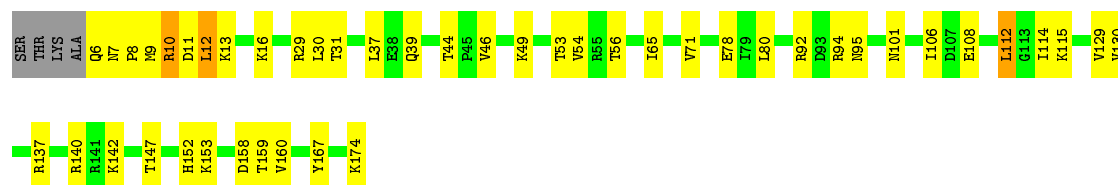
- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 72% 20% 5% .



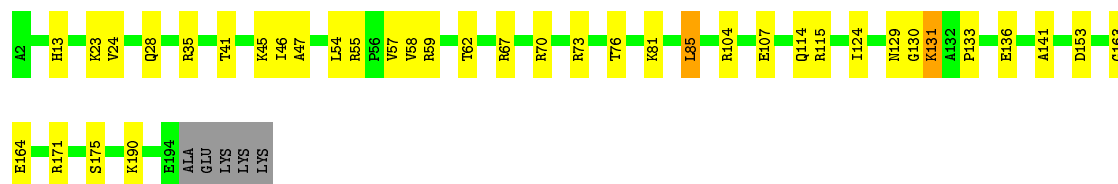
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 71% 25% . .



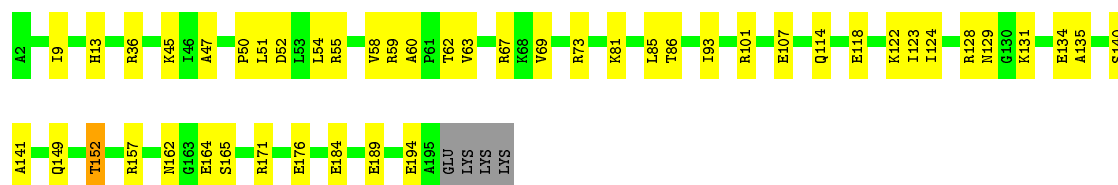
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 78% 18% ..



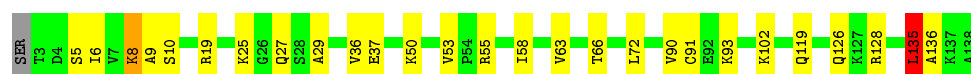
- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 74% 23% ..



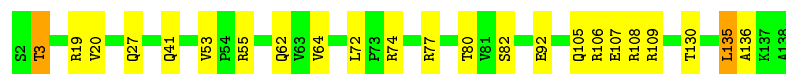
- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 80% 18% ...



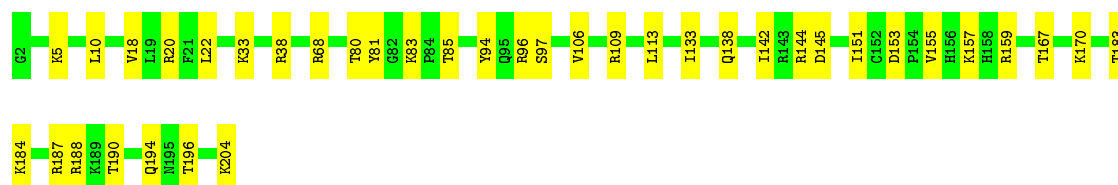
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 83% 15% .

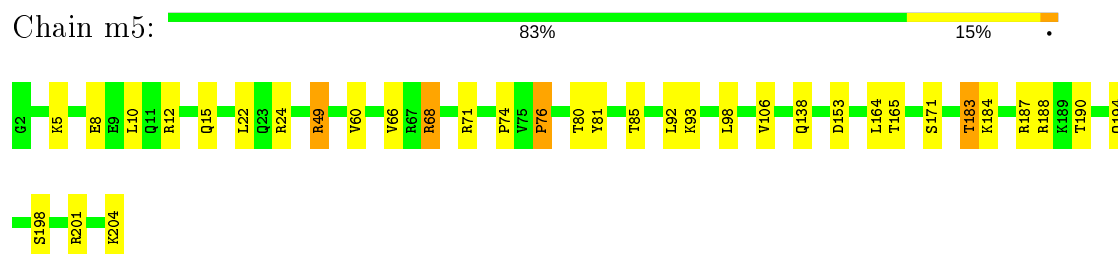


- Molecule 51: 60S ribosomal protein L15-A

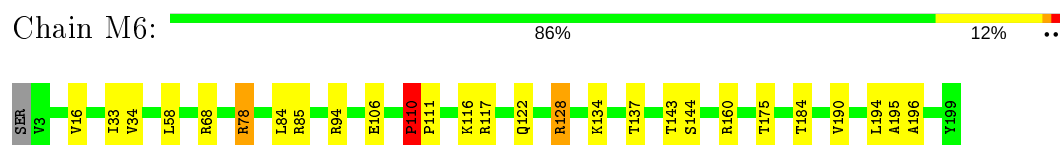
Chain M5: 81% 19%



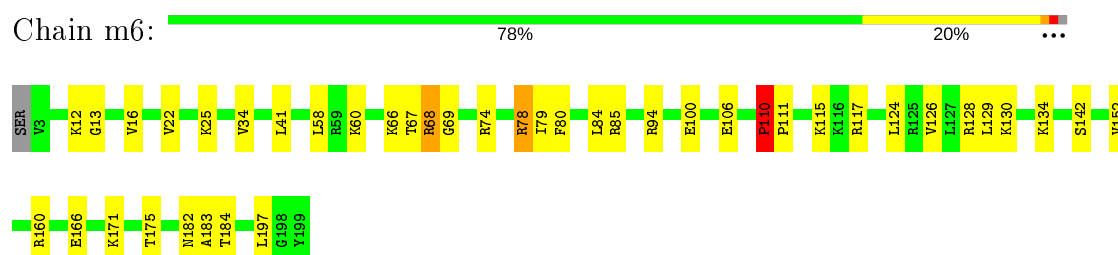
- Molecule 51: 60S ribosomal protein L15-A



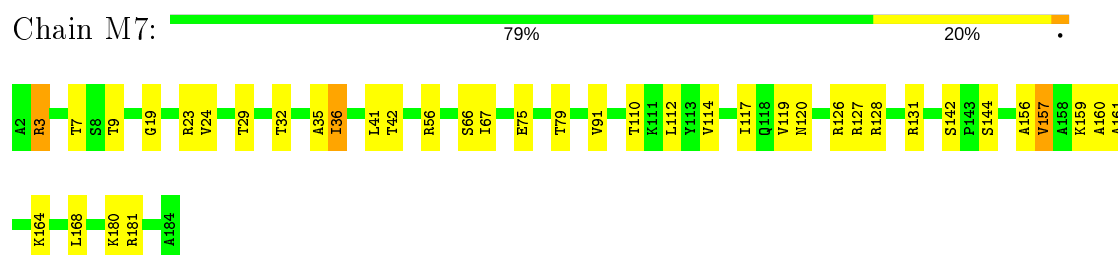
- Molecule 52: 60S ribosomal protein L16-A



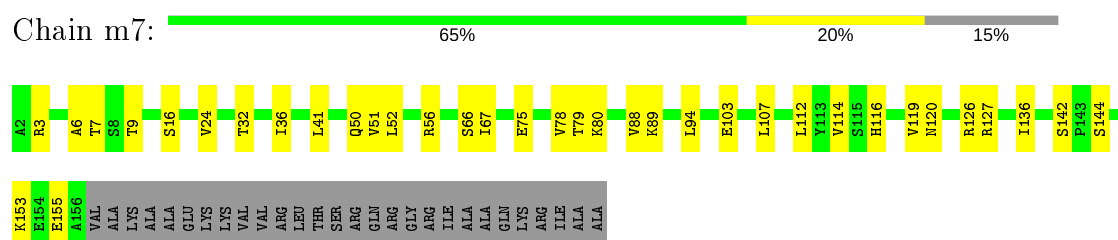
- Molecule 52: 60S ribosomal protein L16-A



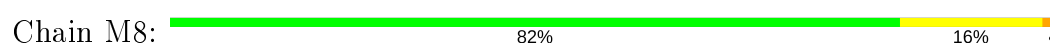
- Molecule 53: 60S ribosomal protein L17-A

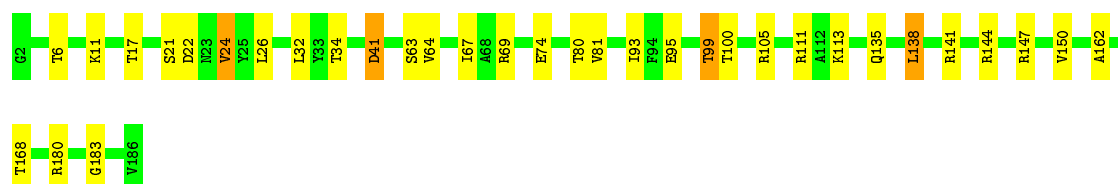


- Molecule 53: 60S ribosomal protein L17-A



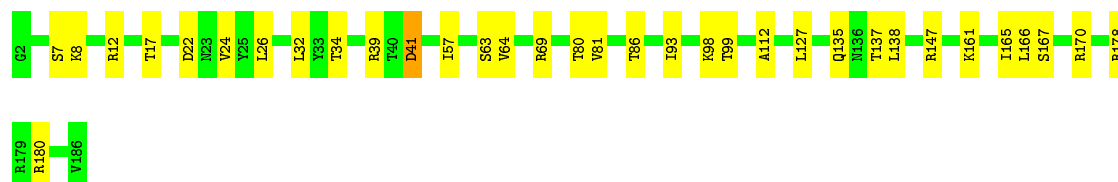
- Molecule 54: 60S ribosomal protein L18-A





- Molecule 54: 60S ribosomal protein L18-A

Chain m8: 82% 18%



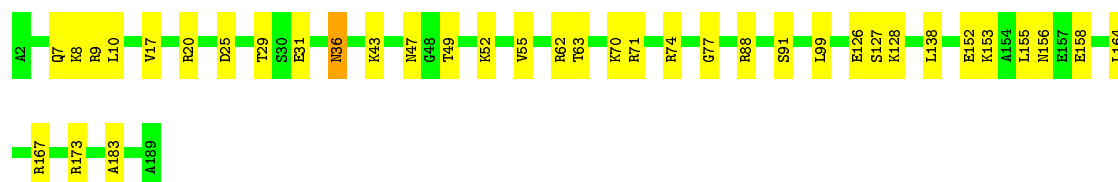
- Molecule 55: 60S ribosomal protein L19-A

Chain M9: 86% 14%



- Molecule 55: 60S ribosomal protein L19-A

Chain m9: 80% 19%



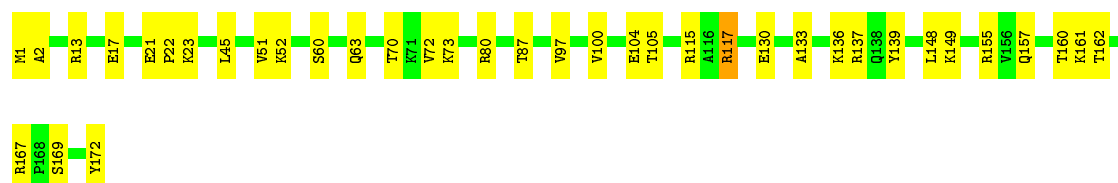
- Molecule 56: 60S ribosomal protein L20-A

Chain N0: 80% 18%

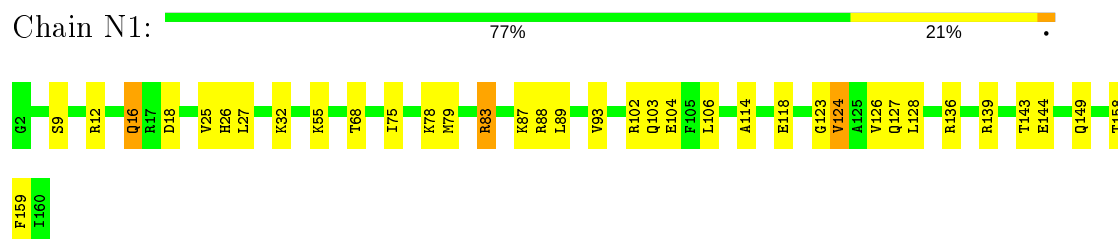


- Molecule 56: 60S ribosomal protein L20-A

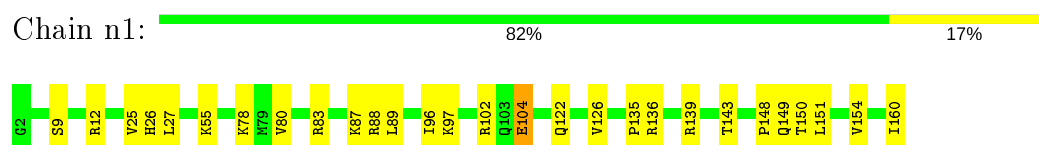
Chain n0: 78% 22%



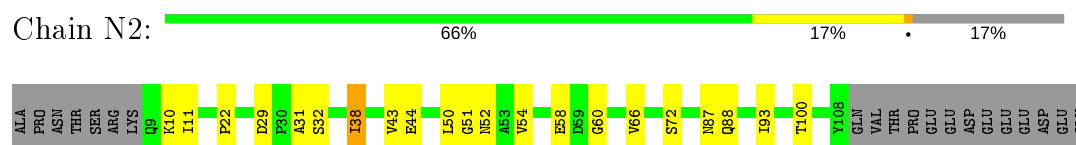
- Molecule 57: 60S ribosomal protein L21-A



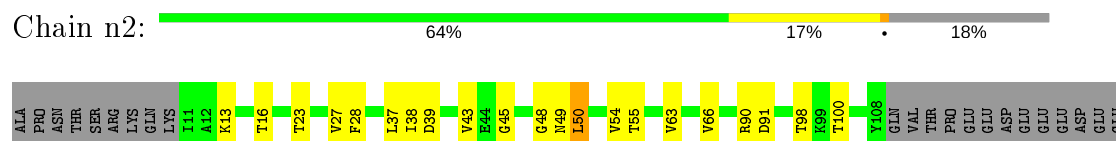
- Molecule 57: 60S ribosomal protein L21-A



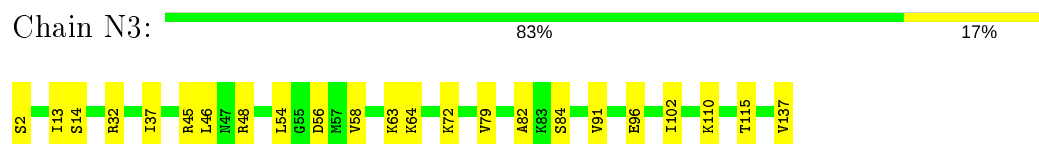
- Molecule 58: 60S ribosomal protein L22-A



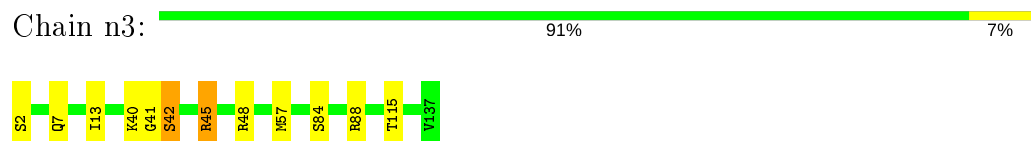
- Molecule 58: 60S ribosomal protein L22-A



- Molecule 59: 60S ribosomal protein L23-A

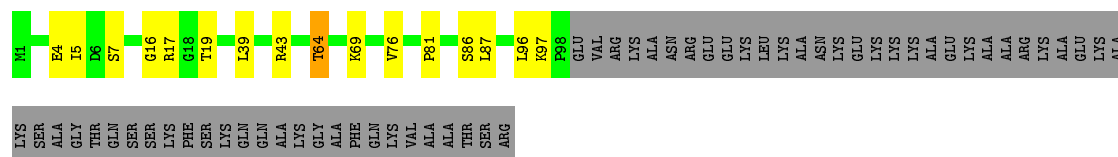


- Molecule 59: 60S ribosomal protein L23-A



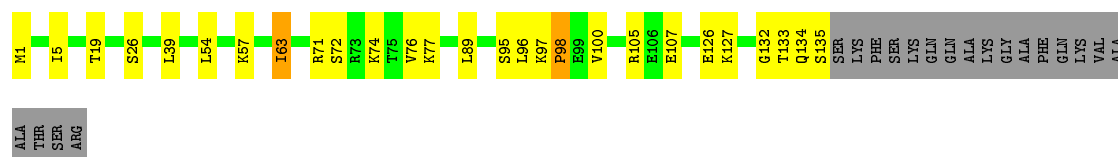
- Molecule 60: 60S ribosomal protein L24-A





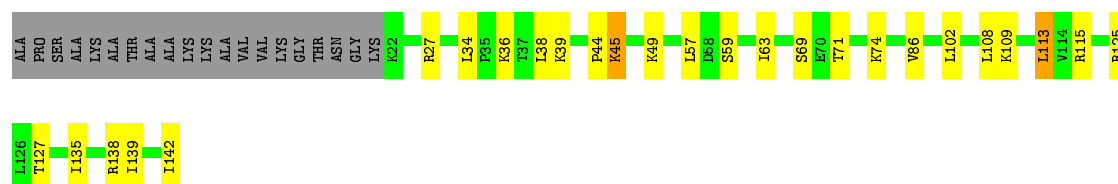
- Molecule 60: 60S ribosomal protein L24-A

Chain n4: 70% 16% 13%



- Molecule 61: 60S ribosomal protein L25

Chain N5: 67% 17% 14%



- Molecule 62: 60S ribosomal protein L26-A

Chain N6: 76% 23%



- Molecule 62: 60S ribosomal protein L26-A

Chain N6: 76% 23%



- Molecule 63: 60S ribosomal protein L27-A

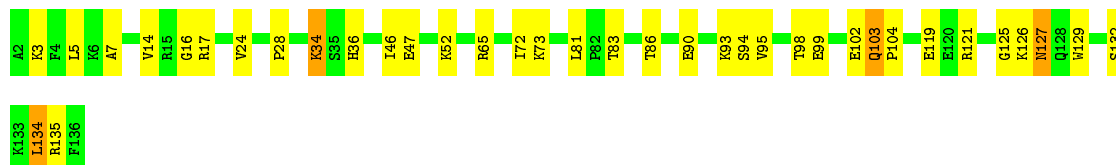
Chain N7: 76% 22%





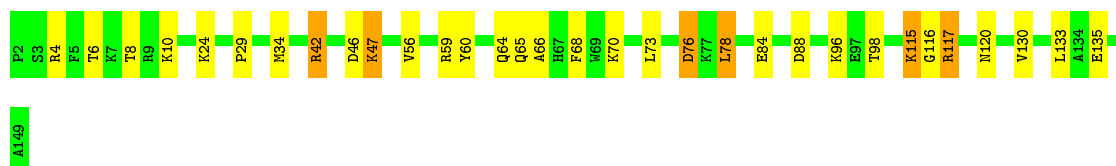
- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 73% 24%



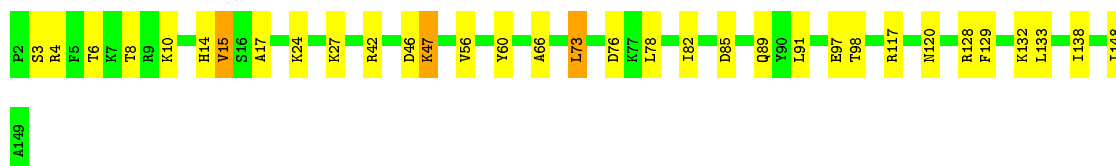
- Molecule 64: 60S ribosomal protein L28

Chain N8: 78% 18%



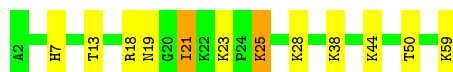
- Molecule 64: 60S ribosomal protein L28

Chain n8: 78% 20%



- Molecule 65: 60S ribosomal protein L29

Chain N9: 79% 17%



- Molecule 65: 60S ribosomal protein L29

Chain n9: 69% 29%

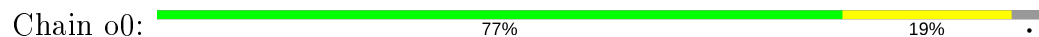


- Molecule 66: 60S ribosomal protein L30

Chain O0: 74% 19% 7%



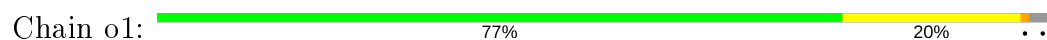
- Molecule 66: 60S ribosomal protein L30



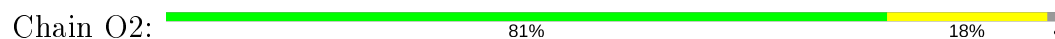
- Molecule 67: 60S ribosomal protein L31-A



- Molecule 67: 60S ribosomal protein L31-A



- Molecule 68: 60S ribosomal protein L32



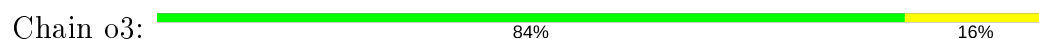
- Molecule 68: 60S ribosomal protein L32

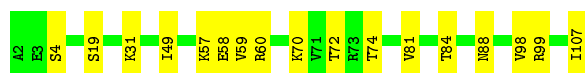


- Molecule 69: 60S ribosomal protein L33-A



- Molecule 69: 60S ribosomal protein L33-A





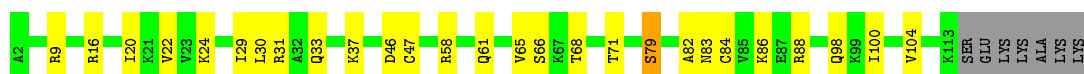
- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 79% 13% 6%



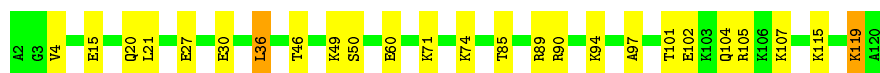
- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 71% 22% 6%



- Molecule 71: 60S ribosomal protein L35-A

Chain O5: 79% 19%



- Molecule 71: 60S ribosomal protein L35-A

Chain o5: 76% 22%



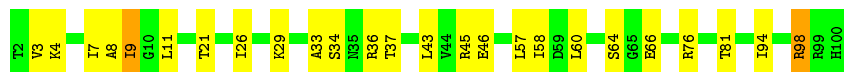
- Molecule 72: 60S ribosomal protein L36-A

Chain O6: 73% 23%



- Molecule 72: 60S ribosomal protein L36-A

Chain o6: 75% 23%



- Molecule 73: 60S ribosomal protein L37-A

Chain O7: 80% 17%



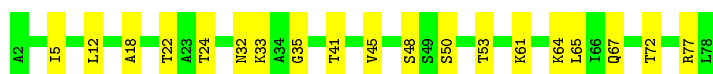
- Molecule 73: 60S ribosomal protein L37-A

Chain o7: 78% 20%



- Molecule 74: 60S ribosomal protein L38

Chain O8: 75% 25%



- Molecule 74: 60S ribosomal protein L38

Chain o8: 79% 21%



- Molecule 75: 60S ribosomal protein L39

Chain O9: 86% 14%



- Molecule 75: 60S ribosomal protein L39

Chain o9: 78% 22%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0: 81% 17%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

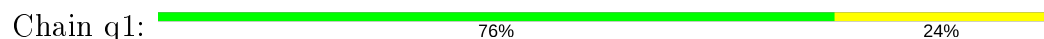
Chain q0: 79% 21%



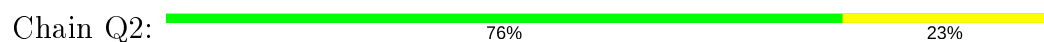
- Molecule 77: 60S ribosomal protein L41-A



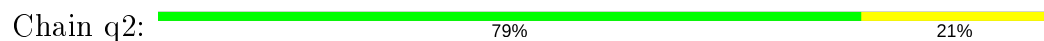
- Molecule 77: 60S ribosomal protein L41-A



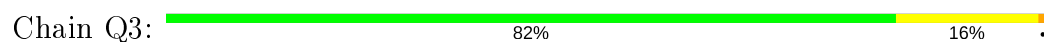
- Molecule 78: 60S ribosomal protein L42-A



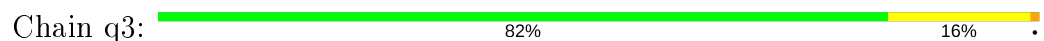
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A

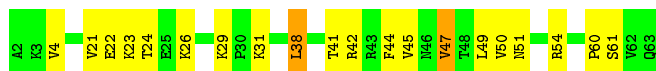


- Molecule 79: 60S ribosomal protein L43-A



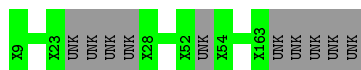
- Molecule 80: 40S ribosomal protein S30-A





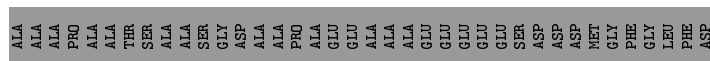
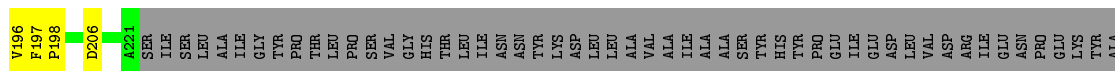
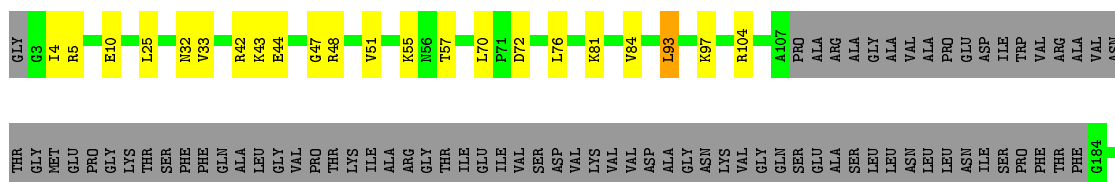
- Molecule 81: Unknown protein m2

Chain m2: 94% 6%



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0: 38% 8% 54%



- Molecule 83: Unknown protein p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 84: Unknown protein p2

Chain p2: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	434.77Å 287.66Å 303.84Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	73.94 – 3.10	Depositor
% Data completeness (in resolution range)	100.0 (73.94-3.10)	Depositor
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.203 , 0.252	Depositor
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.164	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411258	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OHX, MG, EDE

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	0.78	3/41698 (0.0%)	1.36	372/64972 (0.6%)
1	6	0.89	23/42765 (0.1%)	1.41	502/66634 (0.8%)
2	S0	0.49	0/1617	0.70	0/2215
2	s0	0.49	0/1623	0.72	0/2222
3	S1	0.42	0/1735	0.67	2/2335 (0.1%)
3	s1	0.52	0/1748	0.68	1/2352 (0.0%)
4	S2	0.54	0/1665	0.69	0/2263
4	s2	0.61	0/1665	0.77	1/2263 (0.0%)
5	S3	0.52	0/1759	0.67	1/2368 (0.0%)
5	s3	0.45	0/1759	0.64	2/2368 (0.1%)
6	S4	0.50	0/2109	0.73	0/2839
6	s4	0.56	0/2109	0.79	2/2839 (0.1%)
7	S5	0.40	0/1629	0.61	0/2202
7	s5	0.48	0/1629	0.69	1/2202 (0.0%)
8	S6	0.51	0/1823	0.69	0/2439
8	s6	0.58	0/1779	0.74	0/2379
9	S7	0.46	0/1506	0.66	0/2028
9	s7	0.49	0/1516	0.72	0/2043
10	S8	0.57	0/1514	0.75	1/2021 (0.0%)
10	s8	0.66	0/1514	0.77	1/2021 (0.0%)
11	S9	0.52	0/1519	0.72	0/2035
11	s9	0.60	0/1519	0.79	1/2035 (0.0%)
12	C0	0.44	0/790	0.68	1/1069 (0.1%)
12	c0	0.38	0/777	0.65	3/1049 (0.3%)
13	C1	0.62	0/1240	0.69	0/1675
13	c1	0.67	1/1194 (0.1%)	0.80	0/1610
14	C2	0.38	0/900	0.63	0/1224
14	c2	0.30	0/900	0.57	0/1224
15	C3	0.54	0/1215	0.71	2/1638 (0.1%)
15	c3	0.59	0/1215	0.73	0/1638
16	C4	0.43	0/901	0.72	0/1217
16	c4	0.53	0/960	0.75	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.48	0/998	0.68	0/1341
17	c5	0.49	0/1060	0.69	0/1426
18	C6	0.46	0/1125	0.72	2/1510 (0.1%)
18	c6	0.49	0/1131	0.71	0/1518
19	C7	0.49	0/935	0.69	0/1254
19	c7	0.48	0/914	0.73	0/1224
20	C8	0.46	0/1211	0.65	0/1628
20	c8	0.53	0/1211	0.74	2/1628 (0.1%)
21	C9	0.45	0/1130	0.69	0/1517
21	c9	0.50	0/1130	0.67	0/1517
22	D0	0.48	0/865	0.67	0/1169
22	d0	0.50	0/892	0.67	0/1205
23	D1	0.50	0/693	0.67	0/935
23	d1	0.53	0/693	0.76	1/935 (0.1%)
24	D2	0.55	0/1038	0.76	1/1395 (0.1%)
24	d2	0.65	0/1038	0.79	1/1395 (0.1%)
25	D3	0.65	0/1139	0.81	1/1518 (0.1%)
25	d3	0.72	0/1139	0.80	2/1518 (0.1%)
26	D4	0.48	0/1087	0.64	0/1449
26	d4	0.56	0/1087	0.78	0/1449
27	D5	0.44	0/571	0.72	1/768 (0.1%)
27	d5	0.44	0/566	0.68	0/761
28	D6	0.48	0/782	0.70	0/1047
28	d6	0.53	0/782	0.73	0/1047
29	D7	0.50	0/620	0.70	0/838
29	d7	0.50	0/620	0.69	0/838
30	D8	0.40	0/499	0.59	0/670
30	d8	0.44	0/499	0.65	0/670
31	D9	0.55	0/452	0.82	1/600 (0.2%)
31	d9	0.55	0/452	0.69	0/600
32	E0	0.50	0/483	0.65	0/643
33	E1	0.48	0/577	0.77	0/770
33	e1	0.41	0/619	0.73	1/822 (0.1%)
34	SR	0.40	0/2494	0.59	0/3393
34	sR	0.41	0/2495	0.58	0/3395
35	SM	0.56	0/1113	0.78	3/1502 (0.2%)
35	sM	0.51	0/683	0.68	1/923 (0.1%)
36	1	1.22	216/75394 (0.3%)	1.71	2044/117545 (1.7%)
36	5	1.22	222/75414 (0.3%)	1.69	1963/117575 (1.7%)
37	3	0.99	2/2883 (0.1%)	1.42	30/4491 (0.7%)
37	7	1.19	6/2883 (0.2%)	1.73	81/4491 (1.8%)
38	4	1.16	5/3746 (0.1%)	1.70	103/5832 (1.8%)
38	8	0.99	1/3746 (0.0%)	1.51	47/5832 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.75	0/1948	0.86	0/2617
39	l2	0.71	0/1946	0.88	3/2614 (0.1%)
40	L3	0.77	1/3146 (0.0%)	0.85	2/4228 (0.0%)
40	l3	0.87	1/3146 (0.0%)	0.93	7/4228 (0.2%)
41	L4	0.84	0/2800	0.95	4/3790 (0.1%)
41	l4	0.74	0/2800	0.87	2/3790 (0.1%)
42	L5	0.62	0/2425	0.73	1/3271 (0.0%)
42	l5	0.72	0/2408	0.81	0/3248
43	L6	0.84	0/1260	0.87	2/1694 (0.1%)
43	l6	0.80	0/1269	0.84	2/1705 (0.1%)
44	L7	0.84	0/1821	0.91	4/2451 (0.2%)
44	l7	0.85	0/1828	0.93	3/2461 (0.1%)
45	L8	0.60	0/1836	0.72	1/2481 (0.0%)
45	l8	0.54	0/1795	0.69	1/2429 (0.0%)
46	L9	0.70	0/1539	0.79	2/2073 (0.1%)
46	l9	0.81	1/1539 (0.1%)	0.82	0/2073
47	M0	0.81	1/1741 (0.1%)	0.87	2/2335 (0.1%)
47	m0	0.78	0/1758	0.84	0/2358
48	M1	0.55	0/1374	0.74	1/1842 (0.1%)
48	m1	0.66	0/1374	0.79	3/1842 (0.2%)
49	M3	0.80	0/1568	0.85	2/2106 (0.1%)
49	m3	0.68	0/1573	0.82	0/2113
50	M4	0.78	0/1068	0.86	1/1438 (0.1%)
50	m4	0.83	0/1074	0.90	2/1446 (0.1%)
51	M5	0.78	0/1757	0.86	0/2354
51	m5	0.69	0/1757	0.80	1/2354 (0.0%)
52	M6	0.93	0/1585	0.92	4/2128 (0.2%)
52	m6	1.05	2/1585 (0.1%)	1.00	8/2128 (0.4%)
53	M7	0.85	0/1443	0.91	3/1944 (0.2%)
53	m7	0.92	0/1250	0.87	0/1683
54	M8	0.82	0/1465	0.91	2/1965 (0.1%)
54	m8	0.73	0/1465	0.94	1/1965 (0.1%)
55	M9	0.59	0/1538	0.71	0/2050
55	m9	0.66	0/1538	0.72	0/2050
56	N0	0.82	0/1481	0.90	2/1990 (0.1%)
56	n0	0.90	0/1481	0.90	1/1990 (0.1%)
57	N1	0.82	0/1300	0.85	1/1743 (0.1%)
57	n1	0.85	1/1300 (0.1%)	0.82	0/1743
58	N2	0.47	0/812	0.62	0/1099
58	n2	0.55	0/794	0.68	0/1076
59	N3	0.74	0/1018	0.84	1/1369 (0.1%)
59	n3	0.89	0/1018	0.92	1/1369 (0.1%)
60	N4	0.56	0/712	0.69	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.73	0/1052	0.77	0/1398
61	N5	0.64	0/979	0.83	1/1321 (0.1%)
61	n5	0.65	0/974	0.77	0/1314
62	N6	0.72	0/1004	0.88	1/1341 (0.1%)
62	n6	0.65	0/1004	0.84	1/1341 (0.1%)
63	N7	0.56	0/1118	0.71	0/1497
63	n7	0.52	0/1118	0.65	0/1497
64	N8	0.82	0/1204	0.98	4/1612 (0.2%)
64	n8	0.78	0/1204	0.85	1/1612 (0.1%)
65	N9	0.72	0/473	0.82	0/629
65	n9	0.81	0/473	0.97	0/629
66	O0	0.52	0/751	0.72	0/1008
66	o0	0.51	0/775	0.69	0/1040
67	O1	0.65	0/890	0.73	0/1196
67	o1	0.79	0/897	0.88	0/1205
68	O2	0.89	0/1041	0.92	0/1394
68	o2	0.85	0/1041	0.93	3/1394 (0.2%)
69	O3	0.91	0/868	0.87	1/1168 (0.1%)
69	o3	0.92	0/868	0.94	1/1168 (0.1%)
70	O4	0.62	0/890	0.82	2/1189 (0.2%)
70	o4	0.59	0/890	0.78	0/1189
71	O5	0.76	0/978	0.82	1/1301 (0.1%)
71	o5	0.61	0/974	0.73	0/1297
72	O6	0.69	0/778	0.82	0/1034
72	o6	0.57	0/777	0.69	0/1033
73	O7	0.79	0/696	1.00	3/923 (0.3%)
73	o7	0.75	0/696	0.88	2/923 (0.2%)
74	O8	0.54	0/618	0.68	0/826
74	o8	0.48	0/614	0.64	0/822
75	O9	0.87	1/443 (0.2%)	0.93	0/588
75	o9	0.69	0/443	0.81	0/588
76	Q0	0.67	0/423	0.81	0/562
76	q0	0.93	0/423	0.87	0/562
77	Q1	0.63	0/234	0.96	0/300
77	q1	0.77	0/234	0.83	0/300
78	Q2	0.94	1/860 (0.1%)	0.83	0/1136
78	q2	0.84	1/860 (0.1%)	0.79	0/1136
79	Q3	0.78	0/701	0.85	0/934
79	q3	0.74	0/701	0.81	0/934
80	e0	0.59	0/499	0.75	0/665
82	p0	0.48	0/1092	0.62	0/1474
All	All	0.94	489/430074 (0.1%)	1.34	5269/631364 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	s0	0	1
5	s3	0	1
6	S4	0	1
7	s5	0	2
9	S7	0	1
16	C4	0	3
17	c5	0	2
18	c6	0	1
19	C7	0	2
22	d0	0	1
24	D2	0	1
25	d3	0	1
27	D5	0	2
28	D6	0	1
33	E1	0	1
36	1	0	1
39	L2	0	1
39	l2	0	1
41	l4	0	1
42	L5	0	1
42	l5	0	1
43	l6	0	2
44	l7	0	2
45	L8	0	2
48	M1	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
56	n0	0	1
57	N1	0	1
64	n8	0	1
65	N9	0	1
67	O1	0	1
67	o1	0	1
72	O6	0	1
All	All	0	44

All (489) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	16.17	2.09	1.82
36	5	1152	G	N9-C4	-12.64	1.27	1.38
78	q2	17	CYS	CB-SG	12.30	2.03	1.82
36	5	2401	A	N3-C4	10.74	1.41	1.34
36	1	2404	A	N3-C4	10.30	1.41	1.34
36	5	2358	A	N9-C4	-9.40	1.32	1.37
36	1	3181	C	N3-C4	-9.01	1.27	1.33
36	1	804	C	N1-C6	-8.97	1.31	1.37
36	5	970	A	N9-C4	-8.77	1.32	1.37
36	5	2971	A	N9-C4	8.63	1.43	1.37
36	5	953	G	N7-C5	-8.54	1.34	1.39
36	5	3008	A	N9-C4	-8.46	1.32	1.37
36	1	1326	A	N9-C4	-8.43	1.32	1.37
36	5	970	A	N3-C4	-8.41	1.29	1.34
36	5	1152	G	C5-C6	-8.38	1.33	1.42
36	1	699	A	N9-C4	-8.32	1.32	1.37
36	1	2147	A	N9-C4	-8.30	1.32	1.37
36	1	584	G	N7-C5	-8.00	1.34	1.39
36	5	2147	A	C5-C6	-7.97	1.33	1.41
36	1	343	U	C2-N3	-7.90	1.32	1.37
36	5	2636	A	C6-N1	-7.84	1.30	1.35
36	1	716	A	N9-C4	-7.78	1.33	1.37
36	5	1304	A	N3-C4	7.71	1.39	1.34
36	1	2714	G	N9-C4	-7.68	1.31	1.38
36	1	1395	G	C5-C4	-7.61	1.33	1.38
36	1	1369	A	N7-C5	-7.58	1.34	1.39
36	5	2817	A	N3-C4	-7.52	1.30	1.34
36	1	1116	G	N7-C5	-7.50	1.34	1.39
36	5	367	A	N9-C4	-7.43	1.33	1.37
36	1	1399	A	N9-C4	-7.42	1.33	1.37
36	1	1154	A	N7-C5	-7.38	1.34	1.39
36	1	338	A	N7-C5	-7.37	1.34	1.39
36	5	2804	A	N9-C4	-7.36	1.33	1.37
52	m6	80	PHE	CB-CG	-7.35	1.38	1.51
36	1	2147	A	C5-C4	-7.29	1.33	1.38
36	1	2404	A	N9-C4	7.28	1.42	1.37
36	5	2943	G	N7-C5	-7.26	1.34	1.39
36	1	1392	G	C5-C4	-7.22	1.33	1.38
36	5	2401	A	N9-C4	7.21	1.42	1.37
36	1	2356	A	N9-C4	-7.21	1.33	1.37
1	6	163	G	N9-C4	-7.17	1.32	1.38
36	5	1143	A	N3-C4	-7.11	1.30	1.34
36	5	2625	C	N1-C6	-7.06	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	1002	A	N9-C4	-7.05	1.33	1.37
36	1	2726	C	N3-C4	-7.05	1.29	1.33
36	5	3245	A	C5-C6	-7.04	1.34	1.41
36	5	1303	A	N9-C4	-7.04	1.33	1.37
36	1	2147	A	N3-C4	-6.99	1.30	1.34
36	5	3040	A	N9-C4	-6.97	1.33	1.37
36	5	934	G	C5-C4	-6.91	1.33	1.38
36	5	2726	C	N3-C4	-6.89	1.29	1.33
36	1	2762	A	N3-C4	-6.88	1.30	1.34
1	6	623	A	N9-C4	-6.87	1.33	1.37
36	1	884	A	N9-C4	-6.85	1.33	1.37
36	5	649	A	C5-C6	-6.82	1.34	1.41
36	5	934	G	C5-C6	-6.82	1.35	1.42
36	5	1152	G	N3-C4	-6.81	1.30	1.35
36	1	699	A	N3-C4	-6.81	1.30	1.34
36	5	420	G	N9-C8	-6.80	1.33	1.37
36	5	962	A	N7-C5	-6.77	1.35	1.39
36	5	1143	A	N9-C4	-6.77	1.33	1.37
36	5	934	G	N7-C5	-6.74	1.35	1.39
36	1	2406	C	N1-C6	-6.73	1.33	1.37
36	1	919	U	C4-O4	-6.71	1.18	1.23
36	1	2333	C	N3-C4	-6.71	1.29	1.33
36	5	822	G	C2-N3	-6.70	1.27	1.32
36	5	1307	G	N7-C5	-6.70	1.35	1.39
36	5	971	G	N7-C5	-6.70	1.35	1.39
36	1	1133	A	N9-C4	-6.67	1.33	1.37
36	5	2640	A	N9-C4	-6.67	1.33	1.37
36	1	1313	G	C5-C6	-6.66	1.35	1.42
36	5	3240	C	N3-C4	-6.66	1.29	1.33
36	5	2937	G	N7-C5	-6.63	1.35	1.39
36	1	2875	U	C2-N3	6.63	1.42	1.37
36	1	668	G	C6-N1	-6.62	1.34	1.39
36	5	1301	A	C5-C6	-6.61	1.35	1.41
36	1	636	C	N3-C4	-6.60	1.29	1.33
36	5	2364	G	N3-C4	-6.60	1.30	1.35
36	1	925	A	N3-C4	-6.59	1.30	1.34
36	5	3047	U	C2-N3	-6.57	1.33	1.37
36	1	189	G	N7-C5	-6.56	1.35	1.39
36	1	952	A	N7-C5	-6.55	1.35	1.39
36	1	939	U	N1-C2	-6.55	1.32	1.38
36	1	361	A	N9-C4	-6.52	1.33	1.37
36	1	1137	C	N1-C6	-6.51	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2762	A	C6-N1	-6.50	1.30	1.35
36	5	1203	A	C5-C6	-6.50	1.35	1.41
36	5	2401	A	C6-N1	6.50	1.40	1.35
36	1	1445	U	N1-C2	-6.50	1.32	1.38
36	1	2188	A	N9-C4	-6.49	1.33	1.37
36	1	816	A	N9-C4	6.49	1.41	1.37
36	1	1099	A	N7-C5	-6.48	1.35	1.39
36	5	1145	G	N3-C4	-6.47	1.30	1.35
36	1	423	A	N7-C5	-6.47	1.35	1.39
36	5	1332	A	N7-C5	-6.45	1.35	1.39
37	3	82	G	C6-N1	-6.44	1.35	1.39
36	5	2943	G	C5-C6	-6.44	1.35	1.42
36	5	1159	A	N9-C4	-6.43	1.33	1.37
38	4	111	A	C5-C6	-6.42	1.35	1.41
36	5	1462	A	N9-C4	-6.42	1.33	1.37
36	5	2933	A	N3-C4	-6.40	1.31	1.34
47	M0	8	CYS	CB-SG	-6.40	1.71	1.82
36	5	1874	A	N9-C4	-6.39	1.34	1.37
36	5	2138	A	N7-C5	-6.39	1.35	1.39
36	5	437	G	N9-C4	6.38	1.43	1.38
36	5	3052	G	C2-N3	-6.38	1.27	1.32
36	5	2811	A	N9-C4	-6.37	1.34	1.37
36	5	826	G	C2-N3	-6.33	1.27	1.32
38	4	15	G	C5-C4	-6.32	1.33	1.38
36	1	1373	A	N3-C4	-6.32	1.31	1.34
36	5	1159	A	N3-C4	-6.31	1.31	1.34
36	5	2145	A	C6-N1	-6.31	1.31	1.35
36	5	2954	U	N1-C2	6.29	1.44	1.38
36	1	2983	C	N3-C4	-6.28	1.29	1.33
36	1	2887	A	N7-C5	-6.27	1.35	1.39
36	1	695	C	N3-C4	-6.26	1.29	1.33
36	1	3142	A	N3-C4	-6.25	1.31	1.34
36	1	638	C	N1-C6	-6.23	1.33	1.37
36	5	2360	C	C4-C5	-6.22	1.38	1.43
36	1	426	G	N1-C2	-6.21	1.32	1.37
36	5	810	A	N3-C4	6.21	1.38	1.34
36	5	2937	G	C5-C6	-6.21	1.36	1.42
36	5	1304	A	N7-C5	-6.20	1.35	1.39
36	1	2409	G	C5-C4	-6.20	1.34	1.38
40	l3	251	CYS	CB-SG	-6.19	1.71	1.82
36	1	2341	A	N9-C4	-6.17	1.34	1.37
36	5	2375	G	C6-N1	-6.16	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2823	G	N7-C5	-6.15	1.35	1.39
36	1	48	A	N7-C5	-6.15	1.35	1.39
36	1	29	C	N1-C6	-6.15	1.33	1.37
36	1	2356	A	N3-C4	-6.15	1.31	1.34
36	5	2291	A	N9-C4	-6.14	1.34	1.37
36	5	2937	G	C5-C4	-6.14	1.34	1.38
36	5	962	A	C5-C6	-6.13	1.35	1.41
36	1	654	C	N1-C6	-6.13	1.33	1.37
36	5	1338	C	N1-C6	-6.13	1.33	1.37
36	5	2639	G	N7-C5	-6.12	1.35	1.39
36	1	2971	A	N9-C4	6.10	1.41	1.37
36	5	1311	G	C5-C4	-6.09	1.34	1.38
36	5	1456	A	N9-C4	-6.09	1.34	1.37
36	5	1329	U	N1-C6	-6.08	1.32	1.38
36	5	3314	A	N9-C4	-6.07	1.34	1.37
36	1	970	A	C6-N1	-6.07	1.31	1.35
36	5	437	G	C5-C4	6.07	1.42	1.38
36	1	1373	A	C6-N1	-6.06	1.31	1.35
36	1	2598	G	C5-C4	-6.06	1.34	1.38
36	5	416	A	N7-C5	-6.05	1.35	1.39
36	5	2799	A	C6-N1	-6.05	1.31	1.35
36	5	2626	A	N9-C4	-6.03	1.34	1.37
36	5	3382	U	N1-C2	6.02	1.44	1.38
36	1	1103	A	N7-C5	6.02	1.42	1.39
36	5	2872	A	N9-C4	-6.01	1.34	1.37
36	1	2271	A	C5-C6	-6.00	1.35	1.41
36	1	2404	A	C6-N1	6.00	1.39	1.35
36	1	2761	G	N7-C5	-6.00	1.35	1.39
37	7	94	C	C4-C5	-5.98	1.38	1.43
36	1	790	U	C2-N3	-5.98	1.33	1.37
36	5	1103	A	N3-C4	5.98	1.38	1.34
36	5	3095	U	C2-N3	-5.97	1.33	1.37
36	1	337	G	C5-C4	-5.96	1.34	1.38
36	5	1113	G	N3-C4	-5.95	1.31	1.35
36	1	424	G	C5-C4	-5.94	1.34	1.38
36	1	706	A	N9-C4	-5.94	1.34	1.37
1	6	1659	A	N9-C4	-5.93	1.34	1.37
36	5	2139	A	N3-C4	-5.92	1.31	1.34
36	1	34	A	N9-C4	-5.92	1.34	1.37
36	1	343	U	N3-C4	-5.92	1.33	1.38
36	5	2996	U	N1-C2	5.91	1.43	1.38
36	1	2984	C	N3-C4	-5.91	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2885	C	N1-C6	-5.91	1.33	1.37
36	1	3142	A	N9-C4	-5.90	1.34	1.37
1	6	1653	C	N1-C6	-5.90	1.33	1.37
36	5	924	G	N3-C4	-5.90	1.31	1.35
36	1	651	G	N1-C2	-5.89	1.33	1.37
36	1	1667	A	N9-C4	-5.89	1.34	1.37
1	6	44	U	N1-C2	-5.89	1.33	1.38
36	5	1865	A	N9-C4	-5.88	1.34	1.37
36	1	2326	A	N9-C4	-5.88	1.34	1.37
36	5	3209	A	C5-C4	5.87	1.42	1.38
36	1	423	A	N3-C4	-5.87	1.31	1.34
36	1	650	C	N1-C6	-5.87	1.33	1.37
36	1	653	A	C5-C6	-5.87	1.35	1.41
36	5	2395	G	N7-C5	5.85	1.42	1.39
36	1	1377	G	C5-C6	-5.85	1.36	1.42
36	1	1492	G	N7-C5	-5.83	1.35	1.39
36	1	2396	G	N9-C8	-5.83	1.33	1.37
36	5	2404	A	N3-C4	5.82	1.38	1.34
36	1	343	U	N1-C2	-5.81	1.33	1.38
37	3	83	U	C2-N3	-5.81	1.33	1.37
36	5	2892	A	N3-C4	-5.81	1.31	1.34
36	1	1547	G	C5-C4	-5.80	1.34	1.38
36	1	2714	G	N9-C8	5.80	1.42	1.37
40	L3	200	GLU	CG-CD	5.80	1.60	1.51
36	1	919	U	C2-N3	-5.79	1.33	1.37
36	5	1103	A	N9-C4	5.79	1.41	1.37
36	5	1445	U	N1-C2	-5.79	1.33	1.38
36	1	968	G	C6-N1	-5.78	1.35	1.39
37	7	112	G	N7-C5	-5.78	1.35	1.39
36	5	1451	C	N1-C6	-5.77	1.33	1.37
36	5	1902	G	N7-C5	-5.77	1.35	1.39
36	1	100	A	N3-C4	-5.75	1.31	1.34
36	1	2893	C	N3-C4	-5.75	1.29	1.33
36	1	1308	A	C6-N1	-5.75	1.31	1.35
36	1	2761	G	N9-C8	-5.75	1.33	1.37
36	1	2187	G	N7-C5	-5.75	1.35	1.39
36	1	66	A	N9-C4	-5.75	1.34	1.37
36	5	924	G	N9-C4	-5.74	1.33	1.38
36	5	1152	G	N1-C2	5.74	1.42	1.37
57	n1	104	GLU	CB-CG	5.74	1.63	1.52
36	1	1107	C	N1-C6	-5.74	1.33	1.37
36	1	2409	G	N3-C4	-5.74	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2856	G	N7-C5	-5.74	1.35	1.39
36	1	1144	U	C2-N3	-5.73	1.33	1.37
36	5	3362	A	N9-C4	-5.72	1.34	1.37
36	1	895	A	C5-C6	-5.72	1.35	1.41
52	m6	78	ARG	CZ-NH1	5.72	1.40	1.33
1	6	1131	A	N3-C4	-5.71	1.31	1.34
36	1	3273	A	N3-C4	-5.71	1.31	1.34
36	1	1377	G	C5-C4	-5.70	1.34	1.38
36	1	2276	G	N7-C5	-5.70	1.35	1.39
36	5	40	A	N7-C5	-5.69	1.35	1.39
36	5	420	G	C5-C4	-5.69	1.34	1.38
36	5	367	A	N3-C4	-5.67	1.31	1.34
36	5	2931	C	N1-C6	-5.67	1.33	1.37
36	5	883	A	N3-C4	-5.67	1.31	1.34
36	1	1505	C	N3-C4	-5.67	1.29	1.33
1	2	1657	U	N1-C2	5.66	1.43	1.38
36	5	1432	C	C2-N3	-5.66	1.31	1.35
36	5	1116	G	N9-C8	-5.66	1.33	1.37
46	19	11	GLU	CG-CD	5.66	1.60	1.51
36	5	945	C	N1-C6	-5.65	1.33	1.37
36	1	2919	A	N3-C4	-5.65	1.31	1.34
36	1	1305	U	N3-C4	-5.65	1.33	1.38
36	1	658	G	C8-N7	-5.64	1.27	1.30
36	1	2409	G	N9-C8	-5.64	1.33	1.37
37	7	91	G	N7-C5	-5.63	1.35	1.39
36	1	2368	A	N3-C4	-5.63	1.31	1.34
36	5	1891	A	N7-C5	-5.63	1.35	1.39
36	5	2385	G	N9-C4	-5.62	1.33	1.38
36	1	962	A	N7-C5	-5.62	1.35	1.39
1	6	754	A	N9-C4	5.62	1.41	1.37
36	1	870	G	N7-C5	-5.62	1.35	1.39
1	6	426	G	C6-N1	-5.61	1.35	1.39
36	1	1351	U	N1-C2	5.61	1.43	1.38
36	1	49	A	N9-C4	-5.61	1.34	1.37
36	5	1301	A	N7-C5	-5.61	1.35	1.39
36	1	636	C	C4-N4	-5.61	1.28	1.33
36	5	953	G	C5-C4	-5.60	1.34	1.38
36	1	407	A	N7-C5	-5.60	1.35	1.39
36	5	924	G	C2-N3	-5.58	1.28	1.32
36	5	523	A	N9-C4	-5.58	1.34	1.37
36	1	1865	A	N9-C4	-5.58	1.34	1.37
1	6	1000	C	N3-C4	-5.58	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2298	U	N3-C4	-5.57	1.33	1.38
36	1	2954	U	N3-C4	5.57	1.43	1.38
36	1	716	A	C5-C6	-5.57	1.36	1.41
36	5	2976	A	N3-C4	-5.57	1.31	1.34
36	1	828	A	N7-C5	-5.57	1.35	1.39
36	1	1178	G	C6-N1	-5.56	1.35	1.39
36	5	1847	A	N9-C4	-5.56	1.34	1.37
37	7	11	A	N3-C4	-5.56	1.31	1.34
36	1	1401	A	N7-C5	-5.56	1.35	1.39
36	5	424	G	C5-C6	-5.55	1.36	1.42
36	5	818	C	N1-C2	-5.55	1.34	1.40
36	5	2875	U	C2-N3	5.55	1.41	1.37
36	5	2954	U	C4-O4	5.55	1.28	1.23
36	1	1308	A	N3-C4	-5.54	1.31	1.34
36	1	2620	G	N7-C5	5.53	1.42	1.39
36	5	2966	G	N7-C5	-5.53	1.35	1.39
1	6	1537	C	C2-N3	5.53	1.40	1.35
36	5	3095	U	N3-C4	-5.53	1.33	1.38
36	1	2954	U	C2-N3	5.53	1.41	1.37
36	5	938	C	N1-C6	-5.52	1.33	1.37
36	5	981	U	N1-C2	5.51	1.43	1.38
36	5	1332	A	N9-C8	-5.51	1.33	1.37
36	1	2984	C	C2-O2	-5.51	1.19	1.24
36	1	3091	A	N7-C5	-5.51	1.35	1.39
1	6	157	A	N9-C4	-5.51	1.34	1.37
36	1	1103	A	N3-C4	5.50	1.38	1.34
1	6	321	C	N1-C2	5.50	1.45	1.40
36	5	1307	G	C5-C4	-5.50	1.34	1.38
36	1	1507	G	N9-C8	-5.49	1.34	1.37
36	1	610	G	C6-N1	-5.49	1.35	1.39
36	1	1507	G	N7-C5	-5.48	1.35	1.39
36	1	2640	A	C6-N1	-5.48	1.31	1.35
36	5	2280	A	N9-C4	-5.48	1.34	1.37
36	5	2113	A	N9-C4	-5.47	1.34	1.37
36	5	2971	A	N3-C4	5.47	1.38	1.34
1	6	1746	A	N7-C5	-5.47	1.35	1.39
36	5	971	G	N9-C8	-5.47	1.34	1.37
37	7	102	A	N9-C4	-5.47	1.34	1.37
36	1	1369	A	C5-C6	-5.47	1.36	1.41
36	5	647	A	C6-N1	-5.47	1.31	1.35
36	5	1371	G	C5-C4	-5.47	1.34	1.38
36	1	2996	U	N1-C2	5.46	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	790	U	N3-C4	-5.45	1.33	1.38
36	1	1159	A	N3-C4	-5.45	1.31	1.34
36	1	2793	G	C2-N3	-5.45	1.28	1.32
36	5	1175	C	C4-N4	-5.45	1.29	1.33
36	5	2373	A	N7-C5	-5.45	1.35	1.39
36	1	1429	G	C5-C4	-5.45	1.34	1.38
36	5	1912	U	N1-C2	-5.45	1.33	1.38
36	5	3274	A	N9-C4	-5.44	1.34	1.37
36	5	1307	G	P-O5'	-5.43	1.54	1.59
1	6	1736	G	N3-C4	-5.42	1.31	1.35
36	5	2400	G	N9-C4	-5.42	1.33	1.38
36	5	980	A	N7-C5	5.42	1.42	1.39
36	1	900	G	N9-C8	-5.42	1.34	1.37
36	5	1315	U	N1-C6	-5.41	1.33	1.38
36	1	2093	A	N9-C4	5.41	1.41	1.37
36	5	2934	A	C6-N1	-5.41	1.31	1.35
36	5	63	A	N7-C5	-5.41	1.36	1.39
36	5	980	A	N9-C4	5.41	1.41	1.37
36	1	2396	G	C5-C4	-5.41	1.34	1.38
36	5	706	A	N9-C4	-5.41	1.34	1.37
36	5	367	A	C5-C4	-5.40	1.34	1.38
36	5	2942	C	N1-C6	-5.40	1.33	1.37
1	6	352	A	C6-N1	-5.40	1.31	1.35
36	5	2954	U	N3-C4	5.40	1.43	1.38
36	5	1432	C	N3-C4	-5.39	1.30	1.33
36	1	2138	A	N7-C5	-5.39	1.36	1.39
36	5	397	A	N3-C4	-5.39	1.31	1.34
36	5	2825	C	N1-C6	-5.39	1.33	1.37
36	1	693	A	N7-C5	-5.38	1.36	1.39
36	1	909	G	C5-C4	-5.38	1.34	1.38
36	1	1134	G	N9-C8	-5.38	1.34	1.37
36	1	3209	A	N7-C5	5.38	1.42	1.39
36	5	3139	A	N9-C4	-5.38	1.34	1.37
36	1	1192	C	N1-C2	5.37	1.45	1.40
36	1	2418	G	O3'-P	5.37	1.67	1.61
36	5	1851	G	N7-C5	-5.37	1.36	1.39
36	1	282	G	C6-N1	-5.36	1.35	1.39
36	5	1332	A	C5-C4	-5.36	1.34	1.38
36	5	2823	G	N9-C8	-5.36	1.34	1.37
1	6	1746	A	C5-C6	-5.36	1.36	1.41
36	5	3206	C	N1-C6	-5.35	1.33	1.37
36	5	3274	A	N3-C4	-5.35	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2360	C	N3-C4	-5.35	1.30	1.33
36	1	92	G	C6-N1	-5.35	1.35	1.39
36	5	2987	A	N7-C5	-5.35	1.36	1.39
38	4	15	G	C5-C6	-5.34	1.37	1.42
36	1	92	G	N1-C2	-5.34	1.33	1.37
36	1	1305	U	C2-N3	-5.34	1.34	1.37
36	5	2733	A	N9-C4	-5.33	1.34	1.37
36	5	1331	U	C4-C5	-5.33	1.38	1.43
1	6	337	G	C2-N2	5.32	1.39	1.34
36	1	639	G	N9-C8	-5.32	1.34	1.37
36	1	2409	G	N7-C5	-5.32	1.36	1.39
36	1	1452	A	N9-C4	-5.32	1.34	1.37
36	1	407	A	C5-C6	-5.31	1.36	1.41
36	1	1366	A	C5-C6	-5.31	1.36	1.41
36	1	912	G	C5-C4	-5.31	1.34	1.38
36	1	1318	A	N9-C4	-5.31	1.34	1.37
36	5	1192	C	N1-C2	5.31	1.45	1.40
36	1	895	A	N7-C5	-5.31	1.36	1.39
36	5	2910	A	N9-C4	-5.31	1.34	1.37
36	1	2944	U	C4-O4	-5.30	1.19	1.23
36	5	2138	A	N9-C4	-5.30	1.34	1.37
36	1	653	A	C6-N1	-5.30	1.31	1.35
1	2	992	A	N9-C4	-5.29	1.34	1.37
36	5	417	A	N3-C4	-5.29	1.31	1.34
36	1	1415	U	C2-N3	-5.29	1.34	1.37
36	1	2702	A	N7-C5	-5.29	1.36	1.39
36	1	282	G	N1-C2	-5.29	1.33	1.37
36	1	2887	A	C5-C6	-5.28	1.36	1.41
36	5	424	G	N7-C5	-5.28	1.36	1.39
36	5	1151	U	N1-C2	-5.28	1.33	1.38
38	8	80	A	N9-C4	5.28	1.41	1.37
36	1	2811	A	C6-N6	-5.27	1.29	1.33
36	1	923	C	N1-C6	-5.27	1.33	1.37
36	5	2818	U	C2-N3	-5.27	1.34	1.37
36	5	2645	G	C6-N1	-5.27	1.35	1.39
36	5	1195	A	N3-C4	-5.27	1.31	1.34
36	5	3245	A	N7-C5	-5.27	1.36	1.39
36	5	3092	C	N1-C6	-5.27	1.33	1.37
36	1	2145	A	N7-C5	-5.26	1.36	1.39
36	1	3087	A	N3-C4	-5.26	1.31	1.34
36	1	369	A	N3-C4	-5.25	1.31	1.34
1	6	1133	A	N7-C5	-5.25	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	106	A	N9-C4	-5.25	1.34	1.37
36	5	2394	G	N7-C5	-5.25	1.36	1.39
36	5	2814	G	N3-C4	-5.25	1.31	1.35
36	1	343	U	N1-C6	-5.24	1.33	1.38
36	5	1886	A	C5-C6	-5.24	1.36	1.41
36	1	343	U	C2-O2	-5.24	1.17	1.22
36	5	2128	C	N1-C6	-5.23	1.34	1.37
36	5	2911	A	N7-C5	-5.23	1.36	1.39
36	1	2948	C	N3-C4	-5.23	1.30	1.33
13	c1	128	CYS	CB-SG	-5.23	1.73	1.81
36	5	2617	U	N1-C2	-5.22	1.33	1.38
36	1	2958	A	N9-C4	-5.21	1.34	1.37
36	5	1318	A	N3-C4	-5.21	1.31	1.34
36	5	361	A	N7-C5	5.21	1.42	1.39
1	6	1137	A	C5-C4	-5.20	1.35	1.38
36	5	1892	G	C5-C4	-5.20	1.34	1.38
36	5	343	U	N1-C2	-5.20	1.33	1.38
36	1	3216	G	C5-C4	-5.20	1.34	1.38
36	1	1417	G	N3-C4	-5.20	1.31	1.35
36	1	2162	U	C4-O4	-5.20	1.19	1.23
36	1	1364	C	N1-C6	-5.19	1.34	1.37
36	1	342	A	N9-C4	-5.19	1.34	1.37
36	5	3107	U	C2-N3	-5.19	1.34	1.37
36	5	2615	G	C8-N7	-5.19	1.27	1.30
1	2	555	A	N9-C4	5.18	1.41	1.37
36	5	995	U	C2-N3	-5.18	1.34	1.37
36	1	1313	G	N7-C5	-5.17	1.36	1.39
36	1	2986	U	N1-C2	-5.17	1.33	1.38
36	5	981	U	C2-N3	5.17	1.41	1.37
36	5	2338	C	N1-C6	-5.17	1.34	1.37
36	5	2986	U	N1-C6	-5.16	1.33	1.38
36	5	2728	G	C2-N3	-5.16	1.28	1.32
36	5	2825	C	N1-C2	-5.16	1.34	1.40
36	1	2931	C	N1-C6	-5.16	1.34	1.37
36	1	691	A	N9-C4	-5.16	1.34	1.37
36	5	936	A	N7-C5	-5.16	1.36	1.39
36	5	2400	G	C5-C6	-5.16	1.37	1.42
36	1	656	A	N7-C5	-5.15	1.36	1.39
36	5	2404	A	N7-C5	5.15	1.42	1.39
36	5	2862	U	C2-N3	-5.15	1.34	1.37
36	1	100	A	C6-N1	-5.15	1.31	1.35
36	5	2824	G	N7-C5	-5.15	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	908	G	C5-C4	-5.15	1.34	1.38
36	1	361	A	N3-C4	-5.14	1.31	1.34
36	1	358	G	N9-C8	-5.14	1.34	1.37
36	5	1331	U	C5-C6	-5.14	1.29	1.34
36	1	1368	U	N1-C2	-5.14	1.33	1.38
36	5	1173	U	C2-N3	-5.14	1.34	1.37
36	5	960	U	N1-C2	5.13	1.43	1.38
36	5	895	A	N9-C4	-5.13	1.34	1.37
36	1	806	A	N9-C4	-5.13	1.34	1.37
36	5	3084	C	N1-C6	-5.13	1.34	1.37
36	1	1394	A	N9-C4	-5.12	1.34	1.37
36	5	2373	A	C5-C6	-5.12	1.36	1.41
36	1	2919	A	N7-C5	-5.11	1.36	1.39
36	1	1115	G	N3-C4	-5.11	1.31	1.35
36	5	3047	U	N3-C4	-5.11	1.33	1.38
36	1	52	A	N3-C4	-5.11	1.31	1.34
36	1	1416	C	N3-C4	-5.10	1.30	1.33
36	1	2398	A	N3-C4	5.10	1.38	1.34
36	5	2690	G	N3-C4	-5.10	1.31	1.35
36	1	651	G	C8-N7	-5.09	1.27	1.30
1	6	46	A	N7-C5	-5.09	1.36	1.39
36	5	2419	A	P-O5'	5.09	1.64	1.59
36	5	3216	G	N7-C5	-5.09	1.36	1.39
75	O9	2	ALA	CA-CB	-5.09	1.41	1.52
36	5	2913	C	N1-C2	-5.08	1.35	1.40
36	5	3207	U	C2-N3	5.08	1.41	1.37
36	5	3008	A	N3-C4	-5.08	1.31	1.34
36	5	1914	G	N1-C2	-5.08	1.33	1.37
36	5	914	A	N9-C4	-5.07	1.34	1.37
36	1	2363	A	N3-C4	-5.07	1.31	1.34
36	1	2165	G	N7-C5	-5.06	1.36	1.39
36	1	984	G	N7-C5	-5.06	1.36	1.39
36	1	2207	A	N9-C4	5.06	1.40	1.37
37	7	96	U	C4-O4	-5.05	1.19	1.23
36	1	910	G	N7-C5	-5.05	1.36	1.39
36	1	2368	A	N9-C4	-5.05	1.34	1.37
36	1	2394	G	N1-C2	-5.05	1.33	1.37
36	5	2434	U	N3-C4	-5.04	1.33	1.38
38	4	28	C	N1-C6	-5.04	1.34	1.37
36	5	1164	G	N3-C4	-5.04	1.31	1.35
36	5	1432	C	C2-O2	-5.04	1.20	1.24
36	5	969	C	N3-C4	-5.04	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1189	C	N1-C6	-5.04	1.34	1.37
36	1	2406	C	N1-C2	-5.04	1.35	1.40
36	5	1844	C	C2-O2	-5.04	1.20	1.24
36	5	2404	A	C8-N7	5.04	1.35	1.31
36	5	3314	A	N3-C4	-5.03	1.31	1.34
1	6	312	A	N7-C5	-5.03	1.36	1.39
36	1	1795	U	C2-N3	-5.03	1.34	1.37
36	5	2345	A	C5-C6	-5.03	1.36	1.41
36	1	1390	A	N3-C4	-5.02	1.31	1.34
36	5	848	A	N3-C4	-5.02	1.31	1.34
36	1	984	G	C2-N3	5.02	1.36	1.32
1	6	421	A	C6-N1	5.02	1.39	1.35
36	5	2837	A	C5-C4	-5.02	1.35	1.38
36	1	216	G	N7-C5	-5.02	1.36	1.39
36	1	1116	G	C5-C4	-5.02	1.34	1.38
36	1	2881	C	C2-O2	5.02	1.28	1.24
38	4	24	G	N7-C5	-5.01	1.36	1.39
36	1	342	A	N3-C4	-5.01	1.31	1.34
36	5	2762	A	N3-C4	-5.01	1.31	1.34
36	1	826	G	C5-C4	-5.00	1.34	1.38
36	1	2350	C	N1-C6	-5.00	1.34	1.37
1	6	1537	C	C5-C6	5.00	1.38	1.34
36	5	984	G	N7-C5	-5.00	1.36	1.39
36	1	2326	A	N3-C4	-5.00	1.31	1.34
36	5	947	G	N3-C4	-5.00	1.31	1.35
36	5	2910	A	N7-C5	-5.00	1.36	1.39

All (5269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	25.71	141.45	128.60
36	5	1152	G	N3-C4-N9	-21.48	113.11	126.00
36	5	1152	G	C2-N3-C4	-20.82	101.49	111.90
36	1	2714	G	N3-C4-C5	16.25	136.73	128.60
36	1	2714	G	N3-C4-N9	-14.32	117.41	126.00
36	5	424	G	C5-C6-O6	-14.11	120.14	128.60
36	1	86	G	O5'-P-OP2	-14.10	93.02	105.70
1	6	163	G	N3-C4-N9	-14.05	117.57	126.00
36	5	1152	G	C5-N7-C8	-13.71	97.44	104.30
36	5	1902	G	N1-C6-O6	13.70	128.12	119.90
36	5	806	A	O5'-P-OP1	-13.69	93.38	105.70
36	1	794	U	O5'-P-OP2	-13.53	93.52	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	9	A	O5'-P-OP2	-13.34	93.70	105.70
36	5	1152	G	N1-C6-O6	13.26	127.86	119.90
36	1	406	G	O4'-C1'-N9	13.10	118.68	108.20
1	2	553	G	N1-C6-O6	13.05	127.73	119.90
36	5	2364	G	N9-C4-C5	12.98	110.59	105.40
36	1	1495	U	C5-C6-N1	-12.74	116.33	122.70
36	5	2385	G	O5'-P-OP1	-12.73	94.25	105.70
36	1	960	U	C2-N1-C1'	-12.69	102.47	117.70
36	1	2726	C	C6-N1-C2	-12.66	115.23	120.30
36	5	3245	A	N1-C6-N6	12.50	126.10	118.60
36	1	2298	U	N3-C4-O4	-12.34	110.77	119.40
36	1	2617	U	N1-C2-N3	12.33	122.30	114.90
36	1	1308	A	O5'-P-OP2	-12.28	94.65	105.70
36	5	3245	A	C5-N7-C8	-12.17	97.81	103.90
36	5	1513	G	C8-N9-C4	-12.15	101.54	106.40
36	1	2371	G	O5'-P-OP2	-12.10	94.81	105.70
36	1	1838	G	N1-C6-O6	12.09	127.16	119.90
36	1	1377	G	C5-C6-O6	-12.09	121.35	128.60
36	1	2726	C	C5-C4-N4	11.91	128.54	120.20
36	1	672	A	N1-C6-N6	11.83	125.70	118.60
36	5	1301	A	N1-C6-N6	11.80	125.68	118.60
38	8	80	A	C8-N9-C4	-11.74	101.11	105.80
36	1	2846	U	N3-C2-O2	-11.72	114.00	122.20
36	1	2884	C	N3-C4-C5	11.69	126.58	121.90
1	2	1039	A	O4'-C1'-N9	11.69	117.55	108.20
36	1	1157	G	O5'-P-OP2	-11.68	95.19	105.70
36	5	1897	G	N1-C6-O6	11.63	126.88	119.90
36	5	2354	C	N3-C4-C5	-11.56	117.28	121.90
36	1	2694	A	O5'-P-OP2	-11.52	95.33	105.70
36	1	636	C	N3-C4-C5	11.50	126.50	121.90
36	5	437	G	C8-N9-C4	-11.47	101.81	106.40
36	1	2808	A	N1-C6-N6	11.46	125.47	118.60
36	5	2726	C	C6-N1-C2	-11.44	115.72	120.30
36	5	1152	G	C4-C5-N7	11.43	115.37	110.80
36	1	2643	A	C8-N9-C4	11.43	110.37	105.80
36	1	1313	G	C5-C6-O6	-11.36	121.78	128.60
36	1	2726	C	N3-C4-N4	-11.30	110.09	118.00
36	5	877	C	N3-C4-C5	11.25	126.40	121.90
36	5	2726	C	C5-C4-N4	11.18	128.02	120.20
36	5	2400	G	N1-C6-O6	11.16	126.60	119.90
36	5	3245	A	C4-C5-N7	11.09	116.25	110.70
36	5	3245	A	C6-C5-N7	-11.07	124.55	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	C8-N9-C1'	11.01	141.31	127.00
36	1	2617	U	C4-C5-C6	10.97	126.28	119.70
36	1	2726	C	N3-C2-O2	-10.95	114.23	121.90
36	5	1339	C	C6-N1-C2	-10.94	115.93	120.30
36	5	1902	G	C5-C6-O6	-10.93	122.04	128.60
36	5	1110	U	N1-C2-O2	10.90	130.43	122.80
36	1	2714	G	C2-N3-C4	-10.89	106.45	111.90
36	5	2923	U	O5'-P-OP1	-10.89	95.90	105.70
36	5	644	G	C4-C5-N7	-10.87	106.45	110.80
36	5	2954	U	C2-N1-C1'	10.87	130.75	117.70
36	1	716	A	N9-C4-C5	-10.86	101.46	105.80
73	O7	65	ARG	NE-CZ-NH1	10.85	125.72	120.30
36	1	2283	G	N1-C6-O6	10.79	126.37	119.90
36	1	369	A	C8-N9-C4	-10.77	101.49	105.80
36	1	661	G	C8-N9-C4	-10.74	102.10	106.40
36	5	2117	A	N1-C6-N6	-10.72	112.17	118.60
36	1	2617	U	C5-C6-N1	-10.72	117.34	122.70
36	1	1365	G	C8-N9-C4	-10.71	102.11	106.40
36	1	1365	G	N3-C4-C5	-10.70	123.25	128.60
36	1	3278	C	N1-C2-O2	10.69	125.32	118.90
36	5	2943	G	C6-C5-N7	-10.67	124.00	130.40
36	5	1152	G	C4-N9-C1'	-10.66	112.64	126.50
36	5	934	G	C5-C6-O6	-10.65	122.21	128.60
36	1	3306	U	N3-C4-O4	-10.65	111.95	119.40
36	1	1495	U	C4-C5-C6	10.64	126.08	119.70
36	1	2286	U	O5'-P-OP2	-10.64	96.13	105.70
36	5	1203	A	N1-C6-N6	10.61	124.96	118.60
36	1	2617	U	C5-C4-O4	10.56	132.24	125.90
36	5	1902	G	O5'-P-OP1	-10.54	96.22	105.70
36	5	1419	A	O5'-P-OP2	-10.53	96.22	105.70
36	5	424	G	C4-C5-N7	10.52	115.01	110.80
36	5	437	G	N7-C8-N9	10.51	118.35	113.10
1	2	73	U	O4'-C1'-N1	10.50	116.60	108.20
36	5	966	U	N3-C2-O2	-10.49	114.86	122.20
36	5	63	A	N1-C6-N6	10.48	124.89	118.60
36	1	2936	A	O5'-P-OP1	-10.46	96.29	105.70
1	6	815	G	N1-C6-O6	10.45	126.17	119.90
36	1	1495	U	N1-C2-N3	10.43	121.16	114.90
36	5	2354	C	N1-C2-O2	-10.40	112.66	118.90
38	8	80	A	N7-C8-N9	10.39	119.00	113.80
36	5	2928	C	C6-N1-C2	-10.39	116.14	120.30
36	1	1495	U	N1-C2-O2	-10.36	115.55	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2355	G	N1-C6-O6	10.34	126.10	119.90
36	5	2400	G	C5-C6-O6	-10.34	122.40	128.60
36	1	1192	C	N1-C2-O2	10.33	125.10	118.90
36	5	874	U	O5'-P-OP1	-10.33	96.40	105.70
36	1	2831	G	N1-C6-O6	10.31	126.09	119.90
36	5	640	U	N1-C2-O2	-10.28	115.61	122.80
37	7	101	G	N1-C6-O6	10.25	126.05	119.90
36	1	1308	A	C8-N9-C4	-10.22	101.71	105.80
36	1	695	C	C6-N1-C2	10.22	124.39	120.30
36	1	2374	C	N3-C2-O2	-10.22	114.75	121.90
36	5	1481	A	C8-N9-C4	-10.20	101.72	105.80
36	5	2700	G	C5-C6-O6	-10.20	122.48	128.60
36	1	968	G	N1-C6-O6	-10.19	113.79	119.90
36	1	1166	G	N1-C6-O6	10.17	126.00	119.90
36	5	2392	C	C6-N1-C2	10.16	124.36	120.30
36	1	776	U	C4-C5-C6	10.15	125.79	119.70
36	1	3181	C	C5-C4-N4	10.14	127.30	120.20
1	2	1280	C	N3-C4-C5	-10.14	117.84	121.90
1	2	1773	C	C6-N1-C2	-10.13	116.25	120.30
36	1	3181	C	N3-C4-N4	-10.08	110.94	118.00
1	2	639	U	N3-C2-O2	-10.07	115.15	122.20
36	5	2403	G	O5'-P-OP2	-10.04	96.66	105.70
1	6	756	A	N7-C8-N9	10.02	118.81	113.80
1	6	756	A	C8-N9-C4	-10.00	101.80	105.80
38	4	103	G	N3-C4-C5	-9.99	123.61	128.60
1	6	1634	C	C2-N1-C1'	9.98	129.78	118.80
36	5	2364	G	C5-C6-O6	9.97	134.58	128.60
36	5	1307	G	P-O3'-C3'	9.96	131.66	119.70
36	5	776	U	C5-C6-N1	-9.96	117.72	122.70
36	1	716	A	N1-C6-N6	9.96	124.57	118.60
36	1	2959	C	N1-C2-O2	-9.94	112.93	118.90
1	6	1537	C	C6-N1-C2	-9.90	116.34	120.30
36	5	2943	G	C4-C5-N7	9.89	114.76	110.80
36	1	895	A	O5'-P-OP1	-9.85	96.83	105.70
36	5	1321	G	N1-C6-O6	9.83	125.80	119.90
36	1	1303	A	C8-N9-C4	9.83	109.73	105.80
36	5	1119	C	N3-C4-C5	9.82	125.83	121.90
36	1	1313	G	C4-C5-N7	9.81	114.72	110.80
36	1	2617	U	N3-C2-O2	-9.80	115.34	122.20
36	1	2344	U	O5'-P-OP2	-9.80	96.88	105.70
36	5	2761	G	O5'-P-OP1	-9.79	96.89	105.70
36	5	406	G	O4'-C1'-N9	9.78	116.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3245	A	N7-C8-N9	9.78	118.69	113.80
36	1	1381	A	O5'-P-OP2	9.76	122.42	110.70
36	1	86	G	O5'-P-OP1	9.76	122.41	110.70
36	5	1902	G	C6-C5-N7	-9.73	124.56	130.40
36	5	2392	C	N3-C4-C5	9.73	125.79	121.90
36	1	3181	C	N3-C2-O2	-9.72	115.09	121.90
36	1	1838	G	C6-C5-N7	-9.72	124.57	130.40
36	5	424	G	N1-C6-O6	9.71	125.72	119.90
36	5	2189	U	O5'-P-OP1	-9.69	96.97	105.70
36	1	2283	G	C4-C5-N7	9.69	114.68	110.80
1	6	102	U	O5'-P-OP1	-9.69	96.98	105.70
1	6	163	G	N3-C4-C5	9.68	133.44	128.60
36	1	958	C	N3-C4-C5	9.68	125.77	121.90
36	5	2308	C	N1-C2-O2	-9.66	113.10	118.90
36	1	2619	G	O5'-P-OP1	-9.66	97.01	105.70
36	5	3244	A	O5'-P-OP1	-9.65	97.01	105.70
1	2	1762	A	O5'-P-OP1	-9.65	97.02	105.70
36	1	66	A	O5'-P-OP1	-9.63	97.03	105.70
36	1	1445	U	N1-C2-O2	-9.60	116.08	122.80
36	1	680	G	O5'-P-OP2	-9.58	97.08	105.70
36	5	1124	U	N3-C4-O4	-9.58	112.69	119.40
36	5	2364	G	C4-C5-N7	-9.56	106.98	110.80
36	5	2899	C	C6-N1-C2	-9.53	116.49	120.30
36	5	1366	A	C8-N9-C4	-9.53	101.99	105.80
36	1	2197	C	C6-N1-C2	9.50	124.10	120.30
36	5	1152	G	N3-C2-N2	-9.50	113.25	119.90
1	2	1773	C	N3-C4-C5	-9.48	118.11	121.90
36	1	1556	C	C2-N1-C1'	9.47	129.22	118.80
36	5	2937	G	C5-C6-O6	-9.47	122.92	128.60
1	2	639	U	N1-C2-O2	9.46	129.43	122.80
36	1	958	C	N3-C4-N4	-9.46	111.38	118.00
36	1	1377	G	N1-C6-O6	9.45	125.57	119.90
36	5	1055	A	O5'-P-OP2	-9.44	97.20	105.70
1	2	453	U	C2-N1-C1'	9.44	129.02	117.70
36	5	2837	A	O5'-P-OP1	-9.43	97.21	105.70
36	1	1197	A	N1-C6-N6	9.43	124.26	118.60
36	5	2389	C	O5'-P-OP1	-9.43	97.22	105.70
36	1	1422	G	O5'-P-OP1	-9.42	97.22	105.70
1	2	1745	G	C5-C6-O6	-9.41	122.95	128.60
36	5	962	A	C5-C6-N6	-9.41	116.17	123.70
36	5	1113	G	C2-N3-C4	-9.41	107.19	111.90
36	5	1390	A	N9-C4-C5	9.41	109.56	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	111	A	N1-C6-N6	9.39	124.23	118.60
36	1	3306	U	C5-C4-O4	9.38	131.53	125.90
36	1	1115	G	C8-N9-C4	-9.37	102.65	106.40
36	1	1127	G	C5-C6-O6	-9.36	122.99	128.60
36	5	1150	A	O5'-P-OP2	-9.36	97.28	105.70
36	1	2572	C	N1-C2-O2	9.35	124.51	118.90
36	1	2624	G	N1-C6-O6	9.35	125.51	119.90
36	1	344	A	N1-C6-N6	-9.34	113.00	118.60
36	1	395	A	O5'-P-OP2	-9.33	97.30	105.70
36	5	2727	A	C2-N3-C4	9.32	115.26	110.60
36	1	282	G	C8-N9-C4	-9.31	102.67	106.40
36	5	1513	G	N7-C8-N9	9.31	117.76	113.10
36	1	716	A	C8-N9-C4	9.31	109.52	105.80
36	1	1127	G	N1-C6-O6	9.29	125.48	119.90
36	5	3050	U	C5-C4-O4	9.29	131.47	125.90
36	5	2634	U	C5-C4-O4	-9.29	120.33	125.90
36	5	2572	C	N1-C2-O2	9.28	124.47	118.90
1	6	144	U	N3-C2-O2	-9.28	115.71	122.20
36	5	1158	A	N1-C6-N6	9.28	124.17	118.60
36	5	3218	A	N1-C6-N6	9.27	124.16	118.60
36	1	1316	C	N3-C4-N4	9.26	124.48	118.00
36	1	2946	A	N1-C6-N6	9.26	124.16	118.60
36	1	2409	G	N3-C4-C5	-9.25	123.97	128.60
36	5	1473	G	C8-N9-C4	9.24	110.10	106.40
36	1	805	G	C8-N9-C4	9.24	110.10	106.40
1	6	421	A	N1-C6-N6	9.23	124.14	118.60
36	1	2550	U	N3-C2-O2	-9.23	115.74	122.20
36	1	1118	C	C6-N1-C2	-9.22	116.61	120.30
36	1	2987	A	O5'-P-OP2	-9.22	97.40	105.70
36	5	2981	U	N3-C2-O2	-9.21	115.75	122.20
37	7	49	G	N1-C6-O6	9.21	125.42	119.90
36	5	962	A	N1-C6-N6	9.19	124.11	118.60
36	5	2726	C	N3-C2-O2	-9.16	115.49	121.90
36	5	2393	G	O5'-P-OP2	-9.15	97.46	105.70
36	1	1389	G	C4-C5-N7	9.15	114.46	110.80
36	5	1390	A	C8-N9-C4	-9.15	102.14	105.80
36	1	573	C	C6-N1-C2	9.14	123.96	120.30
36	1	2827	U	N1-C2-N3	9.14	120.38	114.90
36	1	1132	C	O5'-P-OP1	-9.13	97.48	105.70
36	1	1377	G	N9-C4-C5	-9.12	101.75	105.40
36	1	776	U	C5-C6-N1	-9.12	118.14	122.70
36	1	1377	G	C4-C5-N7	9.11	114.44	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	829	U	N3-C2-O2	-9.10	115.83	122.20
1	6	815	G	C6-C5-N7	-9.09	124.94	130.40
36	5	2849	C	N3-C2-O2	9.09	128.26	121.90
36	1	3183	A	N1-C6-N6	9.08	124.05	118.60
36	1	343	U	N1-C2-N3	9.04	120.33	114.90
1	6	1773	C	N3-C4-C5	-9.03	118.29	121.90
36	5	1115	G	C8-N9-C4	-9.02	102.79	106.40
36	5	1306	G	C5-C6-O6	-9.02	123.19	128.60
36	5	2372	A	P-O3'-C3'	8.97	130.47	119.70
1	6	163	G	N9-C4-C5	8.97	108.99	105.40
36	5	1316	C	N1-C2-O2	-8.96	113.52	118.90
36	1	2169	G	N1-C6-O6	-8.96	114.53	119.90
36	1	3022	G	O4'-C1'-N9	8.95	115.36	108.20
1	2	553	G	C6-C5-N7	-8.94	125.04	130.40
36	1	2294	U	N1-C2-N3	8.93	120.26	114.90
36	5	642	U	O5'-P-OP2	-8.93	97.66	105.70
36	1	1133	A	N1-C6-N6	8.92	123.95	118.60
36	5	938	C	C5-C4-N4	-8.91	113.96	120.20
1	6	114	C	N1-C2-O2	8.90	124.24	118.90
36	5	1060	U	N3-C4-O4	-8.90	113.17	119.40
1	6	815	G	C4-C5-N7	8.90	114.36	110.80
36	1	1351	U	N3-C2-O2	-8.89	115.97	122.20
36	1	2417	U	C2-N3-C4	-8.89	121.67	127.00
1	6	321	C	N1-C2-O2	8.89	124.23	118.90
36	1	439	C	C2-N1-C1'	8.88	128.57	118.80
36	1	2247	G	N1-C6-O6	8.88	125.23	119.90
37	7	101	G	C6-C5-N7	-8.88	125.07	130.40
36	1	1307	G	N1-C6-O6	-8.86	114.58	119.90
36	5	2971	A	C2-N3-C4	8.86	115.03	110.60
36	1	2417	U	C5-C6-N1	-8.85	118.28	122.70
36	5	2406	C	N1-C2-O2	-8.85	113.59	118.90
36	1	1343	A	O5'-P-OP2	-8.85	97.74	105.70
36	1	2621	G	N3-C2-N2	-8.83	113.72	119.90
36	1	1303	A	O5'-P-OP1	-8.83	97.75	105.70
36	1	2818	U	O5'-P-OP2	-8.83	97.75	105.70
36	1	1399	A	C2-N3-C4	-8.82	106.19	110.60
1	6	1700	C	N1-C2-O2	8.82	124.19	118.90
36	1	2177	G	N3-C4-C5	-8.81	124.19	128.60
1	2	448	C	C6-N1-C2	-8.80	116.78	120.30
36	1	1389	G	C5-C6-O6	-8.79	123.33	128.60
36	1	2699	G	C5-C6-O6	-8.79	123.33	128.60
1	6	1700	C	C2-N1-C1'	8.79	128.47	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	877	C	C4-C5-C6	-8.79	113.01	117.40
1	2	1761	U	C6-N1-C2	-8.78	115.73	121.00
36	1	3278	C	N3-C2-O2	-8.78	115.75	121.90
36	1	226	C	N3-C4-N4	8.78	124.14	118.00
36	1	2622	C	C6-N1-C2	-8.78	116.79	120.30
36	1	2797	C	O5'-P-OP1	-8.77	97.80	105.70
52	M6	110	PRO	C-N-CD	-8.77	101.32	120.60
36	5	1204	A	N1-C6-N6	-8.77	113.34	118.60
36	5	2385	G	N3-C4-C5	8.75	132.98	128.60
36	1	2923	U	O5'-P-OP1	-8.75	97.83	105.70
36	5	2937	G	N1-C6-O6	8.74	125.15	119.90
36	1	2283	G	C5-C6-O6	-8.72	123.37	128.60
36	1	1367	G	N1-C6-O6	8.71	125.13	119.90
36	5	2996	U	N1-C2-O2	8.70	128.89	122.80
36	5	2117	A	N9-C4-C5	8.70	109.28	105.80
36	1	2610	G	N1-C6-O6	8.69	125.11	119.90
1	6	1745	G	C5-C6-O6	-8.69	123.39	128.60
36	1	1316	C	C5-C4-N4	-8.67	114.13	120.20
36	5	2872	A	O5'-P-OP1	-8.67	97.90	105.70
36	1	776	U	N1-C2-N3	8.66	120.10	114.90
36	5	414	U	N1-C2-O2	-8.66	116.73	122.80
36	5	3377	G	C5-C6-O6	-8.66	123.40	128.60
36	1	53	G	O5'-P-OP2	-8.66	97.91	105.70
36	5	2278	C	C4-C5-C6	-8.66	113.07	117.40
36	5	3245	A	C2-N3-C4	-8.66	106.27	110.60
36	5	2616	C	C6-N1-C2	8.64	123.76	120.30
36	5	1124	U	N3-C4-C5	8.63	119.78	114.60
36	1	93	C	C6-N1-C2	-8.62	116.85	120.30
36	5	1301	A	C5-C6-N6	-8.62	116.81	123.70
37	7	98	C	O5'-P-OP2	-8.62	97.94	105.70
36	1	716	A	C4-C5-N7	8.61	115.01	110.70
1	2	966	A	N1-C6-N6	8.60	123.76	118.60
36	1	65	A	P-O3'-C3'	8.60	130.02	119.70
36	5	2364	G	N3-C4-N9	-8.60	120.84	126.00
36	1	2953	U	N1-C2-O2	-8.59	116.78	122.80
36	5	1429	G	C6-C5-N7	-8.59	125.25	130.40
36	5	2985	C	C6-N1-C2	-8.59	116.86	120.30
36	5	641	C	N1-C2-O2	-8.59	113.75	118.90
36	5	1432	C	N3-C4-C5	8.59	125.33	121.90
1	2	75	U	N1-C2-O2	8.58	128.81	122.80
36	5	1481	A	N7-C8-N9	8.55	118.07	113.80
36	1	339	C	OP1-P-OP2	-8.55	106.78	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	200	C	N3-C4-N4	8.54	123.98	118.00
36	1	3306	U	N3-C2-O2	-8.54	116.22	122.20
36	1	608	A	N1-C6-N6	8.54	123.72	118.60
36	5	2524	A	O4'-C1'-N9	8.53	115.03	108.20
36	1	1450	G	O5'-P-OP1	-8.53	98.02	105.70
1	2	1082	C	N1-C2-O2	8.53	124.02	118.90
36	5	3026	G	C5-C6-O6	-8.53	123.48	128.60
36	1	3214	U	C5-C4-O4	8.52	131.01	125.90
1	2	433	C	O5'-P-OP1	-8.52	98.04	105.70
36	5	2351	U	C6-N1-C2	-8.51	115.89	121.00
36	1	374	A	N1-C6-N6	-8.50	113.50	118.60
36	5	404	G	O5'-P-OP2	-8.50	98.05	105.70
36	5	1908	A	C8-N9-C4	-8.50	102.40	105.80
36	1	304	G	N9-C4-C5	8.50	108.80	105.40
36	1	2811	A	C5-C6-N1	8.50	121.95	117.70
36	1	2827	U	C5-C4-O4	8.49	130.99	125.90
36	5	437	G	N3-C4-C5	-8.47	124.36	128.60
36	1	344	A	O5'-P-OP2	-8.47	98.08	105.70
36	1	639	G	N1-C6-O6	8.47	124.98	119.90
1	2	402	C	C6-N1-C2	8.47	123.69	120.30
36	1	2699	G	N1-C6-O6	8.46	124.98	119.90
36	1	2298	U	C5-C4-O4	8.46	130.98	125.90
36	5	1897	G	C4-C5-N7	8.43	114.17	110.80
36	5	578	A	N1-C6-N6	8.43	123.66	118.60
36	5	661	G	O5'-P-OP1	-8.43	98.11	105.70
1	2	580	A	C8-N9-C4	-8.43	102.43	105.80
36	5	2953	U	N3-C4-O4	8.43	125.30	119.40
36	5	644	G	C5-N7-C8	8.42	108.51	104.30
36	5	1313	G	O5'-P-OP2	-8.42	98.12	105.70
36	5	927	C	N1-C2-O2	-8.42	113.85	118.90
36	1	1433	A	O5'-P-OP1	-8.41	98.13	105.70
36	5	2726	C	N1-C2-N3	8.41	125.09	119.20
36	5	2628	A	O5'-P-OP1	8.41	120.79	110.70
36	5	2954	U	O4'-C1'-N1	8.41	114.92	108.20
36	5	3136	G	C2-N3-C4	-8.41	107.70	111.90
1	6	402	C	O5'-P-OP2	-8.40	98.14	105.70
36	5	2937	G	C6-C5-N7	-8.40	125.36	130.40
36	5	2117	A	C5-C6-N6	8.40	130.42	123.70
36	1	1492	G	C5-N7-C8	8.40	108.50	104.30
36	5	1300	G	N1-C6-O6	8.39	124.93	119.90
1	6	1141	G	O5'-P-OP1	-8.38	98.16	105.70
1	6	448	C	C6-N1-C2	-8.37	116.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1484	U	P-O3'-C3'	8.37	129.74	119.70
36	5	1145	G	N9-C4-C5	8.37	108.75	105.40
1	2	1745	G	N3-C4-N9	8.36	131.02	126.00
1	2	1096	C	N1-C2-O2	8.36	123.92	118.90
1	6	321	C	C2-N1-C1'	8.36	127.99	118.80
36	1	2314	U	N1-C2-N3	-8.35	109.89	114.90
36	5	1394	A	N1-C6-N6	-8.35	113.59	118.60
36	5	3188	G	N1-C6-O6	-8.34	114.89	119.90
36	5	881	C	C5-C6-N1	8.34	125.17	121.00
36	5	693	A	O5'-P-OP1	-8.34	98.20	105.70
36	5	3362	A	C5-N7-C8	-8.33	99.73	103.90
36	1	2313	A	O5'-P-OP1	-8.33	98.20	105.70
1	6	638	U	N3-C2-O2	-8.33	116.37	122.20
36	5	3211	C	C6-N1-C2	8.33	123.63	120.30
36	5	2942	C	N3-C4-N4	8.33	123.83	118.00
36	1	651	G	N3-C4-N9	8.32	131.00	126.00
36	5	2909	U	N1-C2-O2	-8.32	116.97	122.80
36	5	2145	A	N1-C6-N6	-8.32	113.61	118.60
36	1	1320	C	O5'-P-OP2	-8.32	98.21	105.70
36	5	2345	A	N1-C6-N6	8.32	123.59	118.60
36	5	2395	G	O5'-P-OP2	-8.31	98.22	105.70
1	6	163	G	N3-C2-N2	-8.31	114.08	119.90
36	1	1428	A	O5'-P-OP2	-8.31	98.22	105.70
1	2	1280	C	C6-N1-C2	-8.30	116.98	120.30
36	1	2621	G	N1-C2-N2	8.30	123.67	116.20
1	6	1522	U	O5'-P-OP2	-8.30	98.23	105.70
1	2	453	U	N3-C2-O2	-8.30	116.39	122.20
1	2	1560	U	N3-C2-O2	-8.29	116.40	122.20
36	1	1450	G	C5-C6-O6	-8.29	123.63	128.60
36	1	1495	U	C2-N1-C1'	-8.29	107.76	117.70
36	5	3209	A	O4'-C1'-N9	8.29	114.83	108.20
36	5	1301	A	C6-C5-N7	-8.28	126.50	132.30
36	1	1390	A	C8-N9-C4	-8.28	102.49	105.80
37	3	75	G	O5'-P-OP1	-8.27	98.25	105.70
38	4	109	A	N1-C6-N6	8.27	123.56	118.60
36	5	2755	C	O5'-P-OP1	-8.27	98.26	105.70
36	1	1308	A	N7-C8-N9	8.26	117.93	113.80
36	5	3154	C	N1-C2-O2	8.25	123.85	118.90
36	1	2812	C	C5-C6-N1	-8.25	116.88	121.00
36	5	3105	U	C5-C4-O4	8.25	130.85	125.90
36	1	895	A	C2-N3-C4	-8.25	106.48	110.60
36	1	897	U	O5'-P-OP1	-8.24	98.28	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1869	C	O5'-P-OP2	-8.24	98.28	105.70
36	1	2695	A	C8-N9-C4	-8.24	102.51	105.80
36	1	3214	U	N3-C2-O2	-8.24	116.44	122.20
36	5	1437	C	C6-N1-C2	-8.23	117.01	120.30
36	5	2278	C	C5-C6-N1	8.23	125.11	121.00
36	5	3098	G	O5'-P-OP2	-8.23	98.30	105.70
1	6	321	C	N3-C2-O2	-8.22	116.15	121.90
37	7	101	G	C5-C6-O6	-8.21	123.68	128.60
36	5	2639	G	C6-C5-N7	-8.20	125.48	130.40
1	6	421	A	N9-C4-C5	-8.20	102.52	105.80
36	1	1133	A	C5-C6-N6	-8.20	117.14	123.70
36	1	887	G	O5'-P-OP2	-8.19	98.33	105.70
36	5	2385	G	C8-N9-C4	8.19	109.68	106.40
36	1	972	A	C8-N9-C4	8.19	109.08	105.80
36	5	2117	A	C4-C5-N7	-8.19	106.61	110.70
36	5	2663	G	O5'-P-OP2	-8.19	98.33	105.70
36	5	2245	C	C6-N1-C2	-8.18	117.03	120.30
38	4	103	G	C8-N9-C4	-8.18	103.13	106.40
36	1	2310	U	O5'-P-OP1	-8.18	98.34	105.70
36	5	2913	C	N1-C2-O2	-8.18	113.99	118.90
40	13	19	ARG	NE-CZ-NH2	-8.17	116.21	120.30
36	1	295	A	C8-N9-C4	-8.17	102.53	105.80
36	5	1392	G	C8-N9-C4	8.16	109.67	106.40
37	7	77	G	C5-C6-O6	-8.16	123.70	128.60
1	2	542	A	O4'-C1'-N9	8.16	114.72	108.20
1	6	371	G	C4-N9-C1'	8.16	137.10	126.50
36	5	922	U	C5-C6-N1	-8.16	118.62	122.70
38	4	94	C	C6-N1-C2	8.15	123.56	120.30
36	1	2942	C	N3-C4-C5	8.15	125.16	121.90
36	1	2349	U	O5'-P-OP2	-8.14	98.37	105.70
1	2	1129	U	N3-C4-O4	-8.14	113.70	119.40
36	5	2364	G	C8-N9-C4	-8.14	103.14	106.40
36	5	3099	C	C4-C5-C6	8.14	121.47	117.40
1	6	1634	C	C6-N1-C2	-8.13	117.05	120.30
36	5	2881	C	C6-N1-C2	8.13	123.55	120.30
36	1	1164	G	N1-C6-O6	-8.13	115.02	119.90
36	1	2823	G	N9-C4-C5	8.13	108.65	105.40
36	1	1351	U	N1-C2-O2	8.12	128.49	122.80
36	1	1390	A	N9-C4-C5	8.12	109.05	105.80
36	1	2873	U	N3-C2-O2	-8.11	116.52	122.20
36	5	2394	G	C2-N3-C4	-8.11	107.84	111.90
36	1	1371	G	C8-N9-C4	8.11	109.64	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	922	U	N1-C2-O2	8.11	128.47	122.80
36	5	1419	A	O5'-P-OP1	8.10	120.42	110.70
36	1	2404	A	C2-N3-C4	8.10	114.65	110.60
36	5	1339	C	C5-C6-N1	8.10	125.05	121.00
1	6	371	G	N3-C4-C5	-8.10	124.55	128.60
36	1	2283	G	C5-N7-C8	-8.10	100.25	104.30
36	5	3214	U	N3-C2-O2	-8.10	116.53	122.20
37	7	98	C	N3-C4-C5	8.10	125.14	121.90
36	1	979	U	N3-C2-O2	-8.09	116.54	122.20
36	1	1901	A	N1-C6-N6	-8.09	113.75	118.60
36	5	2942	C	C5-C4-N4	-8.09	114.54	120.20
36	5	3303	G	N1-C6-O6	-8.09	115.05	119.90
36	5	2234	G	C5-C6-O6	-8.08	123.75	128.60
36	5	2831	G	C5-C6-N1	8.08	115.54	111.50
36	5	2816	G	C8-N9-C4	8.07	109.63	106.40
36	1	2124	G	N1-C6-O6	8.07	124.74	119.90
36	5	385	A	N1-C6-N6	8.06	123.44	118.60
36	1	614	C	C6-N1-C2	8.06	123.52	120.30
36	1	1124	U	N3-C4-C5	8.06	119.43	114.60
36	5	2345	A	C5-C6-N6	-8.05	117.26	123.70
36	5	2354	C	C4-C5-C6	8.05	121.43	117.40
36	1	818	C	N3-C4-C5	-8.04	118.68	121.90
36	5	1116	G	C4-C5-N7	-8.04	107.58	110.80
36	1	439	C	N1-C2-O2	8.04	123.72	118.90
36	1	2374	C	C6-N1-C2	-8.03	117.09	120.30
1	6	453	U	C2-N1-C1'	8.03	127.33	117.70
36	5	2928	C	C2-N1-C1'	8.02	127.62	118.80
1	6	163	G	C8-N9-C1'	8.02	137.42	127.00
36	5	424	G	N9-C4-C5	-8.02	102.19	105.40
36	1	2636	A	C8-N9-C4	-8.01	102.59	105.80
36	5	1110	U	N3-C2-O2	-8.01	116.59	122.20
36	1	1166	G	C5-C6-O6	-8.01	123.79	128.60
36	1	2984	C	C6-N1-C2	-8.01	117.10	120.30
36	5	1380	G	C8-N9-C4	8.01	109.60	106.40
1	6	100	A	N1-C6-N6	8.01	123.40	118.60
1	2	553	G	C5-C6-O6	-8.00	123.80	128.60
1	2	1200	G	N1-C6-O6	7.99	124.70	119.90
36	1	2231	C	C6-N1-C2	7.99	123.50	120.30
36	1	2968	G	C2-N3-C4	-7.99	107.90	111.90
36	5	1844	C	C6-N1-C2	-7.99	117.10	120.30
36	1	1373	A	O5'-P-OP2	-7.99	98.51	105.70
36	1	984	G	C6-C5-N7	-7.98	125.61	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3114	A	O5'-P-OP2	-7.98	98.52	105.70
36	5	2211	U	C4-C5-C6	7.98	124.49	119.70
36	5	915	A	C5-C6-N1	7.98	121.69	117.70
36	1	2777	G	N1-C6-O6	-7.98	115.11	119.90
36	1	3217	C	C2-N1-C1'	7.98	127.58	118.80
1	6	14	C	C6-N1-C2	-7.97	117.11	120.30
52	m6	68	ARG	NE-CZ-NH2	7.97	124.29	120.30
36	1	637	C	P-O3'-C3'	7.97	129.26	119.70
36	5	1429	G	C4-C5-N7	7.97	113.99	110.80
36	5	1308	A	O5'-P-OP2	7.97	120.26	110.70
36	5	2816	G	N9-C4-C5	-7.97	102.21	105.40
36	5	2572	C	N3-C2-O2	-7.96	116.33	121.90
38	4	53	A	N1-C6-N6	-7.96	113.82	118.60
36	5	1006	A	O5'-P-OP2	-7.96	98.54	105.70
36	1	2811	A	C6-N1-C2	-7.96	113.83	118.60
36	1	1449	A	C6-N1-C2	-7.96	113.83	118.60
36	1	2823	G	N3-C2-N2	-7.96	114.33	119.90
36	1	1303	A	N1-C6-N6	7.95	123.37	118.60
36	5	1506	A	C8-N9-C4	-7.95	102.62	105.80
36	1	807	A	C2-N3-C4	-7.95	106.62	110.60
36	1	948	C	N1-C2-O2	-7.95	114.13	118.90
36	5	63	A	C6-C5-N7	-7.95	126.73	132.30
36	5	3105	U	N3-C4-O4	-7.95	113.83	119.40
36	1	942	U	C5-C4-O4	-7.95	121.13	125.90
37	7	98	C	C6-N1-C2	7.95	123.48	120.30
36	1	957	C	N1-C2-O2	-7.95	114.13	118.90
36	1	857	G	N1-C6-O6	7.94	124.67	119.90
36	1	645	A	C6-N1-C2	-7.94	113.83	118.60
1	2	75	U	N3-C2-O2	-7.94	116.64	122.20
36	1	2978	U	O4'-C1'-N1	7.93	114.55	108.20
56	N0	58	ILE	CG1-CB-CG2	-7.93	93.95	111.40
1	6	1137	A	C8-N9-C4	7.93	108.97	105.80
36	5	1176	C	N1-C2-O2	-7.93	114.14	118.90
36	1	2617	U	C2-N3-C4	-7.93	122.24	127.00
36	5	2272	G	O4'-C1'-N9	7.93	114.54	108.20
36	5	3105	U	N1-C2-N3	7.93	119.66	114.90
36	1	1313	G	N1-C6-O6	7.92	124.65	119.90
1	2	1733	C	N3-C4-N4	7.92	123.54	118.00
36	1	1389	G	N1-C6-O6	7.92	124.65	119.90
36	5	922	U	N3-C2-O2	-7.92	116.66	122.20
36	1	399	A	O5'-P-OP1	-7.91	98.58	105.70
36	1	1164	G	C5-C6-O6	7.91	133.35	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2808	A	N9-C4-C5	-7.91	102.64	105.80
1	6	1150	G	C8-N9-C4	7.91	109.56	106.40
36	5	339	C	N1-C2-O2	-7.90	114.16	118.90
36	1	2640	A	N1-C2-N3	7.90	133.25	129.30
36	1	639	G	N3-C2-N2	-7.90	114.37	119.90
48	m1	112	LEU	CA-CB-CG	7.90	133.46	115.30
36	1	3362	A	O4'-C1'-N9	7.89	114.52	108.20
1	6	338	C	C5-C6-N1	7.89	124.95	121.00
36	5	776	U	N1-C2-N3	7.89	119.64	114.90
20	c8	15	LEU	CA-CB-CG	7.89	133.45	115.30
36	1	960	U	C6-N1-C2	7.89	125.73	121.00
36	1	2572	C	C2-N1-C1'	7.88	127.47	118.80
36	5	2372	A	C8-N9-C4	-7.88	102.65	105.80
36	5	2700	G	N1-C6-O6	7.88	124.63	119.90
37	7	94	C	C4-C5-C6	-7.88	113.46	117.40
36	5	861	C	C6-N1-C2	7.88	123.45	120.30
36	5	3075	G	N1-C6-O6	7.88	124.63	119.90
36	1	3362	A	N7-C8-N9	7.87	117.74	113.80
36	5	1152	G	C5-C6-O6	-7.87	123.88	128.60
36	1	1392	G	C2-N3-C4	7.87	115.83	111.90
36	1	2819	A	O5'-P-OP2	-7.86	98.62	105.70
1	2	1600	A	C2-N3-C4	-7.86	106.67	110.60
36	1	636	C	C2-N3-C4	-7.86	115.97	119.90
36	1	1414	G	N1-C6-O6	7.86	124.62	119.90
1	6	453	U	N3-C2-O2	-7.86	116.70	122.20
36	1	1365	G	N7-C8-N9	7.86	117.03	113.10
36	1	979	U	C6-N1-C2	-7.86	116.29	121.00
36	5	3216	G	O5'-P-OP2	-7.86	98.63	105.70
36	5	881	C	N1-C2-O2	7.85	123.61	118.90
1	6	1634	C	N1-C2-O2	7.85	123.61	118.90
36	5	2985	C	C5-C6-N1	7.85	124.92	121.00
36	1	802	C	O5'-P-OP1	-7.85	98.64	105.70
1	6	1670	G	O5'-P-OP2	-7.85	98.64	105.70
36	5	2140	U	C6-N1-C2	-7.84	116.30	121.00
36	1	689	U	N3-C2-O2	-7.84	116.71	122.20
36	1	2870	C	C2-N1-C1'	-7.84	110.18	118.80
36	1	3097	C	O5'-P-OP2	-7.83	98.65	105.70
36	1	439	C	C6-N1-C1'	-7.83	111.40	120.80
36	1	1592	G	C5-C6-O6	7.83	133.30	128.60
36	5	2245	C	O5'-P-OP2	-7.83	98.66	105.70
36	5	2353	G	C5-C6-O6	-7.83	123.90	128.60
36	5	370	U	N3-C2-O2	-7.82	116.73	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1317	A	C5-C6-N6	-7.82	117.45	123.70
36	1	2726	C	N1-C2-N3	7.82	124.67	119.20
1	6	1075	C	N1-C2-O2	-7.81	114.21	118.90
36	5	1329	U	N3-C4-O4	7.81	124.87	119.40
36	1	2606	G	C6-C5-N7	-7.81	125.72	130.40
36	5	1239	C	C5-C6-N1	7.81	124.90	121.00
1	6	982	U	O5'-P-OP1	-7.80	98.68	105.70
36	1	29	C	N3-C4-N4	7.80	123.46	118.00
36	5	2867	C	C6-N1-C2	-7.80	117.18	120.30
41	14	339	LEU	CA-CB-CG	7.80	133.24	115.30
36	5	911	C	C5-C6-N1	-7.80	117.10	121.00
36	1	2378	C	C5-C4-N4	-7.79	114.74	120.20
36	1	2808	A	C6-C5-N7	-7.79	126.84	132.30
36	5	361	A	N1-C6-N6	-7.79	113.92	118.60
36	5	2954	U	C6-N1-C1'	-7.79	110.30	121.20
1	2	1733	C	N3-C2-O2	7.78	127.35	121.90
36	1	939	U	N1-C2-O2	-7.78	117.35	122.80
36	5	38	U	O5'-P-OP2	-7.78	98.70	105.70
36	1	893	C	C6-N1-C2	-7.78	117.19	120.30
36	1	770	G	O4'-C1'-N9	7.78	114.42	108.20
36	1	2884	C	C4-C5-C6	-7.77	113.51	117.40
36	1	2996	U	C2-N1-C1'	7.77	127.03	117.70
36	5	1556	C	C6-N1-C2	-7.77	117.19	120.30
36	5	1851	G	N1-C6-O6	7.77	124.56	119.90
36	1	271	C	N1-C2-O2	7.77	123.56	118.90
36	1	960	U	N3-C4-O4	-7.76	113.97	119.40
36	1	1586	G	O5'-P-OP2	-7.76	98.72	105.70
36	5	2293	C	N1-C2-O2	7.76	123.56	118.90
36	5	3128	G	C8-N9-C4	7.75	109.50	106.40
36	1	1172	G	O5'-P-OP1	-7.75	98.73	105.70
36	1	930	U	C5-C6-N1	-7.75	118.83	122.70
1	2	1568	C	P-O3'-C3'	7.74	128.99	119.70
36	1	221	A	O5'-P-OP2	-7.74	98.74	105.70
36	5	1368	U	N1-C2-O2	-7.74	117.38	122.80
36	1	1520	G	C5-N7-C8	7.74	108.17	104.30
36	5	2331	C	N3-C4-C5	-7.73	118.81	121.90
36	1	2827	U	N3-C2-O2	-7.73	116.79	122.20
36	1	3016	A	N1-C6-N6	7.73	123.24	118.60
1	2	830	U	N3-C2-O2	-7.73	116.79	122.20
36	1	2606	G	N3-C4-N9	7.73	130.64	126.00
36	1	285	A	N1-C6-N6	7.72	123.23	118.60
36	5	2147	A	N1-C6-N6	7.72	123.23	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	125	U	N1-C2-O2	7.72	128.20	122.80
36	1	372	A	O5'-P-OP2	-7.71	98.76	105.70
36	1	2647	A	C6-N1-C2	-7.71	113.97	118.60
36	1	1838	G	C5-C6-O6	-7.71	123.97	128.60
36	5	3107	U	C5-C4-O4	-7.71	121.27	125.90
36	5	2878	G	N1-C6-O6	-7.71	115.28	119.90
36	1	1192	C	C2-N1-C1'	7.71	127.28	118.80
1	6	65	A	C2-N3-C4	-7.71	106.75	110.60
38	8	26	U	N3-C2-O2	-7.71	116.81	122.20
1	2	1339	C	P-O3'-C3'	7.70	128.94	119.70
36	1	1495	U	C2-N3-C4	-7.70	122.38	127.00
36	1	2857	C	C5-C4-N4	-7.70	114.81	120.20
36	5	3218	A	C4-C5-N7	7.70	114.55	110.70
36	1	633	C	N1-C2-O2	-7.70	114.28	118.90
36	5	2572	C	C2-N1-C1'	7.69	127.26	118.80
36	1	695	C	N3-C4-C5	7.69	124.97	121.90
36	5	1306	G	C8-N9-C4	7.69	109.47	106.40
36	5	927	C	C5-C4-N4	-7.68	114.82	120.20
1	6	1596	C	N3-C2-O2	-7.68	116.53	121.90
36	1	2846	U	C5-C4-O4	7.67	130.50	125.90
1	6	782	U	N3-C2-O2	-7.67	116.83	122.20
36	1	2938	G	OP1-P-OP2	7.67	131.11	119.60
36	5	414	U	C5-C4-O4	-7.67	121.30	125.90
36	5	2648	G	C5-C6-N1	7.67	115.33	111.50
36	1	810	A	N1-C6-N6	-7.67	114.00	118.60
36	1	2836	C	C5-C4-N4	7.67	125.57	120.20
36	5	83	U	N3-C2-O2	-7.67	116.83	122.20
1	2	1596	C	N3-C2-O2	-7.67	116.53	121.90
36	1	2624	G	C5-C6-N1	-7.66	107.67	111.50
1	6	815	G	C5-C6-O6	-7.66	124.00	128.60
36	5	966	U	N1-C2-O2	7.66	128.16	122.80
36	5	1449	A	N1-C6-N6	7.66	123.19	118.60
36	1	917	A	N1-C6-N6	-7.66	114.01	118.60
36	5	3143	C	N1-C2-O2	-7.66	114.31	118.90
36	1	1604	G	C4-N9-C1'	7.65	136.45	126.50
36	1	1205	A	O5'-P-OP2	-7.65	98.81	105.70
36	5	2616	C	C5-C4-N4	-7.65	114.84	120.20
36	1	2434	U	C5-C4-O4	7.65	130.49	125.90
38	4	113	U	C5-C6-N1	-7.65	118.88	122.70
36	5	816	A	N9-C4-C5	7.65	108.86	105.80
36	1	2610	G	C6-C5-N7	-7.64	125.81	130.40
36	5	3078	U	N3-C2-O2	-7.64	116.85	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1306	G	N9-C4-C5	-7.64	102.34	105.40
36	1	2305	G	C5-C6-O6	-7.64	124.02	128.60
1	6	337	G	C6-C5-N7	-7.63	125.82	130.40
36	1	2279	A	N1-C6-N6	7.63	123.18	118.60
36	1	2306	C	C6-N1-C2	-7.63	117.25	120.30
36	1	284	A	C8-N9-C4	-7.63	102.75	105.80
36	5	1445	U	N1-C2-O2	-7.62	117.46	122.80
36	5	2726	C	N3-C4-N4	-7.62	112.66	118.00
1	6	371	G	N3-C4-N9	7.62	130.57	126.00
36	1	1052	U	O5'-P-OP2	-7.62	98.84	105.70
36	1	1904	C	C5-C6-N1	7.62	124.81	121.00
36	1	2773	C	O5'-P-OP2	-7.61	98.85	105.70
36	5	2379	U	C5-C6-N1	-7.61	118.89	122.70
36	5	1161	G	N3-C4-N9	7.61	130.57	126.00
36	1	950	G	C4-C5-N7	7.61	113.84	110.80
36	1	422	A	N1-C6-N6	-7.61	114.04	118.60
36	1	2130	G	C5-C6-O6	7.60	133.16	128.60
36	1	2237	C	C6-N1-C2	7.60	123.34	120.30
36	1	2884	C	C6-N1-C2	7.60	123.34	120.30
36	5	1329	U	C5-C4-O4	-7.60	121.34	125.90
36	1	939	U	N3-C2-O2	7.60	127.52	122.20
36	5	2908	G	C8-N9-C4	-7.59	103.36	106.40
1	6	687	G	N3-C2-N2	-7.59	114.58	119.90
36	5	1115	G	C4-N9-C1'	7.59	136.37	126.50
36	1	2308	C	C2-N3-C4	-7.59	116.10	119.90
36	1	2733	A	O5'-P-OP2	-7.59	98.87	105.70
36	5	1148	G	C5-C6-O6	-7.59	124.05	128.60
36	5	2817	A	C8-N9-C4	-7.59	102.76	105.80
36	1	1838	G	N9-C4-C5	-7.59	102.37	105.40
36	5	889	U	N3-C4-C5	7.58	119.15	114.60
36	5	705	A	O5'-P-OP2	-7.58	98.88	105.70
36	5	2727	A	O5'-P-OP2	-7.58	98.88	105.70
36	1	2177	G	N3-C4-N9	7.57	130.54	126.00
36	5	222	A	O5'-P-OP2	-7.57	98.88	105.70
36	5	1520	G	C5-C6-O6	-7.57	124.06	128.60
36	1	701	G	N1-C6-O6	7.57	124.44	119.90
36	1	2812	C	C4-C5-C6	7.57	121.19	117.40
36	1	25	U	N3-C4-O4	7.57	124.70	119.40
36	5	2621	G	N1-C6-O6	7.57	124.44	119.90
36	5	2838	A	O5'-P-OP1	7.57	119.78	110.70
36	1	1377	G	C8-N9-C4	7.56	109.42	106.40
37	3	84	A	N1-C6-N6	7.56	123.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2370	G	C8-N9-C4	-7.56	103.38	106.40
36	5	414	U	N3-C2-O2	7.56	127.49	122.20
36	1	896	A	C8-N9-C4	-7.56	102.78	105.80
1	6	390	G	O5'-P-OP2	-7.56	98.90	105.70
36	5	1931	U	C2-N1-C1'	-7.55	108.63	117.70
36	5	1099	A	N1-C6-N6	7.55	123.13	118.60
36	5	2957	G	O5'-P-OP1	-7.55	98.91	105.70
36	5	1116	G	O5'-P-OP1	-7.55	98.91	105.70
36	5	3374	U	N3-C4-C5	7.55	119.13	114.60
36	1	1192	C	C6-N1-C1'	-7.54	111.75	120.80
36	1	1849	C	C5-C4-N4	-7.54	114.92	120.20
36	1	636	C	O5'-P-OP1	-7.54	98.92	105.70
36	1	1846	C	N1-C2-O2	-7.54	114.38	118.90
36	1	2643	A	N9-C4-C5	-7.54	102.78	105.80
36	5	822	G	N3-C4-N9	-7.54	121.48	126.00
36	5	942	U	C4-C5-C6	7.54	124.22	119.70
36	5	1116	G	C5-C6-N1	-7.54	107.73	111.50
36	5	2996	U	O5'-P-OP2	-7.54	98.92	105.70
36	5	3008	A	C2-N3-C4	-7.54	106.83	110.60
36	1	651	G	N3-C4-C5	-7.54	124.83	128.60
36	1	229	G	C5-C6-O6	-7.54	124.08	128.60
36	1	421	G	N9-C4-C5	-7.53	102.39	105.40
36	1	2279	A	C5-C6-N6	-7.53	117.67	123.70
38	4	32	C	C2-N1-C1'	-7.53	110.51	118.80
1	6	308	C	C5-C6-N1	-7.53	117.23	121.00
37	7	77	G	N1-C6-O6	7.53	124.42	119.90
36	5	426	G	C8-N9-C4	7.53	109.41	106.40
36	5	2800	G	N3-C2-N2	-7.53	114.63	119.90
36	1	2679	A	C2-N3-C4	-7.53	106.84	110.60
36	5	2351	U	N3-C2-O2	-7.52	116.93	122.20
36	5	2400	G	C8-N9-C4	7.52	109.41	106.40
36	5	3362	A	N7-C8-N9	7.52	117.56	113.80
37	7	12	U	C5-C4-O4	-7.52	121.39	125.90
36	1	1334	U	N3-C4-C5	-7.52	110.09	114.60
36	1	2622	C	N3-C4-C5	-7.52	118.89	121.90
1	6	1	U	C2-N1-C1'	7.52	126.72	117.70
1	6	87	C	C6-N1-C2	-7.52	117.29	120.30
36	5	2648	G	C5-C6-O6	-7.52	124.09	128.60
36	5	1897	G	N3-C4-C5	7.51	132.36	128.60
36	5	531	G	O5'-P-OP1	-7.51	98.94	105.70
1	2	61	A	N7-C8-N9	7.51	117.56	113.80
36	5	1516	C	N3-C4-C5	7.51	124.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	343	U	C6-N1-C2	-7.51	116.50	121.00
36	1	2273	G	C8-N9-C4	7.51	109.40	106.40
36	1	1114	U	N3-C4-O4	-7.51	114.15	119.40
36	5	3136	G	N1-C2-N2	-7.50	109.45	116.20
36	1	984	G	N1-C2-N2	-7.50	109.45	116.20
36	5	1306	G	N1-C6-O6	7.50	124.40	119.90
36	1	1197	A	C5-C6-N6	-7.49	117.70	123.70
36	1	1007	U	C5-C4-O4	-7.49	121.41	125.90
36	1	3362	A	C5-N7-C8	-7.49	100.16	103.90
36	1	2836	C	N3-C4-N4	-7.49	112.76	118.00
1	2	75	U	C2-N1-C1'	7.48	126.68	117.70
1	2	17	C	C6-N1-C2	-7.48	117.31	120.30
36	1	573	C	C5-C6-N1	-7.48	117.26	121.00
36	5	1462	A	C2-N3-C4	-7.48	106.86	110.60
36	1	2714	G	C5-N7-C8	-7.48	100.56	104.30
36	1	2915	U	C5-C4-O4	-7.48	121.41	125.90
36	5	2943	G	N1-C6-O6	7.48	124.39	119.90
36	1	803	C	O5'-P-OP1	7.48	119.67	110.70
36	5	2401	A	C2-N3-C4	7.48	114.34	110.60
36	1	829	U	N1-C2-O2	7.47	128.03	122.80
1	6	956	C	C6-N1-C2	7.47	123.29	120.30
36	1	672	A	N9-C4-C5	-7.47	102.81	105.80
36	1	2371	G	C4-C5-N7	7.47	113.79	110.80
36	5	2759	U	N1-C2-N3	7.46	119.38	114.90
36	5	915	A	C6-N1-C2	-7.46	114.12	118.60
36	1	894	G	C5-C6-O6	-7.46	124.13	128.60
36	5	2943	G	C5-C6-O6	-7.46	124.13	128.60
36	1	2808	A	O4'-C1'-N9	-7.45	102.24	108.20
36	1	214	G	N1-C6-O6	7.45	124.37	119.90
36	5	3206	C	N3-C2-O2	-7.45	116.69	121.90
36	1	304	G	N3-C2-N2	-7.44	114.69	119.90
36	5	2643	A	N9-C4-C5	-7.44	102.82	105.80
1	2	1761	U	P-O3'-C3'	7.44	128.63	119.70
1	2	1324	G	N3-C4-N9	-7.44	121.54	126.00
36	1	2870	C	N3-C4-N4	-7.44	112.79	118.00
36	5	1885	U	C6-N1-C2	7.44	125.46	121.00
37	7	37	G	N9-C4-C5	-7.44	102.42	105.40
1	2	1274	C	C2-N1-C1'	7.44	126.98	118.80
36	5	1300	G	C5-C6-O6	-7.43	124.14	128.60
36	5	2872	A	N3-C4-C5	7.43	132.00	126.80
1	2	1175	U	O5'-P-OP1	-7.43	99.01	105.70
36	1	267	G	O5'-P-OP1	-7.43	99.01	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3049	A	C5-C6-N1	-7.43	113.98	117.70
36	1	3107	U	C5-C6-N1	-7.43	118.99	122.70
1	6	338	C	C6-N1-C2	-7.43	117.33	120.30
36	1	435	C	C6-N1-C2	7.42	123.27	120.30
36	5	207	U	N1-C2-O2	-7.42	117.60	122.80
36	5	2950	G	O4'-C1'-N9	7.42	114.14	108.20
1	2	992	A	C2-N3-C4	-7.42	106.89	110.60
36	5	2899	C	N3-C4-C5	-7.42	118.93	121.90
36	1	1303	A	N9-C4-C5	-7.42	102.83	105.80
36	5	1375	G	C8-N9-C4	-7.42	103.43	106.40
1	2	831	U	C6-N1-C2	-7.42	116.55	121.00
38	4	25	G	C5-C6-O6	7.42	133.05	128.60
36	1	2153	U	C6-N1-C2	-7.42	116.55	121.00
36	5	2727	A	C8-N9-C4	-7.42	102.83	105.80
36	5	2904	U	C5-C6-N1	-7.42	118.99	122.70
36	1	1449	A	C5-C6-N1	7.41	121.41	117.70
36	5	3133	C	C6-N1-C2	-7.41	117.33	120.30
36	1	361	A	N1-C6-N6	-7.40	114.16	118.60
1	6	782	U	N1-C2-O2	7.40	127.98	122.80
36	5	1366	A	N9-C4-C5	7.40	108.76	105.80
36	5	2147	A	C5-C6-N6	-7.40	117.78	123.70
36	1	2945	G	O5'-P-OP2	-7.40	99.04	105.70
36	5	315	C	N3-C4-C5	7.40	124.86	121.90
36	1	2945	G	O5'-P-OP1	7.39	119.57	110.70
36	5	2404	A	O4'-C1'-N9	7.39	114.11	108.20
36	1	1515	A	N1-C6-N6	7.39	123.03	118.60
36	1	611	A	O5'-P-OP1	7.39	119.57	110.70
36	5	2404	A	C4-N9-C1'	-7.39	113.00	126.30
36	1	949	C	C6-N1-C2	-7.39	117.34	120.30
36	5	822	G	N3-C4-C5	7.38	132.29	128.60
36	5	1490	A	C8-N9-C4	-7.38	102.85	105.80
1	2	831	U	C2-N1-C1'	7.38	126.56	117.70
36	5	914	A	O5'-P-OP1	-7.38	99.06	105.70
36	5	2392	C	C2-N1-C1'	-7.38	110.68	118.80
36	1	802	C	O5'-P-OP2	7.38	119.56	110.70
36	1	2308	C	N1-C2-O2	-7.38	114.47	118.90
1	6	272	U	N3-C2-O2	-7.38	117.04	122.20
36	1	2403	G	N3-C4-N9	7.37	130.42	126.00
1	6	421	A	C8-N9-C4	7.37	108.75	105.80
1	6	1659	A	O5'-P-OP1	-7.37	99.06	105.70
36	1	2639	G	C4-C5-N7	7.37	113.75	110.80
36	5	1867	A	N1-C6-N6	7.37	123.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1556	C	C6-N1-C2	-7.37	117.35	120.30
36	1	1578	C	C2-N1-C1'	7.37	126.91	118.80
36	5	2868	U	C5-C6-N1	7.37	126.38	122.70
1	6	1634	C	C5-C6-N1	7.37	124.68	121.00
36	1	110	G	O5'-P-OP1	-7.37	99.07	105.70
1	6	1100	G	N3-C4-C5	-7.37	124.92	128.60
36	1	984	G	N3-C2-N2	7.36	125.05	119.90
1	6	194	U	C2-N1-C1'	7.36	126.53	117.70
1	2	453	U	N1-C2-O2	7.36	127.95	122.80
36	1	2367	A	N1-C6-N6	7.36	123.01	118.60
36	5	1834	U	N3-C4-C5	-7.35	110.19	114.60
1	2	310	C	N3-C4-C5	-7.35	118.96	121.90
10	s8	29	LEU	CA-CB-CG	7.35	132.20	115.30
36	1	2871	G	O5'-P-OP2	-7.34	99.09	105.70
37	7	44	C	C6-N1-C2	7.34	123.24	120.30
38	4	80	A	O5'-P-OP2	-7.34	99.09	105.70
36	5	41	G	O5'-P-OP2	-7.34	99.09	105.70
36	5	2400	G	N3-C4-C5	7.34	132.27	128.60
36	5	3382	U	N3-C2-O2	-7.34	117.06	122.20
1	6	453	U	N1-C2-O2	7.34	127.94	122.80
36	1	794	U	O5'-P-OP1	7.34	119.50	110.70
36	5	2870	C	C2-N1-C1'	-7.33	110.73	118.80
36	1	2640	A	C6-N1-C2	-7.33	114.20	118.60
15	C3	22	ALA	C-N-CD	-7.33	104.48	120.60
36	1	808	A	C6-N1-C2	-7.33	114.20	118.60
36	1	886	C	C6-N1-C2	-7.33	117.37	120.30
38	4	43	A	O5'-P-OP1	-7.33	99.11	105.70
36	5	636	C	O5'-P-OP2	-7.33	99.11	105.70
36	5	1660	C	C6-N1-C2	-7.33	117.37	120.30
36	1	1385	C	C6-N1-C2	7.32	123.23	120.30
36	1	2646	C	N3-C4-C5	7.32	124.83	121.90
36	1	1112	A	N9-C4-C5	-7.32	102.87	105.80
36	5	2211	U	N3-C2-O2	-7.32	117.08	122.20
36	5	2982	A	C2-N3-C4	7.32	114.26	110.60
36	1	2373	A	O5'-P-OP1	-7.31	99.12	105.70
36	1	517	G	N7-C8-N9	7.31	116.76	113.10
36	1	1121	U	N1-C2-N3	7.31	119.29	114.90
36	5	2176	U	N3-C2-O2	-7.31	117.08	122.20
36	5	2893	C	N3-C4-C5	-7.31	118.98	121.90
36	1	229	G	N3-C2-N2	-7.30	114.79	119.90
36	1	1556	C	N3-C2-O2	-7.30	116.79	121.90
36	1	2831	G	C5-C6-O6	-7.30	124.22	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	960	U	C2-N3-C4	-7.30	122.62	127.00
36	1	650	C	OP2-P-O3'	7.29	121.25	105.20
36	1	1903	U	C5-C6-N1	7.29	126.35	122.70
36	1	2700	G	C5-C6-O6	-7.29	124.22	128.60
36	1	2777	G	C5-C6-O6	7.29	132.98	128.60
1	2	694	U	C2-N1-C1'	7.29	126.45	117.70
36	1	517	G	C8-N9-C4	-7.29	103.48	106.40
1	6	387	A	O5'-P-OP2	-7.29	99.14	105.70
36	1	2281	A	C8-N9-C4	7.29	108.72	105.80
37	7	104	A	O5'-P-OP2	-7.29	99.14	105.70
36	5	2858	U	C5-C6-N1	7.29	126.34	122.70
36	5	3197	G	N3-C2-N2	-7.29	114.80	119.90
36	5	3388	C	C6-N1-C2	7.29	123.22	120.30
1	2	1560	U	C5-C4-O4	7.28	130.27	125.90
36	5	2908	G	N9-C4-C5	7.28	108.31	105.40
45	18	69	LEU	CA-CB-CG	7.28	132.04	115.30
36	1	2212	C	C6-N1-C2	7.28	123.21	120.30
36	1	54	C	C6-N1-C2	7.28	123.21	120.30
36	1	2937	G	C8-N9-C4	7.28	109.31	106.40
36	5	1208	U	O5'-P-OP1	-7.27	99.15	105.70
36	1	3181	C	C6-N1-C2	-7.27	117.39	120.30
36	5	645	A	N1-C2-N3	7.27	132.93	129.30
36	5	649	A	C5-C6-N6	-7.26	117.89	123.70
36	1	960	U	C5-C6-N1	-7.26	119.07	122.70
36	5	1161	G	C5-C6-O6	-7.26	124.24	128.60
36	5	2821	C	N1-C2-O2	-7.26	114.54	118.90
36	1	3045	G	C2-N3-C4	7.26	115.53	111.90
38	4	40	A	N1-C6-N6	7.25	122.95	118.60
1	6	609	U	C5-C4-O4	7.25	130.25	125.90
36	5	1874	A	C8-N9-C4	7.25	108.70	105.80
36	1	798	G	C8-N9-C4	-7.25	103.50	106.40
36	5	3309	G	N3-C4-C5	-7.25	124.97	128.60
36	5	1124	U	C4-C5-C6	-7.25	115.35	119.70
36	5	2850	G	C5-C6-O6	-7.25	124.25	128.60
36	5	1132	C	O5'-P-OP1	-7.25	99.18	105.70
36	1	1838	G	C4-C5-N7	7.25	113.70	110.80
1	2	581	U	C2-N1-C1'	7.24	126.39	117.70
36	1	939	U	O5'-P-OP2	-7.24	99.18	105.70
36	1	1002	A	C8-N9-C4	7.24	108.70	105.80
36	1	1103	A	O5'-P-OP1	-7.24	99.18	105.70
36	1	2293	C	C5-C4-N4	-7.24	115.13	120.20
36	1	2636	A	N7-C8-N9	7.24	117.42	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	542	A	N7-C8-N9	7.24	117.42	113.80
36	1	2671	A	O5'-P-OP2	-7.24	99.19	105.70
36	1	358	G	C8-N9-C4	7.24	109.29	106.40
36	1	2414	G	O5'-P-OP2	-7.23	99.19	105.70
1	2	145	A	C8-N9-C4	-7.23	102.91	105.80
1	2	1274	C	N3-C2-O2	-7.23	116.84	121.90
36	1	2996	U	N1-C2-O2	7.23	127.86	122.80
36	1	347	G	C5-C6-O6	-7.23	124.26	128.60
36	5	1187	C	N1-C2-O2	7.23	123.24	118.90
36	1	2700	G	C6-C5-N7	-7.23	126.06	130.40
36	5	3188	G	N3-C4-C5	-7.23	124.99	128.60
36	1	2371	G	C5-C6-O6	-7.22	124.27	128.60
36	5	1284	C	C6-N1-C2	-7.22	117.41	120.30
36	5	871	U	C5-C4-O4	7.22	130.23	125.90
36	1	2572	C	N3-C2-O2	-7.22	116.84	121.90
36	5	2699	G	C5-C6-O6	-7.22	124.27	128.60
36	5	1377	G	C5-C6-O6	-7.22	124.27	128.60
36	5	897	U	O5'-P-OP1	-7.22	99.20	105.70
36	1	2878	G	O5'-P-OP1	7.21	119.36	110.70
1	6	696	C	O4'-C1'-N1	7.21	113.97	108.20
36	5	2147	A	C4-C5-N7	7.21	114.30	110.70
36	1	102	C	N1-C2-O2	-7.21	114.58	118.90
36	5	395	A	C5-C6-N6	-7.21	117.94	123.70
36	5	1846	C	C6-N1-C2	7.21	123.18	120.30
36	5	2334	U	O5'-P-OP2	-7.21	99.22	105.70
36	1	54	C	N3-C4-C5	7.21	124.78	121.90
36	1	1741	A	N1-C6-N6	7.20	122.92	118.60
36	5	776	U	C4-C5-C6	7.20	124.02	119.70
36	1	1429	G	C2-N3-C4	7.20	115.50	111.90
36	1	3013	U	O5'-P-OP2	-7.20	99.22	105.70
1	6	1280	C	N3-C4-C5	-7.20	119.02	121.90
36	5	1317	A	N1-C2-N3	-7.20	125.70	129.30
36	1	1310	G	N1-C2-N2	-7.20	109.72	116.20
36	1	2818	U	C5-C6-N1	7.20	126.30	122.70
36	1	410	U	C6-N1-C2	-7.19	116.68	121.00
1	6	1764	C	C6-N1-C2	7.19	123.18	120.30
36	1	2875	U	N3-C4-O4	7.19	124.43	119.40
36	5	1481	A	P-O3'-C3'	7.19	128.33	119.70
35	SM	135	ALA	N-CA-CB	7.19	120.16	110.10
36	5	2249	G	C8-N9-C4	-7.19	103.53	106.40
52	m6	78	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	2	61	A	C5-N7-C8	-7.18	100.31	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1506	A	N1-C6-N6	-7.18	114.29	118.60
36	1	893	C	C5-C6-N1	7.18	124.59	121.00
36	5	2234	G	C8-N9-C4	7.18	109.27	106.40
1	2	602	U	O5'-P-OP1	-7.18	99.24	105.70
36	1	2725	U	C5-C4-O4	7.18	130.21	125.90
36	1	2730	G	N3-C2-N2	-7.18	114.87	119.90
1	6	67	A	N1-C6-N6	7.18	122.91	118.60
36	5	200	C	C5-C4-N4	-7.18	115.17	120.20
36	1	806	A	O5'-P-OP1	-7.18	99.24	105.70
36	5	211	A	O5'-P-OP1	-7.17	99.24	105.70
36	5	1429	G	N3-C4-N9	7.17	130.30	126.00
36	5	225	C	O5'-P-OP1	-7.17	99.25	105.70
36	5	816	A	C8-N9-C4	-7.17	102.93	105.80
38	4	120	C	N1-C2-O2	-7.17	114.60	118.90
36	5	53	G	O5'-P-OP2	-7.17	99.25	105.70
36	5	3060	C	N1-C2-O2	-7.17	114.60	118.90
38	8	26	U	O5'-P-OP2	-7.16	99.25	105.70
36	5	934	G	N1-C6-O6	7.16	124.20	119.90
36	5	2827	U	O4'-C1'-N1	7.16	113.92	108.20
1	2	1749	A	N1-C6-N6	7.15	122.89	118.60
1	6	337	G	C4-N9-C1'	7.15	135.80	126.50
36	5	3105	U	C6-N1-C1'	7.15	131.22	121.20
36	5	1158	A	N9-C4-C5	-7.15	102.94	105.80
36	5	1445	U	N3-C2-O2	7.15	127.20	122.20
36	1	645	A	C5-C6-N1	7.15	121.27	117.70
36	1	637	C	O5'-P-OP2	-7.14	99.27	105.70
36	1	2121	G	N3-C4-C5	-7.14	125.03	128.60
36	5	1140	G	OP1-P-O3'	7.14	120.91	105.20
1	2	1761	U	C5-C4-O4	7.14	130.19	125.90
36	1	2758	A	N7-C8-N9	-7.14	110.23	113.80
36	5	607	A	N1-C6-N6	-7.14	114.32	118.60
36	5	2644	C	N1-C2-O2	-7.14	114.62	118.90
36	1	1180	A	N1-C6-N6	-7.14	114.32	118.60
36	1	2187	G	C6-C5-N7	-7.14	126.12	130.40
36	1	3201	C	C6-N1-C2	-7.14	117.45	120.30
36	5	1911	A	C2-N3-C4	-7.14	107.03	110.60
36	1	2850	G	C4-C5-N7	7.13	113.65	110.80
36	5	63	A	C5-C6-N6	-7.13	118.00	123.70
36	5	960	U	N3-C4-C5	7.13	118.88	114.60
36	5	2366	C	C6-N1-C2	-7.13	117.45	120.30
36	1	1489	A	N1-C6-N6	7.13	122.88	118.60
36	1	1902	G	C4-C5-N7	7.13	113.65	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3154	C	C2-N1-C1'	7.13	126.64	118.80
36	5	2616	C	N3-C4-C5	7.13	124.75	121.90
36	1	1329	U	C2-N1-C1'	7.12	126.25	117.70
1	6	639	U	N3-C2-O2	-7.12	117.21	122.20
36	5	1181	U	C5-C6-N1	-7.12	119.14	122.70
36	1	808	A	N1-C2-N3	7.12	132.86	129.30
37	3	84	A	C5-C6-N6	-7.12	118.00	123.70
36	5	116	A	O4'-C1'-N9	7.12	113.90	108.20
1	6	1641	C	N1-C2-O2	-7.12	114.63	118.90
36	5	2271	A	C8-N9-C4	7.12	108.65	105.80
37	7	77	G	N9-C4-C5	-7.12	102.55	105.40
36	1	2371	G	OP2-P-O3'	7.11	120.85	105.20
36	5	2849	C	N1-C2-O2	-7.11	114.63	118.90
36	1	96	G	C2-N3-C4	-7.11	108.35	111.90
36	5	1367	G	C5-C6-N1	-7.11	107.95	111.50
36	1	3139	A	O5'-P-OP1	-7.11	99.31	105.70
38	4	24	G	N1-C6-O6	7.11	124.16	119.90
36	1	1381	A	O5'-P-OP1	-7.10	99.31	105.70
36	1	960	U	C6-N1-C1'	7.10	131.14	121.20
36	1	1370	G	C4-C5-N7	7.10	113.64	110.80
36	1	2314	U	N3-C2-O2	7.10	127.17	122.20
38	4	113	U	C4-C5-C6	7.10	123.96	119.70
1	6	438	A	O5'-P-OP1	-7.10	99.31	105.70
1	2	1012	U	C2-N3-C4	7.09	131.26	127.00
36	1	2860	U	N3-C2-O2	7.09	127.17	122.20
36	1	2812	C	O5'-P-OP2	7.09	119.21	110.70
36	5	1311	G	C2-N3-C4	7.09	115.45	111.90
36	1	2137	U	O5'-P-OP2	-7.09	99.32	105.70
36	1	2836	C	N3-C2-O2	-7.09	116.94	121.90
36	5	945	C	C6-N1-C2	7.09	123.13	120.30
36	5	1368	U	C5-C4-O4	-7.09	121.65	125.90
36	1	939	U	C5-C4-O4	-7.08	121.65	125.90
36	1	1116	G	OP2-P-O3'	7.08	120.78	105.20
36	1	2372	A	C2-N3-C4	7.08	114.14	110.60
36	5	3078	U	N1-C2-O2	7.08	127.75	122.80
1	6	1568	C	C2-N1-C1'	7.07	126.58	118.80
36	1	1949	G	O5'-P-OP1	-7.07	99.34	105.70
1	2	1129	U	C2-N1-C1'	-7.07	109.22	117.70
10	S8	29	LEU	CA-CB-CG	7.07	131.56	115.30
36	1	341	G	C5-C6-O6	-7.07	124.36	128.60
1	6	610	G	C8-N9-C1'	-7.07	117.81	127.00
1	2	1473	U	N3-C2-O2	-7.06	117.26	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	979	U	O4'-C1'-N1	7.06	113.85	108.20
36	1	2983	C	C4-C5-C6	7.06	120.93	117.40
36	5	1317	A	C2-N3-C4	7.06	114.13	110.60
36	1	1103	A	O5'-P-OP2	7.06	119.17	110.70
36	1	785	G	C2-N3-C4	7.06	115.43	111.90
36	1	2397	A	O5'-P-OP2	-7.05	99.35	105.70
36	1	2964	G	O5'-P-OP2	-7.05	99.35	105.70
36	5	1116	G	C4-C5-C6	7.05	123.03	118.80
36	1	2982	A	C6-N1-C2	-7.05	114.37	118.60
36	5	2831	G	C5-C6-O6	-7.05	124.37	128.60
1	2	831	U	C5-C6-N1	7.05	126.23	122.70
36	1	2366	C	C2-N1-C1'	7.05	126.55	118.80
1	6	337	G	C8-N9-C1'	-7.05	117.84	127.00
36	5	2816	G	C5-C6-O6	-7.05	124.37	128.60
36	1	614	C	N3-C4-C5	7.05	124.72	121.90
36	5	2644	C	O5'-P-OP1	-7.04	99.36	105.70
38	4	32	C	N3-C2-O2	7.04	126.83	121.90
1	2	934	C	C2-N1-C1'	7.04	126.55	118.80
36	5	784	A	N1-C6-N6	7.04	122.83	118.60
36	1	895	A	C4-C5-N7	7.04	114.22	110.70
36	1	2409	G	C2-N3-C4	7.04	115.42	111.90
52	M6	128	ARG	NE-CZ-NH1	-7.04	116.78	120.30
36	5	2112	U	C6-N1-C2	-7.04	116.78	121.00
36	5	2887	A	N1-C6-N6	7.04	122.82	118.60
36	5	645	A	C6-N1-C2	-7.03	114.38	118.60
36	5	2419	A	C8-N9-C4	-7.03	102.99	105.80
37	7	112	G	C8-N9-C4	-7.03	103.59	106.40
36	1	908	G	O4'-C1'-N9	-7.03	102.58	108.20
36	5	1321	G	C5-C6-O6	-7.03	124.38	128.60
36	5	2372	A	OP2-P-O3'	7.03	120.67	105.20
36	1	2700	G	N1-C6-O6	7.03	124.12	119.90
36	5	3082	C	N3-C2-O2	-7.02	116.99	121.90
1	2	310	C	C6-N1-C2	-7.02	117.49	120.30
36	1	693	A	N1-C6-N6	7.02	122.81	118.60
36	1	835	G	O4'-C1'-N9	7.02	113.81	108.20
36	1	810	A	C5-C6-N1	7.01	121.21	117.70
36	5	3055	U	C5-C4-O4	-7.01	121.69	125.90
38	4	125	U	C2-N1-C1'	7.01	126.11	117.70
36	5	410	U	N3-C4-C5	-7.01	110.40	114.60
36	5	2621	G	N3-C2-N2	-7.01	115.00	119.90
36	1	3316	A	C2-N3-C4	-7.00	107.10	110.60
36	1	2385	G	N3-C4-C5	7.00	132.10	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2610	G	C5-C6-O6	-7.00	124.40	128.60
36	5	962	A	N9-C4-C5	-7.00	103.00	105.80
36	5	1101	G	N3-C2-N2	7.00	124.80	119.90
36	5	2400	G	C4-C5-N7	7.00	113.60	110.80
36	1	1279	C	C6-N1-C2	-7.00	117.50	120.30
38	8	84	C	C6-N1-C2	-7.00	117.50	120.30
38	4	19	C	C6-N1-C2	-7.00	117.50	120.30
36	5	3089	C	C5-C6-N1	7.00	124.50	121.00
36	1	2412	G	C5-C6-O6	-6.99	124.40	128.60
1	6	1778	G	C8-N9-C4	-6.99	103.60	106.40
38	4	109	A	C5-C6-N6	-6.99	118.11	123.70
1	6	812	A	N1-C6-N6	6.99	122.79	118.60
36	1	346	C	C5-C6-N1	-6.99	117.51	121.00
36	1	968	G	C8-N9-C4	-6.98	103.61	106.40
37	7	94	C	C5-C6-N1	6.98	124.49	121.00
36	1	699	A	C2-N3-C4	-6.98	107.11	110.60
36	1	1303	A	N7-C8-N9	-6.98	110.31	113.80
36	5	2174	G	N1-C6-O6	6.98	124.09	119.90
36	1	2369	G	N1-C6-O6	6.98	124.09	119.90
36	1	2996	U	C6-N1-C1'	-6.98	111.43	121.20
36	5	2851	A	C2-N3-C4	-6.97	107.11	110.60
36	5	3013	U	O5'-P-OP2	-6.97	99.42	105.70
36	1	793	C	N1-C2-O2	-6.97	114.72	118.90
36	5	2749	G	O5'-P-OP1	-6.97	99.42	105.70
36	1	1741	A	C2-N3-C4	-6.97	107.11	110.60
1	6	1004	U	N1-C2-N3	6.97	119.08	114.90
36	5	952	A	O5'-P-OP2	-6.97	99.43	105.70
36	5	2666	C	O5'-P-OP2	-6.97	99.43	105.70
36	1	1177	G	N3-C4-N9	6.96	130.18	126.00
36	1	2870	C	C6-N1-C1'	6.96	129.16	120.80
36	1	1304	A	O5'-P-OP1	-6.96	99.44	105.70
36	1	217	U	OP1-P-O3'	6.96	120.51	105.20
12	C0	88	PRO	N-CA-CB	6.96	111.65	103.30
36	1	1440	G	O5'-P-OP1	-6.96	99.44	105.70
36	1	1556	C	N1-C2-O2	6.96	123.07	118.90
36	1	2983	C	C5-C4-N4	6.96	125.07	120.20
36	5	1496	C	C2-N1-C1'	6.96	126.45	118.80
36	5	2191	U	N3-C4-O4	-6.96	114.53	119.40
36	1	994	G	N1-C6-O6	-6.95	115.73	119.90
36	5	1513	G	N3-C4-C5	-6.95	125.12	128.60
36	5	3218	A	C5-N7-C8	-6.95	100.42	103.90
36	1	680	G	C8-N9-C4	6.95	109.18	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2146	C	N3-C4-C5	6.95	124.68	121.90
36	1	386	A	N1-C6-N6	6.95	122.77	118.60
36	1	3055	U	C5-C4-O4	-6.95	121.73	125.90
38	4	82	U	N1-C2-O2	-6.95	117.94	122.80
36	1	3120	C	O5'-P-OP2	-6.95	99.45	105.70
36	1	940	G	O5'-P-OP1	-6.94	99.45	105.70
36	1	2620	G	C8-N9-C4	6.94	109.18	106.40
36	1	3210	A	N1-C6-N6	-6.94	114.44	118.60
1	6	609	U	N3-C4-O4	-6.94	114.54	119.40
36	5	1847	A	O5'-P-OP2	-6.94	99.45	105.70
36	5	2287	C	C6-N1-C2	-6.94	117.52	120.30
36	1	1300	G	C5-C6-O6	-6.94	124.44	128.60
36	5	924	G	N1-C6-O6	6.94	124.06	119.90
36	1	116	A	O4'-C1'-N9	6.94	113.75	108.20
36	1	2356	A	C5-N7-C8	-6.94	100.43	103.90
36	5	1450	G	C5-C6-O6	-6.94	124.44	128.60
36	5	1184	A	N1-C6-N6	-6.93	114.44	118.60
36	5	3186	A	N1-C6-N6	-6.93	114.44	118.60
36	1	1902	G	C5-N7-C8	-6.93	100.83	104.30
36	1	2827	U	C5-C6-N1	-6.93	119.23	122.70
36	1	972	A	N7-C8-N9	-6.93	110.33	113.80
36	5	987	U	O5'-P-OP1	-6.93	99.46	105.70
36	1	2827	U	N3-C4-O4	-6.93	114.55	119.40
36	1	1643	A	C8-N9-C4	6.92	108.57	105.80
36	1	286	U	N1-C2-N3	6.92	119.05	114.90
36	1	1904	C	C6-N1-C2	-6.92	117.53	120.30
36	5	530	G	N9-C4-C5	6.92	108.17	105.40
36	5	1149	G	N1-C6-O6	6.92	124.05	119.90
36	1	689	U	N1-C2-O2	6.92	127.64	122.80
36	1	2283	G	C6-C5-N7	-6.92	126.25	130.40
36	5	3245	A	C5-C6-N6	-6.92	118.17	123.70
36	1	802	C	C6-N1-C2	-6.91	117.53	120.30
36	1	2639	G	N9-C4-C5	-6.91	102.64	105.40
36	5	109	A	O5'-P-OP2	-6.91	99.48	105.70
36	5	2601	A	N1-C6-N6	-6.91	114.45	118.60
36	5	2830	G	N1-C2-N3	6.91	128.05	123.90
36	1	3201	C	N3-C4-C5	-6.91	119.14	121.90
38	4	24	G	C5-C6-O6	-6.91	124.46	128.60
1	6	981	U	N1-C2-N3	6.91	119.04	114.90
36	1	919	U	N3-C4-C5	6.90	118.74	114.60
36	1	1849	C	N3-C2-O2	6.90	126.73	121.90
36	5	3115	C	N1-C2-O2	-6.90	114.76	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	15	U	C6-N1-C2	-6.90	116.86	121.00
36	1	2114	C	O5'-P-OP2	-6.90	99.49	105.70
37	7	68	C	N1-C2-O2	6.90	123.04	118.90
36	1	85	A	C2-N3-C4	-6.90	107.15	110.60
36	1	890	C	C6-N1-C2	-6.90	117.54	120.30
36	1	1520	G	N7-C8-N9	-6.90	109.65	113.10
1	2	581	U	C5-C6-N1	6.89	126.15	122.70
36	1	2944	U	N1-C2-O2	6.89	127.63	122.80
1	6	158	U	P-O3'-C3'	6.89	127.97	119.70
37	7	101	G	C4-C5-N7	6.89	113.56	110.80
36	1	2144	A	C5-C6-N1	6.89	121.15	117.70
36	5	682	U	C2-N1-C1'	-6.89	109.43	117.70
1	2	1431	C	C6-N1-C2	6.89	123.06	120.30
36	5	640	U	N3-C2-O2	6.89	127.02	122.20
36	5	962	A	C4-C5-N7	6.89	114.14	110.70
36	5	2881	C	N3-C2-O2	6.89	126.72	121.90
44	17	232	ARG	NE-CZ-NH1	-6.89	116.86	120.30
36	1	1495	U	C6-N1-C1'	6.89	130.84	121.20
36	1	2314	U	C5-C4-O4	-6.89	121.77	125.90
1	2	42	G	N1-C6-O6	-6.88	115.77	119.90
36	1	3144	G	O5'-P-OP1	-6.88	99.50	105.70
37	3	45	A	O5'-P-OP2	-6.88	99.50	105.70
1	6	383	G	C8-N9-C4	-6.88	103.65	106.40
36	5	614	C	N3-C4-C5	6.88	124.65	121.90
36	5	1305	U	N3-C4-O4	6.88	124.22	119.40
36	5	640	U	N3-C4-O4	6.88	124.21	119.40
36	5	2897	A	C6-N1-C2	-6.88	114.47	118.60
36	1	672	A	C8-N9-C4	6.88	108.55	105.80
36	5	857	G	N1-C6-O6	6.88	124.03	119.90
36	5	2377	G	C5-C6-O6	6.88	132.72	128.60
36	1	366	A	O5'-P-OP2	-6.87	99.51	105.70
36	5	96	G	N1-C6-O6	6.87	124.02	119.90
36	1	2249	G	N3-C4-C5	-6.87	125.16	128.60
36	5	1115	G	N7-C8-N9	6.87	116.54	113.10
36	1	49	A	N1-C6-N6	6.87	122.72	118.60
38	4	111	A	N9-C4-C5	-6.87	103.05	105.80
38	4	95	G	C4-N9-C1'	-6.87	117.57	126.50
36	5	1371	G	C2-N3-C4	6.87	115.33	111.90
36	5	1858	A	O4'-C1'-N9	6.87	113.69	108.20
36	1	374	A	N9-C4-C5	6.87	108.55	105.80
36	5	2354	C	N3-C4-N4	6.87	122.81	118.00
36	1	798	G	N3-C2-N2	-6.86	115.09	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2853	A	C8-N9-C4	-6.86	103.06	105.80
36	5	358	G	N1-C6-O6	6.86	124.02	119.90
36	1	609	G	O5'-P-OP2	-6.86	99.52	105.70
36	1	2392	C	C5-C4-N4	-6.86	115.40	120.20
36	5	942	U	N3-C4-O4	6.86	124.20	119.40
36	5	1014	U	C2-N1-C1'	6.86	125.93	117.70
36	1	612	U	C5-C6-N1	-6.85	119.27	122.70
38	4	15	G	N9-C4-C5	-6.85	102.66	105.40
36	1	790	U	N3-C2-O2	-6.85	117.41	122.20
36	1	2550	U	N1-C2-N3	6.85	119.01	114.90
36	1	590	G	N1-C6-O6	6.85	124.01	119.90
36	1	1050	U	N1-C2-O2	6.85	127.59	122.80
36	5	2832	C	N3-C4-N4	-6.85	113.21	118.00
1	2	577	G	C5-N7-C8	-6.84	100.88	104.30
36	1	1392	G	N3-C4-C5	-6.84	125.18	128.60
36	5	2354	C	N3-C2-O2	6.84	126.69	121.90
36	5	3185	U	O5'-P-OP2	-6.84	99.54	105.70
36	5	1134	G	O5'-P-OP2	-6.84	99.54	105.70
1	6	749	U	C6-N1-C2	-6.84	116.89	121.00
36	5	651	G	N3-C4-N9	6.84	130.10	126.00
36	5	1437	C	C2-N1-C1'	6.84	126.33	118.80
36	5	2634	U	N3-C4-O4	6.84	124.19	119.40
38	8	3	A	N1-C2-N3	-6.84	125.88	129.30
36	1	890	C	O5'-P-OP2	-6.84	99.55	105.70
1	6	371	G	C8-N9-C1'	-6.84	118.11	127.00
1	6	392	G	O5'-P-OP2	-6.84	99.55	105.70
36	5	1429	G	N9-C4-C5	-6.84	102.66	105.40
36	5	639	G	N1-C6-O6	6.84	124.00	119.90
36	5	741	U	O5'-P-OP1	-6.84	99.55	105.70
36	1	72	C	C2-N1-C1'	-6.84	111.28	118.80
36	1	2623	G	N1-C2-N2	-6.84	110.05	116.20
36	5	2327	U	C5-C6-N1	-6.84	119.28	122.70
36	5	3049	A	C6-N1-C2	6.84	122.70	118.60
36	1	2729	U	O5'-P-OP1	-6.83	99.55	105.70
36	5	2411	U	N3-C4-C5	6.83	118.70	114.60
36	5	2796	G	N3-C2-N2	6.83	124.68	119.90
36	1	648	C	O5'-P-OP1	-6.83	99.55	105.70
36	1	1661	G	N9-C4-C5	-6.83	102.67	105.40
36	5	2927	C	C6-N1-C2	-6.83	117.57	120.30
1	2	1611	A	N1-C2-N3	6.83	132.72	129.30
36	1	867	G	N3-C2-N2	-6.83	115.12	119.90
1	6	1777	G	C5-C6-O6	-6.83	124.50	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	l3	4	ARG	NE-CZ-NH1	6.83	123.71	120.30
36	5	2945	G	O5'-P-OP1	6.83	118.89	110.70
36	1	820	A	C8-N9-C4	-6.82	103.07	105.80
36	1	3248	C	C6-N1-C2	-6.82	117.57	120.30
1	6	542	A	C8-N9-C4	-6.82	103.07	105.80
36	5	2858	U	C6-N1-C2	-6.82	116.91	121.00
36	5	2813	A	C8-N9-C4	-6.82	103.07	105.80
36	5	227	G	N1-C6-O6	6.82	123.99	119.90
36	5	1897	G	C5-C6-O6	-6.82	124.51	128.60
36	5	2383	C	N1-C2-O2	-6.82	114.81	118.90
38	8	111	A	N1-C6-N6	6.82	122.69	118.60
36	1	979	U	N1-C2-N3	6.81	118.99	114.90
36	5	48	A	C8-N9-C4	-6.81	103.07	105.80
36	5	957	C	C6-N1-C2	-6.81	117.57	120.30
36	5	1335	C	N1-C2-O2	-6.81	114.81	118.90
36	5	2751	G	C4-C5-N7	6.81	113.53	110.80
36	5	1113	G	C5-C6-N1	-6.81	108.09	111.50
1	6	359	A	N1-C2-N3	-6.81	125.90	129.30
36	5	2865	U	C5-C6-N1	6.80	126.10	122.70
36	1	1837	U	N1-C2-O2	-6.80	118.04	122.80
36	1	2699	G	C6-C5-N7	-6.80	126.32	130.40
36	5	1304	A	N1-C6-N6	6.80	122.68	118.60
36	5	1851	G	C6-C5-N7	-6.80	126.32	130.40
36	5	869	G	N1-C6-O6	-6.80	115.82	119.90
36	5	3309	G	C4-N9-C1'	6.80	135.34	126.50
1	6	308	C	N3-C4-N4	-6.80	113.24	118.00
36	5	1886	A	O5'-P-OP2	-6.80	99.58	105.70
36	1	1157	G	C4-C5-N7	-6.79	108.08	110.80
36	5	2727	A	N3-C4-C5	-6.79	122.04	126.80
36	5	2818	U	O5'-P-OP1	-6.79	99.58	105.70
1	2	1773	C	N3-C4-N4	6.79	122.75	118.00
36	1	1157	G	OP2-P-O3'	6.79	120.14	105.20
36	5	3004	C	C6-N1-C2	6.79	123.02	120.30
36	1	226	C	N3-C4-C5	-6.79	119.19	121.90
36	1	2873	U	C5-C4-O4	6.79	129.97	125.90
36	5	43	A	O4'-C1'-N9	6.79	113.63	108.20
36	5	414	U	N3-C4-O4	6.79	124.15	119.40
36	5	3278	C	C2-N1-C1'	-6.79	111.33	118.80
35	SM	167	PRO	N-CA-CB	6.79	111.44	103.30
36	1	2197	C	N1-C2-N3	-6.79	114.45	119.20
36	1	2944	U	N3-C4-C5	6.79	118.67	114.60
36	1	870	G	O5'-P-OP2	-6.78	99.59	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	29	U	C5-C4-O4	6.78	129.97	125.90
36	5	3215	A	N1-C6-N6	6.78	122.67	118.60
36	1	500	C	C4-C5-C6	6.78	120.79	117.40
36	1	1154	A	C8-N9-C4	-6.78	103.09	105.80
36	1	1431	G	C8-N9-C4	6.78	109.11	106.40
36	5	1628	C	C6-N1-C2	-6.78	117.59	120.30
1	6	1640	C	C2-N1-C1'	6.78	126.26	118.80
44	L7	163	LEU	CA-CB-CG	-6.78	99.71	115.30
36	5	710	A	N1-C6-N6	-6.78	114.53	118.60
36	1	3362	A	C6-C5-N7	-6.78	127.56	132.30
1	6	359	A	C4-C5-C6	-6.78	113.61	117.00
36	1	1400	G	O5'-P-OP2	-6.78	99.60	105.70
36	1	2142	A	N1-C6-N6	-6.78	114.53	118.60
36	1	2756	C	C6-N1-C2	-6.78	117.59	120.30
36	5	1302	A	C8-N9-C4	-6.78	103.09	105.80
36	1	1314	C	C6-N1-C2	-6.77	117.59	120.30
36	5	2304	C	O5'-P-OP1	-6.77	99.60	105.70
36	5	1054	A	O5'-P-OP2	-6.77	99.61	105.70
36	5	2873	U	C5-C6-N1	-6.77	119.31	122.70
36	1	1165	A	N7-C8-N9	-6.77	110.42	113.80
36	5	2411	U	C5-C6-N1	-6.77	119.31	122.70
36	5	3343	G	N3-C4-N9	6.77	130.06	126.00
36	1	2846	U	N1-C2-O2	6.77	127.54	122.80
36	1	788	C	C2-N1-C1'	-6.77	111.36	118.80
36	1	2823	G	C8-N9-C4	-6.77	103.69	106.40
36	1	2354	C	N1-C2-O2	-6.76	114.84	118.90
36	5	2404	A	N7-C8-N9	-6.76	110.42	113.80
36	5	2820	A	O5'-P-OP1	6.76	118.81	110.70
36	5	3040	A	C8-N9-C4	6.76	108.50	105.80
36	1	422	A	N9-C4-C5	6.76	108.50	105.80
37	7	104	A	N1-C6-N6	6.76	122.66	118.60
36	1	960	U	N3-C4-C5	6.76	118.65	114.60
1	6	352	A	N1-C6-N6	-6.76	114.55	118.60
36	1	347	G	C4-C5-N7	6.75	113.50	110.80
1	2	577	G	C4-C5-N7	6.75	113.50	110.80
36	1	1481	A	N1-C6-N6	6.75	122.65	118.60
36	5	2351	U	N1-C2-N3	6.75	118.95	114.90
36	5	3217	C	C2-N1-C1'	-6.75	111.37	118.80
36	5	2817	A	C2-N3-C4	6.75	113.97	110.60
1	2	647	G	N3-C4-N9	-6.74	121.95	126.00
36	5	189	G	N1-C6-O6	-6.74	115.85	119.90
36	5	584	G	N9-C4-C5	6.74	108.10	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1175	C	C6-N1-C2	6.74	123.00	120.30
1	6	815	G	C5-N7-C8	-6.74	100.93	104.30
36	5	1429	G	C5-N7-C8	-6.74	100.93	104.30
37	7	87	G	N1-C6-O6	6.74	123.94	119.90
36	5	676	G	N1-C6-O6	-6.74	115.86	119.90
36	5	1131	G	C8-N9-C4	-6.73	103.71	106.40
1	2	1432	U	C5-C4-O4	-6.73	121.86	125.90
36	1	1445	U	N3-C2-O2	6.73	126.91	122.20
38	4	40	A	C5-C6-N6	-6.73	118.31	123.70
70	O4	51	LEU	CA-CB-CG	6.73	130.78	115.30
36	5	1868	G	N9-C4-C5	-6.73	102.71	105.40
36	1	2279	A	N9-C4-C5	-6.73	103.11	105.80
1	2	321	C	N3-C2-O2	-6.73	117.19	121.90
1	2	1596	C	C6-N1-C2	-6.73	117.61	120.30
36	5	218	G	C5-N7-C8	6.73	107.66	104.30
36	5	3306	U	O5'-P-OP2	-6.73	99.65	105.70
1	2	779	U	O4'-C1'-N1	6.72	113.58	108.20
36	1	2372	A	N3-C4-C5	-6.72	122.09	126.80
36	5	1495	U	N3-C4-C5	-6.72	110.57	114.60
36	1	905	U	N1-C2-O2	-6.72	118.09	122.80
38	4	30	C	O5'-P-OP1	-6.72	99.65	105.70
36	1	1520	G	C4-C5-N7	-6.72	108.11	110.80
36	1	2422	C	N1-C2-O2	6.72	122.93	118.90
36	1	3183	A	C5-C6-N6	-6.72	118.33	123.70
1	6	1782	A	C8-N9-C4	-6.72	103.11	105.80
36	5	1301	A	C4-C5-N7	6.72	114.06	110.70
36	1	908	G	C8-N9-C1'	-6.72	118.27	127.00
36	1	3110	C	C6-N1-C2	-6.72	117.61	120.30
36	5	1879	A	C6-C5-N7	-6.72	127.60	132.30
1	2	1033	C	N1-C2-O2	6.71	122.93	118.90
36	1	3182	G	N3-C4-N9	-6.71	121.97	126.00
36	5	2849	C	N3-C4-N4	6.71	122.70	118.00
36	5	1856	C	C6-N1-C2	-6.71	117.61	120.30
36	5	2365	C	C6-N1-C2	6.71	122.98	120.30
36	5	3377	G	N1-C6-O6	6.71	123.93	119.90
36	5	960	U	C5-C6-N1	-6.71	119.34	122.70
36	5	2636	A	N1-C6-N6	-6.71	114.57	118.60
36	1	3305	A	N1-C6-N6	-6.71	114.57	118.60
36	1	2293	C	N3-C4-N4	6.71	122.69	118.00
36	5	3285	C	C2-N1-C1'	6.71	126.18	118.80
37	7	103	A	N1-C6-N6	6.71	122.62	118.60
36	5	3218	A	N9-C4-C5	-6.71	103.12	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2664	C	C6-N1-C2	-6.70	117.62	120.30
18	C6	40	GLU	C-N-CD	-6.70	105.86	120.60
36	1	67	A	N1-C6-N6	6.70	122.62	118.60
36	1	2372	A	C5-C6-N6	-6.70	118.34	123.70
36	1	2889	C	N3-C2-O2	-6.70	117.21	121.90
36	5	360	G	C5-C6-N1	-6.70	108.15	111.50
36	5	640	U	C5-C4-O4	-6.70	121.88	125.90
36	5	2728	G	N9-C4-C5	6.70	108.08	105.40
36	1	2699	G	C4-C5-N7	6.69	113.48	110.80
1	6	272	U	P-O3'-C3'	6.69	127.73	119.70
1	2	1302	U	N1-C2-O2	-6.69	118.12	122.80
36	5	966	U	C6-N1-C2	-6.69	116.98	121.00
36	5	2792	A	C8-N9-C4	-6.69	103.12	105.80
36	5	1390	A	N1-C6-N6	-6.69	114.59	118.60
36	1	2889	C	C6-N1-C2	-6.69	117.62	120.30
1	6	1764	C	N3-C4-C5	6.69	124.58	121.90
36	1	1425	U	N3-C2-O2	-6.69	117.52	122.20
36	5	1329	U	OP1-P-O3'	6.69	119.91	105.20
36	1	797	U	OP2-P-O3'	6.69	119.91	105.20
36	1	820	A	N7-C8-N9	6.69	117.14	113.80
1	6	339	C	N1-C2-O2	-6.69	114.89	118.90
36	5	933	A	N1-C2-N3	6.69	132.64	129.30
36	1	2130	G	N1-C6-O6	-6.68	115.89	119.90
36	1	1180	A	C4-C5-N7	-6.68	107.36	110.70
36	5	592	A	C8-N9-C4	6.68	108.47	105.80
36	5	2377	G	N1-C6-O6	-6.68	115.89	119.90
36	5	3212	C	N1-C2-O2	-6.68	114.89	118.90
36	5	1205	A	O5'-P-OP2	-6.68	99.69	105.70
36	1	2376	G	C8-N9-C4	-6.68	103.73	106.40
1	6	44	U	N1-C2-O2	-6.68	118.13	122.80
1	6	371	G	C6-C5-N7	-6.68	126.39	130.40
36	5	2851	A	N1-C2-N3	6.68	132.64	129.30
73	o7	11	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	2	1600	A	C5-C6-N1	-6.67	114.36	117.70
36	5	2954	U	N1-C2-O2	6.67	127.47	122.80
36	1	894	G	N1-C6-O6	6.67	123.90	119.90
36	1	314	U	N1-C2-O2	6.67	127.47	122.80
36	1	608	A	C6-C5-N7	-6.67	127.63	132.30
36	5	1375	G	C2-N3-C4	6.66	115.23	111.90
36	5	2255	A	O5'-P-OP1	-6.66	99.70	105.70
36	1	2418	G	C2-N3-C4	6.66	115.23	111.90
36	5	2828	G	C4-C5-N7	6.66	113.46	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	969	C	N1-C2-O2	-6.66	114.90	118.90
36	5	63	A	C4-C5-C6	6.66	120.33	117.00
36	5	1454	A	O5'-P-OP2	-6.66	99.71	105.70
36	1	1365	G	N3-C4-N9	6.66	129.99	126.00
36	1	2121	G	N1-C6-O6	-6.65	115.91	119.90
36	1	2373	A	C8-N9-C4	-6.65	103.14	105.80
36	1	2993	G	N9-C4-C5	-6.65	102.74	105.40
1	6	1781	A	C8-N9-C4	-6.65	103.14	105.80
36	5	3335	A	N1-C6-N6	6.65	122.59	118.60
36	1	3361	G	N3-C4-N9	6.65	129.99	126.00
36	1	1124	U	C4-C5-C6	-6.65	115.71	119.70
36	5	691	A	O5'-P-OP1	-6.65	99.72	105.70
36	5	2772	C	P-O3'-C3'	6.65	127.68	119.70
1	2	1324	G	N3-C2-N2	-6.64	115.25	119.90
1	2	1339	C	C5-C6-N1	6.64	124.32	121.00
36	1	2142	A	C6-N1-C2	-6.64	114.61	118.60
36	5	1192	C	N3-C4-C5	6.64	124.56	121.90
36	5	3050	U	N3-C2-O2	-6.64	117.55	122.20
1	6	1773	C	N1-C2-O2	-6.64	114.92	118.90
38	8	43	A	C8-N9-C4	-6.64	103.14	105.80
36	1	2647	A	C8-N9-C4	-6.64	103.14	105.80
36	5	927	C	O5'-P-OP1	-6.64	99.72	105.70
36	5	2365	C	C5-C6-N1	-6.64	117.68	121.00
36	5	1180	A	N9-C4-C5	6.64	108.45	105.80
36	5	2630	C	N1-C2-O2	-6.64	114.92	118.90
36	1	229	G	N1-C6-O6	6.63	123.88	119.90
36	5	1308	A	OP1-P-OP2	-6.63	109.65	119.60
36	1	999	G	C5-C6-N1	6.63	114.82	111.50
36	1	1332	A	N7-C8-N9	6.63	117.12	113.80
36	5	826	G	N3-C4-N9	-6.63	122.02	126.00
1	2	593	U	O5'-P-OP1	-6.63	99.73	105.70
36	1	1339	C	N1-C2-O2	-6.63	114.92	118.90
1	2	507	U	N1-C2-O2	6.63	127.44	122.80
36	1	2389	C	O5'-P-OP1	-6.63	99.74	105.70
53	M7	131	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	2	507	U	N3-C2-O2	-6.62	117.56	122.20
37	7	92	A	N1-C6-N6	6.62	122.57	118.60
36	1	1196	C	C6-N1-C2	6.62	122.95	120.30
36	1	2850	G	C5-C6-O6	-6.62	124.63	128.60
36	1	1300	G	N1-C6-O6	6.62	123.87	119.90
1	2	1198	G	C8-N9-C4	-6.61	103.75	106.40
36	5	3123	A	C8-N9-C4	6.61	108.45	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	971	G	N1-C6-O6	6.61	123.87	119.90
36	1	2419	A	OP1-P-OP2	-6.61	109.69	119.60
36	5	2364	G	N1-C6-O6	-6.61	115.94	119.90
36	1	2373	A	N9-C4-C5	6.61	108.44	105.80
36	1	2968	G	N1-C2-N3	6.61	127.86	123.90
36	5	2700	G	C4-C5-N7	6.61	113.44	110.80
36	5	3212	C	C6-N1-C2	6.61	122.94	120.30
36	1	2700	G	C4-C5-N7	6.61	113.44	110.80
36	5	3339	A	N1-C6-N6	6.61	122.56	118.60
1	6	1747	G	C8-N9-C4	6.60	109.04	106.40
36	1	1403	C	C6-N1-C2	6.60	122.94	120.30
36	1	2371	G	N1-C6-O6	6.60	123.86	119.90
36	5	1152	G	C5-C6-N1	-6.60	108.20	111.50
36	1	1156	C	N3-C2-O2	-6.60	117.28	121.90
38	4	25	G	N1-C6-O6	-6.60	115.94	119.90
36	5	824	C	C6-N1-C2	-6.60	117.66	120.30
36	5	2338	C	N3-C4-N4	6.60	122.62	118.00
36	5	2890	A	C5-C6-N1	-6.60	114.40	117.70
36	1	934	G	C4-N9-C1'	6.60	135.07	126.50
36	1	2839	G	O5'-P-OP2	-6.59	99.76	105.70
52	m6	68	ARG	NE-CZ-NH1	-6.59	117.00	120.30
52	M6	78	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	2	287	G	O4'-C1'-N9	6.59	113.47	108.20
36	5	804	C	N3-C4-C5	-6.59	119.26	121.90
36	5	1370	G	N3-C4-N9	6.59	129.95	126.00
36	1	1507	G	C5-C6-O6	-6.59	124.65	128.60
36	1	2233	A	N1-C6-N6	-6.59	114.65	118.60
36	5	413	U	N3-C4-O4	6.59	124.01	119.40
36	5	3005	A	O5'-P-OP2	-6.59	99.77	105.70
36	5	2643	A	N1-C2-N3	-6.58	126.01	129.30
36	1	808	A	N9-C4-C5	6.58	108.43	105.80
1	6	1700	C	C6-N1-C1'	-6.58	112.90	120.80
36	5	3209	A	N7-C8-N9	6.58	117.09	113.80
36	5	740	G	N1-C6-O6	-6.58	115.95	119.90
1	2	694	U	N1-C2-O2	6.58	127.41	122.80
36	1	76	G	N9-C4-C5	6.58	108.03	105.40
36	1	994	G	N3-C4-C5	-6.58	125.31	128.60
1	6	639	U	C2-N1-C1'	6.58	125.59	117.70
1	6	1537	C	N3-C4-C5	-6.58	119.27	121.90
36	5	2892	A	C6-C5-N7	-6.58	127.70	132.30
36	5	2981	U	N1-C2-O2	6.58	127.40	122.80
37	7	37	G	N3-C4-N9	6.58	129.95	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1014	U	C6-N1-C1'	-6.57	112.00	121.20
36	5	384	A	C8-N9-C4	6.57	108.43	105.80
36	1	49	A	C8-N9-C4	6.57	108.43	105.80
36	1	1173	U	C5-C6-N1	-6.57	119.42	122.70
36	5	417	A	O5'-P-OP2	-6.57	99.79	105.70
36	5	2978	U	N3-C2-O2	-6.57	117.60	122.20
36	5	3204	C	O5'-P-OP2	-6.57	99.79	105.70
36	1	661	G	N9-C4-C5	6.57	108.03	105.40
36	5	83	U	C2-N1-C1'	6.57	125.58	117.70
36	5	1496	C	C6-N1-C1'	-6.57	112.92	120.80
36	5	3142	A	N1-C6-N6	6.56	122.54	118.60
36	1	343	U	OP2-P-O3'	6.56	119.64	105.20
36	1	374	A	C5-C6-N6	6.56	128.95	123.70
36	1	716	A	N3-C4-C5	6.56	131.39	126.80
45	L8	189	LEU	CA-CB-CG	6.56	130.39	115.30
36	5	578	A	O5'-P-OP2	6.56	118.58	110.70
36	1	388	G	N3-C2-N2	-6.56	115.31	119.90
36	1	959	C	C6-N1-C2	6.56	122.92	120.30
36	5	2971	A	N3-C4-N9	6.56	132.65	127.40
36	1	790	U	C6-N1-C2	-6.56	117.06	121.00
36	1	939	U	O5'-P-OP1	6.56	118.57	110.70
36	1	3344	A	N7-C8-N9	6.56	117.08	113.80
36	5	2843	U	N3-C2-O2	-6.56	117.61	122.20
1	6	1641	C	N3-C2-O2	6.56	126.49	121.90
36	5	639	G	C5-C6-N1	-6.56	108.22	111.50
36	5	2142	A	N1-C6-N6	-6.56	114.67	118.60
36	5	2338	C	N3-C4-C5	-6.56	119.28	121.90
36	1	3217	C	N3-C2-O2	-6.55	117.31	121.90
1	6	1514	U	N3-C4-O4	-6.55	114.81	119.40
1	2	399	A	N1-C6-N6	-6.55	114.67	118.60
36	1	1307	G	P-O3'-C3'	6.55	127.56	119.70
36	1	2403	G	O5'-P-OP2	-6.55	99.80	105.70
36	5	2928	C	N3-C4-N4	6.55	122.59	118.00
36	1	2861	U	N3-C4-O4	-6.55	114.81	119.40
36	5	984	G	C6-C5-N7	-6.55	126.47	130.40
37	7	102	A	C2-N3-C4	-6.55	107.33	110.60
36	1	421	G	C5-C6-O6	-6.55	124.67	128.60
36	5	1149	G	C5-C6-O6	-6.55	124.67	128.60
36	5	2407	C	O5'-P-OP2	-6.55	99.81	105.70
36	1	2304	C	C6-N1-C2	-6.55	117.68	120.30
36	1	670	C	C4-C5-C6	6.54	120.67	117.40
1	6	1773	C	N3-C4-N4	6.54	122.58	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	131	C	C6-N1-C2	-6.54	117.68	120.30
36	1	2986	U	N1-C2-O2	-6.54	118.22	122.80
36	5	831	G	C2-N3-C4	6.54	115.17	111.90
36	1	2093	A	C2-N3-C4	6.54	113.87	110.60
36	1	2901	G	N1-C6-O6	6.54	123.82	119.90
36	1	3101	G	C8-N9-C4	6.54	109.02	106.40
38	4	25	G	C4-C5-N7	-6.54	108.18	110.80
36	5	1878	G	C4-N9-C1'	6.54	135.00	126.50
36	5	862	U	O5'-P-OP1	-6.54	99.82	105.70
36	1	24	G	C2-N3-C4	-6.54	108.63	111.90
36	1	922	U	N3-C2-O2	-6.54	117.62	122.20
56	N0	115	ARG	NE-CZ-NH2	-6.53	117.03	120.30
25	d3	16	ARG	NE-CZ-NH2	-6.53	117.03	120.30
48	m1	12	LEU	CA-CB-CG	6.53	130.33	115.30
36	1	793	C	OP2-P-O3'	6.53	119.57	105.20
36	5	944	C	OP2-P-O3'	6.53	119.57	105.20
36	1	963	G	O5'-P-OP1	6.53	118.54	110.70
36	5	395	A	N1-C6-N6	6.53	122.52	118.60
36	5	885	U	O5'-P-OP2	-6.53	99.82	105.70
1	2	1280	C	N3-C4-N4	6.53	122.57	118.00
11	s9	3	ARG	NE-CZ-NH2	6.53	123.56	120.30
36	5	1607	U	C5-C6-N1	-6.53	119.44	122.70
36	5	2323	G	O5'-P-OP1	6.53	118.53	110.70
36	1	2632	G	N1-C6-O6	-6.53	115.98	119.90
36	5	2361	A	OP2-P-O3'	6.53	119.56	105.20
1	2	408	C	O5'-P-OP2	-6.52	99.83	105.70
36	1	646	A	C8-N9-C4	-6.52	103.19	105.80
36	1	743	C	C6-N1-C2	6.52	122.91	120.30
38	4	15	G	C8-N9-C4	6.52	109.01	106.40
36	5	217	U	OP1-P-O3'	6.52	119.55	105.20
36	5	1239	C	C6-N1-C2	-6.52	117.69	120.30
1	2	555	A	P-O3'-C3'	6.52	127.53	119.70
36	1	2245	C	C6-N1-C2	-6.52	117.69	120.30
36	5	3112	G	O5'-P-OP2	-6.52	99.83	105.70
36	5	2625	C	C6-N1-C2	6.52	122.91	120.30
36	1	611	A	O5'-P-OP2	-6.52	99.83	105.70
36	1	962	A	C6-N1-C2	-6.52	114.69	118.60
36	1	2860	U	O5'-P-OP2	-6.52	99.83	105.70
36	1	282	G	N1-C6-O6	-6.52	115.99	119.90
47	M0	57	LEU	CA-CB-CG	6.52	130.29	115.30
36	5	3088	G	N1-C6-O6	6.52	123.81	119.90
1	6	858	G	O4'-C1'-N9	6.51	113.41	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2148	U	N3-C2-O2	6.51	126.76	122.20
36	5	3107	U	C2-N3-C4	-6.51	123.09	127.00
1	2	864	U	N3-C2-O2	-6.51	117.64	122.20
36	1	410	U	C5-C6-N1	6.51	125.96	122.70
36	1	363	G	O5'-P-OP1	-6.51	99.84	105.70
36	5	681	U	OP2-P-O3'	6.51	119.52	105.20
36	5	2637	A	C5-C6-N6	-6.51	118.49	123.70
36	1	695	C	C5-C6-N1	-6.50	117.75	121.00
1	6	337	G	N3-C4-N9	6.50	129.90	126.00
36	5	3154	C	C6-N1-C2	-6.50	117.70	120.30
1	6	1537	C	C6-N1-C1'	6.50	128.60	120.80
36	1	2811	A	N1-C6-N6	-6.50	114.70	118.60
1	2	312	A	C8-N9-C4	-6.50	103.20	105.80
36	1	3362	A	C2-N3-C4	-6.50	107.35	110.60
36	5	2407	C	N3-C4-N4	6.50	122.55	118.00
36	1	124	U	N3-C4-O4	-6.50	114.85	119.40
36	5	915	A	N3-C4-C5	-6.50	122.25	126.80
36	5	2630	C	C2-N3-C4	-6.50	116.65	119.90
36	5	2874	G	C4-C5-N7	-6.50	108.20	110.80
36	5	1316	C	N3-C4-N4	6.49	122.55	118.00
36	5	1370	G	N3-C4-C5	-6.49	125.35	128.60
36	5	1445	U	C5-C4-O4	-6.49	122.00	125.90
36	5	2726	C	N3-C4-C5	-6.49	119.30	121.90
36	5	3382	U	N1-C2-O2	6.49	127.35	122.80
1	6	987	G	C5-C6-O6	-6.49	124.71	128.60
1	2	1324	G	N9-C4-C5	6.49	108.00	105.40
38	4	44	A	N1-C6-N6	6.49	122.49	118.60
36	1	2857	C	N3-C4-C5	6.49	124.50	121.90
1	2	1196	A	P-O3'-C3'	6.49	127.48	119.70
36	5	2407	C	N1-C2-O2	-6.49	115.01	118.90
36	1	2550	U	C6-N1-C2	-6.48	117.11	121.00
36	5	1879	A	C4-C5-N7	6.48	113.94	110.70
36	5	927	C	N3-C4-N4	6.48	122.54	118.00
36	5	2733	A	O5'-P-OP2	-6.48	99.87	105.70
38	8	18	U	O5'-P-OP2	-6.48	99.87	105.70
36	1	984	G	N3-C4-C5	-6.48	125.36	128.60
36	1	1332	A	C8-N9-C4	-6.48	103.21	105.80
36	5	40	A	N1-C6-N6	6.48	122.49	118.60
37	7	108	A	N1-C6-N6	6.48	122.48	118.60
36	1	417	A	N1-C6-N6	6.47	122.48	118.60
36	1	609	G	C5-C6-O6	-6.47	124.72	128.60
36	1	3344	A	O4'-C1'-N9	6.47	113.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3099	C	C5-C6-N1	-6.47	117.76	121.00
36	1	47	C	N3-C4-C5	-6.47	119.31	121.90
36	5	699	A	C2-N3-C4	-6.47	107.36	110.60
36	5	2867	C	C2-N3-C4	6.47	123.13	119.90
36	1	2174	G	N1-C6-O6	6.47	123.78	119.90
36	5	2162	U	O5'-P-OP2	-6.47	99.88	105.70
37	7	47	C	N1-C2-O2	-6.47	115.02	118.90
36	1	2171	G	C2-N3-C4	6.46	115.13	111.90
36	5	3107	U	N3-C4-C5	6.46	118.48	114.60
36	1	1144	U	N3-C4-O4	-6.46	114.88	119.40
36	5	2625	C	N3-C4-C5	6.46	124.48	121.90
36	5	3026	G	N1-C6-O6	6.46	123.78	119.90
36	1	2305	G	N1-C6-O6	6.46	123.78	119.90
36	5	519	A	N1-C6-N6	6.46	122.48	118.60
36	5	1161	G	C5-C6-N1	6.46	114.73	111.50
36	5	1615	C	O5'-P-OP1	-6.46	99.89	105.70
36	5	2392	C	C2-N3-C4	-6.46	116.67	119.90
36	5	2696	A	C6-N1-C2	6.46	122.47	118.60
36	5	2856	G	C6-C5-N7	-6.46	126.53	130.40
36	1	1128	U	N3-C4-O4	-6.46	114.88	119.40
36	5	1146	C	N3-C4-N4	6.46	122.52	118.00
36	1	661	G	C5-C6-O6	6.45	132.47	128.60
36	1	2554	A	C8-N9-C4	6.45	108.38	105.80
36	1	2865	U	N3-C4-C5	6.45	118.47	114.60
36	5	586	C	N3-C4-C5	6.45	124.48	121.90
36	5	1146	C	N3-C4-C5	-6.45	119.32	121.90
36	1	2395	G	C5-C6-O6	-6.45	124.73	128.60
36	5	2748	A	N1-C2-N3	-6.45	126.08	129.30
36	1	2618	G	C5-C6-N1	6.45	114.72	111.50
36	5	1310	G	N1-C6-O6	-6.45	116.03	119.90
36	1	1425	U	N1-C2-N3	6.45	118.77	114.90
36	1	1509	A	C2-N3-C4	-6.45	107.38	110.60
40	13	232	ARG	NE-CZ-NH2	-6.44	117.08	120.30
36	1	2298	U	O5'-P-OP2	-6.44	99.90	105.70
36	5	2133	U	OP2-P-O3'	6.44	119.37	105.20
36	1	3270	U	N3-C4-O4	-6.44	114.89	119.40
36	1	2886	U	C5-C4-O4	-6.44	122.04	125.90
1	6	1535	U	N3-C2-O2	-6.44	117.69	122.20
36	1	2314	U	C6-N1-C2	6.44	124.86	121.00
1	6	1082	C	N3-C4-C5	-6.44	119.33	121.90
36	5	2726	C	C4-C5-C6	6.44	120.62	117.40
36	5	913	A	N1-C2-N3	-6.44	126.08	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1161	G	N9-C4-C5	-6.44	102.83	105.40
36	5	1817	G	O4'-C1'-N9	6.44	113.35	108.20
1	2	136	C	C6-N1-C2	-6.43	117.73	120.30
36	5	33	G	N9-C4-C5	6.43	107.97	105.40
36	5	2362	C	O5'-P-OP2	-6.43	99.91	105.70
40	13	102	LEU	CA-CB-CG	6.43	130.10	115.30
1	2	393	C	C6-N1-C2	6.43	122.87	120.30
36	1	86	G	N9-C4-C5	6.43	107.97	105.40
36	1	1445	U	C5-C4-O4	-6.43	122.04	125.90
36	5	48	A	N9-C4-C5	6.43	108.37	105.80
36	5	1118	C	O5'-P-OP1	-6.43	99.91	105.70
36	5	1203	A	C4-C5-N7	6.43	113.92	110.70
36	5	1473	G	N7-C8-N9	-6.43	109.88	113.10
36	5	2856	G	C5-N7-C8	-6.43	101.08	104.30
36	5	2954	U	N3-C2-O2	-6.43	117.70	122.20
1	2	728	U	C2-N1-C1'	6.43	125.42	117.70
36	1	697	A	C8-N9-C4	6.43	108.37	105.80
1	6	999	U	N3-C4-O4	-6.43	114.90	119.40
1	6	1514	U	C5-C4-O4	6.43	129.76	125.90
36	5	3105	U	C2-N1-C1'	-6.43	109.99	117.70
1	2	1749	A	C2-N3-C4	-6.43	107.39	110.60
36	1	2631	U	N3-C4-C5	6.43	118.45	114.60
36	1	1001	G	C6-C5-N7	-6.42	126.55	130.40
36	1	2946	A	N9-C4-C5	-6.42	103.23	105.80
38	4	32	C	N3-C4-C5	6.42	124.47	121.90
51	m5	164	LEU	CA-CB-CG	-6.42	100.52	115.30
36	5	2358	A	C8-N9-C4	6.42	108.37	105.80
36	1	3133	C	C6-N1-C2	-6.42	117.73	120.30
36	5	1173	U	O5'-P-OP2	-6.42	99.92	105.70
31	D9	36	LEU	CA-CB-CG	6.42	130.06	115.30
36	1	1389	G	C6-C5-N7	-6.42	126.55	130.40
36	5	2639	G	N7-C8-N9	6.42	116.31	113.10
36	5	784	A	C5-C6-N6	-6.42	118.57	123.70
36	5	1495	U	C5-C6-N1	6.42	125.91	122.70
36	1	2658	G	C8-N9-C4	6.41	108.97	106.40
1	6	1634	C	C6-N1-C1'	-6.41	113.11	120.80
1	6	1700	C	N3-C2-O2	-6.41	117.41	121.90
36	5	2761	G	C5-C6-O6	-6.41	124.75	128.60
36	1	2723	U	N1-C2-O2	-6.41	118.31	122.80
1	6	17	C	C6-N1-C2	-6.41	117.74	120.30
36	5	514	G	N1-C6-O6	6.41	123.74	119.90
36	1	3205	G	C2-N3-C4	-6.40	108.70	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1000	C	C4-C5-C6	6.40	120.60	117.40
36	1	898	U	N1-C2-O2	6.40	127.28	122.80
36	5	2376	G	C5-C6-O6	-6.40	124.76	128.60
36	5	2887	A	C5-C6-N6	-6.40	118.58	123.70
1	2	507	U	C2-N1-C1'	6.40	125.38	117.70
36	1	864	G	O5'-P-OP1	-6.40	99.94	105.70
36	1	1437	C	C6-N1-C2	-6.40	117.74	120.30
36	1	2916	U	N1-C2-N3	-6.40	111.06	114.90
36	5	3050	U	C6-N1-C2	-6.40	117.16	121.00
36	1	1891	A	C8-N9-C4	6.40	108.36	105.80
38	4	56	G	C8-N9-C4	6.39	108.96	106.40
36	5	1116	G	N9-C4-C5	6.39	107.96	105.40
36	1	285	A	C5-C6-N6	-6.39	118.59	123.70
36	5	2751	G	C5-N7-C8	-6.39	101.10	104.30
36	5	1504	A	C2-N3-C4	-6.39	107.40	110.60
36	5	2980	U	O5'-P-OP1	6.39	118.37	110.70
36	5	2615	G	N9-C4-C5	-6.39	102.84	105.40
36	5	3154	C	C5-C6-N1	6.39	124.19	121.00
36	5	3200	G	N1-C6-O6	6.39	123.73	119.90
38	8	37	A	O5'-P-OP2	-6.39	99.95	105.70
36	1	2870	C	N3-C4-C5	6.39	124.45	121.90
36	1	3057	U	N3-C2-O2	-6.39	117.73	122.20
36	1	228	U	N3-C2-O2	-6.38	117.73	122.20
36	1	2714	G	C4-C5-C6	-6.38	114.97	118.80
36	1	2814	G	C5-C6-O6	-6.38	124.77	128.60
36	5	2943	G	C5-N7-C8	-6.38	101.11	104.30
37	7	84	A	C2-N3-C4	6.38	113.79	110.60
36	5	340	C	C5-C6-N1	-6.38	117.81	121.00
36	1	911	C	C2-N3-C4	-6.38	116.71	119.90
36	1	2298	U	O4'-C1'-N1	6.38	113.31	108.20
36	1	2372	A	O5'-P-OP2	-6.38	99.96	105.70
36	5	1060	U	C5-C4-O4	6.38	129.73	125.90
36	1	1741	A	C6-C5-N7	-6.38	127.83	132.30
36	1	2209	U	C5-C6-N1	6.38	125.89	122.70
36	1	2294	U	C6-N1-C2	-6.38	117.17	121.00
36	1	2403	G	OP1-P-O3'	6.38	119.23	105.20
36	5	1931	U	C5-C6-N1	-6.38	119.51	122.70
36	5	2113	A	C8-N9-C4	6.38	108.35	105.80
1	2	704	C	N1-C2-O2	6.38	122.73	118.90
36	1	1367	G	O5'-P-OP1	-6.38	99.96	105.70
35	sM	167	PRO	N-CA-CB	6.38	110.95	103.30
36	5	1480	G	N3-C4-C5	6.38	131.79	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	776	U	C5-C4-O4	6.38	129.72	125.90
1	2	1200	G	N3-C2-N2	-6.37	115.44	119.90
36	1	365	A	N1-C6-N6	6.37	122.42	118.60
36	1	2303	A	C2-N3-C4	-6.37	107.41	110.60
38	4	38	U	N3-C2-O2	-6.37	117.74	122.20
36	1	915	A	N1-C6-N6	-6.37	114.78	118.60
36	5	2342	U	N3-C4-C5	6.37	118.42	114.60
36	5	1506	A	N9-C4-C5	6.37	108.35	105.80
36	1	369	A	C2-N3-C4	6.37	113.78	110.60
36	1	1177	G	C6-C5-N7	-6.37	126.58	130.40
36	5	796	U	N1-C2-N3	6.37	118.72	114.90
36	1	1177	G	C8-N9-C1'	-6.37	118.72	127.00
36	1	808	A	N1-C6-N6	-6.37	114.78	118.60
36	5	1284	C	C5-C6-N1	6.37	124.18	121.00
36	5	1855	U	N1-C2-N3	6.37	118.72	114.90
36	1	410	U	N1-C2-O2	-6.36	118.34	122.80
36	5	2920	U	N1-C2-O2	-6.36	118.35	122.80
36	1	2693	C	N3-C4-C5	6.36	124.44	121.90
36	1	2714	G	C8-N9-C1'	6.36	135.27	127.00
36	5	2990	G	N1-C6-O6	6.36	123.72	119.90
36	5	2411	U	C6-N1-C2	6.36	124.82	121.00
36	5	3153	U	N1-C2-O2	6.36	127.25	122.80
38	8	14	C	O5'-P-OP2	-6.36	99.98	105.70
36	1	2625	C	N1-C2-O2	-6.36	115.09	118.90
36	5	651	G	C8-N9-C1'	-6.36	118.74	127.00
36	5	1480	G	O4'-C1'-N9	6.36	113.28	108.20
36	1	963	G	O5'-P-OP2	-6.35	99.98	105.70
36	1	41	G	OP2-P-O3'	6.35	119.17	105.20
36	1	421	G	N3-C4-N9	6.35	129.81	126.00
36	5	1151	U	N3-C4-O4	6.35	123.85	119.40
36	1	1365	G	N1-C2-N2	-6.35	110.49	116.20
36	1	1506	A	N9-C4-C5	6.35	108.34	105.80
36	1	1515	A	C6-C5-N7	-6.35	127.86	132.30
1	6	90	C	N3-C2-O2	-6.34	117.46	121.90
12	c0	83	PRO	N-CA-CB	6.34	110.91	103.30
36	5	437	G	C6-C5-N7	-6.34	126.59	130.40
36	5	1495	U	C6-N1-C2	-6.34	117.19	121.00
36	5	1879	A	N1-C6-N6	6.34	122.41	118.60
38	8	8	C	C6-N1-C2	-6.34	117.76	120.30
1	2	158	U	P-O3'-C3'	6.34	127.31	119.70
36	1	1837	U	N3-C2-O2	6.34	126.64	122.20
36	5	3293	U	C6-N1-C2	6.34	124.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1368	U	N1-C2-N3	6.34	118.70	114.90
36	1	2374	C	N1-C2-O2	6.33	122.70	118.90
36	1	61	A	OP2-P-O3'	6.33	119.13	105.20
36	1	312	C	N3-C4-C5	6.33	124.43	121.90
36	1	958	C	C2-N3-C4	-6.33	116.73	119.90
1	6	57	G	O5'-P-OP2	-6.33	100.00	105.70
36	5	1317	A	N9-C4-C5	-6.33	103.27	105.80
36	5	1384	U	C5-C6-N1	6.33	125.87	122.70
36	5	1724	U	P-O3'-C3'	6.33	127.30	119.70
36	5	2939	G	N7-C8-N9	-6.33	109.93	113.10
36	1	32	U	O5'-P-OP1	6.33	118.30	110.70
36	5	1833	G	N1-C6-O6	-6.33	116.10	119.90
36	5	1204	A	C5-C6-N6	6.33	128.76	123.70
36	5	2285	C	C6-N1-C2	-6.33	117.77	120.30
36	1	954	U	C5-C6-N1	6.33	125.86	122.70
36	1	339	C	N1-C2-N3	6.33	123.63	119.20
1	6	1295	G	C5-C6-O6	-6.33	124.80	128.60
36	5	2626	A	O4'-C1'-N9	-6.33	103.14	108.20
36	1	424	G	C8-N9-C4	6.32	108.93	106.40
36	5	942	U	N3-C4-C5	-6.32	110.81	114.60
36	5	1113	G	N3-C4-C5	6.32	131.76	128.60
36	1	970	A	O5'-P-OP1	-6.32	100.01	105.70
36	1	2138	A	C8-N9-C4	-6.32	103.27	105.80
36	5	1500	G	C8-N9-C4	6.32	108.93	106.40
37	7	79	A	N1-C6-N6	6.32	122.39	118.60
36	1	54	C	N3-C4-N4	-6.32	113.58	118.00
36	1	324	A	C6-N1-C2	-6.32	114.81	118.60
36	1	1849	C	N1-C2-O2	-6.32	115.11	118.90
38	4	74	U	O5'-P-OP1	-6.32	100.01	105.70
36	1	1661	G	C5-C6-O6	-6.32	124.81	128.60
1	2	543	C	N3-C2-O2	-6.32	117.48	121.90
36	1	218	G	C5-C6-O6	-6.32	124.81	128.60
36	1	1545	A	N7-C8-N9	6.32	116.96	113.80
36	5	776	U	C2-N3-C4	-6.32	123.21	127.00
36	1	1547	G	N7-C8-N9	-6.32	109.94	113.10
36	5	2887	A	N3-C4-N9	6.31	132.45	127.40
36	5	2959	C	C2-N3-C4	-6.31	116.74	119.90
38	4	14	C	C6-N1-C2	-6.31	117.78	120.30
38	4	96	A	N1-C6-N6	6.31	122.39	118.60
1	6	347	G	N1-C6-O6	6.31	123.69	119.90
36	5	2892	A	C5-N7-C8	-6.31	100.75	103.90
36	5	3096	C	N3-C2-O2	6.31	126.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	453	U	C6-N1-C1'	-6.31	112.37	121.20
36	1	29	C	C5-C4-N4	-6.31	115.78	120.20
1	6	1744	A	C8-N9-C4	6.31	108.32	105.80
36	1	681	U	N3-C4-O4	6.31	123.81	119.40
36	5	2142	A	C6-N1-C2	-6.31	114.81	118.60
36	5	1433	A	O4'-C1'-N9	-6.31	103.16	108.20
36	5	2870	C	C2-N3-C4	-6.30	116.75	119.90
1	6	1493	A	N7-C8-N9	6.30	116.95	113.80
36	5	1496	C	N1-C2-O2	6.30	122.68	118.90
36	1	2887	A	C6-C5-N7	-6.30	127.89	132.30
36	5	2617	U	N1-C2-O2	-6.30	118.39	122.80
1	6	1657	U	O5'-P-OP2	-6.30	100.03	105.70
36	5	767	U	O4'-C1'-N1	6.30	113.24	108.20
36	5	809	G	C5-C6-O6	-6.30	124.82	128.60
1	6	353	A	N1-C6-N6	-6.30	114.82	118.60
1	2	1636	C	C6-N1-C2	-6.29	117.78	120.30
36	1	1377	G	N3-C4-N9	6.29	129.78	126.00
36	1	2162	U	C4-C5-C6	-6.29	115.92	119.70
36	1	3107	U	C2-N3-C4	-6.29	123.22	127.00
38	4	111	A	C5-C6-N6	-6.29	118.66	123.70
36	5	2874	G	C5-C6-O6	6.29	132.38	128.60
36	1	1604	G	C8-N9-C1'	-6.29	118.82	127.00
1	6	17	C	O5'-P-OP2	-6.29	100.03	105.70
36	5	1330	A	OP1-P-OP2	-6.29	110.16	119.60
36	1	1845	G	OP2-P-O3'	6.29	119.04	105.20
36	1	2639	G	C6-C5-N7	-6.29	126.62	130.40
1	6	606	A	C8-N9-C4	6.29	108.32	105.80
44	17	229	PHE	CB-CG-CD1	6.29	125.20	120.80
36	1	2283	G	C2-N3-C4	-6.29	108.75	111.90
36	5	886	C	N3-C4-C5	6.29	124.42	121.90
36	1	2900	A	C8-N9-C4	6.29	108.31	105.80
1	6	638	U	N1-C2-O2	6.29	127.20	122.80
36	5	1113	G	N1-C6-O6	6.29	123.67	119.90
36	1	2881	C	C6-N1-C2	6.29	122.81	120.30
1	6	622	A	O5'-P-OP1	-6.29	100.04	105.70
1	2	1389	C	N1-C2-O2	6.28	122.67	118.90
36	1	2355	G	N3-C2-N2	-6.28	115.50	119.90
1	6	309	C	O5'-P-OP1	-6.28	100.04	105.70
1	6	1123	C	C5-C4-N4	-6.28	115.80	120.20
36	1	3302	U	C6-N1-C2	6.28	124.77	121.00
53	M7	19	GLY	N-CA-C	-6.28	97.39	113.10
36	1	659	G	OP2-P-O3'	6.28	119.02	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2768	U	O5'-P-OP2	-6.28	100.05	105.70
1	2	1733	C	C5-C4-N4	-6.28	115.81	120.20
36	5	2979	U	C2-N1-C1'	-6.28	110.17	117.70
36	1	2187	G	N1-C6-O6	6.28	123.67	119.90
38	4	15	G	C4-C5-N7	6.28	113.31	110.80
36	1	895	A	C6-C5-N7	-6.28	127.91	132.30
36	5	90	C	N3-C4-N4	6.28	122.39	118.00
36	5	215	G	C8-N9-C4	-6.28	103.89	106.40
36	5	3174	A	C2-N3-C4	-6.28	107.46	110.60
1	6	455	C	N3-C4-N4	6.27	122.39	118.00
36	5	1367	G	N1-C6-O6	6.27	123.66	119.90
36	5	2824	G	C8-N9-C4	-6.27	103.89	106.40
36	5	2709	C	C6-N1-C2	6.27	122.81	120.30
1	2	132	U	P-O3'-C3'	6.27	127.22	119.70
40	l3	19	ARG	NE-CZ-NH1	6.27	123.44	120.30
36	1	1133	A	N9-C4-C5	-6.27	103.29	105.80
36	1	2406	C	C6-N1-C2	6.27	122.81	120.30
1	6	767	U	C5-C4-O4	6.27	129.66	125.90
1	6	1340	U	N3-C2-O2	-6.27	117.81	122.20
36	5	2245	C	N3-C4-C5	-6.27	119.39	121.90
36	1	1322	U	O5'-P-OP2	-6.26	100.06	105.70
1	6	163	G	C8-N9-C4	-6.26	103.89	106.40
38	8	26	U	N1-C2-O2	6.26	127.18	122.80
36	1	1138	U	N3-C2-O2	-6.26	117.82	122.20
36	1	132	C	N1-C2-O2	-6.26	115.14	118.90
36	1	610	G	O5'-P-OP2	-6.26	100.07	105.70
36	1	697	A	C5-C6-N1	6.26	120.83	117.70
36	1	2372	A	N3-C4-N9	6.26	132.41	127.40
36	1	2383	C	N3-C4-C5	6.26	124.40	121.90
36	5	1496	C	O5'-P-OP1	6.26	118.21	110.70
36	5	2142	A	C5-C6-N1	6.26	120.83	117.70
36	5	2572	C	C6-N1-C2	-6.26	117.80	120.30
36	5	1662	G	C5-C6-N1	-6.26	108.37	111.50
36	5	984	G	C4-C5-C6	6.26	122.55	118.80
36	5	1300	G	C6-C5-N7	-6.26	126.65	130.40
36	5	1897	G	C6-C5-N7	-6.26	126.65	130.40
36	5	2994	A	C6-N1-C2	-6.26	114.85	118.60
36	5	3164	C	O4'-C1'-N1	6.26	113.21	108.20
36	1	1197	A	C4-C5-N7	6.25	113.83	110.70
36	1	1507	G	C6-N1-C2	-6.25	121.35	125.10
36	1	1822	C	C6-N1-C2	-6.25	117.80	120.30
73	O7	65	ARG	NE-CZ-NH2	-6.25	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	610	G	C4-N9-C1'	6.25	134.63	126.50
36	5	955	U	N1-C2-O2	-6.25	118.42	122.80
36	5	2937	G	C4-C5-N7	6.25	113.30	110.80
36	1	2901	G	C5-C6-O6	-6.25	124.85	128.60
36	5	2331	C	N1-C2-O2	-6.25	115.15	118.90
1	2	694	U	C5-C6-N1	6.25	125.82	122.70
36	1	801	A	O4'-C1'-N9	-6.25	103.20	108.20
36	1	1846	C	C6-N1-C2	-6.25	117.80	120.30
1	6	1634	C	N3-C2-O2	-6.25	117.53	121.90
36	5	2112	U	C5-C6-N1	6.25	125.83	122.70
36	1	3361	G	N3-C2-N2	6.25	124.27	119.90
36	5	88	A	C8-N9-C4	6.25	108.30	105.80
36	5	2639	G	C4-C5-C6	6.25	122.55	118.80
36	1	295	A	N7-C8-N9	6.24	116.92	113.80
36	1	1168	U	N3-C2-O2	-6.24	117.83	122.20
1	6	1428	G	C8-N9-C4	-6.24	103.90	106.40
36	5	2735	U	C5-C6-N1	6.24	125.82	122.70
36	5	2796	G	O5'-P-OP2	-6.24	100.08	105.70
36	1	48	A	O4'-C1'-N9	6.24	113.19	108.20
1	2	553	G	C4-C5-C6	6.24	122.55	118.80
36	1	1082	U	C6-N1-C2	-6.24	117.26	121.00
36	1	3207	U	C5-C4-O4	6.24	129.64	125.90
36	1	3224	G	N3-C2-N2	-6.24	115.53	119.90
38	4	94	C	N3-C4-C5	6.24	124.40	121.90
1	6	458	G	C8-N9-C4	-6.24	103.90	106.40
36	5	957	C	N3-C2-O2	-6.24	117.53	121.90
36	1	2302	G	OP2-P-O3'	6.24	118.92	105.20
1	6	999	U	N3-C4-C5	6.24	118.34	114.60
36	5	2404	A	C8-N9-C1'	6.24	138.93	127.70
36	5	2821	C	C2-N1-C1'	-6.24	111.94	118.80
38	8	96	A	C8-N9-C4	6.24	108.30	105.80
59	n3	45	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	6	144	U	N1-C2-O2	6.24	127.17	122.80
38	8	9	A	O5'-P-OP2	-6.23	100.09	105.70
1	2	1761	U	N3-C4-C5	-6.23	110.86	114.60
1	6	103	A	P-O3'-C3'	6.23	127.18	119.70
36	5	346	C	O5'-P-OP2	-6.23	100.09	105.70
36	1	24	G	N1-C2-N3	6.23	127.64	123.90
36	1	1590	G	N1-C6-O6	-6.23	116.16	119.90
52	M6	128	ARG	NE-CZ-NH2	6.23	123.41	120.30
36	5	89	A	N1-C6-N6	6.23	122.34	118.60
36	1	590	G	C4-C5-N7	6.23	113.29	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2407	C	C4-C5-C6	6.23	120.51	117.40
36	1	2737	C	N1-C2-O2	-6.23	115.16	118.90
44	17	83	LEU	CA-CB-CG	6.23	129.62	115.30
36	1	398	A	O5'-P-OP2	-6.22	100.10	105.70
36	1	1056	U	C5-C6-N1	6.22	125.81	122.70
36	5	962	A	C6-C5-N7	-6.22	127.94	132.30
36	5	1316	C	N3-C4-C5	-6.22	119.41	121.90
1	2	192	U	C2-N1-C1'	6.22	125.17	117.70
36	1	2687	G	N1-C6-O6	-6.22	116.17	119.90
36	5	366	A	C2-N3-C4	-6.22	107.49	110.60
36	1	3154	C	C2-N1-C1'	6.22	125.64	118.80
1	6	1058	U	OP1-P-O3'	6.22	118.89	105.20
36	5	3218	A	C2-N3-C4	-6.22	107.49	110.60
1	6	542	A	O4'-C1'-N9	6.22	113.17	108.20
36	5	880	G	O5'-P-OP2	-6.22	100.10	105.70
36	5	2113	A	O4'-C1'-N9	-6.22	103.22	108.20
36	5	2639	G	C8-N9-C4	-6.22	103.91	106.40
36	1	968	G	N3-C4-C5	-6.22	125.49	128.60
36	1	350	C	N3-C4-C5	-6.22	119.41	121.90
52	m6	94	ARG	NE-CZ-NH1	-6.22	117.19	120.30
36	1	283	G	O4'-C1'-N9	-6.21	103.23	108.20
36	1	2355	G	C5-C6-O6	-6.21	124.87	128.60
36	1	2758	A	C8-N9-C4	6.21	108.28	105.80
36	1	2942	C	N1-C2-O2	-6.21	115.17	118.90
36	5	950	G	C5-C6-N1	6.21	114.61	111.50
36	5	1329	U	C2-N3-C4	-6.21	123.27	127.00
36	5	1460	A	N1-C6-N6	6.21	122.33	118.60
36	1	1531	C	C6-N1-C2	-6.21	117.82	120.30
36	5	776	U	N3-C2-O2	-6.21	117.85	122.20
1	2	736	C	C2-N1-C1'	6.21	125.63	118.80
36	1	2621	G	OP1-P-OP2	-6.21	110.29	119.60
36	5	1844	C	N1-C2-N3	6.21	123.55	119.20
36	5	2395	G	OP2-P-O3'	6.21	118.86	105.20
36	5	264	G	N1-C6-O6	6.21	123.62	119.90
36	5	635	G	C4-C5-N7	6.21	113.28	110.80
36	5	647	A	C8-N9-C4	6.21	108.28	105.80
1	2	942	G	N1-C6-O6	-6.20	116.18	119.90
36	1	421	G	C4-C5-N7	6.20	113.28	110.80
36	1	920	A	N1-C2-N3	6.20	132.40	129.30
36	1	3304	U	N1-C2-O2	-6.20	118.46	122.80
1	6	139	C	N3-C2-O2	-6.20	117.56	121.90
36	5	216	G	N1-C6-O6	6.20	123.62	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1176	G	N1-C6-O6	6.20	123.62	119.90
36	5	2394	G	N1-C2-N2	-6.20	110.62	116.20
36	1	645	A	N1-C6-N6	-6.20	114.88	118.60
36	1	895	A	C5-N7-C8	-6.20	100.80	103.90
1	6	1493	A	C8-N9-C4	-6.20	103.32	105.80
36	5	1410	U	O5'-P-OP2	-6.20	100.12	105.70
36	5	2843	U	C2-N1-C1'	6.20	125.14	117.70
36	1	2899	C	C2-N1-C1'	6.20	125.62	118.80
1	2	1324	G	N1-C2-N2	6.20	121.78	116.20
36	5	1429	G	N1-C2-N2	-6.20	110.62	116.20
36	5	2877	G	N3-C4-C5	-6.19	125.50	128.60
1	2	1432	U	C6-N1-C2	6.19	124.72	121.00
36	1	1307	G	OP1-P-O3'	6.19	118.83	105.20
36	1	1434	G	O5'-P-OP1	-6.19	100.13	105.70
36	1	3362	A	N1-C2-N3	6.19	132.40	129.30
36	1	638	C	O5'-P-OP2	-6.19	100.13	105.70
36	1	1515	A	C2-N3-C4	-6.19	107.50	110.60
36	5	2797	C	C6-N1-C2	-6.19	117.82	120.30
36	5	641	C	C2-N1-C1'	-6.19	111.99	118.80
36	1	2273	G	N7-C8-N9	-6.19	110.01	113.10
69	O3	73	ARG	NE-CZ-NH2	-6.19	117.21	120.30
36	5	141	C	C5-C6-N1	6.19	124.09	121.00
36	5	1855	U	O5'-P-OP2	-6.19	100.13	105.70
36	5	2678	A	N1-C6-N6	-6.19	114.89	118.60
36	1	358	G	N9-C4-C5	-6.18	102.93	105.40
36	1	1445	U	C2-N3-C4	-6.18	123.29	127.00
1	6	1361	U	C2-N1-C1'	6.18	125.12	117.70
36	5	1075	A	C8-N9-C4	6.18	108.27	105.80
1	2	31	C	C6-N1-C2	-6.18	117.83	120.30
1	2	341	A	C8-N9-C4	-6.18	103.33	105.80
36	1	1849	C	O5'-P-OP1	-6.18	100.14	105.70
36	5	1452	A	N1-C6-N6	6.18	122.31	118.60
36	5	2343	C	N3-C4-C5	6.18	124.37	121.90
36	1	1114	U	C4-C5-C6	-6.18	115.99	119.70
36	1	3205	G	N1-C6-O6	6.18	123.61	119.90
1	6	988	A	C8-N9-C4	-6.18	103.33	105.80
36	5	1897	G	C5-N7-C8	-6.18	101.21	104.30
36	1	28	C	C6-N1-C2	6.18	122.77	120.30
1	6	1629	G	N3-C4-C5	-6.18	125.51	128.60
36	1	640	U	N1-C2-O2	-6.17	118.48	122.80
36	1	2142	A	N1-C2-N3	6.17	132.39	129.30
36	1	2695	A	N9-C4-C5	6.17	108.27	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3108	G	N1-C6-O6	6.17	123.61	119.90
37	7	56	A	N1-C6-N6	6.17	122.30	118.60
1	2	1174	C	N1-C2-O2	6.17	122.60	118.90
36	5	1180	A	C8-N9-C4	-6.17	103.33	105.80
1	2	992	A	N3-C4-C5	6.17	131.12	126.80
36	1	1741	A	N1-C2-N3	6.17	132.38	129.30
36	5	1392	G	N3-C4-N9	6.17	129.70	126.00
36	1	2249	G	N3-C4-N9	6.17	129.70	126.00
36	5	2859	U	O5'-P-OP1	-6.17	100.15	105.70
36	1	96	G	C4-C5-N7	6.17	113.27	110.80
1	6	1106	U	C6-N1-C2	-6.17	117.30	121.00
36	5	385	A	C5-C6-N6	-6.17	118.77	123.70
36	5	1155	C	N3-C4-C5	6.17	124.37	121.90
36	1	1522	U	C2-N3-C4	-6.17	123.30	127.00
36	1	2194	G	C6-C5-N7	-6.17	126.70	130.40
36	1	816	A	C2-N3-C4	6.16	113.68	110.60
36	1	969	C	N3-C4-N4	6.16	122.31	118.00
36	1	646	A	N9-C4-C5	6.16	108.27	105.80
36	1	857	G	C5-C6-N1	-6.16	108.42	111.50
36	1	917	A	C5-C6-N6	6.16	128.63	123.70
1	6	371	G	C4-C5-C6	6.16	122.50	118.80
36	5	1460	A	C5-C6-N6	-6.16	118.77	123.70
36	5	1513	G	C5-N7-C8	-6.16	101.22	104.30
36	1	406	G	C5-C6-N1	6.16	114.58	111.50
36	1	1369	A	N1-C6-N6	6.16	122.30	118.60
64	N8	42	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	6	1031	U	C2-N1-C1'	-6.16	110.31	117.70
36	5	2899	C	N1-C2-N3	6.16	123.51	119.20
1	2	1210	C	N3-C4-C5	-6.16	119.44	121.90
36	5	83	U	N1-C2-O2	6.16	127.11	122.80
36	5	1010	G	O5'-P-OP2	-6.16	100.16	105.70
36	1	2954	U	OP1-P-O3'	6.16	118.75	105.20
36	5	2400	G	N9-C4-C5	-6.16	102.94	105.40
36	1	1481	A	C6-C5-N7	-6.16	127.99	132.30
36	1	3270	U	C2-N1-C1'	-6.15	110.32	117.70
36	5	2648	G	C4-C5-N7	6.15	113.26	110.80
36	1	989	A	C8-N9-C4	6.15	108.26	105.80
36	1	2351	U	N1-C2-N3	6.15	118.59	114.90
36	1	2714	G	C4-N9-C1'	-6.15	118.50	126.50
36	5	366	A	N1-C6-N6	6.15	122.29	118.60
36	5	1305	U	C5-C4-O4	-6.15	122.21	125.90
36	5	2719	U	C2-N1-C1'	-6.15	110.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3326	G	N9-C4-C5	-6.15	102.94	105.40
36	1	2427	U	C5-C4-O4	6.15	129.59	125.90
38	4	113	U	C5-C4-O4	6.15	129.59	125.90
36	5	75	G	O5'-P-OP1	6.15	118.08	110.70
36	1	679	U	O5'-P-OP2	-6.15	100.17	105.70
36	1	2812	C	C6-N1-C2	6.15	122.76	120.30
1	2	110	U	C6-N1-C2	-6.14	117.31	121.00
36	1	406	G	O5'-P-OP2	-6.14	100.17	105.70
36	1	517	G	C6-C5-N7	-6.14	126.71	130.40
36	1	1127	G	C6-C5-N7	-6.14	126.71	130.40
36	5	1869	C	C6-N1-C2	6.14	122.76	120.30
36	5	2905	U	C5-C6-N1	-6.14	119.63	122.70
36	1	1556	C	C6-N1-C1'	-6.14	113.43	120.80
1	2	1027	A	C4-C5-N7	6.14	113.77	110.70
36	5	817	A	C8-N9-C4	-6.14	103.34	105.80
1	6	795	U	N1-C2-O2	6.14	127.10	122.80
36	5	3209	A	C8-N9-C4	-6.14	103.34	105.80
36	1	1131	G	C6-C5-N7	-6.14	126.72	130.40
36	5	659	G	O5'-P-OP1	-6.14	100.18	105.70
36	5	410	U	OP2-P-O3'	6.14	118.70	105.20
36	1	2337	C	C6-N1-C2	-6.13	117.85	120.30
36	5	422	A	C8-N9-C4	-6.13	103.35	105.80
36	1	1376	C	N3-C4-C5	-6.13	119.45	121.90
36	5	1175	C	C2-N1-C1'	-6.13	112.06	118.80
1	6	1028	C	C5-C6-N1	-6.13	117.94	121.00
36	5	1110	U	C2-N1-C1'	6.13	125.06	117.70
36	1	1112	A	C8-N9-C4	6.13	108.25	105.80
36	5	218	G	C4-C5-N7	-6.13	108.35	110.80
36	1	388	G	N9-C4-C5	6.13	107.85	105.40
36	1	2357	A	C5-C6-N6	-6.13	118.80	123.70
36	1	1114	U	C5-C4-O4	6.12	129.57	125.90
36	5	1869	C	C2-N1-C1'	-6.12	112.06	118.80
1	2	12	U	N3-C2-O2	-6.12	117.91	122.20
36	1	776	U	C2-N3-C4	-6.12	123.33	127.00
36	1	2817	A	C5-C6-N1	6.12	120.76	117.70
36	5	2700	G	C6-C5-N7	-6.12	126.73	130.40
36	1	1168	U	O5'-P-OP1	6.12	118.05	110.70
36	1	2383	C	C5-C4-N4	-6.12	115.92	120.20
36	1	3275	U	C5-C6-N1	6.12	125.76	122.70
1	6	1777	G	N1-C6-O6	6.12	123.57	119.90
37	7	85	G	C8-N9-C4	-6.12	103.95	106.40
36	1	634	C	C6-N1-C2	6.12	122.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2764	C	C2-N3-C4	6.12	122.96	119.90
36	5	1151	U	N1-C2-O2	-6.12	118.52	122.80
36	5	1561	G	O4'-C1'-N9	6.12	113.09	108.20
36	1	2938	G	C5-C6-O6	-6.12	124.93	128.60
36	5	1878	G	C8-N9-C4	-6.12	103.95	106.40
36	1	1136	A	C6-N1-C2	-6.12	114.93	118.60
36	1	2642	A	C5-C6-N1	-6.12	114.64	117.70
1	6	1146	G	C4-N9-C1'	6.12	134.45	126.50
1	2	765	G	O4'-C1'-N9	-6.11	103.31	108.20
36	1	2300	G	C8-N9-C4	-6.11	103.95	106.40
36	5	2630	C	C2-N1-C1'	-6.11	112.08	118.80
36	5	3197	G	N3-C4-N9	-6.11	122.33	126.00
36	1	410	U	OP2-P-O3'	6.11	118.64	105.20
36	1	1371	G	N7-C8-N9	-6.11	110.05	113.10
36	1	2747	A	N1-C6-N6	-6.11	114.93	118.60
38	8	96	A	N1-C6-N6	6.11	122.27	118.60
36	1	2859	U	N1-C2-O2	-6.11	118.53	122.80
37	7	49	G	C6-C5-N7	-6.11	126.73	130.40
38	8	111	A	O5'-P-OP2	-6.11	100.20	105.70
36	1	984	G	N7-C8-N9	6.11	116.15	113.10
1	6	1651	A	N1-C6-N6	6.11	122.26	118.60
36	5	567	G	C6-C5-N7	-6.11	126.74	130.40
36	5	955	U	C2-N3-C4	-6.10	123.34	127.00
36	1	96	G	N3-C4-C5	6.10	131.65	128.60
36	1	210	U	N1-C2-N3	6.10	118.56	114.90
36	5	793	C	C2-N1-C1'	6.10	125.51	118.80
36	5	2393	G	N1-C6-O6	6.10	123.56	119.90
36	1	1399	A	N3-C4-C5	6.10	131.07	126.80
36	5	1620	U	N3-C2-O2	-6.10	117.93	122.20
36	1	663	C	N1-C2-O2	-6.10	115.24	118.90
36	1	970	A	N1-C6-N6	-6.10	114.94	118.60
1	6	163	G	C2-N3-C4	-6.10	108.85	111.90
36	5	834	U	C6-N1-C2	6.10	124.66	121.00
36	1	918	C	O5'-P-OP2	-6.10	100.21	105.70
36	1	2162	U	N3-C4-C5	6.10	118.26	114.60
36	1	2144	A	C5-C6-N6	-6.10	118.82	123.70
36	1	2571	U	N1-C2-O2	6.10	127.07	122.80
1	6	163	G	C4-N9-C1'	-6.10	118.58	126.50
36	1	500	C	N3-C4-C5	-6.09	119.46	121.90
36	1	1913	A	N1-C6-N6	6.09	122.26	118.60
36	1	2298	U	N3-C4-C5	6.09	118.26	114.60
36	1	2929	C	C6-N1-C2	-6.09	117.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3176	G	N3-C2-N2	-6.09	115.63	119.90
36	5	2857	C	C5-C4-N4	-6.09	115.94	120.20
1	2	542	A	N7-C8-N9	6.09	116.84	113.80
36	1	1180	A	C5-C6-N6	6.09	128.57	123.70
36	1	2136	C	N1-C2-O2	-6.09	115.25	118.90
36	1	2571	U	N3-C2-O2	-6.09	117.94	122.20
36	5	1321	G	C6-C5-N7	-6.09	126.75	130.40
36	1	93	C	O5'-P-OP1	-6.09	100.22	105.70
36	5	696	C	N3-C4-N4	6.09	122.26	118.00
36	5	1420	C	OP2-P-O3'	6.09	118.60	105.20
36	1	1724	U	O4'-C1'-N1	6.09	113.07	108.20
36	5	218	G	N3-C4-C5	-6.09	125.56	128.60
36	1	337	G	C2-N3-C4	6.09	114.94	111.90
36	1	665	A	C6-N1-C2	-6.09	114.95	118.60
36	1	1197	A	C6-C5-N7	-6.09	128.04	132.30
36	1	1296	C	C6-N1-C2	-6.09	117.86	120.30
36	1	1475	A	N7-C8-N9	-6.09	110.76	113.80
36	1	3263	G	N1-C6-O6	6.08	123.55	119.90
36	5	1151	U	N3-C4-C5	-6.08	110.95	114.60
36	1	683	U	C5-C4-O4	-6.08	122.25	125.90
36	1	1154	A	C4-C5-C6	6.08	120.04	117.00
73	o7	65	ARG	NE-CZ-NH1	6.08	123.34	120.30
36	1	1310	G	N3-C2-N2	6.08	124.16	119.90
36	1	2331	C	O5'-P-OP1	-6.08	100.23	105.70
1	6	795	U	N3-C2-O2	-6.08	117.94	122.20
36	5	217	U	C5-C6-N1	-6.08	119.66	122.70
1	2	73	U	OP1-P-O3'	6.08	118.57	105.20
1	6	1614	A	C5-N7-C8	-6.08	100.86	103.90
36	5	1931	U	N1-C2-O2	-6.08	118.55	122.80
36	5	2763	U	N3-C2-O2	6.08	126.45	122.20
36	1	282	G	C5-C6-O6	6.08	132.25	128.60
36	5	2410	U	N3-C2-O2	6.08	126.45	122.20
36	1	368	G	N1-C2-N2	-6.08	110.73	116.20
36	1	614	C	C5-C4-N4	-6.08	115.95	120.20
1	6	647	G	N3-C2-N2	-6.08	115.65	119.90
36	5	2406	C	N3-C2-O2	6.08	126.15	121.90
1	2	1565	C	C6-N1-C2	-6.07	117.87	120.30
36	1	360	G	N3-C4-N9	6.07	129.64	126.00
36	5	1175	C	N3-C2-O2	6.07	126.15	121.90
36	5	1311	G	N1-C2-N3	-6.07	120.26	123.90
36	5	1902	G	C4-C5-C6	6.07	122.44	118.80
36	5	2245	C	N3-C2-O2	-6.07	117.65	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2271	A	N7-C8-N9	-6.07	110.76	113.80
36	5	938	C	N3-C4-N4	6.07	122.25	118.00
36	1	15	C	C6-N1-C2	-6.07	117.87	120.30
36	1	1620	U	C2-N1-C1'	6.07	124.98	117.70
36	5	1432	C	N3-C2-O2	-6.07	117.65	121.90
36	5	1879	A	C5-N7-C8	-6.07	100.86	103.90
36	1	76	G	C8-N9-C4	-6.07	103.97	106.40
36	1	2522	G	C4-N9-C1'	6.07	134.39	126.50
36	1	2643	A	N7-C8-N9	-6.07	110.77	113.80
36	5	437	G	C4-N9-C1'	6.07	134.39	126.50
36	5	998	A	N1-C6-N6	-6.07	114.96	118.60
1	2	553	G	C5-C6-N1	-6.07	108.47	111.50
36	1	1820	U	P-O3'-C3'	6.07	126.98	119.70
1	6	999	U	C4-C5-C6	-6.07	116.06	119.70
36	5	2845	A	N7-C8-N9	6.06	116.83	113.80
36	1	406	G	C2-N3-C4	6.06	114.93	111.90
36	1	2808	A	C4-C5-N7	6.06	113.73	110.70
1	2	1668	G	N3-C4-N9	-6.06	122.36	126.00
1	2	1536	G	N3-C4-N9	6.06	129.64	126.00
36	1	1069	C	C6-N1-C2	-6.06	117.88	120.30
36	1	1351	U	C2-N1-C1'	6.06	124.97	117.70
1	2	387	A	O5'-P-OP2	-6.06	100.25	105.70
36	1	1131	G	N3-C4-N9	6.06	129.63	126.00
36	1	1370	G	C6-C5-N7	-6.06	126.77	130.40
36	5	587	U	C6-N1-C2	6.06	124.64	121.00
36	5	1336	U	C5-C4-O4	-6.06	122.27	125.90
36	5	2148	U	C2-N1-C1'	-6.06	110.43	117.70
37	3	91	G	C2-N3-C4	-6.06	108.87	111.90
36	5	1101	G	N1-C2-N2	-6.06	110.75	116.20
36	1	2182	A	C8-N9-C4	-6.05	103.38	105.80
36	1	3041	U	O5'-P-OP1	6.05	117.97	110.70
36	5	2145	A	C8-N9-C4	-6.05	103.38	105.80
36	5	2959	C	C5-C6-N1	-6.05	117.97	121.00
1	2	74	U	O5'-P-OP1	-6.05	100.25	105.70
1	6	359	A	C4-N9-C1'	-6.05	115.40	126.30
36	5	2857	C	N3-C4-C5	6.05	124.32	121.90
36	1	726	G	N7-C8-N9	6.05	116.13	113.10
36	5	2306	C	C6-N1-C2	6.05	122.72	120.30
36	1	188	U	C4-C5-C6	6.05	123.33	119.70
36	1	776	U	C5-C4-O4	6.05	129.53	125.90
36	5	3362	A	C8-N9-C4	-6.05	103.38	105.80
36	5	1724	U	OP1-P-O3'	6.05	118.51	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	304	G	N1-C2-N2	6.05	121.64	116.20
36	5	2816	G	O5'-P-OP2	-6.05	100.26	105.70
37	7	69	C	C5-C4-N4	-6.05	115.97	120.20
1	6	767	U	N3-C2-O2	-6.04	117.97	122.20
36	5	1154	A	N9-C4-C5	6.04	108.22	105.80
36	1	1313	G	C5-N7-C8	-6.04	101.28	104.30
36	1	1604	G	N3-C4-C5	-6.04	125.58	128.60
36	1	2514	U	C5-C6-N1	-6.04	119.68	122.70
36	1	57	A	N1-C2-N3	6.04	132.32	129.30
36	1	217	U	N1-C2-O2	-6.04	118.57	122.80
36	1	2826	U	C5-C4-O4	-6.04	122.28	125.90
36	5	955	U	C5-C4-O4	-6.04	122.28	125.90
36	5	2234	G	N9-C4-C5	-6.04	102.98	105.40
1	6	153	G	C4-C5-N7	6.04	113.22	110.80
1	6	1002	G	C8-N9-C4	-6.04	103.98	106.40
36	1	3344	A	C5-N7-C8	-6.04	100.88	103.90
1	6	1600	A	N9-C1'-C2'	6.04	121.85	114.00
36	5	1301	A	C5-N7-C8	-6.04	100.88	103.90
36	5	1309	U	N1-C2-O2	-6.04	118.58	122.80
36	5	2148	U	N1-C2-O2	-6.04	118.58	122.80
36	5	3278	C	C6-N1-C2	6.04	122.71	120.30
1	2	1162	C	C6-N1-C2	-6.03	117.89	120.30
1	6	114	C	N3-C2-O2	-6.03	117.68	121.90
36	5	1878	G	N7-C8-N9	6.03	116.12	113.10
36	5	2904	U	N1-C2-N3	6.03	118.52	114.90
36	1	988	U	C6-N1-C2	6.03	124.62	121.00
36	5	2991	A	N1-C6-N6	-6.03	114.98	118.60
1	2	48	G	OP2-P-O3'	6.03	118.47	105.20
36	1	2973	G	N1-C6-O6	6.03	123.52	119.90
36	5	1308	A	O5'-P-OP1	-6.03	100.27	105.70
1	2	307	G	N3-C4-N9	6.03	129.62	126.00
36	5	3128	G	N7-C8-N9	-6.03	110.08	113.10
36	5	526	C	N3-C4-C5	6.03	124.31	121.90
36	1	24	G	C8-N9-C4	6.03	108.81	106.40
36	1	153	U	C6-N1-C2	-6.03	117.39	121.00
36	1	2413	A	C4-C5-C6	-6.03	113.99	117.00
36	5	2881	C	N3-C4-C5	6.03	124.31	121.90
1	2	1033	C	N3-C2-O2	-6.02	117.68	121.90
1	2	144	U	N3-C2-O2	-6.02	117.98	122.20
36	1	507	U	O5'-P-OP1	6.02	117.93	110.70
36	5	1368	U	N3-C4-O4	6.02	123.61	119.40
36	5	2870	C	N3-C4-C5	6.02	124.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	321	C	C6-N1-C1'	-6.02	113.58	120.80
1	6	1137	A	N7-C8-N9	-6.02	110.79	113.80
1	2	1274	C	C6-N1-C2	-6.02	117.89	120.30
36	1	2764	C	C5-C6-N1	6.02	124.01	121.00
36	1	1346	G	C5-C6-N1	-6.02	108.49	111.50
36	5	1011	A	OP2-P-O3'	6.02	118.44	105.20
36	5	1160	C	C6-N1-C1'	6.02	128.02	120.80
36	5	1187	C	N3-C2-O2	-6.02	117.69	121.90
36	5	1239	C	C2-N1-C1'	6.02	125.42	118.80
36	5	2849	C	C5-C6-N1	6.02	124.01	121.00
36	5	3041	U	C4-C5-C6	-6.02	116.09	119.70
1	2	1489	U	N3-C2-O2	-6.02	117.99	122.20
36	5	1317	A	N1-C6-N6	6.02	122.21	118.60
36	5	1392	G	N9-C4-C5	-6.02	102.99	105.40
46	L9	31	ARG	NE-CZ-NH1	-6.01	117.29	120.30
1	6	755	A	C8-N9-C4	-6.01	103.39	105.80
36	5	2637	A	N1-C6-N6	6.01	122.21	118.60
69	o3	99	ARG	NE-CZ-NH1	-6.01	117.29	120.30
36	1	346	C	C2-N1-C1'	-6.01	112.19	118.80
36	1	807	A	N1-C2-N3	6.01	132.31	129.30
36	1	2142	A	N9-C4-C5	6.01	108.20	105.80
36	1	2647	A	N1-C2-N3	6.01	132.31	129.30
1	6	1025	A	C8-N9-C4	6.01	108.20	105.80
36	5	1337	A	C2-N3-C4	6.01	113.61	110.60
36	5	2107	A	O5'-P-OP1	-6.01	100.29	105.70
1	6	558	U	N1-C2-O2	6.01	127.01	122.80
36	5	2289	U	N1-C2-O2	6.01	127.01	122.80
37	7	77	G	C4-C5-N7	6.01	113.20	110.80
36	1	2917	G	O5'-P-OP2	-6.01	100.29	105.70
1	2	1241	G	O4'-C1'-N9	6.01	113.00	108.20
36	1	281	G	C6-N1-C2	-6.01	121.50	125.10
36	1	439	C	C5-C6-N1	6.01	124.00	121.00
36	1	2942	C	C4-C5-C6	-6.01	114.40	117.40
36	5	952	A	C5-C6-N6	-6.01	118.89	123.70
37	7	1	G	N3-C4-N9	6.01	129.60	126.00
36	5	2891	U	N3-C4-C5	6.00	118.20	114.60
1	2	1339	C	OP1-P-O3'	6.00	118.41	105.20
36	1	895	A	N1-C6-N6	6.00	122.20	118.60
36	5	1461	A	O5'-P-OP2	-6.00	100.30	105.70
1	2	186	C	C5-C6-N1	6.00	124.00	121.00
1	2	734	A	P-O3'-C3'	6.00	126.90	119.70
36	5	1909	A	C8-N9-C4	6.00	108.20	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	90	C	C6-N1-C2	-6.00	117.90	120.30
36	1	388	G	C8-N9-C4	-6.00	104.00	106.40
36	5	966	U	C2-N1-C1'	6.00	124.90	117.70
36	5	2944	U	N1-C2-O2	6.00	127.00	122.80
36	1	386	A	C6-C5-N7	-6.00	128.10	132.30
36	1	2324	A	C8-N9-C4	-6.00	103.40	105.80
36	1	2409	G	C8-N9-C4	-6.00	104.00	106.40
36	5	2856	G	C4-C5-N7	6.00	113.20	110.80
36	5	636	C	N3-C4-C5	5.99	124.30	121.90
36	5	2323	G	OP1-P-OP2	-5.99	110.61	119.60
36	1	2293	C	C2-N1-C1'	5.99	125.39	118.80
1	2	830	U	N1-C2-O2	5.99	126.99	122.80
24	D2	104	LEU	CA-CB-CG	5.99	129.08	115.30
36	1	369	A	N9-C4-C5	5.99	108.20	105.80
36	1	1489	A	N9-C4-C5	-5.99	103.40	105.80
36	1	2376	G	N7-C8-N9	5.99	116.09	113.10
36	5	338	A	OP2-P-O3'	5.99	118.38	105.20
36	5	1852	G	N7-C8-N9	5.99	116.09	113.10
36	5	2405	C	C6-N1-C2	-5.99	117.90	120.30
36	5	3304	U	OP1-P-OP2	5.99	128.59	119.60
36	1	1269	U	C2-N1-C1'	5.99	124.89	117.70
1	6	542	A	C4-N9-C1'	5.99	137.08	126.30
36	1	716	A	C2-N3-C4	-5.99	107.61	110.60
36	1	3212	C	C6-N1-C2	5.99	122.69	120.30
1	6	1673	G	O5'-P-OP2	-5.99	100.31	105.70
36	5	2290	C	C6-N1-C2	5.99	122.69	120.30
1	2	1456	C	N3-C2-O2	-5.98	117.71	121.90
36	5	2899	C	C2-N1-C1'	5.98	125.38	118.80
1	6	536	C	C6-N1-C2	-5.98	117.91	120.30
1	6	1098	U	O5'-P-OP1	-5.98	100.32	105.70
36	5	1203	A	C6-C5-N7	-5.98	128.11	132.30
36	1	618	C	N1-C2-O2	-5.98	115.31	118.90
36	1	1001	G	C5-C6-O6	-5.98	125.01	128.60
36	1	2508	U	C5-C6-N1	5.98	125.69	122.70
1	2	334	G	N3-C4-C5	5.98	131.59	128.60
1	2	354	C	N3-C4-C5	-5.98	119.51	121.90
36	1	2249	G	C5-C6-N1	5.98	114.49	111.50
36	5	1852	G	C8-N9-C4	-5.98	104.01	106.40
36	5	2990	G	C5-C6-O6	-5.98	125.01	128.60
37	7	12	U	C4-C5-C6	-5.98	116.11	119.70
36	1	54	C	C2-N1-C1'	-5.98	112.23	118.80
36	1	132	C	N3-C2-O2	5.98	126.08	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2414	G	N9-C4-C5	5.98	107.79	105.40
36	1	3006	A	N1-C2-N3	5.98	132.29	129.30
36	5	2936	A	C2-N3-C4	5.98	113.59	110.60
36	1	2868	U	N1-C2-O2	5.97	126.98	122.80
36	5	1112	A	C5-C6-N6	-5.97	118.92	123.70
36	5	1300	G	N9-C4-C5	-5.97	103.01	105.40
36	5	2353	G	N1-C6-O6	5.97	123.48	119.90
1	6	1640	C	C6-N1-C1'	-5.97	113.63	120.80
36	5	1592	G	C6-C5-N7	-5.97	126.82	130.40
36	5	425	G	C8-N9-C4	5.97	108.79	106.40
36	1	56	G	C5-C6-N1	5.97	114.48	111.50
36	1	1507	G	N1-C6-O6	5.97	123.48	119.90
1	6	543	C	N3-C2-O2	-5.97	117.72	121.90
36	5	1894	U	C5-C6-N1	-5.97	119.72	122.70
36	5	2728	G	N3-C4-N9	-5.97	122.42	126.00
36	1	984	G	N3-C4-N9	5.97	129.58	126.00
36	1	2550	U	C5-C4-O4	5.97	129.48	125.90
36	1	1876	U	C2-N1-C1'	5.97	124.86	117.70
1	6	864	U	N3-C2-O2	-5.97	118.02	122.20
36	5	936	A	O5'-P-OP2	-5.97	100.33	105.70
36	5	3018	C	C6-N1-C2	-5.97	117.91	120.30
36	1	120	G	C8-N9-C4	5.96	108.79	106.40
36	1	2931	C	N3-C4-N4	5.96	122.17	118.00
36	1	2958	A	C4-C5-C6	-5.96	114.02	117.00
36	5	838	G	C5-C6-O6	5.96	132.18	128.60
36	5	2644	C	N3-C2-O2	5.96	126.07	121.90
36	1	716	A	C5-C6-N6	-5.96	118.93	123.70
36	1	904	A	C2-N3-C4	-5.96	107.62	110.60
36	1	2651	G	C8-N9-C4	5.96	108.78	106.40
1	6	310	C	N3-C4-C5	-5.96	119.52	121.90
36	5	1846	C	C6-N1-C1'	-5.96	113.65	120.80
36	1	350	C	C6-N1-C2	-5.96	117.92	120.30
36	1	590	G	C6-C5-N7	-5.96	126.82	130.40
36	1	3326	G	C5-N7-C8	5.96	107.28	104.30
1	6	323	A	C8-N9-C4	-5.96	103.42	105.80
52	m6	84	LEU	CB-CG-CD1	-5.96	100.87	111.00
38	4	51	G	C5-C6-O6	-5.96	125.03	128.60
36	5	2231	C	C6-N1-C2	-5.96	117.92	120.30
1	2	1765	A	O5'-P-OP1	-5.96	100.34	105.70
36	1	282	G	O5'-P-OP1	-5.96	100.34	105.70
36	1	2413	A	C8-N9-C4	5.96	108.18	105.80
36	5	3004	C	C5-C4-N4	-5.96	116.03	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3036	G	N1-C2-N3	5.96	127.47	123.90
36	1	2374	C	C2-N1-C1'	5.96	125.35	118.80
1	2	597	G	N3-C4-C5	-5.95	125.62	128.60
36	1	1419	A	C5'-C4'-O4'	5.95	116.25	109.10
36	1	1481	A	N9-C4-C5	-5.95	103.42	105.80
36	1	1841	A	O5'-P-OP2	-5.95	100.34	105.70
36	1	3275	U	OP1-P-O3'	5.95	118.30	105.20
36	5	437	G	N3-C4-N9	5.95	129.57	126.00
36	5	2944	U	N3-C4-O4	-5.95	115.23	119.40
36	1	2308	C	N3-C4-C5	5.95	124.28	121.90
1	2	555	A	C8-N9-C4	-5.95	103.42	105.80
36	1	1164	G	N9-C4-C5	5.95	107.78	105.40
36	1	1227	C	C5-C6-N1	5.95	123.97	121.00
38	4	74	U	N1-C2-O2	-5.95	118.64	122.80
36	1	672	A	C5-C6-N1	-5.95	114.73	117.70
36	1	1392	G	C5-C6-N1	5.95	114.47	111.50
36	5	1175	C	C6-N1-C1'	5.95	127.94	120.80
36	5	1483	G	O4'-C1'-N9	5.95	112.96	108.20
36	5	3142	A	O5'-P-OP1	-5.95	100.35	105.70
36	5	2419	A	O5'-P-OP2	5.95	117.84	110.70
36	5	3212	C	N3-C2-O2	5.95	126.06	121.90
36	1	2148	U	N3-C2-O2	5.95	126.36	122.20
36	1	2417	U	N1-C2-N3	5.95	118.47	114.90
36	1	2883	U	O5'-P-OP2	-5.95	100.35	105.70
36	1	2959	C	N3-C2-O2	5.95	126.06	121.90
36	5	2324	A	O5'-P-OP1	-5.95	100.35	105.70
36	1	911	C	N1-C2-O2	-5.94	115.33	118.90
36	1	1507	G	O4'-C1'-N9	-5.94	103.44	108.20
1	2	1190	C	C6-N1-C2	5.94	122.68	120.30
1	2	1202	A	C8-N9-C4	-5.94	103.42	105.80
36	1	2249	G	P-O3'-C3'	5.94	126.83	119.70
36	1	2378	C	C6-N1-C2	5.94	122.68	120.30
36	1	2980	U	N1-C2-N3	5.94	118.47	114.90
1	6	314	C	C6-N1-C2	-5.94	117.92	120.30
1	6	354	C	C5-C6-N1	5.94	123.97	121.00
64	n8	73	LEU	CA-CB-CG	5.94	128.97	115.30
1	2	1486	G	C5-N7-C8	-5.94	101.33	104.30
36	1	1409	G	N3-C4-N9	-5.94	122.44	126.00
36	5	2385	G	C2-N3-C4	-5.94	108.93	111.90
36	5	2611	U	C4-C5-C6	5.94	123.27	119.70
36	5	2639	G	C4-N9-C1'	5.94	134.22	126.50
38	8	48	A	C8-N9-C4	-5.94	103.42	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S3	182	LEU	CA-CB-CG	5.94	128.96	115.30
36	1	314	U	N3-C2-O2	-5.94	118.04	122.20
36	1	726	G	C8-N9-C4	-5.94	104.03	106.40
36	1	2692	A	C8-N9-C4	-5.94	103.42	105.80
36	5	688	G	N1-C6-O6	5.94	123.46	119.90
36	5	1434	G	N9-C4-C5	5.94	107.78	105.40
36	1	2846	U	N1-C2-N3	5.94	118.46	114.90
36	5	2709	C	C5-C4-N4	-5.94	116.05	120.20
1	2	635	A	N1-C6-N6	5.93	122.16	118.60
1	2	1768	G	C4-C5-N7	-5.93	108.43	110.80
36	1	3318	G	C8-N9-C4	-5.93	104.03	106.40
38	4	21	C	C4-C5-C6	-5.93	114.43	117.40
1	6	30	G	N9-C4-C5	5.93	107.77	105.40
1	6	407	A	N1-C2-N3	-5.93	126.33	129.30
36	5	687	U	C6-N1-C2	5.93	124.56	121.00
36	1	92	G	C5-C6-N1	5.93	114.47	111.50
36	1	3112	G	OP1-P-O3'	5.93	118.25	105.20
36	5	913	A	C4-C5-N7	5.93	113.67	110.70
36	5	1517	G	N1-C6-O6	5.93	123.46	119.90
1	6	1614	A	O4'-C1'-N9	5.93	112.94	108.20
36	5	2339	C	O4'-C1'-N1	-5.93	103.45	108.20
36	1	1069	C	C5-C6-N1	5.93	123.97	121.00
36	1	2984	C	N1-C2-N3	5.93	123.35	119.20
36	5	1757	A	C8-N9-C4	-5.93	103.43	105.80
36	1	2915	U	N1-C2-O2	-5.93	118.65	122.80
1	6	275	C	C2-N1-C1'	5.93	125.32	118.80
36	5	2531	C	C2-N1-C1'	5.93	125.32	118.80
37	7	77	G	C8-N9-C4	5.93	108.77	106.40
1	2	2	A	O4'-C1'-N9	-5.93	103.46	108.20
36	5	1905	G	N1-C2-N3	-5.93	120.34	123.90
1	2	877	G	O5'-P-OP2	-5.92	100.37	105.70
36	1	1112	A	N1-C6-N6	5.92	122.15	118.60
1	6	337	G	N3-C2-N2	5.92	124.05	119.90
38	8	2	A	C5-N7-C8	-5.92	100.94	103.90
36	1	271	C	N3-C2-O2	-5.92	117.75	121.90
36	5	2657	A	N1-C6-N6	-5.92	115.05	118.60
38	8	4	C	C2-N3-C4	-5.92	116.94	119.90
36	1	143	G	C5-C6-N1	5.92	114.46	111.50
36	1	334	A	C8-N9-C4	-5.92	103.43	105.80
36	1	1617	G	C8-N9-C4	5.92	108.77	106.40
36	1	1857	C	N1-C2-O2	-5.92	115.35	118.90
36	1	2827	U	C6-N1-C1'	5.92	129.49	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3316	A	OP2-P-O3'	5.92	118.22	105.20
36	1	3092	C	C6-N1-C2	5.92	122.67	120.30
1	6	1	U	C5-C6-N1	5.92	125.66	122.70
37	3	88	G	N1-C6-O6	-5.92	116.35	119.90
36	1	796	U	C5-C6-N1	5.92	125.66	122.70
36	1	2405	C	N3-C4-C5	-5.92	119.53	121.90
1	6	96	G	N9-C4-C5	5.92	107.77	105.40
36	5	398	A	N1-C6-N6	5.92	122.15	118.60
36	5	934	G	N3-C4-N9	5.92	129.55	126.00
36	5	2358	A	N3-C4-C5	5.92	130.94	126.80
36	5	2845	A	C8-N9-C4	-5.92	103.43	105.80
36	1	1159	A	N1-C6-N6	-5.91	115.05	118.60
38	4	15	G	N7-C8-N9	-5.91	110.14	113.10
1	6	543	C	C6-N1-C2	-5.91	117.94	120.30
36	5	2375	G	C5-C6-O6	5.91	132.15	128.60
36	5	3328	G	O5'-P-OP2	-5.91	100.38	105.70
36	5	1867	A	C5-C6-N6	-5.91	118.97	123.70
36	1	1115	G	N7-C8-N9	5.91	116.06	113.10
1	6	470	A	N7-C8-N9	5.91	116.75	113.80
36	5	2273	G	N1-C6-O6	-5.91	116.35	119.90
36	5	3195	U	P-O3'-C3'	5.91	126.79	119.70
36	1	2783	U	OP1-P-O3'	5.91	118.20	105.20
36	1	3268	A	N1-C6-N6	5.91	122.14	118.60
1	6	1097	U	P-O3'-C3'	5.91	126.79	119.70
36	5	1591	G	N3-C2-N2	-5.91	115.76	119.90
36	5	2850	G	C8-N9-C4	5.91	108.76	106.40
1	6	1778	G	N7-C8-N9	5.91	116.05	113.10
36	5	921	A	O5'-P-OP2	-5.91	100.38	105.70
1	2	1150	G	C8-N9-C4	5.91	108.76	106.40
1	2	1611	A	C2-N3-C4	-5.91	107.65	110.60
1	6	297	U	N3-C4-O4	5.91	123.53	119.40
36	5	1157	G	N1-C6-O6	-5.91	116.36	119.90
36	5	2341	A	N1-C6-N6	-5.91	115.06	118.60
36	5	3351	U	N3-C2-O2	-5.91	118.07	122.20
37	7	47	C	C2-N3-C4	-5.91	116.95	119.90
36	5	1367	G	C8-N9-C1'	-5.90	119.33	127.00
36	5	796	U	C4-C5-C6	5.90	123.24	119.70
36	5	1188	U	N1-C2-N3	5.90	118.44	114.90
36	1	908	G	C4-N9-C1'	5.90	134.17	126.50
36	1	1116	G	C8-N9-C4	-5.90	104.04	106.40
36	5	2376	G	N1-C6-O6	5.90	123.44	119.90
36	5	3257	C	O5'-P-OP1	-5.90	100.39	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1113	G	N3-C2-N2	-5.90	115.77	119.90
36	1	1428	A	C5-N7-C8	-5.90	100.95	103.90
36	5	2398	A	N1-C6-N6	-5.90	115.06	118.60
36	1	2629	U	O5'-P-OP2	-5.90	100.39	105.70
37	7	121	U	C2-N1-C1'	5.90	124.78	117.70
1	2	1082	C	N3-C2-O2	-5.89	117.77	121.90
36	1	658	G	C4-N9-C1'	5.89	134.16	126.50
36	1	730	C	C6-N1-C2	5.89	122.66	120.30
36	1	948	C	C5-C6-N1	-5.89	118.05	121.00
36	1	1151	U	N1-C2-O2	-5.89	118.67	122.80
36	5	983	A	C6-N1-C2	-5.89	115.06	118.60
36	5	1371	G	C5-N7-C8	5.89	107.25	104.30
36	5	2751	G	C6-C5-N7	-5.89	126.86	130.40
43	16	30	LEU	CA-CB-CG	5.89	128.86	115.30
36	1	81	C	C2-N3-C4	-5.89	116.95	119.90
36	1	1359	C	C5-C4-N4	-5.89	116.08	120.20
36	5	651	G	C4-N9-C1'	5.89	134.16	126.50
36	5	716	A	O4'-C1'-N9	-5.89	103.49	108.20
36	5	3214	U	C5-C4-O4	5.89	129.44	125.90
36	1	2380	U	N3-C4-C5	5.89	118.13	114.60
71	O5	36	LEU	CA-CB-CG	5.89	128.85	115.30
1	6	866	G	O5'-P-OP2	-5.89	100.40	105.70
1	6	923	A	N1-C6-N6	-5.89	115.07	118.60
1	6	1560	U	N3-C2-O2	-5.89	118.08	122.20
36	5	394	G	C5-C6-O6	5.89	132.13	128.60
36	5	3362	A	O4'-C1'-N9	5.89	112.91	108.20
36	1	23	A	C8-N9-C4	-5.89	103.44	105.80
36	1	2177	G	C2-N3-C4	5.89	114.84	111.90
36	1	2987	A	N1-C6-N6	5.89	122.13	118.60
1	6	1267	G	C8-N9-C4	5.89	108.75	106.40
1	2	1324	G	C8-N9-C1'	5.89	134.65	127.00
36	1	638	C	O5'-P-OP1	5.89	117.77	110.70
36	1	651	G	C8-N9-C1'	-5.89	119.35	127.00
36	1	1342	C	N3-C4-C5	5.89	124.25	121.90
36	1	2606	G	N1-C2-N2	-5.89	110.90	116.20
36	1	3268	A	C6-C5-N7	-5.89	128.18	132.30
1	6	1549	C	N3-C4-C5	-5.89	119.55	121.90
36	1	1001	G	N3-C4-N9	5.88	129.53	126.00
1	6	1515	A	C8-N9-C4	-5.88	103.45	105.80
36	5	2307	G	N3-C2-N2	5.88	124.02	119.90
36	5	2434	U	C5-C6-N1	-5.88	119.76	122.70
40	13	232	ARG	NE-CZ-NH1	5.88	123.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	932	U	N1-C2-O2	-5.88	118.68	122.80
36	1	1406	A	N1-C6-N6	5.88	122.13	118.60
36	1	2418	G	N3-C4-C5	-5.88	125.66	128.60
36	5	1476	G	C5-C6-O6	5.88	132.13	128.60
36	5	2728	G	N3-C2-N2	-5.88	115.78	119.90
1	2	1291	G	N1-C2-N3	5.88	127.43	123.90
36	1	1450	G	N1-C6-O6	5.88	123.43	119.90
36	1	1530	U	C6-N1-C2	5.88	124.53	121.00
36	1	2145	A	C6-C5-N7	-5.88	128.18	132.30
36	1	2379	U	C5-C4-O4	-5.88	122.37	125.90
36	5	1192	C	N1-C2-O2	5.88	122.43	118.90
36	5	2402	A	N9-C4-C5	5.88	108.15	105.80
1	2	1600	A	N1-C6-N6	5.88	122.13	118.60
36	1	2206	G	C5-C6-O6	-5.88	125.07	128.60
36	1	2920	U	OP2-P-O3'	5.88	118.13	105.20
1	6	400	A	N1-C6-N6	5.88	122.12	118.60
1	6	448	C	N3-C4-C5	-5.88	119.55	121.90
6	s4	38	LEU	CA-CB-CG	5.88	128.81	115.30
36	1	1210	U	C5-C6-N1	-5.87	119.76	122.70
36	1	2889	C	N1-C2-O2	5.87	122.42	118.90
37	7	69	C	C6-N1-C2	5.87	122.65	120.30
36	1	1116	G	O5'-P-OP1	-5.87	100.42	105.70
36	1	3209	A	N1-C6-N6	5.87	122.12	118.60
1	6	639	U	N1-C2-O2	5.87	126.91	122.80
36	5	693	A	O5'-P-OP2	5.87	117.75	110.70
36	5	2149	A	N1-C6-N6	5.87	122.12	118.60
36	5	2948	C	OP1-P-OP2	-5.87	110.79	119.60
36	1	1669	C	C6-N1-C2	5.87	122.65	120.30
1	6	1763	A	C8-N9-C4	5.87	108.15	105.80
36	5	1143	A	N9-C4-C5	5.87	108.15	105.80
38	8	80	A	C4-C5-C6	5.87	119.94	117.00
36	1	577	C	N1-C2-O2	-5.87	115.38	118.90
36	1	661	G	N7-C8-N9	5.87	116.03	113.10
1	6	1035	G	N1-C6-O6	-5.87	116.38	119.90
36	5	2375	G	N1-C6-O6	-5.87	116.38	119.90
36	1	1377	G	C6-C5-N7	-5.86	126.88	130.40
36	1	2241	U	O5'-P-OP1	-5.86	100.42	105.70
36	1	2692	A	N1-C6-N6	5.86	122.12	118.60
36	1	3308	C	C6-N1-C2	5.86	122.64	120.30
38	4	24	G	C6-C5-N7	-5.86	126.88	130.40
36	5	529	A	N1-C6-N6	5.86	122.12	118.60
36	5	2916	U	C4-C5-C6	5.86	123.22	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	864	U	C6-N1-C2	-5.86	117.48	121.00
1	2	1291	G	C8-N9-C4	-5.86	104.06	106.40
1	2	1657	U	O4'-C1'-N1	5.86	112.89	108.20
36	1	512	U	C5-C6-N1	-5.86	119.77	122.70
36	1	765	C	N1-C2-O2	5.86	122.42	118.90
36	1	802	C	N3-C2-O2	-5.86	117.80	121.90
36	1	805	G	N7-C8-N9	-5.86	110.17	113.10
36	1	1481	A	C8-N9-C1'	-5.86	117.15	127.70
36	1	2409	G	C6-N1-C2	-5.86	121.58	125.10
36	1	2601	A	C8-N9-C4	5.86	108.14	105.80
37	7	121	U	N1-C2-O2	5.86	126.90	122.80
36	1	1112	A	C5-C6-N6	-5.86	119.02	123.70
36	5	2158	A	N1-C6-N6	-5.86	115.09	118.60
36	5	2754	G	N1-C6-O6	-5.86	116.39	119.90
36	5	3099	C	N1-C2-O2	-5.86	115.39	118.90
36	5	3245	A	C8-N9-C4	-5.86	103.46	105.80
36	1	2124	G	C5-C6-O6	-5.85	125.09	128.60
1	2	284	G	C8-N9-C4	5.85	108.74	106.40
36	1	2805	G	N9-C4-C5	-5.85	103.06	105.40
36	1	2953	U	N3-C2-O2	5.85	126.30	122.20
36	5	2941	A	O4'-C1'-N9	-5.85	103.52	108.20
36	1	1113	G	C5-C6-N1	-5.85	108.58	111.50
36	1	1431	G	N7-C8-N9	-5.85	110.17	113.10
36	1	1906	G	N1-C6-O6	5.85	123.41	119.90
36	1	2388	U	OP2-P-O3'	5.85	118.07	105.20
1	6	884	A	C8-N9-C4	5.85	108.14	105.80
1	6	1004	U	N1-C2-O2	-5.85	118.71	122.80
1	6	1127	G	C8-N9-C4	-5.85	104.06	106.40
36	5	819	U	N1-C2-O2	-5.85	118.70	122.80
36	5	2730	G	C5-C6-O6	-5.85	125.09	128.60
37	7	82	G	OP2-P-O3'	5.85	118.07	105.20
36	1	1144	U	N3-C4-C5	5.85	118.11	114.60
36	1	1338	C	N1-C2-O2	-5.85	115.39	118.90
36	1	1370	G	C5-N7-C8	-5.85	101.38	104.30
36	1	1867	A	C8-N9-C4	5.85	108.14	105.80
1	6	75	U	O4'-C1'-N1	5.85	112.88	108.20
1	6	160	C	N3-C2-O2	-5.85	117.81	121.90
36	1	81	C	C5-C4-N4	-5.84	116.11	120.20
36	1	810	A	C2-N3-C4	5.84	113.52	110.60
36	1	1157	G	N9-C4-C5	5.84	107.74	105.40
36	5	1400	G	O5'-P-OP2	5.84	117.71	110.70
36	5	2358	A	N3-C4-N9	-5.84	122.72	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1848	G	O5'-P-OP1	-5.84	100.44	105.70
36	1	2937	G	N3-C2-N2	-5.84	115.81	119.90
1	2	1473	U	C5-C4-O4	5.84	129.40	125.90
36	1	648	C	C2-N1-C1'	5.84	125.22	118.80
36	1	689	U	C2-N1-C1'	5.84	124.71	117.70
1	6	778	G	N9-C4-C5	-5.84	103.06	105.40
36	5	1112	A	N1-C6-N6	5.84	122.10	118.60
36	5	1609	C	N3-C4-N4	5.84	122.09	118.00
36	5	2843	U	N1-C2-O2	5.84	126.89	122.80
36	5	2927	C	N3-C4-N4	5.84	122.09	118.00
36	1	640	U	N3-C4-O4	5.84	123.49	119.40
36	1	2377	G	C2-N3-C4	-5.84	108.98	111.90
1	2	1745	G	O5'-P-OP2	-5.84	100.45	105.70
36	1	650	C	N1-C2-O2	-5.84	115.40	118.90
36	1	2395	G	O5'-P-OP2	-5.84	100.45	105.70
36	5	369	A	C8-N9-C4	-5.84	103.47	105.80
36	5	1449	A	N9-C4-C5	-5.84	103.47	105.80
36	5	1908	A	N9-C4-C5	5.84	108.14	105.80
36	5	2142	A	C2-N3-C4	5.84	113.52	110.60
36	5	2892	A	N1-C2-N3	5.84	132.22	129.30
37	7	94	C	N1-C2-O2	5.84	122.40	118.90
1	2	297	U	N3-C2-O2	-5.83	118.12	122.20
36	1	2777	G	C4-C5-N7	-5.83	108.47	110.80
1	6	596	C	C6-N1-C2	5.83	122.63	120.30
36	5	41	G	OP2-P-O3'	5.83	118.03	105.20
36	5	2656	A	C8-N9-C4	-5.83	103.47	105.80
36	5	668	G	N3-C4-C5	-5.83	125.68	128.60
36	5	942	U	N1-C2-O2	-5.83	118.72	122.80
36	5	969	C	C5-C6-N1	-5.83	118.08	121.00
36	5	1419	A	N1-C6-N6	-5.83	115.10	118.60
36	5	2761	G	C5-C6-N1	5.83	114.42	111.50
36	1	3197	G	C2-N3-C4	-5.83	108.98	111.90
36	5	2187	G	N3-C4-N9	5.83	129.50	126.00
36	1	2419	A	C5-N7-C8	-5.83	100.99	103.90
36	1	2679	A	N1-C6-N6	5.83	122.10	118.60
1	6	1736	G	C5-C6-N1	-5.83	108.59	111.50
36	5	2953	U	C5-C4-O4	-5.83	122.40	125.90
36	5	3308	C	C2-N3-C4	-5.83	116.98	119.90
36	1	580	C	N1-C2-O2	-5.83	115.40	118.90
36	5	1546	A	O5'-P-OP1	-5.83	100.46	105.70
36	1	1301	A	O5'-P-OP1	-5.83	100.46	105.70
36	1	1365	G	C6-N1-C2	-5.82	121.61	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	336	G	O5'-P-OP2	-5.82	100.46	105.70
1	6	1000	C	C5-C6-N1	-5.82	118.09	121.00
36	5	1730	G	C8-N9-C4	5.82	108.73	106.40
36	1	1054	A	O5'-P-OP2	-5.82	100.46	105.70
1	6	360	A	O5'-P-OP2	-5.82	100.46	105.70
36	5	207	U	N3-C2-O2	5.82	126.28	122.20
36	1	1054	A	O5'-P-OP1	5.82	117.68	110.70
54	M8	138	LEU	CA-CB-CG	5.82	128.69	115.30
36	5	805	G	C8-N9-C4	5.82	108.73	106.40
1	2	554	C	N1-C2-O2	5.82	122.39	118.90
36	1	930	U	C2-N3-C4	-5.82	123.51	127.00
36	1	1349	G	N3-C4-C5	-5.82	125.69	128.60
36	1	2281	A	O5'-P-OP2	-5.82	100.46	105.70
36	1	1094	U	C5-C6-N1	5.82	125.61	122.70
1	6	14	C	C5-C6-N1	5.82	123.91	121.00
1	6	622	A	O5'-P-OP2	5.82	117.68	110.70
36	5	121	A	C8-N9-C4	5.82	108.13	105.80
36	5	1800	A	C8-N9-C4	5.82	108.13	105.80
36	5	2891	U	N3-C4-O4	-5.82	115.33	119.40
36	5	2920	U	C5-C4-O4	-5.82	122.41	125.90
36	1	369	A	N7-C8-N9	5.82	116.71	113.80
36	1	1180	A	C5-N7-C8	5.82	106.81	103.90
36	5	75	G	C5-C6-O6	-5.82	125.11	128.60
36	5	90	C	C6-N1-C2	-5.82	117.97	120.30
36	5	2601	A	OP2-P-O3'	5.82	118.00	105.20
36	5	2920	U	OP1-P-OP2	5.82	128.32	119.60
36	1	2226	U	O5'-P-OP1	-5.81	100.47	105.70
1	2	1777	G	N1-C6-O6	5.81	123.39	119.90
36	1	2805	G	C5-C6-O6	-5.81	125.11	128.60
36	1	2875	U	C6-N1-C2	-5.81	117.51	121.00
37	3	39	C	N3-C4-N4	-5.81	113.93	118.00
36	5	2978	U	C5-C6-N1	-5.81	119.79	122.70
36	5	1665	C	N3-C4-N4	-5.81	113.93	118.00
1	2	934	C	C6-N1-C1'	-5.81	113.83	120.80
36	1	2811	A	C8-N9-C4	-5.81	103.48	105.80
36	1	3043	C	OP2-P-O3'	5.81	117.98	105.20
36	5	922	U	N3-C4-O4	-5.81	115.33	119.40
39	l2	238	ILE	CG1-CB-CG2	-5.81	98.62	111.40
50	m4	19	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	2	794	U	P-O3'-C3'	5.81	126.67	119.70
1	2	1658	G	C4-C5-N7	5.81	113.12	110.80
36	5	934	G	C2-N3-C4	5.81	114.80	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	931	C	N3-C4-C5	5.81	124.22	121.90
36	1	1365	G	C4-N9-C1'	5.81	134.05	126.50
36	5	216	G	C4-C5-N7	5.81	113.12	110.80
25	D3	133	LEU	CA-CB-CG	5.80	128.65	115.30
36	1	974	G	N3-C4-C5	-5.80	125.70	128.60
36	1	2787	G	C8-N9-C4	-5.80	104.08	106.40
1	6	1480	G	C8-N9-C4	-5.80	104.08	106.40
36	5	1188	U	C2-N3-C4	-5.80	123.52	127.00
36	5	1911	A	O5'-P-OP2	-5.80	100.48	105.70
36	5	2866	U	OP1-P-O3'	5.80	117.97	105.20
1	2	1274	C	N1-C2-O2	5.80	122.38	118.90
1	2	321	C	N1-C2-O2	5.80	122.38	118.90
36	1	1368	U	N1-C2-O2	-5.80	118.74	122.80
36	1	2420	C	O5'-P-OP1	-5.80	100.48	105.70
38	4	9	A	N1-C6-N6	-5.80	115.12	118.60
1	6	29	U	N3-C2-O2	-5.80	118.14	122.20
1	6	749	U	N3-C2-O2	-5.80	118.14	122.20
36	5	2980	U	N1-C2-N3	5.80	118.38	114.90
36	1	125	C	N3-C4-C5	5.80	124.22	121.90
36	1	3067	C	O5'-P-OP2	-5.80	100.48	105.70
36	5	1897	G	C5-C6-N1	-5.80	108.60	111.50
36	1	1131	G	N9-C4-C5	-5.80	103.08	105.40
36	1	2937	G	N3-C4-C5	5.80	131.50	128.60
1	6	1535	U	O5'-P-OP1	5.80	117.66	110.70
1	2	794	U	N3-C2-O2	-5.79	118.14	122.20
36	1	2808	A	C5-C6-N6	-5.79	119.07	123.70
1	6	647	G	N3-C4-N9	-5.79	122.52	126.00
36	5	3374	U	N3-C4-O4	-5.79	115.34	119.40
36	1	2993	G	C5-C6-O6	-5.79	125.13	128.60
36	5	424	G	N1-C2-N3	-5.79	120.42	123.90
36	5	581	U	C5-C6-N1	5.79	125.60	122.70
36	5	2549	G	C4-N9-C1'	5.79	134.03	126.50
36	5	2904	U	C2-N3-C4	-5.79	123.53	127.00
36	5	3049	A	C8-N9-C4	5.79	108.12	105.80
37	7	110	G	O5'-P-OP2	-5.79	100.49	105.70
36	5	580	C	N1-C2-O2	-5.79	115.43	118.90
36	5	3184	A	C8-N9-C4	5.79	108.12	105.80
36	5	1851	G	C5-C6-N1	-5.79	108.61	111.50
36	5	3380	U	C5-C4-O4	5.79	129.37	125.90
1	2	307	G	C8-N9-C1'	-5.79	119.48	127.00
36	1	511	G	N1-C2-N3	5.79	127.37	123.90
36	1	1417	G	N3-C4-N9	-5.79	122.53	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2944	U	O5'-P-OP1	-5.79	100.49	105.70
37	3	93	C	N3-C4-C5	5.79	124.21	121.90
38	4	9	A	N9-C4-C5	5.79	108.11	105.80
1	6	678	A	P-O3'-C3'	5.79	126.64	119.70
1	6	1333	C	C6-N1-C2	5.79	122.61	120.30
36	5	2393	G	C5-C6-O6	-5.79	125.13	128.60
36	5	2831	G	C2-N3-C4	5.79	114.79	111.90
36	5	2892	A	C4-C5-C6	5.79	119.89	117.00
36	5	2913	C	C6-N1-C1'	5.79	127.74	120.80
36	1	37	U	N3-C4-C5	-5.78	111.13	114.60
1	6	420	A	N1-C6-N6	5.78	122.07	118.60
36	5	972	A	N1-C6-N6	-5.78	115.13	118.60
36	5	975	C	N3-C4-C5	-5.78	119.59	121.90
36	5	2549	G	C6-C5-N7	-5.78	126.93	130.40
36	1	716	A	C5-N7-C8	-5.78	101.01	103.90
36	1	3038	U	N1-C2-O2	-5.78	118.75	122.80
36	5	2683	U	N1-C2-O2	5.78	126.85	122.80
38	8	110	C	OP2-P-O3'	5.78	117.92	105.20
1	2	532	U	O5'-P-OP1	-5.78	100.50	105.70
1	2	794	U	N1-C2-O2	5.78	126.85	122.80
36	1	1097	G	P-O3'-C3'	5.78	126.64	119.70
1	6	255	U	N3-C2-O2	5.78	126.25	122.20
1	2	1291	G	N7-C8-N9	5.78	115.99	113.10
36	1	347	G	C6-C5-N7	-5.78	126.93	130.40
36	1	1405	U	C6-N1-C2	5.78	124.47	121.00
36	5	1126	G	C8-N9-C4	-5.78	104.09	106.40
36	5	1520	G	N1-C6-O6	5.78	123.37	119.90
36	1	3326	G	N7-C8-N9	-5.78	110.21	113.10
1	6	1027	A	C5-N7-C8	-5.78	101.01	103.90
36	5	2892	A	C8-N9-C4	-5.78	103.49	105.80
36	5	2953	U	N3-C2-O2	5.78	126.24	122.20
38	8	96	A	N9-C4-C5	-5.78	103.49	105.80
36	1	3217	C	C6-N1-C1'	-5.77	113.87	120.80
36	5	1130	A	C2-N3-C4	5.77	113.49	110.60
36	1	672	A	C6-C5-N7	-5.77	128.26	132.30
38	4	142	C	C6-N1-C2	-5.77	117.99	120.30
36	5	1151	U	N3-C2-O2	5.77	126.24	122.20
36	5	2833	A	C8-N9-C4	5.77	108.11	105.80
36	1	1007	U	C6-N1-C2	5.77	124.46	121.00
36	1	3218	A	C8-N9-C4	-5.77	103.49	105.80
36	5	1208	U	N3-C2-O2	-5.77	118.16	122.20
36	5	2142	A	O5'-P-OP1	5.77	117.62	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3095	U	N3-C2-O2	-5.77	118.16	122.20
36	1	422	A	C5-C6-N6	5.77	128.32	123.70
36	1	1474	A	C2-N3-C4	-5.77	107.72	110.60
36	1	3375	A	C8-N9-C4	-5.77	103.49	105.80
1	6	553	G	C5-C6-O6	-5.77	125.14	128.60
1	6	1031	U	C5-C6-N1	-5.77	119.81	122.70
36	5	911	C	C4-C5-C6	5.77	120.28	117.40
36	5	2246	G	C2-N3-C4	5.77	114.78	111.90
36	5	3136	G	N1-C2-N3	5.77	127.36	123.90
36	1	1902	G	C6-C5-N7	-5.77	126.94	130.40
1	6	119	A	C2-N3-C4	-5.77	107.72	110.60
36	5	2202	C	C6-N1-C2	-5.77	117.99	120.30
36	1	420	G	O4'-C1'-N9	5.77	112.81	108.20
36	5	2514	U	C5-C6-N1	5.77	125.58	122.70
36	1	2406	C	N3-C2-O2	5.76	125.94	121.90
36	1	3269	U	C5-C4-O4	5.76	129.36	125.90
36	5	3335	A	C6-C5-N7	-5.76	128.26	132.30
36	1	843	A	C2-N3-C4	-5.76	107.72	110.60
36	5	2121	G	C5-C6-O6	-5.76	125.14	128.60
36	5	2899	C	N3-C4-N4	5.76	122.03	118.00
36	5	2948	C	N3-C4-N4	-5.76	113.97	118.00
1	2	1462	G	N9-C4-C5	-5.76	103.09	105.40
36	1	699	A	N3-C4-N9	-5.76	122.79	127.40
1	6	1632	C	N1-C2-O2	5.76	122.36	118.90
36	5	2392	C	C5-C6-N1	-5.76	118.12	121.00
36	1	1613	A	N1-C6-N6	5.76	122.06	118.60
36	5	661	G	C5-C6-O6	-5.76	125.14	128.60
36	5	2830	G	OP2-P-O3'	5.76	117.87	105.20
36	1	911	C	O5'-P-OP2	5.76	117.61	110.70
36	1	2904	U	O5'-P-OP2	-5.76	100.52	105.70
36	5	2825	C	C6-N1-C2	5.76	122.60	120.30
1	2	380	U	N3-C2-O2	-5.76	118.17	122.20
1	6	361	C	OP1-P-OP2	-5.76	110.97	119.60
36	5	2892	A	N7-C8-N9	5.76	116.68	113.80
36	1	20	A	C8-N9-C4	-5.75	103.50	105.80
1	2	992	A	C5-N7-C8	-5.75	101.02	103.90
36	1	2619	G	OP1-P-OP2	5.75	128.23	119.60
36	1	2624	G	C6-C5-N7	-5.75	126.95	130.40
36	5	981	U	C5-C6-N1	5.75	125.58	122.70
36	5	2351	U	C5-C6-N1	5.75	125.58	122.70
36	5	3392	U	C5-C4-O4	5.75	129.35	125.90
36	1	880	G	C8-N9-C4	5.75	108.70	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2905	U	N3-C2-O2	5.75	126.22	122.20
36	5	2700	G	N9-C4-C5	-5.75	103.10	105.40
36	5	2847	A	C8-N9-C4	5.75	108.10	105.80
36	1	349	A	OP2-P-O3'	5.75	117.84	105.20
36	1	969	C	C4-C5-C6	5.75	120.27	117.40
36	1	2585	G	N3-C4-C5	-5.75	125.73	128.60
1	6	769	A	C8-N9-C4	-5.75	103.50	105.80
1	6	1479	A	N1-C6-N6	5.75	122.05	118.60
36	5	2352	A	C4-C5-C6	5.75	119.87	117.00
36	5	3217	C	C6-N1-C1'	5.75	127.70	120.80
1	6	111	U	C6-N1-C2	-5.75	117.55	121.00
1	6	1765	A	C8-N9-C4	5.75	108.10	105.80
36	1	3217	C	N1-C2-O2	5.74	122.35	118.90
1	6	1670	G	C5-C6-N1	5.74	114.37	111.50
36	5	1902	G	N3-C4-N9	5.74	129.45	126.00
38	8	115	C	N3-C2-O2	5.74	125.92	121.90
1	6	163	G	N1-C2-N2	5.74	121.37	116.20
36	1	49	A	C2-N3-C4	-5.74	107.73	110.60
36	1	1206	G	C5-C6-N1	-5.74	108.63	111.50
37	3	110	G	O5'-P-OP2	-5.74	100.53	105.70
1	6	631	G	C5-C6-O6	-5.74	125.16	128.60
6	s4	222	LEU	CA-CB-CG	5.74	128.50	115.30
36	5	1885	U	C5-C6-N1	-5.74	119.83	122.70
1	2	1597	A	N1-C6-N6	5.74	122.04	118.60
36	1	2617	U	N3-C4-O4	-5.74	115.38	119.40
36	1	3207	U	C2-N1-C1'	-5.74	110.81	117.70
37	7	103	A	C5-C6-N6	-5.74	119.11	123.70
1	2	1258	U	N3-C2-O2	-5.74	118.18	122.20
36	5	2709	C	N3-C4-C5	5.74	124.19	121.90
62	N6	126	LEU	CA-CB-CG	5.74	128.49	115.30
1	6	749	U	N1-C2-N3	5.74	118.34	114.90
36	5	1116	G	C5-C6-O6	5.74	132.04	128.60
36	5	1367	G	C4-C5-C6	5.74	122.24	118.80
36	1	2916	U	C5-C4-O4	-5.73	122.46	125.90
36	5	2994	A	C5-C6-N6	-5.73	119.11	123.70
43	L6	55	LEU	CA-CB-CG	-5.73	102.11	115.30
1	6	543	C	N1-C2-O2	5.73	122.34	118.90
5	s3	202	LEU	CA-CB-CG	5.73	128.48	115.30
36	1	2168	A	C2-N3-C4	5.73	113.47	110.60
36	1	2950	G	O4'-C1'-N9	5.73	112.78	108.20
36	5	1788	C	O5'-P-OP2	-5.73	100.54	105.70
36	5	1931	U	C2-N3-C4	-5.73	123.56	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	646	A	N1-C2-N3	5.73	132.16	129.30
36	1	808	A	C4-C5-N7	-5.73	107.83	110.70
36	1	1414	G	OP1-P-O3'	5.73	117.80	105.20
36	1	2244	A	C8-N9-C4	5.73	108.09	105.80
38	4	79	A	C8-N9-C4	-5.73	103.51	105.80
36	1	829	U	C2-N1-C1'	5.73	124.57	117.70
36	5	2862	U	N3-C2-O2	-5.73	118.19	122.20
36	1	501	A	C5-C6-N6	-5.73	119.12	123.70
36	1	2734	A	N1-C6-N6	5.73	122.04	118.60
44	L7	110	ARG	NE-CZ-NH2	-5.73	117.44	120.30
25	d3	33	LEU	CB-CG-CD1	-5.73	101.27	111.00
36	5	2950	G	C4-C5-N7	5.73	113.09	110.80
36	5	218	G	C2-N3-C4	5.72	114.76	111.90
36	5	1008	U	C2-N1-C1'	-5.72	110.83	117.70
36	5	1380	G	N9-C4-C5	-5.72	103.11	105.40
36	5	2245	C	C2-N1-C1'	5.72	125.10	118.80
1	2	720	G	OP1-P-O3'	5.72	117.79	105.20
36	1	1789	G	N1-C6-O6	-5.72	116.47	119.90
36	5	2892	A	N1-C6-N6	5.72	122.03	118.60
36	5	2164	A	C8-N9-C4	-5.72	103.51	105.80
1	2	11	A	O5'-P-OP1	-5.72	100.55	105.70
1	2	1052	U	C2-N1-C1'	5.72	124.56	117.70
36	1	870	G	N9-C4-C5	5.72	107.69	105.40
36	5	914	A	N1-C6-N6	5.72	122.03	118.60
36	5	399	A	C5-C6-N6	-5.72	119.13	123.70
36	1	49	A	C5-C6-N1	-5.72	114.84	117.70
36	1	544	C	C6-N1-C2	-5.72	118.01	120.30
36	1	2222	A	O4'-C1'-N9	-5.72	103.63	108.20
1	6	1127	G	N7-C8-N9	5.72	115.96	113.10
1	6	1773	C	C4-C5-C6	5.72	120.26	117.40
37	7	92	A	N9-C4-C5	-5.72	103.51	105.80
36	1	934	G	C8-N9-C1'	-5.71	119.57	127.00
36	1	2812	C	C2-N3-C4	-5.71	117.04	119.90
36	1	2820	A	OP1-P-O3'	-5.71	92.63	105.20
1	6	308	C	C2-N1-C1'	-5.71	112.51	118.80
36	5	416	A	C8-N9-C4	-5.71	103.52	105.80
36	5	984	G	N3-C4-C5	-5.71	125.74	128.60
36	5	2187	G	C6-C5-N7	-5.71	126.97	130.40
36	5	3154	C	N3-C2-O2	-5.71	117.90	121.90
1	2	852	C	C5-C6-N1	5.71	123.86	121.00
36	1	410	U	N3-C4-C5	-5.71	111.17	114.60
36	1	2607	G	N1-C2-N2	-5.71	111.06	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1540	G	N1-C6-O6	-5.71	116.47	119.90
36	5	2110	G	N1-C6-O6	5.71	123.33	119.90
37	7	34	C	C6-N1-C2	-5.71	118.02	120.30
1	2	186	C	C6-N1-C2	-5.71	118.02	120.30
36	1	2357	A	N1-C6-N6	5.71	122.03	118.60
36	1	1492	G	N7-C8-N9	-5.71	110.25	113.10
36	1	3079	U	C2-N1-C1'	-5.71	110.85	117.70
36	1	1402	C	N3-C2-O2	-5.71	117.91	121.90
36	1	3362	A	N1-C6-N6	5.71	122.02	118.60
1	6	154	G	C6-C5-N7	-5.71	126.98	130.40
36	5	110	G	N7-C8-N9	-5.71	110.25	113.10
36	5	518	G	O4'-C1'-N9	5.71	112.77	108.20
36	1	910	G	C8-N9-C4	-5.71	104.12	106.40
36	5	835	G	C8-N9-C4	5.71	108.68	106.40
36	5	1400	G	N3-C4-C5	-5.71	125.75	128.60
36	5	2144	A	N1-C6-N6	5.71	122.02	118.60
36	1	1307	G	C5-C6-N1	5.70	114.35	111.50
36	1	1389	G	C5-N7-C8	-5.70	101.45	104.30
36	1	1481	A	O5'-P-OP1	5.70	117.54	110.70
36	1	1902	G	N7-C8-N9	5.70	115.95	113.10
36	5	1307	G	C2'-C3'-O3'	5.70	122.83	113.70
36	5	2983	C	O5'-P-OP1	-5.70	100.57	105.70
38	4	151	C	N3-C4-C5	-5.70	119.62	121.90
36	5	1060	U	N1-C2-O2	5.70	126.79	122.80
36	1	1110	U	C4-C5-C6	-5.70	116.28	119.70
36	1	1838	G	C8-N9-C1'	-5.70	119.59	127.00
36	1	2404	A	C5-C6-N1	5.70	120.55	117.70
1	6	607	G	C4-C5-C6	5.70	122.22	118.80
36	5	568	G	C5-C6-N1	5.70	114.35	111.50
36	5	1180	A	O4'-C1'-N9	-5.70	103.64	108.20
36	5	426	G	O5'-P-OP2	-5.70	100.57	105.70
36	5	708	G	C8-N9-C4	-5.70	104.12	106.40
36	5	2836	C	OP2-P-O3'	5.70	117.74	105.20
36	1	820	A	C5-N7-C8	-5.70	101.05	103.90
36	1	2124	G	C6-C5-N7	-5.70	126.98	130.40
1	6	610	G	N3-C4-N9	5.70	129.42	126.00
1	6	1562	G	N1-C6-O6	5.70	123.32	119.90
20	c8	116	LEU	CA-CB-CG	5.70	128.40	115.30
36	5	3315	G	C5-C6-O6	5.70	132.02	128.60
1	2	137	U	N3-C2-O2	-5.69	118.21	122.20
1	2	1096	C	C2-N1-C1'	5.69	125.06	118.80
36	1	805	G	N9-C4-C5	-5.69	103.12	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	104	A	N1-C6-N6	-5.69	115.18	118.60
36	1	72	C	C6-N1-C1'	5.69	127.63	120.80
36	1	994	G	C5-C6-N1	5.69	114.35	111.50
1	6	1614	A	C4-C5-N7	5.69	113.55	110.70
36	5	2380	U	N1-C2-N3	5.69	118.31	114.90
1	2	901	G	C5-C6-O6	-5.69	125.19	128.60
36	1	2623	G	N1-C2-N3	5.69	127.31	123.90
1	6	1782	A	N7-C8-N9	5.69	116.64	113.80
36	5	810	A	C2-N3-C4	5.69	113.44	110.60
36	5	981	U	C6-N1-C2	-5.69	117.59	121.00
36	1	2702	A	C8-N9-C4	-5.69	103.53	105.80
36	1	2893	C	N3-C4-C5	5.69	124.17	121.90
36	5	23	A	N1-C6-N6	5.69	122.01	118.60
36	1	968	G	C5-C6-N1	5.68	114.34	111.50
36	1	2144	A	C2-N3-C4	5.68	113.44	110.60
36	5	2642	A	N1-C6-N6	-5.68	115.19	118.60
36	5	2651	G	OP2-P-O3'	5.68	117.70	105.20
37	7	91	G	C6-C5-N7	-5.68	126.99	130.40
36	5	3008	A	N3-C4-N9	-5.68	122.86	127.40
36	1	303	G	C8-N9-C4	5.68	108.67	106.40
36	1	635	G	C5-C6-O6	-5.68	125.19	128.60
36	1	885	U	C5-C6-N1	-5.68	119.86	122.70
36	1	2367	A	C6-C5-N7	-5.68	128.32	132.30
36	1	2936	A	O5'-P-OP2	5.68	117.52	110.70
47	M0	24	ARG	NE-CZ-NH1	5.68	123.14	120.30
36	5	2970	C	O5'-P-OP1	-5.68	100.59	105.70
36	1	2850	G	N9-C4-C5	-5.68	103.13	105.40
38	4	113	U	N3-C2-O2	-5.68	118.22	122.20
36	5	2870	C	C6-N1-C1'	5.68	127.61	120.80
36	1	1103	A	P-O3'-C3'	5.68	126.51	119.70
36	1	2283	G	N9-C4-C5	-5.68	103.13	105.40
1	6	1697	G	N3-C4-C5	-5.68	125.76	128.60
37	7	121	U	N3-C2-O2	-5.68	118.23	122.20
36	1	1661	G	N3-C4-N9	5.67	129.40	126.00
36	1	2177	G	N3-C2-N2	5.67	123.87	119.90
38	4	53	A	N9-C4-C5	5.67	108.07	105.80
36	5	3143	C	N3-C2-O2	5.67	125.87	121.90
36	1	2130	G	N3-C2-N2	5.67	123.87	119.90
1	6	1152	A	N1-C6-N6	-5.67	115.20	118.60
1	6	1653	C	N3-C2-O2	-5.67	117.93	121.90
36	5	1184	A	N9-C4-C5	5.67	108.07	105.80
1	2	1490	C	C2-N1-C1'	5.67	125.04	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1746	A	O5'-P-OP1	-5.67	100.60	105.70
36	1	2166	A	O5'-P-OP2	5.67	117.51	110.70
36	1	2677	G	N1-C6-O6	-5.67	116.50	119.90
36	5	758	C	C2-N1-C1'	-5.67	112.56	118.80
1	2	966	A	C6-C5-N7	-5.67	128.33	132.30
36	5	1133	A	C8-N9-C4	-5.67	103.53	105.80
36	1	2369	G	N3-C2-N2	-5.67	115.93	119.90
36	1	3171	U	C6-N1-C2	5.67	124.40	121.00
36	5	559	A	C8-N9-C4	-5.67	103.53	105.80
36	5	1499	C	N1-C2-O2	-5.67	115.50	118.90
36	5	2416	U	C6-N1-C2	-5.67	117.60	121.00
36	5	1003	A	C8-N9-C4	5.67	108.07	105.80
36	5	1190	A	N1-C6-N6	-5.67	115.20	118.60
36	5	1452	A	N9-C4-C5	-5.67	103.53	105.80
54	m8	39	ARG	NE-CZ-NH1	-5.67	117.47	120.30
36	1	1269	U	N1-C2-O2	5.67	126.77	122.80
1	6	1296	A	N1-C6-N6	5.67	122.00	118.60
1	6	1781	A	C4-C5-C6	5.67	119.83	117.00
1	6	426	G	C4-N9-C1'	5.66	133.86	126.50
1	6	1549	C	C6-N1-C2	-5.66	118.03	120.30
36	5	27	C	N1-C2-O2	-5.66	115.50	118.90
1	2	1420	C	N3-C4-N4	5.66	121.96	118.00
36	1	2622	C	N3-C4-N4	5.66	121.96	118.00
36	5	358	G	O5'-P-OP2	-5.66	100.60	105.70
36	1	610	G	N1-C6-O6	-5.66	116.50	119.90
36	5	2817	A	N9-C4-C5	5.66	108.06	105.80
1	2	1018	U	O5'-P-OP1	-5.66	100.61	105.70
36	1	919	U	N3-C4-O4	-5.66	115.44	119.40
38	4	53	A	C2-N3-C4	5.66	113.43	110.60
36	5	2697	A	N1-C6-N6	5.66	122.00	118.60
1	6	523	G	C8-N9-C4	5.66	108.66	106.40
36	5	81	C	N3-C4-C5	5.66	124.16	121.90
1	6	1596	C	N1-C2-O2	5.65	122.29	118.90
36	5	1187	C	O5'-P-OP2	-5.65	100.61	105.70
36	1	1513	G	N3-C4-C5	-5.65	125.77	128.60
38	4	111	A	C6-C5-N7	-5.65	128.34	132.30
38	4	111	A	C4-C5-N7	5.65	113.53	110.70
54	M8	99	THR	N-CA-C	5.65	126.26	111.00
38	8	84	C	N3-C2-O2	-5.65	117.94	121.90
1	2	1027	A	C5-N7-C8	-5.65	101.07	103.90
36	1	1331	U	O4'-C1'-N1	-5.65	103.68	108.20
36	1	2995	A	C8-N9-C4	5.65	108.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1158	A	C5-C6-N6	-5.65	119.18	123.70
36	5	2643	A	C5-C6-N6	-5.65	119.18	123.70
36	5	2887	A	O4'-C1'-N9	-5.65	103.68	108.20
36	5	1116	G	OP2-P-O3'	5.65	117.62	105.20
36	5	2728	G	O5'-P-OP2	-5.65	100.62	105.70
36	1	97	U	N1-C2-O2	-5.64	118.85	122.80
36	1	2355	G	C4-C5-C6	5.64	122.19	118.80
37	3	101	G	N9-C4-C5	-5.64	103.14	105.40
1	6	1119	G	O5'-P-OP2	-5.64	100.62	105.70
36	5	180	C	N3-C2-O2	-5.64	117.95	121.90
36	5	942	U	N1-C2-N3	5.64	118.29	114.90
36	5	2292	U	N3-C2-O2	-5.64	118.25	122.20
36	5	2897	A	C5-C6-N6	-5.64	119.19	123.70
36	5	3218	A	P-O3'-C3'	5.64	126.47	119.70
36	5	360	G	C5-C6-O6	5.64	131.99	128.60
36	5	1429	G	N3-C2-N2	5.64	123.85	119.90
36	5	2916	U	OP1-P-O3'	5.64	117.61	105.20
36	5	2950	G	N1-C2-N3	-5.64	120.51	123.90
36	5	3093	C	O4'-C1'-N1	-5.64	103.69	108.20
1	2	20	G	C2-N3-C4	-5.64	109.08	111.90
1	2	393	C	N3-C4-C5	5.64	124.16	121.90
1	6	472	U	N1-C2-N3	5.64	118.28	114.90
36	5	86	G	C5-C6-O6	-5.64	125.22	128.60
36	5	1399	A	N1-C6-N6	5.64	121.98	118.60
36	1	1376	C	C4-C5-C6	5.64	120.22	117.40
1	6	6	G	N1-C6-O6	5.64	123.28	119.90
36	5	287	G	N3-C4-C5	-5.64	125.78	128.60
36	1	344	A	C6-C5-N7	5.64	136.25	132.30
36	5	646	A	N7-C8-N9	5.64	116.62	113.80
36	5	1789	G	N3-C4-N9	-5.64	122.62	126.00
36	1	3305	A	N9-C4-C5	5.64	108.06	105.80
38	4	9	A	O5'-P-OP1	5.64	117.47	110.70
1	6	1781	A	OP2-P-O3'	5.64	117.60	105.20
36	5	952	A	N1-C6-N6	5.64	121.98	118.60
1	2	187	G	P-O3'-C3'	5.63	126.46	119.70
1	2	380	U	N1-C2-O2	5.63	126.74	122.80
36	1	2404	A	N1-C2-N3	-5.63	126.48	129.30
1	6	66	U	P-O3'-C3'	5.63	126.46	119.70
36	1	1049	C	C5-C4-N4	-5.63	116.26	120.20
37	3	91	G	N1-C2-N3	5.63	127.28	123.90
36	5	1868	G	N3-C2-N2	5.63	123.84	119.90
37	7	120	C	C6-N1-C2	5.63	122.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2719	U	N1-C2-N3	5.63	118.28	114.90
36	5	1158	A	C6-C5-N7	-5.63	128.36	132.30
36	5	2524	A	N9-C1'-C2'	5.63	121.32	114.00
36	5	2700	G	N3-C4-N9	5.63	129.38	126.00
1	2	966	A	C5-C6-N6	-5.63	119.20	123.70
36	1	653	A	O5'-P-OP2	-5.63	100.64	105.70
36	1	793	C	N3-C4-N4	5.63	121.94	118.00
36	1	1307	G	C2'-C3'-O3'	5.63	122.71	113.70
36	1	3183	A	C5-N7-C8	-5.63	101.09	103.90
38	4	73	U	C4-C5-C6	-5.63	116.32	119.70
36	5	1907	C	N3-C4-C5	-5.63	119.65	121.90
1	2	294	C	C6-N1-C2	5.63	122.55	120.30
36	1	1555	U	C2-N1-C1'	-5.63	110.95	117.70
36	1	3050	U	N1-C2-O2	5.63	126.74	122.80
37	3	10	C	N3-C2-O2	-5.63	117.96	121.90
1	6	617	U	C2-N1-C1'	5.63	124.45	117.70
36	5	2856	G	N7-C8-N9	5.63	115.91	113.10
36	5	3331	U	C5-C6-N1	-5.63	119.89	122.70
36	1	658	G	C8-N9-C1'	-5.62	119.69	127.00
36	1	2886	U	N1-C2-O2	-5.62	118.86	122.80
36	1	611	A	N1-C6-N6	5.62	121.97	118.60
36	1	954	U	N1-C2-O2	-5.62	118.86	122.80
36	1	1507	G	C4-C5-C6	5.62	122.17	118.80
36	5	388	G	N1-C6-O6	5.62	123.27	119.90
1	2	913	G	C4-N9-C1'	5.62	133.81	126.50
36	1	709	A	N7-C8-N9	-5.62	110.99	113.80
36	1	3110	C	C2-N1-C1'	5.62	124.98	118.80
1	6	272	U	C2-N1-C1'	5.62	124.45	117.70
1	6	1589	C	C6-N1-C2	-5.62	118.05	120.30
36	5	3140	G	C5-C6-O6	-5.62	125.23	128.60
36	1	685	G	N1-C6-O6	5.62	123.27	119.90
1	2	1324	G	C6-C5-N7	5.62	133.77	130.40
36	1	125	C	C2-N3-C4	-5.62	117.09	119.90
36	1	1835	A	C6-N1-C2	5.62	121.97	118.60
36	1	2332	A	C2-N3-C4	-5.62	107.79	110.60
38	4	97	A	C8-N9-C4	-5.62	103.55	105.80
36	5	1473	G	C5-N7-C8	5.62	107.11	104.30
36	1	688	G	N3-C4-N9	5.62	129.37	126.00
36	5	2837	A	O5'-P-OP2	5.62	117.44	110.70
36	1	1590	G	C5-C6-O6	5.62	131.97	128.60
53	M7	3	ARG	NE-CZ-NH2	-5.62	117.49	120.30
36	5	2730	G	N1-C6-O6	5.62	123.27	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2953	U	N1-C2-O2	-5.62	118.87	122.80
1	2	736	C	C5-C6-N1	5.61	123.81	121.00
36	1	352	A	C2-N3-C4	-5.61	107.79	110.60
36	1	1399	A	N3-C4-N9	-5.61	122.91	127.40
37	3	88	G	C4-C5-N7	-5.61	108.56	110.80
50	M4	135	LEU	CA-CB-CG	5.61	128.21	115.30
36	5	2372	A	N7-C8-N9	5.61	116.61	113.80
37	7	49	G	C4-C5-C6	5.61	122.17	118.80
1	2	1745	G	N3-C4-C5	-5.61	125.79	128.60
36	1	968	G	N3-C2-N2	5.61	123.83	119.90
36	1	2383	C	C2-N3-C4	-5.61	117.09	119.90
36	5	340	C	C6-N1-C2	5.61	122.55	120.30
36	5	644	G	N9-C4-C5	5.61	107.64	105.40
1	2	186	C	C2-N1-C1'	5.61	124.97	118.80
1	2	1560	U	C6-N1-C2	-5.61	117.63	121.00
36	1	1165	A	C8-N9-C4	5.61	108.04	105.80
36	1	1848	G	C5-C6-O6	-5.61	125.23	128.60
36	1	2612	U	C5-C6-N1	-5.61	119.89	122.70
36	1	2918	G	N3-C4-C5	-5.61	125.80	128.60
36	5	2110	G	C6-C5-N7	-5.61	127.03	130.40
36	5	2926	A	N1-C6-N6	5.61	121.97	118.60
36	5	845	G	OP1-P-O3'	5.61	117.54	105.20
36	1	428	A	C5-C6-N1	5.61	120.50	117.70
36	1	2153	U	N1-C2-N3	5.61	118.26	114.90
36	1	2775	U	C5-C6-N1	-5.61	119.90	122.70
1	6	1765	A	N1-C6-N6	-5.61	115.23	118.60
36	5	385	A	N9-C4-C5	-5.61	103.56	105.80
36	5	1813	A	C8-N9-C4	-5.61	103.56	105.80
36	1	2734	A	C8-N9-C4	5.61	108.04	105.80
36	5	2144	A	O4'-C1'-N9	5.61	112.69	108.20
38	8	54	A	N1-C6-N6	5.61	121.96	118.60
1	6	455	C	N1-C2-O2	-5.60	115.54	118.90
1	6	1772	C	C4-C5-C6	5.60	120.20	117.40
36	1	217	U	N3-C4-O4	5.60	123.32	119.40
36	1	614	C	C2-N3-C4	-5.60	117.10	119.90
36	5	283	G	O4'-C1'-N9	-5.60	103.72	108.20
36	5	1160	C	C2-N1-C1'	-5.60	112.64	118.80
36	5	2721	A	O5'-P-OP1	-5.60	100.66	105.70
36	5	2758	A	C5-C6-N1	5.60	120.50	117.70
37	7	50	U	C5-C6-N1	5.60	125.50	122.70
38	8	100	U	C2-N1-C1'	5.60	124.42	117.70
38	8	109	A	OP2-P-O3'	5.60	117.52	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	391	A	C8-N9-C4	5.60	108.04	105.80
36	1	284	A	C4-C5-C6	5.60	119.80	117.00
36	1	2308	C	C5-C6-N1	-5.60	118.20	121.00
36	1	3342	A	N1-C6-N6	5.60	121.96	118.60
41	L4	139	GLY	N-CA-C	-5.60	99.10	113.10
36	1	345	G	C4-C5-C6	5.60	122.16	118.80
36	1	1507	G	N3-C2-N2	-5.60	115.98	119.90
36	1	2414	G	N3-C2-N2	-5.60	115.98	119.90
36	1	2967	A	N1-C6-N6	5.60	121.96	118.60
36	1	3188	G	C8-N9-C4	5.60	108.64	106.40
36	1	3214	U	N1-C2-O2	5.60	126.72	122.80
1	6	1568	C	P-O3'-C3'	5.60	126.42	119.70
36	5	1507	G	N3-C2-N2	-5.60	115.98	119.90
36	5	2179	C	C6-N1-C2	5.60	122.54	120.30
36	5	3102	G	N3-C4-C5	-5.60	125.80	128.60
1	2	21	U	C5-C4-O4	-5.60	122.54	125.90
36	5	3362	A	C2-N3-C4	-5.60	107.80	110.60
36	1	842	G	O5'-P-OP2	-5.59	100.66	105.70
36	1	1316	C	N1-C2-O2	-5.59	115.54	118.90
36	1	2987	A	C6-C5-N7	-5.59	128.38	132.30
42	L5	146	LEU	CA-CB-CG	5.59	128.17	115.30
36	5	1101	G	O5'-P-OP1	5.59	117.41	110.70
36	5	1175	C	N3-C4-C5	5.59	124.14	121.90
36	5	2420	C	N3-C2-O2	5.59	125.82	121.90
36	5	2900	A	OP2-P-O3'	5.59	117.51	105.20
36	1	612	U	N3-C4-O4	-5.59	115.49	119.40
36	1	866	A	N1-C6-N6	5.59	121.95	118.60
36	1	1434	G	C8-N9-C4	-5.59	104.16	106.40
36	1	1520	G	C2-N3-C4	5.59	114.69	111.90
36	5	669	U	C5-C6-N1	-5.59	119.90	122.70
36	5	1929	G	C2-N3-C4	-5.59	109.10	111.90
1	6	364	G	C8-N9-C4	5.59	108.64	106.40
36	5	1420	C	N1-C2-O2	-5.59	115.55	118.90
36	5	2121	G	C4-C5-N7	5.59	113.04	110.80
36	5	3058	U	O4'-C1'-N1	5.59	112.67	108.20
38	8	80	A	N3-C4-C5	-5.59	122.89	126.80
1	2	448	C	N3-C2-O2	-5.59	117.99	121.90
36	1	347	G	N1-C6-O6	5.59	123.25	119.90
36	1	942	U	C2-N3-C4	-5.59	123.65	127.00
36	1	954	U	C6-N1-C2	-5.59	117.65	121.00
36	1	984	G	C4-C5-C6	5.59	122.15	118.80
36	1	2343	C	N3-C4-C5	5.59	124.13	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	542	A	P-O3'-C3'	5.59	126.40	119.70
12	c0	88	PRO	N-CA-CB	5.59	110.00	103.30
36	5	352	A	O5'-P-OP1	-5.59	100.67	105.70
36	5	2400	G	C2-N3-C4	-5.59	109.11	111.90
36	5	2945	G	OP1-P-OP2	-5.59	111.22	119.60
36	5	3326	G	C8-N9-C4	5.59	108.63	106.40
36	1	1419	A	O5'-P-OP1	5.58	117.40	110.70
36	1	2416	U	C6-N1-C2	-5.58	117.65	121.00
68	o2	105	ARG	NE-CZ-NH2	-5.58	117.51	120.30
36	1	1207	G	C5-C6-O6	-5.58	125.25	128.60
36	1	1303	A	C5-C6-N6	-5.58	119.23	123.70
36	1	1507	G	N3-C4-C5	-5.58	125.81	128.60
36	1	2606	G	C8-N9-C1'	-5.58	119.74	127.00
1	6	1796	C	C5-C6-N1	-5.58	118.21	121.00
12	c0	97	PRO	N-CA-CB	5.58	110.00	103.30
52	m6	69	GLY	N-CA-C	-5.58	99.14	113.10
36	1	2968	G	N1-C2-N2	-5.58	111.18	116.20
38	4	125	U	C6-N1-C1'	-5.58	113.39	121.20
49	M3	85	LEU	CA-CB-CG	5.58	128.13	115.30
36	5	1701	C	N3-C4-C5	-5.58	119.67	121.90
36	1	667	C	N3-C4-C5	5.58	124.13	121.90
36	1	936	A	C5-N7-C8	-5.58	101.11	103.90
36	1	1727	G	C2-N3-C4	5.58	114.69	111.90
1	6	858	G	C4-C5-N7	5.58	113.03	110.80
36	5	1359	C	C5-C4-N4	-5.58	116.30	120.20
36	5	3075	G	C6-C5-N7	-5.58	127.05	130.40
68	o2	4	LEU	C-N-CA	-5.58	98.57	122.00
64	N8	116	GLY	N-CA-C	5.58	127.04	113.10
1	6	160	C	N1-C2-O2	5.58	122.25	118.90
36	5	1335	C	N3-C2-O2	5.58	125.80	121.90
36	1	41	G	N1-C2-N3	-5.58	120.56	123.90
36	1	2385	G	C8-N9-C4	5.58	108.63	106.40
36	1	2572	C	C6-N1-C1'	-5.58	114.11	120.80
36	1	2679	A	O4'-C1'-N9	5.58	112.66	108.20
1	6	1680	G	C4-C5-N7	5.58	113.03	110.80
36	1	1177	G	C5-C6-O6	-5.57	125.26	128.60
36	1	1382	G	N1-C6-O6	5.57	123.24	119.90
37	7	88	G	N1-C6-O6	-5.57	116.56	119.90
38	8	39	G	N3-C4-C5	-5.57	125.81	128.60
36	1	58	G	C5-N7-C8	-5.57	101.51	104.30
41	14	134	LEU	CA-CB-CG	5.57	128.12	115.30
36	1	1116	G	C6-C5-N7	-5.57	127.06	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	140	G	C8-N9-C4	-5.57	104.17	106.40
1	6	1266	U	C5-C6-N1	5.57	125.48	122.70
36	1	1017	C	C5-C6-N1	5.57	123.78	121.00
36	1	1049	C	C5-C6-N1	5.57	123.78	121.00
36	1	2688	U	N1-C2-N3	-5.57	111.56	114.90
1	6	581	U	N1-C2-O2	-5.57	118.90	122.80
1	2	1458	G	N9-C4-C5	-5.57	103.17	105.40
36	1	2197	C	C5-C4-N4	-5.57	116.30	120.20
36	1	2712	U	N3-C2-O2	-5.57	118.30	122.20
1	6	1150	G	O5'-P-OP2	-5.57	100.69	105.70
1	6	1680	G	C5-C6-O6	-5.57	125.26	128.60
36	5	1126	G	C5-C6-N1	-5.57	108.72	111.50
36	5	1149	G	C6-C5-N7	-5.57	127.06	130.40
1	2	213	A	C8-N9-C4	5.57	108.03	105.80
36	1	727	G	C5-C6-O6	-5.57	125.26	128.60
36	1	1857	C	C2-N1-C1'	-5.57	112.68	118.80
36	1	2401	A	C2-N3-C4	-5.57	107.82	110.60
36	5	408	A	C6-N1-C2	-5.57	115.26	118.60
36	5	1409	G	N1-C6-O6	-5.57	116.56	119.90
36	5	3121	U	N3-C2-O2	5.57	126.10	122.20
36	1	57	A	C2-N3-C4	-5.56	107.82	110.60
1	6	635	A	OP2-P-O3'	5.56	117.44	105.20
36	1	2617	U	OP2-P-O3'	5.56	117.44	105.20
36	5	824	C	N3-C2-O2	-5.56	118.01	121.90
36	5	1338	C	N3-C4-N4	5.56	121.89	118.00
36	1	282	G	C2'-C3'-O3'	5.56	122.60	113.70
36	5	3217	C	C5-C6-N1	-5.56	118.22	121.00
36	1	520	U	N3-C4-O4	5.56	123.29	119.40
36	1	2639	G	N3-C2-N2	5.56	123.79	119.90
36	1	2710	C	N1-C2-O2	-5.56	115.56	118.90
36	5	398	A	O5'-P-OP2	-5.56	100.70	105.70
36	5	651	G	N3-C4-C5	-5.56	125.82	128.60
36	5	2626	A	C2-N3-C4	-5.56	107.82	110.60
36	5	2704	A	OP2-P-O3'	5.56	117.43	105.20
36	1	1059	G	N1-C6-O6	-5.56	116.57	119.90
36	1	1360	C	C5-C4-N4	-5.56	116.31	120.20
36	1	2756	C	N3-C4-N4	5.56	121.89	118.00
38	4	103	G	C4-N9-C1'	5.56	133.72	126.50
36	1	1743	G	C8-N9-C4	5.56	108.62	106.40
36	1	360	G	C5-C6-O6	-5.55	125.27	128.60
36	1	1901	A	C2-N3-C4	5.55	113.38	110.60
36	1	2600	C	N1-C2-O2	5.55	122.23	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2816	G	O4'-C1'-N9	5.55	112.64	108.20
1	2	1361	U	N1-C2-O2	5.55	126.69	122.80
36	1	1952	G	C8-N9-C4	-5.55	104.18	106.40
1	6	542	A	C6-C5-N7	-5.55	128.41	132.30
7	s5	25	LEU	CA-CB-CG	5.55	128.07	115.30
36	5	924	G	N3-C4-C5	5.55	131.38	128.60
36	5	1662	G	C8-N9-C4	5.55	108.62	106.40
36	5	2625	C	C5-C4-N4	-5.55	116.31	120.20
36	1	870	G	C8-N9-C4	-5.55	104.18	106.40
36	5	932	U	N3-C4-O4	5.55	123.29	119.40
36	5	2553	U	N3-C2-O2	-5.55	118.31	122.20
36	5	2913	C	C2-N1-C1'	-5.55	112.69	118.80
36	1	351	A	OP1-P-OP2	5.55	127.92	119.60
36	1	1165	A	O5'-P-OP2	-5.55	100.71	105.70
36	1	1442	U	N3-C2-O2	5.55	126.08	122.20
38	4	95	G	C8-N9-C1'	5.55	134.21	127.00
1	6	1614	A	N1-C6-N6	5.55	121.93	118.60
36	5	1412	G	C8-N9-C4	-5.55	104.18	106.40
36	1	352	A	O4'-C1'-N9	5.55	112.64	108.20
36	1	2719	U	C6-N1-C1'	5.55	128.97	121.20
38	4	15	G	C5-C6-O6	-5.55	125.27	128.60
36	1	1166	G	C5-N7-C8	-5.54	101.53	104.30
36	1	2968	G	C6-C5-N7	-5.54	127.07	130.40
36	1	3222	U	N3-C2-O2	-5.54	118.32	122.20
36	1	2400	G	C6-C5-N7	-5.54	127.07	130.40
1	6	337	G	C4-C5-N7	5.54	113.02	110.80
36	5	311	C	N3-C4-C5	5.54	124.12	121.90
36	5	2186	U	N3-C2-O2	-5.54	118.32	122.20
36	5	2199	G	C4-C5-N7	5.54	113.02	110.80
1	2	1745	G	N9-C4-C5	-5.54	103.18	105.40
36	1	993	G	C5-C6-N1	5.54	114.27	111.50
36	1	1139	G	C2-N3-C4	-5.54	109.13	111.90
1	6	334	G	C8-N9-C4	5.54	108.62	106.40
36	5	718	G	O4'-C1'-N9	5.54	112.63	108.20
36	5	1416	C	N1-C2-O2	5.54	122.22	118.90
36	1	1159	A	N9-C4-C5	5.54	108.02	105.80
36	1	1417	G	N3-C4-C5	5.54	131.37	128.60
36	1	2370	G	OP2-P-O3'	5.54	117.39	105.20
36	1	1382	G	C5-C6-O6	-5.54	125.28	128.60
36	1	2639	G	N3-C4-N9	5.54	129.32	126.00
36	1	2983	C	C5-C6-N1	-5.54	118.23	121.00
38	4	32	C	C4-C5-C6	-5.54	114.63	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2893	C	N3-C4-N4	5.54	121.88	118.00
36	5	3093	C	C6-N1-C2	5.54	122.52	120.30
36	1	517	G	C4-N9-C1'	5.54	133.70	126.50
36	1	1390	A	N1-C6-N6	-5.54	115.28	118.60
36	5	3228	C	N1-C2-O2	5.54	122.22	118.90
36	1	1545	A	C8-N9-C4	-5.54	103.59	105.80
36	5	337	G	N3-C4-C5	-5.54	125.83	128.60
36	5	1123	U	C4-C5-C6	5.54	123.02	119.70
36	5	1848	G	OP2-P-O3'	5.54	117.38	105.20
36	5	2407	C	C5-C4-N4	-5.54	116.33	120.20
1	2	685	A	P-O3'-C3'	5.53	126.34	119.70
36	1	1000	C	C6-N1-C1'	-5.53	114.16	120.80
36	1	1112	A	C4-C5-N7	5.53	113.47	110.70
36	1	2148	U	N1-C2-O2	-5.53	118.93	122.80
36	1	2983	C	N1-C2-N3	5.53	123.07	119.20
36	1	2993	G	C4-C5-N7	5.53	113.01	110.80
36	1	3178	A	N1-C6-N6	5.53	121.92	118.60
36	5	922	U	N1-C2-O2	5.53	126.67	122.80
36	1	229	G	N1-C2-N2	5.53	121.18	116.20
36	1	498	A	N9-C4-C5	5.53	108.01	105.80
36	1	658	G	C4-C5-C6	5.53	122.12	118.80
36	1	1434	G	N7-C8-N9	5.53	115.87	113.10
64	N8	115	LYS	C-N-CA	-5.53	110.68	122.30
36	5	936	A	O4'-C1'-N9	5.53	112.62	108.20
36	5	3188	G	C5-C6-O6	5.53	131.92	128.60
36	1	3361	G	N3-C4-C5	-5.53	125.83	128.60
36	5	3386	G	N9-C4-C5	5.53	107.61	105.40
1	2	55	A	N1-C6-N6	-5.53	115.28	118.60
1	2	1175	U	OP1-P-O3'	5.53	117.36	105.20
36	5	293	C	O5'-P-OP1	-5.53	100.72	105.70
36	5	895	A	N1-C2-N3	5.53	132.06	129.30
36	5	3178	A	O5'-P-OP1	-5.53	100.72	105.70
1	2	1560	U	N1-C2-N3	5.53	118.22	114.90
36	1	99	A	O4'-C1'-N9	5.53	112.62	108.20
36	1	1481	A	C4-N9-C1'	5.53	136.25	126.30
36	1	2126	A	C8-N9-C4	5.53	108.01	105.80
36	1	2775	U	N3-C2-O2	-5.53	118.33	122.20
36	1	2930	A	O4'-C1'-N9	5.53	112.62	108.20
36	5	416	A	C4-C5-C6	5.53	119.76	117.00
36	5	1054	A	C8-N9-C4	5.53	108.01	105.80
36	5	1163	A	C6-N1-C2	-5.53	115.28	118.60
36	5	1432	C	C2-N3-C4	-5.53	117.14	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	101	G	N9-C4-C5	-5.53	103.19	105.40
36	1	699	A	C5-N7-C8	-5.53	101.14	103.90
36	1	2142	A	C4-C5-N7	-5.53	107.94	110.70
1	6	96	G	C4-C5-N7	-5.53	108.59	110.80
36	5	770	G	O4'-C1'-N9	5.53	112.62	108.20
36	5	845	G	N9-C4-C5	-5.53	103.19	105.40
36	1	359	U	N3-C4-C5	-5.52	111.29	114.60
36	1	2830	G	C5-C6-N1	-5.52	108.74	111.50
36	5	917	A	C2-N3-C4	5.52	113.36	110.60
36	5	1635	G	N3-C4-N9	-5.52	122.69	126.00
36	5	1905	G	C8-N9-C4	5.52	108.61	106.40
62	n6	126	LEU	CA-CB-CG	5.52	128.00	115.30
36	1	349	A	C8-N9-C4	-5.52	103.59	105.80
36	1	394	G	N9-C4-C5	5.52	107.61	105.40
36	1	1152	G	O4'-C1'-N9	5.52	112.62	108.20
36	1	1617	G	N1-C6-O6	5.52	123.21	119.90
1	6	937	C	C6-N1-C2	-5.52	118.09	120.30
36	5	987	U	C5-C4-O4	5.52	129.21	125.90
36	5	1311	G	O5'-P-OP2	-5.52	100.73	105.70
36	1	651	G	C4-N9-C1'	5.52	133.68	126.50
36	1	2762	A	N1-C6-N6	-5.52	115.29	118.60
36	5	2929	C	C6-N1-C2	-5.52	118.09	120.30
36	1	2144	A	C6-N1-C2	-5.52	115.29	118.60
36	1	2298	U	C5-C6-N1	-5.52	119.94	122.70
1	6	308	C	C5-C4-N4	5.52	124.06	120.20
36	5	101	G	O4'-C1'-N9	5.52	112.62	108.20
36	5	338	A	C2-N3-C4	5.52	113.36	110.60
36	5	2919	A	N1-C2-N3	5.52	132.06	129.30
36	1	3227	A	O5'-P-OP2	-5.52	100.73	105.70
1	6	1747	G	N3-C2-N2	5.52	123.76	119.90
1	2	132	U	OP2-P-O3'	5.52	117.33	105.20
1	2	1663	G	O5'-P-OP2	-5.52	100.74	105.70
36	1	583	G	N3-C4-N9	-5.52	122.69	126.00
36	5	1438	U	N1-C2-O2	5.52	126.66	122.80
36	5	2643	A	N1-C6-N6	5.52	121.91	118.60
1	2	829	A	P-O3'-C3'	5.51	126.32	119.70
36	1	983	A	C8-N9-C4	5.51	108.01	105.80
36	1	1351	U	C6-N1-C2	-5.51	117.69	121.00
36	1	2984	C	C5-C4-N4	5.51	124.06	120.20
38	4	95	G	N3-C4-C5	5.51	131.36	128.60
36	5	27	C	N3-C2-O2	5.51	125.76	121.90
36	5	1789	G	N3-C4-C5	5.51	131.36	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1133	A	C6-C5-N7	-5.51	128.44	132.30
36	1	790	U	N1-C2-N3	5.51	118.21	114.90
36	1	2145	A	N1-C6-N6	5.51	121.91	118.60
36	1	2187	G	C4-C5-C6	5.51	122.11	118.80
1	2	720	G	P-O3'-C3'	5.51	126.31	119.70
1	6	942	G	O5'-P-OP1	-5.51	100.74	105.70
36	5	30	G	OP1-P-O3'	5.51	117.32	105.20
36	5	668	G	N1-C6-O6	-5.51	116.59	119.90
36	5	805	G	C5-C6-O6	-5.51	125.29	128.60
36	5	2121	G	N1-C6-O6	5.51	123.21	119.90
38	8	48	A	N9-C4-C5	5.51	108.00	105.80
36	1	672	A	C4-C5-N7	5.51	113.45	110.70
36	1	2513	U	C5-C4-O4	-5.51	122.60	125.90
36	1	2993	G	OP1-P-OP2	5.51	127.86	119.60
1	6	426	G	O5'-P-OP2	-5.51	100.74	105.70
1	6	914	G	C4-C5-N7	5.51	113.00	110.80
36	5	1380	G	O5'-P-OP2	-5.51	100.74	105.70
36	5	2751	G	C8-N9-C4	-5.51	104.20	106.40
36	5	2800	G	N1-C2-N3	5.51	127.20	123.90
1	2	1670	G	O5'-P-OP2	-5.50	100.75	105.70
36	1	1074	U	C5-C4-O4	-5.50	122.60	125.90
36	1	2621	G	N9-C4-C5	5.50	107.60	105.40
36	1	2719	U	N1-C2-O2	-5.50	118.95	122.80
36	1	2983	C	N3-C4-N4	-5.50	114.15	118.00
36	1	3269	U	N3-C2-O2	-5.50	118.35	122.20
1	6	1727	G	O5'-P-OP2	-5.50	100.75	105.70
36	5	931	C	N3-C4-C5	5.50	124.10	121.90
36	5	2144	A	C5-C6-N6	-5.50	119.30	123.70
1	2	1777	G	C6-C5-N7	-5.50	127.10	130.40
36	5	1302	A	N9-C4-C5	5.50	108.00	105.80
36	5	2636	A	C5-C6-N6	5.50	128.10	123.70
36	1	894	G	OP1-P-O3'	5.50	117.31	105.20
36	5	687	U	C5-C6-N1	-5.50	119.95	122.70
36	5	1097	G	C8-N9-C4	5.50	108.60	106.40
36	5	1866	C	O4'-C1'-N1	-5.50	103.80	108.20
36	1	100	A	N1-C2-N3	5.50	132.05	129.30
36	1	1362	G	C5-C6-O6	-5.50	125.30	128.60
1	2	1537	C	C5-C4-N4	-5.50	116.35	120.20
1	2	1745	G	C6-C5-N7	-5.50	127.10	130.40
36	1	231	G	N9-C4-C5	5.50	107.60	105.40
36	1	2817	A	C5-C6-N6	-5.50	119.30	123.70
48	M1	112	LEU	CA-CB-CG	5.50	127.95	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	137	U	C2-N1-C1'	5.50	124.30	117.70
1	6	194	U	N3-C2-O2	-5.50	118.35	122.20
36	5	3214	U	C5-C6-N1	-5.50	119.95	122.70
36	1	653	A	C2-N3-C4	-5.50	107.85	110.60
38	4	58	G	N3-C4-N9	5.50	129.30	126.00
36	5	1149	G	C4-C5-C6	5.50	122.10	118.80
1	2	1761	U	N3-C2-O2	-5.50	118.35	122.20
36	1	75	G	N1-C6-O6	5.50	123.20	119.90
36	5	2887	A	O5'-P-OP1	-5.50	100.75	105.70
36	1	1409	G	N9-C4-C5	5.49	107.60	105.40
36	1	2734	A	N9-C4-C5	-5.49	103.60	105.80
46	L9	166	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	6	1119	G	C8-N9-C4	-5.49	104.20	106.40
36	5	394	G	C4-C5-N7	-5.49	108.60	110.80
36	1	663	C	N3-C4-N4	5.49	121.84	118.00
36	1	1115	G	N9-C4-C5	5.49	107.60	105.40
36	5	672	A	C5-C6-N6	-5.49	119.31	123.70
36	5	1662	G	N9-C4-C5	-5.49	103.20	105.40
1	2	1596	C	N1-C2-O2	5.49	122.19	118.90
36	5	1304	A	C5-C6-N6	-5.49	119.31	123.70
36	5	2988	C	C5-C6-N1	-5.49	118.25	121.00
36	5	3206	C	OP1-P-OP2	5.49	127.83	119.60
1	2	315	A	N1-C6-N6	5.49	121.89	118.60
36	1	1156	C	C2-N3-C4	-5.49	117.16	119.90
36	1	1428	A	N7-C8-N9	5.49	116.54	113.80
36	1	1547	G	C2-N3-C4	5.49	114.64	111.90
36	5	660	A	C5-N7-C8	5.49	106.64	103.90
36	5	1309	U	N1-C2-N3	5.49	118.19	114.90
36	5	3072	C	N3-C4-C5	-5.49	119.70	121.90
37	7	84	A	N3-C4-C5	-5.49	122.96	126.80
36	1	2379	U	O5'-P-OP1	5.49	117.28	110.70
38	4	151	C	C4-C5-C6	5.49	120.14	117.40
1	2	1302	U	N3-C4-O4	5.49	123.24	119.40
36	1	360	G	N9-C4-C5	-5.49	103.21	105.40
36	1	697	A	C5-C6-N6	-5.49	119.31	123.70
36	1	702	C	N3-C2-O2	-5.49	118.06	121.90
1	6	1535	U	N1-C2-O2	5.49	126.64	122.80
36	5	646	A	C8-N9-C4	-5.49	103.61	105.80
36	5	960	U	C6-N1-C2	5.49	124.29	121.00
36	5	1902	G	C4-C5-N7	5.49	112.99	110.80
36	5	2876	C	OP1-P-OP2	5.49	127.83	119.60
36	1	1001	G	C4-N9-C1'	5.48	133.63	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	216	G	C5-C6-O6	-5.48	125.31	128.60
36	5	885	U	N1-C2-O2	-5.48	118.96	122.80
36	5	2367	A	O5'-P-OP2	-5.48	100.77	105.70
1	2	1657	U	C4-C5-C6	5.48	122.99	119.70
36	5	3310	A	N1-C2-N3	5.48	132.04	129.30
1	2	448	C	C5-C6-N1	5.48	123.74	121.00
36	1	286	U	N3-C2-O2	-5.48	118.36	122.20
36	1	984	G	C8-N9-C4	-5.48	104.21	106.40
36	1	2811	A	N9-C4-C5	5.48	107.99	105.80
41	L4	327	LEU	CA-CB-CG	5.48	127.91	115.30
1	6	463	U	N3-C4-O4	5.48	123.24	119.40
36	5	38	U	C6-N1-C2	5.48	124.29	121.00
36	5	329	U	C5-C6-N1	-5.48	119.96	122.70
36	5	590	G	C5-C6-O6	-5.48	125.31	128.60
36	5	2655	U	N1-C2-O2	-5.48	118.96	122.80
1	6	1698	G	P-O3'-C3'	5.48	126.28	119.70
36	5	2920	U	O5'-P-OP1	-5.48	100.77	105.70
1	2	1117	U	N3-C4-O4	5.48	123.23	119.40
1	2	1600	A	N9-C4-C5	-5.48	103.61	105.80
36	1	2820	A	OP2-P-O3'	5.48	117.25	105.20
36	1	2847	A	N1-C6-N6	5.48	121.89	118.60
36	1	3209	A	C5-N7-C8	-5.48	101.16	103.90
1	6	1027	A	N7-C8-N9	5.48	116.54	113.80
36	5	269	G	C5-C6-O6	-5.48	125.31	128.60
36	5	2763	U	C5-C4-O4	-5.48	122.61	125.90
36	5	2832	C	C5-C4-N4	5.48	124.03	120.20
36	1	2275	A	O5'-P-OP1	-5.48	100.77	105.70
1	6	555	A	P-O3'-C3'	5.48	126.27	119.70
36	5	83	U	C6-N1-C2	-5.48	117.72	121.00
36	5	2158	A	C5-C6-N1	5.48	120.44	117.70
36	1	1191	U	N1-C2-O2	-5.47	118.97	122.80
36	1	1396	C	N3-C2-O2	5.47	125.73	121.90
38	4	39	G	N3-C2-N2	5.47	123.73	119.90
1	6	901	G	C4-C5-N7	5.47	112.99	110.80
36	5	2805	G	C8-N9-C4	5.47	108.59	106.40
36	1	47	C	N3-C4-N4	5.47	121.83	118.00
36	1	693	A	C6-C5-N7	-5.47	128.47	132.30
36	1	919	U	N1-C2-O2	5.47	126.63	122.80
36	1	1136	A	C5-C6-N1	5.47	120.44	117.70
36	5	366	A	C6-C5-N7	-5.47	128.47	132.30
36	5	1789	G	C4-N9-C1'	-5.47	119.39	126.50
36	5	2412	G	N3-C4-N9	5.47	129.28	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2541	U	C2-N1-C1'	5.47	124.27	117.70
36	5	2211	U	N1-C2-N3	5.47	118.18	114.90
36	1	1053	A	C8-N9-C4	5.47	107.99	105.80
36	1	1133	A	C4-C5-N7	5.47	113.43	110.70
36	1	1464	G	O5'-P-OP2	-5.47	100.78	105.70
38	4	32	C	C6-N1-C1'	5.47	127.36	120.80
1	6	98	U	C5-C4-O4	5.47	129.18	125.90
36	1	421	G	C8-N9-C4	5.47	108.59	106.40
36	1	612	U	C2-N1-C1'	-5.47	111.14	117.70
36	1	976	U	O5'-P-OP2	-5.47	100.78	105.70
36	1	1326	A	O5'-P-OP1	5.47	117.26	110.70
36	5	104	G	N1-C6-O6	5.47	123.18	119.90
36	5	3014	U	C5-C4-O4	-5.47	122.62	125.90
1	2	610	G	C4-N9-C1'	5.47	133.61	126.50
36	1	343	U	N3-C4-C5	-5.47	111.32	114.60
36	1	1102	A	OP1-P-O3'	5.47	117.23	105.20
36	1	1502	C	C6-N1-C2	5.47	122.49	120.30
36	1	2585	G	C2-N3-C4	5.47	114.63	111.90
1	6	44	U	N3-C2-O2	5.47	126.03	122.20
1	6	1058	U	P-O3'-C3'	5.47	126.26	119.70
36	5	410	U	C5-C6-N1	5.47	125.43	122.70
36	5	1902	G	N3-C2-N2	-5.47	116.07	119.90
36	5	2294	U	C2-N3-C4	-5.47	123.72	127.00
37	7	22	A	N1-C6-N6	5.47	121.88	118.60
36	1	974	G	N3-C4-N9	5.46	129.28	126.00
36	1	1166	G	C4-C5-N7	5.46	112.99	110.80
36	1	1441	G	C5-C6-O6	5.46	131.88	128.60
36	5	1937	U	C5-C6-N1	-5.46	119.97	122.70
36	5	2828	G	C5-N7-C8	-5.46	101.57	104.30
36	5	2951	G	OP1-P-O3'	5.46	117.22	105.20
36	5	3030	G	C4-C5-N7	-5.46	108.61	110.80
1	2	542	A	C4-N9-C1'	5.46	136.13	126.30
36	1	142	C	C6-N1-C2	-5.46	118.11	120.30
36	5	1003	A	N7-C8-N9	-5.46	111.07	113.80
36	5	2971	A	N9-C4-C5	-5.46	103.61	105.80
36	5	3036	G	N1-C2-N2	-5.46	111.28	116.20
36	5	3190	C	C6-N1-C2	-5.46	118.11	120.30
1	2	334	G	C4-N9-C1'	-5.46	119.40	126.50
1	2	782	U	OP2-P-O3'	5.46	117.22	105.20
36	1	668	G	N1-C6-O6	-5.46	116.62	119.90
36	1	2179	C	OP2-P-O3'	5.46	117.22	105.20
36	1	2214	A	O5'-P-OP2	-5.46	100.78	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2719	U	C2-N1-C1'	-5.46	111.15	117.70
38	8	42	G	C8-N9-C4	5.46	108.58	106.40
36	1	628	A	N1-C6-N6	5.46	121.88	118.60
1	6	1744	A	N1-C2-N3	5.46	132.03	129.30
38	8	44	A	N1-C6-N6	5.46	121.88	118.60
1	2	1768	G	N9-C4-C5	5.46	107.58	105.40
36	1	821	U	N1-C2-O2	5.46	126.62	122.80
36	1	2964	G	C8-N9-C4	5.46	108.58	106.40
1	6	981	U	C6-N1-C2	-5.46	117.72	121.00
36	5	967	A	OP2-P-O3'	5.46	117.21	105.20
36	5	1495	U	C2-N1-C1'	5.46	124.25	117.70
36	1	718	G	C5-N7-C8	-5.46	101.57	104.30
36	1	1361	U	C5-C4-O4	-5.46	122.63	125.90
36	1	2169	G	C6-C5-N7	5.46	133.67	130.40
1	6	539	G	N7-C8-N9	5.46	115.83	113.10
1	6	1028	C	C6-N1-C2	5.46	122.48	120.30
1	6	1731	A	C8-N9-C4	-5.46	103.62	105.80
36	5	793	C	C6-N1-C2	-5.46	118.12	120.30
36	5	2310	U	O5'-P-OP2	-5.46	100.79	105.70
36	5	3343	G	N9-C4-C5	-5.46	103.22	105.40
36	1	1177	G	C4-N9-C1'	5.46	133.59	126.50
36	5	359	U	N1-C2-O2	-5.45	118.98	122.80
36	5	2777	G	C4-C5-N7	-5.45	108.62	110.80
36	5	2882	U	C5-C6-N1	5.45	125.43	122.70
36	5	2938	G	OP1-P-O3'	5.45	117.20	105.20
36	5	3012	A	C8-N9-C4	5.45	107.98	105.80
38	8	115	C	N1-C2-O2	-5.45	115.63	118.90
38	8	126	A	OP1-P-O3'	5.45	117.20	105.20
36	1	105	C	C5-C4-N4	-5.45	116.38	120.20
36	1	3143	C	N3-C2-O2	5.45	125.72	121.90
44	L7	107	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	6	194	U	N1-C2-O2	5.45	126.62	122.80
36	5	1449	A	C6-C5-N7	-5.45	128.48	132.30
36	5	1469	C	C6-N1-C2	-5.45	118.12	120.30
36	5	2965	U	N1-C2-O2	-5.45	118.98	122.80
36	5	3186	A	N9-C4-C5	5.45	107.98	105.80
36	1	968	G	C5-C6-O6	5.45	131.87	128.60
36	1	2355	G	C6-C5-N7	-5.45	127.13	130.40
36	1	2869	U	O5'-P-OP2	5.45	117.24	110.70
3	s1	47	LEU	CA-CB-CG	5.45	127.84	115.30
36	5	337	G	C8-N9-C4	-5.45	104.22	106.40
36	5	1392	G	N7-C8-N9	-5.45	110.37	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2646	C	C6-N1-C2	5.45	122.48	120.30
36	5	1185	C	OP2-P-O3'	5.45	117.19	105.20
36	5	1791	C	N3-C2-O2	-5.45	118.09	121.90
36	1	66	A	O5'-P-OP2	5.45	117.24	110.70
1	2	321	C	C6-N1-C2	-5.45	118.12	120.30
1	2	553	G	N3-C2-N2	-5.45	116.09	119.90
36	1	1329	U	C6-N1-C1'	-5.45	113.58	121.20
36	5	1301	A	N9-C4-C5	-5.45	103.62	105.80
36	5	1367	G	C4-N9-C1'	5.45	133.58	126.50
36	5	2926	A	C5-C6-N6	-5.45	119.34	123.70
36	5	2968	G	C5-C6-N1	5.45	114.22	111.50
36	5	3382	U	C2-N1-C1'	5.45	124.23	117.70
36	1	231	G	N3-C4-N9	-5.44	122.73	126.00
36	1	649	A	N7-C8-N9	-5.44	111.08	113.80
36	1	2271	A	C5-C6-N6	-5.44	119.34	123.70
36	1	155	G	C5-C6-N1	5.44	114.22	111.50
36	1	171	G	N3-C4-C5	5.44	131.32	128.60
36	1	693	A	C4-C5-C6	5.44	119.72	117.00
36	1	2610	G	N9-C4-C5	-5.44	103.22	105.40
36	1	3361	G	N1-C2-N2	-5.44	111.30	116.20
37	3	67	G	OP2-P-O3'	5.44	117.17	105.20
1	6	976	G	C4-C5-N7	5.44	112.98	110.80
36	5	342	A	C5-C6-N6	-5.44	119.35	123.70
36	5	2411	U	C2-N3-C4	-5.44	123.73	127.00
36	5	2880	U	C6-N1-C2	-5.44	117.73	121.00
15	C3	22	ALA	C-N-CA	5.44	144.85	122.00
36	1	2964	G	C2-N3-C4	-5.44	109.18	111.90
36	5	1433	A	O5'-P-OP1	-5.44	100.80	105.70
36	5	2366	C	C2-N1-C1'	5.44	124.78	118.80
36	5	2996	U	O5'-P-OP1	5.44	117.23	110.70
36	5	3296	A	OP2-P-O3'	5.44	117.17	105.20
36	5	3388	C	C5-C6-N1	-5.44	118.28	121.00
36	1	938	C	C5-C4-N4	-5.44	116.39	120.20
36	1	1180	A	N9-C4-C5	5.44	107.97	105.80
37	3	84	A	N9-C4-C5	-5.44	103.62	105.80
36	5	1204	A	N9-C4-C5	5.44	107.97	105.80
36	1	335	G	OP1-P-O3'	5.44	117.16	105.20
38	4	155	A	C8-N9-C4	5.44	107.97	105.80
36	1	71	A	N9-C4-C5	5.43	107.97	105.80
36	1	498	A	C8-N9-C4	-5.43	103.63	105.80
36	1	2399	A	C5-C6-N1	5.43	120.42	117.70
36	1	2797	C	N1-C2-O2	-5.43	115.64	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	938	C	C6-N1-C2	5.43	122.47	120.30
36	5	1879	A	O5'-P-OP2	-5.43	100.81	105.70
36	5	2310	U	N1-C2-O2	5.43	126.60	122.80
36	5	2639	G	N3-C4-C5	-5.43	125.88	128.60
36	5	3099	C	N3-C4-C5	-5.43	119.73	121.90
36	5	3232	G	N1-C2-N2	-5.43	111.31	116.20
1	6	751	G	O5'-P-OP1	-5.43	100.81	105.70
37	7	32	U	C5-C6-N1	-5.43	119.98	122.70
36	1	406	G	N1-C6-O6	-5.43	116.64	119.90
36	1	416	A	OP2-P-O3'	5.43	117.14	105.20
36	1	1113	G	N1-C6-O6	5.43	123.16	119.90
36	1	1373	A	OP2-P-O3'	5.43	117.14	105.20
36	1	2603	G	C5-C6-N1	5.43	114.22	111.50
1	6	939	A	O5'-P-OP2	-5.43	100.81	105.70
36	5	98	G	C8-N9-C4	5.43	108.57	106.40
36	5	881	C	C4-C5-C6	-5.43	114.69	117.40
36	5	2355	G	C4-C5-N7	5.43	112.97	110.80
36	5	2816	G	N3-C4-N9	5.43	129.26	126.00
36	5	2868	U	N1-C2-O2	5.43	126.60	122.80
36	5	3115	C	N1-C2-N3	5.43	123.00	119.20
36	1	2823	G	C4-C5-N7	-5.43	108.63	110.80
36	5	2283	G	O5'-P-OP2	-5.43	100.81	105.70
36	5	2737	C	O5'-P-OP2	-5.43	100.81	105.70
36	5	2943	G	O5'-P-OP2	-5.43	100.81	105.70
38	8	66	A	N1-C6-N6	5.43	121.86	118.60
36	1	2846	U	N3-C4-O4	-5.43	115.60	119.40
36	1	2915	U	N3-C2-O2	5.43	126.00	122.20
36	1	3212	C	C2-N1-C1'	-5.43	112.83	118.80
36	5	2904	U	C4-C5-C6	5.43	122.96	119.70
36	5	3126	C	C6-N1-C2	-5.43	118.13	120.30
36	5	3309	G	N3-C4-N9	5.43	129.26	126.00
38	8	33	A	C8-N9-C4	5.43	107.97	105.80
1	2	610	G	C8-N9-C1'	-5.42	119.95	127.00
36	1	810	A	C8-N9-C4	-5.42	103.63	105.80
36	5	2981	U	C2-N1-C1'	5.42	124.21	117.70
36	1	824	C	N3-C4-C5	5.42	124.07	121.90
1	6	1091	A	C2-N3-C4	-5.42	107.89	110.60
36	5	638	C	C2-N3-C4	-5.42	117.19	119.90
1	2	1748	G	O5'-P-OP2	-5.42	100.82	105.70
36	1	1136	A	C5-C6-N6	-5.42	119.36	123.70
36	5	1495	U	OP1-P-O3'	5.42	117.13	105.20
1	2	133	U	O5'-P-OP2	-5.42	100.82	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2222	A	C8-N9-C4	-5.42	103.63	105.80
36	1	2402	A	N1-C6-N6	5.42	121.85	118.60
36	5	96	G	C5-C6-O6	-5.42	125.35	128.60
39	12	208	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	2	1573	A	P-O3'-C3'	5.42	126.20	119.70
36	1	304	G	C4-C5-N7	-5.42	108.63	110.80
36	1	498	A	N1-C6-N6	-5.42	115.35	118.60
36	1	1144	U	C2-N3-C4	-5.42	123.75	127.00
36	1	1483	G	O4'-C1'-N9	5.42	112.53	108.20
36	1	1536	G	O5'-P-OP2	-5.42	100.82	105.70
36	5	96	G	C6-C5-N7	-5.42	127.15	130.40
36	5	2118	C	O5'-P-OP1	-5.42	100.82	105.70
36	5	2872	A	C4-C5-C6	-5.42	114.29	117.00
36	1	2653	C	N3-C2-O2	-5.42	118.11	121.90
36	1	2823	G	N1-C2-N2	5.42	121.07	116.20
36	5	111	C	C6-N1-C2	5.42	122.47	120.30
36	5	329	U	N3-C4-O4	-5.42	115.61	119.40
36	5	971	G	C4-C5-C6	5.42	122.05	118.80
36	1	2366	C	C6-N1-C1'	-5.42	114.30	120.80
36	1	2813	A	C5-C6-N1	-5.42	114.99	117.70
36	5	2870	C	N3-C4-N4	-5.42	114.21	118.00
36	1	101	G	O4'-C1'-N9	5.41	112.53	108.20
36	1	697	A	N9-C4-C5	-5.41	103.64	105.80
36	1	2154	U	C5-C6-N1	5.41	125.41	122.70
1	6	100	A	C6-C5-N7	-5.41	128.51	132.30
1	6	687	G	N3-C4-N9	-5.41	122.75	126.00
36	5	718	G	C4-N9-C1'	5.41	133.54	126.50
36	5	924	G	O5'-P-OP2	5.41	117.20	110.70
36	5	1365	G	C6-C5-N7	-5.41	127.15	130.40
36	5	2794	G	N9-C4-C5	-5.41	103.23	105.40
36	1	1375	G	N1-C6-O6	5.41	123.15	119.90
1	6	463	U	N1-C2-O2	-5.41	119.01	122.80
36	5	2175	U	C2-N3-C4	-5.41	123.75	127.00
1	2	1282	U	N3-C2-O2	-5.41	118.41	122.20
36	1	691	A	C5-N7-C8	-5.41	101.19	103.90
36	1	1406	A	O5'-P-OP2	-5.41	100.83	105.70
36	1	2642	A	C6-N1-C2	5.41	121.85	118.60
36	1	3261	C	N1-C2-O2	-5.41	115.65	118.90
36	5	881	C	C2-N1-C1'	5.41	124.75	118.80
36	1	394	G	C8-N9-C4	-5.41	104.24	106.40
36	1	1180	A	O4'-C1'-N9	-5.41	103.87	108.20
36	1	1658	G	N9-C4-C5	5.41	107.56	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1458	G	C4-N9-C1'	5.41	133.53	126.50
36	5	592	A	N9-C4-C5	-5.41	103.64	105.80
36	5	1373	A	O5'-P-OP2	-5.41	100.83	105.70
36	5	2882	U	O5'-P-OP2	-5.41	100.83	105.70
36	1	2401	A	N3-C4-C5	5.41	130.59	126.80
36	1	693	A	N7-C8-N9	5.41	116.50	113.80
36	1	1197	A	C5-N7-C8	-5.41	101.20	103.90
36	1	1374	G	C5-N7-C8	-5.41	101.60	104.30
36	1	3056	U	O5'-P-OP2	-5.41	100.83	105.70
36	1	75	G	C6-C5-N7	-5.40	127.16	130.40
36	1	410	U	N3-C4-O4	5.40	123.18	119.40
36	1	834	U	O5'-P-OP2	-5.40	100.84	105.70
1	6	470	A	C8-N9-C4	-5.40	103.64	105.80
1	6	1426	C	C6-N1-C2	-5.40	118.14	120.30
36	5	2187	G	N1-C6-O6	5.40	123.14	119.90
1	2	334	G	C2-N3-C4	-5.40	109.20	111.90
36	1	429	U	O5'-P-OP1	-5.40	100.84	105.70
36	1	1374	G	C4-C5-N7	5.40	112.96	110.80
38	4	10	A	OP1-P-O3'	5.40	117.08	105.20
1	6	358	U	O5'-P-OP1	-5.40	100.84	105.70
1	6	467	G	N3-C4-N9	5.40	129.24	126.00
36	1	2627	C	C6-N1-C2	5.40	122.46	120.30
36	5	1100	U	C5-C4-O4	-5.40	122.66	125.90
36	5	2877	G	N1-C6-O6	-5.40	116.66	119.90
36	1	1149	G	O4'-C1'-N9	5.40	112.52	108.20
36	1	1367	G	C5-C6-O6	-5.40	125.36	128.60
36	5	3022	G	O4'-C1'-N9	5.40	112.52	108.20
36	1	214	G	C6-C5-N7	-5.39	127.16	130.40
36	1	2391	G	C4-C5-N7	-5.39	108.64	110.80
37	3	82	G	N1-C2-N3	5.39	127.14	123.90
36	5	329	U	C5-C4-O4	5.39	129.14	125.90
36	5	374	A	N9-C4-C5	5.39	107.96	105.80
36	5	3115	C	C2-N3-C4	-5.39	117.20	119.90
36	5	3141	A	C4-C5-C6	5.39	119.70	117.00
1	2	913	G	C8-N9-C1'	-5.39	119.99	127.00
36	1	608	A	C5-C6-N6	-5.39	119.39	123.70
36	1	1152	G	OP1-P-OP2	5.39	127.69	119.60
36	1	3060	C	C5-C4-N4	-5.39	116.42	120.20
36	5	922	U	C2-N3-C4	-5.39	123.77	127.00
36	5	1468	A	N1-C6-N6	5.39	121.83	118.60
36	1	932	U	C5-C6-N1	5.39	125.39	122.70
36	1	933	A	N1-C2-N3	5.39	132.00	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1406	A	C5-C6-N6	-5.39	119.39	123.70
36	1	2417	U	N1-C2-O2	-5.39	119.03	122.80
36	1	25	U	N3-C4-C5	-5.39	111.37	114.60
36	1	2946	A	C4-C5-N7	5.39	113.39	110.70
36	5	1857	C	N3-C4-C5	5.39	124.06	121.90
36	5	3133	C	N3-C4-C5	-5.39	119.75	121.90
36	5	2166	A	O5'-P-OP1	-5.39	100.85	105.70
36	5	2284	C	C5-C4-N4	-5.39	116.43	120.20
36	1	1181	U	O5'-P-OP2	-5.39	100.85	105.70
36	1	1924	U	N3-C2-O2	5.39	125.97	122.20
1	6	7	G	N3-C4-N9	5.39	129.23	126.00
36	5	879	U	N1-C2-N3	5.39	118.13	114.90
36	5	2340	U	C5-C4-O4	-5.39	122.67	125.90
36	5	2398	A	C6-N1-C2	-5.39	115.37	118.60
36	5	2550	U	N3-C2-O2	-5.39	118.43	122.20
36	5	2759	U	OP1-P-O3'	5.39	117.05	105.20
36	5	2759	U	N1-C2-O2	-5.39	119.03	122.80
1	2	1185	U	N1-C2-O2	5.38	126.57	122.80
1	2	1536	G	C8-N9-C1'	-5.38	120.00	127.00
36	1	637	C	OP2-P-O3'	-5.38	93.35	105.20
36	1	1110	U	N3-C4-C5	5.38	117.83	114.60
36	1	1139	G	C5-C6-O6	5.38	131.83	128.60
1	6	957	G	N3-C2-N2	-5.38	116.13	119.90
1	6	1567	U	C5-C4-O4	-5.38	122.67	125.90
1	2	406	U	O5'-P-OP2	-5.38	100.86	105.70
36	1	349	A	P-O3'-C3'	5.38	126.16	119.70
1	6	1522	U	O4'-C1'-N1	5.38	112.51	108.20
36	5	651	G	C6-C5-N7	-5.38	127.17	130.40
36	1	907	G	O4'-C1'-N9	5.38	112.50	108.20
36	1	1375	G	C5-C6-O6	-5.38	125.37	128.60
44	L7	202	LEU	CB-CG-CD2	-5.38	101.85	111.00
1	6	389	G	N1-C6-O6	-5.38	116.67	119.90
36	5	1170	A	N1-C6-N6	5.38	121.83	118.60
36	5	3354	U	N3-C2-O2	-5.38	118.43	122.20
36	1	960	U	C2-N3-C4	-5.38	123.77	127.00
1	2	1280	C	C4-C5-C6	5.38	120.09	117.40
36	1	3060	C	N3-C4-N4	5.38	121.77	118.00
36	5	1299	U	C5-C4-O4	-5.38	122.67	125.90
1	2	914	G	C4-N9-C1'	5.38	133.49	126.50
36	1	790	U	C5-C4-O4	5.38	129.13	125.90
36	1	3309	G	C6-C5-N7	-5.38	127.17	130.40
1	6	1280	C	C6-N1-C2	-5.38	118.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1488	G	O5'-P-OP2	5.38	117.15	110.70
36	5	617	G	C4-C5-N7	5.38	112.95	110.80
36	5	776	U	N3-C4-O4	-5.38	115.64	119.40
36	5	2887	A	C4-C5-C6	5.38	119.69	117.00
36	1	2160	G	C6-C5-N7	-5.37	127.18	130.40
36	5	410	U	C2-N3-C4	5.37	130.22	127.00
36	5	822	G	O5'-P-OP1	-5.37	100.86	105.70
36	5	835	G	O4'-C1'-N9	5.37	112.50	108.20
36	5	2996	U	N3-C2-O2	-5.37	118.44	122.20
36	1	1131	G	N1-C6-O6	5.37	123.12	119.90
36	5	92	G	C5-C6-N1	5.37	114.19	111.50
36	5	639	G	C4-C5-C6	5.37	122.02	118.80
36	5	2395	G	C4-C5-C6	-5.37	115.58	118.80
36	1	650	C	C4-C5-C6	5.37	120.08	117.40
1	6	23	G	O5'-P-OP2	-5.37	100.87	105.70
36	5	1314	C	C6-N1-C1'	-5.37	114.36	120.80
1	2	1185	U	C2-N1-C1'	5.37	124.14	117.70
36	1	1177	G	N9-C4-C5	-5.37	103.25	105.40
36	1	2618	G	N1-C6-O6	-5.37	116.68	119.90
36	1	2789	U	N1-C2-O2	-5.37	119.04	122.80
36	5	2666	C	N3-C4-N4	5.37	121.76	118.00
1	2	1129	U	N3-C4-C5	5.37	117.82	114.60
36	1	2699	G	C5-N7-C8	-5.37	101.62	104.30
36	1	2731	U	N1-C2-O2	-5.37	119.04	122.80
36	5	3082	C	N1-C2-O2	5.37	122.12	118.90
36	5	3309	G	C8-N9-C1'	-5.37	120.02	127.00
1	2	1131	A	C8-N9-C4	5.36	107.95	105.80
36	1	2706	G	N1-C6-O6	5.36	123.12	119.90
36	5	948	C	N1-C2-O2	-5.36	115.68	118.90
36	1	515	C	N3-C4-C5	-5.36	119.75	121.90
36	1	2182	A	N7-C8-N9	5.36	116.48	113.80
37	3	44	C	N3-C4-C5	-5.36	119.75	121.90
36	5	530	G	O4'-C1'-N9	5.36	112.49	108.20
36	5	2310	U	N3-C2-O2	-5.36	118.45	122.20
36	5	3079	U	C5-C4-O4	5.36	129.12	125.90
1	2	1176	G	C6-C5-N7	-5.36	127.18	130.40
1	2	1733	C	N1-C2-O2	-5.36	115.68	118.90
36	1	1696	A	C8-N9-C4	-5.36	103.66	105.80
1	6	664	U	C2-N1-C1'	5.36	124.13	117.70
36	5	635	G	C5-C6-O6	-5.36	125.38	128.60
36	5	1429	G	C5-C6-O6	-5.36	125.38	128.60
1	6	387	A	C2-N3-C4	5.36	113.28	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	608	U	N1-C2-N3	5.36	118.11	114.90
1	2	864	U	N1-C2-N3	5.36	118.11	114.90
36	1	683	U	N3-C4-O4	5.36	123.15	119.40
36	1	1634	G	C8-N9-C4	-5.36	104.26	106.40
36	1	2141	U	C5-C6-N1	5.36	125.38	122.70
36	1	3181	C	N1-C2-O2	5.36	122.11	118.90
36	5	2116	G	N1-C6-O6	5.36	123.11	119.90
36	1	3134	A	C2-N3-C4	-5.36	107.92	110.60
73	O7	67	LEU	CA-CB-CG	5.36	127.62	115.30
1	6	1752	U	O5'-P-OP1	5.36	117.13	110.70
36	5	838	G	N1-C2-N2	-5.36	111.38	116.20
36	5	1161	G	C4-C5-N7	5.36	112.94	110.80
36	5	2358	A	N1-C6-N6	-5.36	115.39	118.60
36	1	62	A	C5-C6-N6	-5.35	119.42	123.70
36	1	2537	U	P-O3'-C3'	5.35	126.12	119.70
36	1	2396	G	N9-C4-C5	5.35	107.54	105.40
1	6	914	G	C5-C6-O6	-5.35	125.39	128.60
36	5	851	C	P-O3'-C3'	-5.35	113.28	119.70
36	5	2345	A	C4-C5-N7	5.35	113.38	110.70
36	5	2931	C	C5-C4-N4	-5.35	116.45	120.20
36	1	1119	C	C6-N1-C2	5.35	122.44	120.30
36	1	2351	U	C6-N1-C2	-5.35	117.79	121.00
1	6	538	A	O4'-C1'-N9	5.35	112.48	108.20
36	5	1476	G	C8-N9-C4	5.35	108.54	106.40
36	5	2971	A	N1-C2-N3	-5.35	126.62	129.30
36	1	1400	G	C8-N9-C1'	-5.35	120.05	127.00
1	6	696	C	C2-N1-C1'	-5.35	112.92	118.80
1	6	1432	U	O4'-C1'-N1	5.35	112.48	108.20
36	5	2968	G	N1-C6-O6	-5.35	116.69	119.90
1	2	1215	C	C6-N1-C2	-5.35	118.16	120.30
1	2	1458	G	N3-C4-N9	5.35	129.21	126.00
36	1	262	U	N3-C2-O2	5.35	125.94	122.20
36	1	1180	A	N7-C8-N9	-5.35	111.13	113.80
36	5	1885	U	N3-C2-O2	5.35	125.94	122.20
36	5	2211	U	C5-C6-N1	-5.35	120.03	122.70
36	1	501	A	N1-C6-N6	5.34	121.81	118.60
36	5	1321	G	C2-N3-C4	-5.34	109.23	111.90
36	5	1359	C	N3-C4-N4	5.34	121.74	118.00
36	5	2135	U	C6-N1-C2	5.34	124.21	121.00
36	5	512	U	C5-C4-O4	5.34	129.11	125.90
36	5	880	G	C8-N9-C4	5.34	108.54	106.40
36	5	933	A	C6-N1-C2	-5.34	115.39	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1099	A	C5-C6-N6	-5.34	119.43	123.70
1	2	307	G	C4-N9-C1'	5.34	133.44	126.50
36	1	142	C	C5-C6-N1	5.34	123.67	121.00
1	6	1354	G	C4-N9-C1'	5.34	133.44	126.50
36	5	336	A	C8-N9-C4	5.34	107.94	105.80
36	5	3136	G	C5-C6-N1	-5.34	108.83	111.50
36	1	2892	A	N1-C6-N6	-5.34	115.40	118.60
36	5	1154	A	C2-N3-C4	5.34	113.27	110.60
36	5	2190	U	N1-C2-N3	5.34	118.10	114.90
36	5	2991	A	C5-C6-N1	5.34	120.37	117.70
1	2	345	U	N1-C2-N3	5.34	118.10	114.90
1	2	580	A	N9-C4-C5	5.34	107.94	105.80
36	1	1320	C	N3-C4-C5	-5.34	119.77	121.90
36	1	3304	U	N3-C2-O2	5.34	125.94	122.20
1	6	151	G	N3-C2-N2	-5.34	116.17	119.90
36	5	845	G	C5-C6-O6	-5.34	125.40	128.60
36	5	2820	A	N7-C8-N9	5.34	116.47	113.80
36	5	3054	U	N3-C4-C5	-5.34	111.40	114.60
36	1	785	G	N1-C2-N3	-5.33	120.70	123.90
1	2	587	C	C6-N1-C2	-5.33	118.17	120.30
36	1	427	C	C6-N1-C2	-5.33	118.17	120.30
36	1	1901	A	C5-C6-N1	5.33	120.37	117.70
36	1	2375	G	O5'-P-OP2	5.33	117.10	110.70
36	1	2418	G	OP1-P-O3'	5.33	116.93	105.20
36	1	2541	U	P-O3'-C3'	5.33	126.10	119.70
49	M3	46	ILE	CG1-CB-CG2	-5.33	99.67	111.40
1	6	1600	A	O4'-C1'-N9	5.33	112.47	108.20
36	5	971	G	N7-C8-N9	-5.33	110.43	113.10
36	5	1189	C	C6-N1-C2	5.33	122.43	120.30
36	5	1834	U	C6-N1-C2	-5.33	117.80	121.00
36	5	2271	A	N1-C6-N6	-5.33	115.40	118.60
1	2	1761	U	N1-C2-N3	5.33	118.10	114.90
36	1	2163	C	N3-C4-N4	-5.33	114.27	118.00
36	1	2247	G	C5-C6-O6	-5.33	125.40	128.60
36	1	3183	A	C6-C5-N7	-5.33	128.57	132.30
36	5	649	A	N1-C6-N6	5.33	121.80	118.60
36	5	998	A	OP2-P-O3'	5.33	116.93	105.20
36	5	1060	U	C5-C6-N1	-5.33	120.03	122.70
1	2	42	G	C4-C5-N7	-5.33	108.67	110.80
36	1	24	G	N1-C2-N2	-5.33	111.40	116.20
36	1	270	U	N3-C2-O2	-5.33	118.47	122.20
36	1	688	G	N3-C4-C5	-5.33	125.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2622	C	OP2-P-O3'	5.33	116.92	105.20
1	2	190	C	O4'-C1'-N1	5.33	112.46	108.20
36	1	2527	G	N3-C4-N9	-5.33	122.80	126.00
36	1	2881	C	N1-C2-N3	-5.33	115.47	119.20
36	1	3004	C	N3-C4-C5	5.33	124.03	121.90
36	5	587	U	C5-C4-O4	-5.33	122.70	125.90
1	2	1572	G	N9-C4-C5	-5.33	103.27	105.40
36	1	107	A	C5-C6-N6	-5.33	119.44	123.70
36	1	2917	G	N3-C4-C5	-5.33	125.94	128.60
1	2	1745	G	C5-C6-N1	5.33	114.16	111.50
36	1	325	A	OP2-P-O3'	5.33	116.92	105.20
36	1	798	G	N7-C8-N9	5.33	115.76	113.10
36	1	2915	U	C2-N3-C4	-5.33	123.80	127.00
1	6	6	G	C6-C5-N7	-5.33	127.20	130.40
1	6	1000	C	N3-C2-O2	-5.33	118.17	121.90
36	1	392	G	C4-C5-N7	5.32	112.93	110.80
36	1	424	G	N7-C8-N9	-5.32	110.44	113.10
36	1	580	C	N3-C4-C5	5.32	124.03	121.90
36	1	1547	G	N1-C2-N3	-5.32	120.71	123.90
36	1	3046	A	O5'-P-OP1	-5.32	100.91	105.70
36	1	3057	U	N1-C2-N3	5.32	118.09	114.90
1	6	891	A	N1-C6-N6	5.32	121.79	118.60
36	5	2943	G	N9-C4-C5	-5.32	103.27	105.40
36	5	2954	U	N3-C4-O4	5.32	123.13	119.40
27	D5	95	HIS	N-CA-C	5.32	125.37	111.00
36	1	339	C	N3-C4-N4	-5.32	114.28	118.00
36	1	636	C	OP1-P-O3'	5.32	116.91	105.20
36	1	1332	A	N1-C2-N3	5.32	131.96	129.30
36	5	1429	G	N7-C8-N9	5.32	115.76	113.10
36	1	289	A	N1-C6-N6	5.32	121.79	118.60
36	1	2372	A	C5-C6-N1	5.32	120.36	117.70
36	5	1385	C	C5-C4-N4	-5.32	116.48	120.20
36	5	2832	C	C6-N1-C2	5.32	122.43	120.30
36	1	1213	G	C5'-C4'-O4'	-5.32	102.72	109.10
36	1	2800	G	N1-C2-N2	-5.32	111.41	116.20
36	5	949	C	N1-C2-O2	-5.32	115.71	118.90
36	1	2647	A	N9-C4-C5	5.32	107.93	105.80
36	1	2737	C	N3-C2-O2	5.32	125.62	121.90
37	3	10	C	C6-N1-C2	-5.32	118.17	120.30
1	6	1592	A	C2-N3-C4	-5.32	107.94	110.60
36	5	298	U	N1-C2-O2	5.32	126.52	122.80
36	5	641	C	C2-N3-C4	-5.32	117.24	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	820	A	C8-N9-C4	-5.32	103.67	105.80
36	5	1529	A	C8-N9-C4	5.32	107.93	105.80
36	5	2333	C	C6-N1-C2	5.32	122.43	120.30
36	5	2772	C	OP2-P-O3'	5.32	116.90	105.20
36	5	3301	U	O5'-P-OP1	-5.32	100.91	105.70
36	1	938	C	N1-C2-O2	-5.32	115.71	118.90
36	1	2403	G	N3-C2-N2	5.32	123.62	119.90
36	1	2639	G	N1-C2-N2	-5.32	111.42	116.20
1	6	607	G	C6-C5-N7	-5.32	127.21	130.40
1	6	992	A	O5'-P-OP1	-5.32	100.92	105.70
36	5	2643	A	C4-C5-N7	5.32	113.36	110.70
36	5	2704	A	O5'-P-OP1	-5.32	100.92	105.70
36	5	2885	C	N1-C2-N3	5.32	122.92	119.20
36	1	545	U	C2-N1-C1'	5.31	124.08	117.70
36	1	1210	U	N3-C2-O2	-5.31	118.48	122.20
36	1	2836	C	C4-C5-C6	5.31	120.06	117.40
36	5	424	G	C6-C5-N7	-5.31	127.21	130.40
1	2	1781	A	C5-C6-N6	5.31	127.95	123.70
36	1	339	C	C5-C4-N4	5.31	123.92	120.20
36	1	1751	G	N9-C4-C5	-5.31	103.28	105.40
36	1	1913	A	C5-C6-N6	-5.31	119.45	123.70
36	5	1339	C	N3-C4-C5	-5.31	119.78	121.90
36	5	2890	A	C6-N1-C2	5.31	121.79	118.60
37	7	103	A	C4-C5-N7	5.31	113.36	110.70
36	5	370	U	C2-N1-C1'	5.31	124.07	117.70
37	7	49	G	C5-C6-N1	-5.31	108.84	111.50
1	2	301	A	OP2-P-O3'	5.31	116.88	105.20
36	1	224	C	N1-C2-O2	-5.31	115.71	118.90
36	1	1142	G	N3-C4-N9	5.31	129.19	126.00
36	1	2599	U	C6-N1-C2	-5.31	117.81	121.00
36	5	686	G	OP1-P-OP2	-5.31	111.63	119.60
36	1	673	U	C5-C6-N1	-5.31	120.05	122.70
36	1	2276	G	C8-N9-C4	-5.31	104.28	106.40
36	1	2986	U	N1-C2-N3	5.31	118.08	114.90
1	6	65	A	C4-C5-N7	5.31	113.35	110.70
36	5	1449	A	C5-C6-N6	-5.31	119.45	123.70
36	5	2231	C	N3-C4-C5	-5.31	119.78	121.90
36	5	2767	U	O5'-P-OP2	-5.31	100.92	105.70
36	1	423	A	C4-C5-C6	5.31	119.65	117.00
1	6	1082	C	N3-C4-N4	5.31	121.72	118.00
36	5	952	A	C5-N7-C8	-5.31	101.25	103.90
36	1	2196	C	C5-C6-N1	5.30	123.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1565	C	N3-C4-C5	5.30	124.02	121.90
36	5	1175	C	N1-C2-O2	-5.30	115.72	118.90
36	5	3195	U	OP1-P-O3'	5.30	116.87	105.20
38	8	140	G	C5-C6-N1	-5.30	108.85	111.50
36	1	36	C	C5-C6-N1	5.30	123.65	121.00
36	1	1156	C	N1-C2-O2	5.30	122.08	118.90
36	5	1449	A	C8-N9-C4	5.30	107.92	105.80
36	5	3030	G	C5-C6-O6	5.30	131.78	128.60
1	2	75	U	C6-N1-C1'	-5.30	113.78	121.20
1	2	609	U	N1-C2-O2	-5.30	119.09	122.80
1	2	831	U	N3-C4-O4	5.30	123.11	119.40
36	1	107	A	N1-C6-N6	5.30	121.78	118.60
36	1	2968	G	C4-C5-N7	5.30	112.92	110.80
1	6	67	A	C4-C5-N7	5.30	113.35	110.70
36	5	2643	A	C8-N9-C4	5.30	107.92	105.80
36	5	2877	G	C4-C5-N7	-5.30	108.68	110.80
36	1	1329	U	C5'-C4'-O4'	-5.30	102.74	109.10
36	1	3183	A	C4-C5-N7	5.30	113.35	110.70
36	5	426	G	N7-C8-N9	-5.30	110.45	113.10
36	5	714	G	C8-N9-C4	5.30	108.52	106.40
36	5	924	G	N3-C2-N2	-5.30	116.19	119.90
36	5	1385	C	N3-C4-N4	5.30	121.71	118.00
36	5	2818	U	C5'-C4'-O4'	-5.30	102.74	109.10
1	2	1486	G	N7-C8-N9	5.30	115.75	113.10
36	1	2368	A	N3-C4-N9	-5.30	123.16	127.40
36	5	1405	U	N1-C2-N3	5.30	118.08	114.90
52	m6	128	ARG	NE-CZ-NH1	-5.30	117.65	120.30
36	1	2860	U	C4-C5-C6	-5.30	116.52	119.70
1	6	1600	A	C2-N3-C4	-5.30	107.95	110.60
36	5	1148	G	N1-C6-O6	5.30	123.08	119.90
36	5	2645	G	N1-C6-O6	-5.30	116.72	119.90
36	5	2691	A	C8-N9-C4	-5.30	103.68	105.80
36	1	2967	A	C8-N9-C4	5.29	107.92	105.80
1	6	1697	G	N3-C4-N9	5.29	129.18	126.00
36	5	810	A	N1-C2-N3	-5.29	126.65	129.30
36	5	1152	G	N1-C2-N2	5.29	120.97	116.20
1	2	73	U	P-O3'-C3'	5.29	126.05	119.70
1	2	392	G	N1-C6-O6	5.29	123.08	119.90
1	2	1389	C	N3-C2-O2	-5.29	118.19	121.90
36	5	1554	U	OP1-P-O3'	5.29	116.84	105.20
36	5	3144	G	N7-C8-N9	5.29	115.75	113.10
36	1	609	G	C8-N9-C4	-5.29	104.28	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	361	A	C5-C6-N6	5.29	127.93	123.70
36	5	1160	C	O4'-C1'-N1	5.29	112.43	108.20
36	5	1440	G	N9-C4-C5	5.29	107.52	105.40
36	1	421	G	C8-N9-C1'	-5.29	120.12	127.00
36	1	2226	U	N3-C4-C5	-5.29	111.43	114.60
38	4	149	A	N1-C6-N6	-5.29	115.43	118.60
1	6	1665	U	N3-C4-C5	5.29	117.77	114.60
36	5	2353	G	C6-C5-N7	-5.29	127.23	130.40
36	1	2376	G	C5-N7-C8	-5.29	101.66	104.30
36	1	2627	C	N1-C2-O2	-5.29	115.73	118.90
1	6	65	A	N3-C4-C5	5.29	130.50	126.80
1	6	539	G	C8-N9-C4	-5.29	104.28	106.40
1	6	1075	C	N3-C2-O2	5.29	125.60	121.90
1	6	1084	A	O5'-P-OP2	-5.29	100.94	105.70
36	5	971	G	C5-C6-O6	-5.29	125.43	128.60
36	5	1135	A	C8-N9-C4	-5.29	103.69	105.80
36	5	1317	A	C5-C6-N1	5.29	120.34	117.70
36	5	2180	G	N3-C4-C5	5.29	131.24	128.60
36	5	2816	G	N3-C2-N2	5.29	123.60	119.90
36	5	2858	U	N3-C2-O2	-5.29	118.50	122.20
1	2	477	A	N1-C6-N6	5.29	121.77	118.60
36	1	1141	C	C6-N1-C2	-5.29	118.19	120.30
36	1	1581	C	N1-C2-O2	5.29	122.07	118.90
36	1	2969	A	N1-C6-N6	5.29	121.77	118.60
1	6	114	C	C2-N1-C1'	5.29	124.61	118.80
36	5	1604	G	N3-C4-N9	5.29	129.17	126.00
36	5	3144	G	C8-N9-C4	-5.29	104.29	106.40
37	7	50	U	C6-N1-C2	-5.29	117.83	121.00
1	6	1105	C	C6-N1-C2	-5.28	118.19	120.30
36	5	661	G	P-O3'-C3'	5.28	126.04	119.70
36	5	1433	A	N9-C4-C5	5.28	107.91	105.80
36	5	2379	U	C2-N3-C4	-5.28	123.83	127.00
36	5	3008	A	N3-C4-C5	5.28	130.50	126.80
1	2	447	U	C2-N1-C1'	5.28	124.04	117.70
36	1	1428	A	N1-C6-N6	5.28	121.77	118.60
36	1	2620	G	N3-C2-N2	-5.28	116.20	119.90
61	N5	113	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	6	65	A	N1-C6-N6	5.28	121.77	118.60
37	7	42	A	C5-C6-N6	-5.28	119.47	123.70
1	2	734	A	OP1-P-O3'	5.28	116.82	105.20
36	1	153	U	N3-C4-C5	-5.28	111.43	114.60
36	1	667	C	N3-C2-O2	5.28	125.60	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1181	U	O4'-C1'-N1	5.28	112.42	108.20
36	1	36	C	N3-C4-C5	-5.28	119.79	121.90
36	1	518	G	O4'-C1'-N9	5.28	112.42	108.20
36	1	2925	C	C2-N3-C4	-5.28	117.26	119.90
1	6	352	A	O5'-P-OP1	-5.28	100.95	105.70
1	6	470	A	C5-N7-C8	-5.28	101.26	103.90
36	5	682	U	N3-C4-O4	-5.28	115.71	119.40
36	5	1305	U	N3-C2-O2	5.28	125.89	122.20
36	5	2640	A	C2-N3-C4	-5.28	107.96	110.60
36	1	1359	C	N3-C2-O2	5.28	125.59	121.90
36	1	2870	C	O4'-C1'-N1	5.28	112.42	108.20
37	3	84	A	C4-C5-N7	5.28	113.34	110.70
1	6	1772	C	C5-C6-N1	-5.28	118.36	121.00
36	5	1095	U	N3-C2-O2	-5.28	118.51	122.20
36	5	1618	G	C8-N9-C4	5.28	108.51	106.40
36	5	1858	A	O5'-P-OP2	-5.28	100.95	105.70
36	5	1867	A	N9-C4-C5	-5.28	103.69	105.80
36	5	2282	U	N1-C2-O2	-5.28	119.11	122.80
36	5	2994	A	C5-C6-N1	5.28	120.34	117.70
37	7	44	C	N1-C2-O2	-5.28	115.73	118.90
36	1	1847	A	O5'-P-OP2	-5.27	100.95	105.70
36	1	2233	A	N9-C4-C5	5.27	107.91	105.80
36	1	2678	A	N1-C6-N6	-5.27	115.44	118.60
36	5	2213	A	OP2-P-O3'	5.27	116.80	105.20
36	1	880	G	N7-C8-N9	-5.27	110.46	113.10
36	1	1001	G	N1-C6-O6	5.27	123.06	119.90
36	1	2603	G	N3-C2-N2	5.27	123.59	119.90
36	1	2825	C	C6-N1-C2	5.27	122.41	120.30
38	4	65	A	C2-N3-C4	-5.27	107.96	110.60
36	5	644	G	N3-C4-C5	-5.27	125.96	128.60
36	5	659	G	N3-C4-N9	5.27	129.16	126.00
36	5	2616	C	N3-C2-O2	5.27	125.59	121.90
36	5	2877	G	C5-C6-O6	5.27	131.76	128.60
36	5	2889	C	N3-C4-C5	5.27	124.01	121.90
36	5	3301	U	C6-N1-C2	5.27	124.16	121.00
1	2	613	G	N9-C4-C5	-5.27	103.29	105.40
36	1	582	G	C4-C5-N7	5.27	112.91	110.80
36	1	1133	A	C8-N9-C4	5.27	107.91	105.80
36	1	2706	G	C5-C6-O6	-5.27	125.44	128.60
36	1	3171	U	N3-C2-O2	5.27	125.89	122.20
36	1	3362	A	C4-C5-N7	5.27	113.33	110.70
36	5	648	C	OP1-P-OP2	5.27	127.51	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	669	U	C2-N1-C1'	-5.27	111.38	117.70
36	5	2902	A	C6-N1-C2	-5.27	115.44	118.60
37	7	51	A	N1-C6-N6	5.27	121.76	118.60
1	2	1105	C	N3-C4-C5	-5.27	119.79	121.90
36	1	793	C	C6-N1-C2	-5.27	118.19	120.30
36	5	806	A	C4-C5-C6	-5.27	114.37	117.00
36	5	2970	C	N1-C2-O2	-5.27	115.74	118.90
36	1	2297	U	P-O3'-C3'	5.27	126.02	119.70
36	5	993	G	O5'-P-OP2	-5.27	100.96	105.70
1	2	539	G	N7-C8-N9	5.26	115.73	113.10
36	1	956	U	C6-N1-C2	-5.26	117.84	121.00
36	1	3212	C	C5-C6-N1	-5.26	118.37	121.00
36	5	417	A	N1-C6-N6	-5.26	115.44	118.60
36	1	1747	G	N1-C6-O6	5.26	123.06	119.90
36	1	2636	A	C5-N7-C8	-5.26	101.27	103.90
38	4	46	G	C2-N3-C4	5.26	114.53	111.90
36	5	1508	C	OP1-P-OP2	5.26	127.50	119.60
36	5	3108	G	C5-C6-O6	-5.26	125.44	128.60
1	2	7	G	C4-C5-N7	-5.26	108.70	110.80
36	1	1305	U	C5-C4-O4	5.26	129.06	125.90
36	1	2606	G	N9-C4-C5	-5.26	103.30	105.40
1	6	23	G	N9-C4-C5	5.26	107.50	105.40
1	6	466	U	C6-N1-C2	-5.26	117.84	121.00
1	6	1410	A	N1-C6-N6	5.26	121.76	118.60
36	5	183	G	C4-N9-C1'	5.26	133.34	126.50
36	5	2209	U	C2-N1-C1'	-5.26	111.39	117.70
36	5	2932	U	N1-C2-O2	5.26	126.48	122.80
3	S1	181	LEU	CA-CB-CG	5.26	127.39	115.30
36	1	1512	U	N3-C2-O2	-5.26	118.52	122.20
36	1	2309	A	N1-C6-N6	5.26	121.75	118.60
1	6	1141	G	C8-N9-C4	5.26	108.50	106.40
36	5	1548	C	C6-N1-C2	5.26	122.40	120.30
36	5	1892	G	C5-C6-N1	5.26	114.13	111.50
36	5	2639	G	N1-C2-N2	-5.26	111.47	116.20
36	5	2849	C	OP2-P-O3'	5.26	116.77	105.20
36	5	3294	A	C8-N9-C4	-5.26	103.70	105.80
37	7	56	A	C5-C6-N6	-5.26	119.49	123.70
50	m4	77	ARG	NE-CZ-NH1	-5.26	117.67	120.30
36	5	1006	A	OP1-P-OP2	5.26	127.49	119.60
36	1	917	A	N9-C4-C5	5.26	107.90	105.80
36	1	1115	G	C6-N1-C2	-5.26	121.95	125.10
36	1	1838	G	C5-C6-N1	-5.26	108.87	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2551	U	N3-C2-O2	-5.26	118.52	122.20
38	4	10	A	C5-C6-N1	5.26	120.33	117.70
1	6	858	G	C5-N7-C8	-5.26	101.67	104.30
36	5	1238	C	P-O3'-C3'	5.26	126.01	119.70
36	5	2632	G	OP1-P-O3'	5.26	116.77	105.20
36	5	2863	G	N3-C2-N2	5.26	123.58	119.90
36	1	1429	G	C5-N7-C8	5.25	106.93	104.30
36	5	1844	C	N1-C2-O2	-5.25	115.75	118.90
1	2	1199	G	N9-C4-C5	-5.25	103.30	105.40
36	1	627	U	C5-C6-N1	5.25	125.33	122.70
40	L3	35	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	6	453	U	C5-C4-O4	5.25	129.05	125.90
1	6	1459	C	C6-N1-C2	-5.25	118.20	120.30
1	6	1463	C	C6-N1-C2	5.25	122.40	120.30
37	7	1	G	N3-C4-C5	-5.25	125.97	128.60
1	2	1273	G	N1-C6-O6	-5.25	116.75	119.90
1	2	1291	G	C5-N7-C8	-5.25	101.67	104.30
36	1	2827	U	C2-N1-C1'	-5.25	111.40	117.70
36	5	343	U	N1-C2-N3	5.25	118.05	114.90
36	5	643	U	C2-N3-C4	-5.25	123.85	127.00
36	5	1450	G	C5-N7-C8	-5.25	101.67	104.30
36	5	2850	G	N9-C4-C5	-5.25	103.30	105.40
36	1	2192	C	O5'-P-OP2	-5.25	100.97	105.70
36	1	3258	U	OP2-P-O3'	5.25	116.75	105.20
36	5	1602	A	OP2-P-O3'	5.25	116.75	105.20
36	5	1902	G	O5'-P-OP2	5.25	117.00	110.70
36	5	2168	A	O5'-P-OP2	-5.25	100.97	105.70
1	2	966	A	N9-C4-C5	-5.25	103.70	105.80
1	6	14	C	N1-C2-O2	-5.25	115.75	118.90
1	6	314	C	C2-N1-C1'	5.25	124.57	118.80
1	6	408	C	C6-N1-C2	-5.25	118.20	120.30
36	5	392	G	C5-C6-O6	-5.25	125.45	128.60
36	5	1449	A	N1-C2-N3	5.25	131.92	129.30
36	5	1770	G	C4-N9-C1'	5.25	133.32	126.50
36	5	2832	C	N1-C2-O2	5.25	122.05	118.90
36	1	300	G	O5'-P-OP1	-5.25	100.98	105.70
36	1	943	U	N3-C4-C5	5.25	117.75	114.60
36	1	1156	C	N3-C4-C5	5.25	124.00	121.90
36	1	3209	A	N9-C4-C5	-5.25	103.70	105.80
36	1	3391	A	N1-C6-N6	-5.25	115.45	118.60
36	5	3121	U	OP1-P-O3'	5.25	116.74	105.20
37	7	77	G	C6-C5-N7	-5.25	127.25	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2301	U	N3-C2-O2	-5.25	118.53	122.20
36	5	911	C	C2-N3-C4	-5.25	117.28	119.90
36	5	1451	C	N1-C2-O2	-5.25	115.75	118.90
38	8	3	A	C4-C5-C6	-5.25	114.38	117.00
1	2	1573	A	OP2-P-O3'	5.24	116.74	105.20
36	1	363	G	C6-C5-N7	-5.24	127.25	130.40
36	1	1882	G	N3-C2-N2	-5.24	116.23	119.90
36	1	2541	U	C2-N1-C1'	5.24	123.99	117.70
1	6	1675	C	N3-C4-N4	5.24	121.67	118.00
36	5	424	G	C5-C6-N1	5.24	114.12	111.50
36	5	1153	A	C5-N7-C8	-5.24	101.28	103.90
36	5	1292	C	O5'-P-OP1	-5.24	100.98	105.70
36	5	1379	G	C6-C5-N7	-5.24	127.25	130.40
36	5	1688	U	N3-C2-O2	-5.24	118.53	122.20
36	5	1908	A	N7-C8-N9	5.24	116.42	113.80
36	5	2950	G	OP1-P-O3'	5.24	116.73	105.20
36	1	363	G	N1-C6-O6	5.24	123.05	119.90
36	1	719	U	OP1-P-OP2	5.24	127.46	119.60
36	1	1326	A	O5'-P-OP2	-5.24	100.98	105.70
36	1	3201	C	C4-C5-C6	5.24	120.02	117.40
38	4	103	G	N9-C4-C5	5.24	107.50	105.40
36	5	361	A	C6-C5-N7	5.24	135.97	132.30
36	5	1152	G	N7-C8-N9	5.24	115.72	113.10
36	5	2550	U	C5-C4-O4	5.24	129.04	125.90
36	5	2887	A	N3-C4-C5	-5.24	123.13	126.80
36	5	3374	U	C6-N1-C2	5.24	124.14	121.00
36	1	2418	G	N3-C4-N9	5.24	129.14	126.00
36	1	2868	U	C2-N1-C1'	5.24	123.99	117.70
36	1	2946	A	C5-C6-N6	-5.24	119.51	123.70
36	1	2273	G	C4-N9-C1'	-5.24	119.69	126.50
36	1	2378	C	N3-C4-N4	5.24	121.67	118.00
1	2	499	U	C3'-C2'-C1'	5.24	105.69	101.50
36	1	1851	G	C6-C5-N7	-5.24	127.26	130.40
37	3	101	G	C8-N9-C4	5.24	108.49	106.40
1	6	23	G	C8-N9-C4	-5.24	104.31	106.40
1	6	424	C	C6-N1-C1'	-5.24	114.52	120.80
36	5	859	G	C4-C5-N7	5.24	112.89	110.80
36	5	2560	C	N1-C2-O2	5.24	122.04	118.90
36	5	2932	U	C6-N1-C1'	-5.24	113.87	121.20
36	5	3000	A	C2-N3-C4	-5.24	107.98	110.60
36	5	3204	C	C6-N1-C2	5.24	122.39	120.30
1	2	879	G	O5'-P-OP2	-5.23	100.99	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	376	G	C5-C6-N1	-5.23	108.88	111.50
36	1	2121	G	C2-N3-C4	5.23	114.52	111.90
36	1	2291	A	OP1-P-O3'	5.23	116.71	105.20
36	5	3228	C	C2-N1-C1'	5.23	124.56	118.80
36	1	1131	G	C8-N9-C1'	-5.23	120.20	127.00
36	1	2791	G	C8-N9-C4	-5.23	104.31	106.40
1	6	45	U	N1-C2-O2	5.23	126.46	122.80
36	5	63	A	N3-C4-N9	5.23	131.59	127.40
36	1	36	C	C6-N1-C2	-5.23	118.21	120.30
36	1	195	U	N1-C2-N3	5.23	118.04	114.90
36	1	1370	G	N7-C8-N9	5.23	115.72	113.10
36	1	1515	A	C4-C5-C6	5.23	119.61	117.00
36	1	1531	C	C5-C6-N1	5.23	123.62	121.00
36	1	2269	U	C5-C4-O4	-5.23	122.76	125.90
36	1	2615	G	C5-C6-O6	-5.23	125.46	128.60
36	1	2631	U	C2-N3-C4	-5.23	123.86	127.00
1	6	153	G	C6-C5-N7	-5.23	127.26	130.40
1	6	215	A	C8-N9-C4	-5.23	103.71	105.80
36	5	384	A	N7-C8-N9	-5.23	111.19	113.80
36	5	530	G	C8-N9-C1'	5.23	133.80	127.00
36	5	2750	U	N1-C2-N3	5.23	118.04	114.90
36	1	417	A	C5-C6-N6	-5.23	119.52	123.70
37	3	89	G	C8-N9-C4	5.23	108.49	106.40
1	6	347	G	C5-C6-O6	-5.23	125.46	128.60
37	7	93	C	O5'-P-OP1	5.23	116.97	110.70
1	6	30	G	N3-C4-N9	-5.23	122.86	126.00
1	6	128	U	N1-C2-N3	5.23	118.04	114.90
1	6	187	G	P-O3'-C3'	5.23	125.97	119.70
1	6	455	C	C5-C4-N4	-5.23	116.54	120.20
36	5	222	A	C8-N9-C4	5.23	107.89	105.80
36	1	96	G	N1-C6-O6	5.22	123.03	119.90
36	1	1340	G	N3-C4-N9	5.22	129.13	126.00
36	1	2372	A	O4'-C1'-N9	-5.22	104.02	108.20
37	3	96	U	C5-C6-N1	-5.22	120.09	122.70
1	6	782	U	C2-N1-C1'	5.22	123.97	117.70
36	5	1680	G	C4-C5-N7	-5.22	108.71	110.80
36	5	2258	U	N1-C2-O2	5.22	126.46	122.80
36	5	2979	U	C6-N1-C1'	5.22	128.51	121.20
37	7	37	G	C4-C5-N7	5.22	112.89	110.80
36	1	374	A	C4-C5-N7	-5.22	108.09	110.70
36	1	1585	C	N3-C4-C5	5.22	123.99	121.90
36	1	2856	G	O5'-P-OP2	5.22	116.97	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3087	A	C4-C5-C6	5.22	119.61	117.00
38	4	25	G	C5-N7-C8	5.22	106.91	104.30
36	5	1868	G	C8-N9-C4	5.22	108.49	106.40
36	5	2836	C	C2-N3-C4	-5.22	117.29	119.90
36	1	2283	G	N3-C4-C5	5.22	131.21	128.60
36	5	3127	A	C5-C6-N1	5.22	120.31	117.70
1	2	1644	C	C6-N1-C2	-5.22	118.21	120.30
35	SM	134	ASP	CB-CG-OD2	5.22	123.00	118.30
36	1	2142	A	OP1-P-OP2	-5.22	111.77	119.60
36	1	2443	A	C5-C6-N6	-5.22	119.52	123.70
1	6	60	U	C5-C6-N1	5.22	125.31	122.70
1	6	390	G	N3-C4-C5	-5.22	125.99	128.60
1	6	1051	G	C8-N9-C4	-5.22	104.31	106.40
36	5	411	U	C2-N3-C4	-5.22	123.87	127.00
36	5	960	U	N1-C2-O2	5.22	126.45	122.80
36	5	967	A	C5-C6-N6	-5.22	119.53	123.70
36	5	984	G	N3-C4-N9	5.22	129.13	126.00
36	5	1000	C	N3-C4-C5	5.22	123.99	121.90
36	5	3287	U	N1-C2-O2	5.22	126.45	122.80
1	2	694	U	N3-C2-O2	-5.22	118.55	122.20
36	1	1720	U	C5-C4-O4	5.22	129.03	125.90
38	4	102	U	C6-N1-C2	-5.22	117.87	121.00
1	6	558	U	C2-N1-C1'	5.22	123.96	117.70
1	2	782	U	P-O3'-C3'	5.22	125.96	119.70
36	1	2860	U	N1-C2-N3	-5.22	111.77	114.90
1	6	142	G	C8-N9-C1'	-5.22	120.22	127.00
36	5	584	G	C8-N9-C4	-5.22	104.31	106.40
1	2	704	C	C2-N1-C1'	5.21	124.54	118.80
36	1	1421	G	C5-C6-O6	-5.21	125.47	128.60
36	1	2623	G	C6-C5-N7	-5.21	127.27	130.40
41	L4	192	GLY	N-CA-C	-5.21	100.06	113.10
36	5	1321	G	N1-C2-N3	5.21	127.03	123.90
36	5	1688	U	N1-C2-O2	5.21	126.45	122.80
36	5	2127	U	N3-C2-O2	-5.21	118.55	122.20
3	S1	218	LEU	CA-CB-CG	5.21	127.29	115.30
36	1	1082	U	C5-C6-N1	5.21	125.31	122.70
41	L4	136	LEU	CA-CB-CG	-5.21	103.31	115.30
1	6	1021	C	C2-N1-C1'	5.21	124.53	118.80
36	5	526	C	N1-C2-O2	5.21	122.03	118.90
36	5	2234	G	C4-C5-N7	5.21	112.89	110.80
36	1	405	U	C5-C4-O4	-5.21	122.77	125.90
36	1	925	A	C4-C5-C6	5.21	119.61	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1166	G	C6-C5-N7	-5.21	127.27	130.40
36	1	2170	U	C6-N1-C2	-5.21	117.87	121.00
36	1	2281	A	O4'-C1'-N9	5.21	112.37	108.20
36	5	101	G	C4-N9-C1'	5.21	133.28	126.50
36	5	2125	A	C5-C6-N1	5.21	120.31	117.70
1	6	337	G	N9-C4-C5	-5.21	103.32	105.40
36	5	3048	A	N7-C8-N9	5.21	116.41	113.80
1	2	240	U	OP2-P-O3'	5.21	116.66	105.20
36	1	207	U	N1-C2-O2	-5.21	119.15	122.80
36	1	1491	A	O5'-P-OP1	-5.21	101.01	105.70
59	N3	56	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	6	1680	G	N9-C4-C5	-5.21	103.32	105.40
36	5	382	U	O5'-P-OP2	-5.21	101.01	105.70
36	5	649	A	C5-C6-N1	5.21	120.30	117.70
36	5	1500	G	N7-C8-N9	-5.21	110.50	113.10
36	5	2950	G	N3-C2-N2	5.21	123.55	119.90
1	2	378	A	OP2-P-O3'	5.21	116.65	105.20
36	1	1428	A	C5-C6-N6	-5.21	119.53	123.70
36	1	1906	G	C5-C6-O6	-5.21	125.48	128.60
36	1	2348	A	C5-C6-N1	-5.21	115.10	117.70
1	6	606	A	N9-C4-C5	-5.21	103.72	105.80
36	5	578	A	C6-C5-N7	-5.21	128.66	132.30
36	5	1866	C	C2-N1-C1'	5.21	124.53	118.80
36	5	2187	G	N9-C4-C5	-5.21	103.32	105.40
36	5	2648	G	OP1-P-O3'	5.21	116.65	105.20
36	5	2836	C	O4'-C1'-N1	5.21	112.36	108.20
36	5	2837	A	N7-C8-N9	-5.21	111.20	113.80
36	5	2910	A	OP2-P-O3'	5.21	116.66	105.20
38	8	39	G	N3-C4-N9	5.21	129.12	126.00
36	1	633	C	C4-C5-C6	5.21	120.00	117.40
36	1	2607	G	N3-C2-N2	5.21	123.54	119.90
36	1	3176	G	N1-C6-O6	5.21	123.02	119.90
1	6	1127	G	N1-C2-N3	5.21	127.02	123.90
1	6	1389	C	N1-C2-O2	5.21	122.02	118.90
1	2	619	A	OP2-P-O3'	5.20	116.65	105.20
36	1	43	A	C2-N3-C4	-5.20	108.00	110.60
37	3	38	U	N1-C2-O2	-5.20	119.16	122.80
1	6	1113	A	C2-N3-C4	-5.20	108.00	110.60
36	5	227	G	C5-C6-O6	-5.20	125.48	128.60
36	5	1396	C	N3-C4-C5	5.20	123.98	121.90
36	5	1598	G	C8-N9-C4	5.20	108.48	106.40
36	5	2625	C	C2-N3-C4	-5.20	117.30	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3015	G	OP2-P-O3'	5.20	116.65	105.20
36	1	3024	A	O5'-P-OP1	-5.20	101.02	105.70
36	5	1856	C	C5-C6-N1	5.20	123.60	121.00
36	5	2248	C	OP1-P-O3'	5.20	116.64	105.20
36	5	1193	A	C4-C5-C6	5.20	119.60	117.00
36	5	1605	A	O4'-C1'-N9	5.20	112.36	108.20
37	7	85	G	N9-C4-C5	5.20	107.48	105.40
36	1	1294	A	O4'-C1'-N9	5.20	112.36	108.20
36	1	1322	U	N3-C2-O2	5.20	125.84	122.20
36	1	2422	C	N3-C4-N4	-5.20	114.36	118.00
36	1	3319	U	P-O3'-C3'	5.20	125.94	119.70
1	6	154	G	C5-C6-O6	-5.20	125.48	128.60
36	5	1069	C	N1-C2-O2	5.20	122.02	118.90
36	5	816	A	N1-C6-N6	-5.20	115.48	118.60
36	5	1176	C	C5-C4-N4	-5.20	116.56	120.20
1	2	587	C	N3-C4-C5	-5.20	119.82	121.90
36	1	1217	A	OP2-P-O3'	5.20	116.63	105.20
36	1	1661	G	C4-C5-N7	5.20	112.88	110.80
36	1	2988	C	N1-C2-O2	-5.20	115.78	118.90
36	1	3275	U	C6-N1-C2	-5.20	117.88	121.00
36	1	3326	G	C8-N9-C4	5.20	108.48	106.40
1	6	158	U	C2-N1-C1'	5.20	123.94	117.70
1	6	1146	G	C8-N9-C1'	-5.20	120.25	127.00
36	5	830	A	O5'-P-OP1	-5.20	101.02	105.70
36	5	1371	G	N1-C6-O6	-5.20	116.78	119.90
36	5	2618	G	C4-C5-N7	5.20	112.88	110.80
36	5	941	G	N1-C6-O6	-5.19	116.78	119.90
36	5	2365	C	O5'-P-OP1	-5.19	101.03	105.70
1	2	969	C	C6-N1-C2	5.19	122.38	120.30
36	1	245	U	N1-C2-O2	5.19	126.44	122.80
36	1	2379	U	N1-C2-O2	-5.19	119.17	122.80
38	4	47	C	N3-C4-C5	5.19	123.98	121.90
1	6	402	C	O5'-P-OP1	5.19	116.93	110.70
1	6	424	C	C5-C4-N4	-5.19	116.56	120.20
36	5	1303	A	C8-N9-C4	5.19	107.88	105.80
36	5	1395	G	N1-C6-O6	5.19	123.02	119.90
36	5	1897	G	C2-N3-C4	-5.19	109.30	111.90
36	5	2353	G	C6-N1-C2	-5.19	121.98	125.10
36	1	186	U	O5'-P-OP2	5.19	116.93	110.70
36	1	884	A	C8-N9-C4	5.19	107.88	105.80
1	6	1021	C	C6-N1-C2	-5.19	118.22	120.30
1	6	1489	U	C2-N1-C1'	5.19	123.93	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1493	A	C5-N7-C8	-5.19	101.31	103.90
36	5	23	A	C5-C6-N6	-5.19	119.55	123.70
36	5	1100	U	N3-C4-O4	5.19	123.03	119.40
36	5	3024	A	C8-N9-C4	-5.19	103.72	105.80
36	1	2817	A	OP2-P-O3'	5.19	116.62	105.20
36	5	656	A	O5'-P-OP1	-5.19	101.03	105.70
1	2	543	C	P-O3'-C3'	5.19	125.92	119.70
36	1	1669	C	N3-C2-O2	5.19	125.53	121.90
36	1	2354	C	N1-C2-N3	5.19	122.83	119.20
36	1	2599	U	C5-C6-N1	5.19	125.29	122.70
38	4	110	C	OP2-P-O3'	5.19	116.61	105.20
1	6	1144	U	OP2-P-O3'	5.19	116.61	105.20
36	5	191	U	C2-N1-C1'	-5.19	111.47	117.70
36	5	1161	G	C2-N3-C4	5.19	114.49	111.90
36	1	2115	G	C6-C5-N7	-5.19	127.29	130.40
1	6	191	C	O4'-C1'-N1	5.19	112.35	108.20
1	2	95	G	C2-N3-C4	5.18	114.49	111.90
36	1	2154	U	C5-C4-O4	-5.18	122.79	125.90
36	1	2316	G	OP1-P-O3'	5.18	116.61	105.20
1	6	67	A	C5-C6-N6	-5.18	119.55	123.70
36	5	819	U	N3-C2-O2	5.18	125.83	122.20
36	5	991	G	N1-C6-O6	-5.18	116.79	119.90
36	1	98	G	C2-N3-C4	-5.18	109.31	111.90
36	1	1001	G	N3-C4-C5	-5.18	126.01	128.60
36	1	1183	C	N1-C2-O2	-5.18	115.79	118.90
36	1	2418	G	P-O3'-C3'	5.18	125.92	119.70
1	6	1091	A	C5-C6-N1	-5.18	115.11	117.70
1	6	1653	C	OP2-P-O3'	5.18	116.60	105.20
1	6	1737	G	N1-C6-O6	5.18	123.01	119.90
36	5	3166	C	C5-C6-N1	5.18	123.59	121.00
36	5	3225	C	C6-N1-C2	-5.18	118.23	120.30
36	5	869	G	C5-C6-N1	5.18	114.09	111.50
38	8	104	A	C8-N9-C4	5.18	107.87	105.80
1	2	412	A	N1-C6-N6	5.18	121.71	118.60
36	1	894	G	C4-C5-N7	5.18	112.87	110.80
36	1	1111	U	O5'-P-OP1	-5.18	101.04	105.70
36	1	1135	A	C8-N9-C4	5.18	107.87	105.80
36	5	374	A	P-O3'-C3'	5.18	125.92	119.70
36	5	779	G	C5-C6-O6	-5.18	125.49	128.60
36	5	905	U	C5-C4-O4	-5.18	122.79	125.90
36	5	1116	G	N3-C4-C5	-5.18	126.01	128.60
36	5	2404	A	C6-C5-N7	5.18	135.93	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	12	200	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	2	1486	G	C4-C5-N7	5.18	112.87	110.80
36	5	2965	U	N3-C2-O2	5.18	125.83	122.20
1	2	543	C	N1-C2-O2	5.18	122.01	118.90
36	1	718	G	C4-C5-N7	5.18	112.87	110.80
1	2	1479	A	N1-C6-N6	5.17	121.70	118.60
36	1	517	G	C5-N7-C8	-5.17	101.71	104.30
36	1	869	G	N3-C4-C5	-5.17	126.01	128.60
38	4	22	U	C5-C4-O4	5.17	129.00	125.90
1	6	617	U	N3-C2-O2	-5.17	118.58	122.20
36	5	90	C	C5-C6-N1	5.17	123.59	121.00
36	5	96	G	C2-N3-C4	-5.17	109.31	111.90
36	5	682	U	C5-C6-N1	-5.17	120.11	122.70
1	2	933	A	C8-N9-C4	-5.17	103.73	105.80
36	1	1164	G	C8-N9-C4	-5.17	104.33	106.40
36	1	3362	A	C4-N9-C1'	5.17	135.61	126.30
38	4	147	U	C2-N1-C1'	5.17	123.91	117.70
36	1	579	G	OP2-P-O3'	5.17	116.58	105.20
36	1	1383	G	C2-N3-C4	5.17	114.49	111.90
1	6	1491	U	P-O3'-C3'	5.17	125.91	119.70
36	5	659	G	C6-C5-N7	-5.17	127.30	130.40
36	5	1438	U	C2-N1-C1'	5.17	123.91	117.70
36	5	3154	C	C2-N3-C4	5.17	122.49	119.90
36	5	2117	A	C5-N7-C8	5.17	106.48	103.90
36	5	3335	A	C5-C6-N6	-5.17	119.56	123.70
36	1	1146	C	C5-C6-N1	5.17	123.58	121.00
36	1	2619	G	C2-N3-C4	5.17	114.48	111.90
36	5	429	U	N3-C4-C5	5.17	117.70	114.60
36	5	1119	C	OP2-P-O3'	5.17	116.57	105.20
36	5	2339	C	OP1-P-O3'	5.17	116.57	105.20
36	5	3059	G	OP2-P-O3'	5.17	116.57	105.20
36	5	3092	C	C2-N3-C4	-5.17	117.32	119.90
36	5	2849	C	O5'-P-OP1	-5.17	101.05	105.70
36	1	1906	G	C6-C5-N7	-5.17	127.30	130.40
36	1	3242	G	C4-N9-C1'	-5.17	119.78	126.50
1	2	1473	U	N1-C2-O2	5.16	126.42	122.80
36	1	2603	G	C4-C5-N7	5.16	112.86	110.80
1	6	1480	G	N7-C8-N9	5.16	115.68	113.10
36	5	1145	G	C4-C5-N7	-5.16	108.73	110.80
36	5	1148	G	OP2-P-O3'	5.16	116.56	105.20
36	5	1399	A	O5'-P-OP2	-5.16	101.05	105.70
36	5	1408	G	N3-C2-N2	-5.16	116.29	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2886	U	N3-C4-O4	5.16	123.01	119.40
36	1	3362	A	C8-N9-C4	-5.16	103.73	105.80
36	5	75	G	N1-C6-O6	5.16	123.00	119.90
36	1	1113	G	N7-C8-N9	5.16	115.68	113.10
36	5	816	A	C4-C5-N7	-5.16	108.12	110.70
36	5	927	C	N3-C2-O2	5.16	125.51	121.90
36	5	974	G	N3-C4-C5	-5.16	126.02	128.60
36	5	1433	A	C8-N9-C4	-5.16	103.73	105.80
37	7	78	U	N3-C2-O2	-5.16	118.59	122.20
1	2	1307	U	C2-N1-C1'	5.16	123.89	117.70
36	1	1182	A	C8-N9-C4	5.16	107.86	105.80
36	1	2139	A	N1-C6-N6	-5.16	115.50	118.60
36	1	3195	U	N3-C2-O2	-5.16	118.59	122.20
38	4	40	A	C6-C5-N7	-5.16	128.69	132.30
1	6	111	U	O5'-P-OP2	-5.16	101.06	105.70
36	5	2871	G	N3-C2-N2	5.16	123.51	119.90
36	5	2872	A	N3-C4-N9	-5.16	123.27	127.40
36	1	672	A	C5-C6-N6	-5.16	119.57	123.70
36	5	2753	G	N3-C2-N2	-5.16	116.29	119.90
36	1	1615	C	N3-C2-O2	-5.16	118.29	121.90
36	1	3344	A	C8-N9-C4	-5.16	103.74	105.80
1	6	96	G	C5-C6-O6	5.16	131.69	128.60
36	5	1069	C	N3-C2-O2	-5.16	118.29	121.90
36	5	1934	G	N3-C4-N9	-5.16	122.91	126.00
36	5	2872	A	C2-N3-C4	-5.16	108.02	110.60
36	5	2947	G	OP1-P-O3'	5.16	116.54	105.20
36	5	2993	G	O5'-P-OP1	-5.16	101.06	105.70
1	2	1745	G	C6-N1-C2	-5.15	122.01	125.10
36	1	371	G	O5'-P-OP2	-5.15	101.06	105.70
36	1	2135	U	N3-C4-C5	5.15	117.69	114.60
36	5	710	A	C6-C5-N7	5.15	135.91	132.30
36	5	873	C	O5'-P-OP1	5.15	116.88	110.70
36	5	1941	C	N1-C2-O2	-5.15	115.81	118.90
36	5	2258	U	N3-C2-O2	-5.15	118.59	122.20
36	5	2283	G	N1-C6-O6	5.15	122.99	119.90
36	1	1867	A	N1-C6-N6	5.15	121.69	118.60
36	1	2728	G	C2-N3-C4	5.15	114.48	111.90
36	1	2844	C	N3-C4-C5	5.15	123.96	121.90
36	5	419	G	C5-C6-O6	-5.15	125.51	128.60
36	5	826	G	N3-C4-C5	5.15	131.18	128.60
36	5	1462	A	N3-C4-N9	-5.15	123.28	127.40
36	5	2935	U	N3-C4-O4	5.15	123.01	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3343	G	C6-C5-N7	-5.15	127.31	130.40
38	8	25	G	O5'-P-OP2	-5.15	101.06	105.70
38	8	95	G	C4-N9-C1'	-5.15	119.80	126.50
1	2	356	G	N1-C6-O6	5.15	122.99	119.90
36	1	426	G	N3-C4-C5	-5.15	126.03	128.60
36	1	930	U	N3-C4-C5	5.15	117.69	114.60
36	1	1618	G	N1-C6-O6	-5.15	116.81	119.90
36	1	2322	C	N3-C4-N4	-5.15	114.39	118.00
36	5	950	G	N3-C2-N2	5.15	123.50	119.90
36	5	1149	G	N3-C4-C5	-5.15	126.03	128.60
36	5	2145	A	N9-C4-C5	5.15	107.86	105.80
36	5	2819	A	O5'-P-OP2	-5.15	101.06	105.70
43	L6	154	LEU	CA-CB-CG	-5.15	103.46	115.30
36	5	424	G	C5-N7-C8	-5.15	101.73	104.30
36	5	2610	G	C8-N9-C4	-5.15	104.34	106.40
36	5	3218	A	C6-C5-N7	-5.15	128.70	132.30
1	2	1339	C	C6-N1-C2	-5.15	118.24	120.30
36	1	284	A	O5'-P-OP2	-5.15	101.07	105.70
36	1	1502	C	O5'-P-OP2	-5.15	101.07	105.70
36	1	2305	G	C6-C5-N7	-5.15	127.31	130.40
36	1	3209	A	C4-C5-N7	5.15	113.27	110.70
1	6	60	U	N1-C2-O2	5.15	126.40	122.80
36	5	2136	C	N3-C2-O2	-5.15	118.30	121.90
36	5	2939	G	N1-C2-N3	-5.15	120.81	123.90
36	5	1086	C	O5'-P-OP1	5.15	116.88	110.70
36	5	1452	A	C5-C6-N6	-5.15	119.58	123.70
1	2	965	U	N1-C2-O2	5.14	126.40	122.80
1	2	1370	U	P-O3'-C3'	5.14	125.87	119.70
36	1	1830	G	OP1-P-O3'	5.14	116.52	105.20
36	1	2662	G	O5'-P-OP2	-5.14	101.07	105.70
36	1	2887	A	N1-C6-N6	5.14	121.69	118.60
36	1	3093	C	C2-N1-C1'	-5.14	113.14	118.80
1	6	440	U	N1-C2-N3	5.14	117.99	114.90
1	6	956	C	C5-C6-N1	-5.14	118.43	121.00
5	s3	198	GLY	N-CA-C	-5.14	100.24	113.10
36	5	1440	G	C5-C6-O6	5.14	131.69	128.60
36	5	1520	G	C8-N9-C4	-5.14	104.34	106.40
36	5	2899	C	N3-C2-O2	-5.14	118.30	121.90
36	5	3091	A	C6-N1-C2	-5.14	115.51	118.60
36	1	859	G	C6-C5-N7	-5.14	127.31	130.40
36	1	1146	C	C6-N1-C2	-5.14	118.24	120.30
1	6	965	U	C2-N1-C1'	5.14	123.87	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1178	G	C4-N9-C1'	5.14	133.19	126.50
36	5	2191	U	N3-C4-C5	5.14	117.69	114.60
36	1	1520	G	C8-N9-C4	5.14	108.46	106.40
36	1	2403	G	O5'-P-OP1	5.14	116.87	110.70
38	4	102	U	N1-C2-N3	5.14	117.98	114.90
1	6	295	A	C8-N9-C4	5.14	107.86	105.80
1	6	1681	A	N1-C6-N6	5.14	121.68	118.60
36	5	934	G	N3-C4-C5	-5.14	126.03	128.60
36	5	2881	C	C4-C5-C6	-5.14	114.83	117.40
36	1	2974	U	C6-N1-C2	-5.14	117.92	121.00
37	3	91	G	N3-C2-N2	-5.14	116.30	119.90
1	6	755	A	O4'-C1'-N9	5.14	112.31	108.20
36	5	423	A	N7-C8-N9	-5.14	111.23	113.80
36	5	1376	C	OP1-P-OP2	5.14	127.31	119.60
36	5	1378	U	C6-N1-C2	5.14	124.08	121.00
36	1	714	G	OP2-P-O3'	5.14	116.50	105.20
36	1	2946	A	C6-C5-N7	-5.14	128.70	132.30
36	5	1791	C	C6-N1-C2	-5.14	118.25	120.30
38	4	115	C	O5'-P-OP2	-5.14	101.08	105.70
36	5	890	C	O5'-P-OP2	-5.14	101.08	105.70
36	5	936	A	P-O3'-C3'	5.14	125.86	119.70
36	5	2402	A	C8-N9-C4	-5.14	103.75	105.80
36	5	3362	A	C4-C5-N7	5.14	113.27	110.70
1	2	1773	C	C4-C5-C6	5.13	119.97	117.40
36	1	948	C	C2-N3-C4	-5.13	117.33	119.90
36	1	1578	C	C6-N1-C1'	-5.13	114.64	120.80
36	1	2377	G	N1-C2-N3	5.13	126.98	123.90
36	1	3266	G	N9-C4-C5	5.13	107.45	105.40
36	5	788	C	OP2-P-O3'	5.13	116.49	105.20
36	5	1178	G	C6-C5-N7	-5.13	127.32	130.40
36	5	2434	U	C5-C4-O4	5.13	128.98	125.90
36	5	2613	U	N3-C4-C5	-5.13	111.52	114.60
1	2	42	G	C6-C5-N7	5.13	133.48	130.40
1	2	1017	U	C5-C6-N1	-5.13	120.13	122.70
1	2	1633	A	N1-C2-N3	5.13	131.87	129.30
36	1	1056	U	C6-N1-C2	-5.13	117.92	121.00
36	1	1481	A	C4-C5-N7	5.13	113.27	110.70
38	4	116	G	C8-N9-C1'	-5.13	120.33	127.00
1	6	339	C	OP2-P-O3'	5.13	116.49	105.20
1	6	473	A	N1-C6-N6	-5.13	115.52	118.60
36	5	1390	A	C5-C6-N6	5.13	127.81	123.70
36	5	504	A	C8-N9-C4	5.13	107.85	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	641	C	N3-C4-C5	5.13	123.95	121.90
36	5	779	G	N1-C6-O6	5.13	122.98	119.90
36	5	878	G	OP1-P-O3'	5.13	116.48	105.20
1	2	1092	A	N1-C6-N6	5.13	121.68	118.60
36	1	922	U	C2-N1-C1'	5.13	123.85	117.70
36	1	2202	C	C5-C6-N1	5.13	123.56	121.00
38	4	147	U	C5-C4-O4	-5.13	122.82	125.90
1	6	1150	G	N7-C8-N9	-5.13	110.54	113.10
36	5	635	G	C6-C5-N7	-5.13	127.32	130.40
36	5	719	U	N3-C2-O2	-5.13	118.61	122.20
36	5	1154	A	N1-C6-N6	-5.13	115.52	118.60
36	5	2704	A	C8-N9-C4	5.13	107.85	105.80
1	2	1748	G	N3-C4-N9	-5.13	122.92	126.00
36	1	1428	A	C8-N9-C4	-5.13	103.75	105.80
4	s2	229	LEU	CA-CB-CG	5.13	127.09	115.30
36	5	1412	G	C5-N7-C8	-5.13	101.74	104.30
36	5	2366	C	C5-C6-N1	5.13	123.56	121.00
36	1	361	A	N9-C4-C5	5.12	107.85	105.80
36	1	1903	U	N3-C2-O2	5.12	125.79	122.20
36	1	3375	A	C5'-C4'-C3'	-5.12	107.80	116.00
37	3	97	A	N1-C6-N6	-5.12	115.53	118.60
36	5	2126	A	C8-N9-C4	5.12	107.85	105.80
1	2	1657	U	N1-C2-O2	5.12	126.39	122.80
1	2	1730	A	C4-C5-C6	-5.12	114.44	117.00
36	1	225	C	N3-C4-C5	-5.12	119.85	121.90
36	1	1165	A	C5-N7-C8	5.12	106.46	103.90
36	1	1210	U	C2-N3-C4	-5.12	123.93	127.00
36	1	3181	C	N1-C2-N3	5.12	122.79	119.20
36	1	3244	A	O5'-P-OP1	-5.12	101.09	105.70
1	6	1281	G	N1-C6-O6	5.12	122.97	119.90
36	5	3184	A	N1-C2-N3	-5.12	126.74	129.30
36	5	3311	C	N3-C4-C5	-5.12	119.85	121.90
1	2	1570	A	C8-N9-C4	5.12	107.85	105.80
36	1	1043	C	N3-C4-C5	5.12	123.95	121.90
36	1	2878	G	OP1-P-OP2	-5.12	111.92	119.60
36	1	2937	G	N7-C8-N9	-5.12	110.54	113.10
1	6	308	C	C2-N3-C4	-5.12	117.34	119.90
1	6	1726	G	OP2-P-O3'	5.12	116.47	105.20
36	1	1329	U	O4'-C1'-N1	5.12	112.30	108.20
36	1	1482	A	N3-C4-C5	-5.12	123.22	126.80
36	1	2627	C	C2-N3-C4	-5.12	117.34	119.90
36	5	2208	A	O4'-C1'-N9	5.12	112.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	447	U	N3-C2-O2	-5.12	118.62	122.20
36	1	357	A	N1-C2-N3	5.12	131.86	129.30
36	1	427	C	N3-C4-C5	-5.12	119.85	121.90
36	1	2973	G	N3-C2-N2	-5.12	116.32	119.90
36	1	3277	U	N3-C2-O2	-5.12	118.62	122.20
1	6	1537	C	C4-C5-C6	5.12	119.96	117.40
36	5	216	G	C5-N7-C8	-5.12	101.74	104.30
36	5	661	G	OP1-P-O3'	5.12	116.46	105.20
36	5	2419	A	N7-C8-N9	5.12	116.36	113.80
36	1	298	U	N1-C2-O2	5.12	126.38	122.80
36	1	2831	G	C6-C5-N7	-5.12	127.33	130.40
36	5	915	A	N3-C4-N9	5.12	131.49	127.40
36	5	3223	A	C5-C6-N1	5.12	120.26	117.70
36	1	2218	G	N3-C4-C5	-5.12	126.04	128.60
36	1	2689	A	N1-C6-N6	-5.12	115.53	118.60
1	6	677	G	N3-C4-C5	5.12	131.16	128.60
36	5	964	G	C5-C6-O6	-5.12	125.53	128.60
36	5	1329	U	C5-C6-N1	-5.12	120.14	122.70
36	5	1902	G	N9-C4-C5	-5.12	103.35	105.40
36	5	2830	G	C4-C5-C6	5.12	121.87	118.80
36	5	3139	A	C5-N7-C8	-5.12	101.34	103.90
36	1	322	U	N3-C2-O2	-5.11	118.62	122.20
33	e1	100	LEU	CA-CB-CG	5.11	127.06	115.30
36	5	673	U	C4-C5-C6	5.11	122.77	119.70
36	5	793	C	C5-C6-N1	5.11	123.56	121.00
36	5	2299	A	O5'-P-OP2	-5.11	101.10	105.70
36	5	2621	G	C5-C6-O6	-5.11	125.53	128.60
1	6	1092	A	N1-C6-N6	5.11	121.67	118.60
36	5	530	G	C8-N9-C4	-5.11	104.36	106.40
36	5	644	G	C2-N3-C4	5.11	114.46	111.90
36	5	2349	U	OP1-P-O3'	5.11	116.45	105.20
36	1	231	G	N1-C6-O6	-5.11	116.83	119.90
1	6	475	A	N1-C6-N6	5.11	121.67	118.60
38	8	39	G	C4-N9-C1'	5.11	133.14	126.50
38	8	113	U	C5-C6-N1	5.11	125.25	122.70
36	1	374	A	C6-C5-N7	5.11	135.88	132.30
36	1	1924	U	N1-C2-O2	-5.11	119.22	122.80
36	1	2144	A	N3-C4-N9	5.11	131.49	127.40
36	1	3242	G	C6-C5-N7	5.11	133.47	130.40
36	5	1592	G	OP2-P-O3'	5.11	116.44	105.20
1	2	628	G	O5'-P-OP2	-5.11	101.10	105.70
36	1	633	C	N3-C4-C5	-5.11	119.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3015	G	C5-C6-O6	-5.11	125.53	128.60
38	4	24	G	C4-C5-N7	5.11	112.84	110.80
38	4	64	U	N3-C2-O2	-5.11	118.62	122.20
1	6	1696	G	C3'-C2'-C1'	5.11	105.58	101.50
36	5	974	G	C8-N9-C4	-5.11	104.36	106.40
36	5	1396	C	OP2-P-O3'	5.11	116.44	105.20
36	5	2751	G	N7-C8-N9	5.11	115.65	113.10
1	2	1639	C	C6-N1-C2	-5.11	118.26	120.30
36	1	345	G	N3-C4-C5	-5.11	126.05	128.60
36	1	637	C	OP1-P-O3'	5.11	116.43	105.20
36	1	2409	G	N9-C4-C5	5.11	107.44	105.40
36	1	2661	G	C5-C6-O6	-5.11	125.54	128.60
36	1	2993	G	N1-C6-O6	5.11	122.96	119.90
1	6	1478	G	C8-N9-C4	-5.11	104.36	106.40
37	7	92	A	C8-N9-C4	5.11	107.84	105.80
36	1	909	G	C8-N9-C4	5.10	108.44	106.40
36	5	2320	A	C2-N3-C4	-5.10	108.05	110.60
36	5	2754	G	C5-C6-O6	5.10	131.66	128.60
36	1	994	G	N3-C4-N9	5.10	129.06	126.00
36	5	2234	G	C5-C6-N1	5.10	114.05	111.50
1	2	9	U	O5'-P-OP1	-5.10	101.11	105.70
1	2	737	A	O4'-C1'-N9	5.10	112.28	108.20
36	1	125	C	C5-C6-N1	-5.10	118.45	121.00
36	1	519	A	N1-C6-N6	5.10	121.66	118.60
36	1	930	U	C2-N1-C1'	-5.10	111.58	117.70
36	1	1060	U	C5-C6-N1	-5.10	120.15	122.70
36	1	1340	G	C5-C6-N1	5.10	114.05	111.50
36	1	1469	C	C5-C4-N4	-5.10	116.63	120.20
1	6	421	A	C5-C6-N6	-5.10	119.62	123.70
68	o2	44	ARG	NE-CZ-NH2	5.10	122.85	120.30
36	1	1188	U	C5-C4-O4	5.10	128.96	125.90
36	1	1314	C	C5-C6-N1	5.10	123.55	121.00
36	1	1790	G	N1-C6-O6	5.10	122.96	119.90
36	1	2911	A	C8-N9-C4	5.10	107.84	105.80
1	6	1481	C	C6-N1-C2	-5.10	118.26	120.30
36	5	112	U	O4'-C1'-N1	5.10	112.28	108.20
36	5	2281	A	O4'-C1'-N9	5.10	112.28	108.20
36	5	2943	G	C4-N9-C1'	5.10	133.13	126.50
36	5	3243	A	C4-C5-C6	5.10	119.55	117.00
36	1	587	U	N1-C2-O2	-5.10	119.23	122.80
36	1	1815	U	P-O3'-C3'	5.10	125.82	119.70
36	1	3224	G	N1-C2-N2	5.10	120.79	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	11	C	OP2-P-O3'	5.10	116.42	105.20
64	N8	59	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	6	744	U	C5-C4-O4	5.10	128.96	125.90
36	5	641	C	C6-N1-C1'	5.10	126.92	120.80
36	5	661	G	N1-C6-O6	5.10	122.96	119.90
36	5	1408	G	N1-C6-O6	5.10	122.96	119.90
36	5	2389	C	N3-C4-C5	5.10	123.94	121.90
1	2	1241	G	C6-C5-N7	-5.10	127.34	130.40
36	1	1618	G	C5-C6-O6	5.10	131.66	128.60
36	1	1795	U	N1-C2-O2	5.10	126.37	122.80
1	6	106	U	OP2-P-O3'	5.10	116.41	105.20
36	5	2849	C	OP1-P-OP2	5.10	127.24	119.60
37	7	37	G	C6-C5-N7	-5.10	127.34	130.40
36	1	2599	U	C2-N1-C1'	5.09	123.81	117.70
36	1	3079	U	N1-C2-O2	-5.09	119.23	122.80
1	6	372	G	C2-N3-C4	5.09	114.45	111.90
1	6	767	U	N1-C2-N3	5.09	117.96	114.90
1	6	1235	C	C5-C6-N1	5.09	123.55	121.00
36	5	191	U	N3-C2-O2	5.09	125.77	122.20
36	5	681	U	O5'-P-OP2	-5.09	101.11	105.70
36	5	690	A	C8-N9-C4	5.09	107.84	105.80
36	5	2881	C	C5-C4-N4	-5.09	116.63	120.20
36	5	2990	G	C6-C5-N7	-5.09	127.34	130.40
1	2	558	U	N1-C2-O2	5.09	126.36	122.80
36	5	3207	U	N1-C2-O2	-5.09	119.23	122.80
36	1	884	A	C2-N3-C4	-5.09	108.05	110.60
36	1	1522	U	C5-C4-O4	-5.09	122.84	125.90
36	1	2177	G	C5-C6-N1	5.09	114.05	111.50
36	1	2937	G	N1-C2-N2	5.09	120.78	116.20
37	3	38	U	N3-C2-O2	5.09	125.76	122.20
1	6	100	A	C5-C6-N1	-5.09	115.15	117.70
36	5	1490	A	N7-C8-N9	5.09	116.35	113.80
36	5	2263	C	C5-C4-N4	-5.09	116.64	120.20
36	5	2292	U	O5'-P-OP2	-5.09	101.12	105.70
36	5	2889	C	N3-C2-O2	-5.09	118.34	121.90
36	1	519	A	O5'-P-OP1	-5.09	101.12	105.70
36	1	1798	A	C2-N3-C4	-5.09	108.06	110.60
1	6	1629	G	OP2-P-O3'	5.09	116.40	105.20
36	5	504	A	C2-N3-C4	-5.09	108.06	110.60
36	5	1853	U	N1-C2-N3	5.09	117.95	114.90
36	5	3308	C	N1-C2-O2	-5.09	115.85	118.90
36	5	971	G	OP2-P-O3'	5.09	116.39	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1464	G	C8-N9-C4	5.09	108.44	106.40
36	5	3030	G	C5-N7-C8	5.09	106.84	104.30
1	2	31	C	C5-C6-N1	5.09	123.54	121.00
36	1	1193	A	N1-C6-N6	5.09	121.65	118.60
36	1	1414	G	C2-N3-C4	-5.09	109.36	111.90
36	1	1547	G	C8-N9-C4	5.09	108.43	106.40
1	6	756	A	C5-N7-C8	-5.09	101.36	103.90
36	5	1903	U	O5'-P-OP2	5.09	116.80	110.70
36	5	2914	G	C2-N3-C4	5.09	114.44	111.90
1	2	1668	G	N9-C4-C5	5.08	107.43	105.40
36	1	1835	A	C5-C6-N6	5.08	127.77	123.70
36	1	2615	G	C4-C5-N7	5.08	112.83	110.80
36	5	2341	A	C8-N9-C4	5.08	107.83	105.80
36	1	1421	G	OP2-P-O3'	5.08	116.38	105.20
38	4	103	G	C6-N1-C2	-5.08	122.05	125.10
1	6	1465	C	C6-N1-C2	-5.08	118.27	120.30
36	5	410	U	C6-N1-C2	-5.08	117.95	121.00
36	5	1145	G	N3-C2-N2	-5.08	116.34	119.90
36	5	1368	U	N3-C2-O2	5.08	125.76	122.20
36	5	1902	G	C8-N9-C1'	-5.08	120.39	127.00
36	5	2724	U	N3-C2-O2	-5.08	118.64	122.20
36	5	3362	A	C6-C5-N7	-5.08	128.74	132.30
36	1	1150	A	O5'-P-OP2	-5.08	101.13	105.70
36	1	2718	U	N3-C2-O2	-5.08	118.64	122.20
36	1	3375	A	N7-C8-N9	5.08	116.34	113.80
1	6	4	C	N3-C4-C5	5.08	123.93	121.90
36	5	3174	A	N1-C6-N6	5.08	121.65	118.60
36	5	3303	G	C5-C6-O6	5.08	131.65	128.60
38	8	95	G	C8-N9-C1'	5.08	133.61	127.00
1	2	1445	G	O4'-C1'-N9	5.08	112.26	108.20
36	5	1846	C	N3-C4-C5	5.08	123.93	121.90
36	5	2273	G	C6-C5-N7	5.08	133.45	130.40
36	5	2297	U	O5'-P-OP2	-5.08	101.13	105.70
36	1	863	C	OP2-P-O3'	5.08	116.37	105.20
36	1	3016	A	C5-C6-N6	-5.08	119.64	123.70
36	1	3259	U	C6-N1-C2	-5.08	117.95	121.00
38	4	52	A	C8-N9-C4	-5.08	103.77	105.80
1	6	7	G	N3-C4-C5	-5.08	126.06	128.60
23	d1	11	LEU	CA-CB-CG	5.08	126.98	115.30
36	5	170	G	C4-N9-C1'	5.08	133.10	126.50
36	5	329	U	N3-C2-O2	-5.08	118.64	122.20
36	5	932	U	C5-C4-O4	-5.08	122.85	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1189	C	N3-C2-O2	5.08	125.46	121.90
36	5	1456	A	N1-C6-N6	5.08	121.65	118.60
36	5	2114	C	OP1-P-OP2	5.08	127.22	119.60
36	5	3315	G	C4-C5-N7	-5.08	108.77	110.80
36	1	784	A	O4'-C1'-N9	5.08	112.26	108.20
36	1	1879	A	O4'-C1'-N9	5.08	112.26	108.20
36	1	2404	A	N9-C1'-C2'	-5.08	106.42	112.00
38	4	40	A	C4-C5-N7	5.08	113.24	110.70
36	1	212	G	N3-C4-N9	5.08	129.04	126.00
36	1	406	G	N3-C2-N2	5.08	123.45	119.90
36	1	1152	G	O5'-P-OP1	-5.08	101.13	105.70
36	1	1845	G	C8-N9-C4	-5.08	104.37	106.40
36	1	2986	U	C6-N1-C1'	5.08	128.31	121.20
38	4	82	U	N3-C2-O2	5.08	125.75	122.20
57	N1	83	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	6	337	G	O4'-C1'-N9	-5.08	104.14	108.20
1	6	1324	G	N1-C6-O6	5.08	122.94	119.90
36	5	339	C	C6-N1-C1'	5.08	126.89	120.80
36	5	1129	A	O5'-P-OP2	-5.08	101.13	105.70
36	5	2404	A	C5-N7-C8	5.08	106.44	103.90
36	5	2948	C	O5'-P-OP1	5.08	116.79	110.70
1	2	1596	C	C2-N1-C1'	5.07	124.38	118.80
36	1	1191	U	N1-C2-N3	5.07	117.94	114.90
36	1	2294	U	N3-C2-O2	-5.07	118.65	122.20
1	6	1139	A	N1-C6-N6	-5.07	115.56	118.60
36	5	580	C	C6-N1-C2	-5.07	118.27	120.30
36	5	1314	C	C2-N1-C1'	5.07	124.38	118.80
36	5	1662	G	C6-C5-N7	-5.07	127.36	130.40
36	1	2606	G	C4-C5-C6	5.07	121.84	118.80
36	1	2821	C	O5'-P-OP1	-5.07	101.14	105.70
1	6	755	A	N1-C6-N6	5.07	121.64	118.60
36	5	2816	G	N1-C2-N2	-5.07	111.64	116.20
36	1	2353	G	N1-C6-O6	5.07	122.94	119.90
36	1	2606	G	N3-C4-C5	-5.07	126.06	128.60
1	6	1114	G	O4'-C1'-N9	5.07	112.26	108.20
36	5	110	G	C8-N9-C4	5.07	108.43	106.40
36	5	1113	G	C6-C5-N7	-5.07	127.36	130.40
36	5	2121	G	N9-C4-C5	-5.07	103.37	105.40
48	m1	30	LEU	CA-CB-CG	5.07	126.96	115.30
1	2	1291	G	C2-N3-C4	-5.07	109.36	111.90
1	6	89	G	N1-C6-O6	5.07	122.94	119.90
36	5	220	G	OP1-P-O3'	5.07	116.35	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1931	U	N3-C4-O4	-5.07	115.85	119.40
1	2	192	U	N1-C2-O2	5.07	126.35	122.80
1	2	1777	G	C4-C5-N7	5.07	112.83	110.80
18	C6	40	GLU	C-N-CA	5.07	143.28	122.00
36	1	800	G	C5-C6-N1	-5.07	108.97	111.50
36	1	2215	A	N3-C4-C5	5.07	130.35	126.80
36	1	2789	U	N3-C4-C5	-5.07	111.56	114.60
38	4	88	A	N9-C4-C5	-5.07	103.77	105.80
36	5	183	G	C8-N9-C1'	-5.07	120.41	127.00
36	5	831	G	C5-C6-O6	-5.07	125.56	128.60
36	5	1506	A	N7-C8-N9	5.07	116.33	113.80
36	1	969	C	C5-C4-N4	-5.07	116.65	120.20
70	O4	8	ARG	NE-CZ-NH2	-5.07	117.77	120.30
36	5	1203	A	C5-C6-N6	-5.07	119.65	123.70
36	1	58	G	N7-C8-N9	5.06	115.63	113.10
36	1	590	G	C5-C6-O6	-5.06	125.56	128.60
38	4	81	U	N1-C2-O2	-5.06	119.25	122.80
24	d2	93	LEU	CA-CB-CG	5.06	126.95	115.30
36	5	1117	G	N1-C2-N3	-5.06	120.86	123.90
36	5	2849	C	N3-C4-C5	-5.06	119.87	121.90
38	8	44	A	C5-C6-N6	-5.06	119.65	123.70
36	1	305	U	C5-C6-N1	-5.06	120.17	122.70
36	1	806	A	C5-N7-C8	-5.06	101.37	103.90
36	1	2612	U	N3-C4-C5	5.06	117.64	114.60
36	1	2867	C	C2-N3-C4	-5.06	117.37	119.90
36	1	2912	G	C2-N3-C4	5.06	114.43	111.90
1	6	1522	U	C2-N1-C1'	-5.06	111.63	117.70
36	5	517	G	C8-N9-C4	-5.06	104.38	106.40
36	5	1390	A	N1-C2-N3	5.06	131.83	129.30
36	5	2935	U	C5-C6-N1	5.06	125.23	122.70
36	5	3128	G	N9-C4-C5	-5.06	103.38	105.40
36	5	3278	C	C5-C6-N1	-5.06	118.47	121.00
36	1	1396	C	C5-C4-N4	-5.06	116.66	120.20
38	4	52	A	C2-N3-C4	5.06	113.13	110.60
36	5	1311	G	C5-C6-N1	5.06	114.03	111.50
36	5	2215	A	C2-N3-C4	-5.06	108.07	110.60
36	5	2889	C	C2-N3-C4	-5.06	117.37	119.90
36	5	3368	U	O5'-P-OP1	-5.06	101.14	105.70
1	2	1455	G	C5-C6-N1	-5.06	108.97	111.50
36	1	382	U	N3-C2-O2	5.06	125.74	122.20
36	1	1316	C	C2-N3-C4	-5.06	117.37	119.90
36	1	2417	U	OP2-P-O3'	5.06	116.33	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3218	A	P-O3'-C3'	5.06	125.77	119.70
36	1	3224	G	N3-C4-N9	-5.06	122.96	126.00
1	6	359	A	C8-N9-C1'	5.06	136.81	127.70
1	6	1481	C	N3-C2-O2	-5.06	118.36	121.90
36	5	2950	G	C6-N1-C2	5.06	128.13	125.10
1	6	421	A	C4-C5-N7	5.06	113.23	110.70
36	5	617	G	N1-C6-O6	5.06	122.93	119.90
36	5	1394	A	C6-C5-N7	5.06	135.84	132.30
36	5	1903	U	OP1-P-OP2	-5.06	112.01	119.60
36	5	2939	G	C8-N9-C4	5.06	108.42	106.40
36	1	392	G	N1-C6-O6	5.06	122.93	119.90
36	1	1475	A	C8-N9-C4	5.06	107.82	105.80
36	1	2942	C	N3-C2-O2	5.06	125.44	121.90
36	1	3059	G	N1-C6-O6	-5.06	116.87	119.90
1	6	297	U	C5-C4-O4	-5.06	122.87	125.90
1	6	1129	U	N3-C4-O4	-5.06	115.86	119.40
36	5	2213	A	N7-C8-N9	-5.06	111.27	113.80
36	5	2403	G	O5'-P-OP1	5.06	116.77	110.70
37	7	85	G	OP1-P-OP2	-5.06	112.02	119.60
1	2	56	U	N3-C2-O2	-5.05	118.66	122.20
1	2	465	G	O5'-P-OP1	-5.05	101.15	105.70
36	1	1432	C	C6-N1-C2	-5.05	118.28	120.30
36	1	2413	A	C5-C6-N1	5.05	120.23	117.70
37	7	53	U	N3-C4-O4	5.05	122.94	119.40
36	1	3197	G	N3-C4-C5	5.05	131.13	128.60
1	2	142	G	N3-C4-C5	5.05	131.13	128.60
36	1	809	G	N1-C6-O6	5.05	122.93	119.90
36	1	2414	G	N3-C4-N9	-5.05	122.97	126.00
1	6	866	G	C8-N9-C4	5.05	108.42	106.40
1	6	1100	G	C4-N9-C1'	5.05	133.07	126.50
36	5	419	G	N3-C4-N9	5.05	129.03	126.00
36	5	632	G	O5'-P-OP1	5.05	116.76	110.70
36	5	1931	U	C6-N1-C1'	5.05	128.27	121.20
36	5	2346	C	C5-C4-N4	-5.05	116.66	120.20
36	5	3209	A	C5-N7-C8	-5.05	101.38	103.90
36	5	3314	A	C5-N7-C8	-5.05	101.37	103.90
40	13	196	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	2	1783	C	C5-C4-N4	-5.05	116.67	120.20
36	1	660	A	O5'-P-OP1	-5.05	101.16	105.70
36	1	3349	C	C5-C6-N1	5.05	123.53	121.00
1	6	294	C	O5'-P-OP2	-5.05	101.16	105.70
1	6	447	U	C6-N1-C2	-5.05	117.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1119	G	C5-C6-O6	5.05	131.63	128.60
1	6	1123	C	N3-C2-O2	5.05	125.44	121.90
1	6	1778	G	C5-N7-C8	-5.05	101.78	104.30
36	5	672	A	N1-C6-N6	5.05	121.63	118.60
36	5	1203	A	C5-N7-C8	-5.05	101.38	103.90
36	5	2871	G	N1-C6-O6	-5.05	116.87	119.90
36	1	2371	G	N9-C4-C5	-5.05	103.38	105.40
1	6	457	G	N1-C6-O6	5.05	122.93	119.90
36	5	2245	C	C5-C6-N1	5.05	123.52	121.00
37	7	109	G	C4-N9-C1'	-5.05	119.94	126.50
36	1	321	C	N3-C2-O2	-5.05	118.37	121.90
36	1	2401	A	N1-C6-N6	5.05	121.63	118.60
36	1	3127	A	C5-C6-N6	-5.05	119.66	123.70
36	5	1939	G	OP2-P-O3'	5.05	116.30	105.20
36	5	2637	A	N9-C4-C5	-5.05	103.78	105.80
36	5	3265	C	C6-N1-C2	-5.05	118.28	120.30
37	7	81	U	N3-C4-C5	5.05	117.63	114.60
36	1	1578	C	C6-N1-C2	-5.04	118.28	120.30
36	1	2255	A	P-O3'-C3'	5.04	125.75	119.70
1	6	334	G	N7-C8-N9	-5.04	110.58	113.10
1	6	966	A	C2-N3-C4	5.04	113.12	110.60
36	5	197	G	N3-C4-N9	5.04	129.03	126.00
36	5	651	G	C6-N1-C2	-5.04	122.07	125.10
36	5	3089	C	N3-C4-N4	5.04	121.53	118.00
36	1	1095	U	C5-C4-O4	5.04	128.93	125.90
36	1	2169	G	C5-C6-O6	5.04	131.63	128.60
36	1	3316	A	P-O3'-C3'	5.04	125.75	119.70
38	4	40	A	O5'-P-OP2	5.04	116.75	110.70
1	6	901	G	N1-C6-O6	5.04	122.93	119.90
36	5	297	G	N1-C6-O6	-5.04	116.87	119.90
36	5	326	U	N3-C2-O2	5.04	125.73	122.20
36	5	2794	G	C5-C6-O6	-5.04	125.57	128.60
36	5	2936	A	C8-N9-C4	-5.04	103.78	105.80
1	2	1324	G	C4-N9-C1'	-5.04	119.95	126.50
36	1	346	C	C6-N1-C2	5.04	122.32	120.30
36	1	1808	G	N3-C4-C5	-5.04	126.08	128.60
38	4	31	G	O5'-P-OP2	-5.04	101.16	105.70
1	6	484	C	C5-C6-N1	5.04	123.52	121.00
36	5	641	C	N3-C2-O2	5.04	125.43	121.90
36	5	878	G	N3-C2-N2	5.04	123.43	119.90
36	5	1317	A	C4-C5-N7	5.04	113.22	110.70
36	5	2385	G	C4-N9-C1'	-5.04	119.95	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2390	A	OP2-P-O3'	5.04	116.29	105.20
36	5	3196	U	O5'-P-OP1	-5.04	101.16	105.70
36	1	226	C	C5-C4-N4	-5.04	116.67	120.20
36	1	950	G	N3-C4-C5	5.04	131.12	128.60
36	1	1846	C	O5'-P-OP1	-5.04	101.16	105.70
36	1	2630	C	OP1-P-OP2	5.04	127.16	119.60
36	5	101	G	C8-N9-C1'	-5.04	120.45	127.00
36	5	1200	A	C4-C5-C6	5.04	119.52	117.00
36	5	1380	G	OP2-P-O3'	5.04	116.29	105.20
36	5	2412	G	N3-C4-C5	-5.04	126.08	128.60
36	5	2821	C	C5-C6-N1	-5.04	118.48	121.00
1	2	488	G	O5'-P-OP1	5.04	116.75	110.70
36	1	917	A	OP2-P-O3'	5.04	116.28	105.20
36	1	2960	C	N3-C4-C5	5.04	123.92	121.90
36	5	659	G	C5-C6-O6	-5.04	125.58	128.60
36	5	1155	C	C4-C5-C6	-5.04	114.88	117.40
36	5	1300	G	OP1-P-O3'	5.04	116.28	105.20
36	5	2291	A	C8-N9-C4	5.04	107.82	105.80
36	1	961	C	C2-N3-C4	-5.04	117.38	119.90
36	1	1952	G	N3-C4-C5	-5.04	126.08	128.60
36	1	3214	U	N3-C4-C5	-5.04	111.58	114.60
1	6	542	A	C5-N7-C8	-5.04	101.38	103.90
36	5	803	C	N1-C2-O2	5.04	121.92	118.90
36	5	1174	G	C4-N9-C1'	5.04	133.05	126.50
36	1	48	A	C5-C6-N1	5.04	120.22	117.70
36	1	340	C	C2-N3-C4	-5.04	117.38	119.90
36	1	1129	A	N1-C6-N6	5.04	121.62	118.60
36	1	2300	G	N3-C2-N2	-5.04	116.38	119.90
37	3	94	C	N1-C2-O2	-5.04	115.88	118.90
38	4	118	C	N1-C2-O2	-5.04	115.88	118.90
36	5	2693	C	O5'-P-OP1	-5.04	101.17	105.70
36	5	3214	U	N1-C2-O2	5.04	126.33	122.80
1	2	1600	A	C6-C5-N7	-5.03	128.78	132.30
36	1	1365	G	C2-N3-C4	5.03	114.42	111.90
36	1	2887	A	C5-C6-N6	-5.03	119.67	123.70
37	3	86	U	C5-C4-O4	-5.03	122.88	125.90
37	3	105	C	O5'-P-OP1	5.03	116.74	110.70
36	5	335	G	C6-C5-N7	5.03	133.42	130.40
36	5	1219	C	N3-C4-N4	-5.03	114.48	118.00
36	5	2278	C	N1-C2-O2	5.03	121.92	118.90
37	7	68	C	N3-C2-O2	-5.03	118.38	121.90
37	7	102	A	C5-C6-N1	-5.03	115.18	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2399	A	C2-N3-C4	5.03	113.12	110.60
36	5	1902	G	C4-N9-C1'	5.03	133.04	126.50
1	2	1423	U	N1-C2-O2	-5.03	119.28	122.80
36	1	80	G	N7-C8-N9	-5.03	110.58	113.10
36	1	935	U	OP2-P-O3'	5.03	116.27	105.20
36	1	1419	A	C4-C5-C6	5.03	119.52	117.00
36	1	3085	G	N1-C6-O6	5.03	122.92	119.90
1	6	813	U	C2-N1-C1'	5.03	123.74	117.70
1	6	1778	G	N9-C4-C5	5.03	107.41	105.40
36	5	821	U	N3-C2-O2	-5.03	118.68	122.20
36	5	2654	C	N1-C2-O2	-5.03	115.88	118.90
1	2	313	U	N1-C2-O2	-5.03	119.28	122.80
1	2	1768	G	C6-C5-N7	5.03	133.42	130.40
36	1	203	G	C8-N9-C4	5.03	108.41	106.40
36	1	664	U	C6-N1-C2	5.03	124.02	121.00
36	1	2637	A	O5'-P-OP1	-5.03	101.17	105.70
36	1	2818	U	OP2-P-O3'	5.03	116.26	105.20
1	6	106	U	O5'-P-OP1	-5.03	101.17	105.70
36	5	364	G	C4-C5-N7	5.03	112.81	110.80
36	5	1833	G	C6-C5-N7	5.03	133.42	130.40
36	5	1868	G	C4-C5-N7	5.03	112.81	110.80
1	2	36	C	C6-N1-C2	5.03	122.31	120.30
1	2	545	A	OP1-P-O3'	5.03	116.26	105.20
36	1	645	A	N1-C2-N3	5.03	131.81	129.30
36	1	2366	C	C5-C6-N1	5.03	123.51	121.00
36	1	2592	G	C4-C5-N7	5.03	112.81	110.80
36	1	2808	A	C8-N9-C1'	-5.03	118.65	127.70
1	6	829	A	O5'-P-OP1	5.03	116.73	110.70
1	6	1586	A	C8-N9-C4	5.03	107.81	105.80
1	6	1744	A	C2-N3-C4	-5.03	108.09	110.60
36	5	810	A	C5-C6-N1	5.03	120.21	117.70
36	5	1200	A	P-O3'-C3'	5.03	125.73	119.70
36	5	2970	C	OP1-P-OP2	5.03	127.14	119.60
1	6	163	G	C5-N7-C8	-5.02	101.79	104.30
36	5	32	U	N1-C2-O2	-5.02	119.28	122.80
36	5	340	C	N3-C4-C5	5.02	123.91	121.90
37	7	90	U	C5-C4-O4	-5.02	122.89	125.90
36	1	2300	G	N3-C4-N9	-5.02	122.99	126.00
36	1	2869	U	O5'-P-OP1	-5.02	101.18	105.70
36	1	2975	U	N3-C4-C5	5.02	117.61	114.60
36	5	1662	G	N1-C6-O6	5.02	122.91	119.90
36	5	1870	C	N1-C2-O2	-5.02	115.89	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2584	G	OP2-P-O3'	5.02	116.25	105.20
1	2	1497	U	C2-N1-C1'	5.02	123.72	117.70
36	1	649	A	C8-N9-C4	5.02	107.81	105.80
36	1	667	C	C6-N1-C2	5.02	122.31	120.30
36	1	1450	G	C4-C5-N7	5.02	112.81	110.80
36	1	2241	U	C2-N1-C1'	-5.02	111.67	117.70
36	1	2983	C	O5'-P-OP1	-5.02	101.18	105.70
36	5	1513	G	C2-N3-C4	5.02	114.41	111.90
36	5	3245	A	N9-C4-C5	-5.02	103.79	105.80
36	1	394	G	C5-C6-O6	5.02	131.61	128.60
36	1	608	A	C4-C5-C6	5.02	119.51	117.00
36	1	967	A	OP2-P-O3'	5.02	116.24	105.20
36	1	1724	U	P-O3'-C3'	5.02	125.72	119.70
36	1	2944	U	C4-C5-C6	-5.02	116.69	119.70
1	6	417	A	O5'-P-OP2	-5.02	101.18	105.70
1	6	687	G	N1-C2-N2	5.02	120.72	116.20
36	5	514	G	C6-C5-N7	-5.02	127.39	130.40
36	5	1420	C	C2-N1-C1'	-5.02	113.28	118.80
36	5	1528	G	OP2-P-O3'	5.02	116.24	105.20
36	5	2802	A	N1-C2-N3	-5.02	126.79	129.30
37	7	56	A	C4-C5-N7	5.02	113.21	110.70
56	n0	117	ARG	NE-CZ-NH1	-5.02	117.79	120.30
36	1	545	U	N1-C2-O2	5.02	126.31	122.80
36	1	866	A	N1-C2-N3	-5.02	126.79	129.30
36	1	2627	C	N3-C4-C5	5.02	123.91	121.90
36	5	676	G	C5-C6-O6	5.02	131.61	128.60
43	l6	173	MET	CB-CG-SD	-5.02	97.35	112.40
36	1	2621	G	C5-C6-O6	-5.02	125.59	128.60
1	6	1307	U	C2-N1-C1'	-5.02	111.68	117.70
36	5	1698	C	O5'-P-OP2	-5.02	101.19	105.70
52	m6	94	ARG	NE-CZ-NH2	5.02	122.81	120.30
36	1	97	U	C6-N1-C1'	5.01	128.22	121.20
36	1	1143	A	N9-C4-C5	5.01	107.81	105.80
36	1	1196	C	OP1-P-O3'	5.01	116.23	105.20
36	1	2572	C	C6-N1-C2	-5.01	118.29	120.30
1	6	1747	G	O5'-P-OP2	-5.01	101.19	105.70
36	1	577	C	N3-C4-C5	-5.01	119.89	121.90
36	1	1371	G	C8-N9-C1'	-5.01	120.48	127.00
36	1	2169	G	OP2-P-O3'	5.01	116.23	105.20
36	1	2356	A	C4-C5-N7	5.01	113.21	110.70
37	7	57	G	N3-C4-C5	5.01	131.11	128.60
1	2	565	C	N3-C4-C5	5.01	123.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	35	A	N1-C6-N6	5.01	121.61	118.60
36	1	2606	G	C4-N9-C1'	5.01	133.01	126.50
36	1	2619	G	N1-C6-O6	-5.01	116.89	119.90
40	L3	102	LEU	CA-CB-CG	5.01	126.83	115.30
1	6	597	G	O5'-P-OP2	-5.01	101.19	105.70
36	5	1164	G	N9-C4-C5	5.01	107.40	105.40
36	5	2823	G	N1-C6-O6	5.01	122.91	119.90
36	5	2866	U	N3-C2-O2	-5.01	118.69	122.20
1	2	697	C	C6-N1-C2	-5.01	118.30	120.30
1	2	730	G	C4-N9-C1'	5.01	133.01	126.50
1	2	767	U	N3-C2-O2	-5.01	118.69	122.20
36	1	654	C	N1-C2-O2	-5.01	115.89	118.90
36	1	1125	U	OP2-P-O3'	5.01	116.22	105.20
36	1	1849	C	N3-C4-N4	5.01	121.51	118.00
36	1	2309	A	OP1-P-OP2	5.01	127.11	119.60
1	6	1192	C	N1-C2-O2	5.01	121.91	118.90
36	5	972	A	C4-C5-N7	-5.01	108.19	110.70
36	5	1542	G	N3-C2-N2	-5.01	116.39	119.90
1	6	969	C	N1-C2-O2	-5.01	115.89	118.90
36	5	1348	U	C6-N1-C2	-5.01	118.00	121.00
36	1	601	U	N1-C2-O2	5.01	126.31	122.80
36	1	807	A	N1-C6-N6	5.01	121.60	118.60
36	1	1345	G	O4'-C1'-N9	-5.01	104.19	108.20
36	1	1918	C	C6-N1-C2	-5.01	118.30	120.30
36	1	2400	G	N9-C4-C5	-5.01	103.40	105.40
36	1	3361	G	C4-N9-C1'	5.01	133.01	126.50
1	6	858	G	C4-N9-C1'	5.01	133.01	126.50
36	5	1413	G	N3-C4-C5	-5.01	126.10	128.60
36	5	1429	G	C8-N9-C1'	-5.01	120.49	127.00
1	2	1536	G	C4-N9-C1'	5.00	133.01	126.50
36	1	347	G	N3-C4-N9	5.00	129.00	126.00
36	1	917	A	C6-C5-N7	5.00	135.80	132.30
36	1	2861	U	C5-C4-O4	5.00	128.90	125.90
36	5	277	G	C6-C5-N7	5.00	133.40	130.40
36	5	1480	G	N3-C4-N9	-5.00	123.00	126.00
36	5	1604	G	N3-C4-C5	-5.00	126.10	128.60
36	5	2199	G	C6-C5-N7	-5.00	127.40	130.40
36	5	2384	A	OP2-P-O3'	5.00	116.21	105.20
1	2	1120	U	OP2-P-O3'	5.00	116.20	105.20
1	2	1652	C	C5-C6-N1	5.00	123.50	121.00
36	1	1741	A	C4-C5-N7	5.00	113.20	110.70
36	1	2624	G	N3-C2-N2	-5.00	116.40	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2747	A	N9-C4-C5	5.00	107.80	105.80
36	1	2873	U	N1-C2-N3	5.00	117.90	114.90
37	3	39	C	C5-C4-N4	5.00	123.70	120.20
36	5	612	U	N1-C2-N3	5.00	117.90	114.90
36	5	907	G	N9-C4-C5	-5.00	103.40	105.40
36	5	1323	G	O5'-P-OP2	5.00	116.70	110.70
36	5	2873	U	C4-C5-C6	5.00	122.70	119.70

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	1	406	G	Sidechain
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
16	C4	38	THR	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
24	D2	76	SER	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
28	D6	97	PRO	Peptide
33	E1	105	TYR	Peptide
39	L2	142	ASP	Peptide
42	L5	57	ASN	Peptide
45	L8	30	THR	Peptide
45	L8	74	THR	Peptide
48	M1	8	PRO	Peptide
52	M6	110	PRO	Peptide
53	M7	35	ALA	Peptide
57	N1	16	GLN	Peptide
65	N9	19	ASN	Peptide
67	O1	5	LYS	Peptide
72	O6	2	THR	Peptide
6	S4	2	ALA	Peptide
9	S7	131	PHE	Peptide
17	c5	50	THR	Peptide
17	c5	52	LYS	Peptide
18	c6	40	GLU	Peptide
22	d0	70	THR	Peptide
25	d3	44	GLY	Peptide
39	l2	212	GLY	Peptide

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Mol	Chain	Res	Type	Group
41	l4	318	LEU	Peptide
42	l5	270	LYS	Peptide
43	l6	129	GLU	Peptide
43	l6	51	ARG	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
52	m6	110	PRO	Peptide
56	n0	133	ALA	Peptide
64	n8	66	ALA	Peptide
67	o1	90	PHE	Peptide
2	s0	165	ARG	Peptide
5	s3	203	PRO	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	148 (72%)	34 (17%)	22 (11%)	0	2
2	s0	204/251 (81%)	144 (71%)	37 (18%)	23 (11%)	0	2
3	S1	212/254 (84%)	153 (72%)	30 (14%)	29 (14%)	0	1
3	s1	214/254 (84%)	173 (81%)	32 (15%)	9 (4%)	3	16
4	S2	215/253 (85%)	187 (87%)	20 (9%)	8 (4%)	3	19
4	s2	215/253 (85%)	177 (82%)	24 (11%)	14 (6%)	1	8
5	S3	221/239 (92%)	182 (82%)	27 (12%)	12 (5%)	2	12
5	s3	221/239 (92%)	173 (78%)	27 (12%)	21 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S4	258/260 (99%)	200 (78%)	45 (17%)	13 (5%)	2	13
6	s4	258/260 (99%)	215 (83%)	26 (10%)	17 (7%)	1	7
7	S5	204/224 (91%)	161 (79%)	25 (12%)	18 (9%)	1	4
7	s5	204/224 (91%)	158 (78%)	30 (15%)	16 (8%)	1	5
8	S6	224/236 (95%)	188 (84%)	27 (12%)	9 (4%)	3	17
8	s6	216/236 (92%)	189 (88%)	16 (7%)	11 (5%)	2	13
9	S7	182/189 (96%)	135 (74%)	27 (15%)	20 (11%)	0	2
9	s7	184/189 (97%)	145 (79%)	26 (14%)	13 (7%)	1	6
10	S8	184/200 (92%)	150 (82%)	24 (13%)	10 (5%)	2	12
10	s8	184/200 (92%)	159 (86%)	19 (10%)	6 (3%)	4	21
11	S9	183/196 (93%)	144 (79%)	27 (15%)	12 (7%)	1	7
11	s9	183/196 (93%)	144 (79%)	33 (18%)	6 (3%)	4	21
12	C0	94/105 (90%)	66 (70%)	19 (20%)	9 (10%)	0	3
12	c0	92/105 (88%)	66 (72%)	13 (14%)	13 (14%)	0	1
13	C1	153/155 (99%)	127 (83%)	14 (9%)	12 (8%)	1	5
13	c1	144/155 (93%)	123 (85%)	14 (10%)	7 (5%)	2	14
14	C2	122/142 (86%)	73 (60%)	25 (20%)	24 (20%)	0	0
14	c2	122/142 (86%)	71 (58%)	28 (23%)	23 (19%)	0	0
15	C3	148/150 (99%)	127 (86%)	14 (10%)	7 (5%)	2	14
15	c3	148/150 (99%)	117 (79%)	20 (14%)	11 (7%)	1	6
16	C4	125/136 (92%)	88 (70%)	22 (18%)	15 (12%)	0	1
16	c4	126/136 (93%)	103 (82%)	13 (10%)	10 (8%)	1	5
17	C5	122/141 (86%)	87 (71%)	24 (20%)	11 (9%)	1	4
17	c5	133/141 (94%)	92 (69%)	22 (16%)	19 (14%)	0	1
18	C6	139/142 (98%)	116 (84%)	11 (8%)	12 (9%)	1	4
18	c6	140/142 (99%)	115 (82%)	18 (13%)	7 (5%)	2	13
19	C7	116/136 (85%)	87 (75%)	19 (16%)	10 (9%)	1	4
19	c7	113/136 (83%)	84 (74%)	19 (17%)	10 (9%)	1	4
20	C8	143/145 (99%)	112 (78%)	20 (14%)	11 (8%)	1	5
20	c8	143/145 (99%)	116 (81%)	18 (13%)	9 (6%)	1	8
21	C9	141/143 (99%)	119 (84%)	16 (11%)	6 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	c9	141/143 (99%)	118 (84%)	18 (13%)	5 (4%)	3	20
22	D0	105/120 (88%)	85 (81%)	15 (14%)	5 (5%)	2	14
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	0	3
23	D1	85/87 (98%)	67 (79%)	9 (11%)	9 (11%)	0	3
23	d1	85/87 (98%)	67 (79%)	14 (16%)	4 (5%)	2	14
24	D2	127/129 (98%)	104 (82%)	20 (16%)	3 (2%)	6	27
24	d2	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
25	D3	142/144 (99%)	111 (78%)	18 (13%)	13 (9%)	1	4
25	d3	142/144 (99%)	121 (85%)	17 (12%)	4 (3%)	5	25
26	D4	132/134 (98%)	108 (82%)	13 (10%)	11 (8%)	1	5
26	d4	132/134 (98%)	101 (76%)	16 (12%)	15 (11%)	0	2
27	D5	68/107 (64%)	46 (68%)	12 (18%)	10 (15%)	0	0
27	d5	67/107 (63%)	54 (81%)	8 (12%)	5 (8%)	1	6
28	D6	95/97 (98%)	56 (59%)	20 (21%)	19 (20%)	0	0
28	d6	95/97 (98%)	71 (75%)	15 (16%)	9 (10%)	0	3
29	D7	79/81 (98%)	67 (85%)	8 (10%)	4 (5%)	2	13
29	d7	79/81 (98%)	60 (76%)	13 (16%)	6 (8%)	1	5
30	D8	61/66 (92%)	51 (84%)	7 (12%)	3 (5%)	2	14
30	d8	61/66 (92%)	41 (67%)	16 (26%)	4 (7%)	1	7
31	D9	51/55 (93%)	43 (84%)	5 (10%)	3 (6%)	1	10
31	d9	51/55 (93%)	39 (76%)	7 (14%)	5 (10%)	0	3
32	E0	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	2	12
33	E1	69/76 (91%)	33 (48%)	14 (20%)	22 (32%)	0	0
33	e1	74/76 (97%)	36 (49%)	16 (22%)	22 (30%)	0	0
34	SR	316/318 (99%)	270 (85%)	32 (10%)	14 (4%)	2	15
34	sR	316/318 (99%)	271 (86%)	38 (12%)	7 (2%)	6	29
35	SM	155/273 (57%)	107 (69%)	28 (18%)	20 (13%)	0	1
35	sM	98/273 (36%)	65 (66%)	17 (17%)	16 (16%)	0	0
39	L2	250/253 (99%)	223 (89%)	18 (7%)	9 (4%)	3	20
39	l2	250/253 (99%)	200 (80%)	35 (14%)	15 (6%)	1	9
40	L3	384/386 (100%)	332 (86%)	38 (10%)	14 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	l3	384/386 (100%)	337 (88%)	35 (9%)	12 (3%)	4	23
41	L4	359/361 (99%)	292 (81%)	45 (12%)	22 (6%)	1	9
41	l4	359/361 (99%)	298 (83%)	42 (12%)	19 (5%)	2	12
42	L5	294/296 (99%)	233 (79%)	39 (13%)	22 (8%)	1	6
42	l5	292/296 (99%)	251 (86%)	34 (12%)	7 (2%)	6	27
43	L6	152/175 (87%)	127 (84%)	21 (14%)	4 (3%)	5	26
43	l6	153/175 (87%)	121 (79%)	28 (18%)	4 (3%)	5	26
44	L7	220/243 (90%)	193 (88%)	18 (8%)	9 (4%)	3	16
44	l7	221/243 (91%)	189 (86%)	23 (10%)	9 (4%)	3	16
45	L8	231/255 (91%)	189 (82%)	31 (13%)	11 (5%)	2	14
45	l8	229/255 (90%)	176 (77%)	33 (14%)	20 (9%)	1	4
46	L9	189/191 (99%)	164 (87%)	19 (10%)	6 (3%)	4	22
46	l9	189/191 (99%)	162 (86%)	24 (13%)	3 (2%)	9	37
47	M0	207/220 (94%)	171 (83%)	29 (14%)	7 (3%)	3	21
47	m0	209/220 (95%)	168 (80%)	31 (15%)	10 (5%)	2	14
48	M1	167/173 (96%)	123 (74%)	25 (15%)	19 (11%)	0	2
48	m1	167/173 (96%)	138 (83%)	17 (10%)	12 (7%)	1	6
49	M3	191/198 (96%)	159 (83%)	21 (11%)	11 (6%)	1	10
49	m3	192/198 (97%)	156 (81%)	23 (12%)	13 (7%)	1	7
50	M4	134/137 (98%)	118 (88%)	8 (6%)	8 (6%)	1	9
50	m4	135/137 (98%)	120 (89%)	12 (9%)	3 (2%)	6	29
51	M5	201/203 (99%)	182 (90%)	14 (7%)	5 (2%)	5	27
51	m5	201/203 (99%)	182 (90%)	12 (6%)	7 (4%)	3	20
52	M6	195/198 (98%)	179 (92%)	11 (6%)	5 (3%)	5	26
52	m6	195/198 (98%)	178 (91%)	10 (5%)	7 (4%)	3	20
53	M7	181/183 (99%)	152 (84%)	19 (10%)	10 (6%)	2	11
53	m7	153/183 (84%)	135 (88%)	13 (8%)	5 (3%)	4	21
54	M8	183/185 (99%)	158 (86%)	20 (11%)	5 (3%)	5	25
54	m8	183/185 (99%)	152 (83%)	27 (15%)	4 (2%)	6	29
55	M9	186/188 (99%)	167 (90%)	16 (9%)	3 (2%)	9	37
55	m9	186/188 (99%)	163 (88%)	17 (9%)	6 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	N0	170/172 (99%)	147 (86%)	18 (11%)	5 (3%)	4	24
56	n0	170/172 (99%)	155 (91%)	13 (8%)	2 (1%)	13	44
57	N1	157/159 (99%)	136 (87%)	16 (10%)	5 (3%)	4	22
57	n1	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	8	33
58	N2	98/120 (82%)	70 (71%)	19 (19%)	9 (9%)	1	4
58	n2	96/120 (80%)	78 (81%)	12 (12%)	6 (6%)	1	8
59	N3	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	6	29
59	n3	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	10	39
60	N4	96/155 (62%)	70 (73%)	16 (17%)	10 (10%)	0	3
60	n4	133/155 (86%)	108 (81%)	13 (10%)	12 (9%)	1	4
61	N5	119/141 (84%)	107 (90%)	10 (8%)	2 (2%)	9	36
61	n5	118/141 (84%)	99 (84%)	11 (9%)	8 (7%)	1	7
62	N6	124/126 (98%)	108 (87%)	11 (9%)	5 (4%)	3	17
62	n6	124/126 (98%)	112 (90%)	8 (6%)	4 (3%)	4	22
63	N7	133/135 (98%)	111 (84%)	12 (9%)	10 (8%)	1	6
63	n7	133/135 (98%)	97 (73%)	26 (20%)	10 (8%)	1	6
64	N8	146/148 (99%)	119 (82%)	19 (13%)	8 (6%)	2	11
64	n8	146/148 (99%)	117 (80%)	19 (13%)	10 (7%)	1	7
65	N9	56/58 (97%)	47 (84%)	6 (11%)	3 (5%)	2	12
65	n9	56/58 (97%)	42 (75%)	7 (12%)	7 (12%)	0	1
66	O0	95/104 (91%)	83 (87%)	9 (10%)	3 (3%)	4	22
66	o0	98/104 (94%)	86 (88%)	9 (9%)	3 (3%)	4	23
67	O1	107/112 (96%)	92 (86%)	9 (8%)	6 (6%)	2	11
67	o1	107/112 (96%)	87 (81%)	10 (9%)	10 (9%)	0	3
68	O2	125/129 (97%)	112 (90%)	9 (7%)	4 (3%)	4	22
68	o2	125/129 (97%)	101 (81%)	17 (14%)	7 (6%)	2	11
69	O3	104/106 (98%)	96 (92%)	8 (8%)	0	100	100
69	o3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	4	24
70	O4	110/119 (92%)	93 (84%)	16 (14%)	1 (1%)	17	52
70	o4	110/119 (92%)	92 (84%)	14 (13%)	4 (4%)	3	20
71	O5	117/119 (98%)	97 (83%)	18 (15%)	2 (2%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	o5	117/119 (98%)	96 (82%)	15 (13%)	6 (5%)	2	13
72	O6	97/99 (98%)	72 (74%)	16 (16%)	9 (9%)	0	3
72	o6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	1	9
73	O7	85/87 (98%)	74 (87%)	7 (8%)	4 (5%)	2	14
73	o7	85/87 (98%)	76 (89%)	5 (6%)	4 (5%)	2	14
74	O8	75/77 (97%)	62 (83%)	10 (13%)	3 (4%)	3	17
74	o8	75/77 (97%)	60 (80%)	11 (15%)	4 (5%)	2	12
75	O9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	2 (4%)	2 (4%)	3	16
76	Q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	17
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	7	31
77	Q1	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
77	q1	23/25 (92%)	18 (78%)	5 (22%)	0	100	100
78	Q2	103/105 (98%)	86 (84%)	12 (12%)	5 (5%)	2	14
78	q2	103/105 (98%)	94 (91%)	9 (9%)	0	100	100
79	Q3	89/91 (98%)	72 (81%)	13 (15%)	4 (4%)	2	15
79	q3	89/91 (98%)	77 (86%)	9 (10%)	3 (3%)	3	21
80	e0	60/62 (97%)	45 (75%)	8 (13%)	7 (12%)	0	1
82	p0	139/311 (45%)	120 (86%)	13 (9%)	6 (4%)	2	16
All	All	22333/24141 (92%)	18313 (82%)	2695 (12%)	1325 (6%)	1	10

All (1325) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	30	GLN
2	S0	39	ASN
2	S0	66	ALA
2	S0	158	VAL
2	S0	191	ARG
3	S1	49	ASN
3	S1	58	SER
3	S1	79	HIS
3	S1	148	ASN
3	S1	177	GLN

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Mol	Chain	Res	Type
3	S1	179	SER
3	S1	206	PRO
4	S2	148	LEU
5	S3	62	ASN
5	S3	65	ARG
5	S3	93	ASP
5	S3	211	PRO
5	S3	216	PRO
5	S3	220	PRO
6	S4	96	ASN
6	S4	104	ASP
6	S4	242	LYS
7	S5	26	ALA
7	S5	35	GLN
7	S5	39	GLU
7	S5	63	GLN
7	S5	101	GLY
8	S6	20	ASP
8	S6	173	PRO
8	S6	174	LYS
9	S7	31	SER
9	S7	32	PRO
9	S7	64	VAL
9	S7	111	LYS
9	S7	112	ARG
9	S7	116	ARG
9	S7	131	PHE
9	S7	133	THR
9	S7	134	GLU
9	S7	155	ASP
10	S8	22	ARG
11	S9	134	ILE
12	C0	54	TYR
12	C0	60	SER
12	C0	81	ASN
12	C0	88	PRO
13	C1	7	VAL
13	C1	30	ARG
13	C1	147	ALA
14	C2	83	GLU
14	C2	89	ILE
14	C2	90	LYS

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Mol	Chain	Res	Type
14	C2	93	ASP
15	C3	22	ALA
15	C3	68	GLY
16	C4	38	THR
16	C4	39	ILE
16	C4	50	ALA
16	C4	51	ASP
16	C4	124	ASP
16	C4	125	SER
16	C4	126	THR
17	C5	54	ALA
17	C5	80	MET
17	C5	125	PRO
17	C5	126	VAL
18	C6	39	VAL
18	C6	40	GLU
18	C6	41	PRO
18	C6	58	ASP
18	C6	59	LYS
18	C6	113	ASP
18	C6	114	ARG
18	C6	116	LEU
18	C6	138	PHE
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	123	ASN
19	C7	124	VAL
20	C8	14	ILE
20	C8	25	ASN
20	C8	60	GLU
20	C8	91	ASP
20	C8	92	ILE
20	C8	125	ILE
20	C8	144	ARG
21	C9	31	PRO
21	C9	53	TRP
23	D1	7	GLN
23	D1	44	ARG
23	D1	82	VAL
24	D2	66	ASN
24	D2	83	ILE

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Mol	Chain	Res	Type
25	D3	11	SER
25	D3	92	CYS
25	D3	128	SER
25	D3	137	LYS
25	D3	138	GLU
25	D3	144	ARG
26	D4	36	SER
27	D5	39	ALA
27	D5	43	ASP
27	D5	44	GLN
27	D5	56	THR
27	D5	71	ILE
27	D5	97	LYS
28	D6	18	VAL
28	D6	45	VAL
28	D6	47	ALA
28	D6	61	GLU
28	D6	65	PRO
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
29	D7	38	PRO
29	D7	62	ILE
30	D8	36	THR
32	E0	13	LYS
32	E0	47	VAL
33	E1	84	VAL
33	E1	102	VAL
33	E1	103	LEU
33	E1	106	TYR
33	E1	127	GLY
34	SR	51	ASP
34	SR	160	GLU
34	SR	161	LYS
35	SM	17	VAL
35	SM	52	PRO
35	SM	87	THR
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
39	L2	47	GLN

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Mol	Chain	Res	Type
40	L3	140	ASP
40	L3	142	ALA
40	L3	187	SER
40	L3	188	ILE
40	L3	300	ARG
40	L3	347	SER
41	L4	4	PRO
41	L4	130	ALA
41	L4	131	VAL
41	L4	146	PRO
41	L4	291	ASN
41	L4	317	PRO
41	L4	338	LYS
42	L5	20	PHE
42	L5	58	LYS
42	L5	215	ASP
42	L5	233	ALA
42	L5	234	ASP
42	L5	258	LYS
44	L7	24	GLU
44	L7	26	VAL
45	L8	25	PRO
45	L8	31	PRO
45	L8	39	ALA
46	L9	50	ASN
47	M0	145	LYS
47	M0	189	GLU
47	M0	218	ALA
48	M1	8	PRO
48	M1	9	MET
48	M1	11	ASP
48	M1	12	LEU
48	M1	74	PRO
48	M1	140	ARG
48	M1	165	GLN
49	M3	47	ALA
49	M3	129	ASN
49	M3	131	LYS
49	M3	141	ALA
50	M4	8	LYS
50	M4	9	ALA
50	M4	29	ALA

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Mol	Chain	Res	Type
51	M5	144	ARG
51	M5	184	LYS
52	M6	111	PRO
53	M7	157	VAL
54	M8	24	VAL
54	M8	99	THR
56	N0	142	GLN
57	N1	124	VAL
57	N1	159	PHE
60	N4	64	THR
60	N4	81	PRO
61	N5	44	PRO
62	N6	52	ARG
62	N6	84	LYS
62	N6	126	LEU
63	N7	17	ARG
63	N7	35	SER
63	N7	125	GLY
63	N7	129	TRP
64	N8	76	ASP
64	N8	117	ARG
67	O1	5	LYS
67	O1	6	ASP
68	O2	27	ARG
71	O5	119	LYS
72	O6	28	TYR
72	O6	33	ALA
76	Q0	78	ILE
78	Q2	33	ALA
2	s0	4	PRO
2	s0	8	ASP
2	s0	62	ARG
2	s0	95	ALA
2	s0	103	THR
2	s0	164	ASN
2	s0	186	GLY
2	s0	189	VAL
2	s0	206	ASP
3	s1	179	SER
3	s1	206	PRO
3	s1	223	PHE
3	s1	232	HIS

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Mol	Chain	Res	Type
4	s2	40	LYS
4	s2	91	ARG
4	s2	92	ALA
4	s2	163	GLY
5	s3	61	GLU
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
5	s3	221	SER
6	s4	80	THR
6	s4	95	THR
6	s4	104	ASP
6	s4	163	ASP
6	s4	195	ILE
6	s4	196	VAL
7	s5	28	PRO
7	s5	39	GLU
7	s5	184	PHE
7	s5	204	GLY
7	s5	209	TYR
8	s6	70	PRO
8	s6	153	VAL
8	s6	173	PRO
8	s6	174	LYS
9	s7	10	SER
9	s7	64	VAL
9	s7	67	LEU
9	s7	131	PHE
9	s7	185	ILE
10	s8	199	LYS
11	s9	65	LYS
11	s9	134	ILE
12	c0	32	HIS
12	c0	82	LEU
12	c0	83	PRO
12	c0	88	PRO
12	c0	94	GLU
12	c0	97	PRO
13	c1	8	GLN
13	c1	121	ASP
13	c1	144	ALA

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Mol	Chain	Res	Type
14	c2	22	VAL
14	c2	82	PRO
14	c2	89	ILE
14	c2	93	ASP
15	c3	12	SER
15	c3	19	SER
15	c3	60	VAL
15	c3	66	ILE
15	c3	87	ASP
15	c3	139	TRP
15	c3	140	LYS
16	c4	124	ASP
16	c4	132	ARG
17	c5	11	VAL
17	c5	51	SER
17	c5	68	PRO
17	c5	125	PRO
17	c5	126	VAL
17	c5	127	ARG
18	c6	39	VAL
18	c6	42	GLU
18	c6	116	LEU
19	c7	88	VAL
19	c7	99	VAL
20	c8	91	ASP
20	c8	92	ILE
21	c9	28	LEU
21	c9	34	VAL
22	d0	15	GLN
22	d0	49	ASN
22	d0	96	PRO
22	d0	97	VAL
22	d0	118	VAL
26	d4	30	PRO
26	d4	33	ALA
26	d4	35	VAL
26	d4	121	THR
26	d4	123	LYS
26	d4	132	ARG
27	d5	85	LYS
27	d5	104	ALA
28	d6	47	ALA

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Mol	Chain	Res	Type
28	d6	63	ALA
29	d7	38	PRO
29	d7	60	SER
30	d8	57	MET
31	d9	6	VAL
80	e0	51	ASN
80	e0	60	PRO
33	e1	79	LYS
33	e1	83	LYS
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	100	LEU
33	e1	103	LEU
33	e1	106	TYR
33	e1	136	LYS
34	sR	4	ASN
34	sR	163	ASP
34	sR	165	ASP
34	sR	318	ALA
35	sM	50	ASN
35	sM	66	ALA
39	l2	96	LEU
39	l2	194	ASN
40	l3	140	ASP
40	l3	155	ALA
40	l3	347	SER
41	l4	14	GLU
41	l4	120	TYR
41	l4	145	ILE
41	l4	301	PRO
41	l4	329	PRO
41	l4	330	TYR
41	l4	339	LEU
42	l5	260	PHE
43	l6	30	LEU
43	l6	98	VAL
44	l7	54	GLU
44	l7	159	GLN
44	l7	178	ILE
45	l8	25	PRO
45	l8	26	LEU

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Mol	Chain	Res	Type
45	l8	34	PHE
45	l8	81	THR
45	l8	121	SER
45	l8	122	LYS
47	m0	82	ARG
47	m0	101	LYS
47	m0	175	ASN
48	m1	8	PRO
48	m1	9	MET
48	m1	10	ARG
48	m1	39	GLN
48	m1	94	ARG
48	m1	95	ASN
48	m1	108	GLU
49	m3	47	ALA
49	m3	93	ILE
49	m3	134	GLU
49	m3	141	ALA
50	m4	136	ALA
51	m5	183	THR
51	m5	184	LYS
52	m6	12	LYS
52	m6	13	GLY
52	m6	16	VAL
52	m6	110	PRO
53	m7	75	GLU
54	m8	99	THR
59	n3	42	SER
60	n4	26	SER
60	n4	63	ILE
60	n4	76	VAL
60	n4	134	GLN
61	n5	24	LEU
61	n5	44	PRO
62	n6	83	ASP
62	n6	84	LYS
62	n6	125	LYS
62	n6	126	LEU
64	n8	76	ASP
64	n8	120	ASN
65	n9	5	LYS
65	n9	21	ILE

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Mol	Chain	Res	Type
65	n9	25	LYS
65	n9	39	PHE
66	o0	100	ILE
67	o1	7	VAL
67	o1	64	VAL
67	o1	83	GLU
67	o1	99	ALA
68	o2	4	LEU
68	o2	5	PRO
68	o2	27	ARG
69	o3	88	ASN
70	o4	46	ASP
70	o4	79	SER
71	o5	70	TYR
71	o5	119	LYS
72	o6	64	SER
72	o6	98	ARG
74	o8	18	ALA
82	p0	93	LEU
82	p0	198	PRO
2	S0	5	ALA
2	S0	26	ALA
2	S0	49	ASN
2	S0	94	GLY
2	S0	95	ALA
2	S0	189	VAL
2	S0	203	PHE
3	S1	35	PRO
3	S1	51	SER
3	S1	59	ASP
3	S1	60	ALA
3	S1	63	GLY
3	S1	93	GLY
3	S1	221	PRO
4	S2	91	ARG
4	S2	248	SER
5	S3	195	SER
6	S4	3	ARG
6	S4	77	ARG
6	S4	164	LEU
7	S5	43	PHE
7	S5	51	VAL

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Mol	Chain	Res	Type
7	S5	127	GLN
7	S5	153	GLY
7	S5	154	ALA
8	S6	39	GLU
8	S6	154	ARG
9	S7	85	PHE
9	S7	156	SER
10	S8	40	ALA
10	S8	120	THR
10	S8	149	SER
11	S9	98	ALA
11	S9	117	GLY
11	S9	121	SER
12	C0	64	TYR
12	C0	94	GLU
13	C1	29	LYS
13	C1	55	ASP
13	C1	146	ALA
14	C2	91	VAL
14	C2	101	ALA
14	C2	125	ASN
14	C2	127	GLY
15	C3	27	LYS
15	C3	138	ASN
16	C4	33	LEU
16	C4	42	VAL
17	C5	51	SER
19	C7	72	LYS
19	C7	87	GLU
19	C7	113	LEU
20	C8	61	LEU
21	C9	69	LYS
23	D1	2	GLU
23	D1	12	TYR
23	D1	15	ARG
25	D3	3	LYS
25	D3	70	LYS
26	D4	5	VAL
26	D4	34	ASN
26	D4	51	GLU
28	D6	3	LYS
28	D6	5	ARG

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Mol	Chain	Res	Type
28	D6	63	ALA
29	D7	63	LEU
31	D9	6	VAL
31	D9	8	PHE
33	E1	98	VAL
33	E1	110	ALA
33	E1	111	GLU
33	E1	128	ALA
33	E1	138	ARG
33	E1	145	HIS
34	SR	217	ASP
34	SR	318	ALA
35	SM	86	ASN
35	SM	88	ARG
35	SM	89	ARG
35	SM	102	THR
35	SM	116	GLU
35	SM	139	GLU
35	SM	153	ASP
35	SM	172	VAL
39	L2	143	GLU
39	L2	144	ASN
40	L3	4	ARG
40	L3	5	LYS
40	L3	333	LYS
40	L3	351	LEU
40	L3	385	LYS
41	L4	15	ALA
41	L4	190	GLY
41	L4	268	ALA
41	L4	270	SER
41	L4	311	HIS
41	L4	318	LEU
42	L5	137	ASP
42	L5	253	PHE
42	L5	260	PHE
42	L5	295	GLY
44	L7	91	GLY
44	L7	160	ARG
44	L7	163	LEU
45	L8	115	ALA
45	L8	116	VAL

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Mol	Chain	Res	Type
45	L8	156	ASP
45	L8	254	ASP
46	L9	2	LYS
46	L9	164	ILE
47	M0	117	GLY
47	M0	211	ARG
48	M1	94	ARG
48	M1	115	LYS
48	M1	151	SER
48	M1	167	TYR
50	M4	36	VAL
50	M4	135	LEU
50	M4	136	ALA
51	M5	81	TYR
51	M5	145	ASP
52	M6	16	VAL
52	M6	196	ALA
53	M7	161	ALA
53	M7	164	LYS
55	M9	133	LYS
56	N0	167	ARG
57	N1	114	ALA
58	N2	44	GLU
58	N2	51	GLY
58	N2	60	GLY
59	N3	82	ALA
60	N4	16	GLY
60	N4	86	SER
62	N6	53	ASP
62	N6	92	GLY
63	N7	102	GLU
63	N7	128	GLN
64	N8	66	ALA
64	N8	78	LEU
67	O1	84	ASP
68	O2	127	ALA
70	O4	77	GLY
71	O5	97	ALA
72	O6	3	VAL
72	O6	34	SER
73	O7	12	HIS
73	O7	86	ALA

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Mol	Chain	Res	Type
74	O8	18	ALA
78	Q2	94	GLY
78	Q2	100	LYS
79	Q3	21	SER
2	s0	44	GLY
2	s0	66	ALA
2	s0	92	HIS
2	s0	111	ILE
2	s0	185	ARG
3	s1	93	GLY
3	s1	147	ALA
3	s1	154	SER
4	s2	93	GLY
4	s2	107	SER
5	s3	4	LEU
5	s3	59	LEU
5	s3	115	ILE
5	s3	180	GLY
6	s4	12	LEU
6	s4	24	SER
6	s4	164	LEU
7	s5	43	PHE
7	s5	153	GLY
7	s5	171	ALA
7	s5	172	ILE
8	s6	68	LEU
8	s6	126	ASP
8	s6	154	ARG
9	s7	8	ILE
9	s7	66	SER
9	s7	74	GLN
10	s8	101	ILE
11	s9	64	GLU
11	s9	147	MET
12	c0	23	ALA
12	c0	92	ILE
13	c1	114	ALA
14	c2	45	LEU
14	c2	58	LEU
14	c2	101	ALA
14	c2	110	ALA
14	c2	119	SER

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Mol	Chain	Res	Type
14	c2	131	ASP
17	c5	14	THR
17	c5	17	TYR
17	c5	131	ALA
17	c5	132	GLY
18	c6	113	ASP
19	c7	42	GLN
19	c7	67	ARG
19	c7	98	GLY
20	c8	14	ILE
20	c8	18	LEU
20	c8	55	HIS
20	c8	60	GLU
20	c8	61	LEU
21	c9	33	TYR
22	d0	17	GLN
22	d0	51	VAL
22	d0	52	LYS
23	d1	10	GLU
23	d1	44	ARG
25	d3	37	ALA
26	d4	50	ALA
26	d4	51	GLU
26	d4	84	LYS
27	d5	38	HIS
27	d5	44	GLN
28	d6	13	LYS
29	d7	20	LYS
29	d7	62	ILE
30	d8	61	ARG
31	d9	11	PRO
80	e0	47	VAL
33	e1	84	VAL
33	e1	102	VAL
33	e1	112	GLY
33	e1	127	GLY
33	e1	146	SER
34	sR	160	GLU
34	sR	186	PHE
35	sM	48	ARG
35	sM	63	ASP
35	sM	65	THR

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Mol	Chain	Res	Type
35	sM	67	GLY
35	sM	78	ASP
39	l2	13	GLY
39	l2	24	GLN
39	l2	56	ALA
39	l2	213	GLY
39	l2	215	ASN
39	l2	238	ILE
40	l3	22	ALA
40	l3	235	THR
41	l4	90	PHE
41	l4	144	LYS
41	l4	233	LEU
41	l4	302	ALA
41	l4	311	HIS
41	l4	338	LYS
41	l4	342	LYS
42	l5	178	ASN
42	l5	258	LYS
42	l5	270	LYS
43	l6	93	VAL
45	l8	39	ALA
45	l8	82	LEU
45	l8	117	ALA
45	l8	203	VAL
45	l8	239	GLY
45	l8	240	ASN
46	l9	144	ILE
47	m0	176	LEU
49	m3	51	LEU
49	m3	101	ARG
49	m3	129	ASN
49	m3	140	SER
49	m3	152	THR
49	m3	162	ASN
50	m4	135	LEU
51	m5	81	TYR
52	m6	183	ALA
54	m8	41	ASP
55	m9	77	GLY
55	m9	183	ALA
58	n2	49	ASN

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Mol	Chain	Res	Type
58	n2	91	ASP
59	n3	41	GLY
60	n4	98	PRO
61	n5	25	LYS
61	n5	40	LEU
61	n5	45	LYS
63	n7	7	ALA
63	n7	16	GLY
63	n7	129	TRP
64	n8	129	PHE
67	o1	5	LYS
67	o1	45	GLY
67	o1	84	ASP
68	o2	6	HIS
68	o2	12	LYS
68	o2	124	GLY
71	o5	82	ALA
72	o6	4	LYS
72	o6	33	ALA
73	o7	86	ALA
76	q0	78	ILE
79	q3	20	SER
79	q3	51	ALA
82	p0	47	GLY
2	S0	103	THR
2	S0	139	VAL
2	S0	164	ASN
2	S0	195	TRP
4	S2	107	SER
5	S3	59	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	153	ASN
6	S4	195	ILE
7	S5	45	LYS
7	S5	81	ARG
7	S5	156	ARG
8	S6	70	PRO
8	S6	152	ASP
9	S7	5	GLN
9	S7	30	SER
9	S7	36	ALA

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Mol	Chain	Res	Type
9	S7	73	VAL
9	S7	98	ILE
10	S8	52	ASN
10	S8	105	ASP
10	S8	152	ILE
11	S9	118	LEU
11	S9	120	LYS
11	S9	163	PRO
11	S9	164	PHE
11	S9	169	PRO
13	C1	6	THR
13	C1	113	PRO
14	C2	21	GLU
14	C2	25	GLU
14	C2	66	VAL
14	C2	119	SER
14	C2	128	ALA
14	C2	130	THR
15	C3	12	SER
15	C3	28	LEU
16	C4	40	ALA
16	C4	91	THR
17	C5	29	SER
17	C5	52	LYS
17	C5	69	GLU
18	C6	32	ASN
19	C7	115	LEU
20	C8	142	GLY
21	C9	39	THR
21	C9	50	ALA
22	D0	118	VAL
23	D1	28	ASP
25	D3	112	LYS
26	D4	4	ALA
26	D4	6	THR
26	D4	53	ASP
26	D4	104	SER
27	D5	54	VAL
27	D5	55	PRO
27	D5	74	SER
28	D6	10	ARG
28	D6	46	GLU

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Mol	Chain	Res	Type
28	D6	62	TYR
32	E0	51	ASN
33	E1	86	THR
33	E1	87	THR
33	E1	90	LYS
33	E1	124	PRO
34	SR	3	SER
34	SR	117	LYS
34	SR	194	GLY
35	SM	53	ARG
35	SM	111	GLY
35	SM	173	GLU
40	L3	155	ALA
40	L3	386	ASP
41	L4	90	PHE
41	L4	107	ARG
42	L5	21	ARG
42	L5	187	THR
42	L5	221	GLU
42	L5	223	PHE
42	L5	259	LYS
43	L6	97	ASN
43	L6	108	LYS
44	L7	157	ASN
48	M1	108	GLU
48	M1	114	ILE
49	M3	130	GLY
49	M3	136	GLU
53	M7	160	ALA
55	M9	53	LYS
56	N0	2	ALA
57	N1	18	ASP
57	N1	123	GLY
58	N2	31	ALA
58	N2	32	SER
58	N2	38	ILE
58	N2	50	LEU
60	N4	17	ARG
60	N4	97	LYS
61	N5	45	LYS
63	N7	130	PHE
64	N8	24	LYS

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Mol	Chain	Res	Type
65	N9	25	LYS
66	O0	96	GLY
67	O1	60	TRP
67	O1	82	GLU
68	O2	31	ASN
72	O6	27	SER
78	Q2	30	ALA
2	s0	5	ALA
2	s0	14	ALA
4	s2	229	LEU
5	s3	93	ASP
5	s3	196	ARG
6	s4	245	LYS
7	s5	60	ASP
7	s5	100	ASN
8	s6	25	ARG
10	s8	148	ALA
11	s9	22	SER
12	c0	31	LYS
13	c1	7	VAL
13	c1	129	ARG
14	c2	66	VAL
14	c2	90	LYS
14	c2	108	ARG
15	c3	43	LYS
16	c4	92	LYS
17	c5	52	LYS
17	c5	69	GLU
20	c8	33	THR
25	d3	70	LYS
26	d4	58	PHE
28	d6	62	TYR
29	d7	59	CYS
31	d9	7	TRP
80	e0	54	ARG
33	e1	81	LYS
33	e1	131	PHE
33	e1	145	HIS
35	sM	47	ALA
35	sM	64	LYS
35	sM	167	PRO
39	l2	80	GLU

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Mol	Chain	Res	Type
39	l2	127	ALA
39	l2	240	ALA
39	l2	249	SER
40	l3	142	ALA
40	l3	348	ARG
40	l3	386	ASP
41	l4	15	ALA
41	l4	272	VAL
44	l7	32	ALA
44	l7	53	LYS
44	l7	193	PRO
44	l7	229	PHE
45	l8	54	GLU
45	l8	120	LYS
45	l8	123	GLN
45	l8	133	LYS
45	l8	196	ALA
46	l9	2	LYS
47	m0	207	GLU
48	m1	114	ILE
48	m1	115	LYS
49	m3	135	ALA
53	m7	6	ALA
53	m7	66	SER
54	m8	98	LYS
56	n0	2	ALA
56	n0	139	TYR
57	n1	122	GLN
57	n1	136	ARG
60	n4	77	LYS
60	n4	95	SER
60	n4	133	THR
61	n5	47	ALA
61	n5	55	ASN
63	n7	34	LYS
64	n8	17	ALA
64	n8	24	LYS
65	n9	23	LYS
67	o1	47	ASP
69	o3	60	ARG
70	o4	82	ALA
71	o5	40	SER

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Mol	Chain	Res	Type
71	o5	84	LYS
73	o7	85	LYS
73	o7	87	SER
2	S0	102	PHE
2	S0	190	ASP
2	S0	194	PRO
3	S1	54	LEU
3	S1	62	LYS
3	S1	81	PHE
3	S1	132	ASP
3	S1	158	SER
3	S1	207	LEU
3	S1	209	ASN
3	S1	223	PHE
4	S2	150	GLN
5	S3	217	ILE
6	S4	12	LEU
7	S5	64	VAL
8	S6	148	SER
9	S7	110	GLN
9	S7	173	TYR
10	S8	10	LYS
12	C0	34	GLU
13	C1	4	GLU
13	C1	145	ALA
14	C2	106	ILE
14	C2	107	ASP
14	C2	131	ASP
17	C5	46	ALA
17	C5	101	ALA
20	C8	82	PRO
21	C9	28	LEU
22	D0	17	GLN
23	D1	10	GLU
23	D1	11	LEU
25	D3	41	SER
25	D3	89	ASN
26	D4	58	PHE
27	D5	41	ILE
28	D6	36	ILE
28	D6	64	LEU
29	D7	75	GLU

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Mol	Chain	Res	Type
30	D8	20	GLY
30	D8	61	ARG
31	D9	11	PRO
33	E1	83	LYS
33	E1	85	TYR
33	E1	93	HIS
33	E1	118	ARG
34	SR	237	GLN
35	SM	100	THR
39	L2	130	SER
41	L4	5	GLN
41	L4	16	THR
41	L4	232	SER
41	L4	233	LEU
41	L4	292	SER
42	L5	57	ASN
42	L5	107	ARG
42	L5	178	ASN
42	L5	228	ALA
42	L5	239	ILE
43	L6	98	VAL
44	L7	32	ALA
45	L8	36	ILE
45	L8	119	GLY
46	L9	110	LYS
46	L9	190	ASP
47	M0	143	SER
47	M0	220	GLN
48	M1	95	ASN
48	M1	117	ASP
49	M3	13	HIS
52	M6	195	ALA
53	M7	75	GLU
53	M7	110	THR
53	M7	156	ALA
53	M7	159	LYS
54	M8	41	ASP
54	M8	162	ALA
58	N2	11	ILE
59	N3	46	LEU
60	N4	69	LYS
60	N4	87	LEU

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Mol	Chain	Res	Type
60	N4	96	LEU
63	N7	103	GLN
68	O2	12	LYS
72	O6	21	THR
73	O7	84	SER
2	s0	10	THR
2	s0	203	PHE
4	s2	106	ASP
4	s2	150	GLN
4	s2	217	ALA
4	s2	228	ASN
4	s2	235	LEU
4	s2	238	SER
5	s3	43	PRO
5	s3	44	THR
5	s3	45	LYS
5	s3	90	ARG
6	s4	168	LYS
6	s4	242	LYS
7	s5	29	ILE
7	s5	45	LYS
7	s5	74	ALA
8	s6	83	CYS
9	s7	11	GLN
9	s7	83	LYS
9	s7	133	THR
11	s9	162	SER
12	c0	3	MET
12	c0	30	ALA
13	c1	80	MET
14	c2	39	ASP
14	c2	103	LEU
14	c2	106	ILE
14	c2	107	ASP
15	c3	3	ARG
16	c4	12	GLN
17	c5	8	LYS
17	c5	10	ARG
18	c6	13	LYS
19	c7	86	PRO
19	c7	105	GLN
19	c7	120	SER

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Mol	Chain	Res	Type
21	c9	29	GLU
21	c9	100	ILE
25	d3	61	SER
26	d4	4	ALA
26	d4	77	ASN
28	d6	34	LYS
30	d8	6	PRO
31	d9	12	ARG
80	e0	61	SER
33	e1	85	TYR
33	e1	128	ALA
34	sR	149	ASP
35	sM	121	LYS
39	l2	130	SER
40	l3	378	ALA
41	l4	146	PRO
42	l5	119	TYR
42	l5	279	LYS
44	l7	191	VAL
45	l8	150	LEU
45	l8	237	ILE
46	l9	167	VAL
47	m0	170	LYS
47	m0	186	GLU
47	m0	193	ASP
48	m1	167	TYR
49	m3	60	ALA
51	m5	49	ARG
52	m6	68	ARG
55	m9	55	VAL
58	n2	23	THR
58	n2	45	GLY
58	n2	50	LEU
60	n4	72	SER
60	n4	132	GLY
63	n7	125	GLY
63	n7	127	ASN
65	n9	52	LYS
67	o1	82	GLU
69	o3	59	VAL
70	o4	100	ILE
71	o5	79	ASP

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Mol	Chain	Res	Type
73	o7	67	LEU
75	o9	3	ALA
75	o9	39	ALA
82	p0	33	VAL
3	S1	78	ASP
4	S2	235	LEU
5	S3	196	ARG
6	S4	39	ARG
6	S4	245	LYS
7	S5	21	THR
7	S5	100	ASN
11	S9	162	SER
12	C0	30	ALA
13	C1	154	ALA
14	C2	87	PRO
14	C2	129	GLU
16	C4	24	ASN
16	C4	123	SER
16	C4	131	GLY
22	D0	21	LYS
25	D3	5	LYS
25	D3	131	SER
26	D4	60	PHE
26	D4	133	ASN
28	D6	97	PRO
33	E1	100	LEU
33	E1	137	ASP
33	E1	146	SER
34	SR	4	ASN
34	SR	98	GLU
39	L2	70	ARG
39	L2	127	ALA
39	L2	234	LYS
39	L2	246	LEU
39	L2	251	LYS
40	L3	317	ILE
41	L4	14	GLU
42	L5	125	VAL
44	L7	158	LYS
44	L7	178	ILE
48	M1	64	LYS
48	M1	80	LEU

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Mol	Chain	Res	Type
49	M3	76	THR
49	M3	153	ASP
50	M4	10	SER
51	M5	94	TYR
53	M7	66	SER
54	M8	183	GLY
56	N0	13	ARG
56	N0	50	LYS
63	N7	3	LYS
64	N8	47	LYS
65	N9	21	ILE
66	O0	20	SER
67	O1	7	VAL
73	O7	87	SER
74	O8	33	LYS
76	Q0	79	GLU
78	Q2	34	SER
79	Q3	20	SER
79	Q3	51	ALA
2	s0	30	GLN
2	s0	109	ASN
2	s0	139	VAL
2	s0	158	VAL
2	s0	167	LYS
3	s1	94	LYS
5	s3	142	LEU
6	s4	78	THR
6	s4	90	ILE
7	s5	42	LEU
7	s5	127	GLN
8	s6	156	PHE
10	s8	62	THR
10	s8	78	ILE
10	s8	94	ASN
12	c0	35	ILE
12	c0	95	ARG
14	c2	54	ARG
14	c2	87	PRO
15	c3	6	SER
16	c4	32	ASP
16	c4	37	GLU
16	c4	51	ASP

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Mol	Chain	Res	Type
17	c5	7	ALA
17	c5	75	PRO
17	c5	130	ARG
18	c6	4	VAL
19	c7	50	ILE
19	c7	113	LEU
22	d0	72	ASN
23	d1	43	GLY
26	d4	36	SER
28	d6	15	ARG
28	d6	35	ALA
29	d7	53	ALA
30	d8	33	LEU
35	sM	42	ALA
35	sM	43	ASP
35	sM	51	ARG
35	sM	84	LYS
35	sM	122	GLU
39	l2	133	TYR
39	l2	247	ARG
40	l3	3	HIS
43	l6	10	TYR
45	l8	126	SER
47	m0	74	LYS
47	m0	174	THR
48	m1	153	LYS
51	m5	68	ARG
53	m7	88	VAL
54	m8	112	ALA
55	m9	36	ASN
55	m9	155	LEU
61	n5	108	LEU
63	n7	28	PRO
63	n7	104	PRO
63	n7	134	LEU
64	n8	47	LYS
64	n8	78	LEU
72	o6	8	ALA
82	p0	206	ASP
2	S0	205	ARG
3	S1	180	THR
3	S1	210	ILE

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Mol	Chain	Res	Type
4	S2	36	VAL
7	S5	54	LYS
10	S8	9	HIS
10	S8	59	ARG
14	C2	22	VAL
14	C2	112	ALA
15	C3	3	ARG
17	C5	11	VAL
18	C6	42	GLU
19	C7	6	THR
22	D0	106	ILE
35	SM	12	VAL
35	SM	174	LEU
42	L5	6	ASP
43	L6	6	ALA
45	L8	80	TYR
45	L8	157	VAL
46	L9	59	ASN
48	M1	39	GLN
48	M1	152	HIS
52	M6	110	PRO
55	M9	129	GLY
63	N7	16	GLY
64	N8	96	LYS
65	N9	7	HIS
66	O0	27	TYR
72	O6	64	SER
72	O6	97	SER
74	O8	35	GLY
5	s3	219	ALA
6	s4	135	GLY
8	s6	152	ASP
14	c2	40	GLY
14	c2	63	VAL
14	c2	91	VAL
16	c4	50	ALA
16	c4	58	TYR
17	c5	133	ALA
22	d0	59	PRO
26	d4	68	LYS
80	e0	38	LEU
33	e1	148	TYR

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Mol	Chain	Res	Type
40	l3	141	GLY
40	l3	362	ALA
41	l4	328	ASN
42	l5	125	VAL
44	l7	28	ALA
50	m4	3	THR
51	m5	74	PRO
51	m5	76	PRO
52	m6	111	PRO
60	n4	71	ARG
60	n4	74	LYS
63	n7	103	GLN
67	o1	86	LYS
68	o2	31	ASN
74	o8	19	ASP
74	o8	60	GLY
82	p0	197	PHE
3	S1	176	VAL
4	S2	145	GLY
5	S3	199	PRO
9	S7	132	PRO
11	S9	168	ARG
13	C1	130	PRO
14	C2	81	ASP
14	C2	115	VAL
16	C4	79	VAL
20	C8	124	GLY
24	D2	100	GLY
28	D6	75	VAL
41	L4	181	VAL
31	d9	29	GLY
49	m3	50	PRO
58	n2	48	GLY
64	n8	138	ILE
66	o0	10	ILE
5	S3	112	GLY
11	S9	127	VAL
12	C0	86	ILE
34	SR	15	GLY
34	SR	105	GLY
58	N2	22	PRO
60	N4	76	VAL

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Mol	Chain	Res	Type
79	Q3	50	GLY
5	s3	163	PRO
6	s4	30	ARG
6	s4	260	GLY
9	s7	73	VAL
15	c3	22	ALA
20	c8	9	GLY
25	d3	130	VAL
80	e0	50	VAL
33	e1	124	PRO
41	l4	91	GLY
66	o0	96	GLY
72	o6	9	ILE
3	S1	21	VAL
3	S1	48	VAL
7	S5	121	ILE
8	S6	69	LEU
50	M4	6	ILE
53	M7	36	ILE
64	N8	70	LYS
72	O6	52	PRO
3	s1	22	ASP
5	s3	161	GLY
16	c4	131	GLY
17	c5	117	GLY
26	d4	29	HIS
27	d5	87	GLY
33	e1	129	GLY
74	o8	35	GLY
14	C2	55	GLY
18	C6	33	GLY
22	D0	117	VAL
34	SR	28	GLY
49	M3	163	GLY
4	s2	83	ILE
5	s3	203	PRO
9	s7	13	PRO
14	c2	115	VAL
23	d1	77	GLY
28	d6	59	TYR
53	m7	67	ILE
55	m9	25	ASP

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Mol	Chain	Res	Type
57	n1	148	PRO
64	n8	15	VAL
64	n8	148	ILE
65	n9	24	PRO
79	q3	10	ILE
2	S0	117	GLU
3	S1	22	ASP
49	M3	133	PRO
59	N3	58	VAL
18	c6	40	GLU
28	d6	58	VAL
48	m1	7	ASN

5.3.2 Protein sidechains ⓘ

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%)	126 (77%)	38 (23%)	1	3
2	s0	165/209 (79%)	137 (83%)	28 (17%)	2	9
3	S1	191/223 (86%)	150 (78%)	41 (22%)	1	4
3	s1	192/223 (86%)	153 (80%)	39 (20%)	1	5
4	S2	176/204 (86%)	138 (78%)	38 (22%)	1	4
4	s2	176/204 (86%)	133 (76%)	43 (24%)	0	2
5	S3	182/194 (94%)	141 (78%)	41 (22%)	1	3
5	s3	182/194 (94%)	144 (79%)	38 (21%)	1	5
6	S4	221/221 (100%)	166 (75%)	55 (25%)	0	2
6	s4	221/221 (100%)	177 (80%)	44 (20%)	1	5
7	S5	173/190 (91%)	144 (83%)	29 (17%)	2	9
7	s5	173/190 (91%)	134 (78%)	39 (22%)	1	3
8	S6	188/201 (94%)	154 (82%)	34 (18%)	1	7
8	s6	187/201 (93%)	148 (79%)	39 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	S7	165/169 (98%)	136 (82%)	29 (18%)	2	8
9	s7	165/169 (98%)	131 (79%)	34 (21%)	1	5
10	S8	150/161 (93%)	130 (87%)	20 (13%)	4	16
10	s8	150/161 (93%)	123 (82%)	27 (18%)	1	7
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	3
11	s9	158/165 (96%)	127 (80%)	31 (20%)	1	6
12	C0	77/98 (79%)	65 (84%)	12 (16%)	2	11
12	c0	73/98 (74%)	66 (90%)	7 (10%)	8	31
13	C1	129/136 (95%)	108 (84%)	21 (16%)	2	10
13	c1	129/136 (95%)	101 (78%)	28 (22%)	1	4
14	C2	88/118 (75%)	63 (72%)	25 (28%)	0	1
14	c2	88/118 (75%)	68 (77%)	20 (23%)	1	3
15	C3	127/127 (100%)	99 (78%)	28 (22%)	1	4
15	c3	127/127 (100%)	108 (85%)	19 (15%)	3	12
16	C4	81/104 (78%)	61 (75%)	20 (25%)	0	2
16	c4	97/104 (93%)	76 (78%)	21 (22%)	1	4
17	C5	101/117 (86%)	87 (86%)	14 (14%)	3	15
17	c5	103/117 (88%)	83 (81%)	20 (19%)	1	6
18	C6	117/118 (99%)	99 (85%)	18 (15%)	2	11
18	c6	118/118 (100%)	92 (78%)	26 (22%)	1	4
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	5
19	c7	92/124 (74%)	74 (80%)	18 (20%)	1	6
20	C8	128/128 (100%)	103 (80%)	25 (20%)	1	6
20	c8	128/128 (100%)	106 (83%)	22 (17%)	2	9
21	C9	115/115 (100%)	91 (79%)	24 (21%)	1	5
21	c9	115/115 (100%)	91 (79%)	24 (21%)	1	5
22	D0	100/113 (88%)	77 (77%)	23 (23%)	1	3
22	d0	103/113 (91%)	77 (75%)	26 (25%)	0	1
23	D1	74/74 (100%)	57 (77%)	17 (23%)	1	3
23	d1	74/74 (100%)	57 (77%)	17 (23%)	1	3
24	D2	110/110 (100%)	89 (81%)	21 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	d2	110/110 (100%)	94 (86%)	16 (14%)	3	13
25	D3	119/119 (100%)	103 (87%)	16 (13%)	4	16
25	d3	119/119 (100%)	96 (81%)	23 (19%)	1	6
26	D4	112/112 (100%)	88 (79%)	24 (21%)	1	4
26	d4	112/112 (100%)	91 (81%)	21 (19%)	1	6
27	D5	61/88 (69%)	45 (74%)	16 (26%)	0	1
27	d5	61/88 (69%)	52 (85%)	9 (15%)	3	13
28	D6	83/83 (100%)	62 (75%)	21 (25%)	0	1
28	d6	83/83 (100%)	67 (81%)	16 (19%)	1	6
29	D7	70/70 (100%)	60 (86%)	10 (14%)	3	14
29	d7	70/70 (100%)	56 (80%)	14 (20%)	1	5
30	D8	56/59 (95%)	42 (75%)	14 (25%)	0	2
30	d8	56/59 (95%)	41 (73%)	15 (27%)	0	1
31	D9	47/48 (98%)	35 (74%)	12 (26%)	0	1
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	4
32	E0	51/51 (100%)	40 (78%)	11 (22%)	1	4
33	E1	62/66 (94%)	47 (76%)	15 (24%)	0	2
33	e1	66/66 (100%)	53 (80%)	13 (20%)	1	6
34	SR	260/261 (100%)	225 (86%)	35 (14%)	4	16
34	sR	260/261 (100%)	236 (91%)	24 (9%)	9	33
35	SM	97/228 (42%)	78 (80%)	19 (20%)	1	6
35	sM	54/228 (24%)	40 (74%)	14 (26%)	0	1
39	L2	193/195 (99%)	160 (83%)	33 (17%)	2	9
39	l2	192/195 (98%)	148 (77%)	44 (23%)	1	3
40	L3	320/322 (99%)	247 (77%)	73 (23%)	1	3
40	l3	321/322 (100%)	258 (80%)	63 (20%)	1	6
41	L4	288/288 (100%)	236 (82%)	52 (18%)	1	7
41	l4	288/288 (100%)	224 (78%)	64 (22%)	1	4
42	L5	244/244 (100%)	197 (81%)	47 (19%)	1	6
42	l5	243/244 (100%)	196 (81%)	47 (19%)	1	6
43	L6	134/152 (88%)	114 (85%)	20 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	l6	135/152 (89%)	108 (80%)	27 (20%)	1	5
44	L7	186/204 (91%)	161 (87%)	25 (13%)	4	16
44	l7	187/204 (92%)	159 (85%)	28 (15%)	3	12
45	L8	187/207 (90%)	152 (81%)	35 (19%)	1	7
45	l8	177/207 (86%)	145 (82%)	32 (18%)	1	7
46	L9	171/171 (100%)	133 (78%)	38 (22%)	1	4
46	l9	171/171 (100%)	133 (78%)	38 (22%)	1	4
47	M0	177/186 (95%)	143 (81%)	34 (19%)	1	6
47	m0	179/186 (96%)	142 (79%)	37 (21%)	1	5
48	M1	147/150 (98%)	115 (78%)	32 (22%)	1	4
48	m1	147/150 (98%)	113 (77%)	34 (23%)	1	3
49	M3	154/158 (98%)	127 (82%)	27 (18%)	2	8
49	m3	154/158 (98%)	119 (77%)	35 (23%)	1	3
50	M4	107/108 (99%)	86 (80%)	21 (20%)	1	6
50	m4	108/108 (100%)	88 (82%)	20 (18%)	1	7
51	M5	175/175 (100%)	142 (81%)	33 (19%)	1	6
51	m5	175/175 (100%)	144 (82%)	31 (18%)	2	8
52	M6	160/161 (99%)	138 (86%)	22 (14%)	3	16
52	m6	160/161 (99%)	129 (81%)	31 (19%)	1	6
53	M7	140/145 (97%)	112 (80%)	28 (20%)	1	5
53	m7	125/145 (86%)	94 (75%)	31 (25%)	0	2
54	M8	150/150 (100%)	119 (79%)	31 (21%)	1	5
54	m8	150/150 (100%)	120 (80%)	30 (20%)	1	5
55	M9	153/153 (100%)	129 (84%)	24 (16%)	2	11
55	m9	153/153 (100%)	121 (79%)	32 (21%)	1	5
56	N0	156/156 (100%)	126 (81%)	30 (19%)	1	6
56	n0	156/156 (100%)	121 (78%)	35 (22%)	1	3
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1	3
57	n1	136/136 (100%)	111 (82%)	25 (18%)	1	7
58	N2	87/106 (82%)	74 (85%)	13 (15%)	3	13
58	n2	85/106 (80%)	69 (81%)	16 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	N3	104/104 (100%)	85 (82%)	19 (18%)	1	7
59	n3	104/104 (100%)	93 (89%)	11 (11%)	6	26
60	N4	57/129 (44%)	50 (88%)	7 (12%)	4	19
60	n4	100/129 (78%)	83 (83%)	17 (17%)	2	9
61	N5	104/117 (89%)	79 (76%)	25 (24%)	0	2
61	n5	104/117 (89%)	89 (86%)	15 (14%)	3	14
62	N6	109/109 (100%)	84 (77%)	25 (23%)	1	3
62	n6	109/109 (100%)	84 (77%)	25 (23%)	1	3
63	N7	115/115 (100%)	91 (79%)	24 (21%)	1	5
63	n7	115/115 (100%)	84 (73%)	31 (27%)	0	1
64	N8	118/118 (100%)	92 (78%)	26 (22%)	1	4
64	n8	118/118 (100%)	94 (80%)	24 (20%)	1	5
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1	4
65	n9	46/46 (100%)	34 (74%)	12 (26%)	0	1
66	O0	81/87 (93%)	64 (79%)	17 (21%)	1	5
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1	5
67	O1	92/96 (96%)	69 (75%)	23 (25%)	0	2
67	o1	94/96 (98%)	81 (86%)	13 (14%)	3	16
68	O2	109/110 (99%)	90 (83%)	19 (17%)	2	9
68	o2	109/110 (99%)	88 (81%)	21 (19%)	1	6
69	O3	90/90 (100%)	77 (86%)	13 (14%)	3	14
69	o3	90/90 (100%)	77 (86%)	13 (14%)	3	14
70	O4	95/101 (94%)	78 (82%)	17 (18%)	2	8
70	o4	95/101 (94%)	71 (75%)	24 (25%)	0	1
71	O5	104/104 (100%)	80 (77%)	24 (23%)	1	3
71	o5	103/104 (99%)	79 (77%)	24 (23%)	1	3
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0	1
72	o6	80/81 (99%)	59 (74%)	21 (26%)	0	1
73	O7	70/70 (100%)	57 (81%)	13 (19%)	1	7
73	o7	70/70 (100%)	55 (79%)	15 (21%)	1	4
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	8
75	O9	45/45 (100%)	39 (87%)	6 (13%)	4	16
75	o9	45/45 (100%)	36 (80%)	9 (20%)	1	5
76	Q0	47/47 (100%)	38 (81%)	9 (19%)	1	6
76	q0	47/47 (100%)	37 (79%)	10 (21%)	1	4
77	Q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0	1
78	Q2	90/90 (100%)	70 (78%)	20 (22%)	1	4
78	q2	90/90 (100%)	69 (77%)	21 (23%)	1	3
79	Q3	71/71 (100%)	58 (82%)	13 (18%)	1	7
79	q3	71/71 (100%)	57 (80%)	14 (20%)	1	6
80	e0	53/53 (100%)	38 (72%)	15 (28%)	0	1
82	p0	105/253 (42%)	84 (80%)	21 (20%)	1	5
All	All	18729/20239 (92%)	15025 (80%)	3704 (20%)	1	5

All (3704) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	7	PHE
2	S0	27	ARG
2	S0	29	VAL
2	S0	30	GLN
2	S0	32	HIS
2	S0	34	GLU
2	S0	37	VAL
2	S0	43	ASP
2	S0	49	ASN
2	S0	56	LYS
2	S0	59	LEU
2	S0	62	ARG
2	S0	76	ILE
2	S0	84	ARG
2	S0	86	VAL
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	101	ARG

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Mol	Chain	Res	Type
2	S0	103	THR
2	S0	110	TYR
2	S0	111	ILE
2	S0	119	ARG
2	S0	153	SER
2	S0	156	VAL
2	S0	157	ASP
2	S0	162	CYS
2	S0	165	ARG
2	S0	172	LEU
2	S0	177	LEU
2	S0	184	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	189	VAL
2	S0	196	SER
2	S0	198	MET
2	S0	200	ASP
2	S0	202	TYR
3	S1	21	VAL
3	S1	22	ASP
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	46	THR
3	S1	47	LEU
3	S1	51	SER
3	S1	55	LYS
3	S1	58	SER
3	S1	61	LEU
3	S1	70	LEU
3	S1	77	GLU
3	S1	78	ASP
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	110	LEU
3	S1	111	ARG
3	S1	112	SER

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Mol	Chain	Res	Type
3	S1	117	TRP
3	S1	135	LEU
3	S1	149	GLN
3	S1	154	SER
3	S1	170	GLU
3	S1	177	GLN
3	S1	180	THR
3	S1	181	LEU
3	S1	193	ILE
3	S1	198	GLU
3	S1	202	LYS
3	S1	212	VAL
3	S1	214	LYS
3	S1	215	VAL
3	S1	218	LEU
3	S1	219	LYS
3	S1	220	GLN
3	S1	223	PHE
4	S2	41	LEU
4	S2	50	ILE
4	S2	53	ILE
4	S2	58	LEU
4	S2	72	LEU
4	S2	73	LEU
4	S2	76	LEU
4	S2	77	GLN
4	S2	87	GLN
4	S2	89	GLN
4	S2	90	THR
4	S2	91	ARG
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	111	VAL
4	S2	117	THR
4	S2	119	LYS
4	S2	130	ILE
4	S2	134	LEU
4	S2	137	ILE
4	S2	140	ARG
4	S2	141	ARG
4	S2	148	LEU

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Mol	Chain	Res	Type
4	S2	159	THR
4	S2	166	THR
4	S2	174	ARG
4	S2	207	LEU
4	S2	221	THR
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	235	LEU
4	S2	237	VAL
4	S2	240	LEU
4	S2	242	ILE
4	S2	244	SER
4	S2	245	ASP
5	S3	4	LEU
5	S3	7	LYS
5	S3	9	ARG
5	S3	23	GLU
5	S3	41	VAL
5	S3	64	ARG
5	S3	65	ARG
5	S3	66	ILE
5	S3	67	ASN
5	S3	76	ARG
5	S3	84	ILE
5	S3	89	GLU
5	S3	91	VAL
5	S3	92	GLN
5	S3	93	ASP
5	S3	103	GLU
5	S3	105	MET
5	S3	111	ASN
5	S3	117	ARG
5	S3	120	TYR
5	S3	127	MET
5	S3	134	CYS
5	S3	137	VAL
5	S3	139	SER
5	S3	142	LEU
5	S3	143	ARG
5	S3	146	ARG
5	S3	151	LYS

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Mol	Chain	Res	Type
5	S3	158	ILE
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	195	SER
5	S3	202	LEU
5	S3	207	THR
5	S3	210	GLU
5	S3	217	ILE
5	S3	222	VAL
6	S4	6	LYS
6	S4	7	LYS
6	S4	9	LEU
6	S4	11	ARG
6	S4	12	LEU
6	S4	23	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	45	ILE
6	S4	48	LEU
6	S4	54	TYR
6	S4	62	LYS
6	S4	65	LEU
6	S4	68	ARG
6	S4	70	VAL
6	S4	77	ARG
6	S4	92	LEU
6	S4	95	THR
6	S4	96	ASN
6	S4	108	ARG
6	S4	113	ARG
6	S4	123	LEU
6	S4	126	VAL
6	S4	129	VAL
6	S4	131	LEU
6	S4	133	LYS
6	S4	138	TYR
6	S4	151	ASP
6	S4	155	LYS

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Mol	Chain	Res	Type
6	S4	160	VAL
6	S4	164	LEU
6	S4	166	SER
6	S4	180	LEU
6	S4	181	VAL
6	S4	182	TYR
6	S4	187	ARG
6	S4	192	ILE
6	S4	197	HIS
6	S4	198	LYS
6	S4	206	ASP
6	S4	214	LEU
6	S4	221	ARG
6	S4	222	LEU
6	S4	226	PHE
6	S4	227	VAL
6	S4	231	GLN
6	S4	233	LYS
6	S4	236	ILE
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	247	SER
6	S4	248	ILE
6	S4	258	GLN
6	S4	259	GLN
7	S5	23	VAL
7	S5	24	VAL
7	S5	25	LEU
7	S5	38	THR
7	S5	42	LEU
7	S5	43	PHE
7	S5	45	LYS
7	S5	48	PHE
7	S5	49	GLU
7	S5	65	ARG
7	S5	76	ARG
7	S5	79	ASN
7	S5	84	LYS
7	S5	89	ILE
7	S5	92	ARG
7	S5	93	LEU

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Mol	Chain	Res	Type
7	S5	94	THR
7	S5	122	ASN
7	S5	146	THR
7	S5	147	THR
7	S5	149	VAL
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	162	VAL
7	S5	170	GLN
7	S5	194	LEU
7	S5	203	LYS
7	S5	225	ARG
8	S6	6	SER
8	S6	19	ASP
8	S6	21	GLU
8	S6	25	ARG
8	S6	45	PHE
8	S6	58	LYS
8	S6	67	VAL
8	S6	74	LYS
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	82	SER
8	S6	89	ASP
8	S6	94	ARG
8	S6	98	ARG
8	S6	109	LEU
8	S6	120	GLU
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	129	VAL
8	S6	132	ARG
8	S6	133	LEU
8	S6	143	LYS
8	S6	154	ARG
8	S6	155	ASP
8	S6	169	TYR
8	S6	170	THR
8	S6	175	ILE

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Mol	Chain	Res	Type
8	S6	177	ARG
8	S6	178	LEU
8	S6	212	LEU
8	S6	217	SER
8	S6	223	LYS
9	S7	38	LEU
9	S7	46	ILE
9	S7	50	ASP
9	S7	60	ILE
9	S7	67	LEU
9	S7	70	PHE
9	S7	72	LYS
9	S7	77	LEU
9	S7	79	ARG
9	S7	85	PHE
9	S7	87	ASP
9	S7	95	GLU
9	S7	97	ARG
9	S7	104	ARG
9	S7	105	THR
9	S7	107	ARG
9	S7	114	ARG
9	S7	116	ARG
9	S7	123	ASP
9	S7	126	LEU
9	S7	130	VAL
9	S7	131	PHE
9	S7	134	GLU
9	S7	141	ARG
9	S7	147	ASN
9	S7	158	ASP
9	S7	166	LEU
9	S7	167	GLU
9	S7	185	ILE
10	S8	8	ARG
10	S8	10	LYS
10	S8	21	PHE
10	S8	36	THR
10	S8	58	LEU
10	S8	62	THR
10	S8	66	SER
10	S8	70	GLU

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Mol	Chain	Res	Type
10	S8	81	VAL
10	S8	103	GLN
10	S8	107	THR
10	S8	138	ASN
10	S8	149	SER
10	S8	151	LYS
10	S8	152	ILE
10	S8	155	SER
10	S8	158	SER
10	S8	164	ARG
10	S8	184	LEU
10	S8	196	LEU
11	S9	3	ARG
11	S9	7	THR
11	S9	9	SER
11	S9	14	THR
11	S9	28	LEU
11	S9	39	LYS
11	S9	40	LYS
11	S9	46	SER
11	S9	49	LEU
11	S9	60	LEU
11	S9	78	ARG
11	S9	79	ARG
11	S9	82	ARG
11	S9	83	VAL
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	97	LEU
11	S9	99	LEU
11	S9	101	VAL
11	S9	109	LEU
11	S9	110	GLN
11	S9	118	LEU
11	S9	121	SER
11	S9	130	THR
11	S9	132	ARG
11	S9	134	ILE
11	S9	138	LYS
11	S9	140	ILE

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Mol	Chain	Res	Type
11	S9	145	SER
11	S9	149	ARG
11	S9	161	THR
11	S9	162	SER
11	S9	171	ARG
11	S9	172	VAL
11	S9	182	GLU
12	C0	8	ARG
12	C0	20	VAL
12	C0	27	PHE
12	C0	32	HIS
12	C0	46	LEU
12	C0	55	VAL
12	C0	56	LYS
12	C0	71	GLU
12	C0	76	LEU
12	C0	78	GLU
12	C0	81	ASN
12	C0	82	LEU
13	C1	21	ASN
13	C1	27	THR
13	C1	29	LYS
13	C1	40	LEU
13	C1	43	LYS
13	C1	44	THR
13	C1	63	LEU
13	C1	67	ARG
13	C1	69	LYS
13	C1	72	THR
13	C1	74	THR
13	C1	80	MET
13	C1	99	ARG
13	C1	101	GLU
13	C1	109	VAL
13	C1	112	SER
13	C1	118	GLN
13	C1	119	VAL
13	C1	127	GLN
13	C1	129	ARG
13	C1	131	ILE
14	C2	28	LEU
14	C2	33	ARG

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Mol	Chain	Res	Type
14	C2	37	VAL
14	C2	43	ARG
14	C2	45	LEU
14	C2	46	ARG
14	C2	50	LYS
14	C2	52	LEU
14	C2	61	VAL
14	C2	62	LEU
14	C2	66	VAL
14	C2	71	ILE
14	C2	74	LEU
14	C2	83	GLU
14	C2	86	VAL
14	C2	89	ILE
14	C2	103	LEU
14	C2	119	SER
14	C2	121	VAL
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	138	GLU
14	C2	139	HIS
14	C2	140	PHE
15	C3	3	ARG
15	C3	6	SER
15	C3	9	LYS
15	C3	12	SER
15	C3	13	SER
15	C3	16	ILE
15	C3	27	LYS
15	C3	39	LYS
15	C3	45	LEU
15	C3	46	THR
15	C3	64	ARG
15	C3	66	ILE
15	C3	76	LYS
15	C3	83	GLU
15	C3	88	LEU
15	C3	97	SER
15	C3	102	LEU
15	C3	105	ASN
15	C3	110	ASP

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Mol	Chain	Res	Type
15	C3	115	LEU
15	C3	125	LEU
15	C3	127	ARG
15	C3	134	VAL
15	C3	142	GLU
15	C3	143	SER
15	C3	145	THR
15	C3	149	LEU
15	C3	151	ASN
16	C4	14	PHE
16	C4	16	VAL
16	C4	20	TYR
16	C4	29	HIS
16	C4	30	VAL
16	C4	31	THR
16	C4	39	ILE
16	C4	42	VAL
16	C4	43	THR
16	C4	48	VAL
16	C4	51	ASP
16	C4	83	ILE
16	C4	92	LYS
16	C4	102	LEU
16	C4	123	SER
16	C4	125	SER
16	C4	126	THR
16	C4	132	ARG
16	C4	136	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	22	LEU
17	C5	31	GLU
17	C5	35	LYS
17	C5	36	LEU
17	C5	44	ARG
17	C5	47	ARG
17	C5	52	LYS
17	C5	60	LEU
17	C5	89	MET
17	C5	100	LYS
17	C5	110	GLU
17	C5	121	ILE

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Mol	Chain	Res	Type
17	C5	125	PRO
18	C6	4	VAL
18	C6	43	ILE
18	C6	52	LEU
18	C6	53	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	58	ASP
18	C6	66	ARG
18	C6	68	ARG
18	C6	69	VAL
18	C6	98	ASP
18	C6	103	ASN
18	C6	114	ARG
18	C6	116	LEU
18	C6	123	ARG
18	C6	127	LYS
18	C6	137	ARG
18	C6	138	PHE
19	C7	6	THR
19	C7	25	THR
19	C7	26	LEU
19	C7	29	GLN
19	C7	34	LEU
19	C7	38	ILE
19	C7	40	THR
19	C7	45	ARG
19	C7	48	ASN
19	C7	49	LYS
19	C7	62	GLN
19	C7	69	ILE
19	C7	72	LYS
19	C7	78	ARG
19	C7	84	TYR
19	C7	105	GLN
19	C7	113	LEU
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	8	GLN
20	C8	11	PHE
20	C8	12	GLN

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Mol	Chain	Res	Type
20	C8	13	HIS
20	C8	14	ILE
20	C8	17	LEU
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	34	THR
20	C8	54	LEU
20	C8	60	GLU
20	C8	61	LEU
20	C8	71	GLN
20	C8	77	THR
20	C8	80	LYS
20	C8	86	LEU
20	C8	92	ILE
20	C8	97	ASP
20	C8	107	SER
20	C8	116	LEU
20	C8	132	ARG
20	C8	136	GLN
20	C8	143	ARG
21	C9	4	VAL
21	C9	6	VAL
21	C9	18	TYR
21	C9	20	SER
21	C9	22	LEU
21	C9	28	LEU
21	C9	30	VAL
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	41	SER
21	C9	57	ARG
21	C9	63	ARG
21	C9	67	MET
21	C9	70	GLN
21	C9	84	LYS
21	C9	94	ILE
21	C9	110	LYS
21	C9	116	ILE
21	C9	130	ARG

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Mol	Chain	Res	Type
21	C9	131	ASP
21	C9	139	THR
21	C9	144	GLU
22	D0	15	GLN
22	D0	18	GLN
22	D0	23	ARG
22	D0	27	THR
22	D0	31	VAL
22	D0	39	SER
22	D0	42	VAL
22	D0	47	GLN
22	D0	48	HIS
22	D0	51	VAL
22	D0	57	ARG
22	D0	58	LEU
22	D0	60	THR
22	D0	61	LYS
22	D0	70	THR
22	D0	74	GLU
22	D0	76	SER
22	D0	81	THR
22	D0	88	LYS
22	D0	89	ARG
22	D0	99	ILE
22	D0	103	ILE
22	D0	108	ILE
23	D1	1	MET
23	D1	5	LYS
23	D1	7	GLN
23	D1	11	LEU
23	D1	18	SER
23	D1	27	ASP
23	D1	41	GLU
23	D1	49	GLU
23	D1	52	THR
23	D1	61	SER
23	D1	62	ARG
23	D1	69	LEU
23	D1	76	ASP
23	D1	78	LEU
23	D1	80	LYS
23	D1	82	VAL

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Mol	Chain	Res	Type
23	D1	84	SER
24	D2	2	THR
24	D2	7	LEU
24	D2	22	LYS
24	D2	23	ARG
24	D2	24	GLN
24	D2	25	VAL
24	D2	26	LEU
24	D2	27	ILE
24	D2	30	SER
24	D2	47	ILE
24	D2	53	ILE
24	D2	56	HIS
24	D2	65	LEU
24	D2	82	LYS
24	D2	93	LEU
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR
24	D2	121	VAL
24	D2	122	SER
25	D3	7	ARG
25	D3	9	LEU
25	D3	18	HIS
25	D3	19	ARG
25	D3	26	GLU
25	D3	28	ASN
25	D3	33	LEU
25	D3	41	SER
25	D3	73	ARG
25	D3	84	THR
25	D3	103	LEU
25	D3	107	PHE
25	D3	110	LYS
25	D3	114	LYS
25	D3	131	SER
25	D3	138	GLU
26	D4	2	SER
26	D4	10	ARG
26	D4	14	SER
26	D4	17	LEU

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Mol	Chain	Res	Type
26	D4	21	LYS
26	D4	28	LEU
26	D4	32	ARG
26	D4	34	ASN
26	D4	36	SER
26	D4	46	GLU
26	D4	47	VAL
26	D4	51	GLU
26	D4	52	LYS
26	D4	57	VAL
26	D4	61	ARG
26	D4	84	LYS
26	D4	96	LEU
26	D4	98	GLU
26	D4	99	LYS
26	D4	102	LYS
26	D4	105	ARG
26	D4	127	LYS
26	D4	128	LYS
26	D4	129	VAL
27	D5	37	GLN
27	D5	38	HIS
27	D5	42	LEU
27	D5	50	ILE
27	D5	58	ARG
27	D5	59	TYR
27	D5	63	SER
27	D5	67	ASP
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	85	LYS
27	D5	92	ILE
27	D5	93	SER
27	D5	95	HIS
27	D5	100	ILE
28	D6	12	LYS
28	D6	15	ARG
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	44	ILE

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Mol	Chain	Res	Type
28	D6	45	VAL
28	D6	58	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	66	LYS
28	D6	68	TYR
28	D6	69	ASN
28	D6	70	LYS
28	D6	76	SER
28	D6	82	ARG
28	D6	83	ILE
28	D6	85	ARG
28	D6	86	VAL
28	D6	88	SER
28	D6	90	GLU
29	D7	3	LEU
29	D7	20	LYS
29	D7	33	LEU
29	D7	34	ASP
29	D7	38	PRO
29	D7	55	THR
29	D7	60	SER
29	D7	63	LEU
29	D7	67	THR
29	D7	72	LYS
30	D8	5	THR
30	D8	13	ILE
30	D8	15	VAL
30	D8	19	THR
30	D8	32	PHE
30	D8	33	LEU
30	D8	36	THR
30	D8	39	THR
30	D8	49	ARG
30	D8	51	ASN
30	D8	57	MET
30	D8	58	GLU
30	D8	62	GLU
30	D8	64	ARG
31	D9	5	ASN
31	D9	6	VAL
31	D9	7	TRP

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Mol	Chain	Res	Type
31	D9	9	SER
31	D9	10	HIS
31	D9	12	ARG
31	D9	19	ARG
31	D9	22	ARG
31	D9	30	LEU
31	D9	32	ARG
31	D9	36	LEU
31	D9	49	ASP
32	E0	3	LYS
32	E0	20	LYS
32	E0	21	VAL
32	E0	25	GLU
32	E0	28	LYS
32	E0	36	LYS
32	E0	39	LEU
32	E0	42	ARG
32	E0	48	THR
32	E0	49	LEU
32	E0	61	SER
33	E1	89	LYS
33	E1	90	LYS
33	E1	91	ILE
33	E1	97	LYS
33	E1	108	VAL
33	E1	113	LYS
33	E1	118	ARG
33	E1	120	GLU
33	E1	130	VAL
33	E1	137	ASP
33	E1	139	LEU
33	E1	140	TYR
33	E1	146	SER
33	E1	147	VAL
33	E1	151	ASN
34	SR	6	VAL
34	SR	7	LEU
34	SR	48	THR
34	SR	52	GLN
34	SR	59	ARG
34	SR	60	SER
34	SR	62	LYS

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Mol	Chain	Res	Type
34	SR	66	HIS
34	SR	76	ASP
34	SR	81	LEU
34	SR	94	VAL
34	SR	96	THR
34	SR	109	ASP
34	SR	112	SER
34	SR	117	LYS
34	SR	133	VAL
34	SR	136	ILE
34	SR	141	LEU
34	SR	143	THR
34	SR	153	GLN
34	SR	165	ASP
34	SR	166	SER
34	SR	191	ASP
34	SR	195	HIS
34	SR	196	ASN
34	SR	202	LEU
34	SR	238	ASP
34	SR	265	LEU
34	SR	266	ASP
34	SR	268	GLN
34	SR	277	GLU
34	SR	300	THR
34	SR	308	ASN
34	SR	316	MET
34	SR	317	THR
35	SM	24	GLU
35	SM	27	LYS
35	SM	28	SER
35	SM	46	LYS
35	SM	49	LYS
35	SM	51	ARG
35	SM	53	ARG
35	SM	61	ILE
35	SM	64	LYS
35	SM	69	ARG
35	SM	72	ARG
35	SM	82	THR
35	SM	84	LYS
35	SM	89	ARG

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Mol	Chain	Res	Type
35	SM	91	THR
35	SM	97	THR
35	SM	100	THR
35	SM	103	LYS
35	SM	139	GLU
39	L2	8	GLN
39	L2	18	SER
39	L2	20	THR
39	L2	32	LEU
39	L2	44	ILE
39	L2	45	VAL
39	L2	48	ILE
39	L2	62	VAL
39	L2	64	ARG
39	L2	70	ARG
39	L2	73	GLU
39	L2	74	GLU
39	L2	96	LEU
39	L2	104	LEU
39	L2	109	GLU
39	L2	114	SER
39	L2	118	GLU
39	L2	134	VAL
39	L2	137	ILE
39	L2	139	HIS
39	L2	143	GLU
39	L2	157	VAL
39	L2	165	VAL
39	L2	169	ILE
39	L2	177	LYS
39	L2	179	LEU
39	L2	181	LYS
39	L2	190	ARG
39	L2	193	ARG
39	L2	202	VAL
39	L2	204	MET
39	L2	207	VAL
39	L2	227	ARG
40	L3	7	GLU
40	L3	10	ARG
40	L3	17	LEU
40	L3	19	ARG

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Mol	Chain	Res	Type
40	L3	20	LYS
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	50	LYS
40	L3	55	THR
40	L3	56	ILE
40	L3	67	PHE
40	L3	69	LYS
40	L3	70	ARG
40	L3	73	VAL
40	L3	79	VAL
40	L3	84	VAL
40	L3	85	VAL
40	L3	93	VAL
40	L3	94	GLU
40	L3	100	ARG
40	L3	102	LEU
40	L3	103	THR
40	L3	104	THR
40	L3	112	ASP
40	L3	114	VAL
40	L3	116	ARG
40	L3	134	SER
40	L3	139	GLN
40	L3	146	ARG
40	L3	148	LEU
40	L3	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	202	THR
40	L3	207	SER
40	L3	210	GLU
40	L3	212	ASN

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Mol	Chain	Res	Type
40	L3	216	ASP
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	238	LEU
40	L3	241	LYS
40	L3	244	ARG
40	L3	252	ILE
40	L3	264	VAL
40	L3	270	ARG
40	L3	274	SER
40	L3	277	SER
40	L3	296	THR
40	L3	304	THR
40	L3	305	ILE
40	L3	308	MET
40	L3	320	ASP
40	L3	324	VAL
40	L3	328	ILE
40	L3	332	ARG
40	L3	338	LEU
40	L3	347	SER
40	L3	355	SER
40	L3	361	THR
40	L3	365	PHE
40	L3	382	THR
40	L3	385	LYS
41	L4	3	ARG
41	L4	4	PRO
41	L4	16	THR
41	L4	22	LEU
41	L4	47	ARG
41	L4	60	THR
41	L4	71	VAL
41	L4	74	ILE
41	L4	93	MET
41	L4	102	PRO
41	L4	120	TYR
41	L4	124	SER
41	L4	133	SER
41	L4	145	ILE
41	L4	150	LEU

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Mol	Chain	Res	Type
41	L4	152	VAL
41	L4	153	SER
41	L4	156	LEU
41	L4	170	LYS
41	L4	172	VAL
41	L4	176	SER
41	L4	177	ASP
41	L4	179	LEU
41	L4	193	LYS
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	206	LEU
41	L4	220	ARG
41	L4	222	VAL
41	L4	230	VAL
41	L4	246	ARG
41	L4	258	LEU
41	L4	280	ILE
41	L4	283	THR
41	L4	287	THR
41	L4	289	ILE
41	L4	292	SER
41	L4	297	SER
41	L4	306	THR
41	L4	307	GLN
41	L4	310	THR
41	L4	311	HIS
41	L4	323	VAL
41	L4	332	LYS
41	L4	333	VAL
41	L4	339	LEU
41	L4	343	LYS
41	L4	346	LYS
41	L4	349	THR
41	L4	354	VAL
41	L4	359	LEU
42	L5	4	GLN
42	L5	5	LYS
42	L5	17	GLN
42	L5	22	ARG
42	L5	23	ARG

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Mol	Chain	Res	Type
42	L5	41	LYS
42	L5	48	LYS
42	L5	50	ARG
42	L5	58	LYS
42	L5	66	SER
42	L5	67	SER
42	L5	69	ILE
42	L5	80	SER
42	L5	81	HIS
42	L5	89	THR
42	L5	92	LEU
42	L5	101	THR
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	137	ASP
42	L5	140	ARG
42	L5	146	LEU
42	L5	148	ILE
42	L5	152	ARG
42	L5	154	THR
42	L5	155	THR
42	L5	158	ARG
42	L5	163	LEU
42	L5	185	PHE
42	L5	205	SER
42	L5	206	GLN
42	L5	216	GLU
42	L5	222	LEU
42	L5	227	LEU
42	L5	234	ASP
42	L5	242	SER
42	L5	257	GLU
42	L5	259	LYS
42	L5	263	GLU
42	L5	273	ARG
42	L5	277	LEU
42	L5	290	ILE
42	L5	293	LEU

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Mol	Chain	Res	Type
43	L6	5	LYS
43	L6	21	THR
43	L6	31	ARG
43	L6	35	VAL
43	L6	41	ILE
43	L6	52	VAL
43	L6	64	LEU
43	L6	65	ILE
43	L6	84	VAL
43	L6	89	THR
43	L6	90	LYS
43	L6	93	VAL
43	L6	99	GLU
43	L6	129	GLU
43	L6	134	ARG
43	L6	146	ILE
43	L6	152	THR
43	L6	155	LEU
43	L6	160	SER
43	L6	164	SER
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	40	LYS
44	L7	45	LEU
44	L7	53	LYS
44	L7	54	GLU
44	L7	77	VAL
44	L7	80	GLN
44	L7	82	LYS
44	L7	88	ARG
44	L7	93	ASN
44	L7	98	LYS
44	L7	110	ARG
44	L7	118	LYS
44	L7	124	LEU
44	L7	128	LYS
44	L7	143	THR
44	L7	157	ASN
44	L7	158	LYS
44	L7	164	SER
44	L7	175	LYS

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Mol	Chain	Res	Type
44	L7	179	LEU
44	L7	184	LEU
44	L7	239	LEU
45	L8	26	LEU
45	L8	27	THR
45	L8	31	PRO
45	L8	41	GLN
45	L8	63	LYS
45	L8	66	SER
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	92	LYS
45	L8	95	ASN
45	L8	101	THR
45	L8	118	GLU
45	L8	132	VAL
45	L8	136	LEU
45	L8	149	LYS
45	L8	150	LEU
45	L8	155	ASN
45	L8	156	ASP
45	L8	164	VAL
45	L8	169	LEU
45	L8	173	MET
45	L8	185	ARG
45	L8	203	VAL
45	L8	206	GLU
45	L8	208	GLU
45	L8	211	LEU
45	L8	221	ASN
45	L8	238	LEU
45	L8	241	LYS
45	L8	246	MET
45	L8	251	LYS
46	L9	5	GLN
46	L9	6	THR
46	L9	9	GLN
46	L9	12	VAL

Continued on next page...

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Mol	Chain	Res	Type
46	L9	14	GLU
46	L9	18	VAL
46	L9	19	SER
46	L9	20	ILE
46	L9	22	SER
46	L9	33	THR
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	73	SER
46	L9	82	VAL
46	L9	91	ARG
46	L9	113	GLU
46	L9	124	ARG
46	L9	133	THR
46	L9	135	GLU
46	L9	139	ASN
46	L9	141	LYS
46	L9	151	VAL
46	L9	152	GLU
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	164	ILE
46	L9	172	ILE
46	L9	173	ARG
46	L9	189	GLU
46	L9	190	ASP
46	L9	191	LEU
47	M0	3	ARG
47	M0	7	ARG
47	M0	15	LYS
47	M0	24	ARG
47	M0	26	VAL
47	M0	30	LYS
47	M0	31	ILE
47	M0	32	ARG

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Mol	Chain	Res	Type
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	74	LYS
47	M0	78	THR
47	M0	87	LEU
47	M0	91	VAL
47	M0	130	ASP
47	M0	138	VAL
47	M0	139	ARG
47	M0	145	LYS
47	M0	156	ARG
47	M0	163	GLN
47	M0	164	LYS
47	M0	165	ILE
47	M0	166	ILE
47	M0	167	LEU
47	M0	169	LYS
47	M0	177	ASP
47	M0	178	ARG
47	M0	184	LYS
47	M0	185	ARG
47	M0	203	LYS
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	28	ASP
48	M1	31	THR
48	M1	44	THR
48	M1	46	VAL
48	M1	51	ARG
48	M1	53	THR
48	M1	65	ILE
48	M1	70	THR
48	M1	71	VAL
48	M1	80	LEU

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Mol	Chain	Res	Type
48	M1	82	ARG
48	M1	85	LYS
48	M1	94	ARG
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	115	LYS
48	M1	119	SER
48	M1	130	VAL
48	M1	138	VAL
48	M1	140	ARG
48	M1	142	LYS
48	M1	145	LYS
48	M1	147	THR
48	M1	158	ASP
48	M1	166	LYS
49	M3	23	LYS
49	M3	24	VAL
49	M3	28	GLN
49	M3	35	ARG
49	M3	41	THR
49	M3	45	LYS
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	70	ARG
49	M3	73	ARG
49	M3	81	LYS
49	M3	85	LEU
49	M3	104	ARG
49	M3	107	GLU
49	M3	114	GLN
49	M3	115	ARG
49	M3	124	ILE
49	M3	131	LYS
49	M3	164	GLU
49	M3	171	ARG
49	M3	175	SER

Continued on next page...

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Mol	Chain	Res	Type
49	M3	190	LYS
50	M4	5	SER
50	M4	8	LYS
50	M4	19	ARG
50	M4	25	LYS
50	M4	27	GLN
50	M4	37	GLU
50	M4	50	LYS
50	M4	53	VAL
50	M4	55	ARG
50	M4	58	ILE
50	M4	63	VAL
50	M4	66	THR
50	M4	72	LEU
50	M4	90	VAL
50	M4	91	CYS
50	M4	93	LYS
50	M4	102	LYS
50	M4	119	GLN
50	M4	126	GLN
50	M4	128	ARG
50	M4	135	LEU
51	M5	5	LYS
51	M5	10	LEU
51	M5	18	VAL
51	M5	20	ARG
51	M5	22	LEU
51	M5	33	LYS
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	97	SER
51	M5	106	VAL
51	M5	109	ARG
51	M5	113	LEU
51	M5	133	ILE
51	M5	138	GLN
51	M5	142	ILE
51	M5	151	ILE

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Mol	Chain	Res	Type
51	M5	153	ASP
51	M5	155	VAL
51	M5	157	LYS
51	M5	159	ARG
51	M5	167	THR
51	M5	170	LYS
51	M5	183	THR
51	M5	187	ARG
51	M5	188	ARG
51	M5	190	THR
51	M5	194	GLN
51	M5	196	THR
51	M5	204	LYS
52	M6	33	ILE
52	M6	34	VAL
52	M6	58	LEU
52	M6	68	ARG
52	M6	78	ARG
52	M6	84	LEU
52	M6	85	ARG
52	M6	94	ARG
52	M6	106	GLU
52	M6	116	LYS
52	M6	117	ARG
52	M6	122	GLN
52	M6	128	ARG
52	M6	134	LYS
52	M6	137	THR
52	M6	143	THR
52	M6	144	SER
52	M6	160	ARG
52	M6	175	THR
52	M6	184	THR
52	M6	190	VAL
52	M6	194	LEU
53	M7	3	ARG
53	M7	7	THR
53	M7	9	THR
53	M7	23	ARG
53	M7	24	VAL
53	M7	29	THR
53	M7	32	THR

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Mol	Chain	Res	Type
53	M7	36	ILE
53	M7	41	LEU
53	M7	42	THR
53	M7	56	ARG
53	M7	67	ILE
53	M7	79	THR
53	M7	91	VAL
53	M7	112	LEU
53	M7	114	VAL
53	M7	117	ILE
53	M7	119	VAL
53	M7	120	ASN
53	M7	126	ARG
53	M7	127	ARG
53	M7	128	ARG
53	M7	142	SER
53	M7	144	SER
53	M7	157	VAL
53	M7	168	LEU
53	M7	180	LYS
53	M7	181	ARG
54	M8	6	THR
54	M8	11	LYS
54	M8	17	THR
54	M8	21	SER
54	M8	22	ASP
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	34	THR
54	M8	41	ASP
54	M8	63	SER
54	M8	64	VAL
54	M8	67	ILE
54	M8	69	ARG
54	M8	74	GLU
54	M8	80	THR
54	M8	81	VAL
54	M8	93	ILE
54	M8	95	GLU
54	M8	100	THR
54	M8	105	ARG

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Mol	Chain	Res	Type
54	M8	111	ARG
54	M8	113	LYS
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	144	ARG
54	M8	147	ARG
54	M8	150	VAL
54	M8	168	THR
54	M8	180	ARG
55	M9	10	LEU
55	M9	22	VAL
55	M9	25	ASP
55	M9	42	ARG
55	M9	43	LYS
55	M9	44	LEU
55	M9	49	THR
55	M9	55	VAL
55	M9	60	LYS
55	M9	61	SER
55	M9	71	ARG
55	M9	74	ARG
55	M9	81	ARG
55	M9	89	LEU
55	M9	99	LEU
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	110	ARG
55	M9	116	ASP
55	M9	134	HIS
55	M9	138	LEU
55	M9	165	LYS
55	M9	182	ASP
56	N0	1	MET
56	N0	12	ARG
56	N0	17	GLU
56	N0	21	GLU
56	N0	45	LEU
56	N0	51	VAL
56	N0	52	LYS
56	N0	57	GLU

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Mol	Chain	Res	Type
56	N0	61	ILE
56	N0	80	ARG
56	N0	85	SER
56	N0	87	THR
56	N0	105	THR
56	N0	115	ARG
56	N0	117	ARG
56	N0	125	LYS
56	N0	130	GLU
56	N0	132	THR
56	N0	137	ARG
56	N0	138	GLN
56	N0	142	GLN
56	N0	145	THR
56	N0	149	LYS
56	N0	155	ARG
56	N0	156	VAL
56	N0	157	GLN
56	N0	160	THR
56	N0	167	ARG
56	N0	171	PHE
56	N0	172	TYR
57	N1	9	SER
57	N1	12	ARG
57	N1	16	GLN
57	N1	25	VAL
57	N1	26	HIS
57	N1	27	LEU
57	N1	32	LYS
57	N1	55	LYS
57	N1	68	THR
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	83	ARG
57	N1	87	LYS
57	N1	88	ARG
57	N1	89	LEU
57	N1	93	VAL
57	N1	102	ARG
57	N1	103	GLN
57	N1	104	GLU

Continued on next page...

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Mol	Chain	Res	Type
57	N1	106	LEU
57	N1	118	GLU
57	N1	124	VAL
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	136	ARG
57	N1	139	ARG
57	N1	143	THR
57	N1	144	GLU
57	N1	149	GLN
57	N1	158	THR
58	N2	10	LYS
58	N2	29	ASP
58	N2	38	ILE
58	N2	43	VAL
58	N2	52	ASN
58	N2	54	VAL
58	N2	58	GLU
58	N2	66	VAL
58	N2	72	SER
58	N2	87	ASN
58	N2	88	GLN
58	N2	93	ILE
58	N2	100	THR
59	N3	2	SER
59	N3	13	ILE
59	N3	14	SER
59	N3	32	ARG
59	N3	37	ILE
59	N3	45	ARG
59	N3	48	ARG
59	N3	54	LEU
59	N3	63	LYS
59	N3	64	LYS
59	N3	72	LYS
59	N3	79	VAL
59	N3	84	SER
59	N3	91	VAL
59	N3	96	GLU
59	N3	102	ILE
59	N3	110	LYS

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Mol	Chain	Res	Type
59	N3	115	THR
59	N3	137	VAL
60	N4	4	GLU
60	N4	5	ILE
60	N4	7	SER
60	N4	19	THR
60	N4	39	LEU
60	N4	43	ARG
60	N4	64	THR
61	N5	27	ARG
61	N5	34	LEU
61	N5	36	LYS
61	N5	38	LEU
61	N5	39	LYS
61	N5	45	LYS
61	N5	49	LYS
61	N5	57	LEU
61	N5	59	SER
61	N5	63	ILE
61	N5	69	SER
61	N5	71	THR
61	N5	74	LYS
61	N5	86	VAL
61	N5	102	LEU
61	N5	108	LEU
61	N5	109	LYS
61	N5	113	LEU
61	N5	115	ARG
61	N5	125	ARG
61	N5	127	THR
61	N5	135	ILE
61	N5	138	ARG
61	N5	139	ILE
61	N5	142	ILE
62	N6	8	VAL
62	N6	9	SER
62	N6	10	SER
62	N6	13	ARG
62	N6	17	LYS
62	N6	25	SER
62	N6	36	SER
62	N6	37	LYS

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Mol	Chain	Res	Type
62	N6	42	GLN
62	N6	45	ILE
62	N6	50	ILE
62	N6	51	ARG
62	N6	56	VAL
62	N6	57	LEU
62	N6	60	ARG
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	88	GLU
62	N6	94	SER
62	N6	97	ILE
62	N6	105	VAL
62	N6	115	ARG
62	N6	122	LYS
62	N6	127	GLU
63	N7	17	ARG
63	N7	24	VAL
63	N7	25	ILE
63	N7	26	VAL
63	N7	46	ILE
63	N7	52	LYS
63	N7	54	THR
63	N7	64	LYS
63	N7	66	THR
63	N7	72	ILE
63	N7	75	VAL
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	89	VAL
63	N7	99	GLU
63	N7	102	GLU
63	N7	107	ARG
63	N7	108	GLU
63	N7	109	GLU
63	N7	122	HIS
63	N7	123	GLN
63	N7	127	ASN
63	N7	134	LEU
64	N8	4	ARG

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Mol	Chain	Res	Type
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	29	PRO
64	N8	34	MET
64	N8	42	ARG
64	N8	46	ASP
64	N8	47	LYS
64	N8	56	VAL
64	N8	60	TYR
64	N8	64	GLN
64	N8	65	GLN
64	N8	68	PHE
64	N8	73	LEU
64	N8	76	ASP
64	N8	78	LEU
64	N8	84	GLU
64	N8	88	ASP
64	N8	98	THR
64	N8	115	LYS
64	N8	117	ARG
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
64	N8	135	GLU
65	N9	13	THR
65	N9	18	ARG
65	N9	21	ILE
65	N9	23	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	38	LYS
65	N9	44	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	13	LYS
66	O0	14	LEU
66	O0	16	LEU
66	O0	24	THR
66	O0	30	THR
66	O0	34	LEU
66	O0	40	LYS

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Mol	Chain	Res	Type
66	O0	41	LEU
66	O0	48	THR
66	O0	50	VAL
66	O0	61	MET
66	O0	66	LYS
66	O0	76	GLU
66	O0	83	LYS
66	O0	87	VAL
66	O0	100	ILE
66	O0	101	LEU
67	O1	6	ASP
67	O1	13	THR
67	O1	16	LEU
67	O1	26	LYS
67	O1	30	PRO
67	O1	31	ARG
67	O1	47	ASP
67	O1	64	VAL
67	O1	68	GLU
67	O1	75	ILE
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	96	VAL
67	O1	102	LYS
67	O1	104	LEU
67	O1	105	GLN
67	O1	106	THR
67	O1	107	VAL
67	O1	110	GLU
68	O2	4	LEU
68	O2	14	THR
68	O2	18	LYS
68	O2	19	ARG
68	O2	21	HIS
68	O2	30	GLU
68	O2	33	ARG
68	O2	34	LYS
68	O2	41	VAL

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Mol	Chain	Res	Type
68	O2	53	PRO
68	O2	61	LYS
68	O2	67	SER
68	O2	73	THR
68	O2	75	LEU
68	O2	76	VAL
68	O2	82	LEU
68	O2	109	LEU
68	O2	126	LEU
68	O2	128	LEU
69	O3	15	SER
69	O3	20	LYS
69	O3	28	SER
69	O3	45	LEU
69	O3	49	ILE
69	O3	56	SER
69	O3	59	VAL
69	O3	70	LYS
69	O3	80	VAL
69	O3	93	THR
69	O3	98	VAL
69	O3	106	ASN
69	O3	107	ILE
70	O4	3	GLN
70	O4	5	VAL
70	O4	8	ARG
70	O4	20	ILE
70	O4	23	VAL
70	O4	24	LYS
70	O4	29	ILE
70	O4	51	LEU
70	O4	58	ARG
70	O4	65	VAL
70	O4	66	SER
70	O4	71	THR
70	O4	74	ARG
70	O4	81	CYS
70	O4	86	LYS
70	O4	102	LYS
70	O4	104	VAL
71	O5	4	VAL
71	O5	15	GLU

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Mol	Chain	Res	Type
71	O5	20	GLN
71	O5	21	LEU
71	O5	27	GLU
71	O5	30	GLU
71	O5	36	LEU
71	O5	46	THR
71	O5	49	LYS
71	O5	50	SER
71	O5	60	GLU
71	O5	71	LYS
71	O5	74	LYS
71	O5	85	THR
71	O5	89	ARG
71	O5	90	ARG
71	O5	94	LYS
71	O5	101	THR
71	O5	102	GLU
71	O5	104	GLN
71	O5	105	ARG
71	O5	107	LYS
71	O5	115	LYS
71	O5	119	LYS
72	O6	11	LEU
72	O6	18	THR
72	O6	21	THR
72	O6	26	ILE
72	O6	28	TYR
72	O6	34	SER
72	O6	36	ARG
72	O6	43	LEU
72	O6	45	ARG
72	O6	52	PRO
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	62	ARG
72	O6	68	ARG
72	O6	71	LYS
72	O6	76	ARG
72	O6	81	THR
72	O6	88	GLU
72	O6	98	ARG

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Mol	Chain	Res	Type
72	O6	99	ARG
73	O7	5	THR
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	26	SER
73	O7	31	LYS
73	O7	33	THR
73	O7	36	SER
73	O7	55	ARG
73	O7	58	THR
73	O7	65	ARG
73	O7	67	LEU
73	O7	82	SER
74	O8	5	ILE
74	O8	12	LEU
74	O8	22	THR
74	O8	24	THR
74	O8	32	ASN
74	O8	41	THR
74	O8	45	VAL
74	O8	48	SER
74	O8	50	SER
74	O8	53	THR
74	O8	61	LYS
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	72	THR
74	O8	77	ARG
75	O9	21	ARG
75	O9	23	LEU
75	O9	25	GLN
75	O9	29	LEU
75	O9	33	ASN
75	O9	51	ILE
76	Q0	77	ILE
76	Q0	78	ILE
76	Q0	83	LYS
76	Q0	98	LYS
76	Q0	106	ARG
76	Q0	112	LYS

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Mol	Chain	Res	Type
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	127	LEU
77	Q1	2	ARG
77	Q1	4	LYS
77	Q1	5	TRP
77	Q1	6	ARG
77	Q1	9	ARG
77	Q1	11	ARG
77	Q1	16	LYS
77	Q1	19	LYS
77	Q1	21	ARG
78	Q2	2	VAL
78	Q2	8	ARG
78	Q2	13	LYS
78	Q2	21	THR
78	Q2	26	THR
78	Q2	35	LEU
78	Q2	45	ARG
78	Q2	48	SER
78	Q2	55	LYS
78	Q2	60	LYS
78	Q2	76	LYS
78	Q2	78	LYS
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	100	LYS
78	Q2	104	LEU
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	20	SER
79	Q3	45	LYS
79	Q3	46	THR
79	Q3	49	ARG
79	Q3	60	CYS
79	Q3	70	THR
79	Q3	73	THR
79	Q3	82	THR

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Mol	Chain	Res	Type
79	Q3	89	MET
79	Q3	90	VAL
79	Q3	91	GLU
2	s0	10	THR
2	s0	12	GLU
2	s0	29	VAL
2	s0	30	GLN
2	s0	31	VAL
2	s0	41	ARG
2	s0	45	VAL
2	s0	50	VAL
2	s0	59	LEU
2	s0	62	ARG
2	s0	72	ASP
2	s0	87	LEU
2	s0	88	LYS
2	s0	93	THR
2	s0	96	THR
2	s0	106	SER
2	s0	110	TYR
2	s0	119	ARG
2	s0	144	ILE
2	s0	151	SER
2	s0	154	GLU
2	s0	172	LEU
2	s0	183	ARG
2	s0	184	LEU
2	s0	185	ARG
2	s0	189	VAL
2	s0	197	ILE
2	s0	202	TYR
3	s1	21	VAL
3	s1	25	THR
3	s1	36	SER
3	s1	37	THR
3	s1	40	ASN
3	s1	47	LEU
3	s1	51	SER
3	s1	55	LYS
3	s1	62	LYS
3	s1	70	LEU
3	s1	73	LEU

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Mol	Chain	Res	Type
3	s1	74	GLN
3	s1	78	ASP
3	s1	81	PHE
3	s1	83	LYS
3	s1	89	ASP
3	s1	90	GLU
3	s1	97	LEU
3	s1	105	PHE
3	s1	116	LYS
3	s1	119	THR
3	s1	125	VAL
3	s1	126	THR
3	s1	129	THR
3	s1	144	ARG
3	s1	173	THR
3	s1	179	SER
3	s1	180	THR
3	s1	181	LEU
3	s1	184	LEU
3	s1	193	ILE
3	s1	197	ILE
3	s1	202	LYS
3	s1	203	ASP
3	s1	211	HIS
3	s1	214	LYS
3	s1	219	LYS
3	s1	223	PHE
3	s1	225	VAL
4	s2	39	THR
4	s2	41	LEU
4	s2	53	ILE
4	s2	55	GLU
4	s2	58	LEU
4	s2	69	ILE
4	s2	70	ASP
4	s2	72	LEU
4	s2	73	LEU
4	s2	77	GLN
4	s2	79	GLU
4	s2	80	VAL
4	s2	83	ILE
4	s2	87	GLN

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Mol	Chain	Res	Type
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	113	LEU
4	s2	117	THR
4	s2	125	ILE
4	s2	137	ILE
4	s2	141	ARG
4	s2	148	LEU
4	s2	150	GLN
4	s2	159	THR
4	s2	164	SER
4	s2	166	THR
4	s2	170	ILE
4	s2	181	SER
4	s2	194	GLU
4	s2	201	ASN
4	s2	206	THR
4	s2	222	TYR
4	s2	229	LEU
4	s2	233	GLN
4	s2	237	VAL
4	s2	238	SER
4	s2	240	LEU
4	s2	245	ASP
4	s2	248	SER
5	s3	4	LEU
5	s3	10	LYS
5	s3	21	LEU
5	s3	39	VAL
5	s3	41	VAL
5	s3	44	THR
5	s3	56	GLN
5	s3	59	LEU
5	s3	69	LEU
5	s3	83	THR
5	s3	84	ILE
5	s3	89	GLU
5	s3	90	ARG

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Mol	Chain	Res	Type
5	s3	93	ASP
5	s3	111	ASN
5	s3	115	ILE
5	s3	116	ARG
5	s3	124	ARG
5	s3	125	TYR
5	s3	127	MET
5	s3	128	GLU
5	s3	132	LYS
5	s3	134	CYS
5	s3	143	ARG
5	s3	150	MET
5	s3	158	ILE
5	s3	164	VAL
5	s3	168	ILE
5	s3	169	ASP
5	s3	172	THR
5	s3	176	LEU
5	s3	181	VAL
5	s3	185	LYS
5	s3	202	LEU
5	s3	212	LYS
5	s3	213	GLU
5	s3	223	LYS
5	s3	224	ASP
6	s4	6	LYS
6	s4	7	LYS
6	s4	9	LEU
6	s4	11	ARG
6	s4	23	LEU
6	s4	38	LEU
6	s4	42	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	67	GLN
6	s4	68	ARG
6	s4	69	HIS
6	s4	70	VAL
6	s4	72	VAL
6	s4	77	ARG
6	s4	78	THR
6	s4	81	THR

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Mol	Chain	Res	Type
6	s4	96	ASN
6	s4	104	ASP
6	s4	108	ARG
6	s4	113	ARG
6	s4	116	ASP
6	s4	123	LEU
6	s4	126	VAL
6	s4	127	LYS
6	s4	131	LEU
6	s4	146	THR
6	s4	147	ILE
6	s4	148	ARG
6	s4	159	THR
6	s4	160	VAL
6	s4	176	ASP
6	s4	180	LEU
6	s4	182	TYR
6	s4	184	THR
6	s4	208	VAL
6	s4	214	LEU
6	s4	219	VAL
6	s4	221	ARG
6	s4	227	VAL
6	s4	236	ILE
6	s4	245	LYS
6	s4	246	LEU
6	s4	247	SER
7	s5	24	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	32	GLU
7	s5	38	THR
7	s5	39	GLU
7	s5	41	LYS
7	s5	45	LYS
7	s5	47	SER
7	s5	58	LEU
7	s5	59	VAL
7	s5	60	ASP
7	s5	63	GLN
7	s5	64	VAL
7	s5	68	ILE

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Mol	Chain	Res	Type
7	s5	76	ARG
7	s5	79	ASN
7	s5	83	ARG
7	s5	86	GLN
7	s5	93	LEU
7	s5	102	ARG
7	s5	109	LYS
7	s5	112	ARG
7	s5	114	ILE
7	s5	119	ASP
7	s5	125	THR
7	s5	128	ASN
7	s5	143	ARG
7	s5	147	THR
7	s5	148	ARG
7	s5	157	ARG
7	s5	160	VAL
7	s5	166	ARG
7	s5	167	ARG
7	s5	192	GLU
7	s5	194	LEU
7	s5	203	LYS
7	s5	213	LYS
7	s5	216	GLU
8	s6	21	GLU
8	s6	31	ARG
8	s6	39	GLU
8	s6	57	ASP
8	s6	65	GLN
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	93	LYS
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU
8	s6	111	LEU
8	s6	115	LYS
8	s6	120	GLU

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Mol	Chain	Res	Type
8	s6	121	LEU
8	s6	126	ASP
8	s6	127	THR
8	s6	128	THR
8	s6	129	VAL
8	s6	137	ARG
8	s6	143	LYS
8	s6	148	SER
8	s6	150	GLU
8	s6	151	ASP
8	s6	153	VAL
8	s6	154	ARG
8	s6	155	ASP
8	s6	168	THR
8	s6	169	TYR
8	s6	182	GLN
8	s6	193	LEU
8	s6	201	GLN
8	s6	212	LEU
8	s6	215	ARG
8	s6	217	SER
9	s7	10	SER
9	s7	11	GLN
9	s7	14	THR
9	s7	16	LEU
9	s7	22	GLN
9	s7	33	GLU
9	s7	35	LYS
9	s7	41	LEU
9	s7	42	GLN
9	s7	49	ILE
9	s7	50	ASP
9	s7	55	LYS
9	s7	67	LEU
9	s7	77	LEU
9	s7	79	ARG
9	s7	81	LEU
9	s7	97	ARG
9	s7	99	LEU
9	s7	101	LYS
9	s7	103	SER
9	s7	105	THR

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Mol	Chain	Res	Type
9	s7	108	GLN
9	s7	110	GLN
9	s7	114	ARG
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	122	HIS
9	s7	126	LEU
9	s7	139	ARG
9	s7	144	VAL
9	s7	149	ILE
9	s7	166	LEU
9	s7	185	ILE
10	s8	7	SER
10	s8	10	LYS
10	s8	18	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	46	VAL
10	s8	48	THR
10	s8	61	GLU
10	s8	62	THR
10	s8	64	ASN
10	s8	74	LYS
10	s8	76	THR
10	s8	77	ARG
10	s8	82	VAL
10	s8	95	THR
10	s8	111	GLN
10	s8	119	GLN
10	s8	120	THR
10	s8	121	LEU
10	s8	138	ASN
10	s8	151	LYS
10	s8	152	ILE
10	s8	155	SER
10	s8	168	CYS
10	s8	176	SER
10	s8	178	ARG
10	s8	183	ILE
11	s9	3	ARG
11	s9	7	THR

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Mol	Chain	Res	Type
11	s9	9	SER
11	s9	16	LYS
11	s9	21	SER
11	s9	28	LEU
11	s9	37	LYS
11	s9	40	LYS
11	s9	45	ILE
11	s9	46	SER
11	s9	49	LEU
11	s9	78	ARG
11	s9	82	ARG
11	s9	83	VAL
11	s9	87	SER
11	s9	90	LYS
11	s9	93	LEU
11	s9	101	VAL
11	s9	109	LEU
11	s9	111	THR
11	s9	120	LYS
11	s9	130	THR
11	s9	133	HIS
11	s9	134	ILE
11	s9	142	ASN
11	s9	149	ARG
11	s9	161	THR
11	s9	168	ARG
11	s9	172	VAL
11	s9	180	LYS
11	s9	182	GLU
12	c0	5	LYS
12	c0	15	LEU
12	c0	20	VAL
12	c0	36	ASP
12	c0	55	VAL
12	c0	57	THR
12	c0	71	GLU
13	c1	2	SER
13	c1	3	THR
13	c1	5	LEU
13	c1	9	SER
13	c1	10	GLU
13	c1	21	ASN

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Mol	Chain	Res	Type
13	c1	22	ASN
13	c1	26	LYS
13	c1	30	ARG
13	c1	32	LYS
13	c1	33	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	46	LYS
13	c1	47	THR
13	c1	56	LYS
13	c1	60	PHE
13	c1	63	LEU
13	c1	67	ARG
13	c1	72	THR
13	c1	74	THR
13	c1	80	MET
13	c1	83	THR
13	c1	94	ILE
13	c1	99	ARG
13	c1	107	VAL
13	c1	131	ILE
13	c1	140	VAL
14	c2	28	LEU
14	c2	36	LEU
14	c2	39	ASP
14	c2	43	ARG
14	c2	45	LEU
14	c2	59	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	71	ILE
14	c2	74	LEU
14	c2	85	LYS
14	c2	89	ILE
14	c2	97	LEU
14	c2	103	LEU
14	c2	116	VAL
14	c2	121	VAL
14	c2	129	GLU
14	c2	132	GLU
14	c2	136	ILE
14	c2	140	PHE

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Mol	Chain	Res	Type
15	c3	12	SER
15	c3	16	ILE
15	c3	20	ARG
15	c3	21	ASN
15	c3	27	LYS
15	c3	35	GLU
15	c3	39	LYS
15	c3	46	THR
15	c3	62	GLN
15	c3	64	ARG
15	c3	66	ILE
15	c3	70	LYS
15	c3	80	LEU
15	c3	88	LEU
15	c3	115	LEU
15	c3	125	LEU
15	c3	134	VAL
15	c3	138	ASN
15	c3	150	VAL
16	c4	16	VAL
16	c4	18	ARG
16	c4	20	TYR
16	c4	31	THR
16	c4	33	LEU
16	c4	51	ASP
16	c4	52	ARG
16	c4	66	ASP
16	c4	76	ILE
16	c4	79	VAL
16	c4	81	VAL
16	c4	84	ARG
16	c4	92	LYS
16	c4	102	LEU
16	c4	107	ARG
16	c4	114	ARG
16	c4	119	THR
16	c4	125	SER
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
17	c5	10	ARG
17	c5	12	PHE

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Mol	Chain	Res	Type
17	c5	20	VAL
17	c5	24	LYS
17	c5	27	GLU
17	c5	28	MET
17	c5	36	LEU
17	c5	40	ARG
17	c5	43	ARG
17	c5	51	SER
17	c5	69	GLU
17	c5	71	GLU
17	c5	72	LYS
17	c5	92	SER
17	c5	97	TYR
17	c5	107	ILE
17	c5	110	GLU
17	c5	121	ILE
17	c5	127	ARG
17	c5	134	THR
18	c6	7	VAL
18	c6	23	LYS
18	c6	28	LEU
18	c6	36	ILE
18	c6	37	THR
18	c6	43	ILE
18	c6	47	LYS
18	c6	48	VAL
18	c6	53	LEU
18	c6	54	LEU
18	c6	55	VAL
18	c6	57	LEU
18	c6	68	ARG
18	c6	69	VAL
18	c6	81	ILE
18	c6	83	GLN
18	c6	94	GLN
18	c6	101	SER
18	c6	105	LEU
18	c6	107	LYS
18	c6	110	THR
18	c6	111	SER
18	c6	114	ARG
18	c6	115	THR

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Mol	Chain	Res	Type
18	c6	128	LYS
18	c6	137	ARG
19	c7	3	ARG
19	c7	5	ARG
19	c7	8	THR
19	c7	29	GLN
19	c7	34	LEU
19	c7	38	ILE
19	c7	40	THR
19	c7	46	LEU
19	c7	47	ARG
19	c7	49	LYS
19	c7	61	ILE
19	c7	67	ARG
19	c7	69	ILE
19	c7	85	VAL
19	c7	88	VAL
19	c7	105	GLN
19	c7	110	VAL
19	c7	113	LEU
20	c8	3	LEU
20	c8	4	VAL
20	c8	6	GLN
20	c8	12	GLN
20	c8	13	HIS
20	c8	15	LEU
20	c8	20	THR
20	c8	25	ASN
20	c8	28	ILE
20	c8	36	LYS
20	c8	40	ARG
20	c8	55	HIS
20	c8	57	ARG
20	c8	61	LEU
20	c8	63	GLN
20	c8	77	THR
20	c8	93	THR
20	c8	116	LEU
20	c8	119	ILE
20	c8	136	GLN
20	c8	138	THR
20	c8	144	ARG

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Mol	Chain	Res	Type
21	c9	6	VAL
21	c9	20	SER
21	c9	25	GLN
21	c9	27	LYS
21	c9	28	LEU
21	c9	34	VAL
21	c9	68	ARG
21	c9	70	GLN
21	c9	71	VAL
21	c9	75	LYS
21	c9	84	LYS
21	c9	86	ARG
21	c9	91	TYR
21	c9	110	LYS
21	c9	111	ILE
21	c9	116	ILE
21	c9	117	SER
21	c9	123	ARG
21	c9	135	ILE
21	c9	139	THR
21	c9	140	LEU
21	c9	141	GLU
21	c9	142	GLU
21	c9	144	GLU
22	d0	13	GLU
22	d0	22	ILE
22	d0	23	ARG
22	d0	27	THR
22	d0	31	VAL
22	d0	34	LEU
22	d0	39	SER
22	d0	44	ASN
22	d0	57	ARG
22	d0	59	PRO
22	d0	60	THR
22	d0	61	LYS
22	d0	63	LEU
22	d0	67	THR
22	d0	70	THR
22	d0	72	ASN
22	d0	74	GLU
22	d0	77	LYS

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Mol	Chain	Res	Type
22	d0	81	THR
22	d0	88	LYS
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	105	GLN
22	d0	108	ILE
22	d0	115	GLU
23	d1	1	MET
23	d1	2	GLU
23	d1	5	LYS
23	d1	8	LEU
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	24	ILE
23	d1	25	LYS
23	d1	32	VAL
23	d1	41	GLU
23	d1	49	GLU
23	d1	52	THR
23	d1	68	SER
23	d1	69	LEU
23	d1	78	LEU
23	d1	86	SER
24	d2	6	VAL
24	d2	7	LEU
24	d2	15	ASN
24	d2	20	THR
24	d2	23	ARG
24	d2	25	VAL
24	d2	26	LEU
24	d2	43	LYS
24	d2	65	LEU
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	117	ARG
24	d2	121	VAL
24	d2	124	LYS
24	d2	129	VAL
25	d3	3	LYS

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Mol	Chain	Res	Type
25	d3	9	LEU
25	d3	15	LEU
25	d3	19	ARG
25	d3	28	ASN
25	d3	40	SER
25	d3	72	VAL
25	d3	73	ARG
25	d3	78	LYS
25	d3	82	LYS
25	d3	83	VAL
25	d3	84	THR
25	d3	96	VAL
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	109	ARG
25	d3	117	ILE
25	d3	121	ARG
25	d3	128	SER
25	d3	133	LEU
25	d3	139	LYS
25	d3	140	LYS
26	d4	5	VAL
26	d4	10	ARG
26	d4	13	ILE
26	d4	14	SER
26	d4	21	LYS
26	d4	26	ASP
26	d4	29	HIS
26	d4	34	ASN
26	d4	43	LYS
26	d4	49	LYS
26	d4	51	GLU
26	d4	62	THR
26	d4	74	LEU
26	d4	78	SER
26	d4	83	LYS
26	d4	88	THR
26	d4	105	ARG
26	d4	107	GLN
26	d4	116	LYS
26	d4	128	LYS

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Mol	Chain	Res	Type
26	d4	133	ASN
27	d5	46	LYS
27	d5	51	LEU
27	d5	53	GLU
27	d5	57	TYR
27	d5	60	VAL
27	d5	61	SER
27	d5	68	ARG
27	d5	81	ARG
27	d5	88	ILE
28	d6	8	ASN
28	d6	11	ASN
28	d6	18	VAL
28	d6	24	VAL
28	d6	28	LYS
28	d6	29	SER
28	d6	41	ILE
28	d6	44	ILE
28	d6	51	ARG
28	d6	53	LEU
28	d6	55	GLU
28	d6	67	THR
28	d6	82	ARG
28	d6	85	ARG
28	d6	86	VAL
28	d6	90	GLU
29	d7	3	LEU
29	d7	4	VAL
29	d7	11	THR
29	d7	14	SER
29	d7	15	GLU
29	d7	24	LEU
29	d7	26	GLN
29	d7	31	TYR
29	d7	34	ASP
29	d7	43	ILE
29	d7	52	THR
29	d7	55	THR
29	d7	72	LYS
29	d7	81	ARG
30	d8	7	VAL
30	d8	11	LYS

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Mol	Chain	Res	Type
30	d8	16	LEU
30	d8	21	SER
30	d8	22	ARG
30	d8	30	VAL
30	d8	32	PHE
30	d8	33	LEU
30	d8	37	SER
30	d8	38	ARG
30	d8	40	ILE
30	d8	49	ARG
30	d8	54	LEU
30	d8	64	ARG
30	d8	65	ARG
31	d9	10	HIS
31	d9	21	CYS
31	d9	22	ARG
31	d9	28	THR
31	d9	30	LEU
31	d9	36	LEU
31	d9	39	CYS
31	d9	42	CYS
31	d9	49	ASP
31	d9	54	LYS
80	e0	4	VAL
80	e0	21	VAL
80	e0	22	GLU
80	e0	23	LYS
80	e0	24	THR
80	e0	26	LYS
80	e0	29	LYS
80	e0	31	LYS
80	e0	38	LEU
80	e0	41	THR
80	e0	42	ARG
80	e0	44	PHE
80	e0	45	VAL
80	e0	47	VAL
80	e0	49	LEU
33	e1	78	LYS
33	e1	90	LYS
33	e1	93	HIS
33	e1	96	LYS

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Mol	Chain	Res	Type
33	e1	97	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	107	LYS
33	e1	113	LYS
33	e1	115	THR
33	e1	119	ARG
33	e1	120	GLU
34	sR	25	THR
34	sR	29	GLN
34	sR	48	THR
34	sR	52	GLN
34	sR	53	LYS
34	sR	58	VAL
34	sR	59	ARG
34	sR	64	HIS
34	sR	65	SER
34	sR	66	HIS
34	sR	76	ASP
34	sR	96	THR
34	sR	98	GLU
34	sR	145	LEU
34	sR	159	ASN
34	sR	168	THR
34	sR	176	LYS
34	sR	199	ILE
34	sR	228	LYS
34	sR	232	TYR
34	sR	275	ARG
34	sR	286	GLU
34	sR	297	ASP
34	sR	319	ASN
35	sM	23	LYS
35	sM	28	SER
35	sM	30	THR
35	sM	41	SER
35	sM	43	ASP
35	sM	45	SER
35	sM	48	ARG
35	sM	50	ASN
35	sM	61	ILE

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Mol	Chain	Res	Type
35	sM	68	ARG
35	sM	71	ASN
35	sM	74	LYS
35	sM	75	ASP
35	sM	77	THR
39	l2	15	ILE
39	l2	17	THR
39	l2	23	ARG
39	l2	32	LEU
39	l2	44	ILE
39	l2	45	VAL
39	l2	46	LYS
39	l2	48	ILE
39	l2	62	VAL
39	l2	70	ARG
39	l2	71	LEU
39	l2	74	GLU
39	l2	79	ASN
39	l2	80	GLU
39	l2	82	VAL
39	l2	101	VAL
39	l2	104	LEU
39	l2	107	VAL
39	l2	114	SER
39	l2	116	VAL
39	l2	119	LYS
39	l2	128	ARG
39	l2	137	ILE
39	l2	142	ASP
39	l2	147	ARG
39	l2	148	VAL
39	l2	155	LYS
39	l2	158	ILE
39	l2	165	VAL
39	l2	169	ILE
39	l2	179	LEU
39	l2	181	LYS
39	l2	188	LYS
39	l2	193	ARG
39	l2	200	ARG
39	l2	204	MET
39	l2	206	PRO

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Mol	Chain	Res	Type
39	12	207	VAL
39	12	227	ARG
39	12	230	VAL
39	12	238	ILE
39	12	243	THR
39	12	246	LEU
39	12	249	SER
40	13	3	HIS
40	13	4	ARG
40	13	5	LYS
40	13	10	ARG
40	13	17	LEU
40	13	19	ARG
40	13	20	LYS
40	13	34	LYS
40	13	43	LEU
40	13	50	LYS
40	13	56	ILE
40	13	67	PHE
40	13	69	LYS
40	13	85	VAL
40	13	103	THR
40	13	114	VAL
40	13	116	ARG
40	13	139	GLN
40	13	145	GLU
40	13	146	ARG
40	13	148	LEU
40	13	150	ARG
40	13	153	LYS
40	13	157	VAL
40	13	160	VAL
40	13	167	ARG
40	13	169	THR
40	13	188	ILE
40	13	192	VAL
40	13	196	ARG
40	13	197	GLU
40	13	201	LYS
40	13	202	THR
40	13	205	VAL
40	13	208	VAL

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Mol	Chain	Res	Type
40	l3	229	VAL
40	l3	232	ARG
40	l3	235	THR
40	l3	238	LEU
40	l3	249	VAL
40	l3	252	ILE
40	l3	266	ARG
40	l3	274	SER
40	l3	276	THR
40	l3	287	LYS
40	l3	296	THR
40	l3	304	THR
40	l3	308	MET
40	l3	317	ILE
40	l3	324	VAL
40	l3	328	ILE
40	l3	332	ARG
40	l3	334	ARG
40	l3	338	LEU
40	l3	340	LYS
40	l3	346	THR
40	l3	347	SER
40	l3	348	ARG
40	l3	359	ILE
40	l3	363	SER
40	l3	367	LYS
40	l3	380	MET
40	l3	386	ASP
41	l4	3	ARG
41	l4	16	THR
41	l4	18	ASN
41	l4	20	LEU
41	l4	25	VAL
41	l4	27	SER
41	l4	41	SER
41	l4	48	GLN
41	l4	52	VAL
41	l4	67	THR
41	l4	71	VAL
41	l4	73	ARG
41	l4	90	PHE
41	l4	93	MET

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Mol	Chain	Res	Type
41	14	112	LYS
41	14	118	LYS
41	14	120	TYR
41	14	144	LYS
41	14	145	ILE
41	14	148	ILE
41	14	150	LEU
41	14	156	LEU
41	14	158	SER
41	14	170	LYS
41	14	172	VAL
41	14	177	ASP
41	14	179	LEU
41	14	182	LEU
41	14	186	LYS
41	14	187	LEU
41	14	197	ARG
41	14	200	THR
41	14	201	GLN
41	14	203	ARG
41	14	206	LEU
41	14	217	LYS
41	14	220	ARG
41	14	222	VAL
41	14	226	GLU
41	14	230	VAL
41	14	246	ARG
41	14	258	LEU
41	14	265	GLU
41	14	266	THR
41	14	275	THR
41	14	284	SER
41	14	292	SER
41	14	300	ARG
41	14	301	PRO
41	14	306	THR
41	14	307	GLN
41	14	310	THR
41	14	313	LEU
41	14	316	ASN
41	14	319	LYS
41	14	321	LYS

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Mol	Chain	Res	Type
41	14	327	LEU
41	14	333	VAL
41	14	338	LYS
41	14	342	LYS
41	14	345	GLU
41	14	347	THR
41	14	356	THR
41	14	359	LEU
42	15	4	GLN
42	15	5	LYS
42	15	10	SER
42	15	13	SER
42	15	34	LYS
42	15	51	LEU
42	15	58	LYS
42	15	68	THR
42	15	70	THR
42	15	75	LEU
42	15	89	THR
42	15	93	THR
42	15	109	THR
42	15	110	LEU
42	15	112	LYS
42	15	113	LEU
42	15	118	THR
42	15	120	LYS
42	15	132	THR
42	15	133	GLU
42	15	135	VAL
42	15	140	ARG
42	15	144	VAL
42	15	146	LEU
42	15	148	ILE
42	15	155	THR
42	15	158	ARG
42	15	185	PHE
42	15	186	GLU
42	15	187	THR
42	15	190	ILE
42	15	194	LEU
42	15	211	LEU
42	15	218	ARG

Continued on next page...

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Mol	Chain	Res	Type
42	15	227	LEU
42	15	232	ASP
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS
42	15	262	LYS
42	15	268	GLU
42	15	273	ARG
42	15	275	THR
42	15	279	LYS
42	15	282	ARG
42	15	293	LEU
42	15	297	GLN
43	16	8	LYS
43	16	12	SER
43	16	14	ASP
43	16	15	VAL
43	16	21	THR
43	16	23	LYS
43	16	50	LYS
43	16	52	VAL
43	16	64	LEU
43	16	65	ILE
43	16	78	ARG
43	16	79	VAL
43	16	89	THR
43	16	91	VAL
43	16	98	VAL
43	16	102	ASN
43	16	109	GLU
43	16	128	LYS
43	16	129	GLU
43	16	146	ILE
43	16	151	LYS
43	16	152	THR
43	16	155	LEU
43	16	160	SER
43	16	162	SER
43	16	166	LYS
43	16	175	LYS
44	17	22	THR
44	17	24	GLU

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Mol	Chain	Res	Type
44	17	26	VAL
44	17	40	LYS
44	17	41	ARG
44	17	45	LEU
44	17	54	GLU
44	17	56	GLU
44	17	60	ARG
44	17	62	ILE
44	17	77	VAL
44	17	83	LEU
44	17	94	LYS
44	17	98	LYS
44	17	111	ILE
44	17	127	LEU
44	17	130	ILE
44	17	158	LYS
44	17	159	GLN
44	17	173	LEU
44	17	175	LYS
44	17	176	TYR
44	17	179	LEU
44	17	184	LEU
44	17	193	PRO
44	17	219	LYS
44	17	229	PHE
44	17	239	LEU
45	18	26	LEU
45	18	41	GLN
45	18	46	LEU
45	18	50	VAL
45	18	65	LEU
45	18	68	ARG
45	18	70	LYS
45	18	74	THR
45	18	79	GLN
45	18	81	THR
45	18	82	LEU
45	18	89	GLU
45	18	95	ASN
45	18	101	THR
45	18	109	LEU
45	18	136	LEU

Continued on next page...

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Mol	Chain	Res	Type
45	18	146	LYS
45	18	149	LYS
45	18	160	ILE
45	18	164	VAL
45	18	169	LEU
45	18	172	LYS
45	18	185	ARG
45	18	191	ASN
45	18	200	LEU
45	18	208	GLU
45	18	214	LEU
45	18	217	THR
45	18	230	LYS
45	18	241	LYS
45	18	245	LYS
45	18	248	LYS
46	19	1	MET
46	19	5	GLN
46	19	6	THR
46	19	18	VAL
46	19	31	ARG
46	19	33	THR
46	19	34	LEU
46	19	39	LYS
46	19	44	THR
46	19	55	VAL
46	19	62	ARG
46	19	68	LEU
46	19	69	ARG
46	19	70	THR
46	19	80	THR
46	19	82	VAL
46	19	92	TYR
46	19	105	GLU
46	19	106	LYS
46	19	107	ASP
46	19	118	LEU
46	19	121	LYS
46	19	122	LYS
46	19	129	ARG
46	19	133	THR
46	19	138	THR

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Mol	Chain	Res	Type
46	l9	144	ILE
46	l9	151	VAL
46	l9	157	ASN
46	l9	161	LEU
46	l9	162	GLN
46	l9	163	GLN
46	l9	166	ARG
46	l9	170	LYS
46	l9	173	ARG
46	l9	177	ASP
46	l9	179	ILE
46	l9	191	LEU
47	m0	8	CYS
47	m0	24	ARG
47	m0	36	LEU
47	m0	39	LYS
47	m0	42	THR
47	m0	45	GLU
47	m0	52	LEU
47	m0	58	GLU
47	m0	74	LYS
47	m0	76	MET
47	m0	77	THR
47	m0	78	THR
47	m0	83	ASP
47	m0	87	LEU
47	m0	91	VAL
47	m0	99	ILE
47	m0	101	LYS
47	m0	121	LYS
47	m0	139	ARG
47	m0	140	THR
47	m0	144	ASN
47	m0	162	GLN
47	m0	163	GLN
47	m0	166	ILE
47	m0	169	LYS
47	m0	170	LYS
47	m0	174	THR
47	m0	176	LEU
47	m0	177	ASP
47	m0	182	LEU

Continued on next page...

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Mol	Chain	Res	Type
47	m0	193	ASP
47	m0	197	VAL
47	m0	200	LEU
47	m0	205	SER
47	m0	206	LEU
47	m0	211	ARG
47	m0	217	PHE
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	29	ARG
48	m1	31	THR
48	m1	37	LEU
48	m1	44	THR
48	m1	46	VAL
48	m1	49	LYS
48	m1	53	THR
48	m1	54	VAL
48	m1	56	THR
48	m1	65	ILE
48	m1	71	VAL
48	m1	78	GLU
48	m1	80	LEU
48	m1	92	ARG
48	m1	101	ASN
48	m1	106	ILE
48	m1	112	LEU
48	m1	129	VAL
48	m1	130	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	142	LYS
48	m1	147	THR
48	m1	152	HIS
48	m1	158	ASP
48	m1	159	THR
48	m1	160	VAL
48	m1	174	LYS
49	m3	9	ILE

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Mol	Chain	Res	Type
49	m3	13	HIS
49	m3	36	ARG
49	m3	45	LYS
49	m3	52	ASP
49	m3	54	LEU
49	m3	55	ARG
49	m3	58	VAL
49	m3	59	ARG
49	m3	62	THR
49	m3	63	VAL
49	m3	67	ARG
49	m3	69	VAL
49	m3	73	ARG
49	m3	81	LYS
49	m3	85	LEU
49	m3	86	THR
49	m3	107	GLU
49	m3	114	GLN
49	m3	118	GLU
49	m3	122	LYS
49	m3	123	ILE
49	m3	124	ILE
49	m3	128	ARG
49	m3	131	LYS
49	m3	149	GLN
49	m3	152	THR
49	m3	157	ARG
49	m3	164	GLU
49	m3	165	SER
49	m3	171	ARG
49	m3	176	GLU
49	m3	184	GLU
49	m3	189	GLU
49	m3	194	GLU
50	m4	3	THR
50	m4	20	VAL
50	m4	27	GLN
50	m4	41	GLN
50	m4	53	VAL
50	m4	55	ARG
50	m4	62	GLN
50	m4	64	VAL

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Mol	Chain	Res	Type
50	m4	72	LEU
50	m4	74	ARG
50	m4	80	THR
50	m4	82	SER
50	m4	92	GLU
50	m4	105	GLN
50	m4	106	ARG
50	m4	107	GLU
50	m4	108	ARG
50	m4	109	ARG
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	8	GLU
51	m5	10	LEU
51	m5	12	ARG
51	m5	15	GLN
51	m5	22	LEU
51	m5	24	ARG
51	m5	49	ARG
51	m5	60	VAL
51	m5	66	VAL
51	m5	68	ARG
51	m5	71	ARG
51	m5	76	PRO
51	m5	80	THR
51	m5	85	THR
51	m5	92	LEU
51	m5	93	LYS
51	m5	98	LEU
51	m5	106	VAL
51	m5	138	GLN
51	m5	153	ASP
51	m5	165	THR
51	m5	171	SER
51	m5	183	THR
51	m5	187	ARG
51	m5	188	ARG
51	m5	190	THR
51	m5	194	GLN
51	m5	198	SER
51	m5	201	ARG

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Mol	Chain	Res	Type
51	m5	204	LYS
52	m6	22	VAL
52	m6	25	LYS
52	m6	34	VAL
52	m6	41	LEU
52	m6	58	LEU
52	m6	60	LYS
52	m6	66	LYS
52	m6	67	THR
52	m6	74	ARG
52	m6	78	ARG
52	m6	79	ILE
52	m6	85	ARG
52	m6	100	GLU
52	m6	106	GLU
52	m6	110	PRO
52	m6	115	LYS
52	m6	117	ARG
52	m6	124	LEU
52	m6	126	VAL
52	m6	129	LEU
52	m6	130	LYS
52	m6	134	LYS
52	m6	142	SER
52	m6	152	VAL
52	m6	160	ARG
52	m6	166	GLU
52	m6	171	LYS
52	m6	175	THR
52	m6	182	ASN
52	m6	184	THR
52	m6	197	LEU
53	m7	3	ARG
53	m7	7	THR
53	m7	9	THR
53	m7	16	SER
53	m7	24	VAL
53	m7	32	THR
53	m7	36	ILE
53	m7	41	LEU
53	m7	50	GLN
53	m7	51	VAL

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Mol	Chain	Res	Type
53	m7	52	LEU
53	m7	56	ARG
53	m7	78	VAL
53	m7	79	THR
53	m7	80	LYS
53	m7	89	LYS
53	m7	94	LEU
53	m7	103	GLU
53	m7	107	LEU
53	m7	112	LEU
53	m7	114	VAL
53	m7	116	HIS
53	m7	119	VAL
53	m7	120	ASN
53	m7	126	ARG
53	m7	127	ARG
53	m7	136	ILE
53	m7	142	SER
53	m7	144	SER
53	m7	153	LYS
53	m7	155	GLU
54	m8	7	SER
54	m8	8	LYS
54	m8	12	ARG
54	m8	17	THR
54	m8	22	ASP
54	m8	24	VAL
54	m8	26	LEU
54	m8	32	LEU
54	m8	34	THR
54	m8	41	ASP
54	m8	57	ILE
54	m8	63	SER
54	m8	64	VAL
54	m8	69	ARG
54	m8	80	THR
54	m8	81	VAL
54	m8	86	THR
54	m8	93	ILE
54	m8	127	LEU
54	m8	135	GLN
54	m8	137	THR

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Mol	Chain	Res	Type
54	m8	138	LEU
54	m8	147	ARG
54	m8	161	LYS
54	m8	165	ILE
54	m8	166	LEU
54	m8	167	SER
54	m8	170	ARG
54	m8	178	ARG
54	m8	180	ARG
55	m9	7	GLN
55	m9	8	LYS
55	m9	9	ARG
55	m9	10	LEU
55	m9	17	VAL
55	m9	20	ARG
55	m9	29	THR
55	m9	31	GLU
55	m9	36	ASN
55	m9	43	LYS
55	m9	47	ASN
55	m9	49	THR
55	m9	52	LYS
55	m9	62	ARG
55	m9	63	THR
55	m9	70	LYS
55	m9	71	ARG
55	m9	74	ARG
55	m9	88	ARG
55	m9	91	SER
55	m9	99	LEU
55	m9	126	GLU
55	m9	127	SER
55	m9	128	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	167	ARG
55	m9	173	ARG
56	n0	1	MET

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Mol	Chain	Res	Type
56	n0	13	ARG
56	n0	17	GLU
56	n0	21	GLU
56	n0	22	PRO
56	n0	23	LYS
56	n0	45	LEU
56	n0	51	VAL
56	n0	52	LYS
56	n0	60	SER
56	n0	63	GLN
56	n0	70	THR
56	n0	72	VAL
56	n0	73	LYS
56	n0	80	ARG
56	n0	87	THR
56	n0	97	VAL
56	n0	100	VAL
56	n0	104	GLU
56	n0	105	THR
56	n0	115	ARG
56	n0	117	ARG
56	n0	130	GLU
56	n0	136	LYS
56	n0	137	ARG
56	n0	148	LEU
56	n0	149	LYS
56	n0	155	ARG
56	n0	157	GLN
56	n0	160	THR
56	n0	161	LYS
56	n0	162	THR
56	n0	167	ARG
56	n0	169	SER
56	n0	172	TYR
57	n1	9	SER
57	n1	12	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	55	LYS
57	n1	78	LYS
57	n1	80	VAL

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Mol	Chain	Res	Type
57	n1	83	ARG
57	n1	87	LYS
57	n1	88	ARG
57	n1	89	LEU
57	n1	96	ILE
57	n1	97	LYS
57	n1	102	ARG
57	n1	104	GLU
57	n1	126	VAL
57	n1	135	PRO
57	n1	139	ARG
57	n1	143	THR
57	n1	149	GLN
57	n1	150	THR
57	n1	151	LEU
57	n1	154	VAL
57	n1	160	ILE
58	n2	13	LYS
58	n2	16	THR
58	n2	27	VAL
58	n2	28	PHE
58	n2	37	LEU
58	n2	38	ILE
58	n2	39	ASP
58	n2	43	VAL
58	n2	50	LEU
58	n2	54	VAL
58	n2	55	THR
58	n2	63	VAL
58	n2	66	VAL
58	n2	90	ARG
58	n2	98	THR
58	n2	100	THR
59	n3	2	SER
59	n3	7	GLN
59	n3	13	ILE
59	n3	40	LYS
59	n3	42	SER
59	n3	45	ARG
59	n3	48	ARG
59	n3	57	MET
59	n3	84	SER

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Mol	Chain	Res	Type
59	n3	88	ARG
59	n3	115	THR
60	n4	1	MET
60	n4	5	ILE
60	n4	19	THR
60	n4	39	LEU
60	n4	54	LEU
60	n4	57	LYS
60	n4	63	ILE
60	n4	89	LEU
60	n4	96	LEU
60	n4	97	LYS
60	n4	98	PRO
60	n4	100	VAL
60	n4	105	ARG
60	n4	107	GLU
60	n4	126	GLU
60	n4	127	LYS
60	n4	135	SER
61	n5	24	LEU
61	n5	37	THR
61	n5	38	LEU
61	n5	45	LYS
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	74	LYS
61	n5	86	VAL
61	n5	104	GLU
61	n5	115	ARG
61	n5	125	ARG
61	n5	135	ILE
61	n5	137	ASN
61	n5	142	ILE
62	n6	3	LYS
62	n6	9	SER
62	n6	12	ARG
62	n6	13	ARG
62	n6	14	LYS
62	n6	17	LYS
62	n6	36	SER
62	n6	37	LYS

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Mol	Chain	Res	Type
62	n6	40	ARG
62	n6	50	ILE
62	n6	51	ARG
62	n6	55	GLU
62	n6	56	VAL
62	n6	57	LEU
62	n6	66	GLN
62	n6	74	TYR
62	n6	76	LEU
62	n6	83	ASP
62	n6	94	SER
62	n6	103	LYS
62	n6	105	VAL
62	n6	108	LYS
62	n6	111	LEU
62	n6	115	ARG
62	n6	120	GLN
63	n7	3	LYS
63	n7	5	LEU
63	n7	14	VAL
63	n7	17	ARG
63	n7	24	VAL
63	n7	34	LYS
63	n7	36	HIS
63	n7	46	ILE
63	n7	47	GLU
63	n7	52	LYS
63	n7	65	ARG
63	n7	72	ILE
63	n7	73	LYS
63	n7	81	LEU
63	n7	83	THR
63	n7	86	THR
63	n7	90	GLU
63	n7	93	LYS
63	n7	94	SER
63	n7	95	VAL
63	n7	98	THR
63	n7	99	GLU
63	n7	102	GLU
63	n7	103	GLN
63	n7	119	GLU

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Mol	Chain	Res	Type
63	n7	121	ARG
63	n7	126	LYS
63	n7	127	ASN
63	n7	132	SER
63	n7	134	LEU
63	n7	135	ARG
64	n8	3	SER
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	10	LYS
64	n8	14	HIS
64	n8	15	VAL
64	n8	27	LYS
64	n8	42	ARG
64	n8	46	ASP
64	n8	47	LYS
64	n8	56	VAL
64	n8	60	TYR
64	n8	73	LEU
64	n8	82	ILE
64	n8	85	ASP
64	n8	89	GLN
64	n8	91	LEU
64	n8	97	GLU
64	n8	98	THR
64	n8	117	ARG
64	n8	128	ARG
64	n8	132	LYS
64	n8	133	LEU
65	n9	3	LYS
65	n9	22	LYS
65	n9	23	LYS
65	n9	26	THR
65	n9	31	SER
65	n9	33	LYS
65	n9	38	LYS
65	n9	42	ASN
65	n9	50	THR
65	n9	54	LEU
65	n9	58	LYS
65	n9	59	LYS

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Mol	Chain	Res	Type
66	o0	7	GLN
66	o0	8	GLU
66	o0	14	LEU
66	o0	19	LYS
66	o0	28	LYS
66	o0	32	LYS
66	o0	41	LEU
66	o0	55	GLU
66	o0	61	MET
66	o0	64	LYS
66	o0	68	TYR
66	o0	81	VAL
66	o0	84	LEU
66	o0	86	ARG
66	o0	87	VAL
66	o0	99	ASP
66	o0	104	LEU
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	31	ARG
67	o1	34	LYS
67	o1	44	MET
67	o1	70	ARG
67	o1	84	ASP
67	o1	89	LEU
67	o1	102	LYS
67	o1	104	LEU
67	o1	106	THR
67	o1	110	GLU
68	o2	11	LYS
68	o2	24	ARG
68	o2	27	ARG
68	o2	33	ARG
68	o2	34	LYS
68	o2	35	GLN
68	o2	41	VAL
68	o2	51	SER
68	o2	61	LYS
68	o2	62	LYS
68	o2	71	HIS
68	o2	73	THR

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Mol	Chain	Res	Type
68	o2	75	LEU
68	o2	76	VAL
68	o2	82	LEU
68	o2	87	MET
68	o2	89	THR
68	o2	91	THR
68	o2	109	LEU
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	19	SER
69	o3	31	LYS
69	o3	49	ILE
69	o3	57	LYS
69	o3	58	GLU
69	o3	70	LYS
69	o3	72	THR
69	o3	74	THR
69	o3	81	VAL
69	o3	84	THR
69	o3	98	VAL
69	o3	107	ILE
70	o4	9	ARG
70	o4	16	ARG
70	o4	20	ILE
70	o4	22	VAL
70	o4	24	LYS
70	o4	29	ILE
70	o4	30	LEU
70	o4	31	ARG
70	o4	33	GLN
70	o4	37	LYS
70	o4	47	CYS
70	o4	58	ARG
70	o4	61	GLN
70	o4	65	VAL
70	o4	66	SER
70	o4	68	THR
70	o4	71	THR
70	o4	79	SER
70	o4	83	ASN
70	o4	84	CYS

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Mol	Chain	Res	Type
70	o4	86	LYS
70	o4	88	ARG
70	o4	98	GLN
70	o4	104	VAL
71	o5	20	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	36	LEU
71	o5	37	SER
71	o5	38	ARG
71	o5	40	SER
71	o5	46	THR
71	o5	47	VAL
71	o5	48	ARG
71	o5	53	CYS
71	o5	57	VAL
71	o5	69	LEU
71	o5	73	LYS
71	o5	80	LEU
71	o5	81	ARG
71	o5	85	THR
71	o5	86	ARG
71	o5	89	ARG
71	o5	90	ARG
71	o5	100	VAL
71	o5	101	THR
71	o5	107	LYS
71	o5	119	LYS
72	o6	3	VAL
72	o6	7	ILE
72	o6	9	ILE
72	o6	11	LEU
72	o6	21	THR
72	o6	26	ILE
72	o6	29	LYS
72	o6	34	SER
72	o6	36	ARG
72	o6	37	THR
72	o6	43	LEU
72	o6	45	ARG
72	o6	46	GLU
72	o6	57	LEU

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Mol	Chain	Res	Type
72	o6	58	ILE
72	o6	60	LEU
72	o6	66	GLU
72	o6	76	ARG
72	o6	81	THR
72	o6	94	ILE
72	o6	98	ARG
73	o7	17	THR
73	o7	25	ARG
73	o7	33	THR
73	o7	44	THR
73	o7	46	SER
73	o7	55	ARG
73	o7	58	THR
73	o7	59	THR
73	o7	65	ARG
73	o7	67	LEU
73	o7	68	LYS
73	o7	70	VAL
73	o7	72	ARG
73	o7	75	LYS
73	o7	80	THR
74	o8	5	ILE
74	o8	8	ILE
74	o8	24	THR
74	o8	31	LEU
74	o8	41	THR
74	o8	45	VAL
74	o8	53	THR
74	o8	61	LYS
74	o8	63	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	78	LEU
75	o9	4	GLN
75	o9	9	ILE
75	o9	11	GLN
75	o9	17	LYS
75	o9	21	ARG
75	o9	23	LEU
75	o9	27	ILE
75	o9	45	ARG

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Mol	Chain	Res	Type
75	o9	51	ILE
76	q0	79	GLU
76	q0	80	PRO
76	q0	85	LEU
76	q0	88	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	13	LEU
77	q1	19	LYS
77	q1	21	ARG
77	q1	23	ARG
78	q2	6	LYS
78	q2	7	THR
78	q2	8	ARG
78	q2	16	THR
78	q2	38	GLN
78	q2	45	ARG
78	q2	47	GLN
78	q2	48	SER
78	q2	61	LYS
78	q2	64	THR
78	q2	71	ARG
78	q2	73	GLU
78	q2	75	VAL
78	q2	78	LYS
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	93	LEU
78	q2	100	LYS
78	q2	104	LEU
78	q2	105	GLN
79	q3	3	LYS
79	q3	20	SER
79	q3	24	ARG
79	q3	40	SER

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Mol	Chain	Res	Type
79	q3	42	CYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	59	CYS
79	q3	73	THR
79	q3	79	VAL
79	q3	81	SER
79	q3	89	MET
79	q3	90	VAL
82	p0	4	ILE
82	p0	5	ARG
82	p0	10	GLU
82	p0	25	LEU
82	p0	32	ASN
82	p0	42	ARG
82	p0	43	LYS
82	p0	44	GLU
82	p0	48	ARG
82	p0	51	VAL
82	p0	55	LYS
82	p0	57	THR
82	p0	70	LEU
82	p0	72	ASP
82	p0	76	LEU
82	p0	81	LYS
82	p0	84	VAL
82	p0	93	LEU
82	p0	97	LYS
82	p0	104	ARG
82	p0	196	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
3	S1	79	HIS
3	S1	149	GLN
3	S1	177	GLN
3	S1	209	ASN
5	S3	179	GLN
6	S4	36	HIS
7	S5	224	ASN

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Mol	Chain	Res	Type
13	C1	110	HIS
17	C5	103	ASN
18	C6	21	HIS
18	C6	74	HIS
20	C8	25	ASN
20	C8	136	GLN
27	D5	95	HIS
39	L2	209	HIS
40	L3	256	HIS
41	L4	311	HIS
42	L5	40	HIS
44	L7	244	ASN
45	L8	240	ASN
48	M1	109	HIS
53	M7	10	ASN
59	N3	98	ASN
63	N7	36	HIS
63	N7	57	HIS
78	Q2	53	GLN
78	Q2	102	GLN
6	s4	157	ASN
8	s6	197	ASN
8	s6	201	GLN
9	s7	71	HIS
9	s7	122	HIS
11	s9	110	GLN
11	s9	142	ASN
12	c0	32	HIS
13	c1	18	HIS
20	c8	25	ASN
21	c9	64	HIS
26	d4	22	GLN
80	e0	17	GLN
34	sR	299	GLN
42	l5	264	GLN
44	l7	80	GLN
55	m9	7	GLN
61	n5	111	ASN
62	n6	81	GLN
63	n7	127	ASN
64	n8	44	ASN
67	o1	57	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	490 (28%)	72 (4%)
1	6	1793/1800 (99%)	473 (26%)	59 (3%)
36	1	3145/3396 (92%)	702 (22%)	91 (2%)
36	5	3145/3396 (92%)	686 (21%)	84 (2%)
37	3	120/121 (99%)	25 (20%)	2 (1%)
37	7	120/121 (99%)	23 (19%)	1 (0%)
38	4	157/158 (99%)	39 (24%)	5 (3%)
38	8	157/158 (99%)	40 (25%)	2 (1%)
All	All	10384/10950 (94%)	2478 (23%)	316 (3%)

All (2478) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	40	A
1	2	45	U
1	2	46	A
1	2	47	A
1	2	50	C
1	2	57	G
1	2	60	U
1	2	66	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	100	A
1	2	104	A
1	2	114	C
1	2	118	U
1	2	121	U

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Mol	Chain	Res	Type
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	161	U
1	2	167	U
1	2	169	A
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	199	G
1	2	200	A
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	226	A
1	2	227	U
1	2	228	G

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Mol	Chain	Res	Type
1	2	229	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	236	A
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U
1	2	250	C
1	2	253	A
1	2	260	U
1	2	261	U
1	2	265	A
1	2	266	A
1	2	269	G
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	301	A
1	2	309	C
1	2	314	C
1	2	316	A
1	2	319	U
1	2	321	C
1	2	322	G
1	2	333	A
1	2	337	G
1	2	338	C
1	2	341	A
1	2	348	U

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Mol	Chain	Res	Type
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	387	A
1	2	390	G
1	2	397	A
1	2	399	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	403	G
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	448	C
1	2	450	U
1	2	468	A
1	2	471	A
1	2	477	A
1	2	484	C
1	2	485	A
1	2	486	G
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U

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Mol	Chain	Res	Type
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	514	G
1	2	515	A
1	2	516	G
1	2	519	C
1	2	527	A
1	2	532	U
1	2	536	C
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	546	U
1	2	547	U
1	2	548	G
1	2	551	G
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	566	C
1	2	579	A
1	2	580	A
1	2	582	U
1	2	594	A
1	2	595	G
1	2	609	U
1	2	619	A

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Mol	Chain	Res	Type
1	2	620	A
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	650	U
1	2	653	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G

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Mol	Chain	Res	Type
1	2	725	U
1	2	727	U
1	2	728	U
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	743	U
1	2	745	U
1	2	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	793	A
1	2	794	U
1	2	795	U
1	2	811	A
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G

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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	846	G
1	2	848	C
1	2	854	U
1	2	856	A
1	2	860	U
1	2	862	A
1	2	863	A
1	2	864	U
1	2	876	G
1	2	886	U
1	2	898	A
1	2	912	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	916	U
1	2	926	A
1	2	933	A
1	2	935	U
1	2	942	G
1	2	951	A
1	2	960	U
1	2	966	A
1	2	982	U
1	2	988	A
1	2	991	G
1	2	992	A
1	2	993	A
1	2	997	G
1	2	1000	C
1	2	1002	G
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	1029	U
1	2	1031	U
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1066	C
1	2	1073	G
1	2	1080	U
1	2	1082	C
1	2	1083	G
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1101	G
1	2	1138	A
1	2	1139	A
1	2	1143	A
1	2	1146	G
1	2	1149	G
1	2	1150	G
1	2	1151	A
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1176	G
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G

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Mol	Chain	Res	Type
1	2	1200	G
1	2	1202	A
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G
1	2	1226	A
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1256	A
1	2	1257	U
1	2	1258	U
1	2	1259	U
1	2	1276	U
1	2	1286	U
1	2	1288	G
1	2	1301	U
1	2	1307	U
1	2	1314	U
1	2	1315	U
1	2	1320	U
1	2	1321	A
1	2	1337	A
1	2	1339	C
1	2	1340	U
1	2	1344	A
1	2	1345	A
1	2	1354	G
1	2	1355	C
1	2	1361	U
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1370	U
1	2	1371	A
1	2	1372	U

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Mol	Chain	Res	Type
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1412	G
1	2	1413	U
1	2	1414	U
1	2	1427	A
1	2	1428	G
1	2	1432	U
1	2	1433	G
1	2	1435	G
1	2	1446	A
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1461	C
1	2	1462	G
1	2	1469	A
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1475	A
1	2	1482	C
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1499	G
1	2	1506	G
1	2	1514	U
1	2	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1526	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	1539	G
1	2	1540	G
1	2	1550	A
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1574	G
1	2	1584	G
1	2	1590	G
1	2	1591	C
1	2	1601	G
1	2	1604	U
1	2	1614	A
1	2	1616	G
1	2	1619	C
1	2	1624	C
1	2	1631	A
1	2	1634	C
1	2	1639	C
1	2	1657	U
1	2	1658	G
1	2	1680	G
1	2	1683	C
1	2	1684	U
1	2	1731	A
1	2	1756	A
1	2	1757	G
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C

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Mol	Chain	Res	Type
36	1	16	A
36	1	26	A
36	1	40	A
36	1	43	A
36	1	49	A
36	1	57	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	68	C
36	1	76	G
36	1	83	U
36	1	85	A
36	1	92	G
36	1	93	C
36	1	99	A
36	1	109	A
36	1	110	G
36	1	111	C
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	147	U
36	1	156	G
36	1	157	A
36	1	166	C
36	1	172	G
36	1	182	U
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	193	C
36	1	210	U
36	1	218	G
36	1	219	A
36	1	224	C
36	1	235	A
36	1	240	U

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Mol	Chain	Res	Type
36	1	243	G
36	1	245	U
36	1	247	C
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	265	A
36	1	266	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	299	G
36	1	315	C
36	1	323	A
36	1	329	U
36	1	339	C
36	1	347	G
36	1	349	A
36	1	350	C
36	1	351	A
36	1	352	A
36	1	374	A
36	1	376	G
36	1	398	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	417	A
36	1	421	G
36	1	422	A
36	1	438	A
36	1	440	A
36	1	495	G
36	1	520	U
36	1	521	A
36	1	533	A
36	1	535	G

Continued on next page...

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Mol	Chain	Res	Type
36	1	541	U
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G
36	1	551	A
36	1	552	G
36	1	553	U
36	1	555	U
36	1	557	A
36	1	559	A
36	1	569	A
36	1	578	A
36	1	579	G
36	1	592	A
36	1	604	G
36	1	609	G
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A
36	1	625	G
36	1	636	C
36	1	638	C
36	1	643	U
36	1	644	G
36	1	648	C
36	1	649	A
36	1	658	G
36	1	660	A
36	1	667	C
36	1	677	A
36	1	681	U
36	1	682	U
36	1	691	A
36	1	705	A
36	1	708	G
36	1	712	G
36	1	715	A
36	1	716	A
36	1	719	U
36	1	725	G

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Mol	Chain	Res	Type
36	1	726	G
36	1	764	U
36	1	766	U
36	1	767	U
36	1	768	C
36	1	776	U
36	1	777	U
36	1	780	A
36	1	781	G
36	1	785	G
36	1	786	A
36	1	806	A
36	1	817	A
36	1	826	G
36	1	830	A
36	1	849	C
36	1	861	C
36	1	874	U
36	1	879	U
36	1	890	C
36	1	896	A
36	1	897	U
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	920	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	937	G
36	1	944	C
36	1	953	G
36	1	959	C
36	1	960	U
36	1	961	C
36	1	979	U
36	1	981	U
36	1	982	C
36	1	993	G
36	1	994	G

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Mol	Chain	Res	Type
36	1	1000	C
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1014	U
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	1041	U
36	1	1042	U
36	1	1045	C
36	1	1047	A
36	1	1049	C
36	1	1051	U
36	1	1057	A
36	1	1064	A
36	1	1065	A
36	1	1072	G
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1087	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1111	U
36	1	1117	G
36	1	1128	U
36	1	1131	G
36	1	1138	U

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Mol	Chain	Res	Type
36	1	1144	U
36	1	1153	A
36	1	1159	A
36	1	1160	C
36	1	1168	U
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1186	G
36	1	1190	A
36	1	1191	U
36	1	1192	C
36	1	1196	C
36	1	1197	A
36	1	1201	C
36	1	1209	G
36	1	1213	G
36	1	1216	C
36	1	1217	A
36	1	1218	U
36	1	1222	G
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	1238	C
36	1	1241	U
36	1	1242	G
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1251	A
36	1	1253	U
36	1	1258	U
36	1	1259	A
36	1	1262	G

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Mol	Chain	Res	Type
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1267	U
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1272	C
36	1	1274	A
36	1	1277	C
36	1	1278	A
36	1	1279	C
36	1	1280	C
36	1	1285	G
36	1	1286	A
36	1	1287	A
36	1	1292	C
36	1	1298	C
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1323	G
36	1	1330	A
36	1	1331	U
36	1	1348	U
36	1	1349	G
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1379	G
36	1	1386	A
36	1	1392	G
36	1	1399	A
36	1	1400	G
36	1	1406	A
36	1	1418	A
36	1	1419	A

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Mol	Chain	Res	Type
36	1	1422	G
36	1	1429	G
36	1	1434	G
36	1	1437	C
36	1	1446	A
36	1	1448	U
36	1	1450	G
36	1	1455	U
36	1	1465	A
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1488	G
36	1	1490	A
36	1	1508	C
36	1	1525	G
36	1	1526	U
36	1	1527	C
36	1	1528	G
36	1	1533	U
36	1	1534	A
36	1	1554	U
36	1	1555	U
36	1	1556	C
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	1572	U
36	1	1575	A
36	1	1576	G
36	1	1579	C
36	1	1580	A
36	1	1581	C
36	1	1582	C
36	1	1583	A

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Mol	Chain	Res	Type
36	1	1587	A
36	1	1589	A
36	1	1593	A
36	1	1607	U
36	1	1619	A
36	1	1620	U
36	1	1629	U
36	1	1639	C
36	1	1640	G
36	1	1643	A
36	1	1645	U
36	1	1657	C
36	1	1679	A
36	1	1683	A
36	1	1695	U
36	1	1705	U
36	1	1714	A
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1725	C
36	1	1729	A
36	1	1736	G
36	1	1741	A
36	1	1745	C
36	1	1750	A
36	1	1751	G
36	1	1752	A
36	1	1760	A
36	1	1761	C
36	1	1762	C
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1768	U
36	1	1770	G
36	1	1775	G
36	1	1779	C
36	1	1780	G
36	1	1797	A
36	1	1810	A
36	1	1812	G

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Mol	Chain	Res	Type
36	1	1814	A
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1839	A
36	1	1841	A
36	1	1842	A
36	1	1845	G
36	1	1846	C
36	1	1849	C
36	1	1850	A
36	1	1855	U
36	1	1864	A
36	1	1866	C
36	1	1871	U
36	1	1878	G
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1906	G
36	1	1937	U
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	1954	G
36	1	2094	C
36	1	2101	C
36	1	2102	U
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2114	C
36	1	2121	G
36	1	2122	G
36	1	2130	G
36	1	2131	A
36	1	2134	G
36	1	2137	U
36	1	2139	A
36	1	2140	U

Continued on next page...

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Mol	Chain	Res	Type
36	1	2144	A
36	1	2145	A
36	1	2158	A
36	1	2169	G
36	1	2170	U
36	1	2177	G
36	1	2186	U
36	1	2187	G
36	1	2193	U
36	1	2194	G
36	1	2201	G
36	1	2205	U
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2223	A
36	1	2228	A
36	1	2229	A
36	1	2242	A
36	1	2244	A
36	1	2249	G
36	1	2250	G
36	1	2253	G
36	1	2255	A
36	1	2256	A
36	1	2268	U
36	1	2272	G
36	1	2273	G
36	1	2281	A
36	1	2282	U
36	1	2283	G
36	1	2284	C
36	1	2288	G
36	1	2298	U
36	1	2301	U
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2320	A
36	1	2324	A

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Mol	Chain	Res	Type
36	1	2334	U
36	1	2335	G
36	1	2336	U
36	1	2372	A
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2388	U
36	1	2393	G
36	1	2394	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2405	C
36	1	2406	C
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2422	C
36	1	2424	A
36	1	2435	G
36	1	2437	G
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2504	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

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Mol	Chain	Res	Type
36	1	2547	A
36	1	2548	C
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2561	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2576	G
36	1	2585	G
36	1	2586	G
36	1	2593	A
36	1	2594	C
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2618	G
36	1	2628	A
36	1	2637	A
36	1	2638	C
36	1	2652	U
36	1	2655	U
36	1	2656	A
36	1	2664	C
36	1	2672	G
36	1	2674	A
36	1	2677	G
36	1	2681	U
36	1	2689	A
36	1	2691	A
36	1	2693	C
36	1	2694	A
36	1	2696	A
36	1	2705	A
36	1	2709	C
36	1	2714	G
36	1	2728	G

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Mol	Chain	Res	Type
36	1	2729	U
36	1	2737	C
36	1	2752	U
36	1	2753	G
36	1	2762	A
36	1	2772	C
36	1	2773	C
36	1	2777	G
36	1	2778	G
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2810	C
36	1	2817	A
36	1	2818	U
36	1	2829	U
36	1	2838	A
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2847	A
36	1	2849	C
36	1	2853	A
36	1	2860	U
36	1	2869	U
36	1	2871	G
36	1	2872	A
36	1	2875	U
36	1	2886	U
36	1	2887	A
36	1	2889	C
36	1	2893	C
36	1	2898	G
36	1	2899	C
36	1	2914	G
36	1	2923	U
36	1	2935	U
36	1	2936	A
36	1	2942	C
36	1	2945	G

Continued on next page...

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Mol	Chain	Res	Type
36	1	2947	G
36	1	2971	A
36	1	2974	U
36	1	2979	U
36	1	2980	U
36	1	2983	C
36	1	2990	G
36	1	2992	U
36	1	2996	U
36	1	2997	G
36	1	3006	A
36	1	3012	A
36	1	3030	G
36	1	3056	U
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3070	A
36	1	3078	U
36	1	3079	U
36	1	3080	G
36	1	3085	G
36	1	3086	A
36	1	3087	A
36	1	3088	G
36	1	3092	C
36	1	3104	U
36	1	3113	A
36	1	3115	C
36	1	3119	U
36	1	3130	A
36	1	3131	U
36	1	3139	A
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3158	G
36	1	3164	C

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Mol	Chain	Res	Type
36	1	3165	A
36	1	3168	A
36	1	3169	U
36	1	3170	A
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3186	A
36	1	3187	A
36	1	3195	U
36	1	3196	U
36	1	3207	U
36	1	3210	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3228	C
36	1	3229	G
36	1	3235	C
36	1	3238	G
36	1	3243	A
36	1	3244	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3265	C
36	1	3269	U
36	1	3270	U
36	1	3273	A
36	1	3274	A
36	1	3276	G
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3288	G
36	1	3289	G
36	1	3294	A
36	1	3295	A

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Mol	Chain	Res	Type
36	1	3304	U
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3335	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3350	C
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3357	U
36	1	3363	U
36	1	3369	G
36	1	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3386	G
36	1	3389	U
36	1	3390	G
37	3	4	U
37	3	7	G
37	3	8	G
37	3	9	C
37	3	13	A
37	3	14	U
37	3	18	C
37	3	21	G
37	3	22	A
37	3	26	C
37	3	29	C
37	3	42	A

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Mol	Chain	Res	Type
37	3	47	C
37	3	54	U
37	3	59	U
37	3	60	G
37	3	65	G
37	3	76	A
37	3	91	G
37	3	101	G
37	3	102	A
37	3	110	G
37	3	112	G
37	3	114	U
37	3	121	U
38	4	2	A
38	4	20	U
38	4	26	U
38	4	34	U
38	4	35	C
38	4	48	A
38	4	52	A
38	4	53	A
38	4	59	A
38	4	60	U
38	4	62	C
38	4	63	G
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	96	A
38	4	97	A
38	4	102	U
38	4	104	A
38	4	105	A
38	4	106	C

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Mol	Chain	Res	Type
38	4	111	A
38	4	113	U
38	4	116	G
38	4	125	U
38	4	126	A
38	4	127	U
38	4	128	U
38	4	138	A
38	4	152	G
38	4	158	U
1	6	2	A
1	6	4	C
1	6	17	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	47	A
1	6	57	G
1	6	60	U
1	6	61	A
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	95	G
1	6	103	A
1	6	104	A
1	6	114	C
1	6	115	G
1	6	126	A
1	6	127	G
1	6	130	C
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A

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Mol	Chain	Res	Type
1	6	141	U
1	6	144	U
1	6	145	A
1	6	146	U
1	6	158	U
1	6	159	U
1	6	161	U
1	6	167	U
1	6	178	U
1	6	185	U
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	194	U
1	6	195	G
1	6	197	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	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	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

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Mol	Chain	Res	Type
1	6	271	A
1	6	272	U
1	6	273	G
1	6	277	U
1	6	278	U
1	6	280	U
1	6	287	G
1	6	301	A
1	6	308	C
1	6	313	U
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	333	A
1	6	337	G
1	6	338	C
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	381	C
1	6	396	G
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	417	A
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	437	A
1	6	439	U
1	6	444	C
1	6	448	C
1	6	454	U
1	6	470	A

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Mol	Chain	Res	Type
1	6	475	A
1	6	484	C
1	6	486	G
1	6	487	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	495	C
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	507	U
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	514	G
1	6	515	A
1	6	519	C
1	6	527	A
1	6	536	C
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C

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Mol	Chain	Res	Type
1	6	565	C
1	6	566	C
1	6	570	A
1	6	574	G
1	6	578	U
1	6	579	A
1	6	580	A
1	6	582	U
1	6	594	A
1	6	595	G
1	6	597	G
1	6	606	A
1	6	609	U
1	6	611	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	637	C
1	6	639	U
1	6	640	U
1	6	645	C
1	6	648	G
1	6	650	U
1	6	651	G
1	6	652	G
1	6	653	C
1	6	654	C
1	6	658	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	669	G
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	681	U
1	6	682	C

Continued on next page...

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Mol	Chain	Res	Type
1	6	683	C
1	6	684	A
1	6	685	A
1	6	687	G
1	6	691	C
1	6	695	U
1	6	696	C
1	6	697	C
1	6	698	U
1	6	709	C
1	6	710	U
1	6	711	U
1	6	714	G
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	723	G
1	6	730	G
1	6	742	U
1	6	751	G
1	6	753	A
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	789	A
1	6	792	U
1	6	793	A
1	6	794	U
1	6	803	A
1	6	806	A
1	6	811	A
1	6	812	A
1	6	815	G

Continued on next page...

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Mol	Chain	Res	Type
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	828	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	847	A
1	6	856	A
1	6	863	A
1	6	864	U
1	6	873	U
1	6	898	A
1	6	906	A
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	959	U
1	6	960	U
1	6	966	A
1	6	970	A
1	6	971	A
1	6	985	G
1	6	989	U
1	6	991	G
1	6	992	A
1	6	993	A
1	6	997	G
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1021	C
1	6	1026	A

Continued on next page...

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Mol	Chain	Res	Type
1	6	1028	C
1	6	1039	A
1	6	1040	G
1	6	1043	A
1	6	1045	C
1	6	1046	G
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1061	A
1	6	1063	U
1	6	1066	C
1	6	1067	C
1	6	1070	C
1	6	1073	G
1	6	1075	C
1	6	1082	C
1	6	1087	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	1104	U
1	6	1109	G
1	6	1111	G
1	6	1137	A
1	6	1138	A
1	6	1146	G
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1167	G
1	6	1185	U
1	6	1194	A
1	6	1196	A

Continued on next page...

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Mol	Chain	Res	Type
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1217	A
1	6	1218	G
1	6	1220	C
1	6	1221	A
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1239	U
1	6	1241	G
1	6	1242	A
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1262	U
1	6	1285	U
1	6	1286	U
1	6	1288	G
1	6	1291	G
1	6	1297	G
1	6	1305	U
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1331	A
1	6	1338	C
1	6	1341	A
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1348	A
1	6	1354	G

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Mol	Chain	Res	Type
1	6	1361	U
1	6	1363	U
1	6	1364	G
1	6	1371	A
1	6	1372	U
1	6	1383	G
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1413	U
1	6	1415	U
1	6	1425	A
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	1460	A
1	6	1461	C
1	6	1471	A
1	6	1481	C
1	6	1482	C
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1494	C
1	6	1496	U
1	6	1506	G
1	6	1510	U
1	6	1514	U
1	6	1516	A
1	6	1517	U
1	6	1523	G

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Mol	Chain	Res	Type
1	6	1524	A
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1539	G
1	6	1540	G
1	6	1542	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1568	C
1	6	1569	A
1	6	1573	A
1	6	1574	G
1	6	1575	G
1	6	1577	A
1	6	1584	G
1	6	1590	G
1	6	1601	G
1	6	1616	G
1	6	1618	C
1	6	1621	U
1	6	1634	C
1	6	1635	A
1	6	1637	C
1	6	1639	C
1	6	1656	U
1	6	1657	U
1	6	1658	G
1	6	1696	G
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1710	U
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G

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Mol	Chain	Res	Type
1	6	1725	U
1	6	1731	A
1	6	1736	G
1	6	1755	A
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	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	15	C
36	5	26	A
36	5	38	U
36	5	40	A
36	5	43	A
36	5	49	A
36	5	58	G
36	5	60	A
36	5	62	A
36	5	65	A
36	5	66	A
36	5	73	C
36	5	76	G
36	5	92	G
36	5	93	C
36	5	96	G
36	5	97	U
36	5	99	A
36	5	105	C
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	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	148	G
36	5	150	A
36	5	156	G
36	5	157	A
36	5	165	A
36	5	166	C
36	5	170	G
36	5	171	G
36	5	173	G
36	5	174	C
36	5	178	U
36	5	180	C
36	5	181	U
36	5	182	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	200	C
36	5	210	U
36	5	211	A
36	5	213	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	231	G
36	5	234	G
36	5	236	G
36	5	237	G
36	5	238	A
36	5	239	G
36	5	240	U
36	5	244	G
36	5	247	C

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Mol	Chain	Res	Type
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	257	U
36	5	258	G
36	5	269	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	298	U
36	5	322	U
36	5	323	A
36	5	329	U
36	5	339	C
36	5	349	A
36	5	350	C
36	5	370	U
36	5	376	G
36	5	397	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	421	G
36	5	422	A
36	5	426	G
36	5	436	A
36	5	437	G
36	5	439	C
36	5	441	U
36	5	442	G
36	5	443	G
36	5	492	U
36	5	495	G
36	5	519	A
36	5	521	A
36	5	535	G

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Mol	Chain	Res	Type
36	5	542	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	551	A
36	5	552	G
36	5	553	U
36	5	555	U
36	5	557	A
36	5	559	A
36	5	570	A
36	5	578	A
36	5	579	G
36	5	588	G
36	5	589	A
36	5	592	A
36	5	600	G
36	5	604	G
36	5	608	A
36	5	609	G
36	5	611	A
36	5	619	A
36	5	620	U
36	5	621	A
36	5	636	C
36	5	649	A
36	5	651	G
36	5	656	A
36	5	660	A
36	5	675	C
36	5	677	A
36	5	681	U
36	5	683	U
36	5	705	A
36	5	712	G
36	5	715	A
36	5	716	A
36	5	719	U
36	5	725	G
36	5	726	G
36	5	766	U
36	5	767	U

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Mol	Chain	Res	Type
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	807	A
36	5	817	A
36	5	830	A
36	5	851	C
36	5	861	C
36	5	874	U
36	5	875	G
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	937	G
36	5	944	C
36	5	959	C
36	5	960	U
36	5	963	G
36	5	964	G
36	5	979	U
36	5	981	U
36	5	994	G
36	5	1000	C
36	5	1001	G
36	5	1002	A
36	5	1003	A
36	5	1006	A
36	5	1010	G
36	5	1014	U
36	5	1015	U

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Mol	Chain	Res	Type
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1019	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1027	A
36	5	1028	U
36	5	1029	G
36	5	1035	G
36	5	1041	U
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1071	U
36	5	1072	G
36	5	1079	A
36	5	1081	U
36	5	1082	U
36	5	1085	A
36	5	1087	G
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1117	G
36	5	1131	G
36	5	1152	G
36	5	1153	A
36	5	1159	A
36	5	1161	G
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1190	A

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Mol	Chain	Res	Type
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1196	C
36	5	1201	C
36	5	1202	A
36	5	1206	G
36	5	1209	G
36	5	1222	G
36	5	1232	C
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1243	G
36	5	1245	A
36	5	1246	G
36	5	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	1301	A
36	5	1303	A
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1313	G
36	5	1330	A
36	5	1348	U
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1354	G
36	5	1355	A
36	5	1356	U
36	5	1357	G

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Mol	Chain	Res	Type
36	5	1363	A
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1421	G
36	5	1428	A
36	5	1431	G
36	5	1433	A
36	5	1434	G
36	5	1437	C
36	5	1443	G
36	5	1445	U
36	5	1446	A
36	5	1450	G
36	5	1465	A
36	5	1467	A
36	5	1481	A
36	5	1482	A
36	5	1488	G
36	5	1490	A
36	5	1495	U
36	5	1500	G
36	5	1503	A
36	5	1508	C
36	5	1514	G
36	5	1519	G
36	5	1522	U
36	5	1526	U
36	5	1533	U
36	5	1536	G
36	5	1541	G
36	5	1542	G
36	5	1549	U
36	5	1553	U
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1557	A

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Mol	Chain	Res	Type
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1563	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	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1580	A
36	5	1581	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1593	A
36	5	1620	U
36	5	1629	U
36	5	1635	G
36	5	1639	C
36	5	1641	U
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1657	C
36	5	1658	G
36	5	1683	A
36	5	1713	G
36	5	1716	U
36	5	1717	U
36	5	1721	U
36	5	1725	C
36	5	1736	G
36	5	1741	A
36	5	1750	A

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Mol	Chain	Res	Type
36	5	1751	G
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1770	G
36	5	1780	G
36	5	1795	U
36	5	1796	G
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	1839	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1849	C
36	5	1850	A
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1893	A
36	5	1906	G
36	5	1908	A
36	5	1918	C
36	5	1935	G
36	5	1947	G
36	5	1952	G
36	5	1953	G
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2112	U
36	5	2113	A

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Mol	Chain	Res	Type
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2144	A
36	5	2158	A
36	5	2169	G
36	5	2177	G
36	5	2187	G
36	5	2188	A
36	5	2192	C
36	5	2198	A
36	5	2201	G
36	5	2205	U
36	5	2206	G
36	5	2210	G
36	5	2225	U
36	5	2228	A
36	5	2229	A
36	5	2234	G
36	5	2244	A
36	5	2246	G
36	5	2250	G
36	5	2251	G
36	5	2252	A
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2258	U
36	5	2270	A
36	5	2273	G
36	5	2278	C
36	5	2279	A
36	5	2280	A
36	5	2282	U
36	5	2288	G
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2316	G
36	5	2318	U

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Mol	Chain	Res	Type
36	5	2321	A
36	5	2324	A
36	5	2335	G
36	5	2336	U
36	5	2354	C
36	5	2360	C
36	5	2367	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2393	G
36	5	2394	G
36	5	2397	A
36	5	2398	A
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2410	U
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2435	G
36	5	2437	G
36	5	2438	A
36	5	2439	A
36	5	2440	G
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	2509	U
36	5	2510	U
36	5	2511	A
36	5	2512	C
36	5	2514	U
36	5	2515	A

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Mol	Chain	Res	Type
36	5	2518	C
36	5	2523	A
36	5	2526	C
36	5	2530	G
36	5	2532	U
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	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2589	G
36	5	2593	A
36	5	2594	C
36	5	2598	G
36	5	2606	G
36	5	2607	G
36	5	2613	U
36	5	2614	G
36	5	2639	G
36	5	2652	U
36	5	2656	A
36	5	2674	A
36	5	2677	G
36	5	2678	A
36	5	2681	U
36	5	2683	U
36	5	2689	A

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Mol	Chain	Res	Type
36	5	2690	G
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2705	A
36	5	2707	C
36	5	2714	G
36	5	2716	U
36	5	2728	G
36	5	2729	U
36	5	2752	U
36	5	2753	G
36	5	2755	C
36	5	2762	A
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2796	G
36	5	2797	C
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2802	A
36	5	2810	C
36	5	2814	G
36	5	2817	A
36	5	2818	U
36	5	2822	U
36	5	2824	G
36	5	2829	U
36	5	2839	G
36	5	2840	C
36	5	2843	U
36	5	2845	A
36	5	2852	C
36	5	2853	A
36	5	2871	G
36	5	2872	A
36	5	2873	U
36	5	2875	U

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Mol	Chain	Res	Type
36	5	2876	C
36	5	2887	A
36	5	2889	C
36	5	2896	A
36	5	2899	C
36	5	2902	A
36	5	2909	U
36	5	2914	G
36	5	2923	U
36	5	2924	U
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2947	G
36	5	2954	U
36	5	2957	G
36	5	2971	A
36	5	2972	G
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3028	G
36	5	3049	A
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3087	A
36	5	3092	C
36	5	3102	G
36	5	3104	U
36	5	3119	U
36	5	3122	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C

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Mol	Chain	Res	Type
36	5	3153	U
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3159	C
36	5	3164	C
36	5	3165	A
36	5	3167	A
36	5	3168	A
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3175	U
36	5	3176	G
36	5	3178	A
36	5	3179	U
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3198	U
36	5	3199	G
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3224	G
36	5	3228	C
36	5	3229	G
36	5	3239	G
36	5	3242	G
36	5	3243	A
36	5	3244	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3263	G
36	5	3270	U
36	5	3275	U

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Mol	Chain	Res	Type
36	5	3276	G
36	5	3277	U
36	5	3279	A
36	5	3280	U
36	5	3281	U
36	5	3282	U
36	5	3285	C
36	5	3286	G
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3307	A
36	5	3313	U
36	5	3315	G
36	5	3316	A
36	5	3317	U
36	5	3318	G
36	5	3319	U
36	5	3320	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3358	U
36	5	3369	G
36	5	3377	G
36	5	3378	C
36	5	3382	U
36	5	3383	G
36	5	3389	U
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	27	A
37	7	33	U
37	7	38	U
37	7	52	G
37	7	53	U

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Mol	Chain	Res	Type
37	7	54	U
37	7	55	A
37	7	60	G
37	7	63	A
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	78	U
37	7	91	G
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	16	G
38	8	21	C
38	8	34	U
38	8	35	C
38	8	48	A
38	8	50	C
38	8	51	G
38	8	52	A
38	8	59	A
38	8	60	U
38	8	62	C
38	8	63	G
38	8	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
38	8	105	A
38	8	106	C

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Mol	Chain	Res	Type
38	8	110	C
38	8	111	A
38	8	113	U
38	8	116	G
38	8	122	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	136	G
38	8	138	A
38	8	152	G
38	8	156	U
38	8	157	U
38	8	158	U

All (316) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	73	U
1	2	74	U
1	2	103	A
1	2	114	C
1	2	126	A
1	2	130	C
1	2	131	C
1	2	132	U
1	2	136	C
1	2	139	C
1	2	144	U
1	2	158	U
1	2	187	G
1	2	217	A
1	2	218	A
1	2	232	U
1	2	239	C
1	2	240	U
1	2	278	U
1	2	280	U
1	2	400	A

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Mol	Chain	Res	Type
1	2	417	A
1	2	468	A
1	2	484	C
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	555	A
1	2	558	U
1	2	582	U
1	2	609	U
1	2	685	A
1	2	697	C
1	2	704	C
1	2	720	G
1	2	721	U
1	2	734	A
1	2	755	A
1	2	781	U
1	2	782	U
1	2	794	U
1	2	811	A
1	2	815	G
1	2	829	A
1	2	913	G
1	2	1051	G
1	2	1058	U
1	2	1081	A
1	2	1091	A
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	1339	C
1	2	1344	A
1	2	1370	U
1	2	1474	G
1	2	1481	C
1	2	1490	C

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Mol	Chain	Res	Type
1	2	1568	C
1	2	1573	A
1	2	1600	A
1	2	1615	C
1	2	1657	U
1	2	1761	U
36	1	40	A
36	1	43	A
36	1	65	A
36	1	217	U
36	1	223	U
36	1	239	G
36	1	282	G
36	1	349	A
36	1	350	C
36	1	547	G
36	1	588	G
36	1	594	U
36	1	637	C
36	1	715	A
36	1	719	U
36	1	763	G
36	1	816	A
36	1	873	C
36	1	896	A
36	1	908	G
36	1	916	G
36	1	981	U
36	1	993	G
36	1	1000	C
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	1484	U

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Mol	Chain	Res	Type
36	1	1507	G
36	1	1554	U
36	1	1559	A
36	1	1562	C
36	1	1580	A
36	1	1716	U
36	1	1724	U
36	1	1751	G
36	1	1815	U
36	1	1816	A
36	1	1820	U
36	1	1841	A
36	1	1842	A
36	1	1846	C
36	1	1849	C
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2227	C
36	1	2249	G
36	1	2281	A
36	1	2372	A
36	1	2374	C
36	1	2403	G
36	1	2418	G
36	1	2522	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	2689	A
36	1	2728	G
36	1	2772	C
36	1	2801	A
36	1	2817	A
36	1	2818	U
36	1	3056	U
36	1	3078	U
36	1	3139	A

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Mol	Chain	Res	Type
36	1	3157	U
36	1	3195	U
36	1	3218	A
36	1	3228	C
36	1	3242	G
36	1	3269	U
36	1	3275	U
36	1	3316	A
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
37	3	13	A
37	3	49	G
38	4	82	U
38	4	85	G
38	4	111	A
38	4	125	U
38	4	126	A
1	6	25	C
1	6	66	U
1	6	76	A
1	6	103	A
1	6	114	C
1	6	136	C
1	6	139	C
1	6	145	A
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	272	U
1	6	277	U
1	6	313	U
1	6	400	A
1	6	417	A
1	6	454	U
1	6	468	A
1	6	512	A
1	6	541	A

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Mol	Chain	Res	Type
1	6	542	A
1	6	543	C
1	6	555	A
1	6	557	G
1	6	558	U
1	6	651	G
1	6	667	U
1	6	678	A
1	6	697	C
1	6	717	C
1	6	755	A
1	6	829	A
1	6	834	G
1	6	1051	G
1	6	1058	U
1	6	1081	A
1	6	1097	U
1	6	1137	A
1	6	1227	A
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1431	C
1	6	1481	C
1	6	1489	U
1	6	1491	U
1	6	1535	U
1	6	1568	C
1	6	1573	A
1	6	1584	G
1	6	1600	A
1	6	1615	C
1	6	1620	C
1	6	1657	U
1	6	1696	G
1	6	1698	G
1	6	1700	C
36	5	43	A
36	5	122	A
36	5	210	U
36	5	238	A
36	5	397	A

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Mol	Chain	Res	Type
36	5	546	C
36	5	557	A
36	5	588	G
36	5	594	U
36	5	647	A
36	5	715	A
36	5	726	G
36	5	765	C
36	5	786	A
36	5	816	A
36	5	896	A
36	5	916	G
36	5	993	G
36	5	1013	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1160	C
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	1434	G
36	5	1481	A
36	5	1507	G
36	5	1514	G
36	5	1554	U
36	5	1560	G
36	5	1580	A
36	5	1589	A
36	5	1716	U
36	5	1724	U
36	5	1815	U
36	5	1816	A

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Mol	Chain	Res	Type
36	5	1819	U
36	5	1846	C
36	5	2101	C
36	5	2112	U
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2257	C
36	5	2281	A
36	5	2372	A
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2522	G
36	5	2539	C
36	5	2572	C
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2817	A
36	5	2818	U
36	5	2872	A
36	5	2887	A
36	5	2896	A
36	5	2971	A
36	5	3078	U
36	5	3154	C
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3259	U
36	5	3275	U
36	5	3289	G
36	5	3340	G
36	5	3341	U
36	5	3357	U
37	7	49	G
38	8	111	A
38	8	126	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2555 ligands modelled in this entry, 1422 are monoatomic - leaving 1133 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	4009	-	0,6,6	0.00	-	-		
86	OHX	1	4000	-	0,6,6	0.00	-	-		
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	5	4010	-	0,6,6	0.00	-	-		
86	OHX	1	4120	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	5	4122	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		
86	OHX	m6	202	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	5	4092	-	0,6,6	0.00	-	-		
86	OHX	15	303	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4076	-	0,6,6	0.00	-	-		
86	OHX	15	305	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		
86	OHX	1	4063	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	1	3934	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	8	229	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	0,6,6	0.00	-	-		
86	OHX	5	4003	-	0,6,6	0.00	-	-		
86	OHX	M7	206	-	0,6,6	0.00	-	-		
86	OHX	5	4142	-	0,6,6	0.00	-	-		
86	OHX	5	4250	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	1	3928	-	0,6,6	0.00	-	-		
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	o3	202	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	N1	201	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	5	4178	-	0,6,6	0.00	-	-		
86	OHX	1	4014	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	1	4072	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	5	3972	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	5	4016	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	1	4035	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	L3	404	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	5	4208	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	6	2139	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	6	2196	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	n3	204	-	0,6,6	0.00	-	-		
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	1	4045	-	0,6,6	0.00	-	-		
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	0,6,6	0.00	-	-		
86	OHX	1	4020	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	3	217	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	2	2022	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4036	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	1	4019	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	M8	201	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	2	2096	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	6	2142	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	5	4248	-	0,6,6	0.00	-	-		
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	1	3929	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	0,6,6	0.00	-	-		
86	OHX	s1	302	-	0,6,6	0.00	-	-		
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	5	4028	-	0,6,6	0.00	-	-		
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	1	4168	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		
86	OHX	5	4131	-	0,6,6	0.00	-	-		
86	OHX	1	3869	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	1	4191	-	0,6,6	0.00	-	-		
86	OHX	2	2121	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	5	3909	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		
86	OHX	5	3904	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	14	402	-	0,6,6	0.00	-	-		
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	4	239	-	0,6,6	0.00	-	-		
86	OHX	m7	206	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	1	4175	-	0,6,6	0.00	-	-		
86	OHX	5	3942	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	O3	201	-	0,6,6	0.00	-	-		
86	OHX	6	2145	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	2	2106	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4239	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	0,6,6	0.00	-	-		
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	1	4082	-	0,6,6	0.00	-	-		
86	OHX	5	3962	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	5	4143	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		
86	OHX	1	4073	-	0,6,6	0.00	-	-		
86	OHX	n9	103	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	5	4096	-	0,6,6	0.00	-	-		
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	2	2179	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	1	3917	-	0,6,6	0.00	-	-		
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		
86	OHX	1	4091	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4158	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	5	4225	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		
86	OHX	2	2126	-	0,6,6	0.00	-	-		
86	OHX	1	3986	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	5	3915	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	6	2183	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	4	236	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	5	4160	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4217	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	3	215	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	6	2073	-	0,6,6	0.00	-	-		
86	OHX	5	3996	-	0,6,6	0.00	-	-		
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	0,6,6	0.00	-	-		
86	OHX	1	4081	-	0,6,6	0.00	-	-		
86	OHX	1	4053	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	2	2062	-	0,6,6	0.00	-	-		
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	6	2135	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	2	2028	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4057	-	0,6,6	0.00	-	-		
86	OHX	1	3898	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	5	4023	-	0,6,6	0.00	-	-		
86	OHX	5	4252	-	0,6,6	0.00	-	-		
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	5	4024	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	5	4132	-	0,6,6	0.00	-	-		
86	OHX	1	4207	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		
86	OHX	6	2048	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	1	4114	-	0,6,6	0.00	-	-		
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	0,6,6	0.00	-	-		
86	OHX	5	3999	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		
86	OHX	2	2122	-	0,6,6	0.00	-	-		
86	OHX	5	4126	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	1	4165	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	5	4211	-	0,6,6	0.00	-	-		
86	OHX	5	4236	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	5	4167	-	0,6,6	0.00	-	-		
86	OHX	1	4210	-	0,6,6	0.00	-	-		
86	OHX	s4	301	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	1	4215	-	0,6,6	0.00	-	-		
86	OHX	s1	303	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	0,6,6	0.00	-	-		
86	OHX	1	4098	-	0,6,6	0.00	-	-		
87	EDE	6	2202	-	51,55,55	0.72	1 (1%)	57,70,70	1.52	7 (12%)
86	OHX	2	2080	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	0,6,6	0.00	-	-		
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	6	2181	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	C3	201	-	0,6,6	0.00	-	-		
86	OHX	6	2095	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	0,6,6	0.00	-	-		
86	OHX	1	4127	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	2	2178	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	0,6,6	0.00	-	-		
86	OHX	4	237	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	s8	303	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	1	4115	-	0,6,6	0.00	-	-		
86	OHX	5	4222	-	0,6,6	0.00	-	-		
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	6	2105	-	0,6,6	0.00	-	-		
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	l3	403	-	0,6,6	0.00	-	-		
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4125	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	5	4254	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	1	4200	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	6	2198	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	5	4235	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	1	3871	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	2	2149	-	0,6,6	0.00	-	-		
86	OHX	1	3873	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	1	4214	-	0,6,6	0.00	-	-		
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	1	3997	-	0,6,6	0.00	-	-		
86	OHX	6	2184	-	0,6,6	0.00	-	-		
86	OHX	2	2176	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	2	2111	-	0,6,6	0.00	-	-		
86	OHX	2	2024	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	6	2174	-	0,6,6	0.00	-	-		
86	OHX	1	4206	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	5	4149	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	c3	201	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	0,6,6	0.00	-	-		
86	OHX	M7	205	-	0,6,6	0.00	-	-		
86	OHX	5	4234	-	0,6,6	0.00	-	-		
86	OHX	C8	201	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	L3	403	-	0,6,6	0.00	-	-		
86	OHX	1	4023	-	0,6,6	0.00	-	-		
86	OHX	5	4154	-	0,6,6	0.00	-	-		
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	0,6,6	0.00	-	-		
86	OHX	1	3886	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	1	4100	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	5	4247	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4198	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	7	217	-	0,6,6	0.00	-	-		
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	1	4109	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	8	215	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	6	2151	-	0,6,6	0.00	-	-		
86	OHX	3	225	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	0,6,6	0.00	-	-		
86	OHX	5	4161	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	1	3942	-	0,6,6	0.00	-	-		
86	OHX	4	223	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	5	4045	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	2	2138	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	1	3874	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	1	4086	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	M0	303	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	5	3917	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	5	4097	-	0,6,6	0.00	-	-		
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	0,6,6	0.00	-	-		
86	OHX	5	4047	-	0,6,6	0.00	-	-		
86	OHX	2	2087	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		
86	OHX	Q2	503	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	1	3868	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	7	220	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	6	2068	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	6	2123	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	1	3867	-	0,6,6	0.00	-	-		
86	OHX	6	2177	-	0,6,6	0.00	-	-		
86	OHX	2	2170	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	0,6,6	0.00	-	-		
86	OHX	7	222	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	5	3945	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	1	4208	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	5	4055	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	5	4100	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	6	2054	-	0,6,6	0.00	-	-		
86	OHX	2	2144	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		
86	OHX	1	4213	-	0,6,6	0.00	-	-		
86	OHX	5	4226	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	15	304	-	0,6,6	0.00	-	-		
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	m0	301	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	1	4180	-	0,6,6	0.00	-	-		
86	OHX	1	3872	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	1	3884	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	5	4249	-	0,6,6	0.00	-	-		
86	OHX	5	3998	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	1	4087	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	1	3870	-	0,6,6	0.00	-	-		
86	OHX	m4	201	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	6	2074	-	0,6,6	0.00	-	-		
86	OHX	1	4008	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	1	4209	-	0,6,6	0.00	-	-		
86	OHX	o7	502	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	1	4212	-	0,6,6	0.00	-	-		
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		
86	OHX	1	4151	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	5	4168	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	0,6,6	0.00	-	-		
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3885	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	5	3995	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	c8	202	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	0,6,6	0.00	-	-		
86	OHX	8	217	-	0,6,6	0.00	-	-		
86	OHX	1	4153	-	0,6,6	0.00	-	-		
86	OHX	1	3967	-	0,6,6	0.00	-	-		
86	OHX	2	2134	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	0,6,6	0.00	-	-		
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	5	3988	-	0,6,6	0.00	-	-		
86	OHX	O7	103	-	0,6,6	0.00	-	-		
86	OHX	2	2054	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	0,6,6	0.00	-	-		
86	OHX	2	2175	-	0,6,6	0.00	-	-		
86	OHX	4	228	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	5	4026	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	6	2191	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	6	2085	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	0,6,6	0.00	-	-		
86	OHX	2	2073	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	o2	201	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	2	2035	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	5	3966	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	m5	303	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	5	4073	-	0,6,6	0.00	-	-		
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	1	4012	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	1	4156	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		
86	OHX	6	2187	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	5	4232	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	n3	203	-	0,6,6	0.00	-	-		
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	M5	302	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	4	234	-	0,6,6	0.00	-	-		
86	OHX	1	4085	-	0,6,6	0.00	-	-		
86	OHX	n1	201	-	0,6,6	0.00	-	-		
86	OHX	8	219	-	0,6,6	0.00	-	-		
86	OHX	1	4145	-	0,6,6	0.00	-	-		
86	OHX	2	2056	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	5	4241	-	0,6,6	0.00	-	-		
86	OHX	N9	101	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	1	3889	-	0,6,6	0.00	-	-		
86	OHX	l3	404	-	0,6,6	0.00	-	-		
86	OHX	2	2172	-	0,6,6	0.00	-	-		
86	OHX	5	3939	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	2	2032	-	0,6,6	0.00	-	-		
86	OHX	5	4089	-	0,6,6	0.00	-	-		
86	OHX	2	2102	-	0,6,6	0.00	-	-		
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		
86	OHX	7	216	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	6	2116	-	0,6,6	0.00	-	-		
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	s9	201	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	6	2045	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	2	2163	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	1	4170	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	0,6,6	0.00	-	-		
86	OHX	1	4138	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	4	238	-	0,6,6	0.00	-	-		
86	OHX	6	2047	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	0,6,6	0.00	-	-		
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	6	2069	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	1	4150	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	8	214	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4246	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	5	3913	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	5	3982	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	5	4195	-	0,6,6	0.00	-	-		
86	OHX	2	2147	-	0,6,6	0.00	-	-		
86	OHX	5	3955	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	1	3939	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	1	3891	-	0,6,6	0.00	-	-		
86	OHX	m1	202	-	0,6,6	0.00	-	-		
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	1	4013	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	2	2046	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	1	3998	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		
86	OHX	1	4052	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	4	225	-	0,6,6	0.00	-	-		
86	OHX	1	3957	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
86	OHX	6	2046	-	0,6,6	0.00	-	-		
86	OHX	1	4211	-	0,6,6	0.00	-	-		
86	OHX	1	4186	-	0,6,6	0.00	-	-		
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	2	2039	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	0,6,6	0.00	-	-		
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	5	4151	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	5	3941	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3911	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	1	3900	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	5	4227	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	2	2023	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	5	4038	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	1	4030	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	8	216	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	1	4007	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	6	2163	-	0,6,6	0.00	-	-		
86	OHX	1	4037	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		
86	OHX	2	2041	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		
86	OHX	1	4061	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	1	3947	-	0,6,6	0.00	-	-		
86	OHX	1	3920	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	6	2195	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	5	4214	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	1	4216	-	0,6,6	0.00	-	-		
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2050	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	1	4025	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		
86	OHX	l3	405	-	0,6,6	0.00	-	-		
86	OHX	6	2075	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	1	4065	-	0,6,6	0.00	-	-		
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	2	2123	-	0,6,6	0.00	-	-		
86	OHX	7	219	-	0,6,6	0.00	-	-		
86	OHX	1	4004	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	M9	201	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	5	3952	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	5	3924	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	d4	202	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	1	4084	-	0,6,6	0.00	-	-		
86	OHX	5	4153	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	L3	405	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	5	4014	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	5	4253	-	0,6,6	0.00	-	-		
86	OHX	4	224	-	0,6,6	0.00	-	-		
86	OHX	2	2047	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	5	3944	-	0,6,6	0.00	-	-		
86	OHX	6	2082	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	L4	403	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	6	2137	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	8	218	-	0,6,6	0.00	-	-		
86	OHX	19	202	-	0,6,6	0.00	-	-		
86	OHX	o7	503	-	0,6,6	0.00	-	-		
86	OHX	5	4107	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	5	4018	-	0,6,6	0.00	-	-		
86	OHX	2	2094	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	6	2093	-	0,6,6	0.00	-	-		
86	OHX	6	2089	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
87	EDE	2	2180	-	51,55,55	1.10	4 (7%)	57,70,70	1.25	6 (10%)
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	5	4124	-	0,6,6	0.00	-	-		
86	OHX	1	4116	-	0,6,6	0.00	-	-		
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	5	4251	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	1	4083	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	1	3978	-	0,6,6	0.00	-	-		
86	OHX	3	222	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	5	4228	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	1	4183	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	5	4175	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		

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	EDE	2	2180	-	-	18/62/66/66	0/1/1/1
87	EDE	6	2202	-	-	20/62/66/66	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	2	2180	EDE	C3-C4	4.50	1.58	1.52
87	2	2180	EDE	C29-N55	-3.38	1.27	1.33
87	6	2202	EDE	C29-N55	-3.20	1.27	1.33
87	2	2180	EDE	C29-N54	2.22	1.33	1.27
87	2	2180	EDE	C34-C32	-2.06	1.49	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	6	2202	EDE	O42-C3-C4	-5.45	98.09	111.01
87	6	2202	EDE	C32-C31-C30	-5.10	98.00	112.73
87	6	2202	EDE	C2-N1-C30	-4.86	112.11	122.69
87	6	2202	EDE	C2-C3-C4	3.97	116.73	111.05
87	2	2180	EDE	C11-C10-C9	-3.65	102.64	113.90
87	2	2180	EDE	C9-N8-C7	-3.38	118.12	123.19
87	2	2180	EDE	C39-C34-C32	3.16	125.08	120.46
87	2	2180	EDE	O42-C3-C4	-2.95	104.02	111.01
87	6	2202	EDE	C35-C36-C37	-2.29	117.36	119.88
87	2	2180	EDE	C15-C14-C13	-2.22	109.45	112.94
87	6	2202	EDE	O43-C4-C3	-2.14	116.89	120.61
87	2	2180	EDE	C32-C31-C30	2.05	118.67	112.73
87	6	2202	EDE	O43-C4-N5	2.04	126.70	122.93

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	6	2202	EDE	N1-C2-C3-O42
87	6	2202	EDE	O42-C3-C4-N5
87	6	2202	EDE	N46-C45-C6-N5
87	6	2202	EDE	N46-C45-C6-C7
87	6	2202	EDE	C12-C13-C14-C15
87	6	2202	EDE	C12-C13-C14-O51
87	6	2202	EDE	N50-C13-C14-C15
87	6	2202	EDE	N50-C13-C14-O51
87	6	2202	EDE	C13-C14-C15-C16

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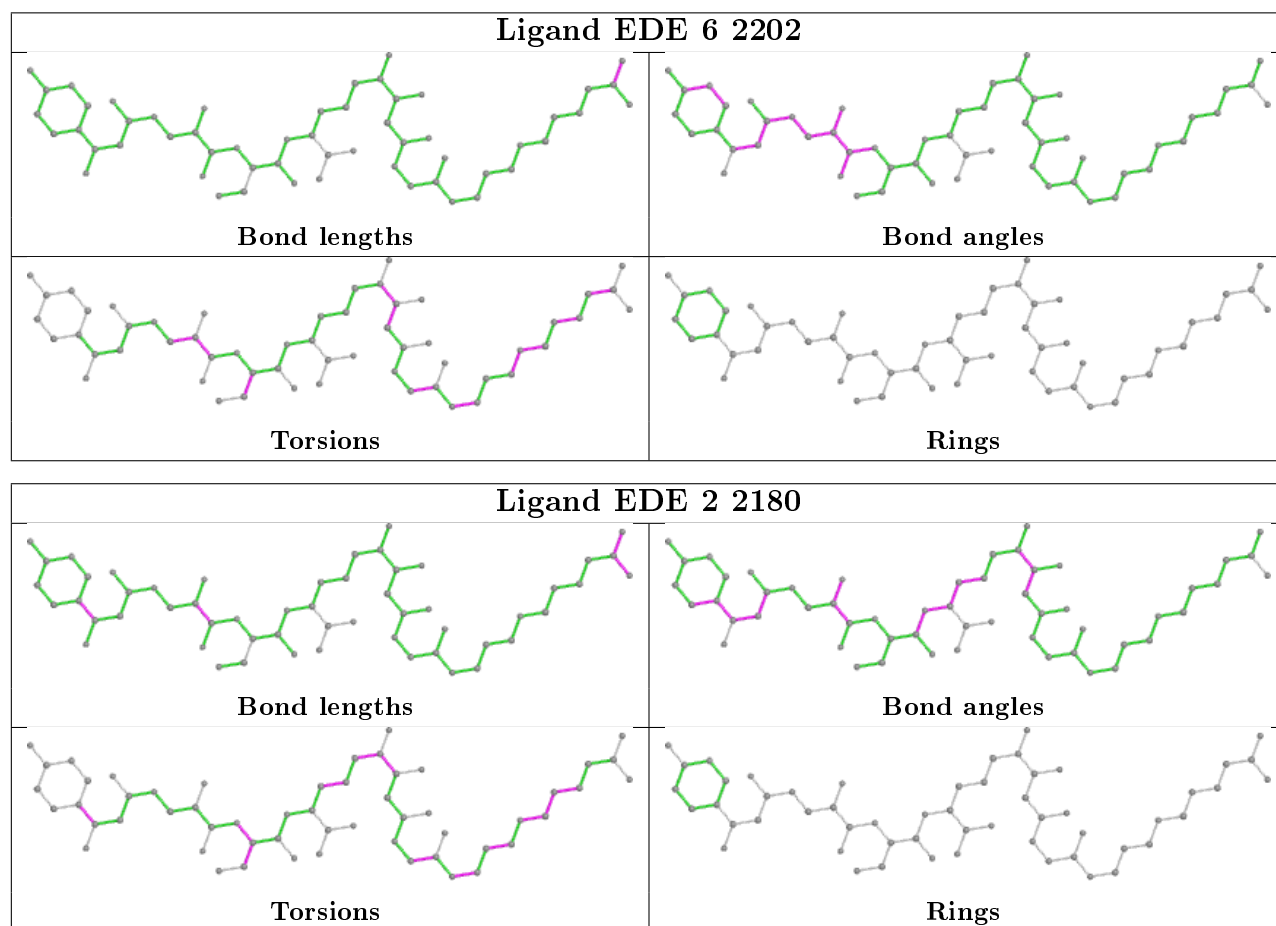
Mol	Chain	Res	Type	Atoms
87	6	2202	EDE	C27-C28-C29-N54
87	2	2180	EDE	N46-C45-C6-C7
87	2	2180	EDE	C12-C13-C14-C15
87	2	2180	EDE	C12-C13-C14-O51
87	2	2180	EDE	N50-C13-C14-O51
87	2	2180	EDE	N33-C32-C34-C35
87	2	2180	EDE	N33-C32-C34-C39
87	6	2202	EDE	C22-C21-N20-C19
87	2	2180	EDE	N17-C18-C19-O53
87	2	2180	EDE	N17-C18-C19-N20
87	6	2202	EDE	N17-C18-C19-O53
87	6	2202	EDE	N17-C18-C19-N20
87	2	2180	EDE	C26-C25-N24-C23
87	6	2202	EDE	C25-C26-C27-C28
87	2	2180	EDE	N24-C25-C26-C27
87	2	2180	EDE	C22-C21-N20-C19
87	6	2202	EDE	O51-C14-C15-C16
87	2	2180	EDE	C21-C22-C23-N24
87	2	2180	EDE	N50-C13-C14-C15
87	2	2180	EDE	C25-C26-C27-C28
87	2	2180	EDE	C11-C12-C13-C14
87	2	2180	EDE	C11-C12-C13-N50
87	6	2202	EDE	O42-C3-C4-O43
87	2	2180	EDE	C9-C10-C11-C12
87	6	2202	EDE	C22-C23-N24-C25
87	2	2180	EDE	C45-C6-N5-C4
87	6	2202	EDE	C2-C3-C4-O43
87	6	2202	EDE	C26-C25-N24-C23
87	6	2202	EDE	C2-C3-C4-N5

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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